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Article

Duality Principles and Numerical Procedures for a Large Class of Non-Convex Models in the Calculus of Variations

Fabio Silva Botelho

Department of Mathematics, Federal University of Santa Catarina, Zip Code 88040-90, Florianópolis - SC, Brazil; fabio.botelho@ufsc.br

Abstract: This article develops duality principles and numerical results for a large class of non-convex variational models. The main results are based on fundamental tools of convex analysis, duality theory and calculus of variations. More specifically the approach is established for a class of non-convex functionals similar as those found in some models in phase transition. Moreover, we develop a general duality principle for quasi-convex relaxed formulations for some models in the vectorial calculus of variations. Concerning applications of such results are presented for a non-linear model of plates and for non-linear elasticity. Finally, in some sections we present concerning numerical examples and the respective softwares.

Keywords: duality theory; non-convex variational analysis; numerical method for a non-smooth model

MSC: 49N15; 35A15; 49J40

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1. Introduction

In this section we establish a dual formulation for a large class of models in non-convex optimization. It is worth highlighting the main duality principle is applied to double well models similar as those found in the phase transition theory.

Such results are based on the works of J.J. Telega and W.R. Bielski [1–4] and on a D.C. optimization approach developed in Toland [5]. About the other references, details on the Sobolev spaces involved are found in [6]. Related results on convex analysis and duality theory are addressed in [7–13].

Similar models on the superconductivity physics may be found in [14–16].

At this point we recall that the duality principles are important since the related dual variational formulations are either convex (in fact concave) or have a large region of convexity around their critical points. These features are relevant considering that, from a concerning strict convexity, the standard Newton, Newton type and similar methods are in general convergent. Moreover, the dual variational formulations are also relevant since in some situations, it is possible to assure the global optimality of some critical points which satisfy certain specific constraints theoretically established.

Among the main results here developed, we highlight the duality principles for the quasi-convex formulations in the context of the vectorial calculus of variations. An important example in non-linear elasticity is addressed along the text in details.

Also, for the applications in physics in the final sections, we believe to have found a path to connect the quantum approach with a more classical one in a unified framework.

Indeed, we have presented a path to model a great variety of chemical reactions through such a connection between the atomic and classical worlds.

Finally, in this text we adopt the standard Einstein convention of summing up repeated indices, unless otherwise indicated.

In order to clarify the notation, here we introduce the definition of topological dual space.

Definition 1.1 (Topological dual spaces)**.** *Let U be a Banach space. We shall define its dual topological space, as the set of all linear continuous functionals defined on U. We suppose such a dual space of U, may be represented by another Banach space U^*, through a bilinear form $\langle \cdot, \cdot \rangle_U : U \times U^* \to \mathbb{R}$ (here we are referring*

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to standard representations of dual spaces of Sobolev and Lebesgue spaces). Thus, given $f : U \to \mathbb{R}$ linear and continuous, we assume the existence of a unique $u^* \in U^*$ such that

$$f(u) = \langle u, u^* \rangle_U, \forall u \in U. \tag{1}$$

The norm of f , denoted by $\|f\|_{U^*}$, is defined as

$$\|f\|_{U^*} = \sup_{u \in U} \{ |\langle u, u^* \rangle_U| \ : \ \|u\|_U \leq 1 \} \equiv \|u^*\|_{U^*}. \tag{2}$$

At this point we start to describe the primal and dual variational formulations.

2. A General Duality Principle Non-Convex Optimization

In this section we present a duality principle applicable to a model in phase transition.

This case corresponds to the vectorial one in the calculus of variations.

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = F(\nabla u_1, \cdots, \nabla u_N) + G(u_1, \cdots, u_N) - \langle u_i, h_i \rangle_{L^2},$$

and where

$$F(\nabla u_1, \cdots, \nabla u_N) = \int_\Omega f(\nabla u_1, \cdots, \nabla u_N) \, dx$$

$f : \mathbb{R}^{N \times n} \to \mathbb{R}$ is a three times Fréchet differentiable function not necessarily convex. Moreover,

$$V = \{ u = (u_1, \cdots, u_N) \in W^{1,p}(\Omega; \mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega \},$$

$h = (h_1, \cdots, h_N) \in L^2(\Omega; \mathbb{R}^N)$, and $1 < p < +\infty$.

We assume there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = \inf_{u \in V} J(u).$$

Furthermore, suppose G is Fréchet differentiable but not necessarily convex. A global optimum point may not be attained for J so that the problem of finding a global minimum for J may not be a solution.

Anyway, one question remains, how the minimizing sequences behave close the infimum of J.

We intend to use duality theory to approximately solve such a global optimization problem.

Define $V_0 = W_0^{1,2}(\Omega; \mathbb{R}^N)$ and

$$V_0(u) = \{ \phi \in V_0 \ : \ \text{supp } \phi \subset B(u) \},$$

where

$$B(u) = \{ x \in \Omega \ : \ f^{**}(\nabla u(x)) < f(\nabla u(x)) \}.$$

Moreover, $Y_1 = Y_1^* = L^2(\Omega; \mathbb{R}^{N \times n})$, $Y_2 = Y_2^* = L^2(\Omega; \mathbb{R}^{N \times n})$, $Y_3 = Y_3^* = L^2(\Omega; \mathbb{R}^N)$, so that at this point we define, $F_1 : V \times V_0 \to \mathbb{R}$, $G_1 : V \to \mathbb{R}$, $G_2 : V \to \mathbb{R}$, $G_3 : V_0 \to \mathbb{R}$ and $G_4 : V \to \mathbb{R}$, by

$$\begin{aligned} F_1(u, \phi) \quad = \quad & F(\nabla u_1 + \nabla \phi_1, \cdots, \nabla u_N + \nabla \phi_N) + \frac{K}{2} \int_\Omega \nabla u_j \cdot \nabla u_j \, dx \\ & + \frac{K_2}{2} \int_\Omega \nabla \phi_j \cdot \nabla \phi_j \, dx \end{aligned} \tag{3}$$

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and

$$G_1(u_1,\cdots,u_n)=G(u_1,\cdots,u_N)+\frac{K_1}{2}\int_\Omega u_j\,u_j\,dx-\langle u_i,f_i\rangle_{L^2},$$

$$G_2(\nabla u_1,\cdots,\nabla u_N)=\frac{K_1}{2}\int_\Omega \nabla u_j\cdot\nabla u_j\,dx,$$

$$G_3(\nabla \phi_1,\cdots,\nabla \phi_N)=\frac{K_2}{2}\int_\Omega \nabla \phi_j\cdot\nabla \phi_j\,dx,$$

and

$$G_4(u_1,\cdots,u_N)=\frac{K_1}{2}\int_\Omega u_j\,u_j\,dx.$$

Define now $J_1: V\times V_0\to\mathbb{R}$,

$$J_1(u,\phi)=F(\nabla u+\nabla\phi)+G(u)-\langle u_i,h_i\rangle_{L^2}.$$

Observe that

$$\begin{aligned}
J_1(u,\phi) &= F_1(u,\phi)+G_1(u)-G_2(\nabla u)-G_3(\nabla\phi)-G_4(u)\\
&\le F_1(u,\phi)+G_1(u)-\langle\nabla u,z_1^*\rangle_{L^2}-\langle\nabla\phi,z_2^*\rangle_{L^2}-\langle u,z_3^*\rangle_{L^2}\\
&\quad+\sup_{v_1\in Y_1}\{\langle v_1,z_1^*\rangle_{L^2}-G_2(v_1)\}\\
&\quad+\sup_{v_2\in Y_2}\{\langle v_2,z_2^*\rangle_{L^2}-G_3(v_2)\}\\
&\quad+\sup_{u\in V}\{\langle u,z_3^*\rangle_{L^2}-G_4(u)\}\\
&= F_1(u,\phi)+G_1(u)-\langle\nabla u,z_1^*\rangle_{L^2}-\langle\nabla\phi,z_2^*\rangle_{L^2}-\langle u,z_3^*\rangle_{L^2}\\
&\quad+G_2^*(z_1^*)+G_3^*(z_2^*)+G_4^*(z_3^*)\\
&= J_1^*(u,\phi,z^*),
\end{aligned}\tag{4}$$

$\forall u\in V,\ \phi\in V_0(u),\ z^*=(z_1^*,z_2^*,z_3^*)\in Y^*=Y_1^*\times Y_2^*\times Y_3^*$.

From the general results in [5], we may infer that

$$\inf_{(u,\phi)\in V\times V_0(u)}J(u,\phi)\quad=\quad\inf_{(u,\phi,z^*)\in V\times V_0(u)\times Y^*}J_1^*(u,\phi,z^*).\tag{5}$$

On the other hand

$$\inf_{u\in V}J(u)\ge\inf_{(u,\phi)\in V\times V_0(u)}J_1(u,\phi).$$

From these last two results we may obtain

$$\inf_{u\in V}J(u)\ge\inf_{(u,\phi,z^*)\in V\times V_0(u)\times Y^*}J_1^*(u,\phi,z^*).$$

Moreover, from standards results on convex analysis, we may have

$$\begin{aligned}
\inf_{u\in V}J_1^*(u,\phi,z^*) &= \inf_{u\in V}\{F_1(u,\phi)+G_1(u)\\
&\quad-\langle\nabla u,z_1^*\rangle_{L^2}-\langle\nabla\phi,z_2^*\rangle_{L^2}-\langle u,z_3^*\rangle_{L^2}\\
&\quad+G_2^*(z_1^*)+G_3^*(z_2^*)+G_4^*(z_3^*)\}\\
&= \sup_{(v_1^*,v_2^*)\in C^*}\{-F_1^*(v_1^*+z_1^*,\phi)-G_1^*(v_2^*+z_3^*)-\langle\nabla\phi,z_2^*\rangle_{L^2}\\
&\quad+G_2^*(z_1^*)+G_3^*(z_2^*)+G_4^*(z_3^*)\},
\end{aligned}\tag{6}$$

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where

$$C^* = \{v^* = (v_1^*, v_2^*) \in Y_1^* \times Y_3^* \ : \ -\operatorname{div}(v_1^*)_i + (v_2^*)_i = \mathbf{0}, \forall i \in \{1, \cdots, N\}\},$$

$$F_1^*(v_1^* + z_1^*, \phi) = \sup_{u \in V}\{\langle u, -\operatorname{div}(z_1^* + v_1^*)\rangle_{L^2} - F_1(u, \phi)\},$$

and

$$G_1^*(v_2^* + z_2^*) = \sup_{u \in V}\{\langle u, v_2^* + z_2^*\rangle_{L^2} - G_1(u)\}.$$

Thus, defining

$$J_2^*(\phi, z^*, v^*) = F_1^*(v_1^* + z_1^*, \phi) - G_1^*(v_2^* + z_3^*) - \langle \nabla\phi, z_2^*\rangle_{L^2} + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*),$$

we have got

$$\begin{aligned} \inf_{u \in V} J(u) &\geq \inf_{(u,\phi) \in V \times V_0} J_1(u, \phi) \\ &= \inf_{(u,\phi,z^*) \in V \times V_0(u) \times Y^*} J_1^*(u, \phi, z^*) \\ &= \inf_{z^* \in Y^*}\left\{\inf_{\phi \in V_0}\left\{\sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*)\right\}\right\}. \end{aligned} \tag{7}$$

Finally, observe that

$$\begin{aligned} &\inf_{u \in V} J(u) \\ \geq\ &\inf_{z^* \in Y^*}\left\{\inf_{\phi \in V_0(u)}\left\{\sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*)\right\}\right\} \\ \geq\ &\sup_{v^* \in C^*}\left\{\inf_{(z^*,\phi) \in Y^* \times V_0(u)} J_2^*(\phi, z^*, v^*)\right\}. \end{aligned} \tag{8}$$

This last variational formulation corresponds to a concave relaxed formulation in v^* concerning the original primal formulation.

3. Another Duality Principle for a Simpler Related Model in Phase Transition with a Respective Numerical Example

In this section we present another duality principle for a related model in phase transition.

Let $\Omega = [0, 1] \subset \mathbb{R}$ and consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = \frac{1}{2}\int_\Omega ((u')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2},$$

and where

$$V = \{u \in W^{1,4}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\}$$

and $f \in L^2(\Omega)$.

A global optimum point is not attained for J so that the problem of finding a global minimum for J has no solution.

Anyway, one question remains, how the minimizing sequences behave close the infimum of J.

We intend to use duality theory to approximately solve such a global optimization problem.

Denoting $V_0 = W_0^{1,4}(\Omega)$, at this point we define, $F : V \to \mathbb{R}$ and $F_1 : V \times V_0 \to \mathbb{R}$ by

$$F(u) = \frac{1}{2}\int_\Omega ((u')^2 - 1)^2\, dx,$$

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and

$$F_1(u,\phi) = \frac{1}{2}\int_\Omega ((u'+\phi')^2 - 1)^2\, dx.$$

Observe that

$$F(u) \geq \inf_{\phi \in V_0} F_1(u,\phi),\ \forall u \in V.$$

In order to restrict the action of ϕ on the region where the primal functional is non-convex, we redefine a not relabeled

$$V_0 = \left\{\phi \in W_0^{1,4}(\Omega)\ :\ (\phi')^2 - 1 \leq 0,\ \text{in}\ \Omega\right\}$$

and define also

$$F_2 : V \times V_0 \to \mathbb{R},$$
$$F_3 : V \times V_0 \to \mathbb{R}$$

and

$$G : V \times V_0 \to \mathbb{R}$$

by

$$F_2(u,\phi) = \frac{1}{2}\int_\Omega ((u'+\phi')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2},$$

$$\begin{aligned} F_3(u,\phi) &= F_2(u,\phi) + \frac{K}{2}\int_\Omega (u')^2\, dx \\ &\quad + \frac{K_1}{2}\int_\Omega (\phi')^2\, dx \end{aligned} \tag{9}$$

and

$$\begin{aligned} G(u,\phi) &= \frac{K}{2}\int_\Omega (u')^2\, dx \\ &\quad + \frac{K_1}{2}\int_\Omega (\phi')^2\, dx \end{aligned} \tag{10}$$

Denoting $Y = Y^* = L^2(\Omega)$ we also define the polar functional $G^* : Y^* \times Y^* \to \mathbb{R}$ by

$$G^*(v^*, v_0^*) = \sup_{(u,\phi)\in V\times V_0} \{\langle u, v^*\rangle_{L^2} + \langle \phi, v_0^*\rangle_{L^2} - G(u,\phi)\}.$$

Observe that

$$\inf_{u\in U} J(u) \geq \inf_{((u,\phi),(v^*,v_0^*))\in V\times V_0\times [Y^*]^2} \{G^*(v^*,v_0^*) - \langle u, v^*\rangle_{L^2} - \langle \phi, v_0^*\rangle_{L^2} + F_3(u,\phi)\}.$$

With such results in mind, we define a relaxed primal dual variational formulation for the primal problem, represented by $J_1^* : V \times V_0 \times [Y^*]^2 \to \mathbb{R}$, where

$$J_1^*(u,\phi,v^*,v_0^*) = G^*(v^*,v_0^*) - \langle u, v^*\rangle_{L^2} - \langle \phi, v_0^*\rangle_{L^2} + F_3(u,\phi).$$

Having defined such a functional, we may obtain numerical results by solving a sequence of convex auxiliary sub-problems, through the following algorithm (in order to obtain the concerning critical points, at first we have neglected the constraint $(\phi')^2 - 1 \leq 0$ in Ω).

1. Set $K \approx 0.1$ and $K_1 = 120.0$ and $0 < \varepsilon \ll 1$.
2. Choose $(u_1, \phi_1) \in V \times V_0$, such that $\|u_1\|_{1,\infty} < 1$ and $\|\phi_1\|_{1,\infty} < 1$.
3. Set $n = 1$.

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4. Calculate $(v_n^*, (v_0^*)_n)$ solution of the system of equations:

$$\frac{\partial J_1^*(u_n, \phi_n, v_n^*, (v_0^*)_n)}{\partial v^*} = \mathbf{0}$$

and

$$\frac{\partial J_1^*(u_n, \phi_n, v_n^*, (v_0^*)_n)}{\partial v_0^*} = \mathbf{0},$$

that is

$$\frac{\partial G^*(v_n^*, (v_0^*)_n)}{\partial v^*} - u_n = 0$$

and

$$\frac{\partial G^*(v_n^*, (v_0^*)_n)}{\partial v_0^*} - \phi_n = 0$$

so that

$$v_n^* = \frac{\partial G(u_n, \phi_n)}{\partial u}$$

and

$$(v_0^*)_n^* = \frac{\partial G(u_n, \phi_n)}{\partial \phi}$$

5. Calculate (u_{n+1}, ϕ_{n+1}) by solving the system of equations:

$$\frac{\partial J_1^*(u_{n+1}, \phi_{n+1}, v_n^*, (v_0^*)_n)}{\partial u} = \mathbf{0}$$

and

$$\frac{\partial J_1^*(u_{n+1}, \phi_{n+1}, v_n^*, (v_0^*)_n)}{\partial \phi} = \mathbf{0}$$

that is

$$-v_n^* + \frac{\partial F_3(u_{n+1}, \phi_{n+1})}{\partial u} = \mathbf{0}$$

and

$$-(v_0^*)_n + \frac{\partial F_3(u_{n+1}, \phi_{n+1})}{\partial \phi} = \mathbf{0}$$

6. If $\max\{\|u_n - u_{n+1}\|_\infty, \|\phi_{n+1} - \phi_n\|_\infty\} \leq \varepsilon$, then stop, else set $n := n + 1$ and go to item 4.

At this point, we present the corresponding software in MAT-LAB, in finite differences and based on the one-dimensional version of the generalized method of lines.

Here the software.

****

1. clear all

m8=300;

d=1/m8;

K=0.1;

K1=120;

for i=1:m8

$uo(i,1) = i^2 * d/2;$

vo(i,1)=i*d/10;

yo(i,1)=sin(i*d*pi)/2;

end;

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k=1;

b12=1.0;

while $(b12 > 10^{-4.3})$ and $(k < 230000)$

k=k+1;

for i=1:m8-1

duo(i,1)=(uo(i+1,1)-uo(i,1))/d;

dvo(i,1)=(vo(i+1,1)-vo(i,1))/d;

end;

m9=zeros(2,2);

m9(1,1)=1;

i=1;

$f1 = 6 * (duo(i,1) + dvo(i,1))^2 - 2;$

m80(1,1,i)=-f1-K;

m80(1,2,i)=-f1;

m80(2,1,i)=-f1;

m80(2,2,i)=-f1-K1;

$y11(1,i) = K * (uo(i+1,1) - 2 * uo(i,1))/d^2 - yo(i,1);$

$y11(2,i) = K1 * (vo(i+1,1) - 2 * vo(i,1))/d^2;$

$m12 = 2 * m80(:,:,i) - m9 * d^2;$

m50(:,:,i)=m80(:,:,i)*inv(m12);

z(:,i)=inv(m12)*y11(:,i)*d^2;

for i=2:m8-1

$f1 = 6 * (duo(i,1) + dvo(i,1))^2 - 2;$

m80(1,1,i)=-f1-K;

m80(1,2,i)=-f1;

m80(2,1,i)=-f1;

m80(2,2,i)=-f1-K1;

$y11(1,i) = K * (uo(i+1,1) - 2 * uo(i,1) + uo(i-1,1))/d^2 - yo(i,1);$

$y11(2,i) = K1 * (vo(i+1,1) - 2 * vo(i,1) + vo(i-1,1))/d^2;$

$m12 = 2 * m80(:,:,i) - m9 * d^2 - m80(:,:,i) * m50(:,:,i-1);$

m50(:,:,i)=inv(m12)*m80(:,:,i);

$z(:,i) = inv(m12) * (y11(:,i) * d^2 + m80(:,:,i) * z(:,i-1));$

end;

U(1,m8)=1/2;

U(2,m8)=0.0;

for i=1:m8-1

U(:,m8-i)=m50(:,:,m8-i)*U(:,m8-i+1)+z(:,m8-i);

end;

for i=1:m8

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```
u(i,1)=U(1,i);
v(i,1)=U(2,i);
end;
b12=max(abs(u-uo))
uo=u;
vo=v;
u(m8/2,1)
end;
for i=1:m8
y(i)=i*d;
end;
plot(y,uo)
**************************************
```

For the case in which $f(x) = 0$, we have obtained numerical results for $K = 0.1$ and $K_1 = 120$. For such a concerning solution u_0 obtained, please see Figure 1. For the case in which $f(x) = \sin(\pi x)/2$, we have obtained numerical results also for $K = 0.1$ and $K_1 = 120$. For such a concerning solution u_0 obtained, please see Figure 2.

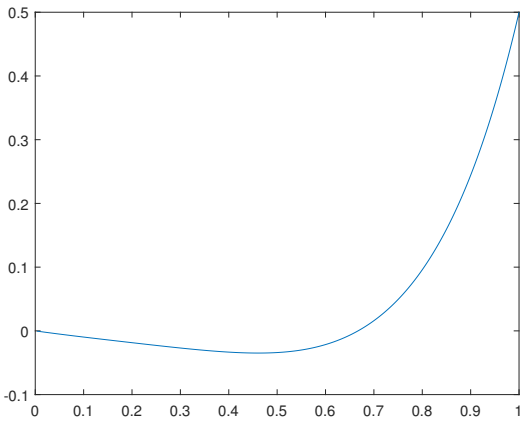

Figure 1. solution $u_0(x)$ for the case $f(x) = 0$.

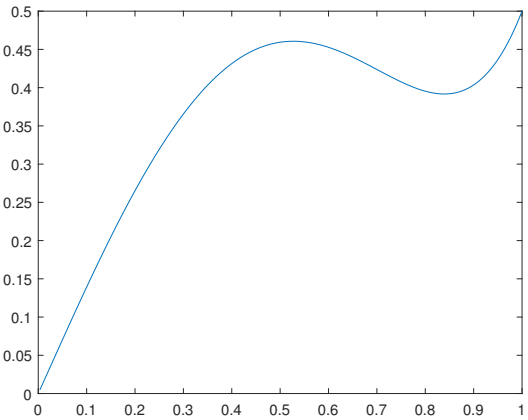

Figure 2. solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

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Remark 3.1. *Observe that the solutions obtained are approximate critical points. They are not, in a classical sense, the global solutions for the related optimization problems. Indeed, such solutions reflect the average behavior of weak cluster points for concerning minimizing sequences.*

3.1. A General Proposal for Relaxation

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = F(\nabla u) + G(u) - \langle u, f_1 \rangle_{L^2},$$

where

$$V = \left\{ u \in W^{1,4}(\Omega; \mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega \right\},$$

$$u_0 \in C^1(\Omega; \mathbb{R}^N),$$

$f_1 \in L^2(\Omega; \mathbb{R}^N)$, $G : V \to \mathbb{R}$ is convex and Fréchet differentiable, and

$$F(\nabla u) = \int_\Omega f(\nabla u)\, dx,$$

where $f : \mathbb{R}^{N\times n} \to \mathbb{R}$ is also Fréchet differentiable.

Assume there exists $\hat{N} \in \mathbb{N}$ such that

$$W_h \equiv \left\{ y \in \mathbb{R}^{N\times n} \ : \ f^{**}(y) < f(y) \right\} = \cup_{j=1}^{\hat{N}} W_j$$

where for each $j \in \{1, \cdots, \hat{N}\}$ $W_j \subset \mathbb{R}^{N\times n}$ is an open connected set such that ∂W_j is regular. We also suppose

$$\overline{W_j} \cap \overline{W_k} = \emptyset, \forall j \neq k.$$

Define

$$\hat{W}_j = \left\{ v_j \in W_0^{1,4}(\Omega; \mathbb{R}^N) \ ; \ \nabla v_j(x) \in W_j, \text{ a.e. in } \Omega \right\}$$

and define also

$$W = \left\{ v = (v_1, \cdots, v_{\hat{N}}) \ : \ v_j \in \hat{W}_j \ \forall j \in \{1, \cdots, \hat{N}\} \text{ and } \text{ supp } v_j \cap \text{ supp } v_k = \emptyset, \forall j \neq k \right\}.$$

At this point we define

$$h_5(u(x), v(x)) = \begin{cases} f(\nabla u(x) + \nabla v_j(x)), & \text{if } \nabla u(x) \in W_j, \\ f(\nabla u(x)), & \text{if } \nabla u(x) \notin W_h, \end{cases} \tag{11}$$

and

$$H(u) = \inf_{v \in W_u} \int_\Omega h_5(u, v)\, dx,$$

where

$$W_u = \{ v \in W \ : \ \nabla u(x) + \nabla v_j(x) \in W_j, \text{ if } \nabla u(x) \in W_j, \text{ a.e. in } \Omega, \ \forall j \in \{1, \cdots, \hat{N}\} \}.$$

Moreover, we propose the relaxed functional

$$J_1(u) = H(u) + G(u) - \langle u, f_1 \rangle_{L^2}.$$

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Observe that clearly

$$\inf_{u\in V} J_1(u) \leq \inf_{u\in V} J(u).$$

4. A Convex Dual Variational Formulation for a Third Similar Model

In this section we present another duality principle for a third related model in phase transition. Let $\Omega = [0,1] \subset \mathbb{R}$ and consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = \frac{1}{2}\int_\Omega \min\{(u'-1)^2, (u'+1)^2\}\, dx + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2},$$

and where

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\}$$

and $f \in L^2(\Omega)$.

A global optimum point is not attained for J so that the problem of finding a global minimum for J has no solution.

Anyway, one question remains, how the minimizing sequences behave close to the infimum of J.

We intend to use the duality theory to solve such a global optimization problem in an appropriate sense to be specified.

At this point we define, $F : V \to \mathbb{R}$ and $G : V \to \mathbb{R}$ by

$$\begin{aligned} F(u) &= \frac{1}{2}\int_\Omega \min\{(u'-1)^2, (u'+1)^2\}\, dx \\ &= \frac{1}{2}\int_\Omega (u')^2\, dx - \int_\Omega |u'|\, dx + 1/2 \\ &\equiv F_1(u'), \end{aligned} \tag{12}$$

and

$$G(u) = \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2}.$$

Denoting $Y = Y^* = L^2(\Omega)$ we also define the polar functional $F_1^* : Y^* \to \mathbb{R}$ and $G^* : Y^* \to \mathbb{R}$ by

$$\begin{aligned} F_1^*(v^*) &= \sup_{v\in Y}\{\langle v, v^*\rangle_{L^2} - F_1(v)\} \\ &= \frac{1}{2}\int_\Omega (v^*)^2\, dx + \int_\Omega |v^*|\, dx, \end{aligned} \tag{13}$$

and

$$\begin{aligned} G^*((v^*)') &= \sup_{u\in V}\{-\langle u', v^*\rangle_{L^2} - G(u)\} \\ &= \frac{1}{2}\int_\Omega ((v^*)' + f)^2\, dx - \frac{1}{2}v^*(1). \end{aligned} \tag{14}$$

Observe this is the scalar case of the calculus of variations, so that from the standard results on convex analysis, we have

$$\inf_{u\in V} J(u) = \max_{v^*\in Y^*}\{-F_1^*(v^*) - G^*(-(v^*)')\}.$$

Indeed, from the direct method of the calculus of variations, the maximum for the dual formulation is attained at some $\hat{v}^* \in Y^*$.

Moreover, the corresponding solution $u_0 \in V$ is obtained from the equation

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$$u_0 = \frac{\partial G((\hat{v}^*)')}{\partial (v^*)'} = (\hat{v}^*)' + f.$$

Finally, the Euler-Lagrange equations for the dual problem stands for

$$\begin{cases} (v^*)'' + f' - v^* - \ \text{sign}(v^*) = 0, & \text{in } \Omega, \\ (v^*)'(0) + f(0) = 0, \ (v^*)'(1) + f(1) = 1/2, \end{cases} \tag{15}$$

where $\text{sign}(v^*(x)) = 1$ if $v^*(x) > 0$, $\text{sign}(v^*(x)) = -1$, if $v^*(x) < 0$ and

$$-1 \leq \ \text{sign}(v^*(x)) \leq 1,$$

if $v^*(x) = 0$.

We have computed the solutions v^* and corresponding solutions $u_0 \in V$ for the cases in which $f(x) = 0$ and $f(x) = \sin(\pi x)/2$.

For the solution $u_0(x)$ for the case in which $f(x) = 0$, please see Figure 3.

For the solution $u_0(x)$ for the case in which $f(x) = \sin(\pi x)/2$, please see Figure 4.

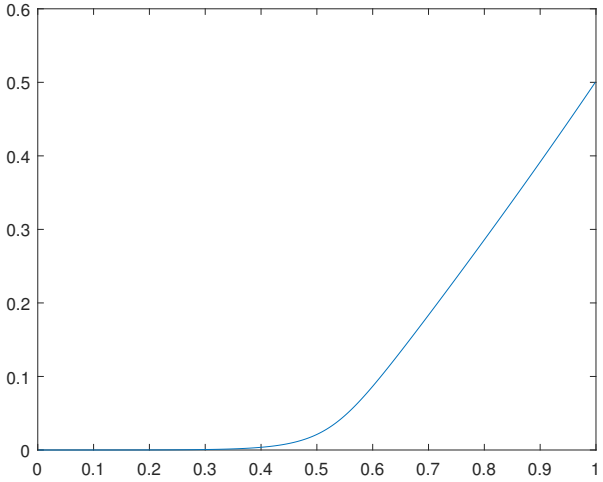

Figure 3. solution $u_0(x)$ for the case $f(x) = 0$.

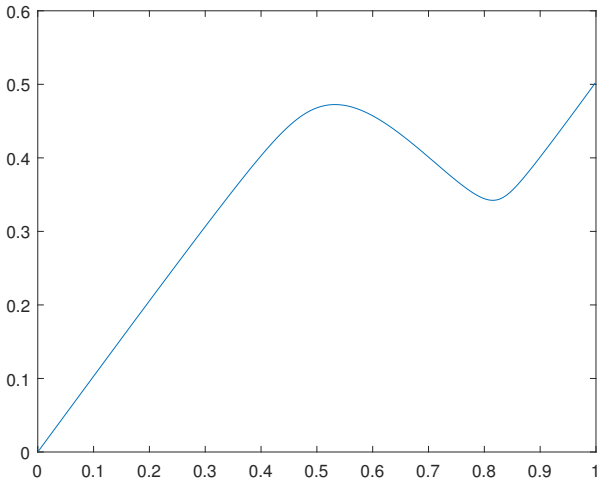

Figure 4. solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

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Remark 4.1. *Observe that such solutions u_0 obtained are not the global solutions for the related primal optimization problems. Indeed, such solutions reflect the average behavior of weak cluster points for concerning minimizing sequences.*

4.1. The Algorithm through Which We Have Obtained the Numerical Results

In this subsection we present the software in MATLAB through which we have obtained the last numerical results.

This algorithm is for solving the concerning Euler-Lagrange equations for the dual problem, that is, for solving the equation

$$\begin{cases} (v^*)'' + f' - v^* - \text{ sign}(v^*) = 0, & \text{in } \Omega, \\ (v^*)'(0) = 0,\ (v^*)'(1) = 1/2. \end{cases} \tag{16}$$

Here the concerning software in MATLAB. We emphasize to have used the smooth approximation

$$|v^*| \approx \sqrt{(v^*)^2 + e_1},$$

where a small value for e_1 is specified in the next lines.

****

1. clear all
2. $m_8 = 800$; (number of nodes)
3. $d = 1/m_8$;
4. $e_1 = 0.00001$;
5. $for\ i = 1 : m_8$

   $yo(i,1) = 0.01$;

   $y_1(i,1) = \sin(\pi * i/m_8)/2$;

   end;
6. $for\ i = 1 : m_8 - 1$

   $dy_1(i,1) = (y_1(i+1,1) - y_1(i,1))/d$;

   end;
7. $for\ k = 1 : 3000$ (we have fixed the number of iterations)

   $i = 1$;

   $h_3 = 1/\sqrt{vo(i,1)^2 + e_1}$;

   $m_{12} = 1 + d^2 * h_3 + d^2$;

   $m_{50}(i) = 1/m_{12}$;

   $z(i) = m_{50}(i) * (dy_1(i,1) * d^2)$;
8. $for\ i = 2 : m_8 - 1$

   $h_3 = 1/\sqrt{vo(i,1)^2 + e_1}$;

   $m_{12} = 2 + h_3 * d^2 + d^2 - m50(i-1)$;

   $m50(i) = 1/m_{12}$;

   $z(i) = m_{50}(i) * (z(i-1) + dy_1(i,1) * d^2)$;

   end;
9. $v(m_8,1) = (d/2 + z(m_8 - 1))/(1 - m_{50}(m_8 - 1))$;
10. $for\ i = 1 : m_8 - 1$

    $v(m_8 - i, 1) = m_{50}(m_8 - i) * v(m_8 - i + 1) + z(m_8 - i)$;

    end;

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11. $v(m_8/2,1)$
12. $vo = v;$

$end;$

13. $for\ i = 1 : m_8 - 1$

$u(i,1) = (v(i+1,1) - v(i,1))/d + y_1(i,1);$

$end;$

14. $for\ i = 1 : m_8 - 1$

$x(i) = i * d;$

$end;$

$plot(x, u(:,1))$

****

5. An Improvement of the Convexity Conditions for a Non-Convex Related Model through an Approximate Primal Formulation

In this section we develop an approximate primal dual formulation suitable for a large class of variational models.

Here, the applications are for the Kirchhoff-Love plate model, which may be found in Ciarlet, [17].

At this point we start to describe the primal variational formulation.

Let $\Omega \subset \mathbb{R}^2$ be an open, bounded, connected set which represents the middle surface of a plate of thickness h. The boundary of Ω, which is assumed to be regular (Lipschitzian), is denoted by $\partial\Omega$. The vectorial basis related to the cartesian system $\{x_1, x_2, x_3\}$ is denoted by $(\mathbf{a}_\alpha, \mathbf{a}_3)$, where $\alpha = 1, 2$ (in general Greek indices stand for 1 or 2), and where $\mathbf{a}_3$ is the vector normal to Ω, whereas $\mathbf{a}_1$ and $\mathbf{a}_2$ are orthogonal vectors parallel to Ω. Also, $\mathbf{n}$ is the outward normal to the plate surface.

The displacements will be denoted by

$$\hat{\mathbf{u}} = \{\hat{u}_\alpha, \hat{u}_3\} = \hat{u}_\alpha \mathbf{a}_\alpha + \hat{u}_3 \mathbf{a}_3.$$

The Kirchhoff-Love relations are

$$\begin{aligned} &\hat{u}_\alpha(x_1, x_2, x_3) = u_\alpha(x_1, x_2) - x_3 w(x_1, x_2)_{,\alpha} \\ &\text{and } \hat{u}_3(x_1, x_2, x_3) = w(x_1, x_2). \end{aligned} \tag{17}$$

Here $-h/2 \leq x_3 \leq h/2$ so that we have $u = (u_\alpha, w) \in U$ where

$$\begin{aligned} U &= \Big\{ u = (u_\alpha, w) \in W^{1,2}(\Omega; \mathbb{R}^2) \times W^{2,2}(\Omega), \\ &\qquad u_\alpha = w = \frac{\partial w}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega \Big\} \\ &= W_0^{1,2}(\Omega; \mathbb{R}^2) \times W_0^{2,2}(\Omega). \end{aligned}$$

It is worth emphasizing that the boundary conditions here specified refer to a clamped plate.

We also define the operator $\Lambda : U \to Y \times Y$, where $Y = Y^* = L^2(\Omega; \mathbb{R}^{2\times 2})$, by

$$\Lambda(u) = \{\gamma(u), \kappa(u)\},$$

$$\gamma_{\alpha\beta}(u) = \frac{u_{\alpha,\beta} + u_{\beta,\alpha}}{2} + \frac{w_{,\alpha} w_{,\beta}}{2},$$

$$\kappa_{\alpha\beta}(u) = -w_{,\alpha\beta}.$$

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The constitutive relations are given by

$$N_{\alpha\beta}(u) = H_{\alpha\beta\lambda\mu}\gamma_{\lambda\mu}(u), \tag{18}$$

$$M_{\alpha\beta}(u) = h_{\alpha\beta\lambda\mu}\kappa_{\lambda\mu}(u), \tag{19}$$

where: $\{H_{\alpha\beta\lambda\mu}\}$ and $\left\{h_{\alpha\beta\lambda\mu} = \frac{h^2}{12}H_{\alpha\beta\lambda\mu}\right\}$, are symmetric positive definite fourth order tensors. From now on, we denote $\{\overline{H}_{\alpha\beta\lambda\mu}\} = \{H_{\alpha\beta\lambda\mu}\}^{-1}$ and $\{\overline{h}_{\alpha\beta\lambda\mu}\} = \{h_{\alpha\beta\lambda\mu}\}^{-1}$.

Furthermore $\{N_{\alpha\beta}\}$ denote the membrane force tensor and $\{M_{\alpha\beta}\}$ the moment one. The plate stored energy, represented by $(G \circ \Lambda) : U \to \mathbb{R}$ is expressed by

$$(G \circ \Lambda)(u) = \frac{1}{2}\int_\Omega N_{\alpha\beta}(u)\gamma_{\alpha\beta}(u)\, dx + \frac{1}{2}\int_\Omega M_{\alpha\beta}(u)\kappa_{\alpha\beta}(u)\, dx \tag{20}$$

and the external work, represented by $F : U \to \mathbb{R}$, is given by

$$F(u) = \langle w, P\rangle_{L^2} + \langle u_\alpha, P_\alpha\rangle_{L^2}, \tag{21}$$

where $P, P_1, P_2 \in L^2(\Omega)$ are external loads in the directions $\mathbf{a}_3$, $\mathbf{a}_1$ and $\mathbf{a}_2$ respectively. The potential energy, denoted by $J : U \to \mathbb{R}$ is expressed by:

$$J(u) = (G \circ \Lambda)(u) - F(u)$$

Define now $J_3 : \tilde{U} \to \mathbb{R}$ by

$$J_3(u) = J(u) + J_5(w).$$

where

$$J_5(w) = 10\int_\Omega \frac{a^{K\,b\,w}}{\ln(a)\,K^{3/2}}\, dx + 10\int_\Omega \frac{a^{-K(b\,w-1/100)}}{\ln(a)\,K^{3/2}}\, dx.$$

In such a case for $a = 2.71$, $K = 185$, $b = P/|P|$ in Ω and

$$\tilde{U} = \{u \in U \ : \ \|w\|_\infty \leq 0.01 \text{ and } P\,w \geq 0 \text{ a.e. in } \Omega\},$$

we get

$$\begin{aligned} \frac{\partial J_3(u)}{\partial w} &= \frac{\partial J(u)}{\partial w} + \frac{\partial J_5(u)}{\partial w} \\ &\approx \frac{\partial J(u)}{\partial w} + \mathcal{O}(\pm 3.0), \end{aligned} \tag{22}$$

and

$$\begin{aligned} \frac{\partial^2 J_3(u)}{\partial w^2} &= \frac{\partial^2 J(u)}{\partial w^2} + \frac{\partial^2 J_5(u)}{\partial w^2} \\ &\approx \frac{\partial^2 J(u)}{\partial w^2} + \mathcal{O}(850). \end{aligned} \tag{23}$$

This new functional J_3 has a relevant improvement in the convexity conditions concerning the previous functional J.

Indeed, we have obtained a gain in positiveness for the second variation $\frac{\partial^2 J(u)}{\partial w^2}$, which has increased of order $\mathcal{O}(700 - 1000)$.

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Moreover the difference between the approximate and exact equation

$$\frac{\partial J(u)}{\partial w} = \mathbf{0}$$

is of order $\mathcal{O}(\pm 3.0)$ which corresponds to a small perturbation in the original equation for a load of $P = 1500\ N/m^2$, for example. Summarizing, the exact equation may be approximately solved in an appropriate sense.

5.1. A Duality Principle for the Concerning Quasi-Convex Envelope

In this section, denoting

$$V_1 = \{\phi = \phi(x,y) \in W^{1,2}(\Omega \times \Omega; \mathbb{R}^2) \ : \ \phi = 0 \text{ on } \Omega \times \partial\Omega\},$$

we define the functional $J_1 : U \times V_1 \to \mathbb{R}$, where

$$\begin{aligned} J_1(u,\phi) &= G_1(\{w_{,\alpha\beta}\}) + G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta} + u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\ &\quad - \langle w, P\rangle_{L^2} - \langle u_\alpha, P_\alpha\rangle_{L^2}. \end{aligned} \tag{24}$$

where

$$G_1(\{w_{,\alpha\beta}\}) = \frac{1}{2}\int_\Omega h_{\alpha\beta\lambda\mu} w_{,\alpha\beta} w_{,\lambda\mu}\, dx$$

and,

$$\begin{aligned} & G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta} + u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\ = \ & \frac{1}{2|\Omega|}\int_\Omega\int_\Omega H_{\alpha\beta\lambda\mu}\left(\frac{1}{2}(u_{\alpha,\beta} + u_{\beta,\alpha}) + \phi_{\alpha,y_\beta}(x,y) + \frac{1}{2}w_{,\alpha}w_{,\beta}\right) \\ & \times\left(\frac{1}{2}(u_{\lambda,\mu} + u_{\lambda,\mu}) + \phi_{\lambda,y_\mu}(x,y) + \frac{1}{2}w_{,\lambda}w_{,\mu}\right) dx\, dy \end{aligned}$$

We define also

$$J_2(\{u_\alpha\},\phi) = \inf_{w \in W_0^{2,2}(\Omega)} J_1(u,\phi),$$

and

$$J_3(\{u_\alpha\}) = \inf_{\phi \in V_1} J_2(\{u_\alpha\},\phi).$$

It is a well known result from the modern Calculus of Variations theory (please, see [18] for details) that

$$\inf_{u \in U} J(u) = \inf_{\{u_\alpha\} \in W_0^{1,2}(\Omega;\mathbb{R}^2)} J_3(\{u_\alpha\}).$$

At this point we denote

$$Y_1 = Y_1^* = Y_3 = Y_3^* \equiv L^2(\Omega \times \Omega; \mathbb{R}^4)$$

and

$$Y_2 = Y_2^* \equiv L^2(\Omega \times \Omega; \mathbb{R}^2).$$

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Observe that

$$
\begin{aligned}
& J(u) \\
= \; & G_1(\{w_{,\alpha\beta}\}) + G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\
& -\langle w, P\rangle_{L^2} - \langle u_\alpha, P_\alpha\rangle_{L^2} \\
= \; & G_1(\{w_{,\alpha\beta}\}) - \langle w_{,\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} + \langle w_{,\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} \\
& + \frac{1}{|\Omega|}\int_\Omega\int_\Omega w_{,\alpha}(x), Q_\alpha(x,y)\; dx\; dy - \langle w, P\rangle_{L^2} \\
& - \frac{1}{|\Omega|}\int_\Omega\int_\Omega w_{,\alpha}(x), Q_\alpha(x,y)\; dx\; dy + G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\
& - \frac{1}{|\Omega|}\int_\Omega\int_\Omega \left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right), v^*_{\alpha\beta}(x,y)\; dx\; dy \\
& + \frac{1}{|\Omega|}\int_\Omega\int_\Omega \left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right), v^*_{\alpha\beta}(x,y)\; dx\; dy - \langle u_\alpha, P_\alpha\rangle_{L^2} \\
\geq \; & \inf_{v_3\in Y_3}\{-\langle (v_3)_{\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} + G_1((v_3)_{\alpha\beta})\} \\
& + \inf_{w\in W_0^{2,2}(\Omega)}\left\{\langle w_{,\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} + \frac{1}{|\Omega|}\int_\Omega\int_\Omega w_{,\alpha}(x)\; Q_\alpha(x,y)\; dx\; dy - \langle w, P\rangle_{L^2}\right\} \\
& + \inf_{v\in Y_1}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega v_{\alpha\beta}\; v^*_{\alpha\beta}\; dx\; dy + G_2(\{v_{\alpha\beta}\})\right\} \\
& + \inf_{(v_2,\{u_\alpha\})\in Y_2\times W_0^{1,2}(\Omega;\mathbb{R}^2)}\left\{\frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}(v_2)_\alpha(x,y)(v_2)_\beta(x,y)\right)\right. \\
& \left.\times v^*_{\alpha\beta}(x,y)\; dx\; dy - \langle u_\alpha, P_\alpha\rangle_{L^2} + \frac{1}{|\Omega|}\int_\Omega\int_\Omega (v_2)_\alpha(x,y) Q_\alpha(x,y)\; dx\; dy\right\} \\
\geq \; & -G_1^*(M) - \frac{1}{2|\Omega|}\int_\Omega\int_\Omega \left(\overline{v^*_{\alpha\beta}}\right) Q_\alpha\; Q_\beta\; dx\; dy - \frac{1}{2|\Omega|}\int_\Omega\int_\Omega \overline{H}_{\alpha\beta\lambda\mu} v^*_{\alpha\beta} v^*_{\lambda\mu}\; dx\; dy, \qquad (25)
\end{aligned}
$$

$\forall u \in U,\ (M,Q) \in C^*, v = \{v_{\alpha\beta}\} \in A^*$ where $A^* = A_1^* \cap A_2^* \cap B^*$,

$$A_1^* = \{\{v^*_{\alpha\beta}\} \in Y_1^* \ :\ (v^*_{\alpha\beta})_{,y_\beta} = 0,\ \text{in } \Omega\},$$

$$A_2^* = \left\{\{v^*_{\alpha\beta}\} \in Y_1^* \ :\ \frac{1}{|\Omega|}\left(\int_\Omega v^*_{\alpha\beta}\; dy\right)_{,x_\beta} + P_\alpha = 0,\ \text{in } \Omega\right\},$$

$$B^* = \left\{\{v^*_{\alpha\beta}\} \in Y_1^* \ :\ \left\{v^*_{\alpha\beta}(x,y)\right\} \text{ is positive definite in } \Omega\times\Omega\right\}.$$

and

$$C^* = \left\{(M,Q) \in Y_3^* \times Y_2^* \ :\ M_{\alpha\beta,\alpha\beta} - \left(\int_\Omega Q_\alpha\; dy\right)_{,x_\alpha} - P = 0,\ \text{in } \Omega\right\}.$$

Also

$$\left\{\overline{v^*_{\alpha\beta}}\right\} = \left\{v^*_{\alpha\beta}\right\}^{-1},$$

and

$$\{\overline{H}_{\alpha\beta\lambda\mu}\} = \{H_{\alpha\beta\lambda\mu}\}$$

in an appropriate tensor sense.

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Here it is worth highlighting we have denoted,

$$\begin{aligned} G_1^*(M) &= \sup_{v_3 \in Y_3} \{\langle (v_3)_{\alpha\beta}, M_{\alpha\beta} \rangle_{L^2} - G_1(v_3)\} \\ &= \frac{1}{2} \int_\Omega \overline{h}_{\alpha\beta\lambda\mu} M_{\alpha\beta} M_{\lambda\mu} \, dx, \end{aligned} \tag{26}$$

where we recall that

$$\{\overline{h}_{\alpha\beta\lambda\mu}\} = \{h_{\alpha\beta\lambda\mu}\}^{-1}$$

in an appropriate tensorial sense.

Summarizing, defining $J^* : C^* \times A^* \to \mathbb{R}$ by

$$\begin{aligned} J^*((M,Q),v^*) &= -G_1^*(M) - \frac{1}{2|\Omega|} \int_\Omega \int_\Omega \left(\overline{v^*_{\alpha\beta}}\right) Q_\alpha \, Q_\beta \, dx \, dy \\ &\quad - \frac{1}{2|\Omega|} \int_\Omega \int_\Omega \overline{H}_{\alpha\beta\lambda\mu} v^*_{\alpha\beta} v^*_{\lambda\mu} \, dx \, dy, \end{aligned} \tag{27}$$

we have got

$$\inf_{u \in U} J(u) \geq \sup_{((M,Q),v^*) \in C^* \times A^*} J^*((M,Q),v^*).$$

Remark 5.1. *This last dual functional is concave and such a concerning inequality corresponds a duality principle for the relaxed primal formulation.*

We emphasize such results are extensions and in some sense complement the original duality principles in the works of Telega and Bielski, [1–3].

Moreover, if $((M_0,Q_0),v_0^*) \in C^* \times A^*$ *is such that*

$$\delta J^*((M_0,Q_0),v_0^*) = \mathbf{0},$$

it is a well known result from the Legendre transform proprieties that the corresponding $(u_0,\phi_0) \in V \times V_1$ *such that*

$$(w_0)_{,\alpha\beta} = \overline{h}_{\alpha\beta\lambda\mu} (M_0)_{\lambda\mu},$$

and

$$(v_0^*)_{\alpha\beta} = H_{\alpha\beta\lambda} \left(\frac{(u_0)_{\lambda,\mu} + (u_0)_{\mu,\lambda}}{2} + \frac{(\phi_0)_{\lambda,y_\mu} + (\phi_0)_{\mu,y_\lambda}}{2} + \frac{1}{2} (v_{2_0})_\lambda (v_{2_0})_\mu \right),$$

$$(v_0^*)_{\alpha\beta,y_\beta} = \mathbf{0},$$

is also such that

$$\delta J_1(u_0,\phi_0) = \mathbf{0}$$

and

$$J_1(u_0,\phi_0) = J^*((M_0,Q_0),v_0^*).$$

From this and

$$\inf_{u \in V} J(u) = \inf_{(u,\phi) \in V \times V_1} J_1(u,\phi) \geq \sup_{((M,Q),v^*) \in C^* \times A^*} J^*((M,Q),v^*),$$

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we obtain

$$\begin{aligned} J_1(u_0,\phi_0) &= \inf_{(u,\phi)\in V\times V_1} J_1(u,\phi) \\ &= \sup_{((M,Q),v^*)\in C^*\times A^*} J^*((M,Q),v^*) \\ &= J^*((M_0,Q_0),v_0^*) \\ &= \inf_{u\in V} J(u). \end{aligned} \tag{28}$$

Also, from the modern calculus of variations theory, there exists a sequence $\{u_n\}\subset V$ *such that*

$$u_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(u_n)\to J_1(u_0,\phi_0)=\inf_{u\in V} J(u).$$

From this and the Ekeland variational principle, there exists $\{v_n\}\subset V$ *such that*

$$\|u_n-v_n\|_V\le 1/n,$$

$$J(v_n)\le \inf_{u\in V} J(u)+1/n,$$

and

$$\|\delta J(v_n)\|_{V^*}\le 1/n,\ \forall n\in\mathbb{N},$$

so that

$$v_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(v_n)\to J_1(u_0,\phi_0)=\inf_{u\in V} J(u).$$

Assume now we are dealing with a finite dimensional version of such a model, in a finite elements of finite differences context, for example.

In such a case we have

$$v_n\to u_0, \text{ strongly in } \mathbb{R}^N$$

for an appropriate $N\in\mathbb{N}$.

From continuity we obtain

$$\delta J(v_n)\to \delta J(u_0)=\mathbf{0},$$

$$J(v_n)\to J(u_0).$$

Summarizing, we have got

$$J(u_0)=\inf_{u\in V} J(u),$$

$$\delta J(u_0)=\mathbf{0}.$$

Here we highlight such last results are valid just for this finite-dimensional model version.

6. A Duality Principle for a Related Relaxed Formulation Concerning the Vectorial Approach in the Calculus of Variations

In this section we develop a duality principle for a related vectorial model in the calculus of variations.

Let $\Omega\subset\mathbb{R}^n$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega=\Gamma$.

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For $1 < p < +\infty$, consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = G(\nabla u) + F(u) - \langle u, f \rangle_{L^2},$$

where

$$V = \Big\{ u \in W^{1,p}(\Omega; \mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega \Big\},$$

$u_0 \in C^1(\overline{\Omega}; \mathbb{R}^N)$ and $f \in L^2(\Omega; \mathbb{R}^N)$.

We assume $G : Y \to \mathbb{R}$ and $F : V \to \mathbb{R}$ are Fréchet differentiable and F is also convex.

Also

$$G(\nabla u) = \int_\Omega g(\nabla u)\, dx,$$

where $g : \mathbb{R}^{N\times n} \to \mathbb{R}$ it is supposed to be Fréchet differentiable. Here we have denoted $Y = L^p(\Omega; \mathbb{R}^{N\times n})$.

We define also $J_1 : V \times Y_1 \to \mathbb{R}$ by

$$J_1(u, \phi) = G_1(\nabla u + \nabla_y \phi) + F(u) - \langle u, f \rangle_{L^2},$$

where

$$Y_1 = W^{1,p}(\Omega \times \Omega; \mathbb{R}^N)$$

and

$$G_1(\nabla u + \nabla_y \phi) = \frac{1}{|\Omega|} \int_\Omega \int_\Omega g(\nabla u(x) + \nabla_y \phi(x, y))\, dx\, dy.$$

Moreover, we define the relaxed functional $J_2 : V \to \mathbb{R}$ by

$$J_2(u) = \inf_{\phi \in V_0} J_1(u, \phi),$$

where

$$V_0 = \{ \phi \in Y_1 \ : \ \phi(x, y) = 0, \ \text{ on } \Omega \times \partial\Omega \}.$$

Now observe that

$$\begin{aligned}
J_1(u,\phi) &= G_1(\nabla u + \nabla_y \phi) + F(u) - \langle u, f \rangle_{L^2} \\
&= -\frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x, y) \cdot (\nabla u + \nabla_y \phi(x, y))\, dy\, dx + G_1(\nabla u + \nabla_y \phi) \\
&\quad + \frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x, y) \cdot (\nabla u + \nabla_y \phi(x, y))\, dy\, dx + F(u) - \langle u, f \rangle_{L^2} \\
&\geq \inf_{v \in Y_2} \left\{ -\frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x, y) \cdot v(x, y)\, dy\, dx + G_1(v) \right\} \\
&\quad + \inf_{(v,\phi) \in V \times V_0} \left\{ \frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x, y) \cdot (\nabla u + \nabla_y \phi(x, y))\, dy\, dx + F(u) - \langle u, f \rangle_{L^2} \right\} \\
&= -G_1^*(v^*) - F^* \left(\text{div}_x \left(\frac{1}{|\Omega|} \int_\Omega v^*(x, y)\, dy \right) + f \right) \\
&\quad + \frac{1}{|\Omega|} \int_{\partial\Omega} \left(\int_\Omega v^*(x, y)\, dy \right) \otimes \mathbf{n} u_0\, d\Gamma,
\end{aligned} \tag{29}$$

$\forall (u, \phi) \in V \times V_0, v^* \in A^*$, where

$$A^* = \{ v^* \in Y_2^* \ : \ \text{div}_y v^*(x, y) = 0, \text{ in } \Omega \}.$$

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Here we have denoted

$$G_1^*(v^*) = \sup_{v \in Y_2} \left\{ \frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot v(x,y)\, dy\, dx - G_1(v) \right\},$$

where $Y_2 = L^p(\Omega \times \Omega; \mathbb{R}^{N\times n})$, $Y_2^* = L^q(\Omega \times \Omega; \mathbb{R}^{N\times n})$, and where

$$\frac{1}{p} + \frac{1}{q} = 1.$$

Furthermore, for $v^* \in A^*$, we have

$$\begin{aligned} & F^*\left(\mathrm{div}_x \left(\frac{1}{|\Omega|} \int_\Omega v^*(x,y)\, dy \right) + f \right) - \frac{1}{|\Omega|} \int_{\partial\Omega} \left(\int_\Omega v^*(x,y)\, dy \right) \otimes \mathbf{n} u_0\, d\Gamma \\ = & \sup_{(v,\phi) \in V \times V_0} \left\{ -\frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot (\nabla u + \nabla_y \phi(x,y))\, dy\, dx - F(u) + \langle u, f \rangle_{L^2} \right\}, \end{aligned} \tag{30}$$

Therefore, denoting $J_3^* : Y_2^* \to \mathbb{R}$ by

$$J_3^*(v^*) = -G_1^*(v^*) - F^*\left(\mathrm{div}_x \left(\int_\Omega v^*(x,y)\, dy \right) + f \right) + \frac{1}{|\Omega|} \int_{\partial\Omega} \left(\int_\Omega v^*(x,y)\, dy \right) \otimes \mathbf{n} u_0\, d\Gamma,$$

we have got

$$\inf_{u \in V} J_2(u) \geq \sup_{v^* \in A^*} J_3^*(v^*).$$

Finally, we highlight such a dual functional J_3^* is convex (in fact concave).

6.1. *An Example in Finite Elasticity*

In this section we develop an application of results obtained in the last section to a model in non-linear elasticity.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Concerning a standard model in non-linear elasticity, consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} & J(u) \\ = & \frac{1}{2} \int_\Omega H_{ijkl} \left(\frac{u_{i,j} + u_{j,i}}{2} + \frac{1}{2} u_{m,i} u_{m,j} \right) \left(\frac{u_{k,l} + u_{j,i}}{2} + \frac{1}{2} u_{m,k} u_{m,l} \right) dx \\ & - \langle u_i, f_i \rangle_{L^2} \end{aligned} \tag{31}$$

where $f \in L^2(\Omega; \mathbb{R}^3)$ and $V = W_0^{1,2}(\Omega; \mathbb{R}^3)$.

Here $\{H_{ijkl}\}$ is a fourth-order and positive definite symmetric tensor (in an appropriate standard sense). Moreover, $u = (u_1, u_2, u_3) \in V$ is a field of displacements resulting from the f load field action on the volume comprised by Ω.

At this point, we define the functional $J_1 : V \times V_1 \to \mathbb{R}$, where

$$\begin{aligned} & J_1(u, \phi) \\ = & \frac{1}{2|\Omega|} \int_\Omega \int_\Omega H_{ijkl} \left(\frac{u_{i,j} + u_{j,i}}{2} + \frac{\phi_{i,y_j} + \phi_{j,y_i}}{2} \frac{1}{2} (u_{m,i} + \phi_{m,y_i})(u_{m,j} + \phi_{m,y_j}) \right) \\ & \times \left(\frac{u_{k,l} + u_{l,k}}{2} + \frac{\phi_{k,y_l} + \phi_{l,y_k}}{2} + \frac{1}{2} (u_{m,k} + \phi_{m,y_k})(u_{m,l} + \phi_{m,y_l}) \right) dx\, dy \\ & - \langle u_i, f_i \rangle_{L^2}, \end{aligned} \tag{32}$$

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where

$$V_1 = \{\phi \in W^{1,2}(\Omega \times \Omega; \mathbb{R}^3) \ : \ \phi = 0 \text{ on } \Omega \times \partial\Omega\}.$$

We define also the quasi-convex envelop of J, denoted by $Q_J : V \to \mathbb{R}$, as

$$Q_J(u) = \inf_{\phi \in V_1} J_1(u, \phi).$$

It is a well known result from the modern calculus of variations theory (please see [18] for details), that

$$\inf_{u \in V} J(u) = \inf_{u \in V} Q_J(u).$$

Observe now that, denoting $Y_1 = Y_1^* = L^2(\Omega \times \Omega; \mathbb{R}^9)$, $Y_2 = Y_2^* = L^2(\Omega \times \Omega; \mathbb{R}^3)$, and

$$\begin{aligned} & G_1\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ = \ & \frac{1}{2|\Omega|}\int_\Omega\int_\Omega H_{ijkl}\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ & \times\left(\frac{u_{k,l}+u_{l,k}}{2} + \frac{\phi_{k,y_l}+\phi_{l,y_k}}{2} + \frac{1}{2}(u_{m,k}+\phi_{m,y_k})(u_{m,l}+\phi_{m,y_l})\right) dx\, dy \end{aligned} \tag{33}$$

we have that

$$\begin{aligned} & J_1(u,\phi) \\ = \ & G_1\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) - \langle u_i, f_i\rangle_{L^2} \\ = \ & -\frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right)\sigma_{ij}\, dx\, dy \\ & + G_1\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ & + \frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right)\sigma_{ij}\, dx\, dy - \langle u_i, f_i\rangle_{L^2} \\ \geq \ & \inf_{v \in Y_1}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega v_{ij}\sigma_{ij}\, dx\, dy - G_1(\{v_{ij}\})\right\} \\ & + \inf_{v_2 \in Y_1}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega (v_2)_{ij}\, Q_{ij}\, dx\, dy + \frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\sigma_{ij}\, \frac{1}{2}((v_2)_{mi}(v_2)_{mj})\right) dx\, dy\right\} \\ & + \inf_{(u,\phi)\in V\times V_1}\left\{\frac{1}{|\Omega|}\int_\Omega\int_\Omega(\sigma_{ij}+Q_{ij})\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2}\right) dx\, dy - \langle u_i, f_i\rangle_{L^2}\right\} \\ \geq \ & -\frac{1}{2|\Omega|}\int_\Omega\int_\Omega \overline{H}_{ijkl}\, \sigma_{ij}\, \sigma_{kl}\, dx\, dy \\ & -\frac{1}{2|\Omega|}\int_\Omega\int_\Omega \overline{\sigma_{ij}}\, Q_{mi}\, Q_{mk}\, dx\, dy, \end{aligned} \tag{34}$$

$\forall (u,\phi) \in V \times V_1, (\sigma, Q) \in A^*$, where $A^* = A_1^* \cap A_2^* \cap A_3^*$,

$$A_1^* = \{(\sigma, Q) \in Y_1^* \times Y_1^* \ : \ \sigma_{ij,y_j} + Q_{ij,y_j} = 0, \text{ in } \Omega \times \Omega\}.$$

$$A_2^* = \left\{(\sigma, Q) \in Y_1^* \times Y_1^* \ : \ \frac{1}{|\Omega|}\left(\int_\Omega(\sigma_{ij})\, dy\right)_{x_j} + \frac{1}{|\Omega|}\left(\int_\Omega(Q_{ij})\, dy\right)_{x_j} + f_i = 0, \text{ in } \Omega\right\},$$

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$$A_3^* = \{(\sigma, Q) \in Y_1^* \times Y_1^* \ : \ \{\sigma_{ij}\} \text{ is positive definite in } \Omega \times \Omega\}.$$

Hence, denoting

$$J^*(\sigma, Q) = -\frac{1}{2|\Omega|}\int_\Omega \int_\Omega \overline{H}_{ijkl}\ \sigma_{ij}\ \sigma_{kl}\ dx\ dy - \frac{1}{2|\Omega|}\int_\Omega \int_\Omega \overline{\sigma_{ij}}\ Q_{mi}\ Q_{mk}\ dx\ dy,$$

we have obtained

$$\inf_{u\in V} J(u) \geq \sup_{(\sigma,Q)\in A^*} J^*(\sigma, Q).$$

Remark 6.1. *This last dual functional is concave and such a concerning inequality corresponds a duality principle for the relaxed primal formulation.*

We emphasize again such results are also extensions and in some sense complement the original duality principles in the works of Telega and Bielski, [1–3].

Moreover, if $(\sigma_0, Q_0) \in A^*$ *is such that*

$$\delta J^*(\sigma_0, Q_0) = \mathbf{0},$$

it is a well known result from the Legendre transform proprieties that the corresponding $(u_0, \phi_0) \in V \times V_1$ *such that*

$$(\sigma_0)_{ij} = H_{ijkl}\left(\frac{u_{k,l} + u_{l,k}}{2} + \frac{\phi_{k,y_l} + \phi_{l,y_k}}{2} + \frac{1}{2}(u_{m,k} + \phi_{m,y_k})(u_{m,l} + \phi_{m,y_l})\right)$$

and

$$(Q_0)_{ij} = (\sigma_0)_{im}(v_{2_0})_{mj},$$

is also such that

$$\delta J_1(u_0, \phi_0) = \mathbf{0}$$

and

$$J_1(u_0, \phi_0) = J^*(\sigma_0, Q_0).$$

From this and

$$\inf_{u\in V} J(u) = \inf_{(u,\phi)\in V\times V_1} J_1(u, \phi) \geq \sup_{(\sigma,Q)A^*} J^*(\sigma, Q),$$

we obtain

$$\begin{aligned} J_1(u_0, \phi_0) &= \inf_{(u,\phi)\in V\times V_1} J_1(u, \phi) \\ &= \sup_{(\sigma,Q)\in A^*} J^*(\sigma, Q) \\ &= J^*(\sigma_0, Q_0) \\ &= \inf_{u\in V} J(u). \end{aligned} \tag{35}$$

Also, from the modern calculus of variations theory, there exists a sequence $\{u_n\} \subset V$ *such that*

$$u_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(u_n) \to J_1(u_0, \phi_0) = \inf_{u\in V} J(u).$$

From this and the Ekeland variational principle, there exists $\{v_n\} \subset V$ *such that*

$$\|u_n - v_n\|_V \leq 1/n,$$

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$$J(v_n) \leq \inf_{u \in V} J(u) + 1/n,$$

and

$$\|\delta J(v_n)\|_{V^*} \leq 1/n, \ \forall n \in \mathbb{N},$$

so that

$$v_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(v_n) \to J_1(u_0, \phi_0) = \inf_{u \in V} J(u).$$

Assume now we are dealing with a finite dimensional version of such a model, in a finite elements of finite differences context, for example.

In such a case we have

$$v_n \to u_0, \text{ strongly in } \mathbb{R}^N$$

for an appropriate $N \in \mathbb{N}$.

From continuity we obtain

$$\delta J(v_n) \to \delta J(u_0) = \mathbf{0},$$

$$J(v_n) \to J(u_0).$$

Summarizing, we have got

$$J(u_0) = \inf_{u \in V} J(u),$$

$$\delta J(u_0) = \mathbf{0}.$$

Here we highlight such last results are valid just for this finite-dimensional model version.

7. An Exact Convex Dual Variational Formulation for a Non-Convex Primal One

In this section we develop a convex dual variational formulation suitable to compute a critical point for the corresponding primal one.

Let $\Omega \subset \mathbb{R}^2$ be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = F(u_x, u_y) - \langle u, f \rangle_{L^2},$$

$V = W_0^{1,2}(\Omega)$ and $f \in L^2(\Omega)$.

Here we denote $Y = Y^* = L^2(\Omega)$ and $Y_1 = Y_1^* = L^2(\Omega) \times L^2(\Omega)$.

Defining

$$V_1 = \{u \in V \ : \ \|u\|_{1,\infty} \leq K_1\}$$

for some appropriate $K_1 > 0$, suppose also F is twice Fréchet differentiable and

$$\det\left\{\frac{\partial^2 F(u_x, u_y)}{\partial v_1 \partial v_2}\right\} \neq 0,$$

$\forall u \in V_1$.

Define now $F_1 : V \to \mathbb{R}$ and $F_2 : V \to \mathbb{R}$ by

$$F_1(u_x, u_y) = F(u_x, u_y) + \frac{\varepsilon}{2}\int_\Omega u_x^2 \, dx + \frac{\varepsilon}{2}\int_\Omega u_y^2 \, dx,$$

and

$$F_2(u_x, u_y) = \frac{\varepsilon}{2}\int_\Omega u_x^2 \, dx + \frac{\varepsilon}{2}\int_\Omega u_y^2 \, dx,$$

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where here we denote $dx = dx_1 dx_2$.

Moreover, we define the respective Legendre transform functionals F_1^* and F_2^* as

$$F_1^*(v^*) = \langle v_1, v_1^* \rangle_{L^2} + \langle v_2, v_2^* \rangle_{L^2} - F_1(v_1, v_2),$$

where $v_1, v_2 \in Y$ are such that

$$v_1^* = \frac{\partial F_1(v_1, v_2)}{\partial v_1},$$

$$v_2^* = \frac{\partial F_1(v_1, v_2)}{\partial v_2},$$

and

$$F_2^*(v^*) = \langle v_1, v_1^* + f_1 \rangle_{L^2} + \langle v_2, v_2^* \rangle_{L^2} - F_2(v_1, v_2),$$

where $v_1, v_2 \in Y$ are such that

$$v_1^* + f_1 = \frac{\partial F_2(v_1, v_2)}{\partial v_1},$$

$$v_2^* = \frac{\partial F_2(v_1, v_2)}{\partial v_2}.$$

Here f_1 is any function such that

$$(f_1)_x = f, \text{ in } \Omega.$$

Furthermore, we define

$$\begin{aligned} J^*(v^*) &= -F_1^*(v^*) + F_2^*(v^*) \\ &= -F_1^*(v^*) + \frac{1}{2\varepsilon} \int_\Omega (v_1^* + f_1)^2 \, dx + \frac{1}{2\varepsilon} \int_\Omega (v_2^*)^2 \, dx. \end{aligned} \tag{36}$$

Observe that through the target conditions

$$v_1^* + f_1 = \varepsilon u_x,$$

$$v_2^* = \varepsilon u_y,$$

we may obtain the compatibility condition

$$(v_1^* + f_1)_y - (v_2^*)_x = 0.$$

Define now

$$A^* = \{v^* = (v_1^*, v_2^*) \in B_r(0,0) \subset Y_1^* \ : \ (v_1^* + f_1)_y - (v_2^*)_x = 0, \text{ in } \Omega\},$$

for some appropriate $r > 0$ such that J^* is convex in $B_r(0,0)$.

Consider the problem of minimizing J^* subject to $v^* \in A^*$.

Assuming $r > 0$ is large enough so that the restriction in r is not active, at this point we define the associated Lagrangian

$$J_1^*(v^*, \varphi) = J^*(v^*) + \langle \varphi, (v_1^* + f)_y - (v_2^*)_x \rangle_{L^2},$$

where φ is an appropriate Lagrange multiplier.

Therefore

$$\begin{aligned} J_1^*(v^*) &= -F_1^*(v^*) + \frac{1}{2\varepsilon} \int_\Omega (v_1^* + f_1)^2 \, dx + \frac{1}{2\varepsilon} \int_\Omega (v_2^*)^2 \, dx \\ &\quad + \langle \varphi, (v_1^* + f)_y - (v_2^*)_x \rangle_{L^2}. \end{aligned} \tag{37}$$

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The optimal point in question will be a solution of the corresponding Euler-Lagrange equations for J_1^*.

From the variation of J_1^* in v_1^* we obtain

$$-\frac{\partial F_1^*(v^*)}{\partial v_1^*}+\frac{v_1^*+f}{\varepsilon}-\frac{\partial \varphi}{\partial y}=0. \tag{38}$$

From the variation of J_1^* in v_2^* we obtain

$$-\frac{\partial F_1^*(v^*)}{\partial v_2^*}+\frac{v_2^*}{\varepsilon}+\frac{\partial \varphi}{\partial x}=0. \tag{39}$$

From the variation of J_1^* in φ we have

$$(v_1^*+f)_y-(v_2^*)_x=0.$$

From this last equation, we may obtain $u\in V$ such that

$$v_1^*+f=\varepsilon u_x,$$

and

$$v_2^*=\varepsilon u_y.$$

From this and the previous extremal equations indicated we have

$$-\frac{\partial F_1^*(v^*)}{\partial v_1^*}+u_x-\frac{\partial \varphi}{\partial y}=0,$$

and

$$-\frac{\partial F_1^*(v^*)}{\partial v_2^*}+u_y+\frac{\partial \varphi}{\partial x}=0.$$

so that

$$v_1^*+f=\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_1},$$

and

$$v_2^*=\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_2}.$$

From this and equation (38) and (39) we have

$$\begin{aligned}&-\varepsilon\left(\frac{\partial F_1^*(v^*)}{\partial v_1^*}\right)_x-\varepsilon\left(\frac{\partial F_1^*(v^*)}{\partial v_2^*}\right)_y\\&+(v_1^*+f_1)_x+(v_2^*)_y\\=\;&-\varepsilon u_{xx}-\varepsilon u_{yy}+(v_1^*)_x+(v_2^*)_y+f=0.\end{aligned} \tag{40}$$

Replacing the expressions of v_1^* and v_2^* into this last equation, we have

$$-\varepsilon u_{xx}-\varepsilon u_{yy}+\left(\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_1}\right)_x+\left(\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_2}\right)_y+f=0,$$

so that

$$\left(\frac{\partial F(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_1}\right)_x+\left(\frac{\partial F(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_2}\right)_y+f=0,\ \text{in }\Omega. \tag{41}$$

Observe that if

$$\nabla^2\varphi=0$$

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then there exists $\hat{u}$ such that u and φ are also such that

$$u_x - \varphi_y = \hat{u}_x$$

and

$$u_y + \varphi_x = \hat{u}_y.$$

The boundary conditions for φ must be such that $\hat{u} \in W_0^{1,2}$.

From this and equation (41) we obtain

$$\delta J(\hat{u}) = \mathbf{0}.$$

Summarizing, we may obtain a solution $\hat{u} \in W_0^{1,2}$ of equation $\delta J(\hat{u}) = \mathbf{0}$ by minimizing J^* on A^*.

Finally, observe that clearly J^* is convex in an appropriate large ball $B_r(0,0)$ for some appropriate $r > 0$

8. Another Primal Dual Formulation for a Related Model

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$.

Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx \\ &\quad -\langle u, f\rangle_{L^2}, \end{aligned} \tag{42}$$

$\alpha > 0,\ \beta > 0,\ \gamma > 0$, $V = W_0^{1,2}(\Omega)$ and $f \in L^2(\Omega)$.

Denoting $Y = Y^* = L^2(\Omega)$, define now $J_1^* : V \times Y^* \to \mathbb{R}$ by

$$\begin{aligned} J_1^*(u, v_0^*) &= -\frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx - \langle u^2, v_0^*\rangle_{L^2} \\ &\quad + \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2 \, dx + \langle u, f\rangle_{L^2} \\ &\quad + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx + \beta\int_\Omega v_0^* \, dx, \end{aligned} \tag{43}$$

Define also

$$A^+ = \{u \in V \ : \ u\, f \geq 0, \text{ a.e. in } \Omega\},$$

$$V_2 = \{u \in V \ : \ \|u\|_\infty \leq K_3\},$$

and

$$V_1 = V_2 \cap A^+$$

for some appropriate $K_3 > 0$ to be specified.

Moreover define

$$B^* = \{v_0^* \in Y^* \ : \ \|v_0^*\|_\infty \leq K\}$$

for some appropriate $K > 0$ to be specified.

Observe that, denoting

$$\varphi = -\gamma\nabla^2 u + 2v_0^* u - f$$

we have

$$\frac{\partial^2 J_1^*(u, v_0^*)}{\partial (v_0^*)^2} = \frac{1}{\alpha} + 4K_1 u^2$$

$$\frac{\partial^2 J_1^*(u, v_0^*)}{\partial u^2} = \gamma\nabla^2 - 2v_0^* + K_1(-\gamma\nabla^2 + 2v_0^*)^2$$

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and

$$\frac{\partial^2 J_1^*(u,v_0^*)}{\partial u \partial v_0^*} = K_1(2\varphi + 2(-\gamma\nabla^2 u + 2v_0^* u)) - 2u$$

so that

$$\begin{aligned} & \det\{\delta^2 J_1^*(u,v_0^*)\} \\ = & \frac{\partial^2 J_1^*(u,v_0^*)}{\partial (v_0^*)^2}\frac{\partial^2 J_1^*(u,v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_1^*(u,v_0^*)}{\partial u \partial v_0^*}\right)^2 \\ = & \frac{K_1(-\gamma\nabla^2 + 2v_0^*)^2}{\alpha} - \frac{\gamma\nabla^2 + 2v_0^* + 4\alpha u^2}{\alpha} \\ & -4K_1^2\varphi^2 - 8K_1\varphi(-\gamma\nabla^2 + 2v_0^*)u + 8K_1\varphi u \\ & +4K_1(-\gamma\nabla^2 u + 2v_0^* u)u. \end{aligned} \tag{44}$$

Observe now that a critical point $\varphi = 0$ and $(-\gamma\nabla^2 u + 2v_0^* u)u = fu \geq 0$ in Ω. Therefore, for an appropriate large $K_1 > 0$, also at a critical point, we have

$$\begin{aligned} & \det\{\delta^2 J_1^*(u,v_0^*)\} \\ = & 4K_1 fu - \frac{\delta^2 J(u)}{\alpha} + K_1\frac{(-\gamma\nabla^2 + 2v_0^*)^2}{\alpha} > \mathbf{0}. \end{aligned} \tag{45}$$

Remark 8.1. *From this last equation we may observe that J_1^* has a large region of convexity about any critical point $(u_0, \hat{v}_0^*)$, that is, there exists a large $r > 0$ such that J_1^* is convex on $B_r(u_0, \hat{v}_0^*)$.*

With such results in mind, we may easily prove the following theorem.

Theorem 8.2. *Assume $K_1 \gg \max\{1, K, K_3\}$ and suppose $(u_0, \hat{v}_0^*) \in V_1 \times B^*$ is such that*

$$\delta J_1^*(u_0, \hat{v}_0^*) = \mathbf{0}.$$

Under such hypotheses, there exists $r > 0$ such that J_1^* is convex in $E^* = B_r(u_0, \hat{v}_0^*) \cap (V_1 \times B^*)$,

$$\delta J(u_0) = \mathbf{0},$$

and

$$-J(u_0) = J_1(u_0, \hat{v}_0^*) = \inf_{(u,v_0^*)\in E^*} J_1^*(u, v_0^*).$$

9. A Third Primal Dual Formulation for a Related Model

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$. Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) = & \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx \\ & -\langle u, f\rangle_{L^2}, \end{aligned} \tag{46}$$

$\alpha > 0,\ \beta > 0,\ \gamma > 0, V = W_0^{1,2}(\Omega)$ and $f \in L^2(\Omega)$.

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Denoting $Y = Y^* = L^2(\Omega)$, define now $J_1^* : V \times Y^* \times Y^* \to \mathbb{R}$ by

$$\begin{aligned} J_1^*(u, v_0^*, v_1^*) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{1}{2}\int_\Omega K\, u^2 \, dx \\ &\quad -\langle u, v_1^*\rangle_{L^2} + \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{(-2v_0^* + K)}\, dx \\ &\quad + \frac{1}{2(\alpha+\varepsilon)}\int_\Omega (v_0^* - \alpha(u^2 - \beta))^2 \, dx + \langle u, f\rangle_{L^2} \\ &\quad -\frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx - \beta\int_\Omega v_0^* \, dx, \end{aligned} \tag{47}$$

where $\varepsilon > 0$ is a small real constant.

Define also

$$A^+ = \{u \in V \ : \ u\, f \geq 0, \text{ a.e. in } \Omega\},$$

$$V_2 = \{u \in V \ : \ \|u\|_\infty \leq K_3\},$$

and

$$V_1 = V_2 \cap A^+$$

for some appropriate $K_3 > 0$ to be specified.

Moreover define

$$B^* = \{v_0^* \in Y^* \ : \ \|v_0^*\|_\infty \leq K_4\}$$

and

$$D^* = \{v_1^* \in Y^* \ : \ \|v_1^*\| \leq K_5\},$$

for some appropriate real constants $K_4, K_5 > 0$ to be specified.

Remark 9.1. *Define now*

$$H_1(u, v_0^*) = -\gamma\nabla^2 + 2v_0^* + 4\alpha u^2$$

For an appropriate function (or, in a more general fashion, an appropriate bounded operator) M_1 define

$$B_1^* = \{v_0^* \in B^* \ : \ 2v_0^* + M_1 \geq \varepsilon_1\},$$

for some small parameter $\varepsilon_1 > 0$.

Moreover, define

$$E^* = \{u \in V_1 \ : \ \sqrt{4\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2|}.$$

Since for $(u, v_0^*) \in V_1 \times B_1^*$ we have $u\, f \geq 0$, in Ω, so that for $u_1, u_2 \in V_1$ we have

$$sign\ (u_1) = \ sign\ (u_2) \text{ in } \Omega,$$

we may infer that E^* is a convex set.

Moreover if $(u, v_0^*) \in E^* \times B_1^*$, then

$$\sqrt{4\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2|}$$

so that

$$4\alpha u^2 \geq M_1 + \gamma\nabla^2$$

and

$$2v_0^* + M_1 \geq \varepsilon_1$$

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so that

$$H_1(u, v_0^*) = -\gamma\nabla^2 + 2v_0^* + 4\alpha u^2 \geq \varepsilon_1.$$

Such a result we will be used many times in the next sections.

Observe that, defining

$$\varphi = v_0^* - \alpha(u^2 - \beta)$$

we may obtain

$$\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial u^2} = -\gamma\nabla^2 + K + \frac{\alpha}{\alpha+\varepsilon}4u^2 - 2\varphi\frac{\alpha}{\alpha+\varepsilon}$$

$$\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial (v_1^*)^2} = \frac{1}{-2v_0^* + K}$$

and

$$\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial u \partial v_1^*} = -1$$

so that

$$\begin{aligned}
& \det\left\{\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial u \partial v_1^*}\right\} \\
= & \frac{\partial^2 J_1^*(u, v_1^*, v_0^*)}{\partial (v_1^*)^2}\frac{\partial^2 J_1^*(u, v_1^*, v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_1^*(u, v_1^*, v_0^*)}{\partial u \partial v_1^*}\right)^2 \\
= & \frac{-\gamma\nabla^2 + 2v_0^* + 4\frac{\alpha^2}{\alpha+\varepsilon}u^2 - 2\frac{\alpha}{\alpha+\varepsilon}\varphi}{-2v_0^* + K} \\
\equiv & H(u, v_0^*). \qquad (48)
\end{aligned}$$

However, at a critical point, we have $\varphi = \mathbf{0}$ so that, for a fixed $v_0^* \in B^*$ we define the non-active but convex restriction

$$(C_1)_{v_0^*}^* = \{u \in V_1 \ : \ (\varphi)^2 \leq \varepsilon\},$$

for a small parameter $\varepsilon > 0$.

From such results, assuming $K \gg \max\{K_3, K_4, K_5\}$, and $0 < \varepsilon \ll \varepsilon_1 \ll 1$, we have that

$$H(u, v_0^*) > \mathbf{0},$$

for $v_0^* \in B_1^*$ and $u \in E^* \cap (C_1)_{v_0^*}^*$.

With such results in mind, we may easily prove the following theorem.

Theorem 9.2. *Suppose* $(u_0, \hat{v}_1^*, \hat{v}_0^*) \in (E^* \cap (C_1)_{\hat{v}_0^*}^*) \times D^* \times B_1^*$ *is such that*

$$\delta J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}.$$

Under such hypotheses, we have that

$$\delta J(u_0) = \mathbf{0}$$

and

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$$\begin{aligned} J(u_0) &= \inf_{u\in(C_1)^*_{\hat{v}_0^*}} J(u) \\ &= J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) \\ &= \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*}\left\{\sup_{v_0^*\in B^*} J_1^*(u,v_1^*,v_0^*)\right\} \\ &= \sup_{v_0^*\in B^*}\left\{\inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,v_0^*)\right\}. \end{aligned} \tag{49}$$

Proof. The proof that

$$\delta J(u_0) = \mathbf{0}$$

and

$$J(u_0) = J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*)$$

may be easily made similarly as in the previous sections.

Moreover, observe that for $K > 0$ sufficiently large, we have

$$\frac{\partial^2 J_1^*(u_0,\hat{v}_1^*,v_0^*)}{\partial (v_0^*)^2} < \mathbf{0},\ \forall v_0^* \in B^*$$

so that this and the other hypotheses, we have also

$$J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) = \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,\hat{v}_0^*)$$

and

$$J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) = \sup_{v_0^*\in B^*} J_1^*(u_0,\hat{v}_1^*,v_0^*).$$

From this, from a standard saddle point theorem and the remaining hypotheses, we may infer that

$$\begin{aligned} J(u_0) &= J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) \\ &= \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*}\left\{\sup_{v_0^*\in B^*} J_1^*(u,v_1^*,v_0^*)\right\} \\ &= \sup_{v_0^*\in B^*}\left\{\inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,v_0^*)\right\}. \end{aligned} \tag{50}$$

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Moreover, observe that

$$\begin{aligned} J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) &= \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,\hat{v}_0^*) \\ &\leq \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx+\frac{K}{2}\int_\Omega u^2\,dx \\ &\quad +\langle u^2,\hat{v}_0^*\rangle_{L^2}-\frac{K}{2}\int_\Omega u^2\,dx \\ &\quad -\frac{1}{2\alpha}\int_\Omega(\hat{v}_0^*)^2\,dx-\beta\int_\Omega\hat{v}_0^*\,dx \\ &\quad +\frac{1}{2(\alpha+\varepsilon)}\int_\Omega(\hat{v}_0^*-\alpha(u^2-\beta))^2\,dx-\langle u,f\rangle_{L^2} \\ &\leq \sup_{v_0^*\in Y^*}\left\{\frac{\gamma}{2}\int_\Omega\nabla u\cdot\nabla u\,dx+\langle u^2,v_0^*\rangle\right. \\ &\quad -\frac{1}{2\alpha}\int_\Omega(v_0^*)^2\,dx-\beta\int_\Omega v_0^*\,dx \\ &\quad \left.+\frac{1}{2(\alpha+\varepsilon)}\int_\Omega(v_0^*-\alpha(u^2-\beta))^2\,dx-\langle u,f\rangle_{L^2}\right\} \\ &= \frac{\gamma}{2}\int_\Omega\nabla u\cdot\nabla u\,dx+\frac{\alpha}{2}\int_\Omega(u^2-\beta)^2\,dx \\ &\quad -\langle u,f\rangle_{L^2},\ \forall u\in(C_1)^*_{\hat{v}_0^*}. \end{aligned} \tag{51}$$

Summarizing, we have got

$$J(u_0)=J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*)\leq\inf_{u\in(C_1)^*_{\hat{v}_0^*}}J(u).$$

From such results, we may infer that

$$\begin{aligned} J(u_0) &= \inf_{u\in(C_1)^*_{\hat{v}_0^*}}J(u) \\ &= J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) \\ &= \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*}\left\{\sup_{v_0^*\in B^*}J_1^*(u,v_1^*,v_0^*)\right\} \\ &= \sup_{v_0^*\in B^*}\left\{\inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*}J_1^*(u,v_1^*,v_0^*)\right\}. \end{aligned} \tag{52}$$

The proof is complete. □

10. An Algorithm for a Related Model in Shape Optimization

The next two subsections have been previously published by Fabio Silva Botelho and Alexandre Molter in [8], Chapter 21.

10.1. Introduction

Consider an elastic solid which the volume corresponds to an open, bounded, connected set, denoted by $\Omega\subset\mathbb{R}^3$ with a regular (Lipschitzian) boundary denoted by $\partial\Omega=\Gamma_0\cup\Gamma_t$ where $\Gamma_0\cap\Gamma_t=\emptyset$. Consider also the problem of minimizing the functional $\hat{J}:U\times B\to\mathbb{R}$ where

$$\hat{J}(u,t)=\frac{1}{2}\langle u_i,f_i\rangle_{L^2(\Omega)}+\frac{1}{2}\langle u_i,\hat{f}_i\rangle_{L^2(\Gamma_t)},$$

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subject to

$$\begin{cases} (H_{ijkl}(t)e_{kl}(u))_{,j} + f_i = 0 \text{ in } \Omega, \\ \\ H_{ijkl}(t)e_{kl}(u)n_j - \hat{f}_i = 0, \text{ on } \Gamma_t, \ \forall i \in \{1,2,3\}. \end{cases} \tag{53}$$

Here $\mathbf{n} = (n_1, n_2, n_3)$ denotes the outward normal to $\partial\Omega$ and

$$U = \{u = (u_1, u_2, u_3) \in W^{1,2}(\Omega; \mathbb{R}^3) \ : \ u = (0,0,0) = \mathbf{0} \text{ on } \Gamma_0\},$$

$$B = \left\{ t : \Omega \to [0,1] \text{ measurable } \ : \ \int_\Omega t(x)\, dx = t_1|\Omega| \right\},$$

where

$$0 < t_1 < 1$$

and $|\Omega|$ denotes the Lebesgue measure of Ω.

Moreover $u = (u_1, u_2, u_3) \in W^{1,2}(\Omega; \mathbb{R}^3)$ is the field of displacements relating the cartesian system $(0, x_1, x_2, x_3)$, resulting from the action of the external loads $f \in L^2(\Omega; \mathbb{R}^3)$ and $\hat{f} \in L^2(\Gamma_t; \mathbb{R}^3)$.

We also define the stress tensor $\{\sigma_{ij}\} \in Y^* = Y = L^2(\Omega; \mathbb{R}^{3\times 3})$, by

$$\sigma_{ij}(u) = H_{ijkl}(t)e_{kl}(u),$$

and the strain tensor $e : U \to L^2(\Omega; \mathbb{R}^{3\times 3})$ by

$$e_{ij}(u) = \frac{1}{2}(u_{i,j} + u_{j,i}), \ \forall i, j \in \{1,2,3\}.$$

Finally,

$$\{H_{ijkl}(t)\} = \{tH^0_{ijkl} + (1-t)H^1_{ijkl}\},$$

where H^0 corresponds to a strong material and H^1 to a very soft material, intending to simulate voids along the solid structure.

The variable t is the design one, which the optimal distribution values along the structure are intended to minimize its inner work with a volume restriction indicated through the set B.

The duality principle obtained is developed inspired by the works in [1,2]. Similar theoretical results have been developed in [7], however we believe the proof here presented, which is based on the min-max theorem is easier to follow (indeed we thank an anonymous referee for his suggestion about applying the min-max theorem to complete the proof). We highlight throughout this text we have used the standard Einstein sum convention of repeated indices.

Moreover, details on the Sobolev spaces addressed may be found in [6]. In addition, the primal variational development of the topology optimization problem has been described in [7].

The main contributions of this work are to present the detailed development, through duality theory, for such a kind of optimization problems. We emphasize that to avoid the check-board standard and obtain appropriate robust optimized structures without the use of filters, it is necessary to discretize more in the load direction, in which the displacements are much larger.

10.2. Mathematical Formulation of the Topology Optimization Problem

Our mathematical topology optimization problem is summarized by the following theorem.

Theorem 10.1. *Consider the statements and assumptions indicated in the last section, in particular those refereing to Ω and the functional $\hat{J} : U \times B \to \mathbb{R}$.*

Define $J_1 : U \times B \to \mathbb{R}$ by

$$J_1(u,t) = -G(e(u),t) + \langle u_i, f_i \rangle_{L^2(\Omega)} + \langle u_i, \hat{f}_i \rangle_{L^2(\Gamma_t)},$$

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where

$$G(e(u),t) = \frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx,$$

and where

$$dx = dx_1dx_2dx_3.$$

Define also $J^* : U \to \mathbb{R}$ *by*

$$\begin{aligned} J^*(u) &= \inf_{t\in B}\{J_1(u,t)\} \\ &= \inf_{t\in B}\{-G(e(u),t) + \langle u_i, f_i\rangle_{L^2(\Omega)} + \langle u_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\}. \end{aligned} \tag{54}$$

Assume there exists $c_0, c_1 > 0$ *such that*

$$H^0_{ijkl}z_{ij}z_{kl} > c_0 z_{ij}z_{ij}$$

and

$$H^1_{ijkl}z_{ij}z_{kl} > c_1 z_{ij}z_{ij},\ \forall z = \{z_{ij}\} \in \mathbb{R}^{3\times 3},\ \text{such that } z \neq \mathbf{0}.$$

Finally, define $J : U \times B \to \mathbb{R}\cup\{+\infty\}$ *by*

$$J(u,t) = \hat{J}(u,t) + Ind(u,t),$$

where

$$Ind(u,t) = \begin{cases} 0, & \text{if } (u,t) \in A^*, \\ +\infty, & \text{otherwise}, \end{cases} \tag{55}$$

where $A^* = A_1 \cap A_2$,

$$A_1 = \{(u,t) \in U\times B\ :\ (\sigma_{ij}(u))_{,j} + f_i = 0,\ \text{in } \Omega,\ \forall i \in \{1,2,3\}\}$$

and

$$A_2 = \{(u,t) \in U\times B\ :\ \sigma_{ij}(u)n_j - \hat{f}_i = 0,\ \text{on } \Gamma_t,\ \forall i \in \{1,2,3\}\}.$$

Under such hypotheses, there exists $(u_0,t_0) \in U\times B$ *such that*

$$\begin{aligned} J(u_0,t_0) &= \inf_{(u,t)\in U\times B} J(u,t) \\ &= \sup_{\hat{u}\in U} J^*(\hat{u}) \\ &= J^*(u_0) \\ &= \hat{J}(u_0,t_0) \\ &= \inf_{(t,\sigma)\in B\times C^*} G^*(\sigma,t) \\ &= G^*(\sigma(u_0),t_0), \end{aligned} \tag{56}$$

where

$$\begin{aligned} G^*(\sigma,t) &= \sup_{v\in Y}\{\langle v_{ij}, \sigma_{ij}\rangle_{L^2(\Omega)} - G(v,t)\} \\ &= \frac{1}{2}\int_\Omega \overline{H}_{ijkl}(t)\sigma_{ij}\sigma_{kl}\,dx, \end{aligned} \tag{57}$$

$$\{\overline{H}_{ijkl}(t)\} = \{H_{ijkl}(t)\}^{-1}$$

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and $C^* = C_1 \cap C_2$, *where*

$$C_1 = \{\sigma \in Y^* \ : \ \sigma_{ij,j} + f_i = 0, \ in \ \Omega, \ \forall i \in \{1,2,3\}\}$$

and

$$C_2 = \{\sigma \in Y^* \ : \ \sigma_{ij} n_j - \hat{f}_i = 0, \ on \ \Gamma_t, \ \forall i \in \{1,2,3\}\}.$$

Proof. Observe that

$$\begin{aligned}
\inf_{(u,t)\in U\times B} J(u,t) &= \inf_{t\in B}\left\{\inf_{u\in U} J(u,t)\right\} \\
&= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{\inf_{u\in U}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx\right.\right.\right. \\
&\quad +\langle \hat{u}_i, (H_{ijkl}(t)e_{kl}(u))_{,j} + f_i\rangle_{L^2(\Omega)} \\
&\quad \left.\left.\left. -\langle \hat{u}_i, H_{ijkl}(t)e_{kl}(u)n_j - \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\}\right\} \\
&= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{\inf_{u\in U}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx\right.\right.\right. \\
&\quad -\int_\Omega H_{ijkl}(t)e_{ij}(\hat{u})e_{kl}(u)\,dx \\
&\quad \left.\left.\left. +\langle \hat{u}_i, f_i\rangle_{L^2(\Omega)} + \langle \hat{u}_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\}\right\} \\
&= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{-\int_\Omega H_{ijkl}(t)e_{ij}(\hat{u})e_{kl}(\hat{u})\,dx\right.\right. \\
&\quad \left.\left. \langle \hat{u}_i, f_i\rangle_{L^2(\Omega)} + \langle \hat{u}_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\} \\
&= \inf_{t\in B}\left\{\inf_{\sigma\in C^*} G^*(\sigma,t)\right\}. \qquad (58)
\end{aligned}$$

Also, from this and the min-max theorem, there exist $(u_0, t_0) \in U \times B$ such that

$$\begin{aligned}
\inf_{(u,t)\in U\times B} J(u,t) &= \inf_{t\in B}\left\{\sup_{\hat{u}\in U} J_1(u,t)\right\} \\
&= \sup_{u\in U}\left\{\inf_{t\in B} J_1(u,t)\right\} \\
&= J_1(u_0,t_0) \\
&= \inf_{t\in B} J_1(u_0,t) \\
&= J^*(u_0). \qquad (59)
\end{aligned}$$

Finally, from the extremal necessary condition

$$\frac{\partial J_1(u_0,t_0)}{\partial u} = \mathbf{0}$$

we obtain

$$(H_{ijkl}(t_0)e_{kl}(u_0))_{,j} + f_i = 0 \text{ in } \Omega,$$

and

$$H_{ijkl}(t_0)e_{kl}(u_0)n_j - \hat{f}_i = 0 \text{ on } \Gamma_t, \ \forall i \in \{1,2,3\},$$

so that

$$G(e(u_0)) = \frac{1}{2}\langle (u_0)_i, f_i\rangle_{L^2(\Omega)} + \frac{1}{2}\langle (u_0)_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}.$$

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Hence $(u_0, t_0) \in A^*$ so that $Ind(u_0, t_0) = 0$ and $\sigma(u_0) \in C^*$.
Moreover

$$\begin{aligned} J^*(u_0) &= -G(e(u_0)) + \langle (u_0)_i, f_i \rangle_{L^2(\Omega)} + \langle (u_0)_i, \hat{f}_i \rangle_{L^2(\Gamma_t)} \\ &= G(e(u_0)) \\ &= G(e(u_0)) + Ind(u_0, t_0) \\ &= J(u_0, t_0) \\ &= G^*(\sigma(u_0), t_0). \end{aligned} \tag{60}$$

This completes the proof. □

10.3. About a Concerning Algorithm and Related Numerical Method

For numerically solve this optimization problem in question, we present the following algorithm

1. Set $t_1 = 0.5$ in Ω and $n = 1$.
2. Calculate $u_n \in U$ such that
$$J_1(u_n, t_n) = \sup_{u \in U} J_1(u, t_n).$$
3. Calculate $t_{n+1} \in B$ such that
$$J_1(u_n, t_{n+1}) = \inf_{t \in B} J_1(u_n, t).$$
4. If $\|t_{n+1} - t_n\|_\infty < 10^{-4}$ or $n > 100$ then stop, else set $n := n + 1$ and go to item 2.

We have developed a software in finite differences for solving such a problem.
Here the software.
****

1. clear all

global P m8 d w u v Ea Eb Lo d1 z1 m9 du1 du2 dv1 dv2 c3

m8=27;

m9=24;

c3=0.95;

d=1.0/m8;

d1=0.5/m9;

Ea=$210 * 10^5$; (stronger material)

Eb=1000; (softer material simulating voids)

w=0.30;

P=-42000000;

z1=(m8-1)*(m9-1);

A3=zeros(z1,z1);

for i=1:z1

A3(1,i)=1.0;

end;

b=zeros(z1,1);

uo=0.000001*ones(z1,1);

u1=ones(z1,1);

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b(1,1)=c3*z1;
for i=1:m9-1
for j=1:m8-1
Lo(i,j)=c3;
end; end;
for i=1:z1
x1(i)=c3*z1;
end;
for i=1:2*m8*m9
xo(i)=0.000;
end;
xw=xo;
xv=Lo;
for k2=1:24
c3=0.98*c3;
b(1,1)=c3*z1;
k2
b14=1.0;
k3=0;
while $(b14 > 10^{-3.5})$ and $(k3 < 5)$
k3=k3+1;
b12=1.0;
k=0;
while $(b12 > 10^{-4.0})$ and $(k < 120)$
k=k+1;
k2
k3
k
X=fminunc('funbeam',xo);
xo=X;
b12=max(abs(xw-xo));
xw=X;
end;
for i=1:m9-1
for j=1:m8-1
$E1 = Lo(i,j)^2 * (Ea - Eb)$;
ex=du1(i,j);
ey=dv2(i,j);
exy=1/2*(dv1(i,j)+du2(i,j));

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$Sx = E1 * (ex + w * ey)/(1 - w^2);$

$Sy = E1 * (w * ex + ey)/(1 - w^2);$

```
Sxy=E1/(2*(1+w))*exy;
dc3(i,j)=-(Sx*ex+Sy*ey+2*Sxy*exy);
end;
end;
for i=1:m9-1
for j=1:m8-1
f(j+(i-1)*(m8-1))=dc3(i,j);
end;
end;
for k1=1:1
k1
X1=linprog(f,[ ],[ ],A3,b,uo,u1,x1);
x1=X1;
end;
for i=1:m9-1
for j=1:m8-1
Lo(i,j)=X1(j+(m8-1)*(i-1));
end;
end;
b14=max(max(abs(Lo-xv)))
xv=Lo;
colormap(gray); imagesc(-Lo); axis equal; axis tight; axis off;pause(1e-6)
end;
end;
```

****

Here the auxiliary Function 'funbeam'

```
function S=funbeam(x)
global P m8 d w u v Ea Eb Lo d1 m9 du1 du2 dv1 dv2
for i=1:m9
for j=1:m8
u(i,j)=x(j+(m8)*(i-1));
v(i,j)=x(m8*m9+(i-1)*m8+j);
end;
end;
for i=1:m9
end;
u(m9-1,1)=0;
v(m9-1,1)=0;
u(m9-1,m8-1)=0;
```

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```
v(m9-1,m8-1)=0;
for i=1:m9-1
for j=1:m8-1
du1(i,j)=(u(i,j+1)-u(i,j))/d;
du2(i,j)=(u(i+1,j)-u(i,j))/d1;
dv1(i,j)=(v(i,j+1)-v(i,j))/d;
dv2(i,j)=(v(i+1,j)-v(i,j))/d1;
end;
end;
S=0;
for i=1:m9-1
for j=1:m8-1
E1 = Lo(i,j)^3 * Ea + (1 - Lo(i,j)^3) * Eb;
ex=du1(i,j);
ey=dv2(i,j);
exy=1/2*(dv1(i,j)+du2(i,j));
Sx = E1 * (ex + w * ey)/(1 - w^2);
Sy = E1 * (w * ex + ey)/(1 - w^2);
Sxy=E1/(2*(1+w))*exy;
S=S+1/2*(Sx*ex+Sy*ey+2*Sxy*exy);
end;
end;
S=S*d*d1-P*v(2,(m8)/3)*d*d1;
```

****

For a two dimensional beam of dimensions $1m \times 0.5m$ and $t_1 = 0.63$ we have obtained the following results:

1. Case A: For the optimal shape for a clamped beam at left (cantilever) and load $P = -4\ 10^6 N\mathbf{j}$ at $(x, y) = (1, 0.25)$, please Figure 5.
2. Case B :For the optimal shape for a simply supported beam at $(0, 0)$ and $(1, 0)$ and load $P = -4\ 10^6 N\mathbf{j}$ at $(x, y) = (1/3, 0.5)$, please Figure 6.

   In the first case the mesh was 28×24. In the second one the mesh was 27×24

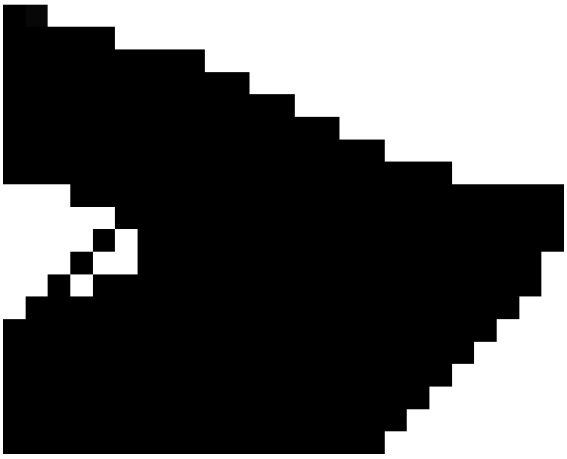

Figure 5. Density $t(x, y)$ for the Case A.

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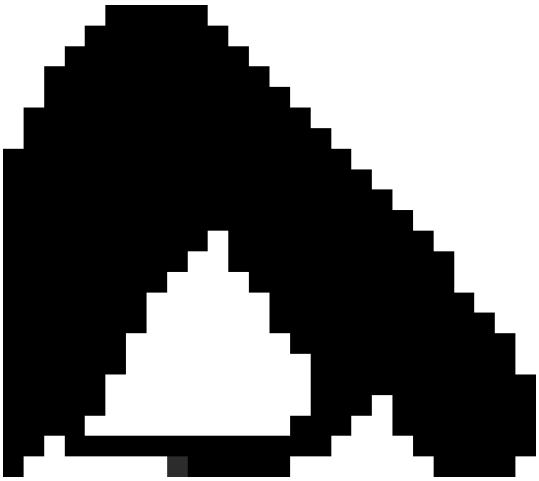

Figure 6. Density $t(x, y)$ for the Case B.

11. A Duality Principle for a General Vectorial Case in the Calculus of Variations

In this section we develop a duality principle for a general vectorial case in variational optimization.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$. Let $J : V \to \mathbb{R}$ be a functional where

$$J(u) = G(\nabla u_1, \cdots, \nabla u_N) - \langle u, f \rangle_{L^2},$$

where

$$V = W_0^{1,2}(\Omega; \mathbb{R}^N)$$

and

$$f = (f_1, \cdots, f_N) \in L^2(\Omega; \mathbb{R}^N).$$

Here we have denoted $u = (u_1, \cdots, u_N) \in V$ and

$$\langle u, f \rangle_{L^2} = \langle u_i, f_i \rangle_{L^2},$$

so that we may also denote

$$J(u) = G(\nabla u) - \langle u, f \rangle_{L^2}.$$

Assume

$$G(\nabla u) = \int_\Omega g(\nabla u)\, dx$$

where $g : \mathbb{R}^{3N} \to \mathbb{R}$ is a differentiable function such that

$$g(y) \to +\infty$$

as $|y| \to \infty$. Moreover, suppose there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = \inf_{u \in V} J(u).$$

It is well known that

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$$\begin{aligned}\alpha &= \inf_{u\in V} J(u)\\ &= \inf_{u\in V} J^{**}(u)\\ &= \inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u, f\rangle_{L^2}\}. \end{aligned} \tag{61}$$

Under some mild hypotheses, from convexity, we have that

$$\begin{aligned}&\inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u, f\rangle_{L^2}\}\\ =\ &\sup_{v^*\in A^*}\{-(G\circ\nabla)^*(-div\ v^*)\} = -(G\circ\nabla)^*(f), \end{aligned} \tag{62}$$

where

$$A^* = \{v^* \in Y = Y^* = L^2(\Omega;\mathbb{R}^{3N})\ :\ div\ v^* + f = 0\}.$$

Now observe that the restriction $v = \nabla u$ for some $u \in V$ is equivalent to the restriction

$$\text{curl}\ v_i = \mathbf{0},\ \text{in}\ \Omega$$

where $v = \{v_i\} = \{v_{ij}\}_{j=1}^3, \forall i \in \{1,\cdots,N\}$, with appropriate boundary conditions, so that with an appropriate Lagrange multiplier $\phi = \{\phi_i\}$, we obtain

$$\begin{aligned}(G\circ\nabla)^*(-div\ v^*) &= \sup_{u\in V}\{\langle u, -div\ v^*\rangle_{L^2} - G(\nabla u)\}\\ &= \sup_{u\in V}\{\langle \nabla u, v^*\rangle_{L^2} - G(\nabla u)\}\\ &\le \inf_{\phi\in Y^*}\left\{\sup_{v\in Y}\{\langle v, v^*\rangle_{L^2} - G(v) + \langle \phi, \text{curl}\ v\rangle_{L^2}\right\}\\ &= \inf_{\phi\in Y^*} G^*(v^* + \text{curl}\ \phi). \end{aligned} \tag{63}$$

where we have denoted

$$\text{curl}\ v = \{\text{curl}\ v_i\}$$

and

$$\text{curl}\ \phi = \{\text{curl}\ \phi_i\}.$$

Joining the pieces, we have got

$$\begin{aligned}\inf_{u\in V} J(u) &= \inf_{u\in V}\{G(\nabla u) - \langle u, f\rangle_{L^2}\}\\ &\ge \sup_{(v^*,\phi)\in A^*\times Y^*}\{-G^*(v^* + \text{curl}\ \phi)\}, \end{aligned} \tag{64}$$

where we recall that $Y = Y^* = L^2(\Omega;\mathbb{R}^{3N})$.

We emphasize such a dual formulation in (v^*, ϕ) is convex (in fact concave).

12. A Note on the Galerkin Functional

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

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Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad -\frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \end{aligned} \tag{65}$$

Here $V = W_0^{1,2}(\Omega)$, $\gamma > 0$, $\alpha > 0$, $\beta > 0$.
We denote also

$$Y = Y^* = L^2(\Omega).$$

At this point we define

$$A^+ = \{u \in V \ : \ u\, f \geq 0, \text{ in } \Omega\},$$

$$V_2 = \{u \in V \ : \ \|u\|_\infty \leq K_3\},$$

for some appropriate real constant $K_3 > 0$ and

$$V_1 = A^+ \cap V_2.$$

Observe that

$$J'(u) = -\gamma\nabla^2 u + \alpha u^3 - \beta - f,$$

so that we define the Galerkin functional $J_1 : V \to \mathbb{R}$ by

$$J_1(u) = \frac{1}{2}\|J'(u)\|_2^2 = \frac{1}{2}\int_\Omega (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2 \, dx.$$

From this, we get

$$\begin{aligned} \frac{\partial^2 J_1(u)}{\partial u^2} &= (-\gamma\nabla u + \alpha u^3 - \beta u - f)6\alpha u \\ &\quad +(-\gamma\nabla^2 + 3\alpha u^2 - \beta)^2. \end{aligned} \tag{66}$$

Define now

$$\varphi_2 = (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)6\alpha u.$$

At this point, for an appropriate small real constant $\varepsilon_1 > 0$ and bounded constant operator $M_1 > \varepsilon_1$, we set the intended non-active restriction

$$\sqrt{3\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2 + \beta|},$$

and define

$$B_1 = \{u \in V_1 \ : \ \sqrt{3\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2 + \beta|}\}.$$

Observe that since for $u \in V_1$ we have $u\, f \geq 0$ in Ω so that if $u_1, u_2 \in V_1$ then

$$\text{sign}(u_1) = \text{sign}(u_2), \text{in } \Omega,$$

we may infer that B_1 is a convex set.

Furthermore, if $u \in B_1$, then

$$\sqrt{3\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2 + \beta|},$$

so that

$$3\alpha u^2 \geq M_1 + \gamma\nabla^2 + \beta,$$

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and hence

$$\delta^2 J(u) = -\gamma\nabla^2 + 3\alpha u^2 - \beta \geq M_1 > \varepsilon_1 > \mathbf{0}.$$

Observe now that

$$\frac{\partial^2 \varphi_2}{\partial u^2} = 12\alpha(-\gamma\nabla^2 + 3\alpha u^2 - \beta).$$

From such a result we may infer that

$$\frac{\partial^2 \varphi_2}{\partial u^2} \geq \mathbf{0}, \text{ on } B_1,$$

so that φ_2 is convex in B_1.

For a small parameter $\varepsilon > 0$ we define the intended non-active restriction

$$|\varphi_2| \leq \varepsilon, \text{ in } \Omega,$$

and define

$$B_3 = \{u \in B_1 \ : \ |\varphi_2| \leq \varepsilon, \text{ in } \Omega\}.$$

Assuming $0 < \varepsilon \ll \varepsilon_1 \ll 1$,

Summarizing, if $u \in B_3$, then

$$\delta^2 J_1(u) \geq \mathbf{0}.$$

With such results in mind, we define the following optimization problem for finding a critical point of J.

Minimize

$$J_1(u) = \frac{1}{2}\|J'(u)\|_2^2 = \frac{1}{2}\int_\Omega (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2 \, dx,$$

subject to

$$u \in B_3.$$

Finally, we may also define the optimization problem of minimizing

$$\begin{aligned} J_3(u) &= K_1 J_1(u) + J(u) \\ &= \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2 \, dx \\ &\quad + \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad - \frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{67}$$

subject to

$$u \in B_3.$$

Here $K_1 > 0$ is a large real constant.

13. A Note on the Legendre-Galerkin Functional

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad - \frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \end{aligned} \tag{68}$$

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Here $V = W_0^{1,2}(\Omega)$, $\gamma > 0$, $\alpha > 0$, $\beta > 0$.
We denote also

$$Y = Y^* = L^2(\Omega)$$

and $F_1 : V \to \mathbb{R}$, $F_2 : V \to \mathbb{R}$ and $F_3 : V \to \mathbb{R}$ by

$$F_1(u) = \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx,$$

$$F_2(u) = \frac{\alpha}{4} \int_\Omega u^4 \, dx,$$

$$F_3(u) = \frac{\beta}{2} \int_\Omega u^2 \, dx.$$

Moreover, we define $F_1^*, F_2^*, F_3^* : Y^* \to \mathbb{R}$ by

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u \in V} \{ \langle u, v_1^* \rangle_{L^2} - F_1(u) \} \\ &= \frac{1}{2} \int_\Omega \frac{(v_1^*)^2}{-\gamma \nabla^2} \, dx, \end{aligned} \tag{69}$$

$$\begin{aligned} F_2^*(v_2^*) &= \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \} \\ &= \frac{3}{4} \int_\Omega \frac{(v_2^*)^{4/3}}{\alpha^{1/3}} \, dx, \end{aligned} \tag{70}$$

$$\begin{aligned} F_3^*(v_3^*) &= \sup_{u \in V} \{ \langle u, v_3^* \rangle_{L^2} - F_3(u) \} \\ &= \frac{1}{2\beta} \int_\Omega (v_3^*)^2 \, dx. \end{aligned} \tag{71}$$

Observe now that these three last suprema are attained through the equations,

$$v_1^* = \frac{\partial F_1(u)}{\partial u} = -\gamma \nabla^2 u,$$

$$v_2^* = \frac{\partial F_2(u)}{\partial u} = \alpha u^3$$

$$v_3^* = \frac{\partial F_3(u)}{\partial u} = \beta u.$$

From such results, at a critical point, we obtain the following compatibility conditions

$$u = \frac{v_1^*}{-\gamma \nabla^2} = \left(\frac{v_2^*}{\beta} \right)^{1/3} = \frac{v_3^*}{\beta}.$$

From such relations we have

$$\frac{v_1^*}{-\gamma \nabla^2} = \frac{v_3^*}{\beta},$$

and

$$v_2^* = \alpha \left(\frac{v_3^*}{\beta} \right)^3,$$

so that

$$v_1^* = -\gamma \nabla^2 \left(\frac{v_3^*}{\beta} \right),$$

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and

$$v_2^* = \alpha\left(\frac{v_3^*}{\beta}\right)^3.$$

Moreover, we define the functional $F_4^* : Y^* \to \mathbb{R}$, by

$$F_4^*(v^*) = \sup_{u\in V}\{\langle u, v_1^* + v_2^* - v_3^*\rangle_{L^2} - \langle u, f\rangle_{L^2}\}.$$

Therefore

$$F_4^*(v^*) = \begin{cases} 0, & \text{if } v_1^* + v_2^* - v_3^* - f = 0, \text{ in } \Omega, \\ +\infty, & \text{otherwise.} \end{cases} \tag{72}$$

Hence, a critical point of J corresponds to the solution of the following system of equations

$$v_1^* = -\gamma\nabla^2\left(\frac{v_3^*}{\beta}\right),$$

$$v_2^* = \alpha\left(\frac{v_3^*}{\beta}\right)^3,$$

and

$$v_1^* + v_2^* - v_3^* - f = 0, \text{ in } \Omega.$$

From this last equation we may obtain

$$v_1^* = -v_2^* + v_3^* + f,$$

so that the final equations to be solved are

$$-v_2^* + v_3^* + f + \gamma\nabla^2\left(\frac{v_3^*}{\beta}\right) = 0$$

and

$$v_2^* - \alpha\left(\frac{v_3^*}{\beta}\right)^3 = 0, \text{ in } \Omega,$$

with the boundary conditions

$$u = \frac{v_3^*}{\beta} = 0, \text{ on } \partial\Omega.$$

With such results in mind, we define the Legendre-Galerkin functional $J^* : [Y^*]^2 \to \mathbb{R}$, where

$$\begin{aligned} J^*(v^*) &= \frac{1}{2}\int_\Omega\left(-v_2^* + v_3^* + f + \frac{\gamma\nabla^2 v_3^*}{\beta}\right)^2 dx \\ &\quad + \frac{1}{2}\int_\Omega\left(v_2^* - \alpha\left(\frac{v_3^*}{\beta}\right)^3\right)^2 dx. \end{aligned} \tag{73}$$

At this point, defining

$$\varphi = v_2^* - \alpha\left(\frac{v_3^*}{\beta}\right)^3,$$

we obtain

$$\frac{\partial^2 J^*(v^*)}{\partial(v_2^*)^2} = 2;$$

$$\frac{\partial^2 J^*(v^*)}{\partial(v_3^*)^2} = \left(-1 - \frac{\gamma\nabla^2}{\beta}\right)^2 + \frac{9\alpha^2(v_3^*)^4}{\beta^6} + \mathcal{O}(\varphi),$$

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$$\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*} = \frac{-3\alpha (v_3^*)^2}{\beta^3} + \left(-1 - \frac{\gamma \nabla^2}{\beta}\right).$$

From such results we may infer that

$$\begin{aligned} \det\left(\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*}\right) &= \frac{\partial^2 J^*(v^*)}{\partial (v_2^*)^2} \frac{\partial^2 J^*(v^*)}{\partial (v_3^*)^2} - \left(\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*}\right)^2 \\ &= \left(-1 - \frac{\gamma \nabla^2}{\beta} + 3\alpha \frac{(v_3^*)^2}{\beta^3}\right)^2 + \mathcal{O}(\varphi) \end{aligned} \tag{74}$$

Observe that a critical point $\varphi = 0$ so that $\delta^2 J^*(v^*) > \mathbf{0}$ at a neighborhood of any critical point.

At this point we define

$$A^+ = \left\{ v^* = (v_2^*, v_3^*) \in [Y^*]^2 \ : \ \frac{v_3^*}{\beta} f \geq 0, \text{ in } \Omega \right\},$$

$$D^* = \{ v^* = (v_2^*, v_3^*) \in [Y^*]^2 \ : \ \|v^*\|_\infty \leq K \},$$

for an appropriate real constant $K > 0$.

Define now $E^* = A^+ \cap D^*$,

$$C_1^* = \{ v^* = (v_2^*, v_3^*) \in E^* \ : \ \varphi^2 \leq \varepsilon, \text{ in } \Omega \},$$

for a small real constant $\varepsilon > 0$,

$$C_2^* = \left\{ v^* = (v_2^*, v_3^*) \in E^* \ : \ \left(-1 - \frac{\gamma \nabla^2}{\beta} + 3\alpha \frac{(v_3^*)^2}{\beta^3}\right) \geq \varepsilon_1 \right\},$$

and

$$C^* = C_1^* \cap C_2^*.$$

Similarly as done in the previous section, we may prove that C^* is a convex set.

Furthermore, for $0 < \varepsilon \ll \varepsilon_1 \ll 1$, we have that J^* is convex on C^*.

Summarizing, we may define the following convex optimization problem to obtain a critical point of the primal functional J,

$$\text{Minimize } J^*(v_2^*, v_3^*) \text{ subject to } v^* = (v_2^*, v_3^*) \in C^*.$$

We call J^* the Legendre-Galerkin functional associated to J.

13.1. Numerical Examples

We have obtained numerical solutions for two one-dimensional examples.

1. For $\gamma = 1.0$, $\alpha = 3.0$, $\beta = 30.0$, $f \equiv 10$, in $\Omega = [0, 1]$.

   For the respective solution please see Figure 7.
2. For $\gamma = 0.01$, $\alpha = 3.0$, $\beta = 30.0$, $f \equiv 10$, in $\Omega = [0, 1]$.

   For the respective solution please see Figure 8.

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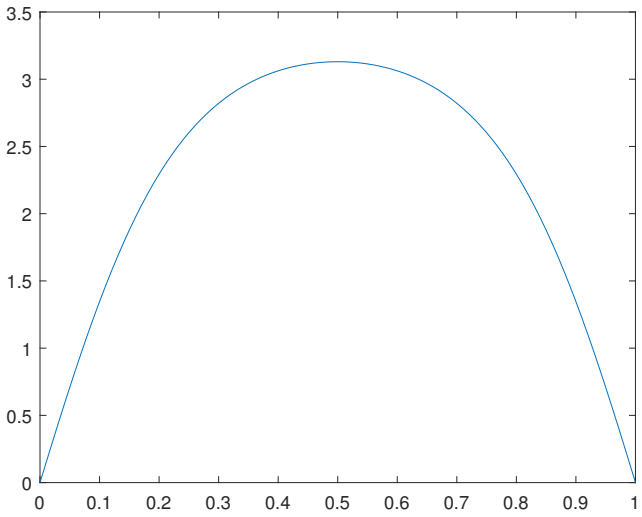

Figure 7. Solution $u(x) = v_3^*(x)/\beta$ for the example 1.

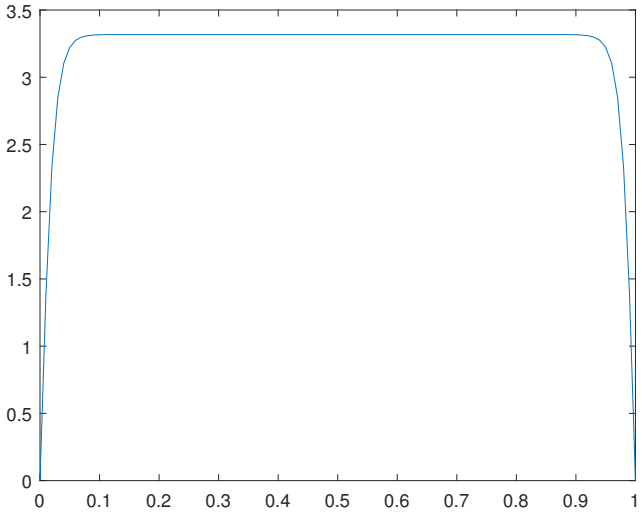

Figure 8. Solution $u(x) = v_3^*(x)/\beta$ for the example 2.

14. A General Concave Dual Variational Formulation for Global Optimization

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = G(u) - \langle u, f \rangle_{L^2}, \ \forall u \in V.$$

Here $V = W_0^{1,2}(\Omega)$, $f \in L^2(\Omega)$ and we also denote $Y = Y^* = L^2(\Omega)$.
Assume there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = \inf_{u \in V} J(u).$$

Furthermore, suppose G is three times Fréchet differentiable and there exists $K > 0$ such that

$$\frac{\partial^2 G(u)}{\partial u^2} + K > \mathbf{0}, \forall u \in V.$$

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Define now $J_1 : V \times Y \to \mathbb{R}$ where,

$$J_1(u,v) = G_1(u,v) + F(u),$$

where

$$G_1(u,v) = G(v) - \frac{\varepsilon}{2}\int_\Omega v^2\,dx + \frac{K}{2}\int_\Omega (v-u)^2\,dx,$$

and

$$F(u) = \frac{\varepsilon}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2}.$$

Moreover, we define the polar functionals $G_1^* : Y^* \times V \to \mathbb{R}$ and $F^* : Y^* \to \mathbb{R}$, where

$$\begin{aligned} G_1^*(v^*,u) &= \sup_{v\in Y}\{\langle v, v^*\rangle_{L^2} - G_1(u,v)\} \\ &= -G_{K_\varepsilon}^*(v^* + Ku) + \frac{K}{2}\int_\Omega u^2\,dx, \end{aligned} \tag{75}$$

$$G_{K_\varepsilon}^*(v^* + Ku) = \sup_{v\in Y}\left\{\langle v, v^*\rangle_{L^2} - G(v) - \frac{K}{2}\int_\Omega v^2\,dx + \frac{\varepsilon}{2}\int_\Omega v^2\,dx\right\},$$

and

$$\begin{aligned} F^*(-v^*) &= \sup_{u\in V}\{-\langle u, v^*\rangle_{L^2} - F(u)\} \\ &= \frac{1}{2\varepsilon}\int_\Omega (v^* - f)^2\,dx. \end{aligned} \tag{76}$$

At this point we define the functional $J_2^* : Y^* \times V \to \mathbb{R}$ by

$$J_2^*(v^*,u) = -G_{K_\varepsilon}^*(v^* + Ku) + \frac{K}{2}\int_\Omega u^2\,dx - F^*(-v^*).$$

With such results in mind we define

$$V_1 = \{u \in V \ : \ \|u\|_\infty \le K_3\},$$

and

$$D^* = \{v^* \in Y^* \ : \ \|v^*\|_\infty \le K_4\},$$

for appropriated real constants $K_3 > 0$ and $K_4 > 0$.

Moreover, we define also the penalized functional $J_3^* : Y^* \times V \to \mathbb{R}$ where

$$J_3^*(v^*,u) = J_2^*(v^*,u) - \frac{K_1}{2}\int_\Omega \left(v^* - \frac{\partial G(u)}{\partial u} + \varepsilon u\right)^2 dx.$$

Finally, we remark that for $\varepsilon > 0$ sufficiently small and $K_1 > 0$ sufficiently large, J_3^* is concave in $D^* \times V_1$ around a concerning critical point. We recall that a critical point

$$v^* - \frac{\partial G(u)}{\partial u} + \varepsilon u = 0, \text{ in } \Omega.$$

15. A Related Restricted Problem in Phase Transition

In this section we develop a convex (in fact concave) dual variational for a model similar to those found in phase transition problems.

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Let $\Omega = [0,1] \subset \mathbb{R}$. Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{1}{2}\int_\Omega \min\{(u'+1)^2,(u'-1)^2\}\,dx \\ &\quad +\frac{1}{2}\int_\Omega u^2\,dx - \langle u,f\rangle_{L^2} \\ &= \frac{1}{2}\int_\Omega (u')^2\,dx - \int_\Omega |u'|\,dx + 1/2 \\ &\quad +\frac{1}{2}\int_\Omega u^2\,dx - \langle u,f\rangle_{L^2}. \end{aligned} \tag{77}$$

Here

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\}.$$

We also denote $V_1 = W_0^{1,2}(\Omega)$, and $Y = Y^* = L^2(\Omega)$.
Furthermore, we define the functionals G and $F : V \times V_1 \to \mathbb{R}$ by

$$G(u',v') = \frac{1}{2}\int_\Omega (u'+v')^2\,dx - \int_\Omega |u'+v'|\,dx + 1/2,$$

and

$$F(u,v) = \frac{1}{2}\int_\Omega u^2\,dx - \langle u,f\rangle_{L^2}.$$

Moreover we define $J_1 : V \times V_1 \to \mathbb{R}$ by

$$J_1(u,v) = G(u',v') + F(u,v),$$

and consider the problem of minimizing J_1 on the set

$$A = \{(u,v) \in V \times V_1 \ : \ (v')^2 \le K_2, \text{ in } \Omega\}.$$

Already including the Lagrange multiplier ϕ concerning such restrictions, we define

$$J_2(u,v,\phi) = J_1(u,v) + \frac{1}{2}\langle \phi^2, (v')^2 - K_2\rangle_{L^2}.$$

Observe now that

$$\begin{aligned} J_2(u,v,\phi) &= J_1(u,v) + \frac{1}{2}\langle \phi^2,(v')^2-K_2\rangle_{L^2} \\ &= G(u',v') + \frac{1}{2}\langle \phi^2,(v')^2-K_2\rangle_{L^2} \\ &\quad +F(u,v) \\ &= -\langle u', v_1^*\rangle_{L^2} - \langle v', v_2^*\rangle_{L^2} + G(u',v') \\ &\quad +\frac{1}{2}\langle \phi^2,(v')^2-K_2\rangle_{L^2} \\ &\quad \langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + F(u,v) \\ &\ge \inf_{(v_1,v_2)\in Y\times Y}\{-\langle v_1,v_1^*\rangle_{L^2} - \langle v_2,v_2^*\rangle_{L^2} + G_1(v_1,v_2,\phi) \\ &\quad +\frac{1}{2}\langle \phi^2,(v_2)^2-K_2\rangle_{L^2}\Big\} \\ &\quad + \inf_{(u,v)\in V\times V_1}\{\langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + F(u,v)\} \\ &= -G_1^*(v_1^*,v_2^*,\phi) - \tilde{F}^*(v_1^*,v_2^*),\ \forall (u,v) \in V\times V_1, (v_1^*,v_2^*,\phi) \in [Y^*]^3, \end{aligned} \tag{78}$$

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where

$$G_1(u', v', \phi) = G(u', v') + \frac{1}{2}\langle \phi^2, (v')^2 - K_2 \rangle_{L^2}.$$

Also,

$$\begin{aligned} G_1^*(v_1^*, v_2^*, \phi) &= \sup_{(v_1, v_2) \in Y \times Y} \{ \langle v_1, v_1^* \rangle_{L^2} + \langle v_1, v_1^* \rangle_{L^2} - G_1(v_1, v_2, \phi) \} \\ &= \frac{1}{2} \int_\Omega (v_1^*)^2 \, dx \\ &\quad + \int_\Omega |v_1^*| \, dx + \frac{1}{2} \int_\Omega \frac{(v_1^* - v_2^*)^2}{\phi^2} \\ &\quad + \frac{K_2}{2} \int_\Omega \phi^2 \, dx, \end{aligned} \tag{79}$$

where

$$\tilde{F}^*(v^*) = \begin{cases} \frac{1}{2} \int_\Omega ((v_1^*)' + f)^2 \, dx - v_1^*(1) u(1), & \text{if } (v_2^*)' = 0, \text{ in } \Omega, \\ +\infty, & \text{otherwise.} \end{cases} \tag{80}$$

From this we may infer that $v_2^* = c$, in Ω, for some $c \in \mathbb{R}$.
Summarizing, denoting $v^* = (v_1^*, v_2^*) = (v_1^*, c)$, and

$$J^*(v^*, \phi) = -G_1^*(v^*, \phi) - \tilde{F}^*(v^*)$$

we have got

$$\inf_{(u,v) \in A} J_1(u, v) \geq \sup_{(v^*, \phi) \in Y^* \times \mathbb{R} \times Y^*} J^*(v^* \phi).$$

We have developed numerical results by maximizing the dual functional J^* for two examples, namely.

1. Example A: In this case, we consider $f(x) = \cos(\pi x)/2$, $K_2 = 10^{-4}$.
   For the optimal
   $$u_0 = (v_1^*)' + f,$$
   please see Figure 9.
2. Example B: In this case, we consider $f(x) = \cos(\pi x)/2$, $K_2 = 30$.
   For the optimal
   $$u_0 = (v_1^*)' + f,$$
   please see Figure 10.

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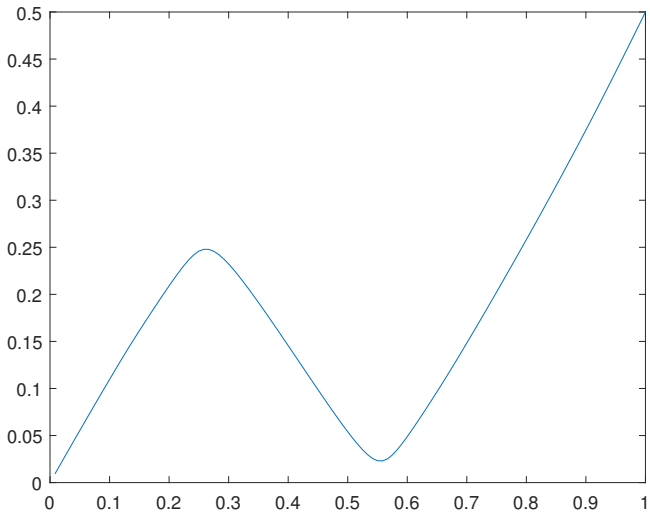

Figure 9. Solution $u_0(x)$ for the example A.

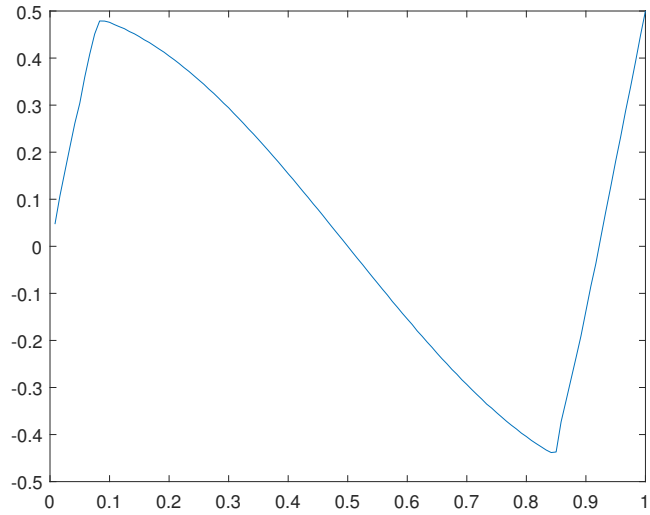

Figure 10. Solution $u_0(x)$ for the example B.

16. One More Dual Variational Formulation

In this section we develop one more dual variational formulation for a related model. Let $\Omega = [0,1] \subset \mathbb{R}$ and consider the functional $J : V \to \mathbb{R}$ defined by

$$J(u) = \frac{1}{2}\int_\Omega ((u')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2},$$

where

$$V = \{u \in W^{1,4}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\}.$$

We define also the relaxed functional $J_1 : V \times V_0 \to \mathbb{R}$, already including a concerning restriction and corresponding non-negative Lagrange multiplier Λ^2, where

$$J_1(u, v, \Lambda) = \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2}.$$

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where

$$V_0 = \{v \in W_0^{1,4}(\Omega) \ : \ (v')^2 - K \leq 0 \text{ in } \Omega\}.$$

Observe that

$$\begin{aligned}
& \frac{1}{2}\int_\Omega ((u'+v')^2-1)^2\,dx + \frac{1}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2} \\
= \ & -\langle v_0^*, (u'+v')^2-1\rangle_{L^2} + \frac{1}{2}\int_\Omega ((u'+v')^2-1)^2\,dx \\
& +\langle v_0^*, (u'+v')^2-1\rangle_{L^2} + \langle \Lambda^2, (v')^2-K\rangle_{L^2} - \langle u', v_1^*\rangle_{L^2} - \langle v', v_2^*\rangle_{L^2} \\
& +\langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + \frac{1}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2} \\
\geq \ & \inf_{w\in Y}\left\{-\langle v_0^*, w\rangle_{L^2} + \frac{1}{2}\int_\Omega (w)^2\,dx\right\} \\
& \inf_{(v_1,v_2)\in Y\times Y}\left\{\langle v_0^*, (v_1+v_2)^2-1\rangle_{L^2} + \langle \Lambda^2, (v_2)^2-K\rangle_{L^2} - \langle v_1, v_1^*\rangle_{L^2} - \langle v_2, v_2^*\rangle_{L^2}\right\} \\
& + \inf_{(u,v)\in V\times V_0}\left\{\langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + \frac{1}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2}\right\} \\
= \ & -\frac{1}{2}\int_\Omega (v_0^*)^2\,dx - \int_\Omega v_0^*\,dx \\
& -\frac{1}{4}\int_\Omega \frac{(v_1^*)^2}{v_0^*}\,dx - \frac{1}{2}\int_\Omega \frac{(v_1^*-v_2^*)^2}{2\Lambda^2}\,dx \\
& -\frac{1}{2}\int_\Omega ((v_1^*)'+f)^2\,dx - \frac{1}{2}\int_\Omega K\Lambda^2\,dx + v_1^*(1)u(1).
\end{aligned} \tag{81}$$

Here, we highlight $v_2^* = c \in \mathbb{R}$ in Ω, for some real constant c.
Hence, denoting

$$\begin{aligned}
J_1^*(v^*,\Lambda) \ = \ & -\frac{1}{2}\int_\Omega (v_0^*)^2\,dx - \int_\Omega v_0^*\,dx \\
& -\frac{1}{4}\int_\Omega \frac{(v_1^*)^2}{v_0^*}\,dx - \frac{1}{2}\int_\Omega \frac{(v_1^*-v_2^*)^2}{2\Lambda^2}\,dx \\
& -\frac{1}{2}\int_\Omega ((v_1^*)'+f)^2\,dx - \frac{1}{2}\int_\Omega K\Lambda^2\,dx + v_1^*(1)u(1)
\end{aligned} \tag{82}$$

and

$$J_2(u,v) = \frac{1}{2}\int_\Omega ((u'+v')^2-1)^2\,dx + \frac{1}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2},$$

we have obtained

$$\inf_{(u,v)\in V\times V_0} J_2(u,v)\} \geq \sup_{(v^*,\Lambda)\in A^*\times[Y^*]\times\mathbb{R}\times Y^*} J_1^*(v^*,\Lambda).$$

Finally, for

$$A^* = \{v_0^* \in Y^* \ : \ v_0^* \geq \varepsilon \text{ in } \Omega\}$$

we emphasize J_1^* is concave on $A^*\times[Y^*]\times\mathbb{R}\times Y^*$.

Here $\varepsilon > 0$ is a small regularizing real constant.

Remark 16.1. *The constraint $(v')^2 - K \leq 0$, in Ω is included to restrict the action of v on the region where the primal functional is non-convex, through an appropriate constant $K > 0$.*

17. A Model in Superconductivity through an Eigenvalue Approach

In this section we intend to model superconductivity through a two phase eigenvalue approach.

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Let $\Omega = [0,5] \subset \mathbb{R}$ be a straight wire corresponding to a one-dimensional super-conducting sample.

Consider the functional $J : V \times V \times \mathbb{R} \to \mathbb{R}$ where

$$\begin{aligned} J(u,v,E) &= \frac{\gamma_1}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha_1}{2}\int_\Omega |u|^4 \, dx \\ &- \frac{\omega^2}{2}\int_\Omega |u|^2 \, dx \\ &+ \frac{\gamma_2}{2}\int_\Omega \nabla v \cdot \nabla v \, dx + \frac{\alpha_2}{2}\int_\Omega |v|^4 \, dx \\ &- \frac{\omega_1^2}{2K_3^2}\int_\Omega |v|^2 \, dx \\ &- \frac{E}{2}\left(\int_\Omega (|u|^2 + |v|^2) \, dx - m_T\right). \end{aligned} \tag{83}$$

Here, in atomic units, m_T is the total electronic charge, $V = W_0^{1,2}(\Omega)$ and we set $\alpha_1 = 10^4$ corresponding to higher self-interacting energy which is related to a normal phase. We also set $\alpha_2 = 10^{-1}$ corresponding to a lower self-interacting energy which is related to a super-conducting phase and respective super-currents.

Moreover, we set $\gamma_1 = \gamma_2 = 1$, and initially $\omega = 1.8$ which is gradually decreased to $\omega = 1.0$.

Furthermore, we define

$$|\phi_N|^2 = \frac{|u|^2}{|u|^2 + |v|^2}$$

and

$$|\phi_S|^2 = \frac{|v|^2}{|u|^2 + |v|^2}$$

where ϕ_N corresponds to a normal phase and ϕ_S to a super-conducting one.

At this point we observe that the temperature $T = T(x,t)$ is proportional the frequency $\omega/(2\pi)$ of vibration for the normal phase.

We start the process with $\omega = 1.8$ which in atomic units corresponds to a higher temperature and gradually decreases it to the value $\omega = 1.0$

Between $\omega = 1.2$ and $\omega = 1.0$ the system changes from an almost total normal phase to an almost total super-conducting phase, as expected.

We highlight that the temperature is proportional to the vibrational kinetics energy

$$E_1(t) = \frac{1}{2}\int_\Omega |u|^2 \frac{\partial \mathbf{r}_N(x,t)}{\partial t} \cdot \frac{\partial \mathbf{r}_N(x,t)}{\partial t} \, dx$$

so that for

$$\mathbf{r}_N(x,t) = e^{i\omega t}\mathbf{w}_5(x)$$

and for a suitable vectorial function $\mathbf{w}_5$, we have

$$T \propto E_1 \propto \omega^2$$

so that we may model the decreasing of temperature T through the decreasing of ω^2.

For $\omega = 1.8$, for the corresponding normal phase ϕ_N and super-conducting phase ϕ_S, please se Figures 11 and 12, respectively.

For $\omega = 1.0$, for the corresponding normal phase ϕ_N and super-conducting phase ϕ_S, please se Figures 13 and 14, respectively.

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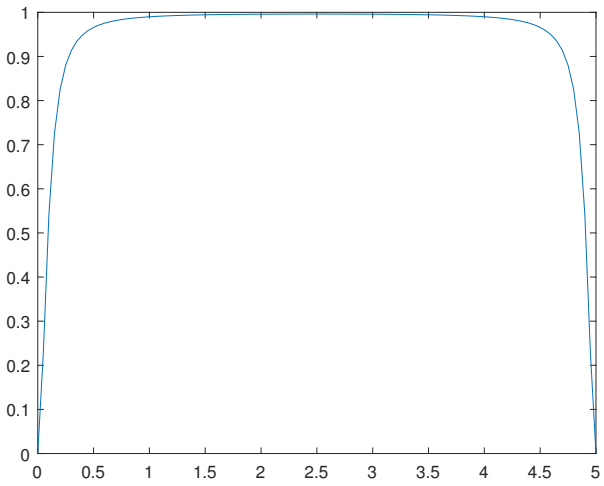

Figure 11. Solution $\phi_N(x)$ for the $\omega = 1.8$.

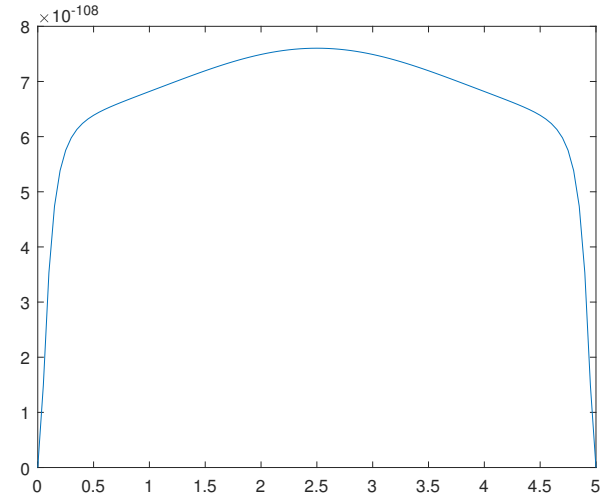

Figure 12. Solution $\phi_S(x)$ for the $\omega = 1.8$.

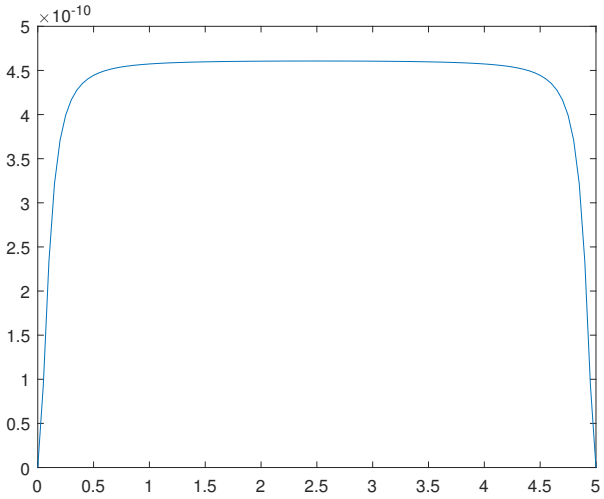

Figure 13. Solution $\phi_N(x)$ for the $\omega = 1.0$.

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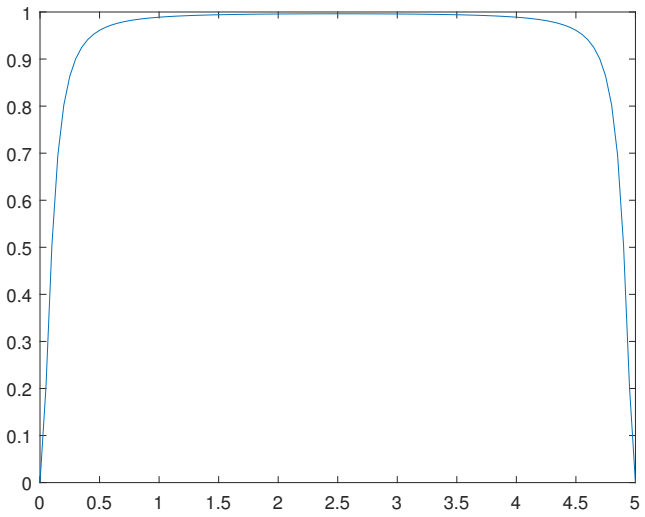

Figure 14. Solution $\phi_S(x)$ for the $\omega = 1.0$.

Finally, we have set $\omega_1/K_3 \approx 1$ which for large ω_1 corresponds to the super-currents.

18. A Simplified Qualitative Many Body Model for the Hydrogen Nuclear Fusion

In this section we develop a qualitative simple model for the hydrogen nuclear fusion.

Let $\Omega = [0, L]^3 \subset \mathbb{R}^3$ be a box in which is confined a gas comprised by an amount of ionized deuterium and tritium isotopes of hydrogen.

Though a suitable increasing in temperature, we intend to develop the following nuclear reaction

$$\text{Deuterium}^+ + \text{Tritium}^+ \rightarrow \text{Helium}^{++} + \text{Neutron (energetic)}.$$

We recall that the ionized Deuterium atom comprises a proton and a neutron and the ionized Tritium atom comprises a proton and two neutrons.

Under certain conditions and at a suitable high temperature the ionized Deuterium and Tritium atoms react chemically resulting in an ionized Helium atom, comprised by two protons and two neutrons and resulting also in one more single energetic neutron. We emphasize the higher kinetics neutron energy level has many potential practical applications, including its conversion in electric energy.

At this point we denote by m_D, m_T, m_{H_e} and m_N the masses of the ionized Deuterium, Tritium and Helium atoms, and the single neutron, respectively.

Therefore, we have the following mass relation

$$m_D + m_T = m_{H_e} + m_N.$$

To simplify our analysis, in such a chemical reaction, denoting the total masses of ionized Deuterium, Tritium, Helium and single Neutrons by $(m_D)_T$, $(m_T)_T$, $(m_{H_e})_T$ and $(m_N)_T$ we assume there is a real constant $c > 0$ such that

$$(m_D)_T = c\, m_D,\ (m_T)_T = c\, m_T,\ (m_{H_e})_T = c\, m_{H_e},\ (m_N)_T = c\, m_N.$$

With such statements and definitions in mind, we define the following functional J, where

$$J(\phi, \mathbf{r}) = J(\phi_D, \phi_T, \phi_{H_e}, \phi_N, \mathbf{r}) = G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}),$$

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where, in a simplified many body context,

$$|\phi_D(x,y)|^2 = |\phi_p^D(y)|^2 + |\phi_N^D(x,y)|^2 |\phi_p^D(y)|^2 \frac{1}{m_p},$$

$$|\phi_T(x,y)|^2 = |\phi_p^T(y)|^2 + (|\phi_{N_1}^T(x,y)|^2 + |\phi_{N_2}^T(x,y)|^2)|\phi_p^T(y)|^2 \frac{1}{m_p},$$

$$|\phi_{H_e}(x,y)|^2 = |\phi_{2P}^{H_e}(y)|^2 + (|\phi_{N_1}^{H_e}(x,y)|^2 + |\phi_{N_2}^{H_e}(x,y)|^2)|\phi_{2P}^{H_e}(y)|^2 \frac{1}{2\, m_p},$$

$$\phi_N = \phi_N(x).$$

Here $x, y \in \Omega \subset \mathbb{R}^3$ refers to the particle densities.

Furthermore, we assume $\gamma_p^D > 0,\ \gamma_p^T > 0,\ \gamma_N^D > 0,\ \gamma_{N_1}^T > 0,\ \gamma_{N_2}^T > 0,\ \gamma_{2p}^{H_e} > 0,\ \gamma_{N_1}^{H_e} > 0,\ \gamma_{N_2}^{H_e} > 0,\ \gamma_N > 0,$ and $\alpha_D > 0,\ \alpha_T > 0,\ \alpha_{H_e} > 0,\ \alpha_N > 0\ , \alpha_{DT} > 0,\ \alpha_{H_e\, N} > 0,$ so that

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2} \int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\, dy \\
& + \frac{\gamma_N^D}{2} \int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\, dx\, dy \\
& \frac{\gamma_p^T}{2} \int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\, dy \\
& + \frac{\gamma_{N_1}^T}{2} \int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\, dx\, dy \\
& + \frac{\gamma_{N_2}^T}{2} \int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\, dx\, dy \\
& + \frac{\gamma_{2p}^{H_e}}{2} \int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\, dy \\
& + \frac{\gamma_{N_1}^{H_e}}{2} \int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\, dx\, dy \\
& + \frac{\gamma_{N_2}^{H_e}}{2} \int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\, dx\, dy \\
& + \frac{\gamma_N}{2} \int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\, dx,
\end{aligned} \tag{84}$$

and,

$$\begin{aligned}
F(\phi) \quad = \quad & \frac{\alpha_D}{2} \int_\Omega \frac{|\phi_D(x-\xi_1, y-\xi_2)|^2 |\phi_D(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\, dx\, dy\, d\xi_1\, d\xi_2 \\
& + \frac{\alpha_T}{2} \int_\Omega \frac{|\phi_T(x-\xi_1, y-\xi_2)|^2 |\phi_T(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\, dx\, dy\, d\xi_1\, d\xi_2 \\
& + \frac{\alpha_{DT}}{2} \int_\Omega \frac{|\phi_D(x-\xi_1, y-\xi_2)|^2 |\phi_T(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\, dx\, dy\, d\xi_1\, d\xi_2 \\
& + \frac{\alpha_{H_e}}{2} \int_\Omega \frac{|\phi_{H_e}(x-\xi_1, y-\xi_2)|^2 |\phi_{H_e}(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\, dx\, dy\, d\xi_1\, d\xi_2 \\
& + \frac{\alpha_N}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_N(x-\xi)|^2 |\phi_N(\xi)|^2}{|x-\xi|}\, dx\, d\xi \\
& + \sum_{j=1}^{2} \frac{\alpha_{H_e\, N}}{2} \int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1, y-\xi_2)|^2 |\phi_N(\xi_j)|^2}{|(x,y)-(\xi_1,\xi_2)|}\, dx\, dy\, d\xi_1\, d\xi_2
\end{aligned} \tag{85}$$

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and the kinetics energy is expressed by

$$\begin{aligned} E_c(\phi,\mathbf{r}) &= \frac{1}{2}\int_\Omega |\phi_D|^2 \frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\,dx\,dy \\ &+\frac{1}{2}\int_\Omega |\phi_T|^2 \frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\,dx\,dy \\ &+\frac{1}{2}\int_\Omega |\phi_{H_e}|^2 \frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\,dx\,dy \\ &+\frac{1}{2}\int_\Omega |\phi_N|^2 \frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\,dx\,dy, \end{aligned} \tag{86}$$

where we also assume

$$\mathbf{r}_D \approx e^{i\omega t}\mathbf{w}_5(x,y),$$
$$\mathbf{r}_T \approx e^{i\omega t}\mathbf{w}_6(x,y),$$

so that considering such a vibrational motion, the temperature T is proportional to ω^2, that is

$$T \propto \omega^2.$$

Therefore, an increasing in T corresponds to a proportional increasing in ω^2.

Summarizing, we have supposed

$$E_c(\phi,\mathbf{r}) \approx \frac{1}{2}\omega^2 \int_\Omega |\phi_D|^2 + |\phi_T|^2\,dx\,C_1 + \frac{1}{2}\omega_1^2 \int_\Omega |\phi_N|^2\,dx\,C_2,$$

so that we represent the increasing in T through an increasing in ω^2.

Moreover, we denote by m_N the mass of a single neutron and by m_p the mass of a single proton.

Thus, denoting also by $\lambda_1,\ \lambda_2$ the proportion of non-reacted and reacted masses respectively, we have the following constraints.

1. $$\int_\Omega |\phi_N^D(x,y)|^2\,dx = m_N,$$
2. $$\int_\Omega |\phi_{N_1}^T(x,y)|^2\,dx = m_N,$$
3. $$\int_\Omega |\phi_{N_2}^T(x,y)|^2\,dx = m_N,$$
4. $$\int_\Omega |\phi_{N_1}^{H_e}(x,y)|^2\,dx = m_N,$$
5. $$\int_\Omega |\phi_{N_2}^{H_e}(x,y)|^2\,dx = m_N,$$
6. $$\int_\Omega |\phi_p^D(y)|^2\,dy = \lambda_1\,cm_p,$$
7. $$\int_\Omega |\phi_p^T(y)|^2\,dy = \lambda_1\,cm_p,$$
8. $$\int_\Omega |\phi_{2P}^{H_e}(y)|^2\,dy = \lambda_2\,(2c\,m_p),$$

Similar constraints are valid corresponding to the charge of a single proton.

We have also the following complementing constraints,

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1. $$\int_\Omega |\phi_D|^2 \, dx \, dy = \lambda_1 (m_D)_T,$$
2. $$\int_\Omega |\phi_T|^2 \, dx \, dy = \lambda_1 (m_T)_T,$$
3. $$\int_\Omega |\phi_{H_e}|^2 \, dx \, dy = \lambda_2 (m_{H_e})_T,$$
4. $$\int_\Omega |\phi_N|^2 \, dx \, dy = \lambda_2 (m_N)_T,$$
5. $$\lambda_1 + \lambda_2 = 1.$$

With such results and statements in mind and simplifying the interacting terms, we re-define the functional J now denoting it by J_1, here already including the Lagrange multipliers concerning the constraints, where

$$\begin{aligned} J_1(\phi, \omega, E, \lambda) \quad = \quad & \frac{\gamma_p^D}{2} \int_\Omega (\nabla \phi_p^D) \cdot (\nabla \phi_p^D) \, dy \\ & + \frac{\gamma_N^D}{2} \int_\Omega (\nabla \phi_N^D) \cdot (\nabla \phi_N^D) \, dx \, dy \\ & \frac{\gamma_p^T}{2} \int_\Omega (\nabla \phi_p^T) \cdot (\nabla \phi_p^T) \, dy \\ & + \frac{\gamma_{N_1}^T}{2} \int_\Omega (\nabla \phi_{N_1}^T) \cdot (\nabla \phi_{N_1}^T) \, dx \, dy \\ & + \frac{\gamma_{N_2}^T}{2} \int_\Omega (\nabla \phi_{N_2}^T) \cdot (\nabla \phi_{N_2}^T) \, dx \, dy \\ & + \frac{\gamma_{2p}^{H_e}}{2} \int_\Omega (\nabla \phi_{2p}^{H_e}) \cdot (\nabla \phi_{2p}^{H_e}) \, dy \\ & + \frac{\gamma_{N_1}^{H_e}}{2} \int_\Omega (\nabla \phi_{N_1}^{H_e}) \cdot (\nabla \phi_{N_1}^{H_e}) \, dx \, dy \\ & + \frac{\gamma_{N_2}^{H_e}}{2} \int_\Omega (\nabla \phi_{N_2}^{H_e}) \cdot (\nabla \phi_{N_2}^{H_e}) \, dx \, dy \\ & + \frac{\gamma_N}{2} \int_\Omega (\nabla \phi_N) \cdot (\nabla \phi_N) \, dx \\ & + \frac{\alpha_D}{2} \int_\Omega |\phi_D|^4 \, dx + \frac{\alpha_T}{2} \int_\Omega |\phi_T|^4 \, dx \\ & + \frac{\alpha_{H_e}}{2} \int_\Omega |\phi_{H_e}|^4 \, dx + \frac{\alpha_N}{2} \int_\Omega |\phi_N|^4 \, dx \\ & - \omega^2 \int_\Omega (|\phi_D|^2 + |\phi_T|^2) \, dx \\ & - \omega_1^2 \int_\Omega |\phi_N|^2 \, dx + J_{Aux}, \end{aligned} \tag{87}$$

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where the functional J_{Aux} stands for

$$\begin{aligned}
J_{Aux} \quad = \quad & -\int_\Omega (E_N^D)_5(y)\left(\int_\Omega |\phi_N^D(x,y)|^2\,dx - m_N\right)dy \\
& -\int_\Omega (E_{N_1}^T)_6(y)\left(\int_\Omega |\phi_{N_1}^T(x,y)|^2\,dx - m_N\right)dy \\
& -\int_\Omega (E_{N_2}^T)_7(y)\left(\int_\Omega |\phi_{N_2}^T(x,y)|^2\,dx - m_N\right)dy \\
& -\int_\Omega (E_{N_1}^{H_e})_8(y)\left(\int_\Omega |\phi_{N_1}^{H_e}(x,y)|^2\,dx - m_N\right)dy \\
& -\int_\Omega (E_{N_2}^{H_e})_9(y)\left(\int_\Omega |\phi_{N_2}^{H_e}(x,y)|^2\,dx - m_N\right)dy \\
& -(E_D)_2\left(\int_\Omega |\phi_p^D(y)|^2\,dy - \lambda_1 c m_p\right) \\
& -(E_T)_3\left(\int_\Omega |\phi_p^T(y)|^2\,dy - \lambda_1 c m_p\right) \\
& -(E_{H_e})_3\left(\int_\Omega |\phi_{2P}^{H_e}(x,y)|^2\,dy - \lambda_2\, 2c m_p\right) \\
& -E_5\left(\int_\Omega |\phi_D|^2\,dx\,dy - \lambda_1 (m_D)_T\right) \\
& -E_6\left(\int_\Omega |\phi_T|^2\,dx\,dy - \lambda_1 (m_T)_T\right) \\
& -E_7\left(\int_\Omega |\phi_{H_e}|^2\,dx\,dy - \lambda_2 (m_{H_e})_T\right) \\
& -E_8\left(\int_\Omega |\phi_N|^2\,dx\,dy - \lambda_2 (m_N)_T\right) \\
& -E_9(\lambda_1 + \lambda_2 - 1).
\end{aligned} \tag{88}$$

Remark 18.1. *In order to obtain consistent results it is necessary to set*

$$(\alpha_N, \alpha_{H_e}) \gg (\alpha_D, \alpha_T).$$

In such a case, a higher temperature corresponding to a large ω^2, though such a nuclear reaction, will result in a small λ_1 and a higher kinetics energy for the neutron field, corresponding to a large ω_1^2 and λ_2 closer to 1.

19. A More Detailed Mathematical Description of the Hydrogen Nuclear Fusion

In this section we develop in more details another model for the hydrogen nuclear fusion.

Remark 19.1. *Denoting by $i \in \mathbb{C}$ the imaginary unit, in this and in the subsequent sections, for the time-dependent case we generically define the gradient of a scalar function $u(x,t)$ with domain in $\mathbb{R}^4$, denoted by $\nabla u(x,t)$, as*

$$\nabla u(x,t) = (iu_t(x,t), u_{x_1}(x,t), u_{x_2}(x,t), u_{x_3}(x,t)),$$

so that

$$\nabla u \cdot \nabla u = -u_t^2 + \sum_{j=1}^{3} u_{x_j}^2.$$

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

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Here such a set Ω stands for a control volume in which an ionized gas (plasma) flows. Such a gas comprises ionized Deuterium and Tritium atoms intended, through a suitable higher temperature, to chemically react resulting in atoms of Hellion and a field of single energetic Neutrons.

Symbolically such a reaction stands for

$$\text{Deuterium}^{+} \ + \ \text{Tritium}^{+} \rightarrow \text{Helium}^{++} \ + \ \text{Neutron (energetic)}.$$

We recall that the ionized Deuterium atom is comprised by a proton and a neutron and the ionized Tritium atom is comprised by a proton and two neutrons.

Moreover, the ionized Helium atom is comprised by two protons and two neutrons.

As previously mentioned, resulting from such a chemical reaction up surges also an energetic neutron which the higher kinetics energy has a great variety of applications, including its conversion in electric energy.

We highlight the model here presented includes electric and magnetic fields and the corresponding potential ones.

Denoting by t the time on the interval $[0, t_f]$, at this point we define the following density functions:

1. For the Deuterium field

$$|\phi_D(x,y,t)|^2 = |\phi_p^D(y,t)|^2 + |\phi_N^D(x,y,t)|^2 |\phi_p^D(y,t)|^2 \frac{1}{m_p},$$

2. For the Tritium field

$$|\phi_T(x,y,t)|^2 = |\phi_p^T(y,t)|^2 + (|\phi_{N_1}^T(x,y,t)|^2 + |\phi_{N_2}^T(x,y,t)|^2) |\phi_p^T(y,t)|^2 \frac{1}{m_p},$$

3. For the Helium field

$$|\phi_{H_e}(x,y,t)|^2 = |\phi_{2p}^{H_e}(y,t)|^2 + (|\phi_{N_1}^{H_e}(x,y,t)|^2 + |\phi_{N_2}^{H_e}(x,y,t)|^2) |\phi_{2p}^{H_e}(y,t)|^2 \frac{1}{2\, m_p},$$

4. For the Neutron field

$$\phi_N = \phi_N(x,t),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t).$$

Furthermore, we define also the related densities

1.
$$\rho_D(y,t) = \int_\Omega |\phi_D(x,y,t)|^2 \, dx,$$

2.
$$\rho_T(y,t) = \int_\Omega |\phi_T(x,y,t)|^2 \, dx,$$

$$\rho_{H_e}(y,t) = \int_\Omega |\phi_{H_e}(x,y,t)|^2 \, dx,$$

$$\rho_N(x,t) = |\phi_N(x,t)|^2,$$

$$\rho_e(y,t) = \int_\Omega |\phi_e(x,y,t)|^2 \, dx.$$

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For the chemical reaction in question we consider that one unit of mass of fractional proportion α_D of ionized Deuterium and α_T of ionized Tritium results in one unit of mass of fractional proportion α_{H_e} of ionized Helium and α_N of neutrons.

Symbolic, this stands for

$$1 = \alpha_D + \alpha_T = \alpha_{H_e} + \alpha_N.$$

Concerning the control volume Ω in question and related surface control $\partial\Omega$, we assume such a volume has an initial (fot $t = 0$) amount of ionized Deuterium of $(m_D)_0$ and an initial amount of ionized Tritium of $(m_T)_0$. The initial amount of ionized Helium and single neutrons are supposed to be zero.

On the other hand, about the surface control $\partial\Omega$, we assume there is a part $\Omega_1 \subset \partial\Omega$ for which is allowed the entrance and exit of Deuterium and Tritium ionized atoms.

We assume also there is another part $\partial\Omega_2 \subset \partial\Omega$ such that $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$ for which is allowed only the exit of ionized Helium atoms and neutrons, but not their entrance.

In $\partial\Omega_2$ is allowed the exit only (not the entrance) of ionized Deuterium and Tritium atoms.

Indeed, we assume the following relations for the masses:

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t)\, dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t)\, dx,$$

5.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

6.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

7.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

8.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D(m_{H_e,N})_T(t),$$

9.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T(m_{H_e,N})_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$

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12.

$$m_e(t) = \int_\Omega |\phi_p^D(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_p^T(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_{2p}^{H_e}(x,t)|^2\, dx \frac{m_e}{m_p}.$$

Here **n** denotes the outward normal vectorial fields to the concerning surfaces.

Having clarified such masses relations, we define the functional

$$J(\phi, \rho, \mathbf{r}, \mathbf{u}, \mathbf{E}, \mathbf{A}, \mathbf{B})$$

where

$$J = G(\nabla u) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3,$$

and where we assume $\gamma_p^D > 0$, $\gamma_p^T > 0$, $\gamma_N^D > 0$, $\gamma_{N_1}^T > 0$, $\gamma_{N_2}^T > 0$, $\gamma_{2p}^{H_e} > 0$, $\gamma_{N_1}^{H_e} > 0$, $\gamma_{N_2}^{H_e} > 0$, $\gamma_N > 0$, $\gamma_e > 0$ and $\alpha_D > 0$, $\alpha_T > 0$, $\alpha_{H_e} > 0$, $\alpha_N > 0$, $\alpha_{DT} > 0$, $\alpha_{H_e\, N} > 0$, $\alpha_{e,e} > 0$, $\alpha_{H_e,e} < 0$ so that

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_p^D) \cdot (\nabla \phi_p^D)\, dy\, dt \\
& + \frac{\gamma_N^D}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_N^D) \cdot (\nabla \phi_N^D)\, dx\, dy\, dt \\
& \frac{\gamma_p^T}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_p^T) \cdot (\nabla \phi_p^T)\, dy\, dt \\
& + \frac{\gamma_{N_1}^T}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_{N_1}^T) \cdot (\nabla \phi_{N_1}^T)\, dx\, dy\, dt \\
& + \frac{\gamma_{N_2}^T}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_{N_2}^T) \cdot (\nabla \phi_{N_2}^T)\, dx\, dy\, dt \\
& + \frac{\gamma_{2p}^{H_e}}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_{2p}^{H_e}) \cdot (\nabla \phi_{2p}^{H_e})\, dy\, dt \\
& + \frac{\gamma_{N_1}^{H_e}}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_{N_1}^{H_e}) \cdot (\nabla \phi_{N_1}^{H_e})\, dx\, dy\, dt \\
& + \frac{\gamma_{N_2}^{H_e}}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_{N_2}^{H_e}) \cdot (\nabla \phi_{N_2}^{H_e})\, dx\, dy\, dt \\
& + \frac{\gamma_N}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_N) \cdot (\nabla \phi_N)\, dx\, dt \\
& + \frac{\gamma_e}{2} \int_0^{t_f} \int_\Omega (\nabla \phi_e) \cdot (\nabla \phi_e)\, dx\, dy\, dt, \qquad (89)
\end{aligned}$$

and

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$$
\begin{aligned}
F(\phi) \quad = \quad & \frac{\alpha_D}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t)|^2|\phi_D(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_T}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2,t)|^2|\phi_T(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{DT}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t)|^2|\phi_T(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{H_e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t)|^2|\phi_{H_e}(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_N}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_N(x-\xi,t)|^2|\phi_N(\xi)|^2}{|x-\xi,t|}\,dx\,d\xi\,dt \\
& +\sum_{j=1}^{2}\frac{\alpha_{H_e}\,N}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2,t)|^2|\phi_N(\xi_j,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{H_e,e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t)|^2|\phi_e(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{e,e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_e(x-\xi_1,y-\xi_2,t)|^2|\phi_e(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \qquad (90)
\end{aligned}
$$

and the internal kinetics energy is expressed by

$$
\begin{aligned}
E_c(\phi,\mathbf{r}) \quad = \quad & \frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_D|^2\,\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_T|^2\,\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_{H_e}|^2\,\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_N|^2\,\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_e|^2\,\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}\,dx\,dy\,dt, \qquad (91)
\end{aligned}
$$

Here it is worth highlighting we have approximated the initially discrete set of indices s of particles as a continuous positive real variable s.

Moreover,

$$F_1 = \frac{1}{4\pi}\int_0^{t_f} \|\operatorname{curl}\mathbf{A}-\mathbf{B}_0\|_2\,dt,$$

$$
\begin{aligned}
F_2 \quad = \quad & \int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)dx\,dy\,dt \\
& +\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)dx\,dy\,dt \\
& +\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)dx\,dy\,dt \\
& +\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_e|\phi_e|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_e}{\partial t}\right)dx\,dy\,dt, \qquad (92)
\end{aligned}
$$

where K_p and K_e are appropriate real constants related to the respective charges.

Here $\mathbf{u}=(u_1,u_2,u_3)$ is the fluid velocity field and

$$\mathbf{r}_D,\ \mathbf{r}_T,\ \mathbf{r}_{H_e},\ \mathbf{r}_N,\ \mathbf{r}_e$$

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are fields of displacements for the corresponding atom fields.

Also **A** denotes the magnetic potential, $\mathbf{B}_0$ an external magnetic field and **B** is the total magnetic field.

Moreover, $\mathbf{E}_{ind}$ is an induced electric field.

Finally,

$$\begin{aligned} F_3 &= \frac{C_D}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_D\cdot\nabla_{(x,y)}\mathbf{r}_D\,dx\,dy\,dt + \frac{C_T}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_T\cdot\nabla_{(x,y)}\mathbf{r}_T\,dx\,dy\,dt \\ &\frac{C_{H_e}}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_{H_e}\cdot\nabla_{(x,y)}\mathbf{r}_{H_e}\,dx\,dy\,dt + \frac{C_N}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_N\cdot\nabla_{(x,y)}\mathbf{r}_N\,dx\,dy\,dt \\ &\frac{C_e}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_e\cdot\nabla_{(x,y)}\mathbf{r}_e\,dx\,dy\,dt, \end{aligned} \tag{93}$$

for appropriate real positive constants C_D C_T, C_{H_e}, C_N, C_e.

Such a functional J is subject to the following constraints:

1. The momentum conservation equation for the fluid motion

$$\rho\left(\frac{\partial u_k}{\partial t} + u_j\frac{\partial u_k}{\partial x_j}\right) = \rho f_k - \frac{\partial P}{\partial x_k} + \tau_{kj,j} + (F_E)_k + (F_M)_k,$$

$\forall k \in \{1,2,3\}$.

Here $\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e$ is the total density and P is the fluid pressure field.

Furthermore,

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\sum_{k=1}^{3}\frac{\partial u_k}{\partial x_k}\right),$$

$\forall i,j \in \{1,2,3\}$,

$$\mathbf{F}_E = \{(F_E)_k\} = \left(K_p(|\phi_p^D|^2 + |\phi_p^T|^2 + |\phi_{2p}^{H_e}|^2) + K_e\int_\Omega |\phi_e|^2\,dx\right)\mathbf{E},$$

and

$$\begin{aligned} \mathbf{F}_M &= \{(F_M)_k\} \\ &= \left(K_p\left(|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)\right.\right. \\ &\quad |\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right) \\ &\quad \left.+|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\right) \\ &\quad \left.+K_e|\phi_e|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_e}{\partial t}\right)\right) \times \mathbf{B}. \end{aligned} \tag{94}$$

2. Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \text{ div } (\rho\mathbf{u}) = 0.$$

3. Energy equation

$$\rho\frac{De}{Dt} + \nabla_x(\hat{E}_1)\cdot\mathbf{u} + \hat{E}_2 + P(\text{ div } \mathbf{u}) = \frac{\partial Q}{\partial t} - \text{ div } \mathbf{q} + \tau_{jk}\frac{\partial u_j}{\partial x_k},$$

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where we assume the Fourier law

$$\mathbf{q} = -K\nabla T,$$

where $T = T(x,t)$ is the scalar field of temperature and Q is a standard heat function.
Also,

$$\begin{aligned} e \approx & \frac{\rho}{2}\mathbf{u}\cdot\mathbf{u} + \frac{\rho_D}{2}\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t} \\ & + \frac{\rho_T}{2}\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t} \\ & + \frac{\rho_{H_e}}{2}\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t} \\ & + \frac{\rho_N}{2}\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t} \\ & + \frac{\rho_e}{2}\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t} \end{aligned} \tag{95}$$

where the densities $\hat{E}_1$ and $\hat{E}_2$ are defined through the expressions of $F(\phi)$ and F_2 so that

$$F(\phi) = \int_0^{t_f}\int_\Omega \hat{E}_1\, dx\, dt$$

and

$$F_2 = \int_0^{t_f}\int_\Omega \hat{E}_2\, dx\, dt.$$

Here we recall that since $\mathbf{r}_D$ is highly oscillating in t we approximately have

$$\mathbf{u}\cdot\mathbf{r}_D \approx 0$$

in a weak or measure sense. The same remark is valid for the other internal velocity fields.
Moreover,

$$\frac{De}{Dt} = \frac{\partial e}{\partial t} + u_j\frac{\partial e}{\partial x_j}.$$

Finally, for a calorically perfect gas we may assume

$$e = C_v T$$

where

$$C_v = \frac{R}{\gamma - 1},$$

for appropriate constants $R > 0$, $\gamma > 1$.

4.

$$P = F_7(\rho, T),$$

for an appropriate scalar function F_7.

5. Mass relations

(a)

$$m_D(t) = \int_\Omega \rho_D(x,t)\, dx,$$

(b)

$$m_T(t) = \int_\Omega \rho_T(x,t)\, dx,$$

(c)

$$m_{He}(t) = \int_\Omega \rho_{H_e}(x,t)\, dx,$$

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(d)
$$m_N(t) = \int_\Omega \rho_N(x,t)\, dx,$$
(e)
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx,$$
(f)
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$
(g)
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$
(h)
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

where,

(a)
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$
(b)
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$
(c)
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D(m_{H_e,N})_T(t),$$
(d)
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T(m_{H_e,N})_T(t),$$
(e)
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau.$$
(f)
$$m_e(t) = \int_\Omega |\phi_p^D(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_p^T(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_{2p}^{H_e}(x,t)|^2\, dx \frac{m_e}{m_p}.$$

6. Other mass constraints

(a)
$$\int_\Omega |\phi_N^D(x,y,t)|^2\, dx = m_N,$$
(b)
$$\int_\Omega |\phi_{N_1}^T(x,y,t)|^2\, dx = m_N,$$
(c)
$$\int_\Omega |\phi_{N_2}^T(x,y,t)|^2\, dx = m_N,$$
(d)
$$\int_\Omega |\phi_{N_1}^{H_e}(x,y,t)|^2\, dx = m_N,$$
(e)
$$\int_\Omega |\phi_{N_2}^{H_e}(x,y,t)|^2\, dx = m_N.$$

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7. For the induced electric field, we must have

$$\begin{aligned}
&\text{curl } \mathbf{E}_{ind} + \frac{1}{c}\,\text{curl}\left(\hat{K}_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)\right.\\
&+\hat{K}_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)\\
&+\hat{K}_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\\
&\left.+\hat{K}_e\int_\Omega|\phi_e(x,y,t)|^2\left(\mathbf{u}(y,t)+\frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\,dx\right)\right)\\
&\times(\,\text{curl }\mathbf{A}-\mathbf{B}_0)-\frac{1}{c}\frac{\partial}{\partial t}(\,\text{curl }\mathbf{A}-\mathbf{B}_0)=\mathbf{0},
\end{aligned} \tag{96}$$

where $\hat{K}_p$ and $\hat{K}_e$ are appropriate real constants related to the respective charges.

8. A Maxwell equation:

$$\text{div } \mathbf{B} = 0,$$

where

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

9. Another Maxwell equation:

$$\text{div } \mathbf{E} = 4\pi\left(K_p(|\phi_p^D|^2+|\phi_p^T|^2+|\phi_{2p}^{H_e}|^2)+K_e\int_\Omega|\phi_e(x,y,t)|^2\,dx\right),$$

where the total electric field $\mathbf{E}$ stands for

$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_\rho,$$

and where generically denoting

$$F(\phi) = \int_0^{t_f}\int_\Omega f_5(\phi,x,\xi,t)\,dx\,d\xi\,dt,$$

we have also

$$\mathbf{E}_\rho = \left\{\int_\Omega \frac{\partial f_5(\phi,x,\xi,t)}{\partial x_k}\,d\xi\right\}.$$

At this point we generically denote

$$\langle h_1,h_2\rangle_{L^2} = \int_0^{t_f}\int_\Omega h_1\,h_2\,dx\,dy\,dt.$$

Thus, already including the Lagrange multipliers concerning the restrictions indicated, the extended functional J_3 stands for

$$\begin{aligned}
&J_3 = J_3(\phi,\mathbf{u},\mathbf{r},P,\mathbf{A},\mathbf{B},\mathbf{E},\Lambda,E)\\
=\;& G(\nabla\phi)+F(\phi)+E_c(\phi,\mathbf{r})+F_1+F_2+F_3\\
&+\left\langle\Lambda_k,\rho\left(\frac{\partial u_k}{\partial t}+u_j\frac{\partial u_k}{\partial x_j}\right)-\rho f_k+\frac{\partial P}{\partial x_k}-\tau_{kj,j}-(F_E)_k-(F_M)_k\right\rangle_{L^2}\\
&+\left\langle\Lambda_4,\ \frac{\partial\rho}{\partial t}+\ \text{div }(\rho\mathbf{u})\right\rangle_{L^2}+J_{Aux_1}+J_{Aux_2}+J_{Aux_3}+J_{Aux_4},
\end{aligned} \tag{97}$$

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where,

$$\begin{aligned} & J_{Aux_1} \\ = & \left\langle \Lambda_5,\ \rho\frac{De}{Dt} + \nabla_x(\hat{E}_1)\cdot\mathbf{u} + \hat{E}_2 + +P(\ \mathrm{div}\ \mathbf{u}) - \frac{\partial Q}{\partial t} + \ \mathrm{div}\ \mathbf{q} - \tau_{jk}\frac{\partial u_j}{\partial x_k}\right\rangle_{L^2} \\ & +\langle \Lambda_6,\ P - F_7(\rho,T)\rangle_{L^2}, \end{aligned} \tag{98}$$

$$\begin{aligned} J_{Aux_2} = & \left\langle \Lambda_7, m_D(t) - \int_\Omega \rho_D(x,t)\ dx\right\rangle_{L^2} \\ & +\left\langle \Lambda_8, m_T(t) - \int_\Omega \rho_T(x,t)\ dx\right\rangle_{L^2} \\ & \left\langle \Lambda_9, m_{H_e}(t) - \int_\Omega \rho_{H_e}(x,t)\ dx\right\rangle_{L^2} \\ & \left\langle \Lambda_{10}, m_N(t) - \int_\Omega \rho_N(x,t)\ dx\right\rangle_{L^2} \\ & \left\langle \Lambda_{11}, m_e(t) - \int_\Omega \rho_e(x,t)\ dx\right\rangle_{L^2} \\ & \int_0^{t_f} E_12(t)(\alpha_N m_{H_e})_T(t) - \alpha_{H_e}(m_N)_T(t))\ dt, \end{aligned} \tag{99}$$

$$\begin{aligned} J_{Aux_3} = & -\int_0^{t_f}\int_\Omega (E_N^D)_5(y,t)\left(\int_\Omega |\phi_N^D(x,y,t)|^2\ dx - m_N\right)\ dy\ dt \\ & -\int_0^{t_f}\int_\Omega (E_{N_1}^T)_6(y,t)\left(\int_\Omega |\phi_{N_1}^T(x,y,t)|^2\ dx - m_N\right)\ dy\ dt \\ & -\int_0^{t_f}\int_\Omega (E_{N_2}^T)_7(y,t)\left(\int_\Omega |\phi_{N_2}^T(x,y,t)|^2\ dx - m_N\right)\ dy\ dt \\ & -\int_0^{t_f}\int_\Omega (E_{N_1}^{H_e})_8(y,t)\left(\int_\Omega |\phi_{N_1}^{H_e}(x,y,t)|^2\ dx - m_N\right)\ dy\ dt \\ & -\int_0^{t_f}\int_\Omega (E_{N_2}^{H_e})_9(y,t)\left(\int_\Omega |\phi_{N_2}^{H_e}(x,y,t)|^2\ dx - m_N\right)\ dy\ dt, \end{aligned} \tag{100}$$

$$\begin{aligned} J_{Aux_4} = & \langle \Lambda_{12},\ \mathrm{curl}\ \mathbf{E}_{ind} \\ & +\frac{1}{c}\ \mathrm{curl}\left(\hat{K}_p|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)\right. \\ & +\hat{K}_p|\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right) \\ & +\hat{K}_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right) \\ & \left.+\hat{K}_e\int_\Omega |\phi_e(x,y,t)|^2\left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\ dx\right)\right) \\ & \times(\ \mathrm{curl}\ \mathbf{A} - \mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\ \mathrm{curl}\ \mathbf{A} - \mathbf{B}_0)\Big\rangle_{L^2} \\ & +\langle \Lambda_{13},\ \mathrm{div}\ \mathbf{B}\rangle_{L^2} \\ & +\left\langle \Lambda_{14},\ \mathrm{div}\ \mathbf{E} - 4\pi\left(K_p(|\phi_p^D|^2 + |\phi_p^T|^2 + |\phi_{2p}^{H_e}|^2) + K_e\int_\Omega |\phi_e(x,y,t)|^2\ dx\right)\right\rangle_{L^2}. \end{aligned} \tag{101}$$

Here we recall the following definitions and relations:

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1. For the Deuterium field

$$|\phi_D(x,y,t)|^2 = |\phi_p^D(y,t)|^2 + |\phi_N^D(x,y,t)|^2|\phi_p^D(y,t)|^2\frac{1}{m_p},$$

2. For the Tritium field

$$|\phi_D(x,y,t)|^2 = |\phi_p^D(y,t)|^2 + (|\phi_{N_1}^D(x,y,t)|^2 + |\phi_{N_2}^D(x,y,t)|^2)|\phi_p^D(y,t)|^2\frac{1}{m_p},$$

3. For the Helium field

$$|\phi_{H_e}(x,y,t)|^2 = |\phi_{2p}^{H_e}(y,t)|^2 + (|\phi_{N_1}^{H_e}(x,y,t)|^2 + |\phi_{N_2}^{H_e}(x,y,t)|^2)|\phi_{2p}^{H_e}(y,t)|^2\frac{1}{2\,m_p},$$

4. For the Neutron field

$$\phi_N = \phi_N(x,t),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t).$$

1.
$$\rho_D(y,t) = \int_\Omega |\phi_D(x,y,t)|^2\,dx,$$

2.
$$\rho_T(y,t) = \int_\Omega |\phi_T(x,y,t)|^2\,dx,$$

$$\rho_{H_e}(y,t) = \int_\Omega |\phi_{H_e}(x,y,t)|^2\,dx,$$

$$\rho_N(x,t) = |\phi_N(x,t)|^2,$$

$$\rho_e(y,t) = \int_\Omega |\phi_e(x,y,t)|^2\,dx.$$

Also,

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e,$$

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u}\cdot\mathbf{n}\,dS\,d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t)\,dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t)\,dx,$$

5.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\,dS\,d\tau - \alpha_D(m_{H_e,N})_T(t),$$

6.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\,dS\,d\tau - \alpha_T(m_{H_e,N})_T(t),$$

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7.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

8.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

9.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that
$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) - \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$

12.
$$m_e(t) = \int_\Omega |\phi_p^D(x,t)|^2\, dx\frac{m_e}{m_p} + \int_\Omega |\phi_p^T(x,t)|^2\, dx\frac{m_e}{m_p} + \int_\Omega |\phi_{2p}^{H_e}(x,t)|^2\, dx\frac{m_e}{m_p}.$$

Finally,
$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_\rho,$$

and where generically denoting
$$F(\phi) = \int_\Omega f_5(\phi,x,\xi)\, dx\, d\xi,$$

we have also
$$\mathbf{E}_\rho = \left\{ \int_\Omega \frac{\partial f_5(\phi,x,\xi)}{\partial x_k}\, d\xi \right\}.$$

and,

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

20. A Final Mathematical Description of the Hydrogen Nuclear Fusion

In this section we develop in even more details another model for the hydrogen nuclear fusion.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Here such a set Ω stands for a control volume in which an ionized gas (plasma) flows. Such a gas comprises ionized Deuterium and Tritium atoms intended, through a suitable higher temperature, to chemically react resulting in atoms of Helium and a field of single energetic Neutrons.

Symbolically such a reaction stands for

$$\text{Deuterium}^+ \ + \ \text{Tritium}^+ \rightarrow \text{Helium}^{++} \ + \ \text{Neutron (energetic)}.$$

We recall that the ionized Deuterium atom is comprised by a proton and a neutron and the ionized Tritium atom is comprised by a proton and two neutrons.

Moreover, the ionized Helium atom is comprised by two protons and two neutrons.

As previously mentioned, resulting from such a chemical reaction up surges also an energetic neutron which the higher kinetics energy has a great variety of applications, including its conversion in electric energy.

We highlight the model here presented includes electric and magnetic fields and the corresponding potential ones.

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Denoting by t the time on the interval $[0, t_f]$, at this point we define the following density functions:

1. For a single Deuterium atom indexed by s:

$$|\phi_D(x,y,t,s)|^2 = |\phi_p^D(y,t,s)|^2 + |\phi_N^D(x,y,t,s)|^2 |\phi_p^D(y,t,s)|^2 \frac{1}{m_p},$$

2. For a single Tritium atom indexed by s:

$$|\phi_T(x,y,t,s)|^2 = |\phi_p^T(y,t,s)|^2 + (|\phi_{N_1}^T(x,y,t,s)|^2 + |\phi_{N_2}^T(x,y,t,s)|^2) |\phi_p^T(y,t,s)|^2 \frac{1}{m_p},$$

3. For a single Helium atom indexed by s:

$$|\phi_{H_e}(x,y,t,s)|^2 = |\phi_{2p}^{H_e}(y,t,s)|^2 + (|\phi_{N_1}^{H_e}(x,y,t,s)|^2 + |\phi_{N_2}^{H_e}(x,y,t,s)|^2) |\phi_{2p}^{H_e}(y,t,s)|^2 \frac{1}{2\, m_p},$$

4. For the Neutron field:

$$\phi_N = \phi_N(x,t,s),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t,s).$$

Furthermore, we define also the related densities

1.
$$\rho_D(y,t) = \int_0^{N_D(t)} \int_\Omega |\phi_D(x,y,t,s)|^2 \, dx \, ds,$$

2.
$$\rho_T(y,t) = \int_0^{N_T(t)} \int_\Omega |\phi_T(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_{H_e}(y,t) = \int_0^{N_{H_e}(t)} \int_\Omega |\phi_{H_e}(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_N(x,t) = \int_0^{N_N(t)} |\phi_N(x,t,s)|^2 \, ds,$$

$$\rho_e(y,t) = \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \, dx \, ds.$$

For the chemical reaction in question we consider that one unit of mass of fractional proportion α_D of ionized Deuterium and α_T of ionized Tritium results in one unit of mass of fractional proportion α_{H_e} of ionized Helium and α_N of neutrons.

Symbolically, this stands for

$$1 = \alpha_D + \alpha_T = \alpha_{H_e} + \alpha_N.$$

Concerning the control volume Ω in question and related surface control $\partial\Omega$, we assume such a volume has an initial (fot $t = 0$) amount of ionized Deuterium of $(m_D)_0$ and an initial amount of ionized Tritium of $(m_T)_0$. The initial amount of ionized Helium and single neutrons are supposed to be zero.

On the other hand, about the surface control $\partial\Omega$, we assume there is a part $\Omega_1 \subset \partial\Omega$ for which is allowed the entrance and exit of Deuterium and Tritium ionized atoms.

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We assume also there is another part $\partial\Omega_2 \subset \partial\Omega$ such that $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$ for which is allowed only the exit of ionized Helium atoms and neutrons, but not their entrance.

In $\partial\Omega_2$ is allowed the exit only (not the entrance) of ionized Deuterium and Tritium atoms.

Indeed, we assume the following relations for the masses:

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t)\, dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t)\, dx,$$

5.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D(m_{H_e,N})_T(t),$$

6.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T(m_{H_e,N})_T(t),$$

7.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

8.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

9.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$

12.
$$\begin{aligned} m_e(t) \quad = \quad & \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p} \\ & + \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p}. \end{aligned} \tag{102}$$

Here $\mathbf{n}$ denotes the outward normal vectorial fields to the concerning surfaces.

Having clarified such masses relations, denoting by $N_D(t)$ $N_T(t)$, $N_{H_e}(t)$, $N_N(t)$, $N_e(t)$ the respective indexed number of particles at time t, we define the functional

$$J(\phi, \rho, \mathbf{r}, \mathbf{u}, \mathbf{E}, \mathbf{A}, \mathbf{B}, \{N_D, N_T, N_{H_e}, N_N, N_e\})$$

where

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$$J = G(\nabla u) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 + F_4,$$

and where we assume $\gamma_p^D > 0,\ \gamma_p^T > 0,\ \gamma_N^D > 0,\ \gamma_{N_1}^T > 0,\ \gamma_{N_2}^T > 0,\ \gamma_{2p}^{H_e} > 0,\ \gamma_{N_1}^{H_e} > 0,\ \gamma_{N_2}^{H_e} > 0,\ \gamma_N > 0,\ \gamma_e > 0$ and $\alpha_D > 0,\ \alpha_T > 0,\ \alpha_{H_e} > 0,\ \alpha_N > 0\ , \alpha_{DT} > 0,\ \alpha_{H_e\,N} > 0,\ \alpha_{e,e} > 0,\ \alpha_{H_e,e} < 0$ so that

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\,dy\,ds\,dt \\
& + \frac{\gamma_N^D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\,dx\,dy\,ds\,dt \\
& \frac{\gamma_p^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\,dy\,ds\,dt \\
& + \frac{\gamma_{N_1}^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\,dx\,dy\,ds\,dt \\
& + \frac{\gamma_{N_2}^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\,dx\,dy\,ds\,dt \\
& + \frac{\gamma_{2p}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\,dy\,ds\,dt \\
& + \frac{\gamma_{N_1}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\,dx\,dy\,ds\,dt \\
& + \frac{\gamma_{N_2}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\,dx\,dy\,ds\,dt \\
& + \frac{\gamma_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\,dx\,ds\,dt \\
& + \frac{\gamma_e}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega (\nabla\phi_e)\cdot(\nabla\phi_e)\,dx\,dy\,ds\,dt, \qquad (103)
\end{aligned}$$

and

$$\begin{aligned}
& F(\phi) = \\
& \frac{\alpha_D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_0^{N_D(t)}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_D(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& + \frac{\alpha_T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_0^{N_T(t)}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_T(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& + \frac{\alpha_{DT}}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_0^{N_T(t)}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_T(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& + \frac{\alpha_{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_{H_e}(t)}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_{H_e}(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2,s_1)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& + \frac{\alpha_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_0^{N_N(t)}\int_\Omega \frac{|\phi_N(x-\xi,t,s-s_1)|^2|\phi_N(\xi,t,s_1)|^2}{|x-\xi|}\,dx\,d\xi\,ds\,ds_1\,dt \\
& + \sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_D(t)}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2,t)|^2|\phi_N(\xi_j,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& + \frac{\alpha_{H_e,\,e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_e(t)}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_e(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& + \frac{\alpha_{e,e}}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_0^{N_e(t)}\int_\Omega \frac{|\phi_e(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_e(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \qquad (104)
\end{aligned}$$

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and the internal kinetics energy is expressed by

$$\begin{aligned} E_c(\phi,\mathbf{r}) &= \frac{1}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega |\phi_D|^2\,\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega |\phi_T|^2\,\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega |\phi_{H_e}|^2\,\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega |\phi_N|^2\,\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega |\phi_e|^2\,\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}\,dx\,dy\,ds\,dt, \end{aligned} \tag{105}$$

Moreover,

$$F_1 = \frac{1}{4\pi}\int_0^{t_f} \|\operatorname{curl}\mathbf{A}-\mathbf{B}_0\|_2\,dt,$$

$$\begin{aligned} F_2 &= \int_0^{t_f}\int_0^{N_D(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)dx\,dy\,ds\,dt \\ &+\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)dx\,dy\,ds\,dt \\ &+\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)dx\,dy\,ds\,dt \\ &+\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_e|\phi_e|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_e}{\partial t}\right)dx\,dy\,ds\,dt, \end{aligned} \tag{106}$$

where K_p and K_e are appropriate real constants related to the respective charges.

Here $\mathbf{u}=(u_1,u_2,u_3)$ is the fluid velocity field and

$$\mathbf{r}_D,\ \mathbf{r}_T,\ \mathbf{r}_{H_e},\ \mathbf{r}_N,\ \mathbf{r}_e$$

are fields of displacements for the corresponding particle fields.

Also $\mathbf{A}$ denotes the magnetic potential, $\mathbf{B}_0$ an external magnetic field and $\mathbf{B}$ is the total magnetic field.

Moreover, $\mathbf{E}_{ind}$ is an induced electric field.

Also,

$$\begin{aligned} F_3 &= \frac{C_D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_D\cdot\nabla_{(x,y)}\mathbf{r}_D\,dx\,dy\,ds\,dt \\ &+\frac{C_T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_T\cdot\nabla_{(x,y)}\mathbf{r}_T\,dx\,dy\,ds\,dt \\ &+\frac{C_{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_{H_e}\cdot\nabla_{(x,y)}\mathbf{r}_{H_e}\,dx\,dy\,ds\,dt \\ &+\frac{C_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_N\cdot\nabla_{(x,y)}\mathbf{r}_N\,dx\,dy\,ds\,dt \\ &\frac{C_e}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_e\cdot\nabla_{(x,y)}\mathbf{r}_e\,dx\,dy\,ds\,dt, \end{aligned} \tag{107}$$

for appropriate real positive constants C_D C_T, C_{H_e}, C_N, C_e.

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Finally,

$$\begin{aligned} F_4 &= \frac{\varepsilon_D}{2}\int_0^{t_f}\left(\frac{\partial N_D(t)}{\partial t}\right)^2 dt + \frac{\varepsilon_T}{2}\int_0^{t_f}\left(\frac{\partial N_D(t)}{\partial t}\right)^2 dt \\ &+ \frac{\varepsilon_N}{2}\int_0^{t_f}\left(\frac{\partial N_N(t)}{\partial t}\right)^2 dt + \frac{\varepsilon_{H_e}}{2}\int_0^{t_f}\left(\frac{\partial N_{H_e}(t)}{\partial t}\right)^2 dt \\ &+ \frac{\varepsilon_e}{2}\int_0^{t_f}\left(\frac{\partial N_e(t)}{\partial t}\right)^2 dt, \end{aligned} \tag{108}$$

where ε_D, ε_T, ε_N, ε_{H_e}, ε_e are small real positive constants.

Such a functional J is subject to the following constraints:

1. The momentum conservation equation for the fluid motion

$$\rho\left(\frac{\partial u_k}{\partial t} + u_j\frac{\partial u_k}{\partial x_j}\right) = \rho f_k - \frac{\partial P}{\partial x_k} + \tau_{kj,j} + (F_E)_k + (F_M)_k,$$

$\forall k \in \{1,2,3\}$.

Here $\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e$ is the total density and P is the fluid pressure field.

Furthermore,

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\sum_{k=1}^{3}\frac{\partial u_k}{\partial x_k}\right),$$

$\forall i,j \in \{1,2,3\}$,

$$\mathbf{F}_E = \{(F_E)_k\} = \left(K_p\left(\int_0^{N_D(t)}|\phi_p^D|^2\,ds + \int_0^{N_T(t)}|\phi_p^T|^2\,ds + \int_0^{N_{H_e}(t)}|\phi_{2p}^{H_e}|^2\,ds\right) + K_e\int_0^{N_e(t)}|\phi_e|^2\,ds\right)\mathbf{E},$$

and

$$\begin{aligned} \mathbf{F}_M &= \{(F_M)_k\} \\ &= \left(K_p\left(\int_0^{N_D(t)}|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)ds\right.\right. \\ &\int_0^{N_T(t)}|\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right)ds \\ &\left.+ \int_0^{N_{H_e}(t)}|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)ds\right) \\ &\left.+K_e\int_0^{N_e(t)}|\phi_e|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_e}{\partial t}\right)ds\right) \times \mathbf{B}. \end{aligned} \tag{109}$$

2. Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \text{ div } (\rho\mathbf{u}) = 0.$$

3. Energy equation

$$\rho\frac{De}{Dt} + \nabla_x(\hat{E}_1)\cdot\mathbf{u} + \hat{E}_2 + P(\text{ div } \mathbf{u}) = \frac{\partial Q}{\partial t} - \text{ div } \mathbf{q} + \tau_{jk}\frac{\partial u_j}{\partial x_k},$$

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where we assume the Fourier law

$$\mathbf{q} = -K\nabla T,$$

where $T = T(x,t)$ is the scalar field of temperature and Q is a standard heat function.
Also,

$$\begin{aligned} e &= \frac{\rho}{2}\mathbf{u}\cdot\mathbf{u} + \frac{\rho_D}{2}\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t} \\ &+ \frac{\rho_T}{2}\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t} \\ &+ \frac{\rho_{H_e}}{2}\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t} \\ &+ \frac{\rho_N}{2}\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t} \\ &+ \frac{\rho_e}{2}\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}, \end{aligned} \tag{110}$$

where the densities $\hat{E}_1$ and $\hat{E}_2$ are defined through the expressions of $F(\phi)$ and F_2 so that

$$F(\phi) = \int_0^{t_f}\int_\Omega \hat{E}_1\, dx\, dt$$

and

$$F_2 = \int_0^{t_f}\int_\Omega \hat{E}_2\, dx\, dt.$$

Here we recall that since $\mathbf{r}_D$ is highly oscillating in t we approximately have

$$\mathbf{u}\cdot\mathbf{r}_D \approx 0$$

in a weak or measure sense. The same remark is valid for the other internal velocity fields.
Moreover,

$$\frac{De}{Dt} = \frac{\partial e}{\partial t} + u_j\frac{\partial e}{\partial x_j}.$$

4.

$$P = F_7(\rho, T),$$

for an appropriate scalar function F_7.

5. Mass relations

(a)

$$m_D(t) = \int_\Omega \rho_D(x,t)\, dx,$$

(b)

$$m_T(t) = \int_\Omega \rho_T(x,t)\, dx,$$

(c)

$$m_{He}(t) = \int_\Omega \rho_{H_e}(x,t)\, dx,$$

(d)

$$m_N(t) = \int_\Omega \rho_N(x,t)\, dx,$$

(e)

$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx,$$

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where,

(a)
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

(b)
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

(c)
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D(m_{H_e,N})_T(t),$$

(d)
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T(m_{H_e,N})_T(t),$$

(e)
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

(f)
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

(g)
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that
$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

(h)
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau.$$

(i)
$$\begin{aligned} m_e(t) \quad = \quad & \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\, dy\, dy\, ds \frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p} \\ & + \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p}. \end{aligned} \tag{111}$$

6. Other mass constraints

(a)
$$\int_\Omega |\phi_N^D(x,y,t,s)|^2\, dx = m_N,$$

(b)
$$\int_\Omega |\phi_{N_1}^T(x,y,t,s)|^2\, dx = m_N,$$

(c)
$$\int_\Omega |\phi_{N_2}^T(x,y,t,s)|^2\, dx = m_N,$$

(d)
$$\int_\Omega |\phi_{N_1}^{H_e}(x,y,t,s)|^2\, dx = m_N,$$

(e)
$$\int_\Omega |\phi_{N_2}^{H_e}(x,y,t,s)|^2\, dx = m_N,$$

(f)
$$\int_\Omega |\phi_p^D(x,t,s)|^2\, dx = m_p,$$

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(g)

$$\int_\Omega |\phi_p^T(x,t,s)|^2\, dx = m_p,$$

(h)

$$\int_\Omega |\phi_{2p}^{H_e}(x,t,s)|^2\, dx = 2\, m_p,$$

7.

$$m_D(t) = m_p\, N_D(t) + m_N\, N_D(t)$$
$$m_T(t) = m_p\, N_T(t) + m_N\, N_T(t),$$
$$m_{H_e}(t) = 2m_p\, N_{H_e}(t) + 2m_N\, N_{H_e}(t),$$
$$m_e(t) = m_e\, N_D(t) + m_e\, N_T(t) + 2\, m_e\, N_{H_e}(t).$$

8. For the induced electric field, we must have

$$\begin{aligned}
&\text{curl}\, \mathbf{E}_{ind} + \frac{1}{c}\, \text{curl} \left(\hat{K}_p \int_0^{N_D(t)} |\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t} \right) ds \right. \\
&+ \hat{K}_p \int_0^{N_T(t)} |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t} \right) ds \\
&+ \hat{K}_p \int_0^{N_{He}(t)} |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t} \right) ds \\
&\left. + \hat{K}_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\, dx \right) ds \right) \\
&\times (\, \text{curl}\, \mathbf{A} - \mathbf{B}_0) - \frac{1}{c} \frac{\partial}{\partial t} (\, \text{curl}\, \mathbf{A} - \mathbf{B}_0) = \mathbf{0}, \qquad (112)
\end{aligned}$$

where $\hat{K}_p$ and $\hat{K}_e$ are appropriate real constants related to the respective charges.

9. A Maxwell equation:

$$\text{div}\, \mathbf{B} = 0,$$

where

$$\mathbf{B} = \mathbf{B}_0 - \text{curl}\, \mathbf{A}.$$

10. Another Maxwell equation:

$$\begin{aligned}
\text{div}\, \mathbf{E} \;=\; & 4\pi \left(K_p \left(\int_0^{N_D(t)} |\phi_p^D|^2\, ds + \int_0^{N_T(t)} |\phi_p^T|^2\, ds + \int_0^{N_{He}(t)} |\phi_{2p}^{H_e}|^2\, ds \right) \right. \\
& \left. + K_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2\, dx\, ds \right), \qquad (113)
\end{aligned}$$

where the total electric field $\mathbf{E}$ stands for

$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_\rho,$$

and where generically denoting

$$F(\phi) = \int_0^{t_f} \int_\Omega f_5(\phi, x, t\xi, s)\, dx\, d\xi\, ds\, dt,$$

we have also

$$\mathbf{E}_\rho = \left\{ \int_\Omega \frac{\partial f_5(\phi, x, t, \xi, s)}{\partial x_k}\, d\xi\, ds \right\}.$$

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At this point we generically denote

$$\langle h_1, h_2 \rangle_{L^2} = \int_0^{t_f} \int_\Omega h_1 \, h_2 \, dx \, dy \, dt.$$

Thus, already including the Lagrange multipliers concerning the restrictions indicated, the extended functional J_3 stands for

$$\begin{aligned} & J_3 = J_3(\phi, \mathbf{u}, \mathbf{r}, P, \mathbf{A}, \mathbf{B}, \mathbf{E}, \Lambda, E, \{N_D, N_T, N_{H_e}, N_N, N_e\}) \\ = \; & G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 + F_4 \\ & + \left\langle \Lambda_k, \rho \left(\frac{\partial u_k}{\partial t} + u_j \frac{\partial u_k}{\partial x_j} \right) - \rho f_k + \frac{\partial P}{\partial x_k} - \tau_{kj,j} - (F_E)_k - (F_M)_k \right\rangle_{L^2} \\ & + \left\langle \Lambda_4, \; \frac{\partial \rho}{\partial t} + \text{ div } (\rho \mathbf{u}) \right\rangle_{L^2} + J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5}, \end{aligned} \tag{114}$$

where,

$$\begin{aligned} J_{Aux_1} \; = \; & \left\langle \Lambda_5, \; \rho \frac{De}{Dt} + \nabla_x(\hat{E}_1) \cdot \mathbf{u} + P(\text{ div } \mathbf{u}) - \frac{\partial Q}{\partial t} + \text{ div } \mathbf{q} - \tau_{jk} \frac{\partial u_j}{\partial x_k} \right\rangle_{L^2} \\ & + \langle \Lambda_6, \; P - F_7(\rho, T) \rangle_{L^2}, \end{aligned} \tag{115}$$

$$\begin{aligned} J_{Aux_2} \; = \; & \left\langle \Lambda_7, m_D(t) - \int_\Omega \rho_D(x,t) \, dx \right\rangle_{L^2} \\ & + \left\langle \Lambda_8, m_T(t) - \int_\Omega \rho_T(x,t) \, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_9, m_{H_e}(t) - \int_\Omega \rho_{H_e}(x,t) \, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_{10}, m_N(t) - \int_\Omega \rho_N(x,t) \, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_{11}, m_e(t) - \int_\Omega \rho_e(x,t) \, dx \right\rangle_{L^2} \\ & \int_0^{t_f} E_{12}(t)(\alpha_N m_{H_e})_T(t) - \alpha_{H_e}(m_N)_T(t)) \, dt, \end{aligned} \tag{116}$$

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$$
\begin{aligned}
J_{Aux_3} \;=\; & -\int_0^{t_f}\int_\Omega (E_N^D)_5(y,t,s)\left(\int_\Omega |\phi_N^D(x,y,t,s)|^2\,dx - m_N\right) dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_1}^T)_6(y,t,s)\left(\int_\Omega |\phi_{N_1}^T(x,y,t,s)|^2\,dx - m_N\right) dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_2}^T)_7(y,t,s)\left(\int_\Omega |\phi_{N_2}^T(x,y,t,s)|^2\,dx - m_N\right) dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_1}^{H_e})_8(y,t,s)\left(\int_\Omega |\phi_{N_1}^{H_e}(x,y,t,s)|^2\,dx - m_N\right) dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_2}^{H_e})_9(y,t,s)\left(\int_\Omega |\phi_{N_2}^{H_e}(x,y,t,s)|^2\,dx - m_N\right) dy\,dt, \\
& -\int_0^{t_f}\int_\Omega (E_p^D)(t,s)\left(\int_\Omega |\phi_p^D(y,t,s)|^2\,dy - m_p\right) ds\,dt, \\
& -\int_0^{t_f}\int_\Omega (E_p^T)(t,s)\left(\int_\Omega |\phi_p^T(y,t,s)|^2\,dy - m_p\right) ds\,dt, \\
& -\int_0^{t_f}\int_\Omega (E_{2p}^{H_e})(t,s)\left(\int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\,dy - 2m_p\right) ds\,dt, \qquad (117)
\end{aligned}
$$

$$
\begin{aligned}
J_{Aux_4} \;=\; & \langle \Lambda_{12},\ \text{curl}\,\mathbf{E}_{ind} \\
& +\frac{1}{c}\,\text{curl}\left(\hat{K}_p\int_0^{N_D(t)} |\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right) ds\right. \\
& +\hat{K}_p\int_0^{N_T(t)} |\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right) ds \\
& +\hat{K}_p\int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right) ds \\
& \left.+\hat{K}_e\int_0^{N_e(t)}\int_\Omega |\phi_e(x,y,t,s)|^2\left(\mathbf{u}(y,t)+\frac{\partial \mathbf{r}_e(x,y,t,s)}{\partial t}\,dx\right) ds\right) \\
& \times(\,\text{curl}\,\mathbf{A}-\mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\,\text{curl}\,\mathbf{A}-\mathbf{B}_0)\Big\rangle_{L^2} \\
& +\langle \Lambda_{13},\ \text{div}\,\mathbf{B}\rangle_{L^2} \\
& +\left\langle \Lambda_{14},\ \text{div}\,\mathbf{E} - 4\pi\left(K_p\left(\int_0^{N_D(t)} |\phi_p^D|^2\,ds + \int_0^{N_T(t)} |\phi_p^T|^2\,ds + \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2\,ds\right)\right.\right. \\
& \left.\left.+K_e\int_\Omega |\phi_e|^2\,dx\,ds\right)\right\rangle_{L^2}. \qquad (118)
\end{aligned}
$$

$$
\begin{aligned}
J_{Aux_5} \;=\; & \langle \Lambda_{15},\ m_D(t) - (m_p\ N_D(t) + m_N\ N_D(t))\rangle_{L^2} \\
& +\langle \Lambda_{16},\ m_T(t) - (m_p\ N_T(t) + m_N\ N_T(t))\rangle_{L^2} \\
& +\langle \Lambda_{17},\ m_{H_e}(t) - (2m_p\ N_{H_e}(t) + 2m_N\ N_{H_e}(t))\rangle_{L^2} \\
& +\langle \Lambda_{18},\ m_e(t) - (m_e\ N_D(t) + m_e\ N_T(t) + 2\ m_e\ N_{H_e}(t))\rangle_{L^2}. \qquad (119)
\end{aligned}
$$

Here we recall the following definitions and relations:

1. For the Deuterium field

$$
|\phi_D(x,y,t,s)|^2 = |\phi_p^D(y,t,s)|^2 + |\phi_N^D(x,y,t,s)|^2|\phi_p^D(y,t,s)|^2\frac{1}{m_p},
$$

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2. For the Tritium field

$$|\phi_T(x,y,t,s)|^2 = |\phi_p^T(y,t,s)|^2 + (|\phi_{N_1}^T(x,y,t,s)|^2 + |\phi_{N_2}^T(x,y,t,s)|^2)|\phi_p^D(y,t,s)|^2 \frac{1}{m_p},$$

3. For the Helium field

$$|\phi_{H_e}(x,y,t,s)|^2 = |\phi_{2p}^{H_e}(y,t,s)|^2 + (|\phi_{N_1}^{H_e}(x,y,t,s)|^2 + |\phi_{N_2}^{H_e}(x,y,t,s)|^2)|\phi_{2p}^{H_e}(y,t,s)|^2 \frac{1}{2\, m_p},$$

4. For the Neutron field

$$\phi_N = \phi_N(x,t,s),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t,s).$$

1.
$$\rho_D(y,t) = \int_0^{N_D(t)} \int_\Omega |\phi_D(x,y,t,s)|^2 \, dx \, ds,$$

2.
$$\rho_T(y,t) = \int_0^{N_T(t)} \int_\Omega |\phi_T(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_{H_e}(y,t) = \int_0^{N_{H_e}(t)} \int_\Omega |\phi_{H_e}(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_N(x,t) = \int_0^{N_N(t)} |\phi_N(x,t,s)|^2 \, ds,$$

$$\rho_e(y,t) = \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \, dx \, ds.$$

Also,

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e,$$

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t) \, dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t) \, dx,$$

5.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1 \cup \partial\Omega_2} (\rho_D(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau - \alpha_D (m_{H_e,N})_T(t),$$

6.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1 \cup \partial\Omega_2} (\rho_T(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau - \alpha_T (m_{H_e,N})_T(t),$$

7.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t) \, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u} \cdot \mathbf{n} \, d\Gamma d\tau,$$

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8.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\,dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\,d\Gamma d\tau,$$

9.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that
$$\alpha_N(m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) - \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\,d\Gamma\,d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\,dx.$$

12.
$$\begin{aligned} m_e(t) &= \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\,dy\,dy\,ds\frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p} \\ &+ \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p}. \end{aligned} \tag{120}$$

Finally,
$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_\rho,$$

and where generically denoting
$$F(\phi) = \int_0^{t_f} \int_\Omega f_5(\phi,x,t,\xi,s)\,dx\,d\xi\,ds,$$

we have also
$$\mathbf{E}_\rho = \left\{ \int_\Omega \frac{\partial f_5(\phi,x,t,\xi,s)}{\partial x_k}\,d\xi\,ds \right\}.$$

and,
$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

21. A Qualitative Modeling for a General Phase Transition Process

In this section we develop a general qualitative modeling for a phase transition process.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Such a set Ω is supposed to a be a fixed volume in which an amount of mass of a substance A with a density function u will develop phase a transition for another phase with corresponding density function v. The total mass m_T is suppose to be kept constant throughout such a process.

We model such transition in phase through a functional $J : V \times V \to \mathbb{R}$ where

$$\begin{aligned} J(u,v) &= \frac{\gamma_1}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{\alpha_1}{2}\int_\Omega u^4\,dx \\ &\frac{\gamma_2}{2}\int_\Omega \nabla v\cdot\nabla v\,dx + \frac{\alpha_2}{2}\int_\Omega v^4\,dx \\ &-\frac{1}{2}\int_\Omega \omega^2(u^2+v^2)\,dx - \frac{E}{2}\left(\int_\Omega (u^2+v^2)\,dx - m_T\right). \end{aligned} \tag{121}$$

Here $\gamma_1 > 0,\ \gamma_2 > 0,\ \alpha_1 > 0,\ \alpha_2 > 0$ and $V = W^{1,2}(\Omega)$.

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The phases corresponding to u and v are connected through a Lagrange multiplier E, which represents the chemical potential of the chemical process in question.

We assume the temperature is directly proportional to the internal kinetics E_C energy where

$$E_C = \frac{1}{2}\int_\Omega u^2 \frac{\partial \mathbf{r}_u}{\partial t}\cdot\frac{\partial \mathbf{r}_u}{\partial t}\,dx.$$

For a internal vibrational motion, we assume approximately

$$\mathbf{r}_u \approx e^{i\omega t}\mathbf{w}_5(x),$$

for an appropriate frequency ω and vectorial function $\mathbf{w}_5$.

Thus, the temperature $T = T(x,t)$ is indeed proportional to ω^2, that is, symbolically, we may write

$$T \propto E_1 \propto \omega^2.$$

Therefore, we start with the system with a phase corresponding to $u \approx 1$ and $v \approx 0$ at $\omega = 1$. Gradually increasing the temperature to a corresponding $\omega = 15$, we obtain a transition to a phase corresponding to $u \approx 0$ and $v \approx 1$.

At this point, we also define the index normalized corresponding densities

$$\phi_u = \frac{u^2}{u^2+v^2}$$

and

$$\phi_v = \frac{v^2}{u^2+v^2}.$$

Finally, we have obtained some numerical results for the following parameters:
$\Omega = [0,1] \subset \mathbb{R}$, $\gamma_1 = \gamma_2 = 1$, $\alpha = 0.1$, $\alpha_2 = 10^3$.

1. We start with $\omega = 1$ corresponding to $\phi_u \approx 1$ and $\phi_v \approx 0$ in Ω.

   For the corresponding solutions ϕ_u and ϕ_v, please see Figures 15 and 16, respectively.
2. We end the process with $\omega = 15$ corresponding to $\phi_u \approx 0$ and $\phi_v \approx 1$ in Ω.

   For the corresponding solutions ϕ_u and ϕ_v, please see Figures 17 and 18, respectively.

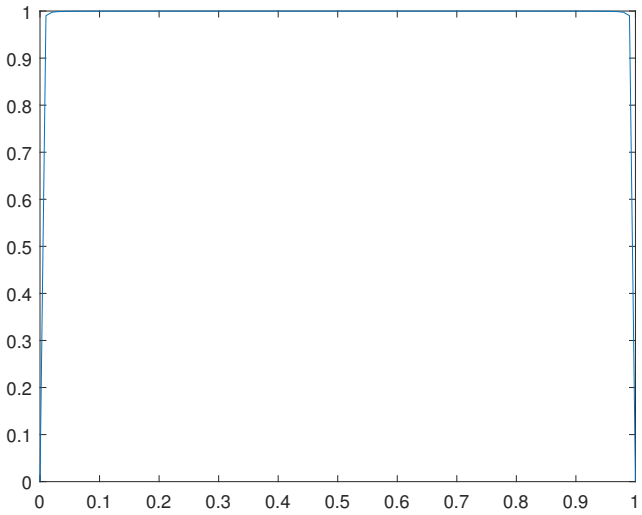

Figure 15. Solution $\phi_u(x)$ for $\omega = 1$.

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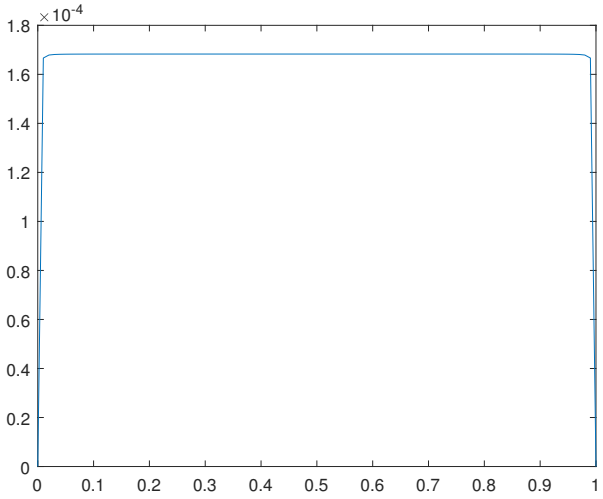

Figure 16. Solution $\phi_v(x)$ for $\omega = 1$.

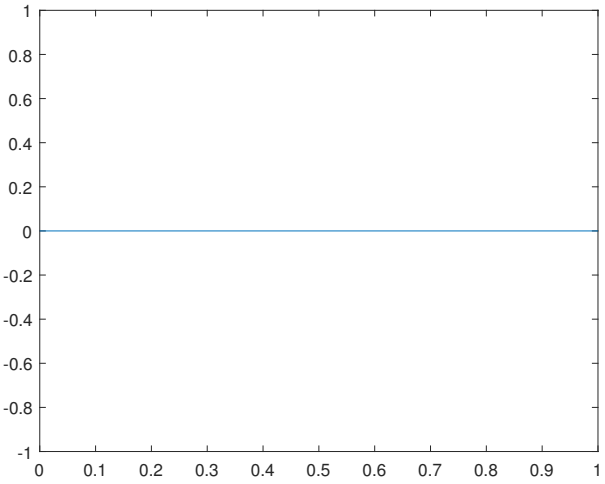

Figure 17. Solution $\phi_u(x)$ for $\omega = 15$.

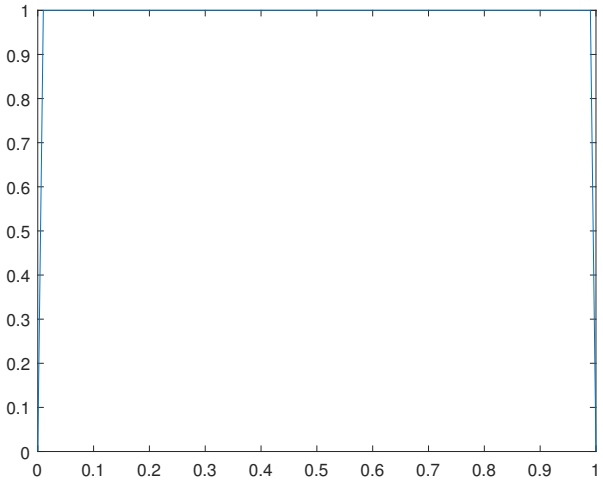

Figure 18. Solution $\phi_v(x)$ for $\omega = 15$.

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22. A Mathematical Description of a Hydrogen Molecule in a Quantum Mechanics Context

In this section we develop a mathematical description for a hydrogen molecule.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Observe that a single hydrogen molecule comprises two hydrogen atoms physically linked through their electrons.

We recall that each hydrogen atom comprises one proton, one neutron and one electron.

Since the electric charge interaction effects are much higher than those related to the respective masses, in a first analysis we neglect the single neutron densities.

Denoting $(x,y,z) \in \Omega \times \Omega \times \Omega$ and time $t \in [0,t_f]$, generically, for a particle p_{jkl} at the atom A_{kl} in the molecule M_l, we define the following general density:

$$|\phi_{(p_{jkl})_T}(x,y,z,t)|^2 = \frac{|\phi_{p_{jkl}}(x,y,z,t)|^2|\phi_{A_{kl}}(y,z,t)|^2|\phi_{M_l}(z,t)|^2}{m_{A_{jk}}m_{M_l}}.$$

Here we have the particle density $|\phi_{p_{jkl}}(x,y,z,t)|^2$ in the atom A_{kl} with density $|\phi_{A_{kl}}(y,z,t)|^2$, at the molecule M_l with a global density $|\phi_{M_l}(z,t)|^2$.

Here we have also denoted, $m_{p_{jkl}}$ the particle mass, $m_{A_{kl}}$ the mass of atom A_{kl} and m_{M_l} the mass of molecule M_l, so that we set the following constraints:

1.
$$\int_\Omega |\phi_{p_{jkl}}(x,y,z,t)|^2\,dx = m_{p_{jkl}},$$

2.
$$\int_\Omega |\phi_{A_{kl}}(y,z,t)|^2\,dy = m_{A_{kl}},$$

3.
$$\int_\Omega |\phi_{M_l}(z,t)|^2\,dz = m_{M_l}.$$

At this point we denote for the atoms A_1 e A_2 of a hydrogen molecule:

1. $m_{e_j} = m_e$: mass of electron e_j in the atom A_j, where $j \in \{1,2\}$.
2. $m_{p_j} = m_p$: mass of proton p_j in the atom A_j, where $j \in \{1,2\}$.

Therefore, considering the respective indexed densities for the particles in question, we define the total hydrogen molecule density, denoted by $|\phi_{H_2}(x,y,z,t)|^2$ as

$$\begin{aligned}|\phi_{H_2}(x,y,z,t)|^2 \quad = \quad & \frac{|\phi_{p_1}(x,y,z,t)|^2|\phi_{A_1}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_1}m_M} \\ & + \frac{|\phi_{e_1}(x,y,z,t)|^2|\phi_{A_1}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_1}m_M} \\ & + \frac{|\phi_{p_2}(x,y,z,t)|^2|\phi_{A_2}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_2}m_M} \\ & + \frac{|\phi_{e_2}(x,y,z,t)|^2|\phi_{A_2}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_2}m_M}. \end{aligned} \tag{122}$$

Such system is subject to the following constraints:

1. From the proton p_1 in the atom A_1:

$$\int_\Omega |\phi_{p_1}(x,y,z,t)|^2\,dx = m_p,$$

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2. For the proton p_2 in the atom A_2:

$$\int_\Omega |\phi_{p_2}(x,y,z,t)|^2\, dx = m_p,$$

3. For the atom A_1:

$$\int_\Omega |\phi_{A_1}(y,z,t)|^2\, dy = m_{A_1},$$

4. For the atom A_2:

$$\int_\Omega |\phi_{A_2}(y,z,t)|^2\, dy = m_{A_2},$$

5. For the electrons e_1 and e_2, concerning the physical electronic link between the atoms:

$$\int_\Omega |\phi_{e_1}(x,y,z,t)|^2\, dx + \int_\Omega |\phi_{e_2}(x,y,z,t)|^2\, dx = 2m_e.$$

6. For the total molecular density:

$$\int_\Omega |\phi_M(z,t)|^2\, dz = m_M.$$

Therefore, already including the Lagrange multipliers, the corresponding variational formulation for such a system stands for $J : V \to \mathbb{R}$, where

$$J(\phi, E) = G(\nabla\phi) + F(\phi) + J_{Aux}(\phi, E).$$

Here we denote

$$|(\phi_{p_j})_T|^2 = \frac{|\phi_{p_j}(x,y,z,t)|^2 |\phi_{A_j}(y,z,t)|^2 |\phi_M(z,t)|^2}{m_{A_j} m_M},$$

$$|(\phi_{e_j})_T|^2 = \frac{|\phi_{e_j}(x,y,z,t)|^2 |\phi_{A_j}(y,z,t)|^2 |\phi_M(z,t)|^2}{m_{A_j} m_M},\ \forall j \in \{1,2\}$$

we assume $\gamma_{(p_j)} > 0,\ \gamma_{e_j} > 0,\ \gamma_{A_j} > 0,\ \gamma_M > 0,\ \alpha_{(p_j)_T} > 0,\ \alpha_{(e_j)_T} > 0\ \alpha_{(p_j\, e_k)_T} < 0,\ \forall j,k \in \{1,2\},$

$$\begin{aligned} G(\nabla\phi) \quad = \quad & \frac{\gamma_{p_j}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{p_j}) \cdot (\nabla\phi_{p_j})\, dx\, dy\, dz\, dt \\ & + \frac{\gamma_{e_j}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{e_j}) \cdot (\nabla\phi_{e_j})\, dx\, dy\, dz\, dt \\ & \frac{\gamma_{A_j}}{2} \int_\Omega (\nabla\phi_{A_j}) \cdot (\nabla\phi_{A_j})\, dy\, dz\, dt \\ & + \frac{\gamma_M}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_M) \cdot (\nabla\phi_M)\, dz\, dt \end{aligned} \tag{123}$$

and

$$\begin{aligned} & F(\phi) = \\ & \frac{\alpha_{(p_j)_T}}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_{(p_j)_T}(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_{(p_j)_T}(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z) - (\xi_1,\xi_2,\xi_3)|}\, dx\, dy\, dz; d\xi_1\, d\xi_2\, d\xi_3\, dt \\ & + \frac{\alpha_{(e_j)_T}}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_{(e_j)_T}(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_{(e_j)_T}(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z) - (\xi_1,\xi_2,\xi_3)|}\, dx\, dy\, dz\, d\xi_1\, d\xi_2\, d\xi_3\, dt \\ & + \frac{\alpha_{(p_j\, e_k)_T}}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_{(p_j)_T}(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_{(e_k)_T}(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z) - (\xi_1,\xi_2,\xi_3)|}\, dx\, dy\, dz\, d\xi_1\, d\xi_2\, d\xi_3\, dt \end{aligned}$$

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Finally,

$$\begin{aligned} J_{Aux}(\phi, E) &= \int_0^{t_f} \int_\Omega (E_p)_j(y,z,t) \left(\int_\Omega |\phi_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\ & \int_0^{t_f} \int_\Omega (E_e)(y,z,t) \left(\int_\Omega (|\phi_{e_1}(x,y,z,t)|^2 + |\phi_{e_2}(x,y,z,t)|^2) \, dx - 2m_e \right) dy \, dz \, dt \\ & \int_0^{t_f} \int_\Omega (E_A)_j(z,t) \left(\int_\Omega |\phi_{A_j}(y,z,t)|^2 \, dy - m_{A_j} \right) dz \, dt \\ & \int_0^{t_f} (E_M)(t) \left(\int_\Omega |\phi_M(z,t)|^2 \, dz - m_M \right) dt. \end{aligned} \tag{124}$$

Remark 22.1. *We highlight the two electrons which link the atoms are at same level of energy E_e. Morever, each atom has its energy level E_{A_j} and the molecule as a whole has also its energy level E_M.*

23. A Mathematical Model for the Water Hydrolysis

In this section we develop a modeling for a chemical reaction known as the water hydrolysis.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

In such a volume Ω containing a total mass m_T of water initially at the temperature 25 C with pressure 1 atm, we intend to model the following reaction

$$H_2O \rightleftharpoons OH^- + H^+$$

which as previously mentioned is the well known water hydrolysis.

We highlight H_2O stand for a water molecule which subject to an appropriate electric potential is decomposed into a ionized OH^- molecule and ionized H^+ atom.

It is also well known that the water symbol H_2O corresponds to a molecule with two hydrogen (H) atoms and one oxygen (O) atom.

Moreover, the oxygen atom O has 8 protons, 8 neutrons and 8 electrons whereas the hydrogen atom H has one proton, one neutron and one electron.

Remark 23.1. *Here we have assumed that a unit mass of H_2O reacts into a fractional mass α_B of OH^- and a fractional mass α_C of H^+.*

Symbolically, we have:

$$1 = \alpha_B + \alpha_C.$$

To clarify the notation we set the conventions:

1. H_2O molecule generically corresponds to wave function ϕ_1.
2. OH^- molecule corresponds to wave function ϕ_2.
3. H^+ hydrogen atom corresponds to wave function ϕ_3.

At this point we define the following densities:

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1. For the H_2O water density (for charges), denoted by $|\phi_1|^2$, we have

$$\begin{aligned}|\phi_1(x,y,z,t)|^2 &= K_p\sum_{j=1}^{2}|(\phi_1^H)_{p_j}(x,y,z,t)|^2\frac{|(\phi_1^H)_{A_j}(y,z,t)|^2|(\phi_1)_M(z,t)|^2}{(m)_{A_j}^H\,(m_1)_M}\\ &+K_e\sum_{j=1}^{2}|(\phi_1^H)_{e_j}(x,y,z,t)|^2\frac{|(\phi_1^H)_{A_j}(y,z,t)|^2|(\phi_1)_M(z,t)|^2}{(m_1)_{A_j}^H\,(m_1)_M}\\ &+K_p\sum_{j=1}^{8}|(\phi_1^O)_{p_j}(x,y,z,t)|^2\frac{|(\phi_1^O)_{A}(y,z,t)|^2|(\phi_1)_M(z,t)|^2}{(m)_{A}^O\,(m_1)_M}\\ &+K_e\sum_{j=1}^{8}|(\phi_1^O)_{e_j}(x,y,z,t)|^2\frac{|(\phi_1^O)_{A}(y,z,t)|^2|(\phi_1)_M(z,t)|^2}{(m)_{A}^O\,(m_1)_M}\end{aligned}\tag{125}$$

where $(m_1)_M$ is the mass of a single water molecule and generically $|(\phi_1^H)_{p_j}(x,y,z,t)|^2$ refers to the hydrogen proton p_j at the hydrogen atom A_j concerning the H_2O molecular density and so on.

2. For the OH^- density, denoted by $|\phi_2|^2$, we have

$$\begin{aligned}|\phi_2(x,y,z,t)|^2 &= K_p|(\phi_2^H)_p(x,y,z,t)|^2\frac{|(\phi_2^H)_{A}(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_{A}^H\,(m_2)_M}\\ &+K_e|(\phi_2^H)_{e_1}(x,y,z,t)|^2\frac{|(\phi_2^H)_{A}(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_{A}^H\,(m_2)_M}\\ &+K_e|(\phi_2^{OH^-})_{e_2}(x,z,t)|^2\frac{|(\phi_2)_M(z,t)|^2}{(m_2)_M}\\ &+K_p\sum_{j=1}^{8}|(\phi_2^O)_{p_j}(x,y,z,t)|^2\frac{|(\phi_2^O)_{A}(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_{A}^O\,(m_2)_M}\\ &+K_e\sum_{j=1}^{8}|(\phi_2^O)_{e_j}(x,y,z,t)|^2\frac{|(\phi_2^O)_{A}(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_{A}^O\,(m_2)_M},\end{aligned}\tag{126}$$

where $(m_2)_M$ is the mass of a single molecule of OH^-.

3. For the ionized hydrogen atom have

$$|\phi_3(x,y,t)|^2 = K_p|(\phi_3^H)_p(x,y,t)|^2\frac{|(\phi_3^H)_{A}(y,t)|^2}{(m_3)_A}.$$

where we have denoted $(m_3)_A$ is the mass of a single atom of H^+.

Here $K_p > 0$ and $K_e < 0$ are appropriate real constants concerning a proton and an electron charge, respectively.

The system is subject to the following constraints:

1. $$\int_\Omega |(\phi_1^H)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j\in\{1,2\},$$

2. $$\int_\Omega |(\phi_1^H)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j\in\{1,2\},$$

3. $$\int_\Omega |(\phi_1^O)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j\in\{1,8\},$$

4. $$\int_\Omega |(\phi_1^O)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j\in\{1,8\},$$

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5. $$\int_{\Omega} |(\phi_2^H)_p(x,y,z,t)|^2 \, dx = m_p,$$

6. $$\int_{\Omega} |(\phi_2^H)_{e_1}(x,y,z,t)|^2 \, dx = m_e,$$

7. $$\int_{\Omega} |(\phi_2^H)_{e_2}(x,y,z,t)|^2 \, dx = m_e,$$

8. $$\int_{\Omega} |(\phi_2^O)_{p_j}(x,y,z,t)|^2 \, dx = m_p, \ \forall j \in \{1,8\},$$

9. $$\int_{\Omega} |(\phi_2^O)_{e_j}(x,y,z,t)|^2 \, dx = m_e, \ \forall j \in \{1,8\},$$

10. $$\int_{\Omega} |(\phi_3^H)_p(x,z,t)|^2 \, dx = m_p,$$

11. $$\int_{\Omega} |(\phi_1^H)_{A_j}(y,z,t)|^2 \, dy = m_A^H, \forall j \in \{1,2\},$$

12. $$\int_{\Omega} |(\phi_1^O)_A(y,z,t)|^2 \, dy = m_A^O,$$

13. $$\int_{\Omega} |(\phi_2^H)_A(y,z,t)|^2 \, dy = m_A^H,$$

14. $$\int_{\Omega} |(\phi_2^O)_A(y,z,t)|^2 \, dy = m_A^O,$$

15. $$\int_{\Omega} |(\phi_3^H)_A(y,z,t)|^2 \, dy = m_A^H,$$

16. $$\int_{\Omega} (|(\phi_1)_M(z,t)|^2 + |(\phi_2)_M(z,t)|^2 + |(\phi_3)_M(z,t)|^2) \, dz = m_T,$$

17. $$\int_{\Omega} (\alpha_C |(\phi_2)_M(z,t)|^2 - \alpha_B |(\phi_3)_M(z,t)|^2) \, dz = 0.$$

Already including the Lagrange multipliers for the constraints, the variational formulation for such system. denoted by the functional $J(\phi, E)$ stands for

$$J(\phi, E) = G(\nabla\phi) + F(\phi) + F_1(\phi) - J_{Aux}(\phi, E),$$

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where

$$
\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^H)_{p_j}\cdot\nabla(\phi_1^H)_{p_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^H)_{e_j}\cdot\nabla(\phi_1^H)_{e_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_p}{2}\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^O)_{p_j}\cdot\nabla(\phi_1^O)_{p_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^O)_{e_j}\cdot\nabla(\phi_1^O)_{e_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_p}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{p}\cdot\nabla(\phi_2^H)_{p}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{e_1}\cdot\nabla(\phi_2^H)_{e_1}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^{OH^-})_{e_2}\cdot\nabla(\phi_1^{OH^-})_{e_2}\,dx\,dz\,dt \\
& +\frac{\gamma_p}{2}\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^O)_{p_j}\cdot\nabla(\phi_2^O)_{p_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^O)_{e_j}\cdot\nabla(\phi_2^O)_{e_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_p}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{p}\cdot\nabla(\phi_2^O)_{p}\,dx\,dy\,dt \\
& +\frac{\gamma_{A^H}}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^H)_{A_j}\cdot\nabla(\phi_1^H)_{A_j}\,dy\,dz\,dt \\
& +\frac{\gamma_{A^O}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^O)_{A}\cdot\nabla(\phi_1^O)_{A}\,dy\,dz\,dt \\
& +\frac{\gamma_{A^H}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{A}\cdot\nabla(\phi_2^H)_{A}\,dy\,dz\,dt \\
& +\frac{\gamma_{A^O}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^O)_{A}\cdot\nabla(\phi_2^O)_{A}\,dy\,dz\,dt \\
& +\frac{\gamma_{M_1}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1)_{M}\cdot\nabla(\phi_1)_{M}\,dz\,dt \\
& +\frac{\gamma_{M_2}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2)_{M}\cdot\nabla(\phi_2)_{M}\,dz\,dt \\
& \frac{\gamma_{A_3}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_3)_{A}\cdot\nabla(\phi_3)_{A}\,dy\,dt.
\end{aligned}
$$

Here $\gamma_p > 0$, $\gamma_e > 0$, $\gamma_A^H > 0$,, $\gamma_A^O > 0$, $\gamma_{M_1} > 0$, $\gamma_{M_2} > 0$, $\gamma_{A_3} > 0$.

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Moreover,

$$
\begin{aligned}
& F(\phi) \\
= \; & \frac{\alpha_1}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_1(x-\xi_1,y-\xi_2,z-\xi_3,t)|^2|\phi_1(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_2\,dx_3\,dt \\
& +\frac{\alpha_2}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_2(x-\xi_1,y-\xi_2,z-\xi_3,t)|^2|\phi_2(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_2\,dx_3\,dt \\
& +\frac{\alpha_3}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_3(x-\xi_1,z-\xi_3,t)|^2|\phi_3(\xi_1,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_3\,dt \\
& +\frac{\alpha_{23}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_2(x-\xi_1,y-\xi_2,z-\xi_3,t)|^2|\phi_3(\xi_1,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_2\,dx_3\,dt
\end{aligned}
$$

where $\alpha_1 > 0$, $\alpha_2 > 0$, $\alpha_3 > 0$ and $\alpha_{23} > 0$.

Furthermore,

$$
F_1(\phi) \;=\; \int_0^{t_f}\int_\Omega V(x,y,z,t)(|\phi_1|^2+|\phi_2|^2+|\phi_3|^2)\,dx\,dy\,dz\,dt, \tag{127}
$$

where $V = V(x,y,z,t)$ is an electric potential originated from an external electric field $\mathbf{E}$ applied on Ω.

Finally,

$$
\begin{aligned}
& J_{Aux}(\phi,E) \\
= \; & \sum_{j=1}^{2}\int_0^{t_f}\int_\Omega (E_1)^H_{p_j}(y,z,t)\left(\int_\Omega |(\phi_1^H)_{p_j}(x,y,z,t)|^2\,dx - m_p\right)dy\,dz\,dt \\
& +\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega (E_1)^H_{e_j}(y,z,t)\left(\int_\Omega |(\phi_1^H)_{e_j}(x,y,z,t)|^2\,dx - m_e\right)dy\,dz\,dt \\
& +\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega (E_1)^O_{p_j}(y,z,t)\left(\int_\Omega |(\phi_1^O)_{p_j}(x,y,z,t)|^2\,dx - m_p\right)dy\,dz\,dt \\
& +\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega (E_1)^O_{e_j}(y,z,t)\left(\int_\Omega |(\phi_1^O)_{e_j}(x,y,z,t)|^2\,dx - m_e\right)dy\,dz\,dt \\
& +\int_0^{t_f}\int_\Omega (E_2)^H_{p}(y,z,t)\left(\int_\Omega |(\phi_2^H)_{p}(x,y,z,t)|^2\,dx - m_p\right)dy\,dz\,dt \\
& +\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega (E_2)^O_{p_j}(y,z,t)\left(\int_\Omega |(\phi_2^O)_{p_j}(x,y,z,t)|^2\,dx - m_p\right)dy\,dz\,dt \\
& +\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega (E_2)^O_{e_j}(y,z,t)\left(\int_\Omega |(\phi_2^O)_{e_j}(x,y,z,t)|^2\,dx - m_e\right)dy\,dz\,dt \\
& +\int_0^{t_f}\int_\Omega (E_3)^H_{p}(y,t)\left(\int_\Omega |(\phi_3^H)_{p}(x,y,t)|^2\,dx - m_p\right)dy\,dt \\
& +\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega (E_4)^H_{A_j}(z,t)\left(\int_\Omega (|(\phi_1)^H_{A_j}(y,z,t)|^2\,dy - m^H_{A_j}\right)dz\,dt \\
& +\int_0^{t_f}\int_\Omega\int_\Omega (E_4)^O_{A}(z,t)\left(\int_\Omega (|(\phi_1)^O_{A}(y,z,t)|^2\,dy - m^O_{A}\right)dz\,dt \\
& +\int_0^{t_f}\int_\Omega (E_5)^H_{A}(z,t)\left(\int_\Omega (|(\phi_2)^H_{A}(y,z,t)|^2\,dy - m^H_{A}\right)dz\,dt \\
& +\int_0^{t_f}\int_\Omega (E_5)^O_{A}(z,t)\left(\int_\Omega (|(\phi_2)^O_{A}(y,z,t)|^2\,dy - m^O_{A}\right)dz\,dt \\
& \int_0^{t_f}(E_6)^H_{A}(t)\left(\int_\Omega (|(\phi_3)^H_{A}(y,t)|^2\,dy - m^H_{A}\right)dt \\
& +\int_0^{t_f}(E_7)(t)\left(\int_\Omega (|(\phi_1)_M(z,t)|^2+|(\phi_2)_M(z,t)|^2+|(\phi_3)_M(z,t)|^2)\,dz - m_T\right)dt \\
& +\int_0^{t_f}(E_8)(t)\left(\int_\Omega (\alpha_C|(\phi_2)_M(z,t)|^2-\alpha_B|(\phi_3)_M(z,t)|^2)\,dz\right)dt.
\end{aligned} \tag{128}
$$

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24. A Mathematical Model for the Austenite and Martensite Phase Transition

In this section we consider a phase transition of a solid solution of $\gamma - Fe$ ($\gamma - iron$) and carbon with a $0.75/100$ proportion of carbon, known as austenite, initially at a temperature above and close to $723\ C$ and rapidly cooled to a temperature of about $25\ C$, developing a phase transition which generates a solid solution of $\alpha - Fe$ ($\alpha - iron$) and carbon known as martensite.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$ which contains an amount of austenite at $723\ C$ and which, as previously mentioned, is rapidly cooled to a temperature $25\ C$ on a time interval $[0, t_f]$, resulting a phase known as martensite.

We recall the $\gamma - Fe$ of austenite phase presents a multi-faced cubic crystalline structure in a micro-structure with carbon atoms.

On the other hand, $\alpha - F_e$ structure of the martensite phase has a CCC cubic centralized crystalline structure in a micro-structure with carbon atoms.

At this point, we also recall that the F_e (iron) atom has 26 protons, 26 electrons and 30 neutrons.

On the other hand a $Carbon_{12}$ atom has 6 protons and this same number of electrons and neutrons.

Here we define the density function ϕ_1, representing the Austenite phase, where:

$$\begin{aligned}
|\phi_1(x,y,z,t)|^2 &= \sum_{j=1}^{26} |\phi_{p_j}^{\gamma-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\gamma})^2} \\
&+ \sum_{j=1}^{26} |\phi_{e_j}^{\gamma-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\gamma})^2} \\
&+ \sum_{j=1}^{30} |\phi_{N_j}^{\gamma-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\gamma})^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^C)_{p_j}(x,y,z,t)|^2 |(\phi_1^C)_A(y,z,t)|^2 |\phi_1^C(z,t)|^2 \frac{1}{(m_A^C)^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^C)_{e_j}(x,y,z,t)|^2 |(\phi_1^C)_A(y,z,t)|^2 |\phi_1^C(z,t)|^2 \frac{1}{(m_A^C)^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^C)_{N_j}(x,y,z,t)|^2 |(\phi_1^C)_A(y,z,t)|^2 |\phi_1^C(z,t)|^2 \frac{1}{(m_A^C)^2}. \qquad (129)
\end{aligned}$$

Similarly, we define the density function for the Martensite phase, which is denoted by ϕ_2, where:

$$\begin{aligned}
|\phi_2(x,y,z,t)|^2 &= \sum_{j=1}^{26} |\phi_{p_j}^{\alpha-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\alpha}(z,t)|^2 \frac{1}{(m_A^{\alpha})^2} \\
&+ \sum_{j=1}^{26} |\phi_{e_j}^{\alpha-F_e}(x,y,z,t)|^2 |\phi_A^{\alpha-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\alpha})^2} \\
&+ \sum_{j=1}^{30} |\phi_{N_j}^{\alpha-F_e}(x,y,z,t)|^2 |\phi_A^{\alpha-F_e}(y,z,t)|^2 |\phi_1^{\alpha}(z,t)|^2 \frac{1}{(m_A^{\alpha})^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^C)_{p_j}(x,y,z,t)|^2 |(\phi_1^C)_A(y,z,t)|^2 |\phi_1^C(z,t)|^2 \frac{1}{(m_A^C)^2} \\
&+ \sum_{j=1}^{6} |(\phi_2^C)_{e_j}(x,y,z,t)|^2 |(\phi_2^C)_A(y,z,t)|^2 |\phi_2^C(z,t)|^2 \frac{1}{(m_A^C)^2} \\
&+ \sum_{j=1}^{6} |(\phi_2^C)_{N_j}(x,y,z,t)|^2 |(\phi_2^C)_A(y,z,t)|^2 |\phi_2^C(z,t)|^2 \frac{1}{(m_A^C)^2}. \qquad (130)
\end{aligned}$$

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For the CFC $\gamma - F_e$ $(\gamma - iron)$ corresponding to the Austenite phase, such density functions are subject to the following constraints:

Defining

$$C_\gamma = \{(\varepsilon_1, 0, 0),\ (0, \varepsilon_2, 0),\ (0, 0, \varepsilon_3),\ :\ \varepsilon_j \in \{+1, -1\},\ \forall j \in \{1, 2, 3\}\},$$

$$(C_\gamma)_1 = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3),\ :\ \varepsilon_j \in \{+1, -1\},\ \forall j \in \{1, 2, 3\}\},$$

and

$$(C_\gamma)_2 = \{(\varepsilon_1, \varepsilon_2, 0),\ (\varepsilon_1, 0, \varepsilon_3), (0, \varepsilon_2, \varepsilon_3),\ :\ \varepsilon_j \in \{+1, -1\},\ \forall j \in \{1, 2, 3\}\},$$

we must have

$$\phi_A^{\gamma - F_e}(y, z_1 + \varepsilon_1\delta_z, z_2 + \varepsilon_2\delta_z, z_3 + \varepsilon_3\delta_z, t) = \phi_A^{\gamma - F_e}(y, z_1 + \tilde{\varepsilon}_1\delta_z, z_2 + \tilde{\varepsilon}_2\delta_z, z_3 + \tilde{\varepsilon}_3\delta_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in C_\gamma$, where $\delta_z \in \mathbb{R}^+$ is a small real parameter related to $\gamma - F_e$ crystalline structure dimensions.

We must have also,

$$\phi_A^{\gamma - F_e}(y, z_1 + \varepsilon_1\delta_z, z_2 + \varepsilon_2\delta_z, z_3 + \varepsilon_3\delta_z, t) = \phi_A^{\gamma - F_e}(y, z_1 + \tilde{\varepsilon}_1\delta_z, z_2 + \tilde{\varepsilon}_2\delta_z, z_3 + \tilde{\varepsilon}_3\delta_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in (C_\gamma)_1$ and,

$$(\phi_1^C)_A(y, z_1 + \varepsilon_1\delta_z, z_2 + \varepsilon_2\delta_z, z_3 + \varepsilon_3\delta_z, t) = (\phi_1^C)_A(y, z_1 + \tilde{\varepsilon}_1\delta_z, z_2 + \tilde{\varepsilon}_2\delta_z, z_3 + \tilde{\varepsilon}_3\delta_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in (C_\gamma)_2$.

For the CCC $\alpha - F_e$ $(\alpha - iron)$ corresponding to the Austenite phase, such density functions are subject to the following constraints:

Defining

$$C_\alpha = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3),\ :\ \varepsilon_j \in \{+1, -1\},\ \forall j \in \{1, 2, 3\}\},$$

$$(C_\alpha)_1 = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3),\ :\ \varepsilon_1,\ \varepsilon_2 \in \{+1, -1\} \text{ and } \varepsilon_3 = 0\},$$

$$(C_\alpha)_2 = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3),\ :\ \varepsilon_1 = \varepsilon_2 = 0 \text{ and } \varepsilon_3 \in \{+1, -1\}\},$$

we must have

$$\phi_A^{\alpha - F_e}(y, z_1 + \varepsilon_1\hat{\delta}_z, z_2 + \varepsilon_2\hat{\delta}_z, z_3 + \varepsilon_3\hat{\delta}_z, t) = \phi_A^{\alpha - F_e}(y, z_1 + \tilde{\varepsilon}_1\hat{\delta}_z, z_2 + \tilde{\varepsilon}_2\hat{\delta}_z, z_3 + \tilde{\varepsilon}_3\hat{\delta}_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in C_\alpha$, where $\hat{\delta}_z \in \mathbb{R}^+$ is a small real parameter related to $\alpha - F_e$ crystalline structure dimensions.

We must have also,

$$(\phi_2^C)_A(y, z_1 + \varepsilon_1\hat{\delta}_z, z_2 + \varepsilon_2\hat{\delta}_z, z_3 + \varepsilon_3\hat{\delta}_z, t) = (\phi_2^C)_A(y, z_1 + \tilde{\varepsilon}_1\hat{\delta}_z, z_2 + \tilde{\varepsilon}_2\hat{\delta}_z, z_3 + \tilde{\varepsilon}_3\hat{\delta}_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in (C_\alpha)_1 \cup (C_\alpha)_2$.

The other constraints for the densities are given by:

1. For the Austenite phase:

   (a)

$$\int_\Omega |\phi_{p_j}^{\gamma - F_e}(x, y, z, t)|^2\, dx = m_p,\ \forall j \in \{1, 26\},$$

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(b)
$$\int_\Omega |\phi_{e_j}^{\gamma-F_e}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,26\},$$
(c)
$$\int_\Omega |\phi_{N_j}^{\gamma-F_e}(x,y,z,t)|^2\,dx = m_N,\ \forall j \in \{1,30\},$$
(d)
$$\int_\Omega |\phi_A^{\gamma-F_e}(x,y,z,t)|^2\,dx = m_A^\gamma,$$
(e)
$$\int_\Omega |(\phi_1^C)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j \in \{1,6\},$$
(f)
$$\int_\Omega |(\phi_1^C)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,6\},$$
(g)
$$\int_\Omega |(\phi_1^C)_{N_j}(x,y,z,t)|^2\,dx = m_N,\ \forall j \in \{1,6\},$$
(h)
$$\int_\Omega |(\phi_1^C)_A(x,y,z,t)|^2\,dx = m_A^C,$$

2. For the Martensite phase:

(a)
$$\int_\Omega |\phi_{p_j}^{\alpha-F_e}(x,y,z,t)|^2\,dx = m_p,\ \forall j \in \{1,26\},$$
(b)
$$\int_\Omega |\phi_{e_j}^{\alpha-F_e}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,26\},$$
(c)
$$\int_\Omega |\phi_{N_j}^{\alpha-F_e}(x,y,z,t)|^2\,dx = m_N,\ \forall j \in \{1,30\},$$
(d)
$$\int_\Omega |\phi_A^{\alpha-F_e}(x,y,z,t)|^2\,dx = m_A^\alpha,$$
(e)
$$\int_\Omega |(\phi_2^C)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j \in \{1,6\},$$
(f)
$$\int_\Omega |(\phi_2^C)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,6\},$$
(g)
$$\int_\Omega |(\phi_2^C)_{N_j}(x,y,z,t)|^2\,dx = m_N,\ \forall j \in \{1,6\},$$
(h)
$$\int_\Omega |(\phi_2^C)_A(x,y,z,t)|^2\,dx = m_A^C.$$

3. For the total F_e (iron) mass,
$$\int_\Omega |\phi_1^\gamma(z,t)|^2\,dz + \int_\Omega |\phi_2^\gamma(z,t)|^2\,dz = (m_{F_e})_T,$$
4. For the total Carbon mass
$$\int_\Omega |\phi_1^C(z,t)|^2\,dz + \int_\Omega |\phi_2^C(z,t)|^2\,dz = (m_C)_T.$$

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At this point we define the functional J which models such a pahse transition in question, where

$$J(\phi, E) = G(\nabla\phi) + F(\phi) + F_1(\phi) + J_{Aux}(\phi, E)$$

where

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \sum_{j=1}^{26} \frac{\hat{\gamma}_p^{\gamma-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{p_j}^{\gamma-F_e} \cdot \nabla\phi_{p_j}^{\gamma-F_e} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{26} \frac{\hat{\gamma}_e^{\gamma-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{e_j}^{\gamma-F_e} \cdot \nabla\phi_{e_j}^{\gamma-F_e} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{30} \frac{\hat{\gamma}_N^{\gamma-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{N_j}^{\gamma-F_e} \cdot \nabla\phi_{N_j}^{\gamma-F_e} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{26} \frac{\hat{\gamma}_p^{\alpha-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{p_j}^{\alpha-F_e} \cdot \nabla\phi_{p_j}^{\alpha-F_e} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{26} \frac{\hat{\gamma}_e^{\alpha-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{e_j}^{\alpha-F_e} \cdot \nabla\phi_{e_j}^{\gamma-F_e} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{30} \frac{\hat{\gamma}_N^{\alpha-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{N_j}^{\alpha-F_e} \cdot \nabla\phi_{N_j}^{\alpha-F_e} \, dx \, dy \, dz \, dt \\
& + \frac{\hat{\gamma}_A^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_A^{\gamma-F_e}(y,z,t) \cdot \nabla\phi_A^{\gamma-F_e}(y,z,t)) \, dy \, dz \, dt \\
& + \frac{\hat{\gamma}_A^{\alpha}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_A^{\alpha-F_e}(y,z,t) \cdot \nabla\phi_A^{\alpha-F_e}(y,z,t)) \, dy \, dz \, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_p^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_1^C)_{p_j} \cdot \nabla(\phi_1^C)_{p_j} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_e^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_1^C)_{e_j} \cdot \nabla(\phi_1^C)_{e_j} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_N^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_1^C)_{N_j} \cdot \nabla(\phi_1^C)_{N_j} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_p^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_2^C)_{p_j} \cdot \nabla(\phi_2^C)_{p_j} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_e^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_2^C)_{e_j} \cdot \nabla(\phi_2^C)_{e_j} \, dx \, dy \, dz \, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_N^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_2^C)_{N_j} \cdot \nabla(\phi_2^C)_{N_j} \, dx \, dy \, dz \, dt \\
& + \frac{\hat{\gamma}_A^{C}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^C)_A \cdot \nabla(\phi_1^C)_A) \, dy \, dz \, dt + \frac{\hat{\gamma}_A^{C}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_2^C)_A \cdot \nabla(\phi_2^C)_A) \, dy \, dz \, dt \\
& + \frac{\hat{\gamma}_T^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^\gamma) \cdot \nabla(\phi_1^\gamma)) \, dz \, dt + \frac{\hat{\gamma}_T^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^\alpha) \cdot \nabla(\phi_1^\alpha)) \, dz \, dt \\
& + \frac{\hat{\gamma}_T^{C}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^C) \cdot \nabla(\phi_1^C)) \, dz \, dt + \frac{\hat{\gamma}_T^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_2^C) \cdot \nabla(\phi_2^C)) \, dz \, dt \qquad (131)
\end{aligned}$$

Also,

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$$
\begin{aligned}
& F(\phi) \\
= \; & \frac{\hat{\alpha}_1}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_1(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_1(\xi_1, \xi_2, \xi_3, t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|} \, dx \, dy \, dz \, d\xi_1 \, d\xi_2 \, d\xi_3 \, dt \\
& + \frac{\hat{\alpha}_2}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_2(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_2(\xi_1, \xi_2, \xi_3, t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|} \, dx \, dy \, dz \, d\xi_1 \, d\xi_2 \, d\xi_3 \, dt,
\end{aligned}
$$

$$
F_1(\phi) = -\int_0^{t_f} \int_\Omega w^2(z,t)(|\phi_1(z,t)|^2 + \phi_2(z,t)|^2) \, dz \, dt,
$$

Finally, $J_{Aux} = J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5}$, where

$$
\begin{aligned}
J_{Aux_1} \; = \; & \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{p_j}^{\gamma - F_e}(y,z,t) \left(\int_\Omega |\phi_{p_j}^{\gamma - F_e}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& + \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{e_j}^{\gamma - F_e}(y,z,t) \left(\int_\Omega |\phi_{e_j}^{\gamma - F_e}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& + \sum_{j=1}^{30} \int_0^{t_f} \int_\Omega E_{N_j}^{\gamma - F_e}(y,z,t) \left(\int_\Omega |\phi_{N_j}^{\gamma - F_e}(x,y,z,t)|^2 \, dx - m_N \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{p_j}^{\alpha - F_e}(y,z,t) \left(\int_\Omega |\phi_{p_j}^{\alpha - F_e}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& + \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{e_j}^{\alpha - F_e}(y,z,t) \left(\int_\Omega |\phi_{e_j}^{\alpha - F_e}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& + \sum_{j=1}^{30} \int_0^{t_f} \int_\Omega E_{N_j}^{\alpha - F_e}(y,z,t) \left(\int_\Omega |\phi_{N_j}^{\alpha - F_e}(x,y,z,t)|^2 \, dx - m_N \right) dy \, dz \, dt \\
& + \int_0^{t_f} \int_\Omega E_A^{\gamma - F_e}(y,t) \left(\int_\Omega |\phi_A^{\gamma - F_e}(y,z,t)|^2 \, dy - m_A^\gamma \right) dz \, dt \\
& + \int_0^{t_f} \int_\Omega E_A^{\alpha - F_e}(y,t) \left(\int_\Omega |\phi_A^{\alpha - F_e}(y,z,t)|^2 \, dy - m_A^\alpha \right) dz \, dt
\end{aligned} \tag{132}
$$

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$$
\begin{aligned}
J_{Aux_2} \;=\; & \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_1^C)_{p_j}(y,z,t) \left(\int_\Omega |(\phi_1^C)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_1^C)_{e_j}(y,z,t) \left(\int_\Omega |(\phi_1^C)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_1^C)_{N_j}(y,z,t) \left(\int_\Omega |(\phi_1^C)_{N_j}(x,y,z,t)|^2 \, dx - m_N \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_2^C)_{p_j}(y,z,t) \left(\int_\Omega |(\phi_2^C)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_2^C)_{e_j}(y,z,t) \left(\int_\Omega |(\phi_2^C)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_2^C)_{N_j}(y,z,t) \left(\int_\Omega |(\phi_2^C)_{N_j}(x,y,z,t)|^2 \, dx - m_N \right) dy \, dz \, dt \\
& \int_0^{t_f} \int_\Omega (E_1^C)_A(y,t) \left(\int_\Omega |(\phi_1^C)_A(y,z,t)|^2 \, dy - m_A^C \right) dz \, dt \\
& + \int_0^{t_f} \int_\Omega (E_2^C)_A(y,t) \left(\int_\Omega |(\phi_2^C)_A(y,z,t)|^2 \, dy - m_A^C \right) dz \, dt
\end{aligned} \tag{133}
$$

and,

$$
\begin{aligned}
J_{Aux_3} \;=\; & \int_0^{t_f} E_3^{\gamma,\alpha}(t) \left(\int_\Omega (|\phi_1^\gamma(z,t)|^2 + |\phi_2^\alpha(z,t)|^2) \, dz - (m_{F_e})_T \right) dt \\
& + \int_0^{t_f} E_3^C(t) \left(\int_\Omega (|\phi_1^C(z,t)|^2 + |\phi_2^C(z,t)|^2) \, dz - (m_C)_T \right) dt.
\end{aligned} \tag{134}
$$

$$
\begin{aligned}
& J_{Aux_4} \\
= \; & + \sum_{\varepsilon,\, \tilde{\varepsilon} \in C_\gamma} \int_0^{t_f} \int_\Omega E_4^{\varepsilon,\tilde{\varepsilon}}(y,z,t) (\phi_A^{\gamma - F_e}(y, z_1 + \varepsilon_1 \delta_z, z_2 + \varepsilon_2 \delta_z, z_3 + \varepsilon_3 \delta_z, t) \\
& - \phi_A^{\gamma - F_e}(y, z_1 + \tilde{\varepsilon}_1 \delta_z, z_2 + \tilde{\varepsilon}_2 \delta_z, z_3 + \tilde{\varepsilon}_3 \delta_z, t)) \, dy \, dz \, dt \\
& \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\gamma)_1} \int_0^{t_f} \int_\Omega E_5^{\varepsilon,\tilde{\varepsilon}}(y,z,t) \phi_A^{\gamma - F_e}(y, z_1 + \varepsilon_1 \delta_z, z_2 + \varepsilon_2 \delta_z, z_3 + \varepsilon_3 \delta_z, t) \\
& - \phi_A^{\gamma - F_e}(y, z_1 + \tilde{\varepsilon}_1 \delta_z, z_2 + \tilde{\varepsilon}_2 \delta_z, z_3 + \tilde{\varepsilon}_3 \delta_z, t)) \, dy \, dz \, dt \\
& + \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\gamma)_2} \int_0^{t_f} \int_\Omega E_6^{\varepsilon,\tilde{\varepsilon}}(y,z,t) (\phi_1^C)_A(y, z_1 + \varepsilon_1 \delta_z, z_2 + \varepsilon_2 \delta_z, z_3 + \varepsilon_3 \delta_z, t) \\
& - (\phi_1^C)_A(y, z_1 + \tilde{\varepsilon}_1 \delta_z, z_2 + \tilde{\varepsilon}_2 \delta_z, z_3 + \tilde{\varepsilon}_3 \delta_z, t)) \, dy \, dz \, dt \\
& + \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\alpha)} \int_0^{t_f} \int_\Omega E_7^{\varepsilon,\tilde{\varepsilon}}(y,z,t) (\phi_A^{\alpha - F_e}(y, z_1 + \varepsilon_1 \hat{\delta}_z, z_2 + \varepsilon_2 \hat{\delta}_z, z_3 + \varepsilon_3 \hat{\delta}_z, t) \\
& - \phi_A^{\alpha - F_e}(y, z_1 + \tilde{\varepsilon}_1 \hat{\delta}_z, z_2 + \tilde{\varepsilon}_2 \hat{\delta}_z, z_3 + \tilde{\varepsilon}_3 \hat{\delta}_z, t)) \, dy \, dz \, dt \\
& + \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\alpha)_1 \cup (C_\alpha)_2} \int_0^{t_f} \int_\Omega E_8^{\varepsilon,\tilde{\varepsilon}}(y,z,t) ((\phi_2^C)_A(y, z_1 + \varepsilon_1 \hat{\delta}_z, z_2 + \varepsilon_2 \hat{\delta}_z, z_3 + \varepsilon_3 \hat{\delta}_z, t) \\
& - (\phi_2^C)_A(y, z_1 + \tilde{\varepsilon}_1 \hat{\delta}_z, z_2 + \tilde{\varepsilon}_2 \hat{\delta}_z, z_3 + \tilde{\varepsilon}_3 \hat{\delta}_z, t)) \, dy \, dz \, dt.
\end{aligned} \tag{135}
$$

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Finally, for a field of displacements $u = (u_1, u_2, u_3)$ resulting from the action of a external load field $f = (f_1, f_2, f_3)$ and temperature variations, we define

$$\begin{aligned} & J_{Aux_5} \\ = \; & \frac{1}{2}\int_0^{t_f}\int_\Omega \Big(\Lambda_1(x,t)H^1_{ijkl}((e_{ij}(u)-e^1_{ij}(w))(e_{kl}(u)-e^1_{kl}(w))) \\ & +\Lambda_2(z,t)H^2_{ijkl}((e_{ij}(u)-e^2_{ij}(w))(e_{kl}(u)-e^2_{kl}(w)))\Big)\,dx\,dt \\ & -\frac{1}{2}\int_0^{t_f}\int_\Omega \rho(x,t)u_t(x,t)\cdot u_t(x,t)\,dx\,dt \\ & -\langle u_i, f_i\rangle_{L^2}, \end{aligned} \tag{136}$$

where

$$e_{ij}(u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

$$\rho_1(z,t) = \int_\Omega |\phi_1(x,y,z,t)|^2\,dx\,dy,$$

$$\rho_2(z,t) = \int_\Omega |\phi_2(x,y,z,t)|^2\,dx\,dy,$$

$$\rho(z,t) = \rho_1(z,t) + \rho_2(z,t),$$

and

$$\Lambda_1(z,t) = \frac{\rho_1(z,t)}{\rho_1(z,t)+\rho_2(z,t)},$$

$$\Lambda_2(z,t) = \frac{\rho_2(z,t)}{\rho_1(z,t)+\rho_2(z,t)}.$$

Remark 24.1. *The system temperature is supposed to be directly proportional to $w(z,t)^2$, which in this model is a known function obtained experimentally. Finally, the strain tensors $\{e^1_{ij}(w)\}$ and $\{e^2_{ij}(w)\}$ refer to austenite and martensite phases, respectively. Such tensors also depend on the temperature and must be also obtained experimentally.*

25. A Note on Classical Free Fields through a Variational Perspective

This section is strongly based on the first chapter of the book [20], by N.N. Bogoliubov and D.V. Shirkov.

Therefore, the credit for this section is of these mentioned authors. This section is a kind of review of such a book chapter indicated. In fact, what we have done is simply to open more and clarify some calculations, specially about the first variation of the functional L, in order to improve their understanding.

Let $\Omega = \hat{\Omega} \times [0,T] \subset \mathbb{R}^4$ where $\hat{\Omega} \subset \mathbb{R}^3$ is a bounded, open and connected set with a regular boundary denoted by $\partial\hat{\Omega}$.

Consider the Lagrangian density $L : \mathbb{R}^N \times \mathbb{R}^{N\times n} \to \mathbb{R}$ and an action $A : V \to \mathbb{R}$ where

$$A(u) = \int_\Omega L(u, \nabla u)\,dx,$$

$V = W^{1,2}_0(\Omega;\mathbb{R}^N)$.

We denote

$$\nabla u = \left\{\frac{\partial u_i}{\partial x_j}\right\}$$

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and

$$\frac{\partial u_i}{\partial x_j} = (u_i)_{x_j}.$$

Assume $u \in V$ is such that

$$\delta L(u, \nabla u) = \mathbf{0},$$

so that

$$\frac{\partial L(u,\nabla u)}{\partial u_i} - \sum_{k=1}^{n} \frac{d}{dx_k}\left(\frac{\partial L(u,\nabla u)}{\partial (u_i)_{x_k}}\right) = 0, \text{ in } \Omega, \ \forall i \in \{1, \cdots, N\}.$$

We define a change of variables

$$(x')_k = x_k + \delta x_k,$$

where $x_k = (x_0, x_1, x_2, x_3)$ and $x_0 = t$ (here t denotes time).

Also

$$g_{jk} = 0, \text{ if } j \neq k, \ g_{00} = -1 \text{ and } g_{11} = g_{22} = g_{33} = 1, \{g^{jk}\} = \{g_{jk}\}^{-1},$$

$$\delta x_k = \sum_{j=1}^{N} X_j^k \varepsilon \, w^j,$$

where $|\varepsilon| \ll 1$ denotes a small real parameter.

We define also

$$u_i'(x') = u_i(x) + \delta u_i(x),$$

where

$$\delta u_i(x) = \sum_{j=1}^{N} \psi_{ij} \varepsilon \, w^j,$$

and

$$\overline{\delta u_i} = u_i'(x) - u_i(x).$$

Observe that

$$\begin{aligned} \delta u_i(x) &= u_i'(x) - u_i(x) \\ &= u_i'(x') - u_i'(x) + u_i'(x) - u_i(x), \end{aligned} \tag{137}$$

so that

$$\begin{aligned} \overline{\delta u_i(x)} &= u_i'(x) - u_i(x) \\ &= \delta u_i(x) - (u_i'(x') - u_i'(x)) \\ &\quad \sum_{j=1}^{N} \psi_{ij} \varepsilon \, w^j - \sum_{k=1}^{n} \frac{\partial u_i'(\bar{x}^i)}{dx_k} \delta x_k \\ &= \sum_{j=1}^{N} \psi_{ij} \varepsilon \, w^j - \sum_{k=1}^{n} \frac{\partial u_i(x)}{dx_k} \delta x_k + \mathcal{O}(\varepsilon^2). \end{aligned} \tag{138}$$

Summarizing, we have got

$$\overline{\delta u_i(x)} = \varepsilon \left(\sum_{j=1}^{N} \left(\psi_{ij} w^j - \sum_{k=1}^{n} \frac{\partial u_i(x)}{dx_k} X_j^K w^j \right) \right) + \mathcal{O}(\varepsilon^2).$$

Define now

$$\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon) = \int_{\Omega} L[u(x + \varepsilon \varphi_2(x)) + \varepsilon \varphi_1(x)] \ \det J(x) \ dx.$$

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where we have generically denoted

$$L[u] \equiv L(u, \nabla u),$$

$$L[u(x+\varepsilon\varphi_2(x))+\varepsilon\varphi_1(x)] \equiv L(u(x+\varepsilon\varphi_2(x))+\varepsilon\varphi_1(x), \nabla u(x+\varepsilon\varphi_2(x))+\varepsilon\nabla\varphi_1(x)),$$

and

$$\begin{aligned} J(x) &= \left\{\frac{\partial x_j'}{\partial x_k}\right\} \\ &= \left\{\frac{\partial(x_j+\varepsilon(\varphi_2)_j(x))}{\partial x_k}\right\} \\ &= \left\{\delta_{jk}+\varepsilon\frac{\partial(\varphi_2)_j(x)}{\partial x_k}\right\}. \end{aligned} \tag{139}$$

From such a last definition we have

$$\det J(x) = 1+\varepsilon\sum_{k=1}^{n}\frac{\partial(\varphi_2)_k(x)}{\partial x_k}+\mathcal{O}(\varepsilon^2).$$

so that

$$\frac{\partial \det J(x)}{\partial\varepsilon}|_{\varepsilon=0} = \sum_{k=1}^{n}\frac{\partial(\varphi_2)_k(x)}{\partial x_k},$$

At this point we define

$$\delta A(u,\varphi_1,\varphi_2) = \frac{d}{d\varepsilon}\left(\tilde{A}(u,\varphi_1,\varphi_2,\varepsilon)\right)|_{\varepsilon=0},$$

so that

$$\begin{aligned} \delta A(u,\varphi_1,\varphi_2) &= \int_\Omega\left(\sum_{i=1}^{N}\left(\frac{\partial L(u,\nabla u)}{\partial u_i}(\varphi_1)_i\right.\right. \\ &\quad +\sum_{k=1}^{n}\left(\frac{\partial L(u,\nabla u)}{\partial(u_i)_{x_k}}((\varphi_1)_i)_{x_k}\right) \\ &\quad \left.\left.+\sum_{k=1}^{n}\frac{\delta L[u]}{\delta u_i}\frac{\partial u_i}{\partial x_k}(\varphi_2)_k\right)+\sum_{k=1}^{n}L[u]\frac{\partial(\varphi_2)_k}{\partial x_k}\right)dx. \end{aligned} \tag{140}$$

From this and

$$\frac{\partial L(u,\nabla u)}{\partial u_i}-\frac{d}{dx_k}\left(\frac{\partial L(u,\nabla u)}{\partial u_{x_k}}\right) = 0, \text{ in } \Omega, \ \forall i\in\{1,\cdots,N\},$$

we obtain

$$\begin{aligned} \delta A(u,\varphi_1,\varphi_2) &= \sum_{i=1}^{N}\sum_{k=1}^{n}\left(\int_\Omega\frac{d}{dx_k}\left(\frac{\partial L[u]}{\partial(u_i)_{x_k}}(\varphi_1)_k\right)\right)dx \\ &\quad +\sum_{k=1}^{n}\int_\Omega\frac{d(L[u](\varphi_2)_k)}{dx_k}\,dx. \end{aligned} \tag{141}$$

In particular, for

$$(\varphi_2)_k = \sum_{j=1}^{N}X_j^k w^j$$

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and

$$(\varphi_1)_i = \sum_{j=1}^{N}\left(\psi_{ij}w^j - \sum_{k=1}^{n}\frac{\partial u_i}{\partial x_k}X_j^k w^j\right),$$

we obtain

$$\begin{aligned}
& \delta A(u,\varphi_1,\varphi_2) \\
= & \sum_{i=1}^{N}\sum_{k=1}^{n}\int_\Omega\left(\frac{d}{dx_k}\left(\frac{\partial L[u]}{\partial (u_i)_k}\left(\sum_{j=1}^{N}\left(\psi_{ij}-\sum_{l=1}^{n}\frac{\partial u_i(x)}{\partial x_l}X_j^l w^j\right)\right)\right)\right)dx \\
& + \sum_{k=1}^{n}\int_\Omega \frac{\partial L[u]X_j^k w^j}{dx_k}\,dx \\
= & \sum_{j=1}^{N}\left(\sum_{k=1}^{n}\left(\int_\Omega \frac{d}{dx_k}\left(\sum_{i=1}^{N}\frac{\partial L[u]}{\partial (u_i)_k}\left(\sum_{j=1}^{N}\left(\psi_{ij}-\sum_{l=1}^{n}\frac{\partial u_i(x)}{\partial x_l}X_j^l w^j\right)\right)\right.\right.\right. \\
& \left.\left.\left. + L[u]X_j^k w^j\right)\,dx\right)\right).
\end{aligned} \tag{142}$$

Moreover, we define

$$\theta_k^j = \sum_{i=1}^{N}\left(\frac{\partial L[u]}{\partial (u_i)_{x_k}}\left(-\psi_{ij}+\sum_{l=1}^{n}\frac{\partial u_i}{\partial x_l}X_j^l\right)\right) - L(u)X_j^k$$

so that

$$\delta A(u,\varphi_1,\varphi_2) = -\int_\Omega \sum_{j=1}^{N}\sum_{k=1}^{n}\frac{d(\theta_j^k w^j)}{dx_k}\,dx,$$

$\forall\{w^j\} \in C_c^\infty(\Omega;\mathbb{R}^N)$.

In particular, for

$$\psi_{ij} = 0$$

and

$$X_j^k = \delta_j^k$$

we obtain the Energy-Momentum tensor T_k^j, where

$$T_k^j \equiv \theta_k^j = \sum_{i=1}^{N}\sum_{l=1}^{n}\left(\frac{\partial L[u]}{\partial (u_i)_{x_k}}\frac{\partial u_i}{\partial x_l}\delta_j^l\right) - L[u]\delta_j^k.$$

25.1. The Angular-Momentum Tensor

In this subsection we define the following change of variables

$$x_k' = x_k + \sum_{m\neq k} g^{mm}x_m\varepsilon\, w^{km},$$

where

$$w^{km} = -w^{mk}.$$

With such relations in mind, we set

$$\begin{aligned}
\delta x_k &= x_k' - x_k \\
&= \varepsilon\sum_{l=1}^{n}\sum_{m<l} w^{ml}(g^{ll}x_l g_m^k - g^{mm}x_m g_l^k).
\end{aligned} \tag{143}$$

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We define also,

$$u_i'(x') = u_i(x) + \delta u_i(x)$$

where

$$\delta u_i(x) = \sum_{l=1}^{n} \sum_{j,p<l} A^j_{i(pl)} u_j(x) \varepsilon \, w^{pl}.$$

Moreover, we define

$$\psi_{i(mn)} = \sum_{j=1}^{n} A^j_{i(mn)},$$

where

$$A^j_{i(pl)} = g_{ip}\delta^j_l - g^l_i \delta^j_p.$$

Hence,

$$\psi_{i(mn)} = \sum_{j=1}^{n} A^j_{i(mn)} u_j(x) = g_{in}u_m(x) - g_{jm}u_n(x).$$

For the general variation, we define again

$$\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon) = \int_\Omega L[u(x + \varepsilon\varphi_2(x)) + \varepsilon\varphi_1(x)] \ \det J(x) \ dx.$$

where we have generically denoted

$$L[u] \equiv L(u, \nabla u),$$

$$L[u(x + \varepsilon\varphi_2(x)) + \varepsilon\varphi_1(x)] \equiv L(u(x + \varepsilon\varphi_2(x)) + \varepsilon\varphi_1(x), \nabla u(x + \varepsilon\varphi_2(x)) + \varepsilon\nabla\varphi_1(x)),$$

$$\begin{aligned} J(x) &= \left\{ \frac{\partial x_j'}{\partial x_k} \right\} \\ &= \left\{ \frac{\partial (x_j + \varepsilon(\varphi_2)_j(x))}{\partial x_k} \right\} \\ &= \left\{ \delta_{jk} + \varepsilon \frac{\partial (\varphi_2)_j(x)}{\partial x_k} \right\}. \end{aligned} \tag{144}$$

and

$$\delta A(u, \varphi_1, \varphi_2) = \frac{d}{d\varepsilon}(\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon))|_{\varepsilon=0},$$

Moreover, we set

$$(\varphi_2)^{ml}_k = w^{ml}(g^{ll}x_l\delta^k_m - g^{mm}x_m\delta^k_l),$$

and

$$\overline{\delta u_i} = u_i'(x) - u_i(x).$$

Thus,

$$\begin{aligned} \delta u_i(x) &= u_i'(x) - u_i(x) \\ &= u_i'(x') - u_i'(x) + u_i'(x) - u_i(x), \end{aligned} \tag{145}$$

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so that

$$\begin{aligned}
&\overline{\delta u_i(x)} = u_i'(x) - u_i(x)\\
=\;& \delta u_i(x) - (u_i'(x') - u_i'(x))\\
&\delta u_i(x) - \sum_{k=1}^{n} \frac{\partial u_i(x)}{dx_k}\delta x_k + \mathcal{O}(\varepsilon^2)\\
=\;& \delta u_i(x) - \sum_{l=1}^{n}\sum_{m<l}\sum_{k=1}^{n} \frac{\partial u_i(x)}{\partial x_k}\varepsilon w^{ml}(g^{ll}x_l\delta_m^k - g^{mm}x_m\delta_l^k) + \mathcal{O}(\varepsilon^2)\\
=\;& \varepsilon\left(\sum_{l=1}^{n}\sum_{j,k<l} A^j_{i(kl)}u_j(x)w^{kl} - \sum_{l=1}^{n}\sum_{m<l}\sum_{k=1}^{n} \frac{\partial u_i(x)}{\partial x_k}w^{ml}(g^{ll}x_l\delta_m^k - g^{mm}x_m\delta_l^k)\right) + \mathcal{O}(\varepsilon^2),
\end{aligned}$$

With such results in mind, we define

$$\begin{aligned}
(\varphi_1)_i^{ml} \;=\;& \sum_{j,k<l} A^j_{i(kl)}u_j(x)w^{ml}\\
&- \sum_{k=1}^{n}\left(\frac{\partial u_i(x)}{\partial x_k}w^{ml}(g^{ll}x_l\delta_m^k - g^{mm}x_m\delta_l^k)\right).
\end{aligned} \tag{146}$$

Similarly as in the previous section, we may obtain

$$\begin{aligned}
&\delta A(u,\varphi_1,\varphi_2)\\
=\;& \frac{d\tilde{A}(u,\varphi_1,\varphi_2,\varepsilon)}{d\varepsilon}|_{\varepsilon=0}\\
=\;& \sum_{l=1}^{n}\sum_{j,m<l}\sum_{k=1}^{n}\sum_{i=1}^{N}\int_\Omega \frac{d}{dx_k}\left(\frac{\partial L[u]}{\partial(u_i)_{x_k}}(A_{i(l,m)^j}u_j(x) + \frac{\partial u_i}{\partial x_p}g^{mm}x_m\delta_l^p - \frac{\partial u_i}{\partial x_p}g^{ll}x_l\delta_m^p)w^{ml}\right)dx\\
&+\sum_{k=1}^{n}\sum_{l=1}^{n}\sum_{j,m<l}\sum_{i=1}^{N}\int_\Omega \frac{d}{dx_k}\left(L[u](g^{ll}x_l\delta_m^k - g^{mm}x_m\delta_l^k)w^{ml}\right)dx
\end{aligned} \tag{147}$$

Thus,

$$\delta A(u,\varphi_1,\varphi_2) = -\sum_{k=1}^{n}\sum_{m<l}\int_\Omega \frac{d}{dx_k}\left(M^k_{ml}w^{ml}\right)dx,$$

where

$$\begin{aligned}
M^k_{ml} \;=\;& \sum_{i=1}^{N}\sum_{j<l}\frac{\partial L[u]}{\partial(u_i)_{x_k}}\left(A^j_{ilm}u_j - \frac{\partial u_i}{\partial x_l}g^{mm}x_m + \frac{\partial u_i}{\partial x_m}g^{ll}x_l\right)\\
&+L[u](g^{ll}x_l\delta_m^k + g^{mm}x_m\delta_l^k),
\end{aligned} \tag{148}$$

so that

$$\begin{aligned}
M^k_{lm} \;=\;& (g^{mm}x_mT^k_l - g^{ll}x_lT^k_m)\\
&-\sum_{i=1}^{n}\sum_{j<l}\frac{\partial L[u]}{\partial(u_i)_{x_k}}A^j_{i(lm)}u_j(x)\\
=\;& L^k_{ml} + S^k_{ml},
\end{aligned} \tag{149}$$

where

$$L^k_{ml} = (g^{mm}x_mT^k_l - g^{ll}x_lT^k_m)$$

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and

$$S^k_{ml} = -\sum_{i=1}^{N}\sum_{j<l}\frac{\partial L[u]}{\partial(u_i)_{x_k}}A^j_{i(lm)}u_j(x).$$

The tensor $\{L^k_{ml}\}$ is said to be the Orbital angular momentum tensor and $\{S^k_{ml}\}$ is said to be Spin one.

25.2. A Note on the Solution of the Klein-Gordon Equation

For $\Omega = \mathbb{R}^4$, $\Omega_1 = \mathbb{R}^3$ and denoting as usual by $i \in \mathbb{C}$ the imaginary unit, consider the Klein-Gordon equation in distributional sense

$$-\frac{\partial^2 u}{\partial t^2} + \sum_{j=1}^{3}\frac{\partial^2 u}{\partial x_j^2} - m^2 u = 0, \text{ in } \Omega,$$

where $u \in V = W^{1,2}(\Omega)$.

Defining the Fourier transform of u, by

$$\phi(p) = \frac{1}{(2\pi)^{3/2}}\int_\Omega e^{-ip\cdot x}u(x)\,dx,$$

in the momenta space, the last equation is equivalent to

$$\left(p_0^2 - \sum_{j=1}^{3}p_j^2 - m^2\right)\phi(p) = 0, \text{ in } \Omega,$$

where we have denoted $p = (p_0, p_1, p_2, p_3) \in \mathbb{R}^4$, and $x = (x_0, x_1, x_2, x_3) \in \mathbb{R}\,4$

Observe that a general solution for this last equation is given by the wave function

$$\hat{\phi}(p) = \delta\left(p_0^2 - \sum_{j=1}^{3}p_j^2 - m^2\right)\phi(p),$$

where $\phi \in W^{1,2}(\Omega)$.

Indeed,

$$\begin{aligned}\left(p_0^2 - \sum_{j=1}^{3}p_j^2 - m^2\right)\hat{\phi}(p) &= \left(p_0^2 - \sum_{j=1}^{3}p_j^2 - m^2\right)\delta\left(p_0^2 - \sum_{j=1}^{3}p_j^2 - m^2\right)\phi(p)\\ &= 0, \text{ in } \Omega.\end{aligned} \tag{150}$$

Here, we recall that generically for the Dirac delta function $\delta(t)$, we have

$$\delta(t) = \begin{cases} 0, & \text{if } t \neq 0,\\ +\infty, & \text{if } t = 0.\end{cases} \tag{151}$$

Observe that, for the scalar case in the previous section, we have

$$2T^{00} = \sum_{j=0}^{3}\left(\frac{\partial u}{\partial x_j}\right)^2 + m^2 u.$$

Also, from

$$-\frac{\partial^2 u}{\partial t^2} + \sum_{j=1}^{3}\frac{\partial^2 u}{\partial x_j^2} - m^2 u = 0, \text{ in } \Omega,$$

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we get

$$\int_\Omega \left(\frac{\partial u}{\partial t}\right)^2 dx - \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx - m^2 \int_\Omega u^2 \, dx = 0,$$

so that

$$\int_\Omega \left(\frac{\partial u}{\partial t}\right)^2 dx = \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx + m^2 \int_\Omega u^2 \, dx.$$

From such results, we may infer that

$$\begin{aligned} \int_\Omega T^{00} \, dx &= \int_\Omega \left(\frac{\partial u}{\partial t}\right)^2 dx \\ &= \left\| \frac{\partial u}{\partial t} \right\|_{L^2}^2 \\ &= \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx + m^2 \int_\Omega u^2 \, dx. \end{aligned} \tag{152}$$

On the other hand,

$$\begin{aligned} & \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx \\ = \; & \frac{1}{(2\pi)^3} \sum_{j=1}^{3} \int_\Omega \left(\int_\Omega i \, p_j \, \hat{\phi}(p) \, e^{ip\cdot x} dp \right) \left(\int_\Omega i \, p'_j \hat{\phi}(p') \, e^{ip'\cdot x} \, dp' \right) dx \\ = \; & \frac{1}{(2\pi)^3} \sum_{j=1}^{3} \int_\Omega \int_\Omega \left(-p_j \, p'_j \, \hat{\phi}(p) \, \hat{\phi}(p') \int_\Omega e^{i(p+p')\cdot x} \, dx \right) dp \, dp' \\ = \; & \frac{1}{(2\pi)^{3/2}} \sum_{j=1}^{3} \int_\Omega \int_\Omega \left(-p_j \, p'_j \, \hat{\phi}(p) \, \hat{\phi}(p') \, \delta(p+p') \right) dp \, dp' \\ = \; & \frac{1}{(2\pi)^{3/2}} \sum_{j=1}^{3} \int_\Omega \left(p_j^2 \, \hat{\phi}(p) \, \hat{\phi}(-p) \right) dp. \end{aligned} \tag{153}$$

Thus, denoting $\hat{p} = (p_1, p_2, p_3)$, $d\hat{p} = dp_1 \, dp_2 \, dp_3$, and

$$p_0(\hat{p}) = \sqrt{\sum_{j=1}^{3} p_j^2 + m^2},$$

we may infer that

$$\begin{aligned} \int_\Omega T^{00} \, dx &= \frac{1}{(2\pi)^{3/2}} \int_\Omega \left(\sum_{j=1}^{3} p_j^2 + m^2 \right) \hat{\phi}(p) \, \hat{\phi}(-p)) \, dp \\ &= \frac{1}{(2\pi)^{3/2}} \int_\Omega \left(\sum_{j=1}^{3} p_j^2 + m^2 \right) \delta \left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2 \right) \phi(p) \, \phi(-p)) \, dp \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\Omega_1} \left(p_0(\hat{p})^2 \, \phi(p_0(\hat{p}), \hat{p}) \, \phi(-p_0(\hat{p}), -\hat{p}) \right) d\hat{p}. \end{aligned} \tag{154}$$

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Summarizing we have got

$$\begin{aligned}\int_\Omega T^{00}\,dx &= \frac{1}{(2\pi)^{3/2}}\int_{\Omega_1}\left(p_0(\hat{p})^2\,\phi(p_0(\hat{p}),\hat{p})\,\phi(-p_0(\hat{p}),-\hat{p})\right)d\hat{p}\\ &= \left\|\frac{\partial u}{\partial t}\right\|^2_{L^2},\end{aligned}\tag{155}$$

so that

$$\int_\Omega T^{00}\,dx = \left\|\frac{\partial u}{\partial t}\right\|^2_{L^2}$$

may be expressed as a kind of average expectance of p_0^2 related to the function $\phi(p)$.

25.3. A Note on the Dirac Equation

In this subsection we denote

$$\Delta^2 = \sum_{j=0}^{3} g^{jj} L_j\,L_j,$$

where

$$L_j = i\,g^{jj}\frac{\partial}{\partial x_j},\ \forall j\in\{0,1,2,3\}.$$

We recall that the relativistic Klein-Gordon equation may be written as

$$(\Delta^2 - m^2)u = 0,\ \text{in}\ \Omega=\mathbb{R}^4.$$

Moreover, for 4×4 matrices γ^k indicated in the subsequent lines, we may obtain

$$\{D_{ij}\}u = \left[-i\left(\sum_{j=0}^{3}\gamma^j\frac{\partial}{\partial x_j}\right)-m\right]\left[-i\left(\sum_{j=0}^{3}\gamma^j\frac{\partial}{\partial x_j}\right)+m\right]u,$$

where

$$D_{ii} = \Delta^2 - m^2$$

and

$$D_{ij} = 0,\ \text{if}\ i\neq j,\ \forall i,j\in\{0,1,2,3\}.$$

Here

$$u = (u_0,u_1,u_2,u_3)^T \in V = W^{1,2}(\Omega;\mathbb{C}^4).$$

In such a case the fundamental Dirac equation stands for

$$\left[i\left(\sum_{j=0}^{3}\gamma^j\frac{\partial}{\partial x_j}\right)-m\right]u = \mathbf{0}\in\mathbb{R}^4,\ \text{in}\ \Omega.$$

Summarizing, if $(u_0,u_1,u_2,u_3)^T\in V$ is a solution of this last Dirac equation, then u_0,u_1,u_2,u_3 are four solutions of the Klein-Gordon equation.

In the momentum configuration space, through the Fourier transform proprieties, the Dirac equation stands for

$$(\hat{p}+m)\hat{u}(p) = \mathbf{0},\ \text{in}\ \mathbb{R}^4,$$

where

$$\hat{p} = \sum_{j=0}^{3} g^{jj}p_j\gamma^j.$$

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Observe that

$$\tilde{u}(p) = \delta(\hat{p} + m)u(p)$$

corresponds to a general solution of the Dirac equation.

Indeed,

$$(\hat{p} + m)\tilde{u}(p) = (\hat{p} + m)\delta(\hat{p} + m)u(p) = \mathbf{0} \in \mathbb{R}^4, \text{ in } \Omega.$$

On the other hand

$$\hat{u}(p) = \delta\left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right)u(p)$$

correspond to four solutions of the Klein-Gordon equation.

At this point, we assume such a $\hat{u}(p)$ corresponds to a solution of the Dirac equation as well.

Furthermore, here we recall that (please see the first chapter of the book [20], by N.N. Bogoliubov and D.V. Shirkov for details):

$$\gamma^0 = \begin{Bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{Bmatrix}, \tag{156}$$

$$\gamma^1 = \begin{Bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{Bmatrix}, \tag{157}$$

$$\gamma^2 = \begin{Bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{Bmatrix}, \tag{158}$$

$$\gamma^3 = \begin{Bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{Bmatrix} \tag{159}$$

and

$$\gamma^5 = \begin{Bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{Bmatrix} \tag{160}$$

where we also denote

$$\alpha_j = \gamma^0\gamma^j, \ \forall j \in \{1,2,3\},$$

$$\sigma_j = i\gamma^5\gamma^0\gamma^j, \ \forall j \in \{1,2,3\},$$

and

$$\beta = \gamma^0.$$

On the other hand, a variational formulation for the Dirac equation corresponds to the functional $A : V \to \mathbb{R}$ where

$$A(u) = \frac{1}{2}\int_{\Omega} L(u, \nabla u)\, dx,$$

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where

$$L(u,\nabla u)=i\sum_{j=0}^{3}\left(u^*\gamma^j\frac{\partial u}{\partial x_j}-\frac{\partial u^*}{\partial x_j}\gamma^j u\right)-m^2u^*u,$$

where here

$$u=(u_0,u_1,u_2,u_3)^T\in W^{1,2}(\Omega;\mathbb{C}^4).$$

From such statements and definitions, similarly as in the previous sections (please see [20] for details), we may obtain

$$T^{kl}=\frac{i}{2}g^{ll}\left(u^*\gamma^k\frac{\partial u}{\partial x_l}-\frac{\partial u^*}{\partial x_l}\gamma^k u\right),$$

and

$$S^{k,lm}=-\left(\frac{\partial L(u,\nabla u)}{\partial u_{x_k}}A^{u,lm}u-u^*A^{u^*,lm}\frac{\partial L(u,\nabla u)}{\partial u_{x_k}}\right),$$

where

$$A^{u,lm}=\frac{i}{2}\sigma^{ml},$$

$$A^{u^*,lm}=\frac{i}{2}\sigma^{lm},$$

and where

$$\sigma^{lm}=\frac{\gamma^l\gamma^k-\gamma^k\gamma^l}{2},$$

so that

$$S^{k,lm}=\frac{1}{4}u^*\left(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k\right)u.$$

Thus,

$$\begin{aligned}
&\int_\Omega S^{k,lm}\,dx\\
=\;&\frac{1}{4}\int_\Omega\left(u^*\left(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k\right)u\right)\,dx\\
=\;&\frac{1}{4}\frac{1}{(2\pi)^3}\int_\Omega\left(\int_\Omega\int_\Omega\left(\hat{u}(p)e^{ip\cdot x}(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k)\hat{u}(p')e^{ip'\cdot x}\right)\,dp\,dp'\right)\,dx\\
=\;&\frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_\Omega\int_\Omega\left(\hat{u}(p)(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k)\delta(p+p')\hat{u}(p')\right)\,dp\,dp'\\
=\;&\frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_\Omega\left(\hat{u}(p)(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k)\hat{u}(-p)\right)\,dp\\
=\;&\frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_\Omega\left(u(p)(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k)\delta\left(p_0^2-\sum_{j=1}^{3}p_j^2-m^2\right)u(-p)\right)\,dp\\
=\;&\frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_{\Omega_1}\left(u(p_0(\hat{p}),\hat{p})(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k)u(-p_0(\hat{p}),-\hat{p})\right)\,d\hat{p},
\end{aligned}\tag{161}$$

where

$$p_0(\hat{p})=\sqrt{\sum_{j=1}^{3}p_j^2+m^2}.$$

Summarizing, we have got

$$\int_\Omega S^{k,lm}\,dx=\frac{1}{4(2\pi)^{3/2}}\int_{\Omega_1}\left(u(p_0(\hat{p}),\hat{p})(\gamma^k\sigma^{lm}-\sigma^{lm}\gamma^k)u(-p_0(\hat{p}),-\hat{p})\right)\,d\hat{p},$$

where $\Omega_1=\mathbb{R}^3$, $\hat{p}=(p_1,p_2,p_3)$ and $d\hat{p}=dp_1\,dp_2\,dp_3$.

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26. A Note on Quantum Field Operators

This section is strongly based on the chapter 3, page 53 of the book [21], by G.B. Folland.

Therefore, here we have done a kind of review of these pages of such a book chapter indicated. In fact, we have simply opened more and clarified some calculations, in order to improve their understanding.

Let $\Omega = \hat{\Omega} \times [0,T] \subset \mathbb{R}^4$ where $\hat{\Omega} \subset \mathbb{R}^3$ is a open, bounded and connected set with a regular boundary denoted $\partial\hat{\Omega}$.

Define $V = W^{1,2}(\Omega)$ and

$$V_0 = W_0^{1,2}(\Omega).$$

Consider an operator $H : V_1 = V_0 \cap W^{2,2}(\Omega) \to Y$ where in a distributional sense,

$$H(u) = -\frac{\partial^2 u}{\partial t^2} + \nabla^2 u - m^2 u,$$

and where

$$Y = Y^* = L^2(\Omega).$$

Suppose there exists operators $B_1 : Y \to Y$ and $B_2 : Y \to Y$ such that

$$B_1 B_2(u) = H(u) + \frac{1}{2}u$$

and

$$B_2 B_1(u) = H(u) - \frac{1}{2}u, \ \forall u \in V_1.$$

Assume also $\phi_0 \in V_1$ is such that

$$\|\phi_0\|_{L^2} = 1,$$

and $B_1\phi_0 = 0$.

Now define

$$\phi_k = \frac{B_2^k(\phi_0)}{\sqrt{k!}}, \ \forall k \in \mathbb{N}.$$

Observe that

$$[B_1 B_2] = B_1 B_2 - B_2 B_1 = I_d.$$

We shall prove by induction that

$$[B_1, B_2^k] = k B_2^{k-1}, \ \forall k \in \mathbb{N}. \tag{162}$$

Indeed, for $k = 1$

$$[B_1, B_2] = I_d = 1 B_2^0,$$

so that (162) holds for $k = 1$.

Suppose now (162) holds for $k \in \mathbb{N}$, so that

$$[B_1, B_2^k] = k B_2^{k-1}.$$

In order to complete the induction, it suffices to prove that (162) holds for $k+1$.

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Observe that

$$\begin{aligned}
[B_1, B_2^{k+1}] &= (B_1 B_2^{k+1} - B_2^{k+1} B_1) \\
&= (B_1 B_2^k) B_2 - B_2^{k+1} B_1 \\
&= (B_2^k B_1 + k B_2^{k-1}) B_2 - B_2^{k+1} B_1 \\
&= B_2^k (B_1 B_2) + k B_2^k - B_2^{k+1} B_1 \\
&= B_2^k (B_2 B_1 + I_d) + k B_2 - B_2^{k+1} B_1 \\
&= B_2^{k+1} B_1 + B_2^k + k B_2^k - B_2^{k+1} B_1 \\
&= (k+1) B_2^k. \qquad (163)
\end{aligned}$$

Thus, the induction is complete, so that

$$[B_1, B_2^k] = k B_2^{k-1}, \ \forall k \in \mathbb{N}.$$

Moreover, we recall that

$$B_1 \phi_0 = 0,$$

so that

$$\begin{aligned}
B_1 \phi_k &= B_1 \left(\frac{B_2^k \phi_0}{\sqrt{k!}} \right) \\
&= \frac{(B_2^k B_1 + k B_2^{k-1}) \phi_0}{\sqrt{k!}} \\
&= \frac{k \phi_{k-1} \sqrt{(k-1)!}}{\sqrt{k!}} \\
&= \frac{k \phi_{k-1}}{\sqrt{k}} \\
&= \sqrt{k} \phi_{k-1}, \ \forall k \in \mathbb{N}. \qquad (164)
\end{aligned}$$

Summarizing, we have got

$$B_1 \phi_k = \sqrt{k} \phi_{k-1}, \ \forall k \in \mathbb{N}.$$

Now, we shall prove that

$$B_2 \phi_k = \sqrt{k+1} \phi_{k+1}, \ \forall k \in \mathbb{N}.$$

Observe that

$$\begin{aligned}
B_2^{k+1} \phi_0 &= \phi_{k+1} (\sqrt{(k+1)!} \\
&= B_2 (B_2^k \phi_0) \\
&= (B_2 \phi_k) \sqrt{k!}. \qquad (165)
\end{aligned}$$

Summarizing, we have got

$$(B_2 \phi_k) \sqrt{k!} = \phi_{k+1} (\sqrt{(k+1)!},$$

so that

$$(B_2 \phi_k) = \sqrt{k+1} \phi_{k+1}, \ \forall k \in \mathbb{N}.$$

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Finally, from such results, we may infer that

$$\begin{aligned} B_1B_2\phi_k &= B_1(\sqrt{k+1}\phi_{k+1}) \\ &= \sqrt{k+1}B_1\phi_{k+1} \\ &= \sqrt{k+1}\sqrt{k+1}\phi_k \\ &= (k+1)\phi_k,\ \forall k \in \mathbb{N}. \end{aligned} \tag{166}$$

Similarly,

$$\begin{aligned} B_2B_1\phi_k &= B_2(\sqrt{k}\phi_{k-1}) \\ &= \sqrt{k}B_2\phi_{k-1} \\ &= \sqrt{k}\sqrt{k}\phi_k \\ &= k\phi_k. \end{aligned} \tag{167}$$

Therefore we have got

$$H\,\phi_k = B_1B_2\phi_k - \frac{1}{2}\phi_k = (k+1)\phi_k - \frac{1}{2}\phi_k = \left(k+\frac{1}{2}\right)\phi_k,$$

that is

$$H\phi_k = \left(k+\frac{1}{2}\right)\phi_k,\ \forall k \in \mathbb{N}.$$

Thus, for each $k \in \mathbb{N}$, $k+\frac{1}{2}$ is an eigenvalue of H with corresponding eigenvector ϕ_k.

26.1. An Application Concerning the Harmonic Oscillator Operator in Quantum Mechanics

In this section we have the aim of representing the relativistic Klein-Gordon equation through the creation and annihilation operations related to the harmonic oscillator in quantum mechanics.

Consider first the one-dimensional Hamiltonian, corresponding to the harmonic oscillator, namely

$$H = -\frac{\hbar}{2m}\frac{d^2}{dx^2} + K\frac{x^2}{2},$$

which through an appropriate re-scale results into the following related Hamiltonian H_0, where

$$H_0 = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right).$$

Define now the operators

$$B_1 = A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right),$$

and

$$B_2 = A^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right).$$

Clearly,

$$H_0 = B_1B_2 - \frac{I_d}{2} = B_2B_1 + \frac{I_d}{2},$$

so that

$$[A, A^*] = [B_1, B_2] = B_1B_2 - B_2B_1 = I_d.$$

Similarly, as in the previous sections, by induction, we may obtain

$$[B_1, B_2^k] = kB_2^{k-1},\ \forall k \in \mathbb{N}.$$

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For

$$\phi_0 = \pi^{-1/4} e^{-\frac{x^2}{2}},$$

we define

$$\phi_k = \frac{1}{\sqrt{k}} B_2^k \phi_0, \ \forall k \in \mathbb{N}.$$

Also from the previous section, we may obtain

$$B_2\phi_k = A^*\phi_k = \sqrt{k+1}\phi_{k+1},$$

$$B_1\phi_k = A\phi_k = \sqrt{k}\phi_{k-1}, \ \forall k \in \mathbb{N}.$$

$$B_2B_1 = A^*A\phi_k = k\phi_k,$$

and

$$B_1B_2\phi_k = AA^*\phi_k = (k+1)\phi_k, \forall k \in \mathbb{N} \cup \{0\}.$$

so that

$$H_0\phi_k = (k+1/2)\phi_k, \ \forall k \in \mathbb{N}.$$

Here we recall that

$$B_1\phi_0 = A\phi_0 = 0,$$

and

$$\|\phi_0\|_{L^2} = 1.$$

In reference [21], page 54 it is proven that such a sequence $\{\phi_k\}$ is an ortho-normal basis for $L^2(\mathbb{R})$.

Finally, observe that for $\mathbb{R}^4$ we may define

$$(B_1)_j = A_j = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x_j} + x_j\right),$$

and

$$(B_2)_j = A_j^* = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial x_j} + x_j\right), \ \forall j \in \{0,1,2,3\}.$$

Here generically,

$$\mathbf{x} = (x_0, x_1, x_2, x_3) \in \mathbb{R}^4.$$

Observe that clearly

$$\frac{\partial}{\partial x_j} = \frac{\sqrt{2}}{2}(A_j - A_j^*),$$

and

$$x_j I_d = \frac{\sqrt{2}}{2}(A_j + A_j^*), \ \forall j \in \{0,1,2,3\}.$$

Denoting $x_0 = t$ where t stands for time, consider the relativistic Klein-Gordon equation,

$$-\frac{\partial^2\phi}{\partial t^2} + \sum_{j=1}^{3}\frac{\partial^2\phi}{\partial x_j^2} - m^2\phi = 0.$$

From the previous results, we may represent such an equation by

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$$\left(-\frac{1}{2}(A_0 - A_0^*)^2 + \sum_{j=1}^{3}\frac{1}{2}(A_j - A_j^*)^2 - m^2 I_d\right)\phi = 0.$$

We highlight from the previous results we know the action of A_j and A_j^* on an appropriate basis of $L^2(\mathbb{R}^4)$ obtained though an appropriate tensorial product of the bases

$$\{\{\phi_k(x_j)\}, \text{ for } j \in \{0,1,2,3\}\}.$$

We shall call the operators A_j^* and A_j as the creation and annihilation operators concerning the original harmonic operator in quantum mechanics.

To justify such a nomenclature, we recall that $A_j^*\phi_0(x_j) = \phi_1(x_j)$ and $A_j\phi_0(x_j) = 0$, $\forall j \in \{0,1,2,3\}$.

27. A Dual Variational Formulation for a Related Model

In this section we develop a concave dual variational formulation for a Ginzburg-Landau type equation.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ defined by

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx \\ &\quad + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{168}$$

where $\gamma > 0$, $\alpha > 0$, $\beta > 0$, $f \in L^2(\Omega)$, and

$$V = W_0^{1,2}(\Omega).$$

We also denote $Y = Y^* = L^2(\Omega)$.

Define now

$$V_1 = \{u \in V \ : \ \|u\|_\infty \leq K_3\},$$

for some appropriate $K_3 > 0$ and, $J_1 : V \times Y \to \mathbb{R}$ by

$$J_1(u, v_0^*) = J(u) + \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2 \, dx,$$

where

$$K_1 = \frac{1}{4\,\alpha K_3^2 + \varepsilon}$$

for some small parameter $0 < \varepsilon \ll 1$.

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Observe that

$$\begin{aligned} J(u,v_0^*) &= \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx+\langle u^2,v_0^*\rangle_{L^2} \\ &\quad +\frac{K_1}{2}\int_\Omega(-\gamma\nabla^2u+2v_0^*u-f)^2\,dx-\langle u,f\rangle_{L^2} \\ &\quad -\langle u^2,v_0^*\rangle_{L^2}+\frac{\alpha}{2}\int_\Omega(u^2-\beta)^2\,dx \\ &\geq \inf_{u\in V_1}\left\{\frac{\gamma}{2}\int_\Omega\nabla u\cdot\nabla u\,dx+\langle u^2,v_0^*\rangle_{L^2}\right. \\ &\quad \left.+\frac{K_1}{2}\int_\Omega(-\gamma\nabla^2u+2v_0^*u-f)^2\,dx-\langle u,f\rangle_{L^2}\right\} \\ &\quad +\inf_{v\in Y}\left\{-\langle v,v_0^*\rangle_{L^2}+\frac{\alpha}{2}\int_\Omega(v-\beta)^2\,dx\right\} \\ &= -F^*(v_0^*)-G^*(v_0^*) \\ &\equiv J^*(v_0^*),\forall u\in V_1,\ v_0^*\in Y^*, \end{aligned} \tag{169}$$

where we have denoted

$$F^*(v_0^*)=\sup_{u\in V_1}\{-\langle u^2,v_0^*\rangle_{L^2}-F(u,v_0^*)\},$$

$$F(u,v_0^*)=\frac{\gamma}{2}\int_\Omega\nabla u\cdot\nabla u\,dx+\frac{K_1}{2}\int_\Omega(-\gamma\nabla^2u+2v_0^*u-f)^2\,dx-\langle u,f\rangle_{L^2},$$

and

$$G(v)=\frac{\alpha}{2}\int_\Omega(v-\beta)^2\,dx,$$

$$\begin{aligned} G^*(v_0^*) &= \sup_{v\in Y}\{\langle v,v_0^*\rangle_{L^2}-G(v)\} \\ &= \frac{1}{2\alpha}\int_\Omega(v_0^*)^2\,dx+\beta\int_\Omega v_0^*\,dx. \end{aligned} \tag{170}$$

Observe that

$$\frac{\partial F(u,v_0^*)}{\partial u^2}=-\gamma\nabla^2+2v_0^*+K_1(-\nabla^2+2v_0^*)^2,$$

so that we define

$$B^*=\{v_0^*\in Y^*\ :\ -\gamma\nabla^2+2v_0^*+K_1(-\nabla^2+2v_0^*)^2>\mathbf{0}\}.$$

With such assumptions and definitions in mind, we may prove the following theorem:

Theorem 27.1. *For $J^*(v_0^*)=-F^*(v_0^*)-G^*(v_0^*)$, suppose $\hat{v}_0^*\in B^*$ is such that*

$$\delta J^*(\hat{v}_0^*)=\mathbf{0}.$$

Let $u_0\in Y$ be such that

$$\frac{\partial H(u_0,\hat{v}_0^*)}{\partial u}=\mathbf{0},$$

where

$$H(u,v_0^*)=F(u,v_0^*)+\langle u^2,v_0^*\rangle_{L^2}.$$

Suppose

$$u_0\in V_1.$$

Under such hypotheses,

$$F^*(\hat{v}_0^*)=H(u_0,\hat{v}_0^*),$$

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$$\delta J(u_0) = \mathbf{0},$$

and

$$\begin{aligned} J(u_0) &= J_1(u_0, \hat{v}_0^*) \\ &= \inf_{u \in V_1} J_1(u, \hat{v}_0^*) \\ &= \sup_{v_0^* \in Y^*} J^*(v_0^*) \\ &= J^*(\hat{v}_0^*). \end{aligned} \tag{171}$$

Proof. The proof that

$$F^*(\hat{v}_0^*) = H(u_0, \hat{v}_0^*),$$

is immediate from $\hat{v}_0 \in B^*$.

Moreover, the proof that

$$\delta J(u_0) = \mathbf{0},$$

and

$$J(u_0) = J_1(u_0, \hat{v}_0^*) = J^*(\hat{v}_0^*)$$

may be done similarly as in the previous sections.

Observe that

$$J^*(v_0^*) = -F^*(v_0^*) - G^*(v_0^*) = \inf_{u \in V_1} \{H(u, v_0^*) - G^*(v_0^*)\},$$

so that J^* is concave in v_0^* as the infimum of a family of concave functionals in v_0^*.

From this and $\delta J^*(\hat{v}_0^*) = \mathbf{0}$ we get

$$J^*(\hat{v}_0^*) = \sup_{v_0^* \in Y^*} J^*(v_0^*).$$

Furthermore observe that

$$\begin{aligned} J(u_0) &= J_1(u_0, \hat{v}_0^*) \\ &\leq J_1(u, v_0^*) \\ &= F(u, \hat{v}_0^*) + \langle u^2, \hat{v}_0^* \rangle_{L^2} - G^*(\hat{v}_0^*) \\ &\leq F(u, \hat{v}_0^*) + \sup_{v_0^* \in Y^*} \left\{ \langle u^2, \hat{v}_0^* \rangle_{L^2} - G^*(\hat{v}_0^*) \right\} \\ &= F(u, \hat{v}_0^*) + G(u^2) \\ &= J_1(u, \hat{v}_0^*), \ \forall u \in V_1. \end{aligned} \tag{172}$$

Hence

$$J(u_0) = J_1(u_0, \hat{v}_0^*) = \inf_{u \in V_1} J_1(u, \hat{v}_0^*).$$

Joining the pieces, we have got

$$\begin{aligned} J(u_0) &= J_1(u_0, \hat{v}_0^*) \\ &= \inf_{u \in V_1} J_1(u, \hat{v}_0^*) \\ &= \sup_{v_0^* \in Y^*} J^*(v_0^*) \\ &= J^*(\hat{v}_0^*). \end{aligned} \tag{173}$$

The proof is complete. □

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28. The Generalized Method of Lines Applied to Fourth Order Differential Equations

In this sections we develop an application of the generalized method of lines to a fourth order equation.

We start by addressing the following ordinary differential equation (ode):

$$\varepsilon \frac{d^4u(x)}{dx^4} - f = 0, \text{ in } [0,1],$$

with the boundary conditions

$$u(0) = u'(0) = 0$$

and

$$u(1) = u'(1) = 0.$$

In terms of linear elasticity, such a boundary conditions corresponds to a bi-clamped beam.

In a finite difference context, this last equation corresponds to

$$\varepsilon \left(\frac{u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2}}{d^4} \right) - f_n = 0, \ \forall n \in \{1, \cdots N-2\},$$

where N is the number of nodes and $d = 1/N$.

Considering that, from the boundary conditions, $u_{-1} = u_0 = 0$, for $n = 1$ we get

$$6u_1 - 4u_2 + u_3 = \frac{f_1 d^4}{\varepsilon},$$

so that

$$u_1 = a_1 u_2 + b_1 u_3 + c_1,$$

where

$$a_1 = 2/3, \ \ b_1 - 1/6 \text{ and } c_1 = \frac{f_1 d^4}{6\varepsilon}.$$

Similarly, for $n = 2$, we obtain

$$-4u_1 + 6u_2 - 4u_3 + u_4 = \frac{f_2 d^4}{\varepsilon}.$$

Hence, replacing the value of u_1 previously obtained in this last equation, we have

$$-4(a_1 u_2 + b_1 u_3 + c_1) + 6u_2 - 4u_3 + u_4 = \frac{f_2 d^4}{\varepsilon},$$

so that

$$u_2 = a_2 u_3 + b_2 u_4 + c_2,$$

where defining $m_{12} = (6 - 4a_1)$, we have also

$$a_2 = \frac{4b_1 + 4}{m_{12}},$$

$$b_2 = -\frac{1}{m_{12}},$$

$$c_2 = \frac{1}{m_{12}} \left(\frac{f_2 d^4}{\varepsilon} + 4c_1 \right).$$

Now reasoning inductively, for n, having

$$u_{n-1} = a_{n-1} u_n + b_{n-1} u_{n+1} + c_{n-1},$$

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and

$$u_{n-2} = a_{n-2}u_{n-1} + b_{n-2}u_n + c_{n-2}$$

we obtain

$$u_{n-2} = a_{n-2}(a_{n-1}u_n + b_{n-1}u_{n+1} + c_{n-1}) + b_{n-2}u_n + c_{n-2},$$

so that from this and

$$u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2} = \frac{f_n d^4}{\varepsilon},$$

we obtain

$$\begin{aligned} &a_{n-2}(a_{n-1}u_n + b_{n-1}u_{n+1} + c_{n-1}) + b_{n-2}u_n + c_{n-2} \\ &-4(a_{n-1}u_n + b_{n-1}u_{n+1} + c_{n-1}) + 6u_n - 4u_{n+1} + u_{n+2} = \frac{f_n d^4}{\varepsilon}, \end{aligned} \tag{174}$$

so that

$$u_n = a_n u_{n+1} + b_n u_{n+1} + c_n$$

where defining

$$m_{12} = (a_{n-2}(a_{n-1}) + b_{n-2} - 4a_{n-1} + 6)$$

we obtain

$$a_n = -\frac{1}{m_{12}}(a_{n-2}b_{n-1} - 4b_{n-1} - 4)$$

$$b_n = -\frac{1}{m_{12}},$$

and

$$c_n = \frac{1}{m_{12}}\left(a_{n-2}c_{n-1} + c_{n-2} - 4c_{n-1} - \frac{f_n d^4}{\varepsilon}\right).$$

Summarizing, we have got

$$u_n = a_n u_{n+1} + b_n u_{n+2} + c_n, \forall n \in \{1, \cdot N - 2\}.$$

Observe now that from the boundary conditions,

$$u_{N-1} = u_N = 0.$$

From these last two equations, we may obtain

$$u_{N-2} = c_{N_2},$$

and

$$u_{N-3} = a_{N-3}u_{N-2} + b_{N-3}u_{N-1} + c_{N-3},$$

and so on up to obtaining

$$u_1 = a_1 u_2 + b_1 u_3 + c_1.$$

The problem is then solved.

28.1. A Numerical Example

We develop a numerical example considering

$$\varepsilon = 1,$$

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and

$$f \equiv 1, \text{ in } [0,1].$$

Thus, we have solved the equation

$$\varepsilon \frac{d^4u(x)}{dx^4} - f = 0, \text{ in } [0,1],$$

with the boundary conditions

$$u(0) = u'(0) = 0$$

and

$$u(1) = u'(1) = 0.$$

In a finite differences context, we have used $N = 100$ nodes and $d = 1/N$. For a solution $u(x)$, please see Figure 19.

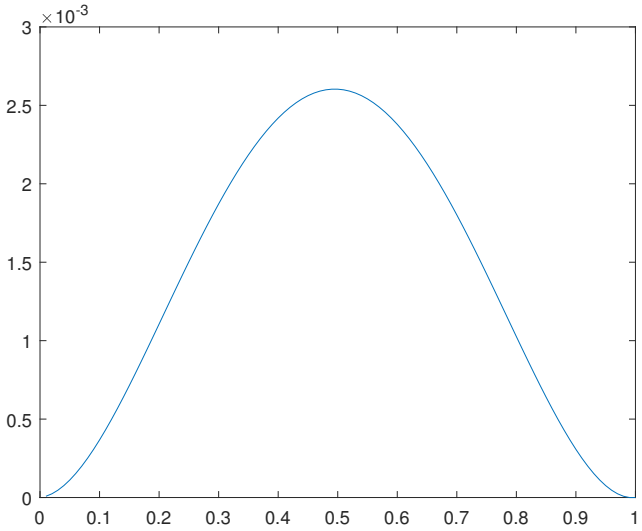

Figure 19. Solution $u(x)$ for the example B.

In the next lines, we present the concerning software in MAT-LAB

****

1. clear all

   m8=100;

   d=1/m8;

   e1=1.0;

   for i=1:m8

   f(i,1)=1.0;

   end;

   a(1)=2/3;

   b(1)=-1/6;

   c(1)=f(1,1)*d^4/(6e1);

   m12=(6-4*a(1));

   a(2)=(4*b(1)+4)/m12;

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```
b(2)=-1/m12;
c(2)=1/m12*(4*c(1)+f(2,1)*d^4/e1);
for i=3:m8-2
m12=(a(i-2)*a(i-1)+b(i-2)-4*a(i-1)+6);
a(i)=-1/m12*(a(i-2)*b(i-1)-4*b(i-1)-4);
b(i)=-1/m12;
c(i)=1/m12*(f(i,1)*d^4/e1-c(i-2)-a(i-2)*c(i-1)+4*c(i-1));
end;
u(m8,1)=0;
u(m8-1,1)=0;
for i=2:m8-1;
u(m8-i,1)=a(m8-i)*u(m8-i+1,1)+b(m8-i)*u(m8-i+2,1)+c(m8-i);
end;
for i=1:m8
x(i)=i*d;
end;
plot(x,u)
**********
```

29. A Note on Hyper-Finite Differences for the Generalized Method of Lines

In this section we develop an application of the hyper finite differences method through an approximation of the generalized method of lines.

Consider the equation

$$\begin{cases} -\varepsilon u''(x) + \alpha u^3 - \beta u - f = 0, & \text{in } \Omega = [0,1], \\ u(0) = 0, & u(1) = 0 \end{cases} \tag{175}$$

As $\varepsilon > 0$ is small, in order to decrease the error concerning the approximations used we propose to divide the domain $\Omega = [0,1]$ into N_1 sub-intervals of same measure. Thus we define

$$x_k = \frac{k}{N_1},\ \forall k \in \{0, 1, \cdots, N_1\}.$$

For each sub-interval $I_k = [x_{k-1}, x_k]$ we are going to obtain an approximate solution of the equation in question with the general boundary conditions

$$u((k-1)/N_1) = U[k-1],$$

and

$$u(k/N_1) = U[k].$$

Denoting such a solution by

$$\{u[i,k]\}$$

where

$$x_i = \frac{k-1}{N_1} + i\ d,$$

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and

$$d = \frac{1}{m_8\ N_1},$$

where m_8 is the fixed number of nodes in each interval I_k.

Observe that in a finite differences context, linearizing it about a initial solution $\{u_0[i,k]\}$, the equation in question stands for:

$$\begin{aligned} &-\varepsilon\frac{(u[i+1,k]-2u[i,k]+u[i-1,k])}{d^2}+3\alpha u_0[i,k]^2u[i,k]-2\alpha u_0[i,k]^3\\ &-\beta u[i,k]-f[i,k]=0,\ \forall i\in\{1,\cdots,m_8-1\}. \end{aligned} \tag{176}$$

In particular, for $i=1$, we obtain

$$\begin{aligned} &-\varepsilon\frac{(u[2,k]-2u[1,k]+u[0,k])}{d^2}+3\alpha u_0[1,k]^2u[1,k]-2\alpha u_0[1,k]^3\\ &-\beta u[1,k]-f[1,k]=0, \end{aligned} \tag{177}$$

so that

$$\begin{aligned} u[1,k] &= a[1,k]u[2,k]+b[1,k]u[0,k]+c[1,k]T[1,k]\\ &\quad +e[1,k]+E_r[1,k], \end{aligned} \tag{178}$$

where

$$a[1,k]=1/2,$$

$$b[1,k]=1/2,$$

$$c[1,k]=1/2,$$

$$e[1,k]=f[1,k]\ \frac{d^2}{2\varepsilon},$$

$$T[1,k]=(-3\alpha u_0[1,k]^2u[i,k]+2\alpha u_0[1,k]^3-\beta u[1,k])\frac{d^2}{\varepsilon},$$

and

$$E_r[1,k]=0.$$

Now reasoning inductively, having

$$\begin{aligned} u[i-1,k] &= a[i-1,k]u[i,k]+b[i-1,k]u[0,k]+c[i-1,k]T[i-1,k]\\ &\quad +e[i-1,k]+E_r[i-1,k], \end{aligned} \tag{179}$$

and

$$\begin{aligned} &-\varepsilon\frac{(u[i+1,k]-2u[i,k]+u[i-1,k])}{d^2}+3\alpha u_0[i,k]^2u[i,k]-2\alpha u_0[i,k]^3\\ &-\beta u[i,k]-f[i,k]=0, \end{aligned} \tag{180}$$

so that

$$(u[i+1,k]-2u[i,k]+u[i-1,k])+T[i,k]+f[i,k]\frac{d^2}{\varepsilon}=0,$$

where,

$$T[i,k]=(-3\alpha u_0[i,k]^2u[i,k]+2\alpha u_0[i,k]^3+\beta u[i,k])\frac{d^2}{\varepsilon},$$

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we obtain

$$\begin{aligned} u[i,k] &= a[i,k]u[i,k] + b[i,k]u[0,k] + c[i,k]T[i,k] \\ &\quad + e[i,k] + E_r[i,k], \end{aligned} \tag{181}$$

where,

$$a[i,k] = (2 - a[i-1,k])^{-1},$$

$$b[i,k] = a[i,k]b[i-1,k],$$

$$c[i,k] = a[i,k](c[i-1,k] + 1),$$

$$e[i,k] = a[i,k]\left(e[i-1,k] + \frac{f[i,k]d^2}{\varepsilon}\right),$$

and

$$E_r[i,k] = a[i,k](E_r[i-1,k]) + c[i,k](T[i-1,k] - T[i,k]).$$

Observe that in particular for $i = m_8 - 1$, we have $u[m8,k] = U[k]$ and $u[0,k] = U[k-1]$, so that from above, neglecting $E_r[1,k]$, we also obtain

$$\begin{aligned} & u[m_8 - 1,k] \approx a[m_8 - 1]u[m_8,k] + b[m_8 - 1,k]u[0,k] \\ & + c[m_8 - 1,k]T[m8 - 1,k](u[m_8,k], u[0,k]) + e[m_8 - 1,k] \\ = \quad & H_{m_8-1}(U[k], U[k-1]). \end{aligned} \tag{182}$$

Similarly, for $i = m8 - 2$ we may obtain

$$\begin{aligned} & u[m_8 - 2,k] \approx a[m_8 - 2]u[m_8 - 1,k] + b[m_8 - 2,k]u[0,k] \\ & + c[m_8 - 2,k]T[m8 - 2,k](u[m_8 - 1,k], u[0,k]) + e[m_8 - 2,k] \\ = \quad & H_{m_8-2}(U[k], U[k-1]), \end{aligned} \tag{183}$$

and so on, up to finding

$$u[1,k] = H_1(U[k], U[k-1]),\ \forall k \in \{1, \cdots, N_1\}.$$

At this point we connect the sub-intervals by setting

$$U[0] = U[N_1] = 0$$

and obtaining $\{U[1], \cdots, U[N_1 - 1]\}$, by solving the equations

$$\begin{aligned} & -\varepsilon\frac{(u[m_8 - 1,k] - 2U[k] + u[1,k+1])}{d^2} + 3\alpha u_0[m8,k]^2 U[k] - 2\alpha u_0[m8,k]^3 \\ & -\beta U[k] - f[m_8,k] = 0,\ \forall k \in \{1, \cdots, N_1 - 1\}. \end{aligned} \tag{184}$$

Having obtained $\{U[k],\ \forall k \in \{1, \cdots, N_1 - 1\}\}$ we may obtain the solution $\{u[i,k]\}$ where $i \in \{0, \cdots, m_8\}$ and $k \in \{1, \cdots, N_1\}$.

The next step is to replace $\{u_0[i,k]\}$ by $\{u[i,k]\}$ and then to repeat the process until an appropriate convergence criterion is satisfied.

The problem is then approximately solved.

We have obtained numerical results for $\varepsilon = 0.001$, $f \equiv 1$, on Ω, $N_1 = 10$, $m_8 = 100$ and $\alpha = \beta = 1$.

For the related software in MATHEMATICA we have obtained $U[1], \cdots, U[9]$,

Here the software and results:

****

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1.
```
Clear[u, U, z, N1];
m8 = 100;
N1 = 10;
d = 1/m8/N1;
e1 = 0.001;
For[k = 1, k < N1 + 1, k++,
For[i = 0, i < m8 + 1, i++,
uo[i, k] = 1.01]];
A = 1.0;
B = 1.0;
a[1] = 1.0/2;
b[1] = 1.0/2;
c[1] = 1/2.0;
e[1] = d^2/e1/2.0;
For[i = 2, i < m8, i++,
a[i] = 1/(2.0 - a[i - 1]);
b[i] = b[i - 1]*a[i];
c[i] = a[i]*(c[i - 1] + 1.0);
e[i] = a[i] * (e[i - 1] + d^2/e1);
];
For[k1 = 1, k1 < 10, k1++,
Print[k1];
Clear[U, z];
For[k = 1, k < N1 + 1, k++,
u[0, k] = U[k - 1];
u[m8, k] = U[k];
For[i = 1, i < m8, i++,
z = a[m8 - i]*u[m8 - i + 1, k] + b[m8 - i]*u[0, k] +
c[m8 - i]*(-3*A*uo[m8 - i + 1, k]^2*u[m8 - i + 1, k] +
2*A*uo[m8 - i + 1, k]^3 + B*u[m8 - i + 1, k])*d^2/e1 +
e[m8 - i];
u[m8 - i, k] = Expand[z]]];
U[0] = 0.0;
U[N1] = 0.0;
S = 0;
For[k = 1, k < N1, k++,
S = S + (e1*(-u[m8 - 1, k] + 2*U[k] - u[1, k + 1])/d^2 +
3*A*U[k]*uo[m8, k]^2 - 2*A*uo[m8, k]^3 - B*U[k] - 1)^2];
Sol = NMinimize[S, U[1], U[2], U[3], U[4], U[5], U[6], U[7], U[8], U[9]];
```

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```
For[k = 1, k < N1, k++,
w4[k] = U[k] Ṡol[[2, k]]];
For[k = 1, k < N1, k++,
U[k] = w4[k]];
For[k = 1, k < N1 + 1, k++,
For[i = 0, i < m8 + 1, i++,
uo[i, k] = u[i, k]]];
Print[U[5]]];
For[k = 0, k < N1 + 1, k++,
Print["U[", k, "]=", U[k]]]
U[0]=0.
U[1]=1.27567
U[2]=1.32297
U[3]=1.32466
U[4]=1.32472
U[5]=1.32472
U[6]=1.32472
U[7]=1.32472
U[8]=1.32472
U[9]=1.32471
U[10]=0.
**********
```

Remark 29.1. *Observe that along the domain we have obtained approximately the constant value* $u = 1.32472$. *This is expected since* $\varepsilon = 0.001$ *is small and such a value* u *is approximately the solution of equation*

$$\alpha u^3 - \beta u - 1 = 0.$$

30. Applications to the Optimal Shape Design for a Beam Model

In this section, we present a numerical procedure for the shape optimization concerning the Bernoulli beam model.

Let $\Omega = [0,1] \subset \mathbb{R}$ corresponds to the horizontal axis of a straight beam with rectangular cross section $b \times h(x)$, that is, the beam has a variable thickness $h(x)$ distributed along such a horizontal axis x, where $x \in [0,1]$.

Define now

$$V = \{w \in W^{2,2}(\Omega) \ : \ w(0) = w(1) = 0\},$$

which corresponds to a simply supported beam.

Consider the problem of minimizing in $V \times B$ the functional

$$J(w,h) = \frac{1}{2}\int_\Omega H(x) w_{xx}(x)^2 \, dx$$

subject to

$$(H(x)w_{xx}(x))_{xx} - P(x) = 0, \text{ in } \Omega,$$

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where

$$H(x) = \frac{h(x)^3 b}{12} E,$$

$h(x)$ is variable beam thickness, $A(x) = bh(x)$ corresponds to a rectangular cross section perpendicular to the x axis, and E is the young elasticity model.

Also, we define

$$B = \left\{ h : [0,1] \to \mathbb{R} \text{ measurable } : \ h_{min} \leq h(x) \leq h_{max} \text{ and } \int_0^1 h(x) \leq c_0 h_{max} \right\},$$

where $0 < c_0 < 1$ and

$$C^* = \{ w \in V \ : \ (H(x) w_{xx}(x))_{xx} - P(x) = 0, \text{ in } \Omega \}.$$

Observe that

$$\begin{aligned}
& \inf_{(w,h) \in C^* \times B} J(w,h) \\
= & \inf_{h \in B} \left\{ \inf_{w \in C^*} J(w,h) \right\} \\
= & \inf_{h \in B} \left\{ \sup_{\hat{w} \in V} \left\{ \inf_{w \in V} \left\{ \frac{1}{2} \int_\Omega H(x) w_{xx}(x)^2 \, dx - \langle \hat{w}, (H(x) w_{xx}(x))_{xx} - P(x) \rangle_{L^2} \right\} \right\} \right\} \\
= & \inf_{h \in B} \left\{ \sup_{\hat{w} \in V} \left\{ -\frac{1}{2} \int_\Omega H(x) \hat{w}_{xx}^2 \, dx + \langle \hat{w}, P \rangle_{L^2} \right\} \right\} \\
= & \inf_{h \in B} \left\{ \inf_{M \in D^*} \left\{ \frac{1}{2} \int_\Omega \frac{M^2}{H(x)} \, dx \right\} \right\}.
\end{aligned} \tag{185}$$

where

$$D^* = \{ M \in Y^* \ : \ M_{xx} - P = 0, \text{ in } \Omega, \text{ and } M(0) = M(1) = 0 \}.$$

Summarizing, we have got

$$\inf_{(w,h) \in C^* \times B} J(w,h) = \inf_{(M,h) \in D^* \times B} \left\{ \frac{1}{2} \int_\Omega \frac{M^2}{H(x)} \, dx \right\}.$$

In order to obtain numerical results, we suggest the following primal dual procedure:

1. Set $n = 1$ and
$$h_n(x) = c_0 h_{max}.$$
2. Calculate $w_n \in V$ solution of equation
$$(H_n(x)(w_n)_{xx})_{xx} = P(x),$$
where
$$H_n(x) = \frac{E b h_n(x)^3}{12}.$$
3. Calculate $h_{n+1}(x) \in B$ such that
$$J^*(M_n, h_{n+1}) = \inf_{h \in B} J^*(M_n, h),$$
where
$$M_n = H_n(w_n)_{xx},$$

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$$J^*(M,h) = \frac{1}{2}\int_\Omega \frac{M^2}{H(x)}\,dx.$$

4. Set $n := n+1$ and go to step 2 until an appropriate convergence criterion is satisfied.

We have developed numerical results for $c_0 = 0.65$, $E = 210\ 10^7$, $b = 0.1\ m$, $P(x) = 36\ 10^2\ N$, $h_{min} = 0.072\ m$ and $h_{max} = 0.18\ m$.

We have also defined

$$h(x) = t(x)h_{max},$$

where

$$0.4 \leq t(x) \leq 1, \text{ a.e. in } \Omega.$$

For the optimal solution $w = w(x)$, please see Figure 20.

For a corresponding optimal solution $t = t(x)$, please see Figure 21.

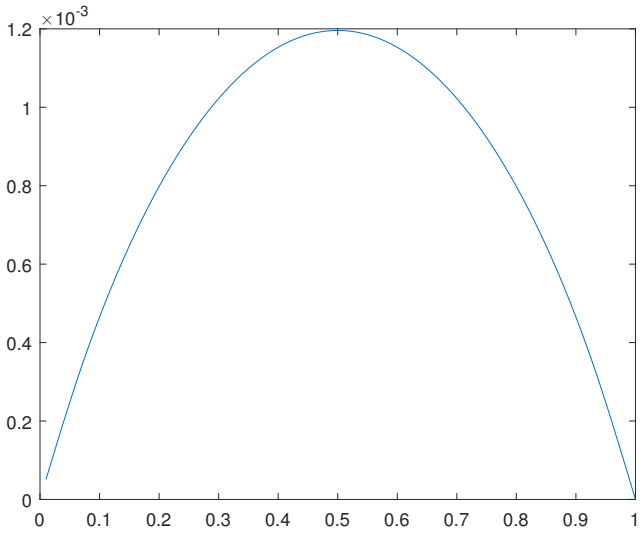

Figure 20. Optimal solution $w(x)$ for a simply supported beam.

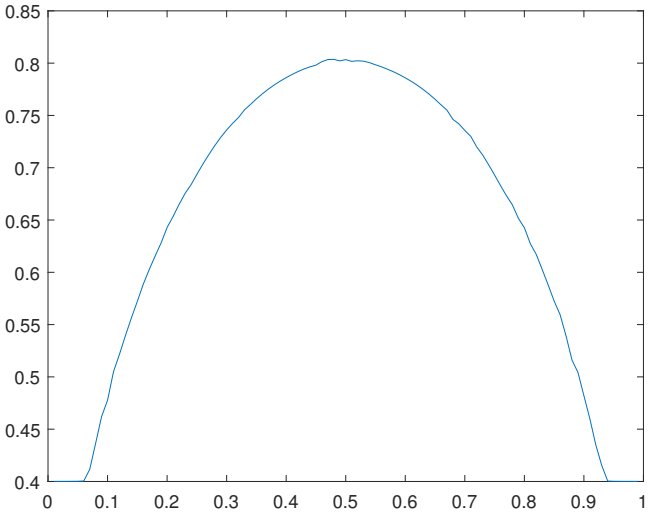

Figure 21. Optimal shape solution $t(x)$ for a simply supported beam.

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Remark 30.1. *For such a simply-supported beam model, for the numerical solution of equation*

$$(H(x)w_{xx})_{xx} = P,$$

with the boundary conditions

$$w(0) = w(1) = w''(0) = w''(1) = 0$$

firstly we have solved the equation

$$v_{xx} - P = 0$$

with the boundary conditions

$$v(0) = v(1) = 0.$$

Subsequently, we have solved the equation

$$H(x)w_{xx} = v$$

with the boundary conditions

$$w(0) = w(1) = 0.$$

Here we present the software developed in MAT-LAB.

****

```
clear all
global m8 d d2wo H e1 ho h1 xo b5
m8=100;
d=1.0/m8;
b5=0.1;
e1=210*10^7;
ho=0.18;
A=zeros(m8-1,m8-1);
for i=1:m8-1
A(1,i)=1.0;
xo(i,1)=0.55;
x3(i,1)=0.55;
end;
lb=0.4*ones(m8-1,1);
ub=ones(m8-1,1);
b=zeros(m8-1,1);
b(1,1)=0.65*(m8-1);
for i=1:m8
f(i,1)=1.0;
L(i,1)=1/2;
P(i,1)=36.0*10^2;
end;
i=1;
```

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m12=2;

m50(i)=1/m12;

z(i)=1/m50(i)*(-P(i,1)*d^2);

for i=2:m8-1

m12=2-m50(i-1);

m50(i)=1/m12;

z(i)=m50(i)*(-P(i,1)*d^2+z(i-1));

end;

v(m8,1)=0;

for i=1:m8-1

v(m8-i,1)=m50(m8-i)*v(m8-i+1,1)+z(m8-i);

end;

k=1;

b12=1.0;

while $(b12 > 10^{-4})$ and $(k < 10)$

k

k=k+1;

for i=1:m8-1

H(i,1)=b5*$L(i,1)^3 * ho^3$/12*e1;

f1(i,1)=v(i,1)/H(i,1);

end;

i=1;

m12=2;

m70(i)=1/m12;

z1(i)=m70(i)*(-f1(i,1)*d^2);

for i=2:m8-1

m12=2-m70(i-1);

m70(i)=1/m12;

z1(i)=m70(i)*(-f1(i,1)*d^2+z1(i-1));

end;

w(m8,1)=0;

for i=1:m8-1

w(m8-i,1)=m70(m8-i)*w(m8-i+1,1)+z1(m8-i);

end;

d2wo(1,1)=(-2*w(1,1)+w(2,1))/d^2;

for i=2:m8-1

d2wo(i,1)=(w(i+1,1)-2*w(i,1)+w(i-1,1))/d^2;

end;

k9=1;

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b14=1.0;

while $(b14 > 10^{-4})$ and $(k9 < 120)$

k9

k9=k9+1;

X=fmincon('beamNov2023',xo,A,b,[ ], [ ],lb,ub);

b14=max(abs(xo-X))

xo=X;

end;

b12=max(abs(xo-x3))

x3=xo;

for i=1:m8-1

L(i,1)=xo(i,1);

end;

end;

****

With the auxiliary function "beamNov2023":

****

1. function S=beamNov2023(x)

global m8 d d2wo H e1 ho h1 xo b5

S=0;

for i=1:m8-1

S=S+1/$(x(i,1)^3)$/ho^3/b5/e1*(H(i,1)*$d2wo(i,1))^2$*12;

end;

****

We develop numerical results also for

$$V = W_0^{2,2}(\Omega) = \{w \in W^{2,2}(\Omega) \text{ such that } w(0) = w(1) = w'(0) = w'(1) = 0\}.$$

Such boundary conditions corresponds to bi-clamped beam. The remaining data is equal to the previous example

For the optimal solution $w = w(x)$, please see Figure 22.

For a corresponding optimal solution $t = t(x)$, please see Figure 23.

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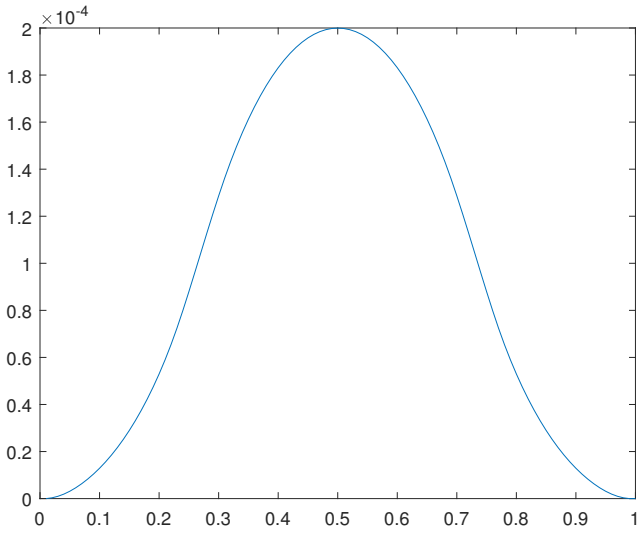

Figure 22. Optimal solution $w(x)$ for a bi-clamped beam.

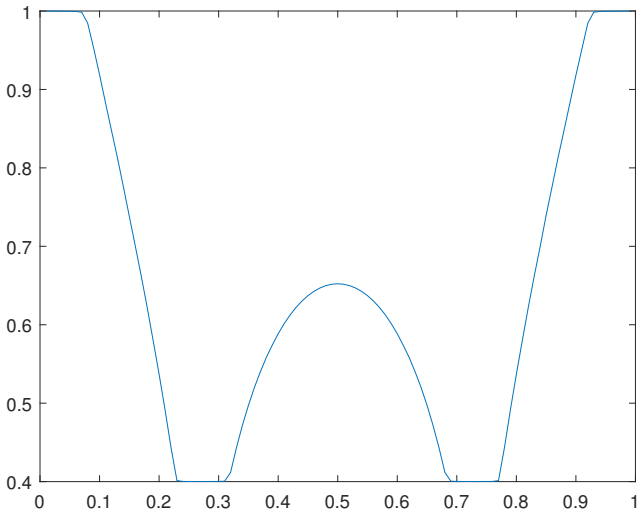

Figure 23. Optimal shape solution $t(x)$ for a bi-clamped beam.

Remark 30.2. *For such a bi-clamped beam model, for the numerical solution of equation*

$$(H(x)w_{xx})_{xx} = P,$$

with the boundary conditions

$$w(0) = w(1) = w'(0) = w'(1) = 0,$$

firstly we have solved the equation

$$v_{xx} - P = 0$$

with the boundary conditions

$$v(0) = v(1) = 0.$$

Subsequently, we solved the equation

$$H(x)w_{xx} = v + ax + b$$

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with the boundary conditions

$$w(0) = w(1) = 0,$$

obtaining $a, b \in \mathbb{R}$ *such that the boundary conditions*

$$w'(0) = w'(1) = 0$$

are also satisfied.

Here we present the software developed in MAT-LAB.

****

```
clear all
global m8 d d2wo H e1 ho h1 xo b5
m8=100;
d=1.0/m8;
b5=0.1;
e1=210*10^7;
ho=0.18;
A=zeros(m8-1,m8-1);
for i=1:m8-1
A(1,i)=1.0;
xo(i,1)=0.55;
x3(i,1)=0.55;
end;
lb=0.4*ones(m8-1,1);
ub=ones(m8-1,1);
b=zeros(m8-1,1);
b(1,1)=0.65*(m8-1);
for i=1:m8
f(i,1)=1.0;
L(i,1)=1/2;
P(i,1)=36.0*10^2;
end;
i=1;
m12=2;
m50(i)=1/m12;
z(i)=1/m50(i)*(-P(i,1)*d^2);
for i=2:m8-1
m12=2-m50(i-1);
m50(i)=1/m12;
z(i)=m50(i)*(-P(i,1)*d^2+z(i-1));
end;
```

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v(m8,1)=0;

for i=1:m8-1

v(m8-i,1)=m50(m8-i)*v(m8-i+1,1)+z(m8-i);

end;

k=1;

b12=1.0;

while $(b12 > 10^{-4})$ and $(k < 10)$

k

k=k+1;

for i=1:m8-1

H(i,1)=b5*$L(i,1)^3 * ho^3$/12*e1;

f1(i,1)=v(i,1)/H(i,1);

f2(i,1)=i*d/H(i,1);

f3(i,1)=1/H(i,1);

end;

i=1;

m12=2;

m70(i)=1/m12;

z1(i)=m70(i)*(-f1(i,1)*d^2);

z2(i)=m70(i)*(-f2(i,1)*d^2);

z3(i)=m70(i)*(-f3(i,1)*d^2);

for i=2:m8-1

m12=2-m70(i-1);

m70(i)=1/m12;

z1(i)=m70(i)*(-f1(i,1)*d^2+z1(i-1));

z2(i)=m70(i)*(-f2(i,1)*d^2+z2(i-1));

z3(i)=m70(i)*(-f3(i,1)*d^2+z3(i-1));

end;

w1(m8,1)=0;

w2(m8,1)=0;

w3(m8,1)=0;

for i=1:m8-1

w1(m8-i,1)=m70(m8-i)*w1(m8-i+1,1)+z1(m8-i);

w2(m8-i,1)=m70(m8-i)*w2(m8-i+1,1)+z2(m8-i);

w3(m8-i,1)=m70(m8-i)*w3(m8-i+1,1)+z3(m8-i);

end;

m3(1,1)=w2(1,1);

m3(1,2)=w3(1,1);

m3(2,1)=w2(m8-1,1);

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m3(2,2)=w3(m8-1,1);

h3(1,1)=-w1(1,1);

h3(2,1)=-w1(m8-1,1);

h5(:,1)=inv(m3)*h3;

for i=1:m8

wo(i,1)=w1(i,1)+h5(1,1)*w2(i,1)+h5(2,1)*w3(i,1);

end;

d2wo(1,1)=(-2*wo(1,1)+wo(2,1))/d^2;

for i=2:m8-1

d2wo(i,1)=(wo(i+1,1)-2*wo(i,1)+wo(i-1,1))/d^2;

end;

k9=1;

b14=1.0;

while ($b14 > 10^{-4}$) and ($k9 < 120$)

k9

k9=k9+1;

X=fmincon('beamNov2023',xo,A,b,[ ], [ ],lb,ub);

b14=max(abs(xo-X))

xo=X;

end;

b12=max(abs(xo-x3))

x3=xo;

for i=1:m8-1

L(i,1)=xo(i,1);

end;

end;

****

Remark 30.3. *About the numerical results obtained for these two beam models, a final word of caution is necessary.*

Indeed, the full convergence in such cases is hard to obtain so that we have obtained just approximations of critical points with the functionals close to their optimal values. It is also worth emphasizing we have fixed the number of iterations so that the solutions and shapes obtained are just approximate ones.

31. Applications to the Optimal Shape Design for a Plate Model

In this section, we present a numerical procedure for the shape optimization concerning a thin plate model.

Let $\Omega = [0,1] \times [0,1] \subset \mathbb{R}^2$ corresponds to the middle surface of a thin plate with a variable thickness $h(x,y)$.

Define now

$$V = \{w \in W^{2,2}(\Omega) \ : \ w = 0 \text{ on } \partial\Omega\},$$

which corresponds to a simply supported plate.

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Consider the problem of minimizing in $V \times B$ the functional

$$J(w,h) = \frac{1}{2}\int_\Omega H(x,y)(\nabla^2 w(x,y))^2\, dx$$

subject to

$$\nabla^2[(H(x,y)\nabla^2 w(x,y))] - P(x,y) = 0, \text{ in } \Omega,$$

where

$$H(x,y) = \frac{h(x,y)^3}{12} E/(1-w_5^2),$$

$h = h(x,y)$ is variable plate thickness, E is the young elasticity model and $w_5 = 0.3$.

Also, we define

$$B = \left\{ h : \Omega \to \mathbb{R} \text{ measurable } : \ h_{min} \le h(x,y) \le h_{max} \text{ and } \int_\Omega h(x,y) \le c_0 h_{max} \right\},$$

where $0 < c_0 < 1$ and

$$C^* = \{w \in V \ : \ \nabla^2[H(x,y)\nabla^2 w(x,y))] - P(x,y) = 0, \text{ in } \Omega\}.$$

Observe that

$$\begin{aligned}
&\inf_{(w,h)\in C^*\times B} J(w,h) \\
=\ &\inf_{h\in B}\left\{\inf_{w\in C^*} J(w,h)\right\} \\
=\ &\inf_{h\in B}\left\{\sup_{\hat{w}\in V}\left\{\inf_{w\in V}\left\{\frac{1}{2}\int_\Omega H(x,y)[\nabla^2\, w(x,y)]^2\, dx - \langle \hat{w}, \nabla^2[H(x,y)\nabla^2 w(x,y)] - P(x,y)\rangle_{L^2}\right\}\right\}\right\} \\
=\ &\inf_{h\in B}\left\{\sup_{\hat{w}\in V}\left\{-\frac{1}{2}\int_\Omega H(x,y)[\nabla^2\hat{w}(x,y)]^2\, dx + \langle \hat{w}, P\rangle_{L^2}\right\}\right\} \\
=\ &\inf_{h\in B}\left\{\inf_{\tilde{M}\in D^*}\left\{\frac{1}{2}\int_\Omega \frac{\tilde{M}^2}{H(x,y)}\, dx\right\}\right\}. \qquad (186)
\end{aligned}$$

where

$$D^* = \{\tilde{M} \in Y^* \quad \nabla^2\tilde{M} - P = 0, \text{ in } \Omega, \text{ and } \tilde{M} = 0, \text{ on } \Omega\}.$$

Summarizing, we have got

$$\inf_{(w,h)\in C^*\times B} J(w,h) = \inf_{(\tilde{M},h)\in D^*\times B}\left\{\frac{1}{2}\int_\Omega \frac{\tilde{M}^2}{H(x,y)}\, dx\right\}.$$

In order to obtain numerical results, we suggest the following primal dual procedure:

1. Set $n = 1$ and
$$h_n(x) = c_0 h_{max}.$$
2. Calculate $w_n \in V$ solution of equation
$$\nabla^2(H_n(x,y)\nabla^2 w_n(x,y)) = P(x,y),$$
where
$$H_n(x,y) = \frac{E h_n(x)^3}{12(1-w_5^2)}.$$

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3. Calculate $h_{n+1} \in B$ such that

$$J^*(\tilde{M}_n, h_{n+1}) = \inf_{h \in B} J^*(\tilde{M}_n, h),$$

where

$$\tilde{M}_n = H_n(x,y)\nabla^2 w_n,$$

$$J^*(\tilde{M}, h) = \frac{1}{2}\int_\Omega \frac{\tilde{M}^2}{H(x,y)}\, dx.$$

4. Set $n := n+1$ and go to step 2 until an appropriate convergence criterion is satisfied.

We have developed numerical results for $c_0 = 0.75$, $E = 200\ 10^5$, $P(x,y) = 2\ 10^2\ N$, $h_{min} = 0.45 * (0.12)\ m$ and $h_{max} = 0.12\ m$.

We have also defined

$$h(x,y) = t(x,y)h_{max},$$

where

$$0.45 \leq t(x,y) \leq 1, \text{ a.e. in } \Omega.$$

For the optimal solution $w = w(x,y)$, please see Figure 24.

For a corresponding optimal solution $t = t(x,y)$, please see Figure 25.

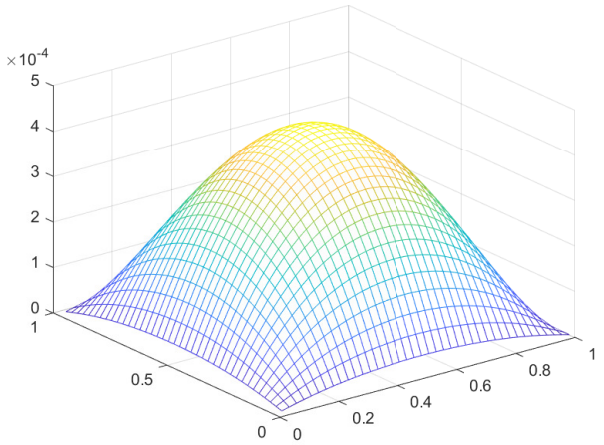

Figure 24. Optimal solution $w(x,y)$ for a simply supported plate.

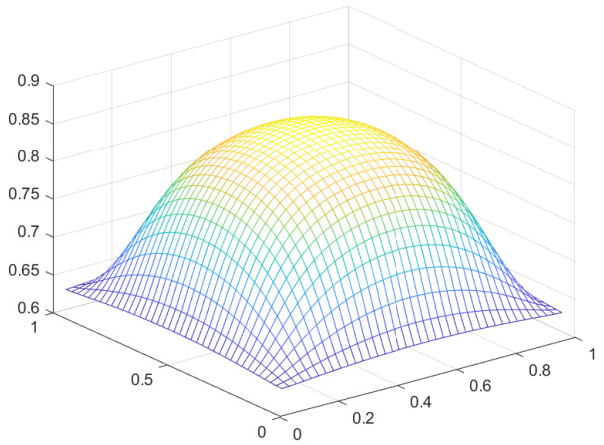

Figure 25. Optimal shape solution $t(x,y)$ for a simply supported plate.

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Remark 31.1. *For such a simply-supported plate model, for the numerical solution of equation*

$$\nabla^2[H(x,y)\nabla^2\, w(x,y)] = P,$$

with the boundary conditions

$$w = 0 \text{ on } \partial\Omega,$$

firstly we have solved the equation

$$\nabla^2 v - P = 0$$

with the boundary conditions

$$v = 0 \text{ on } \partial\Omega.$$

Subsequently, we have solved the equation

$$H(x,y)\nabla^2 w(x,y) = v(x,y)$$

with the boundary conditions

$$w = 0 \text{ on } \partial\Omega.$$

Here we present the software developed in MAT-LAB.

****

1. clear all
   global m8 d d2xwo d2ywo H e1 ho xo b5
   m8=40;
   d=1.0/m8;
   w5=0.3;
   e1=200*10^5/(1 − w5^2);
   ho=0.12;
   A=zeros((m8 − 1)^2, (m8 − 1)^2);
   for i=1:(m8 − 1)^2
   A(1,i)=1.0;
   xo(i,1)=0.55;
   x3(i,1)=0.55;
   end;
   lb=0.45*ones((m8 − 1)^2,1);
   ub=ones((m8 − 1)^2,1);
   b=zeros((m8 − 1)^2,1);
   b(1,1)=0.75*(m8 − 1)^2;
   for i=1:(m8-1)
   for j=1:m8-1
   f(i,j,1)=1.0;
   L(i,j,1)=1/2;
   P(i,j,1)=2*10^2; end;
   end;

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for i=1:m8

wo(:,i)=0.001*ones(m8-1,1);

end;

m2=zeros(m8-1,m8-1);

for i=2:m8-2

m2(i,i)=-2.0;

m2(i,i-1)=1.0;

m2(i,i+1)=1.0;

end;

m2(1,1)=-2.0;

m2(1,2)=1.0;

m2(m8-1,m8-1)=-2.0;

m2(m8-1,m8-2)=1.0;

Id=eye(m8-1);

i=1;

m12=2*Id-m2*d^2/d^2; m50(:,:,i)=inv(m12);

z(:,i)=m50(:,:,i)*(-P(:,i,1)*d^2);

for i=2:m8-1

m12=2*Id-m2*d^2/d^2-m50(:,:,i-1);

m50(:,:,i)=inv(m12);

z(:,i)=m50(:,:,i)*(-P(:,i,1)*d^2+z(:,i-1));

end; v(:,m8)=zeros(m8-1,1);

for i=1:m8-1

v(:,m8-i)=m50(:,:,m8-i)*v(:,m8-i+1)+z(:,m8-i);

end;

k=1;

b12=1.0;

while ($b12 > 10^{-4}$) and ($k < 12$)

k

k=k+1;

for i=1:m8-1

for j=1:m8-1

H(j,i,1)=$L(j,i,1)^3 * ho^3/12$*e1;

f1(j,i,1)=v(j,i)/H(j,i,1);

end;

end;

i=1;

m12=2*Id-m2*d^2/d^2;

m70(:,:,i)=inv(m12);

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z1(:,i)=m70(:,:,i)*(-f1(:,i,1)*d^2);
for i=2:m8-1
m12=2*Id-m2*d^2/d^2-m70(:,:,i-1);
m70(:,:,i)=inv(m12);
z1(:,i)=m70(:,:,i)*(-f1(:,i,1)*d^2+z1(:,i-1));
end;
w(:,m8)=zeros(m8-1,1);
for i=1:m8-1
w(:,m8-i)=m70(:,:,m8-i)*w(:,m8-i+1)+z1(:,m8-i);
end;
d2xwo(:,1)=(-2*w(:,1)+w(:,2))/d^2;
for i=2:m8-1
d2xwo(:,i)=(w(:,i+1)-2*w(:,i)+w(:,i-1))/d^2;
end;
for i=1:m8-1
d2ywo(:,i)=m2*w(:,i)/d^2;
end;
k9=1; b14=1.0;
while ($b14 > 10^{-4}$) and ($k9 < 30$)
k9
k9=k9+1;
X=fmincon('beamNov2023A3',xo,A,b,[ ], [ ],lb,ub);
b14=max(abs(xo-X))
xo=X;
end;
b12=max(max(abs(w-wo)))
wo=w;
x3=xo;
for i=1:m8-1
for j=1:m8-1
L(j,i,1)=xo((i-1)*(m8-1)+j,1);
end;
end;
end;
for i=1:m8-1
x8(i,1)=i*d;
end;
mesh(x8,x8,L);
****

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With the auxiliary function "beamNov2023A3', where

****

```
1.  function S=beamNov2023A3(x)
    global m8 d d2xwo d2ywo H e1 ho xo b5
    S=0;
    for i=1:m8-1
    for j=1:m8-1
    x1(j,i)=x((m8-1)*(i-1)+j,1);
    end;
    end;
    for i=1:m8-1
    for j=1:m8-1
    S=S+1/((x1(j,i))^3)/ho^3/e1*(H(j,i,1))^2*(d2xwo(j,i)+d2ywo(j,i))^2*12;
    end;
    end;
    ********************************
```

Remark 31.2. *About the numerical results obtained for this plate model, a final word of caution is necessary.*

Indeed, the full convergence in such a case is hard to obtain so that we have obtained just approximations of critical points with the functional close to its optimal value. It is also worth emphasizing we have fixed the number of iterations so that the solution and shape obtained are just approximate ones.

32. A Note on the First Maxwell Equation of Electromagnetism

Let $\Omega_1 \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega_1$.

Suppose $\mathbf{E} : \Omega_1 \to \mathbb{R}^3$ is an electric field of C^1 class in Ω.

Let $\Omega \subset \Omega_1$ be also an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $S = \partial\Omega$.

Observe that there exists a scalar field $V : \Omega \to \mathbb{R}$ such that

$$\nabla^2 V = \text{ div } \mathbf{E}, \text{ in } \Omega,$$

and

$$\nabla V \cdot \mathbf{n} = 0, \text{ on } S = \partial\Omega.$$

Here $\mathbf{n}$ denotes the normal outward field to S.

Observe also that

$$\nabla^2 V = \text{ div } \nabla V = \text{ div } \mathbf{E},$$

so that defining

$$\mathbf{h} = \nabla V - \mathbf{E},$$

we have that

$$\text{div } \mathbf{h} = 0, \text{ in } \Omega.$$

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Hence, from such results and the divergence Theorem, we get

$$\begin{aligned}\int_S \mathbf{E}\cdot\mathbf{n}\,dS &= \int_S (\nabla V)\cdot\mathbf{n}\,dS - \int_S \mathbf{h}\cdot\mathbf{n}\,dS \\ &= -\int_\Omega \operatorname{div}\mathbf{h}\,dV = 0. \end{aligned} \tag{187}$$

Summarizing, we have got

$$\int_S \mathbf{E}\cdot\mathbf{n}\,dS = 0.$$

Consider now a charge q_0 localized at the center of a sphere Ω_2 of radius $R > 0$ and boundary $S_2 = \partial\Omega_2$.

The electric field on the sphere surface generated by q_0 is given by

$$\mathbf{E}_2 = \frac{1}{4\pi\varepsilon_0}\frac{q_0}{R^2}\mathbf{n}_2,$$

where $\mathbf{n}_2$ is the normal outward field to S_2.

Clearly

$$\int_{S_2} \mathbf{E}_2\cdot\mathbf{n}_2\,dS_2 = \frac{1}{4\pi\varepsilon_0}\frac{q_0}{R^2}(4\pi R^2) = \frac{q_0}{\varepsilon_0}.$$

Consider again the set Ω but now with a charge q_0 localized at a point $\mathbf{x}$ inside the interior of Ω, which is denoted by Ω^0.

At first the electric field $\mathbf{E}$ generated by q_0 is not of C^1 class on Ω.

However, there exists $R > 0$ such that

$$B_R(\mathbf{x}) \subset \Omega = \Omega^0.$$

Define $\Omega_3 = \Omega \setminus B_R(\mathbf{x})$.

Therefore, $\mathbf{E}$ is of C^1 class on Ω_3.

Denoting the boundary of Ω_3 by S_3, from the previous results, we may infer that

$$\int_{S_3} \mathbf{E}\cdot\mathbf{n}\,dS_3 = 0,$$

so that

$$\begin{aligned}\int_{S_3} \mathbf{E}\cdot\mathbf{n}\,dS_3 &= \int_S \mathbf{E}\cdot\mathbf{n}\,dS - \int_{\partial B_R(\mathbf{x})} \mathbf{E}\cdot\mathbf{n}\,dS_2 \\ &= \int_S \mathbf{E}\cdot\mathbf{n}\,dS - \frac{q_0}{\varepsilon_0} \\ &= 0. \end{aligned} \tag{188}$$

Therefore, we have got

$$\int_S \mathbf{E}\cdot\mathbf{n}\,dS = \frac{q_0}{\varepsilon_0}.$$

Assume now on Ω we have a density of charges $\rho(\mathbf{x})$.

For a small volume ΔV consider a punctual charge q_0 localized in $\mathbf{x} \in \Omega$ such that

$$q_0 \approx \rho(x)\Delta V.$$

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Denoting by $\Delta\mathbf{E}$ the electric field generated by q_0, from the previous results we may infer that

$$\int_S \Delta\mathbf{E}\cdot\mathbf{n}\,dS = \frac{q_0}{\varepsilon_0} \approx \frac{\rho(\mathbf{x})\Delta V}{\varepsilon_0}.$$

Such an equation in its differential form, stands for:

$$\int_S d\mathbf{E}\cdot\mathbf{n}\,dS = \frac{\rho(\mathbf{x})\,dV}{\varepsilon_0}.$$

Integrating in Ω we may obtain

$$\begin{aligned}\int_S \mathbf{E}\cdot\mathbf{n}\,dS &= \int_S\int_\Omega d\mathbf{E}\cdot\mathbf{n}\,dV\,dS \\ &= \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0}\,dV,\end{aligned} \tag{189}$$

so that

$$\int_S \mathbf{E}\cdot\mathbf{n}\,dS = \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0}\,dV.$$

From this and the Divergence Theorem, we have

$$\int_S \mathbf{E}\cdot\mathbf{n}\,dS = \int_\Omega \operatorname{div}\mathbf{E}\,dV = \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0}\,dV.$$

Summarizing, we have got

$$\int_\Omega \operatorname{div}\mathbf{E}\,dV = \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0}\,dV.$$

This is the integral form of the first Maxwell equation of electromagnetism.

For this last equation, the set $\Omega \subset \Omega_1$ is rather arbitrary so that for Ω as a ball of small radius $r > 0$ with center at a point $\mathbf{x} \in \Omega_1$, from the Mean Value Theorem fot integrals and letting $r \to 0^+$, we obtain

$$\operatorname{div}\mathbf{E} = \frac{\rho}{\varepsilon_0}, \text{ in } \Omega_1.$$

This last equation stands for the differential form of the first Maxwell equation of electromagnetism.

Remark 32.1. *Summarizing, in this section we have formally obtained a mathematical deduction of the first Maxwell equation of electromagnetism.*

33. A Note on Relaxation for a General Model in the Vectorial Calculus of Variations

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a function $g : \mathbb{R}^{N\times n} \to \mathbb{R}$ twice differentiable and such that

$$g(y) \to +\infty, \text{ as } |y| \to +\infty.$$

Define a functional $G : V \to \mathbb{R}$ by

$$G(\nabla u) = \frac{1}{2}\int_\Omega g(\nabla u)\,dx,$$

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where

$$V = \{W^{1,2}(\Omega;\mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega\}.$$

Moreover, for $f \in L^2(\Omega;\mathbb{R}^N)$, define also

$$J(u) = G(\nabla u) - \langle u, f\rangle_{L^2}.$$

We assume there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = \inf_{u\in V} J(u).$$

Observe that from the convex analysis basic theory, we have that

$$\begin{aligned} \alpha &= \inf_{u\in V} J(u) \\ &= \inf_{u\in V} J^{**}(u) \\ &= \inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u, f\rangle_{L^2}\}. \end{aligned} \tag{190}$$

On the other hand

$$\begin{aligned} (G\circ\nabla)^{**}(u) &\leq H(u) \\ &\equiv \inf_{(\lambda,(v,w))\in[0,1]\times B(u,\lambda)} \{\lambda G(\nabla w) + (1-\lambda)G(\nabla v)\} \\ &\leq G(\nabla u), \end{aligned} \tag{191}$$

where

$$B(u,\lambda) = \{(v,w) \in V \ : \ \lambda w + (1-\lambda)v = u\}.$$

From such results, we may infer that

$$\inf_{u\in V} J^{**}(u) = \inf_{u\in V}\{H(u) - \langle u, f\rangle_{L^2}\} = \inf_{u\in V} J(u).$$

Furthermore, observe that

$$\lambda\nabla w + (1-\lambda)\nabla v = \nabla u,$$

so that

$$\begin{aligned} \nabla v &= \nabla u + \lambda(\nabla v - \nabla w) \\ &= \nabla u + \lambda\nabla\phi, \end{aligned} \tag{192}$$

where $\phi = v - w \in W_0^{1,2}(\Omega;\mathbb{R}^N)$ so that

$$\nabla\phi = \nabla v - \nabla w,$$

and

$$\nabla w = \nabla v - \nabla\phi.$$

Therefore,

$$\nabla w = \nabla v - \nabla\phi = \nabla u + \lambda\nabla\phi - \nabla\phi = \nabla u - (1-\lambda)\nabla\phi.$$

Replacing such results into the expression of H, we have

$$H(u) = \inf_{(\lambda,\phi)\in[0,1]\times V_0} \{\lambda G(\nabla u - (1-\lambda)\nabla\phi) + (1-\lambda)G(\nabla u + \lambda\nabla\phi)\},$$

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where

$$V_0 = W_0^{1,2}(\Omega;\mathbb{R}^N).$$

Joining the pieces, we have got

$$\begin{aligned}\inf_{u\in V} J(u) &= \inf_{u\in V} J^{**}(u)\\ &= \inf_{u\in V}\{H(u) - \langle u, f\rangle_{L^2}\}\\ &= \inf_{(\lambda,\phi,u)\in[0,1]\times V_0\times V}\{\lambda G(\nabla u - (1-\lambda)\nabla\phi) + (1-\lambda)G(\nabla u + \lambda\nabla\phi) - \langle u, f\rangle_{L^2}\}.\end{aligned}$$

This last functional corresponds to a relaxation for the original non-convex functional.
The note is complete.

33.1. Some Related Numerical Results

In this subsection we present numerical results for an one-dimensional model and related relaxed formulation.

For $\Omega = [0,1] \subset \mathbb{R}$, consider the functional $J : V \to \mathbb{R}$ where

$$J(u) = \frac{1}{2}\int_\Omega ((u')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega (u-f)^2\, dx,$$

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\},$$

$f \in Y = Y^* = L^2(\Omega)$.

Based on the results of the previous section, denoting $V_0 = W_0^{1,2}(\Omega)$, we define the following relaxed functional $J_1 : [0,1]\times V\times V_0 \to \mathbb{R}$, where

$$J_1(\lambda,u,\phi) = \frac{\lambda}{2}\int_\Omega ((u' - (1-\lambda)\phi')^2 - 1)^2\, dx + \frac{1-\lambda}{2}\int_\Omega ((u' + \lambda\phi')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega (u-f)^2\, dx.$$

Indeed, we have developed an algorithm for minimizing the following regularized functional $J_2 : [0,1]\times V\times V_0 \to \mathbb{R}$, where

$$J_2(\lambda,u,\phi) = J_1(\lambda,u,\phi) + \frac{\varepsilon_3}{2}\int_\Omega (u'')^2\, dx,$$

for a small parameter $\varepsilon_3 > 0$.

For the case in which $f(x) = \sin(\pi x)/2$, for the optimal solution u, please see Figure 26.
For the case in which $f(x) = \cos(\pi x)/2$, for the optimal solution u, please see Figure 27.
For the case in which $f(x) = 0$, for the optimal solution u, please see Figure 28.

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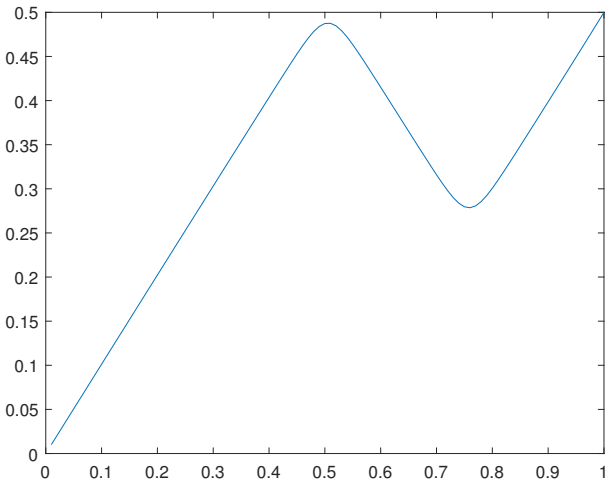

Figure 26. Optimal solution $u(x)$ for the case $f(x) = \sin(\pi x)/2$.

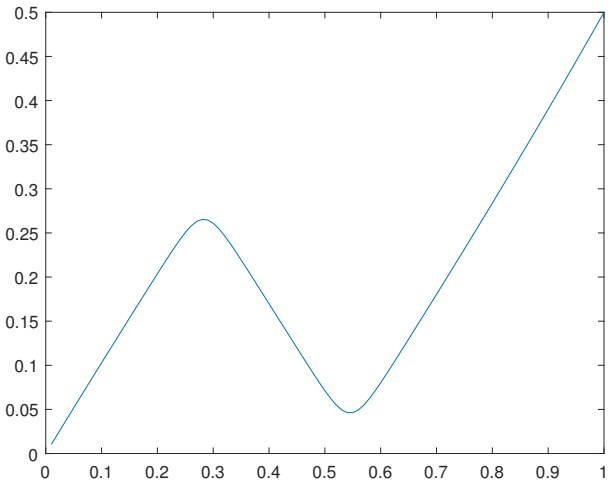

Figure 27. Optimal solution $u(x)$ for the case $f(x) = \cos(\pi x)/2$.

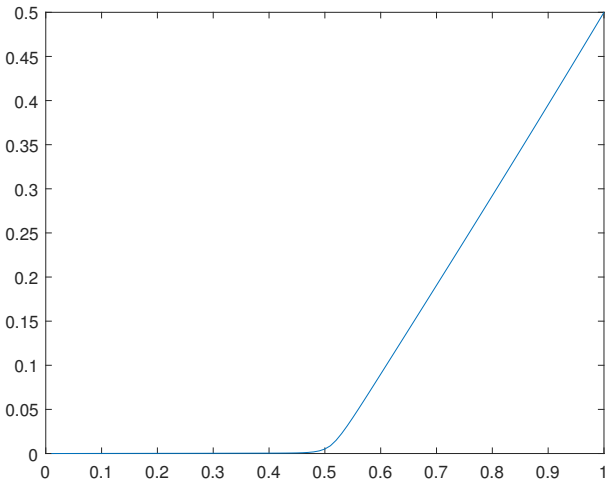

Figure 28. Optimal solution $u(x)$ for the case $f(x) = 0$.

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We highlight to obtain the solution for this last case which $f = 0$ is harder. A good solution was possible only using

$$x_0 = 0$$

as the initial solution concerning the iterative process.

Here we present the software in MAT-LAB developed.

****

```
clear all
global m8 d u e3
m8=100;
d=1/m8;
e3=0.0005;
for i=1:2*m8+1
xo(i,1)=0.36;
end;
b12=1.0;
k=1;
while (b12 > 10^-7) and (k < 60)
k
k=k+1;
X=fminunc('funDecember2023',xo);
b12=max(abs(xo-X))
xo=X;
u(m8/2)
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u);
```

****

With the main function "funDecember2023"

****

```
function S=funDecember2023(x)
global m8 d u e3
for i=1:m8
u(i,1)=x(i,1);
v(i,1)=x(i+m8,1);
yo(i,1)=sin(pi*i*d)/2;
end;
L=(1+sin(x(2*m8+1,1)))/2;
```

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u(m8,1)=1/2;

v(m8,1)=0.0;

du(1,1)=u(1,1)/d;

dv(1,1)=v(1,1)/d;

for i=2:m8

du(i,1)=(u(i,1)-u(i-1,1))/d;

dv(i,1)=(v(i,1)-v(i-1,1))/d;

end;

d2u(1,1)=(-2*u(1,1)+u(2,1))/d^2;

for i=2:m8-1

d2u(i,1)=(u(i-1,1)-2*u(i,1)+u(i+1,1))/d^2;

end;

S=0;

for i=1:m8

S=S+1/2 $*$ $L*((du(i,1)-(1-L)*dv(i,1))^2-1)^2$;

S=S+1/2 $*(1-L)*((du(i,1)+L*dv(i,1))^2-1)^2$;

S=S+$(u(i,1)-yo(i,1))^2$;

end;

for i=1:m8-1

S=S+e3*$d2u(i,1)^2$;

end;

****

33.2. A Related Duality Principle and Concerning Convex Dual Formulation

With the notation and statements of the previous sections in mind, consider the functionals $J : V \to \mathbb{R}$ and $J_3 : [0,1] \times V \times V_0 \to \mathbb{R}$ where

$$J(u) = G(\nabla u) + \frac{1}{2}\int_\Omega u \cdot u \, dx - \langle u, f\rangle_{L^2},$$

and

$$\begin{aligned} J_3(\lambda, u, \phi) \quad = \quad & \lambda G(\nabla u - (1-\lambda)\nabla\phi) + (1-\lambda)G(\nabla u + \lambda\nabla\phi) \\ & + \frac{\lambda}{2}\int_\Omega (u-(1-\lambda)\phi)\cdot(u-(1-\lambda)\phi)\, dx \\ & + \frac{(1-\lambda)}{2}\int_\Omega (u+\lambda\phi)\cdot(u+\lambda\phi)\, dx \\ & - \lambda\langle u-(1-\lambda)\phi, f\rangle_{L^2} - (1-\lambda)\langle u+\lambda\phi, f\rangle_{L^2}. \end{aligned} \tag{193}$$

Here we have denoted

$$V = \{u \in W^{1,2}(\Omega;\mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega = S\},$$

$$V_0 = W_0^{1,2}(\Omega;\mathbb{R}^N),$$

$$Y = Y^* = L^2(\Omega;\mathbb{R}^{N\times n})$$

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and

$$Y_1 = Y_1^* = L^2(\Omega;\mathbb{R}^N).$$

Observe that

$$J^{**}(u) \leq \min_{(\lambda,\phi)\in[0,1]\times V_0} J_3(\lambda,u,\phi).$$

Moreover,

$$\begin{aligned} J_3(\lambda,u,\phi) &= -\langle \nabla u-(1-\lambda)\nabla\phi, v_1^*\rangle_{L^2} + \lambda G(\nabla u-(1-\lambda)\nabla\phi) \\ &\quad -\langle \nabla u-(1-\lambda)\nabla\phi, v_2^*\rangle_{L^2} + (1-\lambda)G(\nabla u+\lambda\nabla\phi) \\ &\quad -\langle u-(1-\lambda)\phi, v_3^*\rangle_{L^2} + \frac{\lambda}{2}\int_\Omega (u-(1-\lambda)\phi)\cdot(u-(1-\lambda)\phi)\,dx \\ &\quad -\langle u+\lambda\phi, v_4^*\rangle_{L^2} + \frac{(1-\lambda)}{2}\int_\Omega (u+\lambda\phi)\cdot(u+\lambda\phi)\,dx \\ &\quad +\langle \nabla u-(1-\lambda)\nabla\phi, v_1^*\rangle_{L^2} + \langle \nabla u-(1-\lambda)\nabla\phi, v_1^*\rangle_{L^2} \\ &\quad +\langle u-(1-\lambda)\phi, v_3^*\rangle_{L^2} + \langle u+\lambda\phi, v_4^*\rangle_{L^2} \\ &\quad -\lambda\langle u-(1-\lambda)\phi, f\rangle_{L^2} - (1-\lambda)\langle u+\lambda\phi, f\rangle_{L^2}. \end{aligned} \tag{194}$$

Therefore,

$$\begin{aligned} J_3(\lambda,u,\phi) &\geq \inf_{v_1\in Y}\{-\langle v_1, v_1^*\rangle_{L^2} + \lambda G(v_1)\} \\ &\quad + \inf_{v_2\in Y}\{-\langle v_2, v_2^*\rangle_{L^2} + (1-\lambda)G(v_2)\} \\ &\quad + \inf_{v_3\in Y_1}\left\{-\langle v_3, v_3^*\rangle_{L^2} + \frac{\lambda}{2}\int_\Omega (v_3)\cdot(v_3)\,dx\right\} \\ &\quad + \inf_{v_4\in Y_1}\left\{-\langle v_4, v_4^*\rangle_{L^2} + \frac{(1-\lambda)}{2}\int_\Omega (v_4)\cdot(v_4)\,dx\right\} \\ &\quad + \inf_{(u,\phi)\in V\times V_0}\{\langle \nabla u-(1-\lambda)\nabla\phi, v_1^*\rangle_{L^2} + \langle \nabla u-(1-\lambda)\nabla\phi, v_1^*\rangle_{L^2} \\ &\quad +\langle u-(1-\lambda)\phi, v_3^*\rangle_{L^2} + \langle u+\lambda\phi, v_4^*\rangle_{L^2} \\ &\quad -\lambda\langle u-(1-\lambda)\phi, f\rangle_{L^2} - (1-\lambda)\langle u+\lambda\phi, f\rangle_{L^2}\} \\ &= -\lambda G^*\left(\frac{v_1^*}{\lambda}\right) - (1-\lambda)G^*\left(\frac{v_2^*}{(1-\lambda)}\right) \\ &\quad -F_3^*(v_3^*,\lambda) - F_4^*(v_4^*,\lambda) \\ &\quad + \int_S (v_1^*)_{ij}n_j(u_0)_i\,dS + \int_S (v_2^*)_{ij}n_j(u_0)_i\,dS, \\ &\quad \forall\lambda\in(0,1), u\in V,\ \phi\in V_0, v^*\in A^*, \end{aligned} \tag{195}$$

where

$$G^*(v^*) = \sup_{v\in Y}\{\langle v, v^*\rangle_{L^2} - G(v)\},$$

$$\begin{aligned} F_3^*(v_3^*,\lambda) &= \sup_{v_3\in Y_1}\left\{\langle v_3, v_3^*\rangle_{L^2} - \frac{\lambda}{2}\int_\Omega v_3\cdot v_3\,dx\right\} \\ &= \frac{1}{2\lambda}\int_\Omega v_3^*\cdot v_3^*\,dx, \end{aligned} \tag{196}$$

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$$\begin{aligned} F_4^*(v_4^*,\lambda) &= \sup_{v_4\in Y_1}\left\{\langle v_4,v_4^*\rangle_{L^2}-\frac{(1-\lambda)}{2}\int_\Omega v_4\cdot v_4\,dx\right\} \\ &= \frac{1}{2(1-\lambda)}\int_\Omega v_4^*\cdot v_4^*\,dx. \end{aligned} \tag{197}$$

Furthermore, $A^* = A_1^* \cap A_2^*$ where

$$A_1^* = \{v^* = (v_1^*, v_2^*, v_3^*, v_4^*) \in [Y^*]^2 \times [Y_1^*]^2 \ : \ -\text{div}\,(v_1^*)_i - \text{div}\,(v_2^*)_i + (v_3^*)_i + (v_4^*)_i - f_i = 0, \text{ in } \Omega\},$$

and

$$\begin{aligned} A_2^* &= \{v^* = (v_1^*, v_2^*, v_3^*, v_4^*) \in [Y^*]^2 \times [Y_1^*]^2 \ : \\ &\quad -(-1+\lambda)\,\text{div}\,(v_1^*)_i - \lambda\,\text{div}\,(v_2^*)_i + (-1+\lambda)(v_3^*)_i + \lambda(v_4^*)_i = 0, \text{ in } \Omega\}. \end{aligned} \tag{198}$$

Summarizing, we have got

$$\begin{aligned} &\inf_{(\lambda,u\phi)\in(0,1)\times V\times V_0} J_3(\lambda,u,\phi) \\ \geq\ &\sup_{v^*\in A^*}\left\{\inf_{\lambda\in(0,1)}\left\{-\lambda G^*\left(\frac{v_1^*}{\lambda}\right)-(1-\lambda)G^*\left(\frac{v_2^*}{(1-\lambda)}\right)\right.\right. \\ &\left.\left.-F_3^*(v_3^*,\lambda)-F_4^*(v_4^*,\lambda)+\int_{\partial\Omega}(v_1^*)_{ij}n_j(u_0)_i\,dS+\int_{\partial\Omega}(v_2^*)_{ij}n_j(u_0)_i\,dS\right\}\right\}. \end{aligned} \tag{199}$$

Remark 33.1. *We highlight this last dual function in v^* is convex (in fact concave) on the convex set A^*.*

33.3. A Numerical Example

For $\Omega = [0,1] \subset \mathbb{R}$ consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{1}{2}\int_\Omega \min\{(u'(x)-1)^2,(u'(x)+1)^2\}\,dx+\frac{1}{2}\int_\Omega (u-f)^2\,dx \\ &= \frac{1}{2}\int_\Omega (u')^2\,dx-\int_\Omega |u'|\,dx+\frac{1}{2}\int_\Omega (u-f)^2\,dx, \end{aligned} \tag{200}$$

where

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\},$$

$Y = Y^* = L^2(\Omega)$ and $f \in Y$.

Define $G : Y \to \mathbb{R}$ and $F : V \to \mathbb{R}$ by

$$G(u') = \frac{1}{2}\int_\Omega (u')^2\,dx - \int_\Omega |u'|\,dx,$$

and

$$F(u) = \frac{1}{2}\int_\Omega u^2\,dx,$$

respectively.

Denoting $V_0 = W_0^{1,2}(\Omega)$, define also $J_1 : V \times V_0 \times (0,1) \to \mathbb{R}$ by

$$\begin{aligned} J_1(u,\phi,\lambda) &= \lambda G(u'-(1-\lambda)\phi')+(1-\lambda)G(u'+\lambda\phi') \\ &\quad +\lambda F(u-(1-\lambda)\phi)+(1-\lambda)F(u+\lambda\phi) \\ &\quad -\langle u,f\rangle_{L^2}. \end{aligned} \tag{201}$$

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Observe that

$$\begin{aligned}(\lambda G)^*(v_1^*) &= \sup_{v_1\in Y}\{\langle v_1, v_1^*\rangle_{L^2} - \lambda G(v_1)\}\\ &= \lambda G^*\left(\frac{v_1^*}{\lambda}\right)\\ &= \frac{1}{2\lambda}\int_\Omega (v_1^*)^2\,dx + \int_\Omega |v_1^*|\,dx, \end{aligned} \tag{202}$$

$$\begin{aligned}((1-\lambda)G)^*(v_2^*) &= \sup_{v_2\in Y}\{\langle v_2, v_2^*\rangle_{L^2} - (1-\lambda) G(v_2)\}\\ &= (1-\lambda)G^*\left(\frac{v_2^*}{(1-\lambda)}\right)\\ &= \frac{1}{2(1-\lambda)}\int_\Omega (v_2^*)^2\,dx + \int_\Omega |v_2^*|\,dx, \end{aligned} \tag{203}$$

$$\begin{aligned}(\lambda F)^*(v_3^*) &= \sup_{v_3\in Y}\{\langle v_3, v_3^*\rangle_{L^2} - \lambda F(v_3)\}\\ &= \lambda F^*\left(\frac{v_3^*}{\lambda}\right)\\ &= \frac{1}{2\lambda}\int_\Omega (v_3^*)^2\,dx, \end{aligned} \tag{204}$$

and

$$\begin{aligned}((1-\lambda)F)^*(v_4^*) &= \sup_{v_4\in Y}\{\langle v_4, v_4^*\rangle_{L^2} - (1-\lambda) F(v_4)\}\\ &= (1-\lambda)F^*\left(\frac{v_4^*}{(1-\lambda)}\right)\\ &= \frac{1}{2(1-\lambda)}\int_\Omega (v_4^*)^2\,dx. \end{aligned} \tag{205}$$

Denoting $v^* = (v_1^*, \cdots, v_4^*) \in [Y^*]^4$, define $J^* : [Y^*]^4 \times (0,1) \to \mathbb{R}$ by

$$\begin{aligned}J_1^*(v^*, \lambda) &= -\lambda G^*\left(\frac{v_1^*}{\lambda}\right) - (1-\lambda)G^*\left(\frac{v_2^*}{(1-\lambda)}\right)\\ &\quad -\lambda F^*\left(\frac{v_3^*}{\lambda}\right) - (1-\lambda)F^*\left(\frac{v_4^*}{(1-\lambda)}\right)\\ &\quad +v_1^*(1)u(1) + v_2^*(1)u(1). \end{aligned} \tag{206}$$

Similarly as in the previous section, we may obtain

$$\inf_{u\in V} J(u) \geq \inf_{\lambda\in(0,1)}\left\{\sup_{v^*\in A^*} J^*(v^*, \lambda)\right\},$$

where $A^* = A_1^* \cap A_2^*$,

$$A_1^* = \{v^* \in Y^* \ : \ (v_1^*)' + (v_2^*)' - v_3^* - v_4^* + f = 0, \text{ in } \Omega\},$$

and

$$A_2^* = \{(v^*, \lambda) \in [Y^*]^4 \times (0,1) \ : \ -(1-\lambda)(v_1^*)' + \lambda(v_2^*)' + (1-\lambda)v_3^* - \lambda v_4^* = 0, \text{ in } \Omega\}.$$

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From such expressions of A_1^* and A_2^* we may obtain

$$v_3^* = (v_1^*)' + \lambda f,$$

and

$$v_4^* = (v_2^*)' + (1-\lambda) f.$$

Replacing such expressions for v_3^* and v_4^* into the expression of J^*, and from now and on denoting $v^* = (v_1^*, v_2^*) \in [Y^*]^2$, we may obtain $J_1^* : [Y^*]^2 \times (0,1] \to \mathbb{R}$ where

$$\begin{aligned} J_1^*(v^*, \lambda) &= -\frac{1}{2\lambda} \int_\Omega (v_1^*)^2 \, dx - \int_\Omega |v_1^*| \, dx \\ &\quad -\frac{1}{2(1-\lambda)} \int_\Omega (v_2^*)^2 \, dx - \int_\Omega |v_2^*| \, dx \\ &\quad -\frac{1}{2\lambda} \int_\Omega ((v_1^*)' + \lambda f)^2 \, dx \\ &\quad -\frac{1}{2(1\lambda)} \int_\Omega ((v_2^*)' + (1-\lambda) f)^2 \, dx \\ &\quad + v_1^*(1) u(1) + v_2^*(1) u(1). \end{aligned} \tag{207}$$

Consequently, we have got

$$\inf_{u \in V} J(u) \geq \sup_{v^* \in [Y^*]^2} \left\{ \inf_{\lambda \in (0,1)} J_1^*(v^*, \lambda) \right\}.$$

In order to obtain numerical results we have designed the following algorithm:

1. Set $n = 1$ and $\lambda_n = 1/2$.
2. Calculate $(v^*)_n \in [Y^*]^2$ such that

$$J_1^*((v^*)_n, \lambda_n) = \sup_{v^* \in [Y^*]^2} J_1^*(v^*, \lambda_n).$$

3. Calculate $\lambda_{n+1} \in (0,1)$ such that

$$J_1^*((v^*)_n, \lambda_{n+1}) = \inf_{\lambda \in (0,1)} J_1^*((v^*)_n, \lambda).$$

4. Set $n := n + 1$ and go to item (2) until the satisfaction of an appropriate convergence criterion.

We have developed numerical results for the following cases

1.
$$f(x) = \sin(\pi x)/2,$$

2.
$$f(x) = \cos(\pi x)/2,$$

3.
$$f(x) = 0.$$

Observe that for the optimal point we have

$$v_3^* = u - (1-\lambda)\phi,$$

and

$$v_4^* = u + \lambda \phi,$$

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so that

$$u = \lambda v_3^* + (1-\lambda)v_4^*.$$

For the optimal solution $u_0(x)$ found for the cases (1), (2) and (3), please see the Figures 29, 30 and 31, respectively.

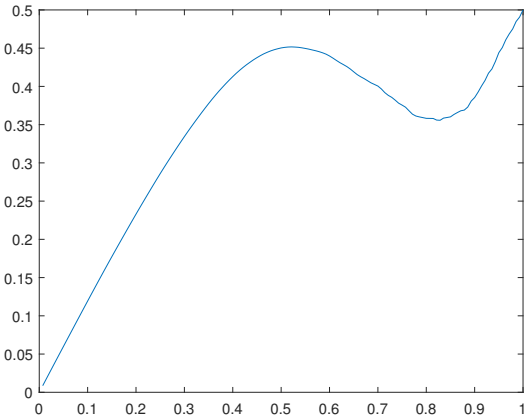

Figure 29. Optimal solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

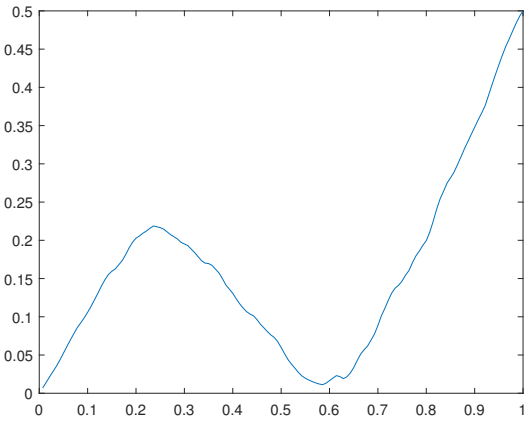

Figure 30. Optimal solution $u_0(x)$ for the case $f(x) = \cos(\pi x)/2$.

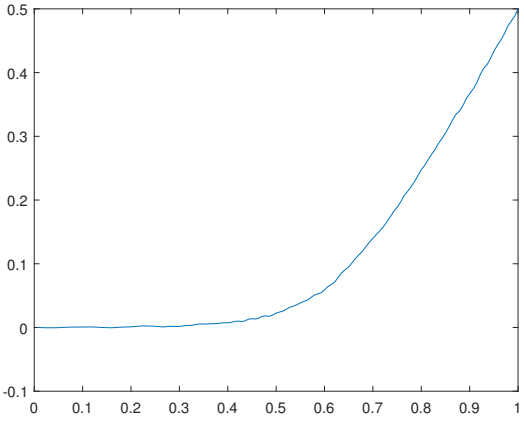

Figure 31. Optimal solution $u_0(x)$ for the case $f(x) = 0$.

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Here we present the concerning software in MAT-LAB.

****

1. clear all
   global m8 d L v1 v2 v3 v4 yo dv1 dv2 e1
   m8=140;
   d=1/m8;
   e1=0.0001;
   L=1/2;
   for i=1:2*m8
   xo(i,1)=0.01;
   end;
   for i=1:m8
   yo(i,1)=sin(pi*i*d)/2;
   end;
   x1=1/2;
   k=1;
   b12=1;
   while $(b12 > 10^{-4})$ and $(k < 100)$
   k
   k=k+1;
   X1=fminunc('funFeb24',xo);
   b12=max(abs(X1-xo))
   xo=X1;
   X2=fminunc('funFeb24A',x1);
   x1=X2;
   L=(sin(x1)+1)/2;
   L
   end;
   u(m8,1)=1/2;
   for i=1:m8-1
   u(i,1)=L*v3(i,1)+(1-L)*v4(i,1);
   end;
   for i=1:m8
   x(i,1)=i*d;
   end;
   plot(x,u);

****

Here the auxiliary function "funFeb24"

****

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```
function S=funFeb24(x)
global m8 d L v1 v2 v3 v4 yo dv1 dv2 e1
for i=1:m8
v1(i,1)=x(i,1);
v2(i,1)=x(m8+i,1);
end;
for i=1:m8-1
dv1(i,1)=(v1(i+1,1)-v1(i,1))/d;
dv2(i,1)=(v2(i+1,1)-v2(i,1))/d;
end;
S=0;
for i=1:m8
S=S+1/2/sqrt(L^2+e1)*v1(i,1)^2+sqrt(v1(i,1)^2+e1);
S=S+1/2/sqrt((1-L)^2+e1)*v2(i,1)^2+sqrt(v2(i,1)^2+e1);
end;
for i=1:m8-1
v3(i,1)=dv1(i,1)+L*yo(i,1);
v4(i,1)=dv2(i,1)-(L-1)*yo(i,1);
S=S+1/2/sqrt(L^2+e1)*v3(i,1)^2+1/2/sqrt((1-L)^2+e1)*v4(i,1)^2;
end;
S=S-(v1(m8,1)+v2(m8,1))/d/2;
```

****

Finally, the auxiliary function "funFeb24A"

****

```
function S1=funFeb24A(y)
global m8 d L v1 v2 v3 v4 yo e1
L=(sin(y)+1)/2;
for i=1:m8-1
dv1(i,1)=(v1(i+1,1)-v1(i,1))/d;
dv2(i,1)=(v2(i+1,1)-v2(i,1))/d;
end;
S=0;
for i=1:m8
S=S+1/2/sqrt(L^2+e1)*v1(i,1)^2+sqrt(v1(i,1)^2+e1);
S=S+1/2/sqrt((1-L)^2+e1)*v2(i,1)^2+sqrt(v2(i,1)^2+e1);
end;
for i=1:m8-1
v3(i,1)=dv1(i,1)+L*yo(i,1);
v4(i,1)=dv2(i,1)-(L-1)*yo(i,1);
```

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S=S+1/2/$sqrt(L^2+e1)*v3(i,1)^2+1/2/sqrt((1-L)^2+e1)*v4(i,1)^2$;

end;

S=S-(v1(m8,1)+v2(m8,1))/d/2;

S1=-S;

****

34. One More Note on Relaxation for a General Model in the Vectorial Calculus of Variations

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a function $g : \mathbb{R}^{N\times n} \to \mathbb{R}$ twice differentiable and such that

$$g(y) \to +\infty, \text{ as } |y| \to +\infty.$$

Define a functional $G : V \to \mathbb{R}$ by

$$G(\nabla u) = \frac{1}{2}\int_\Omega g(\nabla u)\, dx,$$

where

$$V = \{W^{1,2}(\Omega;\mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega\}.$$

Moreover, for $f \in L^2(\Omega;\mathbb{R}^N)$, define also

$$J(u) = G(\nabla u) - \langle u, f\rangle_{L^2}.$$

We assume there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = \inf_{u\in V} J(u).$$

Observe that from the convex analysis basic theory, we have that

$$\begin{aligned} \alpha &= \inf_{u\in V} J(u) \\ &= \inf_{u\in V} J^{**}(u) \\ &= \inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u, f\rangle_{L^2}\}. \end{aligned} \tag{208}$$

On the other hand

$$\begin{aligned} (G\circ\nabla)^{**}(u) &\le H(u) \\ &\equiv \inf_{(\lambda,(v_1,\cdots,v_m))\in B\times B_1(u,\lambda)} \left\{\sum_{j=1}^m \lambda_j G(\nabla v_j)\right\} \\ &\le G(\nabla u), \end{aligned} \tag{209}$$

where

$$B = \left\{\lambda = (\lambda_1,\cdots,\lambda_m) \in \mathbb{R}^m \ : \ \lambda_j \ge 0, \ \forall j \in \{1,\cdots,m\}, \text{ and } \sum_{j=1}^m \lambda_j = 1\right\},$$

and

$$B_1(u,\lambda) = \left\{v = (v_1,\cdots,v_m) \in [V]^m \ : \ \sum_{j=1}^m \lambda_j v_j = u\right\}.$$

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From such results, we may infer that

$$\inf_{u\in V} J^{**}(u) = \inf_{u\in V}\{H(u) - \langle u, f\rangle_{L^2}\} = \inf_{u\in V} J(u).$$

Furthermore, observe that

$$\sum_{j=1}^{m} \lambda_j \nabla v_j = \nabla u,$$

and

$$\lambda_m = 1 - \sum_{j=1}^{m-1} \lambda_j,$$

so that

$$\begin{aligned} \nabla v_m &= \nabla u - \sum_{j=1}^{m-1} \lambda_j (\nabla v_j - \nabla v_m) \\ &= \nabla u + \sum_{j=1}^{m-1} \lambda_j \nabla \phi_j, \end{aligned} \tag{210}$$

where $\phi_j = -v_j + v_m \in W_0^{1,2}(\Omega;\mathbb{R}^N)$ so that

$$\nabla \phi_j = -\nabla v_j + \nabla v_m,$$

and

$$\nabla v_m = \nabla v_j + \nabla \phi_j,\ \forall j \in \{1,\cdots,m\}.$$

Therefore,

$$\nabla v_j = \nabla v_m - \nabla \phi_j = \nabla u + \sum_{k=1}^{m-1} \lambda_k \nabla \phi_k - \nabla \phi_j.$$

Replacing such results into the expression of H, we have

$$H(u) = \inf_{(\lambda,\phi)\in B\times (V_0)^{m-1}} \left\{ \sum_{j=1}^{m-1} \lambda_j G\left(\nabla u + \sum_{k=1}^{m-1} \nabla \phi_k - \nabla \phi_j\right) + \lambda_m G\left(\nabla u + \sum_{k=1}^{m-1} \lambda_k \nabla \phi_k\right)\right\},$$

where we recall that

$$V_0 = W_0^{1,2}(\Omega;\mathbb{R}^N).$$

Joining the pieces, we have got

$$\begin{aligned} \inf_{u\in V} J(u) &= \inf_{u\in V} J^{**}(u) \\ &= \inf_{u\in V}\{H(u) - \langle u, f\rangle_{L^2}\} \\ &= \inf_{(u,\lambda,\phi)\in V\times B\times (V_0)^{m-1}} \left\{ \sum_{j=1}^{m-1} \lambda_j G\left(\nabla u + \sum_{k=1}^{m-1} \lambda_k \nabla \phi_k - \nabla \phi_j\right)\right. \\ &\quad + \lambda_m G\left(\nabla u + \sum_{k=1}^{m} \lambda_k \nabla \phi_k\right) \\ &\quad \left. - \langle u, f\rangle_{L^2}\right\}. \end{aligned}$$

This last functional corresponds to a relaxation for the original non-convex functional.

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The note is complete.

34.1. A Related Duality Principle and Concerning Convex Dual Formulation

With the notation and statements of the previous sections in mind, consider the functionals $J : V \to \mathbb{R}$ and $J_3 : B \times V \times [V_0]^m \to \mathbb{R}$ where

$$J(u) = G(\nabla u) + \frac{1}{2}\int_\Omega u \cdot u \, dx - \langle u, f \rangle_{L^2},$$

and

$$\begin{aligned} J_3(\lambda, u, \phi) \quad = \quad & \sum_{j=1}^{m} \lambda G\left(\nabla u + \sum_{k=1}^{m-1} \lambda_k \phi_k - \nabla \phi_j\right) \\ & + \lambda_m G\left(\nabla u + \sum_{k=1}^{m-1} \lambda_k \nabla \phi_k\right) \\ & + \sum_{j=1}^{m-1} \frac{\lambda_j}{2} \int_\Omega \left(u + \sum_{k=1}^{m-1} \lambda_k \phi_k - \nabla \phi_j\right) \cdot \left(u + \sum_{k=1}^{m-1} \lambda_k \phi_k - \nabla \phi_j\right) dx \\ & + \frac{(\lambda_m)}{2} \int_\Omega \left(u + \sum_{k=1}^{m-1} \lambda_k \phi_k\right) \cdot \left(u + \sum_{k=1}^{m-1} \lambda_k \phi_k\right) dx \\ & - \sum_{j=1}^{m-1} \lambda_j \left\langle u + \sum_{k=1}^{m-1} \lambda_k \phi_k - \phi_j, f \right\rangle_{L^2} \\ & - (\lambda_m) \left\langle u + \sum_{k=1}^{m-1} \lambda_k \phi_k, f \right\rangle_{L^2}. \end{aligned} \tag{211}$$

Here we have denoted

$$V = \{u \in W^{1,2}(\Omega; \mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega = S\},$$

$$V_0 = W_0^{1,2}(\Omega; \mathbb{R}^N),$$

$$Y = Y^* = L^2(\Omega; \mathbb{R}^{N \times n})$$

and

$$Y_1 = Y_1^* = L^2(\Omega; \mathbb{R}^N).$$

Observe that

$$J^{**}(u) \leq \min_{(\lambda, \phi) \in B \times (V_0)^{m-1}} J_3(\lambda, u, \phi).$$

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Moreover,

$$
\begin{aligned}
J_3(\lambda,u,\phi) \quad = \quad & -\sum_{j=1}^{m-1}\left\langle \nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k-\nabla\phi_j,(v_1^*)_j\right\rangle_{L^2} \\
& +\sum_{j=1}^{m-1}\lambda_j G\left(\nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k-\nabla\phi_j\right) \\
& -\left\langle \nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k,(v_1^*)_m\right\rangle_{L^2}+\lambda_m G\left(\nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k\right) \\
& -\sum_{j=1}^{m-1}\left\langle u+\sum_{k=1}^{m-1}\lambda_k\phi_k-\phi_j,(v_3^*)_j\right\rangle_{L^2} \\
& +\sum_{j=1}^{m-1}\frac{\lambda_j}{2}\int_\Omega\left(u+\sum_{k=1}^{m-1}\lambda_k\phi_k-\phi_j\right)\cdot\left(u+\sum_{k=1}^{m-1}\lambda_k\phi_k-\phi_j\right)dx \\
& -\left\langle u+\sum_{k=1}^{m-1}\lambda_k\phi_k,(v_3^*)_m\right\rangle_{L^2} \\
& +\frac{\lambda_m}{2}\int_\Omega\left(u+\sum_{k=1}^{m-1}\lambda_k\phi_k\right)\cdot\left(u+\sum_{k=1}^{m-1}\lambda_k\phi_k\right)dx \\
& +\sum_{j=1}^{m-1}\left\langle \nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k-\nabla\phi_j,(v_1^*)_j\right\rangle_{L^2} \\
& +\left\langle \nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k,(v_1^*)_m\right\rangle_{L^2} \\
& +\sum_{j=1}^{m-1}\left\langle u+\sum_{k=1}^{m-1}\lambda_k\phi_k-\phi_j,(v_3^*)_j\right\rangle_{L^2} \\
& +\left\langle u+\sum_{k=1}^{m-1}\lambda_k\phi_k,(v_3^*)_m\right\rangle_{L^2}-\langle u,f\rangle_{L^2}
\end{aligned}
\tag{212}
$$

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Therefore,

$$\begin{aligned}
J_3(\lambda,u,\phi) \quad \geq \quad & \inf_{v_1\in[Y]^{m-1}}\left\{\sum_{j=1}^{m-1}\left(-\langle (v_1)_j,(v_1^*)_j\rangle_{L^2}+\lambda_j G((v_1)_j)\right)\right\}\\
& +\inf_{(v_1)_m\in Y}\{-\langle (v_1)_m,(v_1^*)_m\rangle_{L^2}+\lambda_m G((v_1)_m)\}\\
& +\inf_{v_3\in[Y_1]^{m-1}}\left\{\sum_{j=1}^{m-1}\left(-\langle (v_3)_j,(v_3^*)_j\rangle_{L^2}+\frac{\lambda_j}{2}\int_\Omega (v_3)_j\cdot(v_3)_j\,dx\right)\right\}\\
& +\inf_{(v_3)_m\in Y_1}\left\{-\langle (v_3)_m,(v_3^*)_m\rangle_{L^2}+\frac{\lambda_m}{2}\int_\Omega (v_3)_j\cdot(v_3)_j\,dx\right\}\\
& +\inf_{(u,\phi)\in V\times(V_0)^{m-1}}\left\{\sum_{j=1}^{m-1}\left\langle \nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k-\phi_j,(v_1^*)_j\right\rangle_{L^2}\right.\\
& +\left\langle \nabla u+\sum_{k=1}^{m-1}\lambda_k\nabla\phi_k,(v_1^*)_m\right\rangle_{L^2}\\
& +\sum_{j=1}^{m-1}\left\langle u+\sum_{k=1}^{m-1}\nabla\phi_k-\phi_j,v_3^*\right\rangle_{L^2}\\
& \left.+\left\langle u+\sum_{k=1}^{m-1}\lambda_k\phi_k,(v_3^*)_m\right\rangle_{L^2}-\langle u,f\rangle_{L^2}\right\}\\
= \quad & -\sum_{j=1}^{m-1}\lambda_j G^*\left(\frac{(v_1^*)_j}{\lambda_j}\right)-\lambda_m G^*\left(\frac{(v_1^*)_m}{\lambda_m}\right)\\
& -\sum_{j=1}^{m-1}(F_3)_j^*((v_3^*)_j,\lambda_j)-(F_3)_m^*((v_3^*)_m,\lambda_m)\\
& +\sum_{k=1}^{m}\int_S((v_1^*)_k)_{ij}n_j(u_0)_i\,dS,\\
& \forall\lambda\in B,u\in V,\ \phi\in(V_0)^{m-1},v^*\in A^*,
\end{aligned}\tag{213}$$

where

$$G^*(v^*)=\sup_{v\in Y}\{\langle v,v^*\rangle_{L^2}-G(v)\},$$

$$\begin{aligned}
(F_3)_j^*((v_3^*)_j,\lambda_j) \quad &= \quad \sup_{v_3\in Y_1}\left\{\langle (v_3)_j,(v_3^*)_j\rangle_{L^2}-\frac{\lambda_j}{2}\int_\Omega (v_3)_j\cdot(v_3)_j\,dx\right\}\\
&= \quad \frac{1}{2\lambda_j}\int_\Omega (v_3)_j^*\cdot(v_3)_j^*\,dx,\ \forall j\in\{1,\cdots,m\}.
\end{aligned}\tag{214}$$

Furthermore, $A^*=A_1^*\cap A_2^*(\lambda)$ where

$$A_1^*=\left\{v^*=(v_1^*,v_3^*)\in[Y^*]^m\times[Y_1^*]^m\ :\ -\sum_{j=1}^{m}(\ \mathrm{div}\ ((v_1^*)_j)_i+((v_3^*)_j)_i)-f_i=0,\ \text{in }\Omega\right\},$$

and

$$\begin{aligned}
A_2^*(\lambda) \quad = \quad & \{v^*=(v_1^*,v_3^*)\in[Y^*]^m\times[Y_1^*]^m\ :\\
& \lambda_k\sum_{j=1}^{m}\ \mathrm{div}\ ((v_1^*)_j)_i-\ \mathrm{div}\ ((v_1^*)_k)_i-\lambda_k\sum_{j=1}^{m}((v_3^*)_j)_i+((v_3^*)_k)_i=0,\\
& \text{in }\Omega,\ \forall k\in\{1,\cdots,m-1\},\ \forall i\in\{1,\cdots,N\}\}.
\end{aligned}\tag{215}$$

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Summarizing, we have got

$$\begin{aligned} & \inf_{(\lambda,u\phi)\in B\times V\times (V_0)^{m-1}} J_3(\lambda,u,\phi) \\ \geq & \inf_{\lambda\in B}\left\{\sup_{v^*\in A^*}\left\{-\sum_{j=1}^m \lambda_j G^*\left(\frac{(v_1^*)_j}{\lambda_j}\right)\right.\right. \\ & \left.\left.-\sum_{j=1}^m (F_3^*)_j((v_3^*)_j,\lambda_j)+\sum_{k=1}^m\int_{\partial\Omega}((v_1^*)_k)_{ij}n_j(u_0)_i\,dS\right\}\right\}. \end{aligned} \tag{216}$$

Remark 34.1. *We highlight this last dual function in v^* is convex (in fact concave) on the convex set A^*.*

35. A General Convex Primal Dual Formulation with a Restriction for an Originally Non-Convex Primal One

Let $\Omega \subset \mathbb{R}^3$ be an open bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx+\frac{\alpha}{2}\int_\Omega (u^2-\beta)^2\,dx \\ &\quad -\langle u,f\rangle_{L^2}, \end{aligned} \tag{217}$$

where $\alpha>0,\beta>0,\gamma>0$, $V=W_0^{1,2}(\Omega)$ and $Y=Y^*=L^2(\Omega)$.

Define $F_1 : V \to \mathbb{R}$ and $F_2 : V\times Y^* \to \mathbb{R}$ by

$$F_1(u)=\frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx+\frac{K}{2}\int_\Omega u^2\,dx-\langle u,f\rangle_{L^2},$$

and

$$\begin{aligned} F_2(u,v_0^*) &= -\langle u^2,v_0^*\rangle_{L^2}+\frac{K}{2}\int_\Omega u^2\,dx \\ &\quad +\frac{1}{2\alpha}\int_\Omega (v_0^*)^2\,dx+\beta\int_\Omega v_0^*\,dx. \end{aligned} \tag{218}$$

Define also $F_1^* : Y^* \to \mathbb{R}$ and $F_2^* : Y^*\times Y^* \to \mathbb{R}$ by

$$\begin{aligned} F^*(v_1^*) &= \sup_{u\in V}\{\langle u,v_1^*\rangle_{L^2}-F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*+f)^2}{-\gamma\nabla^2+K}\,dx, \end{aligned} \tag{219}$$

and

$$\begin{aligned} F_2^*(v_1^*,v_0^*) &= \sup_{u\in V}\{-\langle u,v_1^*\rangle_{L^2}-F_2(u,v_0^*)\} \\ &= -\frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{2v_0^*-K}\,dx \\ &\quad -\frac{1}{2\alpha}\int_\Omega (v_0^*)^2\,dx-\beta\int_\Omega v_0^*\,dx. \end{aligned} \tag{220}$$

if $v_0^* \in B^*$, where

$$B^*=\{v_0^*\in Y^* \ : \ \|v_0^*\|_\infty \leq K/2\},$$

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for some appropriate $K > 0$ to be specified.

At this point we define

$$V_2 = \{u \in V \ : \ \|u\|_\infty \leq K_3\},$$
$$A^+ = \{u \in V \ : \ uf \geq 0, \text{ in } \Omega\},$$
$$V_1 = V_2 \cap A^+,$$
$$D^* = \{v_1^* \in Y^* \ : \ \|v_1^*\|_\infty \leq 5/4K\},$$

for appropriate $K_3 > 0$ to be specified, and $J_1^* : D^* \times B^* \to \mathbb{R}$ by

$$J_1^*(v_1^*, v_0^*) = -F_1^*(v_1^*) + F_2^*(v_1^*, v_0^*).$$

Moreover, we define $J_2^* : V_1 \times D^* \times B^* \to \mathbb{R}$ by

$$\begin{aligned} J_2^*(u, v_1^*, v_0^*) &= J_1^*(v_1^*, v_0^*) + \frac{K_1}{2}\|v_1^* - (-\gamma\nabla^2 + K)u\|_2^2 \\ &\quad + \frac{1}{10\alpha K_3^2}\|v_1^* - (-2v_0^* + K)u\|_2^2 \end{aligned} \tag{221}$$

Observe that

$$\frac{\partial^2 J_2^*(u, v_1^*, v_0^*)}{\partial (v_1^*)^2} = -\frac{1}{-\gamma\nabla^2 + K} - \frac{1}{2v_0^* - K} + K_1 + \frac{1}{5\alpha K_3^2},$$
$$\frac{\partial^2 J_2^*(u, v_1^*, v_0^*)}{\partial u^2} = K_1(-\gamma\nabla^2 + K)^2 + \frac{1}{5\alpha K_3^2}(-2v_0^* + K)^2,$$

and

$$\frac{\partial^2 J_2^*(u, v_1^*, v_0^*)}{\partial u \partial v_1^*} = -K_1(-\gamma\nabla^2 + K) - \frac{1}{5\alpha K_3^2}(-2v_0^* + K).$$

Now we set K_1, K, K_3 such that

$$K_1 \gg \max\{K, K_3, 1, \alpha, \beta, \gamma, 1/\alpha, 1/\gamma, 1/\beta\},$$
$$K \gg \max\{K_3, 1, \alpha, \beta, \gamma, 1/\alpha, 1/\gamma, 1/\beta\},$$

and $K_3 \approx 3$.

From such results and constant choices, we may obtain

$$\begin{aligned} \det\{\delta^2_{u,v_1^*} J_2^*(u, v_1^*, v_0^*)\} &= \frac{\partial^2 J_2^*(u, v_1^*, v_0^*)}{\partial (v_1^*)^2}\frac{\partial^2 J_2^*(u, v_1^*, v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_2^*(u, v_1^*, v_0^*)}{\partial u \partial v_1^*}\right)^2 \\ &= \mathcal{O}\left(\frac{K_1(-\gamma\nabla^2 + 2v_0^*)^2}{5\alpha K_3^2} + 2K_1(-\gamma\nabla^2 + 2v_0^*)\right) + \mathcal{O}\left(\frac{K_1}{K}\right), \\ &\quad \text{in } V_1 \times D^* \times B^*. \end{aligned} \tag{222}$$

Define now

$$C^* = \left\{v_0^* \in Y^* \ : \ \frac{(-\gamma\nabla^2 + 2v_0^*)^2}{5\alpha K_3^2} + 2(-\gamma\nabla^2 + 2v_0^*) > \frac{c_0}{K} I_d\right\},$$

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where we assume that $c_0 > 0$ is such that if $v_0^* \in C^*$, then

$$\det\{\delta^2_{u,v_1^*} J_2^*(u, v_1^*, v_0^*)\} > \mathbf{0}, \text{ in } B^* \cap C^*.$$

Finally, we also suppose the concerning constants are such that $B^* \cap C^*$ is convex.
With such statements, definitions and results in mind, we may prove the following theorem.

Theorem 35.1. *Let $(u_0, \hat{v}_1^*, \hat{v}_0^*) \in V_1 \times D^* \times (B^* \cap C^*)$ be such that*

$$\delta J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}.$$

Under such hypotheses,

$$\delta J(u_0) = \mathbf{0},$$

and

$$\begin{aligned} J(u_0) &= J(u_0) + \frac{K_1}{2} \| - \gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f\|_2^2 \\ &= \inf_{u \in V_1} \left\{ J(u) + \frac{K_1}{2} \| - \gamma \nabla^2 u + 2\hat{v}_0^* u - f\|_2^2 \right\} \\ &= \sup_{v_0^* \in B^*} \left\{ \inf_{(u, v_1^*) \in V_1 \times D^*} J_2^*(u, v_1^*, v_0^*) \right\} \\ &= J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*). \end{aligned} \tag{223}$$

Proof. The proof that

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f = \mathbf{0}$$

and

$$J(u_0) = J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*),$$

may be done similarly as in the previous sections and will not be repeated.

Furthermore, since

$$\delta J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0},$$

$v_0^* \in B^* \times C^*$ and J_2^* is concave in v_0^* on $V_1 \times D^* \times B^*$, we have

$$J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \inf_{(u, v_1^*) \in V_1 \times D^*} J_2^*(u, v_1^*, \hat{v}_0^*),$$

and

$$J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \sup_{v_0^* \in B^*} J_2^*(u_0, \hat{v}_1^*, v_0^*).$$

From such results and the Saddle Point Theorem we may infer that

$$\begin{aligned} J(u_0) &= J(u_0) + \frac{K_1}{2} \| - \gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f\|_2^2 \\ &= \sup_{v_0^* \in B^*} \left\{ \inf_{(u, v_1^*) \in V_1 \times D^*} J_2^*(u, v_1^*, v_0^*) \right\} \\ &= J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*). \end{aligned} \tag{224}$$

Finally, from evident convexity,

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$$\begin{aligned} J(u_0) &= J(u_0) + \frac{K_1}{2}\| - \gamma\nabla^2 u_0 + 2\hat{v}_0^* u_0 - f\|_2^2 \\ &= \inf_{u\in V_1}\left\{J(u) + \frac{K_1}{2}\| - \gamma\nabla^2 u + 2\hat{v}_0^* u - f\|_2^2\right\}. \end{aligned} \tag{225}$$

Joining the pieces, we have got

$$\begin{aligned} J(u_0) &= J(u_0) + \frac{K_1}{2}\| - \gamma\nabla^2 u_0 + 2\hat{v}_0^* u_0 - f\|_2^2 \\ &= \inf_{u\in V_1}\left\{J(u) + \frac{K_1}{2}\| - \gamma\nabla^2 u + 2\hat{v}_0^* u - f\|_2^2\right\} \\ &= \sup_{v_0^*\in B^*}\left\{\inf_{(u,v_1^*)\in V_1\times D^*} J_2^*(u, v_1^*, v_0^*)\right\} \\ &= J_2^*(u_0, \hat{v}_1^*, \hat{v}_0^*). \end{aligned} \tag{226}$$

The proof is complete.

□

36. A General Convex Dual Formulation for an Originally Non-Convex Primal One

In this section we develop a convex dual formulation for an originally non-convex primal formulation.

Let $\Omega \subset \mathbb{R}^3$ be an open bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\, dx + \frac{\alpha}{2}\int_\Omega (u^2-\beta)^2\, dx \\ &\quad -\langle u, f\rangle_{L^2}, \end{aligned} \tag{227}$$

where $\alpha > 0, \beta > 0, \gamma > 0$, $V = W_0^{1,2}(\Omega)$ and $Y = Y^* = L^2(\Omega)$.

At the moment, fix a matrix $K_1 > 0$ and $K > 0$ to be specified.

Define $F_1 : V \to \mathbb{R}$, $F_2 : V \to \mathbb{R}$ and $F_3 : V \times Y^* \to \mathbb{R}$, by

$$\begin{aligned} F_1(u) &= \frac{\gamma}{4}\int_\Omega \nabla u\cdot\nabla u\, dx + \frac{K}{2}\int_\Omega u^2\, dx \\ &\quad -\langle u, f\rangle_{L^2}, \end{aligned} \tag{228}$$

$$F_2(u) = \frac{\gamma}{4}\int_\Omega \nabla u\cdot\nabla u\, dx + \frac{K}{2}\int_\Omega u^2\, dx, \tag{229}$$

$$F_3(u, v_0^*) = -\langle u^2, v_0^*\rangle_{L^2} + K\int_\Omega u^2\, dx + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2\, dx + \beta\int_\Omega v_0^*\, dx + \langle u, f\rangle_{L^2}.$$

Define also $F_1^* : Y^* \to \mathbb{R}$ and $F_2^* : Y^* \to \mathbb{R}$,

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u\in V}\{\langle u, v_1^*\rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{-\frac{\gamma}{2}\nabla^2 + K}\, dx, \end{aligned} \tag{230}$$

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$$\begin{aligned} F_2^*(v_2^*) &= \sup_{u\in V}\{\langle u, v_2^*\rangle_{L^2} - F_2(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_2^*)^2}{-\frac{\gamma}{2}\nabla^2 + K}\,dx, \end{aligned} \tag{231}$$

At this point we also define

$$B^* = \{v_0^* \in Y^* \ : \ \|v_0^*\|_\infty \le K/2\},$$

$$V_2 = \{u \in V \ : \ \|u\|_\infty \le K_3\},$$

$$A^+ = \{u \in V \ : \ uf \ge 0, \text{ in } \Omega\},$$

$$V_1 = V_2 \cap A^+,$$

$$D^* = \{v^* \in Y^* \ : \ \|v^*\|_\infty \le 5/4K\},$$

for an appropriate $K_3 > 0$ to be specified.

Furthermore, we define $F_3^* : D^* \times D^* \times B^* \to \mathbb{R}$ by

$$\begin{aligned} F_3^*(v_1^*, v_2^*, v_0^*) &= \sup_{u\in V}\{-\langle u, v_1^* + v_2^*\rangle_{L^2} - F_3(u, v_0^*)\} \\ &= -\frac{1}{2}\int_\Omega \frac{(v_1^* + v_2^* - f)^2}{2v_0^* - 2K}\,dx \\ &\quad -\frac{1}{2\alpha}\int_\Omega (v_0^*)^2\,dx - \beta\int_\Omega v_0^*\,dx. \end{aligned} \tag{232}$$

Moreover, we define $J_1^* : D^* \times D^* \times B^* \to \mathbb{R}$ by

$$J_1^*(u, v_1^*, v_0^*) = -F_1^*(v_1^*) - F_2(v_2^*) + F_3^*(v_1^*, v_2^*, v_0^*)$$

and $J_2^* : D^* \times D^* \times B^* \to \mathbb{R}$ by

$$\begin{aligned} J_2^*(v_1^*, v_2^*, v_0^*) &= J_1^*(v_1^*, v_2^*, v_0^*) \\ &\quad + \frac{K_1}{2}\int_\Omega (v_1^* - v_2^*)^2\,dx \\ &\quad + \frac{K^2}{2}\int_\Omega \left(\frac{v_1^*}{-\frac{\gamma}{2}\nabla^2 + K} - \frac{v_1^* + v_2^* - f}{-2v_0^* + 2K}\right)^2 dx. \end{aligned} \tag{233}$$

Now observe that

$$\frac{\partial^2 J_2^*(v_1^*, v_2^*, v_0^*)}{\partial (v_1^*)^2} = -\frac{1}{-\frac{\gamma}{2}\nabla^2 + K} + K_1 + K^2\left(\frac{1}{-\frac{\gamma}{2}\nabla^2 + K} - \frac{1}{2K - 2v_0^*}\right)^2 - \frac{1}{-2K + 2v_0^*},$$

and

$$\frac{\partial^2 J_2^*(v_1^*, v_2^*, v_0^*)}{\partial (v_2^*)^2} = -\frac{1}{-\frac{\gamma}{2}\nabla^2 + K} + K_1 + \frac{K^2}{(-2K + 2v_0^*)^2} - \frac{1}{-2K + 2v_0^*},$$

and

$$\frac{\partial^2 J_2^*(v_1^*, v_2^*, v_0^*)}{\partial v_1^*\,\partial v_2^*} = -K_1 - K^2\frac{\left(\frac{1}{-\frac{\gamma}{2}\nabla^2 + K} - \frac{1}{2K - 2v_0^*}\right)^2}{2K - 2v_0^*} - \frac{1}{-2K + 2v_0^*}.$$

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We set $K_1 \gg K$,

$$K \gg K_3,$$

and $K_3 \approx \sqrt{3}$. Moreover, after a re-scale if necessary, we assume $\alpha \approx 0.15$.

From such results and constant choices, with the help of the software MATHEMATICA, we may obtain

$$\begin{aligned} \det\{\delta^2_{v_1^*,v_2^*} J_2^*(v_1^*, v_2^*, v_0^*)\} &= \frac{\partial^2 J_2^*(v_1^*, v_2^*, v_0^*)}{\partial (v_1^*)^2} \frac{\partial^2 J_2^*(v_1^*, v_2^*, v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_2^*(v_1^*, v_2^*, v_0^*)}{\partial u \partial v_1^*} \right)^2 \\ &= \mathcal{O}\Big(2K_1((-\gamma\nabla^2 + 2v_0^*)^2 + 4(-\gamma\nabla^2 + 2v_0^*))\Big). \end{aligned} \tag{234}$$

Define now

$$H(v_0^*) \equiv 2((-\gamma\nabla^2 + 2v_0^*)^2 + 4(-\gamma\nabla^2 + 2v_0^*)),$$

Observe that we may obtain $c_0 > 0$ such that if $v_0^* \in (C^* \times B^*)$, then

$$\det\{\delta^2_{v_1^*,v_2^*} J_2^*(v_1^*, v_2^*, v_0^*)\} > \mathbf{0},$$

where

$$C^* = \{v_0^* \in Y^* \ : \ H(v_0^*) \geq c_0 I_d\}.$$

Furthermore, we assume $K > 0$ and $c_0 > 0$ are such that $C^* \cap B^*$ is convex.

With such statements, definitions and results in mind, we may prove the following theorem.

Theorem 36.1. *Let $(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*) \in D^* \times D^* \times (B^* \cap C^*)$ be such that*

$$\delta J_2^*(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*) = \mathbf{0}.$$

Under such hypotheses,

$$\delta J(u_0) = \mathbf{0},$$

and

$$\begin{aligned} & J(u_0) \\ = & \sup_{v_0^* \in B^*} \left\{ \inf_{(v_1^*, v_2^*) \in D^* \times D^*} J_2^*(v_1^*, v_2^*, v_0^*) \right\} \\ = & J_2^*(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*). \end{aligned} \tag{235}$$

Proof. The proof that

$$J(u_0) = \mathbf{0},$$

$$-\gamma\nabla^2 u_0 + 2\hat{v}_0^* u_0 - f = \mathbf{0},$$

and

$$J(u_0) = J_2^*(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*),$$

may be done similarly as in the previous sections and will not be repeated.

Furthermore, since

$$\delta J_2^*(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*) = \mathbf{0},$$

$v_0^* \in B^* \cap C^*$ and J_2^* is concave in v_0^* on $D \times D^* \times B^*$, we have

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$$J_2^*(\hat{v}_1^*, \hat{v}_2^*\hat{v}_0^*) = \inf_{(v_1^*, v_2^*) \in D^* \times D^*} J_2^*(v_1^*, v_2^*, \hat{v}_0^*),$$

and

$$J_2^*(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*) = \sup_{v_0^* \in B^*} J_2^*(\hat{v}_1^*, \hat{v}_2^*, v_0^*).$$

From such results and the Saddle Point Theorem we may infer that

$$\begin{aligned} J(u_0) &= J_2^*(\hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*) \\ &= \sup_{v_0^* \in B^*} \left\{ \inf_{(v_1^*, v_2^*) \in D^* \times D^*} J_2^*(v_1^*, v_2^*, v_0^*) \right\} \\ &= J_2^* \hat{v}_1^*, \hat{v}_2^*, \hat{v}_0^*). \end{aligned} \tag{236}$$

The proof is complete.

□

37. A Note on the Special Relativistic Physics

Consider in $\mathbb{R}^3$ two observers O and O' and related referential Cartesian frames $O(x, y, z)$ and $O'(x', y', z')$ respectively.

Suppose a particle moves from a point (x_0, y_0, z_0) to a point $(x_0 + \Delta x, y_0 + \Delta y, z_0 + \Delta z)$ related to $O(x, y, z)$ on a time interval Δt.

Denote

$$I_1 = \Delta x^2 + \Delta y^2 + \Delta z^2,$$

and $I_2 = \Delta t$.

In a Newtonian physics context, we have

$$I_1 = \Delta x^2 + \Delta y^2 + \Delta z^2 = \Delta x'^2 + \Delta y'^2 + \Delta z'^2,$$

and

$$I_2 = \Delta t = \Delta t',$$

that is, I_1 and I_2 remain invariant.

However, through experiments in higher energy physics, it was discovered that in fact is I_3 which remains invariant (this had been previously proposed in the Einstein special relativity theory in 1905), where

$$I_3 = -c^2\Delta t^2 + \Delta x^2 + \Delta y^2 + \Delta z^2,$$

so that

$$-c^2\Delta t^2 + \Delta x^2 + \Delta y^2 + \Delta z^2 = -c^2\Delta t'^2 + \Delta x'^2 + \Delta y'^2 + \Delta z'^2 = I_3,$$

for any pair of observers O and O'. Here c denotes the speed of light, and in the case in which $v, v' \ll c$ we have the Newtonian approximation

$$\Delta t' \approx \Delta t.$$

From the expression of I_3 we obtain

$$\begin{aligned} & -c^2\frac{\Delta t'^2}{\Delta t^2} + \frac{\Delta x'^2}{\Delta t^2} + \frac{\Delta y'^2}{\Delta t^2} + \frac{\Delta z'^2}{\Delta t^2} \\ = \; & -c^2\frac{\Delta t^2}{\Delta t^2} + \frac{\Delta x^2}{\Delta t^2} + \frac{\Delta y^2}{\Delta t^2} + \frac{\Delta z^2}{\Delta t^2}. \end{aligned} \tag{237}$$

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Thus,

$$\begin{aligned} & -c^2\frac{\Delta t'^2}{\Delta t^2}+\left(\frac{\Delta x'^2}{\Delta t'^2}+\frac{\Delta y'^2}{\Delta t'^2}+\frac{\Delta z'^2}{\Delta t'^2}\right)\frac{\Delta t'^2}{\Delta t^2} \\ = \quad & -c^2+\frac{\Delta x^2}{\Delta t^2}+\frac{\Delta y^2}{\Delta t^2}+\frac{\Delta z^2}{\Delta t^2} \end{aligned} \tag{238}$$

so that

$$\left(\frac{\Delta t'}{\Delta t}\right)^2=\frac{c^2-\left(\frac{\Delta x^2}{\Delta t^2}+\frac{\Delta y^2}{\Delta_t^2}+\frac{\Delta z^2}{\Delta t^2}\right)}{c^2-\left(\frac{\Delta x'^2}{\Delta t'^2}+\frac{\Delta y'^2}{\Delta t'^2}+\frac{\Delta z'^2}{\Delta t'^2}\right)}.$$

Letting $\Delta t,\ \Delta t' \to 0$, we obtain

$$\left(\frac{\partial t'}{\partial t}\right)^2=\frac{1-\frac{v^2}{c^2}}{1-\frac{(v')^2}{c^2}}.$$

In particular for constant v and $v'=0$ we have

$$\left(\frac{\Delta t'}{\Delta t}\right)^2=1-\frac{v^2}{c^2},$$

so that

$$\Delta t'=\sqrt{1-\frac{v^2}{c^2}}\Delta t.$$

Consider now that O is at rest and O' has a constant velocity

$$v\,e_1$$

where $\{e_1,e_2,e_3\}$ is the canonical basis for $\mathbb{R}^3$ related to O.

Consider $O(x,y,z)$ and $O'(x,y,z)$ such that the axis x' coincide with the axis x, axis y' is parallel to axis y and axis z' is parallel to z.

Since v is constant, we have

$$v=\frac{\Delta x}{\Delta t},$$

and

$$v'=0.$$

Assuming $x(0)=0$, and the initial time $t=0$, we have $\Delta x=x$, and $\Delta t=t$ so that

$$t'=\sqrt{1-\frac{v^2}{c^2}}\,t,$$

so that

$$t'=\frac{1-\frac{v^2}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}\,t=\frac{\left(t-\frac{vvt}{c^2}\right)}{\sqrt{1-\frac{v^2}{c^2}}},$$

and thus

$$t'=\frac{\left(t-\frac{vx}{c^2}\right)}{\sqrt{1-\frac{v^2}{c^2}}}.$$

On the other hand we have $v'=0$.

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We may easily check that the solution

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}},$$

lead us to $v' = 0$.

Indeed,

$$\frac{\Delta x' \sqrt{1 - \frac{v^2}{c^2}}}{\Delta t'} = \frac{\Delta x'}{\Delta t},$$

so that, considering that v is constant, we obtain

$$\frac{dx'}{dt} = \frac{\frac{d(x-vt)}{dt}}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{\frac{dx}{dt} - v}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{v - v}{\sqrt{1 - \frac{v^2}{c^2}}} = 0,$$

that is,

$$\frac{dx'}{dt} = 0.$$

Thus,

$$\frac{d\left(x' \sqrt{1 - \frac{v^2}{c^2}}\right)}{dt'} = 0,$$

so that

$$x' \sqrt{1 - \frac{v^2}{c^2}} = c_1$$

for some constant $c_1 \in \mathbb{R}$ so that

$$x' = c_2,$$

for some $c_2 \in \mathbb{R}$.

Therefore

$$v' = \frac{dx'}{dt'} = 0.$$

Summarizing, for the Newton mechanics we have

$$t' = t$$

,

$$x' = x - vt,$$

$$y' = y,$$

and

$$z' = z.$$

On the other hand, for the special relativity context, we have the following Lorentz relations

$$t' = \frac{\left(t - \frac{vx}{c^2}\right)}{\sqrt{1 - \frac{v^2}{c^2}}}.$$

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}},$$

$$y' = y,$$

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and

$$z' = z.$$

37.1. The Kinetics Energy for the Special Relativity Context

Consider the motion of a particle system described by the position field

$$\mathbf{r} : \Omega \times [0,T] \to \mathbb{R}^4,$$

where $\Omega \subset \mathbb{R}^3$, $[0,T]$ is a time interval and

$$\mathbf{r}(x,y,z,t) = (ct, X_1(x,y,z,t), X_2(x,y,z,t), X_3(x,y,z,t)).$$

In my understanding, this is the special relativity theory context.
The related density field is denoted by

$$\rho : \Omega \times [0,T] \to \mathbb{R}^+,$$

where

$$\rho(x,y,z,t) = m_0 |\phi(x,y,z,t)|^2,$$

m_0 is total system mass at rest, and $\phi : \Omega \times [0,T] \to \mathbb{C}$ is a wave function such that

$$\int_\Omega |\phi(x,y,z,t)|^2 \, dx = 1, \ \forall t \in [0,T].$$

The Kinetics energy differential is given by

$$dE_c = -dm \, \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial t},$$

where

$$\begin{aligned} \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial t} &= \left(c, \frac{\partial X_1}{\partial t}, \frac{\partial X_2}{\partial t}, \frac{\partial X_3}{\partial t}\right) \cdot \left(c, \frac{\partial X_1}{\partial t}, \frac{\partial X_2}{\partial t}, \frac{\partial X_3}{\partial t}\right) \\ &= -c^2 + \left(\frac{\partial X_1}{\partial t}\right)^2 + \left(\frac{\partial X_2}{\partial t}\right)^2 + \left(\frac{\partial X_3}{\partial t}\right)^2 \\ &= -c^2 + v^2, \end{aligned} \tag{239}$$

where

$$v^2 = \left(\frac{\partial X_1}{\partial t}\right)^2 + \left(\frac{\partial X_2}{\partial t}\right)^2 + \left(\frac{\partial X_3}{\partial t}\right)^2.$$

Moreover,

$$dm = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} |\phi(x,y,z,t)|^2 \, dxdydz,$$

so that

$$\begin{aligned} dE_c &= \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} (c^2 - v^2) |\phi(x,y,z,t)|^2 \, dxdydz \\ &= m_0 c \sqrt{c^2 - v^2} |\phi|^2 \, dxdydz. \end{aligned} \tag{240}$$

Thus,

$$E_c(t) = \int_\Omega dE_c = \int_\Omega m_0 c \sqrt{c^2 - v^2} |\phi|^2 \, dxdydz.$$

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In particular for a constant v (not varying in (x,y,z,t)), we obtain

$$E_c(t) = m_0 c\sqrt{c^2 - v^2}.$$

Hence if $v \ll c$, we have

$$E_c(t) \approx m_0\, c^2.$$

This is the most famous Einstein equation previously published in his article of 1905.

37.2. The Kinetics Energy for the General Relativity Context

In a general relativity theory context, the motion of a particle system will be specified by a field

$$(\mathbf{r} \circ \hat{u}) : \Omega \times [0,T] \to \mathbb{R}^4$$

where

$$(\mathbf{r} \circ \hat{u})(x,t) = (ct, X_1(\hat{u}(x,t)), X_2(\hat{u}(x,t)), X_3(\hat{u}(x,t))),$$

where

$$\hat{u}(x,t) = (u_0(t), u_1(x,t), u_2(x,t), u_3(x,t)),$$

$$u_0(t) = t,$$

$$x = (x_1, x_2, x_3) \in \Omega \subset \mathbb{R}^3,$$

and $t \in [0,T]$, where $[0,T]$ is a time interval.

The corresponding density is represented by

$$(\rho \circ \hat{u}) : \Omega \times [0,T] \to \mathbb{R}^+,$$

where

$$(\rho \circ \hat{u})(x,t) = m_0 |\phi(\hat{u}(x,t))|^2,$$

m_0 is total system mass at rest and $\phi : \Omega \times [0,T] \to \mathbb{C}$ is a complex wave function such that

$$\int_\Omega |\phi(\hat{u}(x,t))|^2 \sqrt{-g}\, |\det\{\hat{u}'(x,t)\}|\, dx = 1, \forall t \in [0,T]$$

where

$$dx = dx_1\, dx_2\, dx_3,$$

$$\mathbf{g}_j = \frac{\partial \mathbf{r}}{\partial u_j}$$

$$g_{jk} = \mathbf{g}_j \cdot \mathbf{g}_k, \forall j,k \in \{0,1,2,3\}.$$

and $g = \det\{g_{jk}\}$.

Now observe that

$$\begin{aligned} \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial t} &= \frac{\partial \mathbf{r}}{\partial u_j}\frac{\partial u_j}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial u_k}\frac{\partial u_k}{\partial t} \\ &= \frac{\partial \mathbf{r}}{\partial u_j} \cdot \frac{\partial \mathbf{r}}{\partial u_k}\frac{\partial u_j}{\partial t}\frac{\partial u_k}{\partial t} \\ &= g_{jk}\frac{\partial u_j}{\partial t}\frac{\partial u_k}{\partial t}. \end{aligned} \tag{241}$$

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Observe that

$$\frac{\partial \mathbf{r}}{\partial t}\cdot\frac{\partial \mathbf{r}}{\partial t} = g_{jk}\frac{\partial u_j}{\partial t}\frac{\partial u_k}{\partial t} = -c^2+v^2.$$

Moreover, the Kinetics energy differential is given by

$$dE_c = -dm\ \frac{\partial \mathbf{r}}{\partial t}\cdot\frac{\partial \mathbf{r}}{\partial t},$$

where

$$dm = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}|\phi(\hat{u}(x,t))|^2\sqrt{-g}|\det\{\hat{u}'(x,t)\}|\ dx,$$

so that the total Kinetics energy is expressed by

$$E_c = \int_0^T\int_\Omega dE_c\ dt,$$

that is,

$$\begin{aligned} E_c &= \int_0^T\int_\Omega \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}(c^2-v^2)|\phi(\hat{u}(x,t)|^2\sqrt{-g}|\det\{\hat{u}'(x,t)\}|\ dxdt \\ &= \int_0^T\int_\Omega m_0c\sqrt{c^2-v^2}|\phi(\hat{u}(x,t))|^2\sqrt{-g}|\det\{\hat{u}'(x,t)\}|\ dxdt \\ &= \int_0^T\int_\Omega m_0c\sqrt{-g_{jk}\frac{\partial u_j}{\partial t}\frac{\partial u_k}{\partial t}}|\phi(\hat{u}(x,t))|^2\sqrt{-g}|\det\{\hat{u}'(x,t)\}|\ dxdt. \end{aligned} \tag{242}$$

Summarizing, for the general relativity theory context

$$E_c = \int_0^T\int_\Omega m_0c\sqrt{-g_{jk}\frac{\partial u_j}{\partial t}\frac{\partial u_k}{\partial t}}|\phi(\hat{u}(x,t))|^2\sqrt{-g}|\det\{\hat{u}'(x,t)\}|\ dxdt.$$

38. About an Energy Term Related to the Manifold Curvature Variation

In this section we consider a particle system motion represented by a field

$$\mathbf{r}:\Omega\to\mathbb{R}^4$$

of C^2 class where here $\Omega=\hat{\Omega}\times[0,T]$, $\hat{\Omega}\subset\mathbb{R}^3$ is an open, bounded and connected set, and $[0,T]$ is a time interval.

More specifically, point-wise we denote

$$\mathbf{r}(\mathbf{u}) = (c\ t, X_1(\mathbf{u}), X_2(\mathbf{u}), X_3(\mathbf{u})),$$

where $u_0=t$, and $\mathbf{u}=(u_0,u_1,u_2,u_3)\in\Omega$.

Now, define

$$\mathbf{g}_j = \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j},$$

and

$$g_{jk} = \mathbf{g}_j\cdot\mathbf{g}_k,\ \forall j,k\in\{0,1,2,3\}.$$

Moreover

$$\{g^{jk}\} = \{g_{jk}\}^{-1},$$

and

$$g = \det\{g_{jk}\}.$$

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We assume

$$\left\{\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j},\ \text{for } j \in \{0,1,2,3\}\right\}$$

is a basis for $\mathbb{R}^4$, $\forall \mathbf{u} \in \Omega$.

At this point we define the Christofel symbols, denoted by Γ^l_{jk}, by

$$\Gamma^l_{jk} = \frac{1}{2} g^{lp}\left\{\frac{\partial g_{kp}}{\partial u_j} + \frac{\partial g_{jp}}{\partial u_k} - \frac{\partial g_{jk}}{\partial u_p}\right\},\ \forall j,k,l \in \{0,1,2,3\}.$$

Theorem 38.1. *Considering these last previous statements and definitions, we have that*

$$\frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k} = \Gamma^l_{jk}\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_l},\ \forall j,k \in \{0,1,2,3\},\ \forall \mathbf{u} \in \Omega.$$

Proof. Fix $\mathbf{u} \in \Omega$ and $j,k,m \in \{0,1,2,3\}$.

Observe that

$$\begin{aligned}
\Gamma^l_{jk} g_{lm} &= \frac{1}{2} g_{ml} g^{lp}\left\{\frac{\partial g_{kp}}{\partial u_j} + \frac{\partial g_{jp}}{\partial u_k} - \frac{\partial g_{jk}}{\partial u_p}\right\} \\
&= \frac{1}{2}\delta^p_m\left\{\frac{\partial g_{kp}}{\partial u_j} + \frac{\partial g_{jp}}{\partial u_k} - \frac{\partial g_{jk}}{\partial u_p}\right\} \\
&= \frac{1}{2}\left\{\frac{\partial g_{km}}{\partial u_j} + \frac{\partial g_{jm}}{\partial u_k} - \frac{\partial g_{jk}}{\partial u_m}\right\} \\
&= \frac{1}{2}\left\{\frac{\partial}{\partial u_j}\left(\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m}\right) + \frac{\partial}{\partial u_k}\left(\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m}\right) - \frac{\partial}{\partial u_m}\left(\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k}\right)\right\} \\
&= \frac{1}{2}\left\{\frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_k \partial u_j}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m} + \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_m \partial u_j}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k}\right. \\
&\quad + \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m} + \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_m \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j} \\
&\quad \left. - \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_m \partial u_j}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k} - \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_m \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j}\right\} \\
&= \frac{1}{2}\left\{\frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m} + \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m}\right\} \\
&= \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m}.
\end{aligned} \tag{243}$$

Summarizing, we have got

$$\Gamma^l_{jk}\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_l}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m} = \Gamma^l_{jk} g_{lm} = \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k}\cdot\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_m}.$$

Since

$$\left\{\frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_j},\ \text{for } j \in \{0,1,2,3\}\right\},$$

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is a basis for $\mathbb{R}^4$, we may infer that

$$\frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k} = \Gamma_{jk}^l \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_l}, \ \forall j,k \in \{0,1,2,3\}, \ \forall \mathbf{u} \in \Omega.$$

The proof is complete.

□

38.1. The Energy Term Related to Curvature Variation

We define such an energy term, denoted by E_q, as

$$E_q(\phi, \mathbf{r}) = \frac{1}{2} \int_\Omega g^{jk} g^{lp} \frac{\partial}{\partial u_j} \left(\phi \, \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k} \right) \cdot \frac{\partial}{\partial u_l} \left(\phi^* \, \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_p} \right) \sqrt{-g} \, du,$$

where $du = du_1 du_2 du_3 du_0$.

Here $\phi : \Omega \to \mathbb{C}$ is a complex wave function representing the scalar density field.

Now observe that

$$\begin{aligned}
& \frac{\partial}{\partial u_j} \left(\phi \, \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k} \right) \cdot \frac{\partial}{\partial u_l} \left(\phi^* \, \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_p} \right) \\
= & \left(\frac{\partial \phi}{\partial u_j} \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k} + \phi \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k} \right) \cdot \left(\frac{\partial \phi^*}{\partial u_l} \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_p} + \phi^* \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_l \partial u_p} \right) \\
= & \frac{\partial \phi}{\partial u_j} \frac{\partial \phi^*}{\partial u_j} g_{kp} + |\phi|^2 \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k} \cdot \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_l \partial u_p} \\
& + \phi \frac{\partial \phi^*}{\partial u_l} \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_j \partial u_k} \cdot \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_p} \\
& + \phi^* \frac{\partial \phi}{\partial u_j} \frac{\partial^2 \mathbf{r}(\mathbf{u})}{\partial u_l \partial u_p} \cdot \frac{\partial \mathbf{r}(\mathbf{u})}{\partial u_k} \\
= & \frac{\partial \phi}{\partial u_j} \frac{\partial \phi^*}{\partial u_j} \, g_{kp} + |\phi|^2 \Gamma_{jk}^m \Gamma_{lp}^o \, g_{mo} \\
& + \phi \frac{\partial \phi^*}{\partial u_l} \Gamma_{jk}^s \, g_{sp} + \phi^* \frac{\partial \phi}{\partial u_j} \Gamma_{lp}^r \, g_{rk}.
\end{aligned} \tag{244}$$

From such results, we may infer that

$$\begin{aligned}
E_q(\phi, \mathbf{r}) = & \frac{1}{2} \int_\Omega g^{jk} \frac{\partial \phi}{\partial u_j} \frac{\partial \phi^*}{\partial u_k} \sqrt{-g} \, du \\
& + \frac{1}{2} \int_\Omega g^{jk} \, g^{lp} \, \Gamma_{jk}^r \, \Gamma_{lp}^s \, g_{rs} \, |\phi|^2 \sqrt{-g} \, du \\
& + \frac{1}{2} \int_\Omega g^{jk} \Gamma_{jk}^l \left(\phi \frac{\partial \phi^*}{\partial u_l} + \phi^* \frac{\partial \phi}{\partial u_l} \right) \sqrt{-g} \, du.
\end{aligned} \tag{245}$$

39. A Note on the Definition of Temperature

The main results in this section may be found in similar form in the book [16], page 261.

Consider a system with $N = \sum_{j=1}^{N_0} N_j$ and suppose each set of N_j particles has a set of C_j possible states.

Therefore, the number of states of such N_j particles is given by

$$\Delta \Gamma_j = \frac{(C_j)^{N_j}}{N_j!},$$

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where we have considered simple permutations as equivalent states.

Define

$$S_j = \ln(\Delta\Gamma_j),$$

and define the system entropy, denoted by S, as

$$S = A\left(\sum_{j=1}^{N_0} S_j\right),$$

where $A > 0$ is a normalizing constant.

Thus,

$$S = A\sum_{j=1}^{N_0} \ln\left(\frac{(C_j)^{N_j}}{N_j!}\right),$$

so that

$$S = A\left(\sum_{j=1}^{N_0} (N_j \ln(C_j) - \ln(N_j!))\right).$$

If N_j is large enough, we have the following approximation

$$\ln(N_j!) \approx N_j \ln(N_j).$$

In particular for $C_j = 1,\ \forall j \in \{1, \cdots, N_0\}$ we obtain

$$S = A\left(\sum_{j=1}^{N_0} S_j\right) \approx -A\left(\sum_{j=1}^{N_0} N_j \ln(N_j)\right),$$

At this point we define the following local density $\hat{N}_j$ where

$$\hat{N}_j(x,t) = \frac{|\phi_j(x,t)|^2}{|\phi(x,t)|^2} N,$$

where

$$|\phi(x,t)|^2 = \sum_{j=1}^{N_0} |\phi_j(x,t)|^2.$$

Here, $\phi_j : \Omega \to \mathbb{C}$ denotes the wave function of the particles corresponding to the system part N_j.

The final definition of Entropy is given by

$$S(x,t) = A\left(\sum_{j=1}^{N_0} S_j(x,t)\right)$$

where

$$\begin{aligned} S_j(x,t) &= -\hat{N}_j(x,t)\ln(\hat{N}_j(x,t)) \\ &= -\frac{|\phi_j(x,t)|^2}{\phi(x,t)|^2} N \ln\left(\frac{|\phi_j(x,t)|^2}{\phi(x,t)|^2} N\right). \end{aligned} \tag{246}$$

Here we highlight the position field for each particle system part N_j is given by

$$\hat{\mathbf{r}}_j(x,t) = \mathbf{x} + \mathbf{r}_j(x,t),$$

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where $\mathbf{r}_j$ is related to the internal energy, that is, related to the atomic/electronic vibrational motion linked with the concept of temperature, as specified in the next lines.

The total kinetics energy is given by

$$E(x,t) = -\frac{1}{2}\sum_{j=1}^{N_0} m_{p_j}|\phi_j(x,t)|^2 \frac{\partial \mathbf{r}_j(x,t)}{\partial t}\cdot\frac{\partial \mathbf{r}_j(x,t)}{\partial t}.$$

At this point, we define the scalar field of temperature, denoted by $T(x,t)$, such as symbolically

$$\frac{\partial S}{\partial E} = \frac{1}{T(x,t)}.$$

More specifically, we define

$$T(x,t) = \sum_{j=1}^{N_0} \frac{\frac{\partial E}{\partial \phi_j}}{\frac{\partial S}{\partial \phi_j}},$$

so that

$$T(x,t) = \frac{-\frac{1}{2}\sum_{j=1}^{N_0} m_{p_j}\,\phi_j(x,t)\,\frac{\partial \mathbf{r}_j(x,t)}{\partial t}\cdot\frac{\partial \mathbf{r}_j(x,t)}{\partial t}}{-A\frac{\phi_j N}{|\phi|^2}\ln\left(\frac{|\phi_j|^2 N}{|\phi|^2}+1\right)}.$$

39.1. A Note on Basic Thermodynamics

Consider a solid $\Omega \subset \mathbb{R}^3$ where such a Ω is an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Denoting by $[0,T]$ a time interval, consider a particle system where the field of displacements is given by

$$\mathbf{r}_j(x,t) = \mathbf{r}(x,t) + \mathbf{u}(x,t) + (\mathbf{r}_3)_j(x,t),$$

where $\mathbf{r} : \Omega\times[0,T] \to \mathbb{R}$ is a macroscopic displacement field, $\mathbf{u} : \Omega\times[0,T] \to \mathbb{R}$ is the elastic displacement field and $(\mathbf{r}_3)_j : \Omega\times[0,T] \to \mathbb{R}$ denotes the displacement field related to the atomic and electronic vibration motion concerning the concept of temperature, as specified in the previous section.

In particular for the case in which

$$\mathbf{r}(x,t) = x,$$

we define the heat functional, denoted by W, as

$$\begin{aligned} W \;=\; & \frac{1}{2}\int_0^T\int_\Omega \rho(x,t)\frac{\partial \mathbf{u}(x,t)}{\partial t}\cdot\frac{\partial \mathbf{u}(x,t)}{\partial t}\,dx\,dt \\ & -\int_0^T\int_\Omega \mathbf{F}\cdot\,\mathbf{u}\,dx\,dt \\ & +\frac{1}{2}\int_0^T\int_\Omega H_{ijkl}e_{ij}(\mathbf{u})e_{kl}(\mathbf{u})\,dx\,dt \\ & +\frac{1}{2}\sum_{j=1}^{N_0}\int_0^T\int_\Omega m_{p_j}|\phi_j(x,t)|^2\frac{\partial (\mathbf{r}_3)_j(x,t)}{\partial t}\cdot\frac{\partial (\mathbf{r}_3)_j(x,t)}{\partial t}\,dx\,dt, \end{aligned} \tag{247}$$

where

$$\rho(x,t) = \sum_{j=1}^{N_0} m_{p_j}|\phi_j(x,t)|^2$$

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is the point wise total density,

$$\frac{1}{2}\int_0^T\int_\Omega H_{ijkl}e_{ij}(\mathbf{u})e_{kl}(\mathbf{u})\,dx\,dt$$

is a standard elastic inner energy for small displacements $\mathbf{u}$, $\mathbf{F}(x,t)$ is the resulting field of external forces acting point wise on Ω, and for the term

$$\frac{1}{2}\sum_{j=1}^{N_0}\int_0^T\int_\Omega m_{p_j}|\phi_j(x,t)|^2\frac{\partial(\mathbf{r}_3)_j(x,t)}{\partial t}\cdot\frac{\partial(\mathbf{r}_3)_j(x,t)}{\partial t}\,dx\,dt$$

we are refereing to the definitions and notations of the previous section.

At this point we denote

$$E_{in}=\frac{1}{2}\sum_{j=1}^{N_0}\int_0^T\int_\Omega m_{p_j}|\phi_j(x,t)|^2\frac{\partial(\mathbf{r}_3)_j(x,t)}{\partial t}\cdot\frac{\partial(\mathbf{r}_3)_j(x,t)}{\partial t}\,dx\,dt,$$

and

$$\begin{aligned}E_T &= \frac{1}{2}\int_0^T\int_\Omega \rho(x,t)\frac{\partial\mathbf{u}(x,t)}{\partial t}\cdot\frac{\partial\mathbf{u}(x,t)}{\partial t}\,dx\,dt\\ &-\int_0^T\int_\Omega \mathbf{F}\cdot\,\mathbf{u}\,dx\,dt\\ &+\frac{1}{2}\int_0^T\int_\Omega H_{ijkl}e_{ij}(\mathbf{u})e_{kl}(\mathbf{u})\,dx\,dt.\end{aligned}\tag{248}$$

Hence $W=E_T+E_{in}$ and from the previous section we may generically denote

$$\delta\,E_{in}=T\,\delta S,$$

Therefore

$$\delta W=\delta E_T+\delta E_{in}=\delta E_T+T\,\delta S.$$

For a standard reversible process we must have $\delta\,E_T=\mathbf{0}$.
so that

$$\delta\,W=T\,\delta S.$$

For a general case in which other types of internal energy (such as E_q indicated in the previous sections and even E_{in}) are partially and irreversibly converted into a E_T type of energy, in which

$$\delta\,E_T\neq\mathbf{0},$$

we may have

$$\delta\,W<T\,\delta S.$$

Remark 39.1. *Indeed, in general the vibrational motion related to E_{in} is of relativistic nature so that in fact we would need to consider*

$$E_{in}=\frac{1}{2}\sum_{j=1}^{N_0}\int_0^T\int_\Omega m_{p_j}\,c\,|\phi_j(x,t)|^2\sqrt{c^2-\frac{\partial(\mathbf{r}_3)_j(x,t)}{\partial t}\cdot\frac{\partial(\mathbf{r}_3)_j(x,t)}{\partial t}}\sqrt{-g_j}\,dx\,dt.$$

40. A Formal Proof of Castigliano Theorem

In this section we present the mathematical formalism of a result in elasticity theory known as the Castigliano's Theorem.

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Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipischitzian) boundary denoted by $\partial\Omega$.

In a context of linear elasticity, consider the functional $J : V \to \mathbb{R}$ where

$$J(u) = E_{in} - \langle u_i, f_i \rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j) P_{ij},$$

$u = (u_1, u_2, u_3) \in W_0^{1,2}(\Omega; \mathbb{R}^3) \equiv V$, $f = (f_1, f_2, f_3) \in L^2(\Omega; \mathbb{R}^3)$, $Y = Y^* = L^2(\Omega; \mathbb{R}^3)$, and

$$P_{ij} \in \mathbb{R},\ \forall i \in \{1,2,3\},\ j \in \{1, \cdots, N\}$$

for some $N \in \mathbb{N}$.

Here we have denoted

$$E_{in} = \frac{1}{2} \int_\Omega H_{ijkl} e_{ij}(u) e_{kl}(u)\ dx,$$

$$e_{ij}(u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$

Moreover H_{ijkl} is a fourth order positive definite and constant tensor.

Observe that the variation of J in u_i give us the following Euler-Lagrange equation

$$-(H_{ijkl} e_{kl}(u))_{,j} - f_i - \sum_{j=1}^{N} P_{ij} \delta(x_j) = \mathbf{0},\ \text{in } \Omega. \tag{249}$$

Symbolically such a system stands for

$$\frac{\partial J(u)}{\partial u_i} = \mathbf{0}, \forall i \in \{1,2,3\},$$

so that

$$\frac{\partial (E_{in} - \langle u_i, f_i \rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j) P_{ij})}{\partial u_i} = \mathbf{0},\ \forall i \in \{1,2,3\}. \tag{250}$$

We denote $u \in V$ solution of (249) by $u = u(f, P)$, so that multiplying the concerning extremal equation by u_i and integrating by parts, we get

$$\begin{aligned} H_1(u(f,P), f, P) &= 2E_{in}(u(f,P)) - \langle u_i(f,P), f_i \rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j, f, P) P_{ij} \\ &= 0,\ \forall f \in Y^*,\ P \in \mathbb{R}^{3N}. \end{aligned} \tag{251}$$

Therefore

$$\frac{d}{dP_{ij}} (H_1(u(f,P), f, P)) = 0,$$

so that

$$2\frac{dE_{in}}{dP_{ij}} - \frac{d}{dP_{ij}} \left(\langle u_i(f,P), f_i \rangle_{L^2} + \sum_{j=1}^{N} u_i(x_j, f, p) P_{ij} \rangle_{L^2} \right) = 0,$$

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that is

$$\begin{aligned} & \frac{dE_{in}}{dP_{ij}} + \left\langle \frac{\partial(E_{in} - \langle u_i, f_i\rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j)P_{ij})}{\partial u_k}, \frac{\partial u_k}{\partial P_{ij}} \right\rangle_{L^2} \\ & - \frac{\partial}{\partial P_{ij}} \left(\langle u_i, f_i\rangle_{L^2} + \sum_{j=1}^{N} u_i(x_j)P_{ij} \right) \\ = \; & 0. \end{aligned} \tag{252}$$

From this and (249) we obtain

$$\frac{dE_{in}}{dP_{ij}} - u_i(x_j) = 0,$$

so that

$$u_i(x_j) = \frac{dE_{in}}{dP_{ij}} = \frac{d}{dP_{ij}} \left(\frac{1}{2} \int_\Omega H_{ijkl} e_{ij}(u(f,P)) e_{kl}(u(f,P)) \, dx \right),$$

$\forall i \in \{1,2,3\}, \forall j \in \{1, \cdots, N\}$.

With such results in mind, we have proven the following theorem.

Theorem 40.1 (Castigliano)**.** *Considering the notations and definitions in this section, we have*

$$u_i(x_j) = \frac{dE_{in}}{dP_{ij}} = \frac{d}{dP_{ij}} \left(\frac{1}{2} \int_\Omega H_{ijkl} e_{ij}(u(f,P)) e_{kl}(u(f,P)) \, dx \right),$$

$\forall i \in \{1,2,3\}, \forall j \in \{1, \cdots, N\}$.

40.1. A Generalization of Castigliano Theorem

In this subsection we present a more general version of the Castigliano theorem. Considering the context of last section, we recall that

$$\begin{aligned} H_1(u(f,P),f,P) &= 2E_{in}(u(f,P)) - \langle u_i(f,P), f_i\rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j,f,P)P_{ij} \\ &= 0, \; \forall f \in Y^*, \; P \in \mathbb{R}^{3N}. \end{aligned} \tag{253}$$

Therefore, for $x_k \in \Omega$ such that

$$x_k \neq x_j, \; \forall j \in \{1, \cdots, N\},$$

we have

$$\left\langle \frac{d}{df_i}(H_1(u(f,P),f,P)), \delta(x_k) \right\rangle_{L^2} = 0,$$

so that

$$\begin{aligned} & 2\left\langle \frac{d}{df_i}(E_{in}(u(f,P))), \delta(x_k) \right\rangle_{L^2} \\ & - \left\langle \frac{d}{df_i} \left(\langle u_i(f,P), f_i\rangle_{L^2} + \sum_{j=1}^{N} u_i(x_j,f,p)P_{ij}\rangle_{L^2} \right), \delta(x_k) \right\rangle_{L^2} \\ = \; & 0, \end{aligned} \tag{254}$$

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that is

$$\begin{aligned}
&\left\langle \frac{d}{df_i}(E_{in}(u(f,P))), \delta(x_k) \right\rangle_{L^2} \\
&+\left\langle \frac{d}{du_k}\left(E_{in}(u(f,P)) - \langle u_i(f,P), f_i\rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j,f,p)P_{ij} \right)\frac{du_k}{df_i}, \delta(x_k) \right\rangle_{L^2} \\
&-\left\langle \frac{\partial}{\partial f_i}\left(\langle u_i(f,P), f_i\rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j,f,p)P_{ij} \right), \delta x(x_k) \right\rangle_{L^2} \\
=\ & 0. \qquad (255)
\end{aligned}$$

From such results, we may obtain

$$\left\langle \frac{d}{df_i}(E_{in}(u(f,P))), \delta(x_k) \right\rangle_{L^2} - \langle u_i(x), \delta(x_k)\rangle_{L^2} = 0,$$

so that

$$\left\langle \frac{d}{df_i}(E_{in}(u(f,P))), \delta(x_k) \right\rangle_{L^2} - u_i(x_k) = 0,$$

that is

$$u_i(x_k) = \left\langle \frac{d}{df_i}(E_{in}(u(f,P))), \delta(x_k) \right\rangle_{L^2},$$

$\forall i \in \{1,2,3\},\ \forall x_k \in \Omega$ such that $x_k \neq x_j,\ \forall j \in \{1,\cdots,N\}$.

With such results in mind, we have proven the following theorem.

Theorem 40.2 (The Generalized Castigliano Theorem)**.** *Considering the notations and definitions in this section, we have*

$$u_i(x_k) = \left\langle \frac{d}{df_i}(E_{in}(u(f,P))), \delta(x_k) \right\rangle_{L^2},$$

$\forall i \in \{1,2,3\},\ \forall x_k \in \Omega$ *such that* $x_k \neq x_j,\ \forall j \in \{1,\cdots,N\}$.

40.2. The Virtual Work Principle

Considering the definitions, results and statements of the previous section and subsection, we may easily prove the following theorem.

Theorem 40.3 (The virtual work principle)**.** *Let* $x_l \in \Omega$ *such that* $x_l \neq x_j, \forall j \in \{1,\cdots,N\}$.

For a virtual constant load $P_{lk} \in \mathbb{R}$ *on* x_l *at the direction of* $u_k(x_l)$*, define now* $J : V \to \mathbb{R}$ *where*

$$J(u) = E_{in} - \langle u_i, f_i\rangle_{L^2} - \sum_{j=1}^{N} u_i(x_j)P_{ij} - P_{lk}u_k(x_l).$$

Under such hypotheses,

$$u_k(x_l) = \left(\frac{d\ E_{in}(u(f,P,P_{lk}))}{dP_{lk}} \right)_{P_{lk}=0},$$

$\forall k \in \{1,2,3\},\ \forall x_l \in \Omega$ *such that* $x_l \neq x_j,\ \forall j \in \{1,\cdots,N\}$.

Proof. The proof is exactly the same as in the Castigliano Theorem in the previous section except by setting the virtual load $P_{lk} = 0$ in the end of this calculation and will not be repeated. □

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41. Duality for a General Relaxed Primal Variational Formulation

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$. Consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2}\int_\Omega (u^2-\beta)^2 \, dx - \langle u, f\rangle_{L^2},$$

where $V = W_0^{1,2}(\Omega)$, $\gamma > 0$, $\alpha > 0$, $\beta > 0$, $Y = Y^* = L^2(\Omega)$, $Y_1 = Y_1^* = L^2(\Omega;\mathbb{R}^3)$, and $f \in L^2(\Omega)$.

We define the associated relaxed functional $J_1 : V \times V \times (0,1)$, by

$$\begin{aligned} J_1(u,\phi,\lambda) &= \frac{\lambda\gamma}{2}\int_\Omega (\nabla u - (1-\lambda)\nabla\phi)\cdot(\nabla u - (1-\lambda)\nabla\phi)\, dx \\ &+\frac{(1-\lambda)\gamma}{2}\int_\Omega (\nabla u + \lambda\nabla\phi)\cdot(\nabla u + \lambda\nabla\phi)\, dx \\ &+\frac{\lambda\alpha}{2}\int_\Omega ((u-(1-\lambda)\phi)^2-\beta)^2\, dx + \frac{(1-\lambda)\alpha}{2}\int_\Omega ((u+\lambda\phi)^2-\beta)^2\, dx \\ &-\lambda\langle u-(1-\lambda)\phi, f\rangle_{L^2} - (1-\lambda)\langle u+\lambda\phi, f\rangle_{L^2}. \end{aligned} \tag{256}$$

Moreover, we define, $F_1 : V \times V \times (0,1) \to \mathbb{R}$, $F_2 : V \times V \times (0,1) \to \mathbb{R}$, $F_3 : V \times V \times (0,1) \to \mathbb{R}$, $F_4 : V \times V \times (0,1) \to \mathbb{R}$, $F_5 : V \times V \times (0,1) \to \mathbb{R}$, and $F_6 : V \times V \times (0,1) \to \mathbb{R}$, by

$$F_1(u,\phi,\lambda) = \frac{\lambda\gamma}{2}\int_\Omega (\nabla u - (1-\lambda)\nabla\phi)\cdot(\nabla u - (1-\lambda)\nabla\phi)\, dx,$$

$$F_2(u,\phi,\lambda) = \frac{(1-\lambda)\gamma}{2}\int_\Omega (\nabla u + \lambda\nabla\phi)\cdot(\nabla u + \lambda\nabla\phi)\, dx,$$

$$F_3(u,\phi,\lambda) = \frac{\lambda\alpha}{2}\int_\Omega ((u-(1-\lambda)\phi)^2-\beta)^2\, dx,$$

$$F_4(u,\phi,\lambda) = \frac{(1-\lambda)\alpha}{2}\int_\Omega ((u+\lambda\phi)^2-\beta)^2\, dx,$$

$$F_5(u,\phi,\lambda) = -\lambda\langle u-(1-\lambda)\phi, f\rangle_{L^2},$$

$$F_6(u,\phi,\lambda) = -(1-\lambda)\langle u+\lambda\phi, f\rangle_{L^2},$$

respectively.

Observe that

$$\begin{aligned} J_1(u,\phi,u) &= F_1(u,\phi,\lambda) + F_2(u,\phi,\lambda) \\ &\quad F_3(u,\phi,\lambda) + F_4(u,\phi,\lambda) \\ &\quad F_5(u,\phi,\lambda) + F_6(u,\phi,\lambda), \end{aligned} \tag{257}$$

Thus,

$$\begin{aligned} J_1(u,\phi,u) &\geq F_1(u,\phi,\lambda) + F_2(u,\phi,\lambda) \\ &\quad +\langle (u-(1-\lambda)\phi)^2-\beta, v_3^*\rangle_{L^2} \\ &\quad +\langle (u+\lambda\phi)^2-\beta, v_4^*\rangle_{L^2} \\ &\quad F_5(u,\phi,\lambda) + F_6(u,\phi,\lambda) \\ &\quad F_3(u,\phi,\lambda) + F_4(u,\phi,\lambda) \\ &\quad + \inf_{v_3\in Y}\{-\langle v_3, v_3^*\rangle_{L^2} + \tilde{F}_3(v_3,\lambda)\} \\ &\quad + \inf_{v_4\in Y}\{-\langle v_4, v_4^*\rangle_{L^2} + \tilde{F}_4(v_4,\lambda)\} \end{aligned} \tag{258}$$

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where

$$\tilde{F}_3(v_3,\lambda)=\frac{\lambda\alpha}{2}\int_\Omega v_3^2\,dx,$$

$$\tilde{F}_4(v_4,\lambda)=\frac{(1-\lambda)\alpha}{2}\int_\Omega v_4^2\,dx,$$

Therefore, defining $\tilde{F}_3^*:Y^*\times(0,1)\to\mathbb{R}$ and $\tilde{F}_4^*:Y^*\times(0,1)\to\mathbb{R}$ by

$$\begin{aligned}\tilde{F}_3^*(v_3^*,\lambda) &= \sup_{v_3\in Y}\{\langle v_3.v_3^*\rangle_{L^2}-F_3(v_3,\lambda)\\ &= \frac{1}{2\alpha\lambda}\int_\Omega (v_3^*)^2\,dx,\end{aligned}\tag{259}$$

and

$$\begin{aligned}\tilde{F}_4^*(v_4^*,\lambda) &= \sup_{v_4\in Y}\{\langle v_4.v_4^*\rangle_{L^2}-F_4(v_4,\lambda)\\ &= \frac{1}{2\alpha(1-\lambda)}\int_\Omega (v_4^*)^2\,dx,\end{aligned}\tag{260}$$

we may also infer that

$$\begin{aligned}J_1(u,\phi,\lambda) \geq\ & \inf_{v_1\in Y_1}\{\langle v_1,v_1^*\rangle_{L^2}+\tilde{F}_1(v_1,\lambda)\}\\ &+\inf_{v_2\in Y_1}\{\langle v_2,v_2^*\rangle_{L^2}+\tilde{F}_2(v_2,\lambda)\}\\ &+\inf_{v_5\in Y}\left\{-\langle v_5,\ \mathrm{div}\ v_1^*\rangle_{L^2}+\int_\Omega (v_5^2-\beta)v_3^*\,dx-\lambda\langle v_5,f\rangle_{L^2}\right\}\\ &+\inf_{v_6\in Y}\left\{-\langle v_6,\ \mathrm{div}\ v_2^*\rangle_{L^2}+\int_\Omega (v_6^2-\beta)v_4^*\,dx-(1-\lambda)\langle v_6,f\rangle_{L^2}\right\}\\ &-\tilde{F}_3^*(v_3^*,\lambda)-\tilde{F}_4^*(v_4^*,\lambda)\\ =\ & -\tilde{F}_1^*(v_1^*,\lambda)-\tilde{F}_2^*(v_2^*,\lambda)\\ &-F_5^*(v_1^*,v_3^*,\lambda)-F_6^*(v_2^*,v_4^*,\lambda)\\ &-\tilde{F}_3^*(v_3^*,\lambda)-\tilde{F}_4^*(v_4^*,\lambda),\end{aligned}\tag{261}$$

if $v^*=(v_1^*,\cdots,v_4^*)\in A^*$ where,

$$A^*=\{v^*\in[Y_1^*]^2\times[Y^*]^2\ :\ v_3^*>0 \text{ and } v_4^*>0,\ \text{in}\ \Omega\},$$

$$\tilde{F}_1(v_1,\lambda)=\frac{\lambda\gamma}{2}\int_\Omega v_1\cdot v_1\,dx,$$

$$\tilde{F}_2(v_2,\lambda)=\frac{\lambda\gamma}{2}\int_\Omega v_2\cdot v_2\,dx,$$

$$\tilde{F}_5(v_5,v_3^*,\lambda)=\int_\Omega (v_5^2-\beta)v_3^*\,dx-\lambda\langle v_5,f\rangle_{L^2},$$

$$\tilde{F}_6(v_6,v_4^*,\lambda)=\int_\Omega (v_6^2-\beta)v_4^*\,dx-(1-\lambda)\langle v_6,f\rangle_{L^2},$$

and

$$\begin{aligned}\tilde{F}_1^*(v_1^*,\lambda) &= \sup_{v_1\in Y_1}\{\langle v_1,v_1^*\rangle_{L^2}-\tilde{F}_1(v_1,\lambda)\}\\ &= \frac{1}{2\gamma\lambda}\int_\Omega v_1^*\cdot v_1^*\,dx,\end{aligned}\tag{262}$$

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$$\begin{aligned}\tilde{F}_2^*(v_2^*,\lambda) &= \sup_{v_2\in Y_1}\{\langle v_2,v_2^*\rangle_{L^2}-\tilde{F}_2(v_2,\lambda)\}\\ &= \frac{1}{2\gamma(1-\lambda)}\int_\Omega v_2^*\cdot v_2^*\,dx,\end{aligned}\tag{263}$$

$$\begin{aligned}\tilde{F}_5^*(v_1^*,v_3^*,\lambda) &= \sup_{v_5\in Y}\{\langle v_5,v_1^*\rangle_{L^2}-\tilde{F}_5(v_5,v_3^*,\lambda)\}\\ &= \frac{1}{2}\int_\Omega\frac{(\operatorname{div} v_1^*+\lambda f)^2}{4v_3^*}\,dx+\beta\int_\Omega v_3^*\,dx,\end{aligned}\tag{264}$$

and

$$\begin{aligned}\tilde{F}_6^*(v_2^*,v_4^*,\lambda) &= \sup_{v_6\in Y}\{\langle v_6,v_1^*\rangle_{L^2}-\tilde{F}_6(v_6,v_4^*,\lambda)\}\\ &= \frac{1}{2}\int_\Omega\frac{(\operatorname{div} v_2^*+(1-\lambda)f)^2}{4v_4^*}\,dx+\beta\int_\Omega v_4^*\,dx.\end{aligned}\tag{265}$$

Denoting, as above indicated, $v^*=(v_1^*,v_2^*,v_3^*,v_4^*)\in[Y_1^*]^2\times[Y^*]^2$, we define $J^*:[Y_1^*]^2\times[Y^*]^2\times(0,1)\to\mathbb{R}$ by

$$\begin{aligned}J^*(v^*,\lambda) &= -\tilde{F}_1^*(v_1^*,\lambda)-\tilde{F}_2^*(v_2^*,\lambda)\\ &\quad -F_5^*(v_1^*,v_3^*,\lambda)-F_6^*(v_2^*,v_4^*,\lambda)\\ &\quad -\tilde{F}_3^*(v_3^*,\lambda)-\tilde{F}_4^*(v_4^*,\lambda),\end{aligned}\tag{266}$$

Observe that we have got

$$\begin{aligned}\inf_{u\in V}J(u) &\geq \inf_{(u,\phi,\lambda)\in V\times V\times[0,1]}J_1(u,\phi,\lambda)\\ &\geq \inf_{\lambda\in(0,1)}\left\{\sup_{v^*\in A^*}J^*(v^*,\lambda)\right\}.\end{aligned}\tag{267}$$

41.1. A Numerical Example

We have obtained numerical results for $\gamma=0.1$, $\alpha=3.0$, $\beta=5.0$ and $f\equiv 10,$ in Ω, for the special case in which $\Omega=[0,1]\subset\mathbb{R}$.

Such results have been performed through the following algorithm:

1. Set $n=1$ and $\lambda_n=1/2$.
2. Calculate $v_n^*\in A^*$ such that
$$J^*(v_n^*,\lambda_n)=\sup_{v^*\in A^*}J^*(v^*,\lambda_n),$$
3. Calculate $\lambda_{n+1}\in(0,1)$ such that
$$J^*(v_n^*,\lambda_{n+1})=\inf_{\lambda\in(0,1)}J^*(v_n^*,\lambda),$$
4. Set $n:=n+1$ and go to step 2 until the satisfaction of an appropriate convergence criterion.

Here, we recall that for the optimal points

$$\frac{\operatorname{div} v_1^*+\lambda f}{2v_3^*}=u-(1-\lambda)\phi,$$

and

$$\frac{\operatorname{div} v_2^*+(1-\lambda)\,f}{2v_4^*}=u+\lambda\phi,$$

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so that

$$u = \lambda\left(\frac{\text{div } v_1^* + \lambda f}{2v_3^*}\right) + (1-\lambda)\left(\frac{\text{div } v_2^* + (1-\lambda)f}{2v_4^*}\right).$$

For such a corresponding optimal u_0 please see Figure 32.

For the solution u_1 of the primal problem obtained through the generalized method of lines, please see Figure 33.

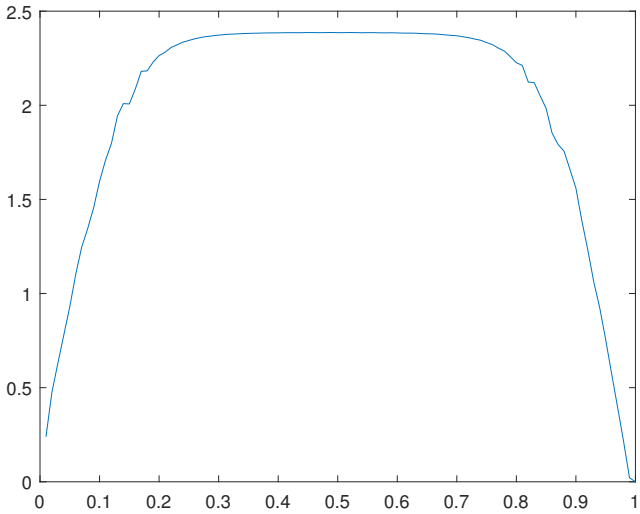

Figure 32. Optimal solution $u_0(x)$ through the concerning dual formulation.

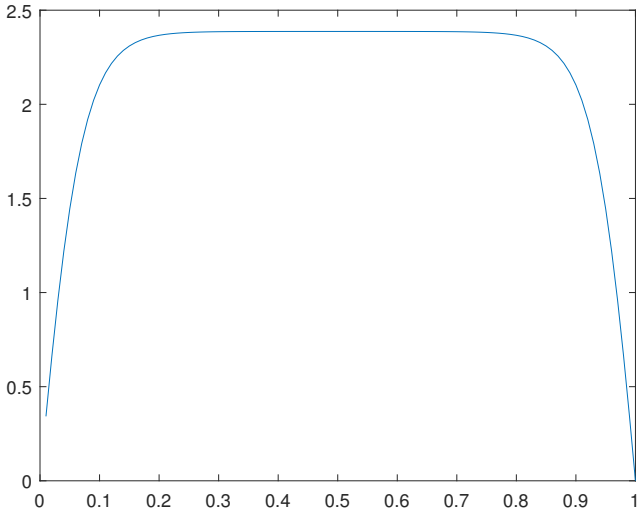

Figure 33. Optimal solution $u_1(x)$ through the concerning primal formulation.

We may observe the solutions u_0 and u_1 are qualitatively similar, as expected.

Here we present the software developed to perform such numerical results.

****

1. clear all

   global m8 d L A3 A B yo u v e1 dv1 dv2 dv3 v5 v6 v3 v4 v1 v2 K5 e5 L1 L2 L3

   m8=100;

   d=1/m8;

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e1=0.00001;

e5=0.001;

K5=10000.0;

A3=0.1;

A=3.0;

B=5.0;

for i=1:m8

uo(i,1)=5;

yo(i,1)=10.0;

end;

L=1/2;

for k=1:50

k

i=1;

m12=$2+6*A*uo(i,1)^2*d^2/A3-2*A*B/A3*d^2$;

m50(i)=1/m12;

z(i)=$m50(i)*(yo(i,1)*d^2/A3+4*A*uo(i,1)^3*d^2/A3)$;

for i=2:m8-1

m12=$2+6*A*uo(i,1)^2*d^2/A3-2*A*B/A3*d^2-m50(i-1)$;

m50(i)=1/m12;

z(i)=$m50(i)*(yo(i,1)*d^2/A3+4*A*uo(i,1)^3*d^2/A3+z(i-1))$;

end;

w(m8,1)=0;

for i=1:m8-1

w(m8-i,1)=m50(m8-i)*w(m8-i+1)+z(m8-i);

end;

uo=w;

uo(m8/2,1)

end;

for i=1:4*m8

xo(i,1)=3.0;

end;

for i=1:1

x1(i,1)=1/2;

end;

for k1=1:10

k1

k=1;

b12=1.0;

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while $(b12 > 10^{-4})$ && $(k < 50)$

k

k=k+1;

X=fminunc('funFeb30LG',xo);

b12=max(abs(xo-X))

xo=X;

end;

X1=fminunc('funFeb31LG',x1);

x1=X1;

end;

u(m8,1)=0;

for i=1:m8

x(i,1)=i*d;

end;

plot(x,u);

****

With the auxiliary function "funFeb30LG", where

****

1. function S=funFeb30LG(x)

global m8 d L A3 A B yo u v e1 dv2 dv1 dv3 v3 v4 v5 v6 v1 v2 K5 e5 L1 L2 L3

for i=1:m8

v1(i,1)=x(i,1);

v2(i,1)=x(m8+i,1);

v3(i,1)=x(2*m8+i,1);

v4(i,1)=x(3*m8+i,1);

end; for i=1:m8-1

dv1(i,1)=(v1(i+1,1)-v1(i,1))/d;

dv2(i,1)=(v2(i+1,1)-v2(i,1))/d;

end;

S=0;

for i=1:m8-1

S=S+$(yo(i,1)^2 * L^2 + 2 * yo(i,1) * L * dv1(i,1) + dv1(i,1)^2 + 4 * B * v3(i,1)^4)/(4 * v3(i,1)^2)$;

S=S+$(yo(i,1)^2 * (1-L)^2 + 2 * yo(i,1) * (1-L) * dv2(i,1) + dv2(i,1)^2 + 4 * B * v4(i,1)^4)/(4 * v4(i,1)^2)$;

S=S+$v1(i,1)^2/sqrt(L^2+e1)/2/A3 + v2(i,1)^2/sqrt((1-L)^2+e1)/2/A3$;

S=S+$v3(i,1)^4/2/sqrt(L^2+e1)/A + v4(i,1)^4/2/sqrt((1-L)^2+e1)/A$;

end;

for i=1:m8-1

u(i,1)=$L * (yo(i,1) * L + dv1(i,1))/(v3(i,1)^2)/2$;

u(i,1)=u(i,1)+$(1-L) * ((1-L) * yo(i,1) + dv2(i,1))/2/(v4(i,1)^2)$;

end;

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****

Finally, we present the auxiliary function "funFeb31LG"

****

```
function S1=funFeb31LG(x)
global m8 d L L1 L2 L3 A3 A B yo u v e1 dv2 dv1 dv3 v5 v6 v3 v4 v1 v2 K5 e5
L=(sin(x(1,1))+1)/2;
for i=1:m8-1
dv1(i,1)=(v1(i+1,1)-v1(i,1))/d;
dv2(i,1)=(v2(i+1,1)-v2(i,1))/d;
end;
S=0;
for i=1:m8-1
S=S+(yo(i,1)^2*L^2+2*yo(i,1)*L*dv1(i,1)+dv1(i,1)^2+4*B*v3(i,1)^4)/(4*v3(i,1)^2);
S=S+(yo(i,1)^2*(1-L)^2+2*yo(i,1)*(1-L)*dv2(i,1)+dv2(i,1)^2+4*B*v4(i,1)^4)/(4*
v4(i,1)^2);
S=S+v1(i,1)^2/sqrt(L^2+e1)/2/A3+v2(i,1)^2/sqrt((1-L)^2+e1)/2/A3;
S=S+v3(i,1)^4/2/sqrt(L^2+e1)/A+v4(i,1)^4/2/sqrt((1-L)^2+e1)/A;
end;
S1=-S;
```

****

Remark 41.1. *Observe that the functional J^* is convex in A^* however, the restrictions $v_3^* > 0$ and $v_4^* > 0$ in Ω may cause a difference between the solution obtained through J^* and the solution got through the primal formulation J, a so-called duality gap.*

Anyway, through such a relaxation process, utilizing the dual functional J^* we may still obtain a good qualitative approximation of the global optimal point for the primal formulation J.

Indeed, such a global solution obtained through the dual functional J^* may be an excellent initial solution for obtaining a more accurate one through the standard Newton Method, for example.

42. A Global Existence Result for a Model in Non-Linear Elasticity

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega = S$.

Define a functional $J : V \to \mathbb{R}$ by

$$J(u) = \frac{1}{2}\int_\Omega H_{ijkl}\gamma_{ij}(u)\gamma_{kl}(u)\,dx - \langle u_i, f_i\rangle_{L^2},$$

where

$$\gamma_{ij}(u) = \frac{u_{i,j}+u_{j,i}}{2} + \frac{1}{2}u_{m,i}u_{m,j},$$

$$V = \{u \in W^{1,2}(\Omega;\mathbb{R}^3) \ : \ u = \hat{v}_0 \text{ on } S_1 \subset \partial\Omega\}.$$

We also denote $Y = Y^* = L^2(\Omega;\mathbb{R}^3)$, so that $f = (f_1, f_2, f_3) \in Y$.

Here $\{H_{ijkl}\}$ is a fourth order constant, positive definite and symmetric tensor.

With such assumptions and statements in mind, we may prove the following theorem.

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Theorem 42.1. *Assume* $\{H_{ijkl}\}$ *is such that*

$$\lim_{\|u\|_V \to \infty} J(u) = +\infty.$$

Under such hypothesis, there exists $u_0 \in V$ *such that*

$$J(u_0) = \min_{u \in V} J(u).$$

Proof. From the hypotheses, there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = \inf_{u \in V} J(u).$$

Let $\{u_n\} \subset V$ be a sequence such that

$$\alpha \leq J(u_n) < \alpha + \frac{1}{n}, \forall n \in \mathbb{N}.$$

Suppose, to obtain contradiction, there exists a subsequence $\{n_k\} \subset \mathbb{N}$, such that

$$\|u_{n_k}\|_V \to \infty.$$

From the hypotheses, we have

$$J(u_{n_k}) \to +\infty, \text{ as } k \to \infty.$$

This contradicts

$$\lim_{k \to \infty} J(u_{n_k}) = \alpha \in \mathbb{R}.$$

From such results we may infer that there exists $K > 0$ such that

$$\|u_n\|_V \leq K, \ \forall n \in \mathbb{N}.$$

Consequently, from this, the Sobolev Embedding and Rellich Kondrashov theorems, there exists $u_0 \in V \cap L^\infty(\Omega; \mathbb{R}^3)$ for which, up to a not relabelled subsequence, we have

$$u_n \rightharpoonup u_0, \text{ weakly in } W^{1,4}(\Omega; \mathbb{R}^3),$$

$$u_n \to u_0, \text{ strongly in } L^4(\Omega),$$

$$u_n \to u_0, \text{ strongly in } L^\infty(\Omega; \mathbb{R}^3).$$

Let $\varphi \in C_c^\infty(\Omega)$.
Thus,

$$\begin{aligned} & \left| \left\langle \frac{\partial (u_n)_i}{\partial x_j} - \frac{\partial (u_0)_i}{\partial x_j}, \varphi \right\rangle_{L^2} \right| \\ = & \left| \left\langle (u_n)_i - (u_0)_i, \frac{\partial \varphi}{\partial x_j} \right\rangle_{L^2} \right| \\ \leq & \|(u_n)_i - (u_0)_i\|_\infty \left\| \frac{\partial \varphi}{\partial x_j} \right\|_1 \\ \to & \ 0, \text{ as } n \to \infty. \end{aligned} \tag{268}$$

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Since $\varphi \in C_c^\infty(\Omega)$ is arbitrary and $C_c^\infty(\Omega)$ is dense in $L^4(\Omega)$ we may infer that

$$\frac{\partial (u_n)_i}{\partial x_j} \rightharpoonup \frac{\partial (u_0)_i}{\partial x_j}, \text{ weakly in } L^4(\Omega),$$

$\forall i, j \in \{1,2,3\}$.

Define $W = L^4(\Omega)$ with the norm

$$\|v\|_W = \sup\{\langle v, \varphi\rangle_{L^2},\ \varphi \in C_c^\infty(\Omega), \|\varphi\|_{1,2} \leq 1\}.$$

We may easily verify that

$$\frac{\partial (u_n)_i}{\partial x_j} \to \frac{\partial (u_0)_i}{\partial x_j}, \text{ strongly in } W,$$

$\forall i, j \in \{1,2,3\}$.

Thus,

$$\left\{\frac{\partial (u_n)_i}{\partial x_j}\right\}$$

is a Cauchy sequence in W.

Hence, for each $n \in \mathbb{N}$ there exists $n_k \in \mathbb{N}$ such that $m, l \geq n_k$, then

$$\left\|\frac{\partial (u_m)_i}{\partial x_j} - \frac{\partial (u_l)_i}{\partial x_j}\right\|_W < \frac{1}{k^2}.$$

where n_k may be taken as an increasing subsequence in $\mathbb{N}$.

In particular, we have got

$$\left\|\frac{\partial (u_{n_{k+1}})_i}{\partial x_j} - \frac{\partial (u_{n_k})_i}{\partial x_j}\right\|_W < \frac{1}{k^2}.$$

Define now

$$g_l = \left|\frac{\partial (u_{n_1})_i}{\partial x_j}\right| + \sum_{k=1}^{l-1}\left|\frac{\partial (u_{n_{k+1}})_i}{\partial x_j} - \frac{\partial (u_{n_k})_i}{\partial x_j}\right|,$$

and

$$g = \left|\frac{\partial (u_{n_1})_i}{\partial x_j}\right| + \sum_{k=1}^{\infty}\left|\frac{\partial (u_{n_{k+1}})_i}{\partial x_j} - \frac{\partial (u_{n_k})_i}{\partial x_j}\right|.$$

Observe that

$$\begin{aligned} \|g\|_W &\leq \left\|\frac{\partial (u_{n_1})_i}{\partial x_j}\right\|_W + \sum_{k=1}^{\infty}\left\|\frac{\partial (u_{n_{k+1}})_i}{\partial x_j} - \frac{\partial (u_{n_k})_i}{\partial x_j}\right\|_W \\ &\leq \left\|\frac{\partial (u_{n_1})_i}{\partial x_j}\right\|_W + \sum_{k=1}^{\infty}\frac{1}{k^2} \\ &< +\infty. \end{aligned} \tag{269}$$

From such results we may infer that $g(x) \in \mathbb{R}$, a.e. in Ω.

Moreover, since an absolutely convergent series is also convergent, we may infer that

$$\frac{\partial (u_{n_l})_i}{\partial x_j} = \frac{\partial (u_{n_1})_i}{\partial x_j} + \sum_{k=1}^{l-1}\left(\frac{\partial (u_{n_{k+1}})_i}{\partial x_j} - \frac{\partial (u_{n_k})_i}{\partial x_j}\right) \to h_{ij}, \text{ a.e. in } \Omega,$$

for some $h_{ij} \in L^4(\Omega)$, $\forall i, j \in \{1,2,3\}$.

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From such results, we have

$$\frac{\partial (u_{n_l})_i}{\partial x_j} \to h_{ij}, \text{ a.e. in } \Omega$$

and

$$\frac{\partial (u_{n_l})_i}{\partial x_j} \rightharpoonup \frac{\partial (u_0)_i}{\partial x_j}, \text{ weakly in } L^4(\Omega),$$

so that

$$\frac{\partial (u_0)_i}{\partial x_j} = h_{ij}, \text{ a.e. in } \Omega.$$

Consequently, we have got

$$\frac{\partial (u_{n_l})_i}{\partial x_j} \to \frac{\partial (u_0)_i}{\partial x_j}, \text{ a.e. in } \Omega.$$

Now fix $i, j, m \in \{1, 2, 3\}$.

Observe that from the Cauchy-Schwarz inequality, we have

$$\begin{aligned} & \int_\Omega \left(\frac{\partial (u_{n_l})_m}{\partial x_j} \frac{\partial (u_{n_l})_m}{\partial x_j} \right)^2 dx \\ \leq & \left\| \frac{\partial (u_{n_l})_m}{\partial x_i} \right\|_4^2 \left\| \frac{\partial (u_{n_l})_m}{\partial x_j} \right\|_4^2 \\ \leq & K_1, \ \forall l \in \mathbb{N} \end{aligned} \tag{270}$$

for some appropriate real constant $K_1 > 0$.

Therefore, up to a not relabeled subsequence there exists $v_0 \in L^2(\Omega)$ such that

$$\frac{\partial (u_{n_l})_m}{\partial x_i} \frac{\partial (u_{n_l})_m}{\partial x_j} \rightharpoonup v_0, \text{ weakly in } L^2(\Omega),$$

Since

$$\frac{\partial (u_{n_l})_m}{\partial x_i} \frac{\partial (u_{n_l})_m}{\partial x_j} \to \frac{\partial (u_0)_m}{\partial x_i} \frac{\partial (u_0)_m}{\partial x_j}, \text{ a.e. in } \Omega,$$

we obtain

$$v_0 = \frac{\partial (u_0)_m}{\partial x_i} \frac{\partial (u_0)_m}{\partial x_j}, \text{ a.e. in } \Omega,$$

so that

$$\frac{\partial (u_{n_l})_m}{\partial x_i} \frac{\partial (u_{n_l})_m}{\partial x_j} \rightharpoonup \frac{\partial (u_0)_m}{\partial x_i} \frac{\partial (u_0)_m}{\partial x_j}, \text{ weakly in } L^2(\Omega),$$

$\forall i, j, m \in \{1, 2, 3\}$.

Therefore, from such results we may infer that

$$\gamma_{ij}(u_{n_l}) \rightharpoonup \gamma_{ij}(u_0), \text{ weakly in } L^2(\Omega), \forall i, j \in \{1, 2, 3\}.$$

Moreover, since J is convex in $\{\gamma_{ij}\}$ we finally obtain

$$\alpha = \liminf_{l \to \infty} J(u_{n_l}) \geq J(u_0),$$

so that

$$J(u_0) = \min_{u \in V} J(u).$$

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The proof is complete.
□

43. A Note on a General Relaxation Procedure for the Vectorial Case in the Calculus of Variation

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$. Consider a continuous and bounded below functional $F : V \to \mathbb{R}$ where

$$V = \{u \in W^{1,2}(\Omega;\mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega\}.$$

Define $H_1 : V \to \mathbb{R}$ by

$$H_1(u) = \inf\{\lambda_1 F(v_1) + (1-\lambda_1)F(w_1) \ ; \ 0 \leq \lambda_1 \leq 1, \ v_1, w_1 \in V, \ \lambda_1 v_1 + (1-\lambda_1)w_1 = u\}.$$

Observe that as it has been shown in a previous section, we have

$$F^{**}(u) \leq H_1(u) \leq F(u), \ \forall u \in V.$$

Moreover, also as indicated in a previous section, we may obtain

$$H_1(u) = \inf_{(\phi_1,\lambda_1)\in V_0\times[0,1]} \{\lambda_1 F(u-(1-\lambda_1)\phi_1) + (1-\lambda_1)F(u+\lambda_1\phi_1)\},$$

where $V_0 = W_0^{1,2}(\Omega;\mathbb{R}^N)$.

Reasoning inductively, having $H_k : V \to \mathbb{R}$, define $H_{k+1} : V \to \mathbb{R}$ by

$$\begin{aligned} H_{k+1}(u) \quad = \quad & \inf\{\lambda_{k+1} H_k(v_{k+1}) + (1-\lambda_{k+1})H_k(w_{k+1}) \ ; \\ & 0 \leq \lambda_{k+1} \leq 1, \ v_{k+1}, w_{k+1} \in V, \ \lambda_{k+1} v_{k+1} + (1-\lambda_{k+1})w_{k+1} = u\}. \end{aligned} \tag{271}$$

Thus

$$H_{k+1}(u) = \inf_{(\phi_{k+1},\lambda_{k+1})\in V_0\times[0,1]} \{\lambda_{k+1} H_k(u-(1-\lambda_{k+1})\phi_{k+1}) + (1-\lambda_{k+1})H_k(u+\lambda_{k+1}\phi_{k+1})\}.$$

Observe that

$$F^{**}(u) \leq H_{k+1}(u) \leq H_k(u) \leq F(u), \ \forall k \in \mathbb{N}.$$

Define $H_0 : V \to \mathbb{R}$ by

$$H_0(u) = \lim_{k\to+\infty} H_k(u) = \inf_{k\in\mathbb{N}} H_k(u), \ \forall u \in V.$$

Suppose, to obtain contradiction, that H_0 is not convex.

Hence, there exists $\hat{u} \in V$ such that

$$(H_0)_1(\hat{u}) < H_0(\hat{u}),$$

where

$$(H_0)_1(u) = \inf\{\lambda_1 H_0(v_1) + (1-\lambda_1)H_0(w_1) \ ; \ 0 \leq \lambda_1 \leq 1, \ v_1, w_1 \in V, \ \lambda_1 v_1 + (1-\lambda_1)w_1 = u\}.$$

This contradicts

$$H_0(u) = \lim_{k\to+\infty} H_k(u) = \inf_{k\in\mathbb{N}} H_k(u), \ \forall u \in V.$$

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Therefore H_0 is convex on V so that from this and

$$F^{**}(u) \leq H_0(u) \leq F(u),\ \forall u \in V$$

we may infer that

$$H_0(u) = F^{**}(u),\ \forall u \in V.$$

44. A Note on Another General Relaxation Procedure for the Vectorial Case in the Calculus of Variation

Let $\Omega \subset \mathbb{R}^n$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$. Consider a continuous and bounded below functional $F : V \to \mathbb{R}$ where

$$V = \{u \in W^{1,2}(\Omega;\mathbb{R}^N)\ :\ u = u_0 \text{ on } \partial\Omega\}.$$

Fix $k \in \mathbb{N}$.
Define $(H_1)_k : V \to \mathbb{R}$ by

$$\begin{aligned}(H_1)_k(u) \quad = \quad & \inf\Big\{\sum_{j=1}^{k}\lambda_j F(v_j)\ :\ 0 \leq \lambda_j \leq 1 \text{ and } v_j \in V,\ \forall j \in \{1,\cdots,k\},\\ & \sum_{j=1}^{k}\lambda_j = 1 \text{ and } \sum_{j=1}^{k}\lambda_j v_j = u\Big\}.\end{aligned} \tag{272}$$

Observe that

$$F^{**}(u) \leq (H_1)_{k+1}(u) \leq (H_1)_k(u) \leq F(u),\ \forall u \in V.$$

Define $H_2 : V \to \mathbb{R}$ by

$$H_2(u) = \lim_{k\to\infty}(H_1)_k(u) = \inf_{k\in\mathbb{N}}\{(H_1)_k(u)\}, \forall u \in V.$$

Reasoning inductively, having $H_m : V \to \mathbb{R}$, we may obtain $(H_m)_k : V \to \mathbb{R}$ by

$$\begin{aligned}(H_m)_k(u) \quad = \quad & \inf\Big\{\sum_{j=1}^{k}\lambda_j H_m(v_j)\ :\ 0 \leq \lambda_j \leq 1 \text{ and } v_j \in V,\ \forall j \in \{1,\cdots,k\},\\ & \sum_{j=1}^{k}\lambda_j = 1 \text{ and } \sum_{j=1}^{k}\lambda_j v_j = u\Big\}.\end{aligned} \tag{273}$$

Observe that

$$F^{**}(u) \leq (H_m)_{k+1}(u) \leq (H_m)_k(u) \leq F(u),\ \forall u \in V.$$

Now we define

$$H_{m+1}(u) = \lim_{k\to\infty}(H_m)_k(u) = \inf_{k\in\mathbb{N}}\{(H_m)_k(u)\},\ \forall u \in V,$$

$\forall m \in \mathbb{N}$.
Therefore, we have obtained a sequence $\{H_m : V \to \mathbb{R}\}$ such that

$$F^{**}(u) \leq H_{m+1}(u) \leq H_m(u) \leq F(u),\ \forall u \in V.$$

Thus, we may define $H^0 : V \to \mathbb{R}$ by

$$H^0(u) = \lim_{m\to\infty} H_m(u) = \inf_{m\in\mathbb{N}}\{H_m(u)\},\ \forall u \in V.$$

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Suppose, to obtain contradiction, that $H^0 : V \to \mathbb{R}$ is not convex on V.
Hence, there exists $\hat{u} \in V$ such that

$$(H^0)_1(\hat{u}) < H^0(\hat{u}),$$

where

$$(H^0)_1(u) = \inf\{\lambda_1 H^0(v_1) + (1-\lambda_1)H^0(w_1) \ : \ 0 \leq \lambda_1 \leq 1, \ v_1, w_1 \in V, \ \lambda_1 v_1 + (1-\lambda_1)w_1 = u\},$$

$\forall u \in V$.

This contradicts

$$H^0(u) = \lim_{m\to\infty} H_m(u) = \inf_{m\in\mathbb{N}}\{H_m(u)\}, \ \forall u \in V.$$

Therefore, H^0 is convex on V so that from this and

$$F^{**}(u) \leq H^0(u) \leq F(u), \ \forall u \in V,$$

we may infer that

$$H^0(u) = F^{**}(u), \ \forall u \in V.$$

45. A Proximal Relaxed General Approach Also Suitable for the Vectorial Case in the Calculus of Variations

Let $\Omega = [0,1] \subset \mathbb{R}$ and consider a proximal relaxed functional $J_1 : V \times V_0 \times [0,1] \times Y^* \to \mathbb{R}$ where

$$\begin{aligned} J_1(u,\phi,\lambda,z^*) \quad = \quad & \frac{\lambda}{2}\int_\Omega ((u' - (1-\lambda)\phi')^2 - 1)^2 \, dx \\ & \frac{(1-\lambda)}{2}\int_\Omega ((u' + \lambda\phi')^2 - 1)^2 \, dx \\ & + \frac{1}{2}\int_\Omega (u-f)^2 \, dx + \frac{K}{2}\int_\Omega (u-f)^2 \, dx \\ & - \int_\Omega z^*(u-f) \, dx + \frac{1}{2K}\int_\Omega (z^*)^2 \, dx, \end{aligned} \tag{274}$$

where

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\},$$

$V_0 = W_0^{1,2}(\Omega)$, and $Y = Y^* = L^2(\Omega)$.

In order to obtain a critical point of such a proximal relaxed primal formulation, we propose the following algorithm:

1. Set $n = 1$, $\varepsilon = 10^{-4}$ and $z_n^* \equiv 0$.
2. Calculate $(u_n, \phi_n, \lambda_n) \in V \times V_0 \times [0,1]$ such that

$$J_1(u_n, \phi_n, \lambda_n, z_n^*) = \inf_{(u,\phi,\lambda)\in V\times V_0\times[0,1]} J_1(u,\phi,\lambda,z_n^*).$$

3. Calculate $z_{n+1}^* \in Y^*$ such that

$$J_1(u_n, \phi_n, \lambda_n, z_{n+1}^*) = \inf_{z^*\in Y^*} J_1(u_n, \phi_n, \lambda_n, z^*),$$

so that indeed,

$$z_{n+1}^* = K(u_n - f).$$

4. If $\|z_{n+1}^* - z_n^*\|_\infty < \varepsilon$, then stop. Otherwise set $n := n+1$ and go to item 2.

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We have obtained numerical results for $K = 100$ and

$$f(x) = \sin(\pi x)/2.$$

For the optimal solution $u(x)$ obtained, please see Figure 34.

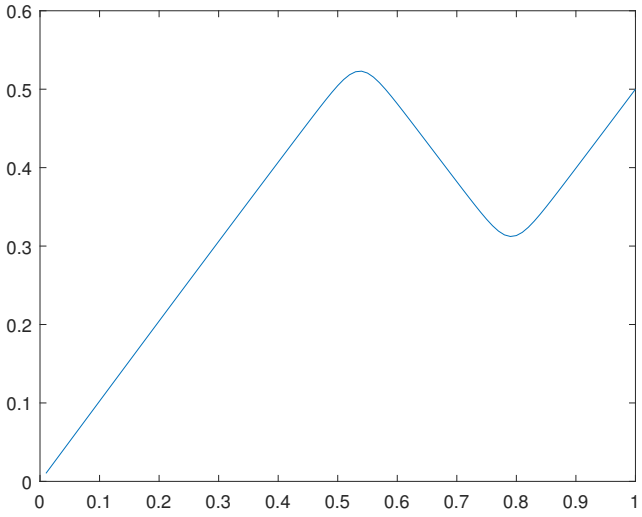

Figure 34. Optimal solution $u(x)$ for the case $f(x) = \sin(\pi x)/2$.

At this point we present the software in MAT-LAB we have developed to obtain such numerical results.

****

1. clear all

   global m8 d u v yo e1 K z

   m8=100;

   d=1/m8;

   e1=0.0005;

   K=100.0;

   for i=1:m8

   yo(i,1)=sin(pi*i*d)/2;

   z(i,1)=0;

   end;

   for i=1:2*m8+1

   xo(i,1)=0.3;

   x1(i,1)=0.3;

   end;

   k1=1;

   b14=1.0;

   while $(b14 > 10^{-4})$ && $(k1 < 11)$

   k1

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k1=k1+1;

k=1;

b12=1.0;

while $(b12 > 10^{-4})$ && $(k < 16)$

k

k=k+1;

X=fminunc('funMarch24PhaseT',xo);

b12=max(abs(X-xo))

xo=X;

u(m8/2,1)

end;

b14=max(abs(x1-xo));

z=K*(u-yo);

x1=xo;

u(m8/2,1)

end;

for i=1:m8

x(i,1)=i*d;

end;

plot(x,u)

****

Here the auxiliary function "funMarch24PhaseT"

****

1. function S=funMarch24PhaseT(x)

global m8 d u v L yo e1 K z

for i=1:m8

u(i,1)=x(i,1);

v(i,1)=x(i+m8,1);

end;

L=(sin(x(2*m8+1,1))+1)/2;

u(m8,1)=1/2;

v(m8,1)=0.0;

du(1,1)=u(1,1)/d;

dv(1,1)=v(1,1)/d;

for i=2:m8

du(i,1)=(u(i,1)-u(i-1,1))/d;

dv(i,1)=(v(i,1)-v(i-1,1))/d;

end;

d2u(1,1)=$(-2 * u(1,1) + u(2,1))/d^2$;

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for i=2:m8-1

d2u(i,1)=$(u(i+1,1)-2*u(i,1)+u(i-1,1))/d^2$;

end;

S=0;

for i=1:m8

S=S+$L*((du(i,1)-(1-L)*dv(i,1))^2-1)^2/2$;

S=S+$(1-L)*((du(i,1)+L*dv(i,1))^2-1)^2/2$;

S=S+$(u(i,1)-yo(i,1))^2/2$;

S=S+$K*(u(i,1)-yo(i,1))^2/2-z(i,1)*(u(i,1)-yo(i,1))$;

end;

for i=1:m8-1

S=S+$e1*d2u(i,1)^2$;

end;

****

46. Another Proximal Relaxed General Approach Also Suitable for the Vectorial Case in the Calculus of Variations

Let $\Omega=[0,1]\subset\mathbb{R}$ and consider a proximal relaxed functional $J_1: V\times[V_0]^3\times B\times Y^*\to\mathbb{R}$ where

$$\begin{aligned} J_1(u,\phi,\lambda,z^*) &= \frac{\lambda_1}{2}\int_\Omega((u'+\lambda_1\phi_1'+\lambda_2\phi_2'+\lambda_3\phi_3'-\phi_1')^2-1)^2\,dx \\ &+\frac{\lambda_2}{2}\int_\Omega((u'+\lambda_1\phi_1'+\lambda_2\phi_2'+\lambda_3\phi_3'-\phi_2')^2-1)^2\,dx \\ &+\frac{\lambda_3}{2}\int_\Omega((u'+\lambda_1\phi_1'+\lambda_2\phi_2'+\lambda_3\phi_3'-\phi_3')^2-1)^2\,dx \\ &+\frac{\lambda_4}{2}\int_\Omega((u'+\lambda_1\phi_1'+\lambda_2\phi_2'+\lambda_3\phi_3')^2-1)^2\,dx \\ &+\frac{1}{2}\int_\Omega(u-f)^2\,dx+\frac{K}{2}\int_\Omega(u-f)^2\,dx \\ &-\int_\Omega z^*(u-f)\,dx+\frac{1}{2K}\int_\Omega(z^*)^2\,dx, \end{aligned} \tag{275}$$

where

$$V=\{u\in W^{1,2}(\Omega)\ :\ u(0)=0 \text{ and } u(1)=1/2\},$$

$V_0=W_0^{1,2}(\Omega)$, $Y=Y^*=L^2(\Omega)$, $f\in L^2(\Omega)$ and

$$B=\left\{\lambda=(\lambda_1,\cdots,\lambda_4)\in\mathbb{R}^4\ :\ \lambda_j\geq 0,\ \forall j\in\{1,\cdots,4\} \text{ and } \sum_{j=1}^4\lambda_j=1\right\}.$$

In order to obtain a critical point of such a proximal relaxed primal formulation, we propose the following algorithm:

1. Set $n=1$, $\varepsilon=10^{-4}$ and $z_n^*\equiv 0$.
2. Calculate $(u_n,\phi_n,\lambda_n)\in V\times[V_0]^3\times B$ such that

$$J_1(u_n,\phi_n,\lambda_n,z_n^*)=\inf_{(u,\phi,\lambda)\in V\times[V_0]^3\times B}J_1(u,\phi,\lambda,z_n^*).$$

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3. Calculate $z_{n+1}^* \in Y^*$ such that

$$J_1(u_n, \phi_n, \lambda_n, z_{n+1}^*) = \inf_{z^* \in Y^*} J_1(u_n, \phi_n, \lambda_n, z^*),$$

so that indeed,

$$z_{n+1}^* = K(u_n - f).$$

4. If $\|z_{n+1}^* - z_n^*\|_\infty < \varepsilon$, then stop. Otherwise set $n := n + 1$ and go to item 2.

We have obtained numerical results for $K = 100$ and

$$f(x) = 0.0.$$

For the optimal solution $u(x)$ obtained, please see Figure 35.

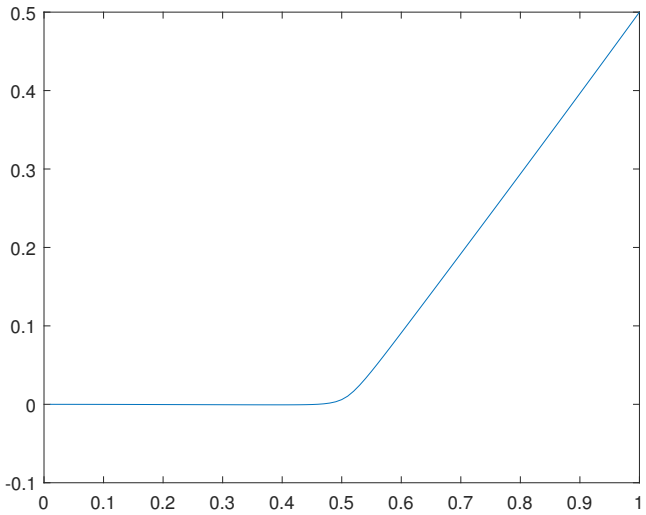

Figure 35. Optimal solution $u(x)$ for the case $f(x) = 0$.

At this point we present the software in MAT-LAB we have developed to obtain such numerical results.

****

1. clear all

global m8 d u v yo e1 K z

m8=100;

d=1/m8;

e1=0.0007;

K=100.0;

for i=1:m8

yo(i,1)=0.0*sin(pi*i*d)/2;

z(i,1)=0;

end;

for i=1:4*m8+3

xo(i,1)=0.3;

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```
x1(i,1)=0.3;
end;
k1=1;
b14=1.0;
while (b14 > 10^-4) && (k1 < 11)
k1
k1=k1+1;
k=1;
b12=1.0;
while (b12 > 10^-4) && (k < 16)
k
k=k+1;
X=fminunc('funMarch24PhaseTC',xo);
b12=max(abs(X-xo))
xo=X;
u(m8/2,1)
end;
b14=max(abs(x1-xo));
z=K*(u-yo);
x1=xo;
u(m8/2,1)
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u)
```

****

With the auxiliary function "funMarch24PhaseTC"

****

1.

```
function S=funMarch24PhaseTC(x)
global m8 d u v L yo e1 K z
for i=1:m8
u(i,1)=x(i,1);
v(i,1)=x(i+m8,1);
v1(i,1)=x(i+2*m8,1);
v2(i,1)=x(i+3*m8,1);
end;
L1=(sin(x(4*m8+1,1))+1)/2;
L2=min((sin(x(4*m8+2,1))+1)/2,1-L1);
```

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L3=min((sin(x(4*m8+3,1))+1)/2,1-L1-L2);

L4=1-L1-L2-L3;

u(m8,1)=1/2;

v(m8,1)=0.0;

v1(m8,1)=0.0;

v2(m8,1)=0.0;

du(1,1)=u(1,1)/d;

dv(1,1)=v(1,1)/d;

dv1(1,1)=v1(1,1)/d;

dv2(1,1)=v2(1,1)/d;

for i=2:m8

du(i,1)=(u(i,1)-u(i-1,1))/d;

dv(i,1)=(v(i,1)-v(i-1,1))/d;

dv1(i,1)=(v1(i,1)-v1(i-1,1))/d;

dv2(i,1)=(v2(i,1)-v2(i-1,1))/d;

end;

d2u(1,1)=$(-2*u(1,1)+u(2,1))/d^2$;

for i=2:m8-1

d2u(i,1)=$(u(i+1,1)-2*u(i,1)+u(i-1,1))/d^2$;

end;

S=0;

for i=1:m8

S=S+$L1*((du(i,1)+L1*dv(i,1)+L2*dv1(i,1)+L3*dv2(i,1)-dv(i,1))^2-1)^2/2$;

S=S+$L2*((du(i,1)+L1*dv(i,1)+L2*dv1(i,1)+L3*dv2(i,1)-dv1(i,1))^2-1)^2/2$;

S=S+$L3*((du(i,1)+L1*dv(i,1)+L2*dv1(i,1)+L3*dv2(i,1)-dv2(i,1))^2-1)^2/2$;

S=S+$L4*((du(i,1)+L1*dv(i,1)+L2*dv1(i,1)+L3*dv2(i,1))^2-1)^2/2$;

S=S+$(u(i,1)-yo(i,1))^2/2$;

S=S+$K*(u(i,1)-yo(i,1))^2/2-z(i,1)*(u(i,1)-yo(i,1))$;

end;

for i=1:m8-1

S=S+$e1*d2u(i,1)^2$;

end;

****

47. A Dual Variational Formulation for a Non-Convex Primal One

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$. Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx \\ &\quad + \frac{\alpha}{2}\int_\Omega (u^2-\beta)^2 \, dx - \langle u, f\rangle_{L^2}. \end{aligned} \tag{276}$$

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Here $V = W_0^{1,2}(\Omega)$, $\alpha > 0$, $\beta > 0$, $\gamma > 0$, and $f \in L^2(\Omega) \equiv Y = Y^*$.
Denoting $Y_1 = Y_1^* = L^2(\Omega; \mathbb{R}^3)$, define $F_1 : Y_1 \to \mathbb{R}$, $F_2 : V \times Y \to \mathbb{R}$ and $F_3 : Y \to \mathbb{R}$ by

$$F_1(\nabla u) = \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx,$$

$$F_2(u, v) = \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx + \frac{K}{2} \int_\Omega u^2 \, dx - \langle u, f \rangle_{L^2},$$

and

$$F_3(u) = \frac{K}{2} \int_\Omega u^2 \, dx.$$

Define also, $F_1 : Y_1^* \to \mathbb{R}$, $\tilde{F}_2 : Y_1^* \times Y^* \times Y^* \to \mathbb{R}$ and $F_3 : Y^* \to \mathbb{R}$, by

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{v_1 \in Y_1} \{\langle v_1, v_1^* \rangle_{L^2} - F_1(v_1)\} \\ &= \frac{1}{2\gamma} \int_\Omega |v_1^*|^2 \, dx, \end{aligned} \tag{277}$$

$$\begin{aligned} \tilde{F}_2^*(v_1^*, v_0^*, z^*) &= \sup_{(u,v) \in V \times Y} \{-\langle \nabla u, v_1^* \rangle_{L^2} + \langle u, z^* \rangle_{L^2} \\ &\quad + \langle v, v_0^* \rangle_{L^2} - F_2(u, v)\} \\ &= \frac{1}{2} \int_\Omega \frac{(\operatorname{div} v_1^* + z^* + f)^2}{2v_0^* + K} \, dx + \frac{1}{2\alpha} \int_\Omega (v_0^*)^2 \, dx \\ &\quad + \beta \int_\Omega v_0^* \, dx, \end{aligned} \tag{278}$$

if $v_0^* \in B^*$, where

$$B^* = \{v_0^* \in Y^* \ : \ \|2v_0^*\|_\infty \leq K/2\}.$$

Moreover,

$$\begin{aligned} F_3^*(z^*) &= \sup_{u \in V} \{\langle u, z^* \rangle_{L^2} - F_3(u)\} \\ &= \frac{1}{2K} \int_\Omega (z^*)^2 \, dx. \end{aligned} \tag{279}$$

At this point we define $J^* : Y_1^* \times B^* \times Y^* \to \mathbb{R}$ by

$$J_1^*(v_1^*, v_0^*, z^*) = -F_1^*(v_1^*) - \tilde{F}_2^*(v_1^*, v_0^*, z^*) + F_3^*(z^*).$$

Assume $(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \in Y_1^* \times B^* \times Y^*$ is such that

$$\delta J^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) = \mathbf{0}.$$

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Observe that

$$\begin{aligned} J^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) &= -F_1^*(v_1^*) - \tilde{F}_2^*(v_1^*, v_0^*, z^*) + F_3^*(z^*) \\ &\leq -\langle \nabla u, \hat{v}_1^* \rangle_{L^2} + F_1(\nabla u) \\ &\quad + \langle \nabla u, \hat{v}_1^* \rangle_{L^2} + \langle u^2, \hat{v}_0^* \rangle_{L^2} + \frac{K}{2} \int_\Omega u^2 \, dx \\ &\quad - \frac{1}{2\alpha} \int_\Omega \hat{v}_0^* \, dx - \beta \int_\Omega \hat{v}_0^* \, dx \\ &\quad - \langle u, f \rangle_{L2} - \langle u, \hat{z}^* \rangle_{L^2} + \frac{1}{2K} \int_\Omega (\hat{z}^*)^2 \, dx \\ &\leq F_1(\nabla u) + \sup_{v_0^* \in Y^*} \left\{ \langle u^2, v_0^* \rangle_{L^2} - \frac{1}{2\alpha} \int_\Omega v_0^* \, dx - \beta \int_\Omega v_0^* \, dx \right\} \\ &\quad - \langle u, f \rangle_{L2} + \frac{K}{2} \int_\Omega u^2 \, dx - \langle u, \hat{z}^* \rangle_{L^2} + \frac{1}{2K} \int_\Omega (\hat{z}^*)^2 \, dx \\ &= F_1(\nabla u) + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L2} \\ &\quad + \frac{K}{2} \int_\Omega \left(u - \frac{\hat{z}^*}{K} \right)^2 dx \\ &= J(u) + \frac{K}{2} \int_\Omega \left(u - \frac{\hat{z}^*}{K} \right)^2 dx, \ \forall u \in V. \end{aligned} \tag{280}$$

Define now $u_0 \in V$ by

$$u_0 = \frac{\hat{z}^*}{K}.$$

From this and (280) we have

$$J^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \leq \inf_{u \in V} \left\{ J(u) + \frac{K}{2} \int_\Omega (u - u_0)^2 \, dx \right\}.$$

Furthermore, from the variation of J^* in v_1^* we obtain

$$-\frac{\hat{v}_1^*}{\gamma} + \nabla \left(\frac{\operatorname{div} \hat{v}_1^* + \hat{z}^* + f}{2\hat{v}_0^* + K} \right) = \mathbf{0},$$

so that

$$\hat{v}_1^* = \gamma \nabla \left(\frac{\operatorname{div} \hat{v}_1^* + \hat{z}^* + f}{2\hat{v}_0^* + K} \right).$$

From the variation of J^* in z^*, we get

$$\frac{\hat{z}^*}{K} - \left(\frac{\operatorname{div} \hat{v}_1^* + \hat{z}^* + f}{2\hat{v}_0^* + K} \right) = \mathbf{0}$$

so that

$$u_0 = \frac{\hat{z}^*}{K} = \left(\frac{\operatorname{div} \hat{v}_1^* + \hat{z}^* + f}{2\hat{v}_0^* + K} \right).$$

From the variation of J^* in v_0^*, we obtain

$$\frac{\hat{v}_0^*}{\alpha} - \left(\frac{\operatorname{div} \hat{v}_1^* + \hat{z}^* + f}{2\hat{v}_0^* + K} \right)^2 + \beta = \mathbf{0}$$

so that

$$\hat{v}_0^* = \alpha(u_0^2 - \beta).$$

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Joining the pieces, we have also

$$\hat{v}_1 = \gamma \nabla u_0,$$

$$\hat{z} = K u_0,$$

so that from this and

$$\text{div } \hat{v}_1^* + \hat{z}^* + f = (2\hat{v}_0^* + K)u_0,$$

we obtain

$$\gamma \nabla^2 u_0 + K u_0 + f = \alpha(u_0^2 - \beta)2u_0 + K u_0,$$

so that

$$-\gamma \nabla^2 u_0 + \alpha(u_0^2 - \beta)2u_0 - f = \mathbf{0},$$

that is,

$$\delta J(u_0) = \mathbf{0}.$$

Finally, from the Legendre transform proprieties, we also obtain

$$F_1^*(\hat{v}_1^*) = \langle \nabla u_0, \hat{v}_1^* \rangle_{L^2} - F_1(\nabla u_0),$$

$$\begin{aligned} \tilde{F}_2(\hat{v}_1, \hat{v}_0^*, \hat{z}^*) &= -\langle \nabla u_0, \hat{v}_1^* \rangle_{L^2} + \langle u_0, \hat{z}^* \rangle_{L^2} \\ &\quad + \langle 0, \hat{v}_0^* \rangle_{L^2} - F_2(u_0, 0) \end{aligned} \tag{281}$$

and

$$F_3^*(z^*) = \langle u_0, \hat{z}^* \rangle_{L^2} - F_3(u_0).$$

Therefore

$$\begin{aligned} J^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) &= -F_1^*(\hat{v}_1^*) - \tilde{F}_2^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) + F_3^*(\hat{z}^*) \\ &= F_1(\nabla u_0) + F_2(u_0, 0) - F_3(u_0) \\ &= J(u_0). \end{aligned} \tag{282}$$

Observe now that from $\delta J(u_0) = \mathbf{0}$, for $K > 0$ sufficiently large, we have

$$J(u_0) = \inf_{u \in V} \left\{ J(u) + \frac{K}{2} \int_\Omega (u - u_0)^2 \, dx \right\}.$$

Joining the pieces we have got

$$\begin{aligned} J(u_0) &= \inf_{u \in V} \left\{ J(u) + \frac{K}{2} \int_\Omega (u - u_0)^2 \, dx \right\} \\ &= J^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*). \end{aligned} \tag{283}$$

We have obtained numerical results for the case A, where $\gamma = 0.1$, $\alpha = 3.0$, $\beta = 5.0$, $f(x) = 10.0$ and $K = 120$.

For the optimal solution $u(x)$, where

$$u(x) = \frac{(v_1 *)' + z^* + f}{2\, v_0^* + K},$$

please see Figure 36.

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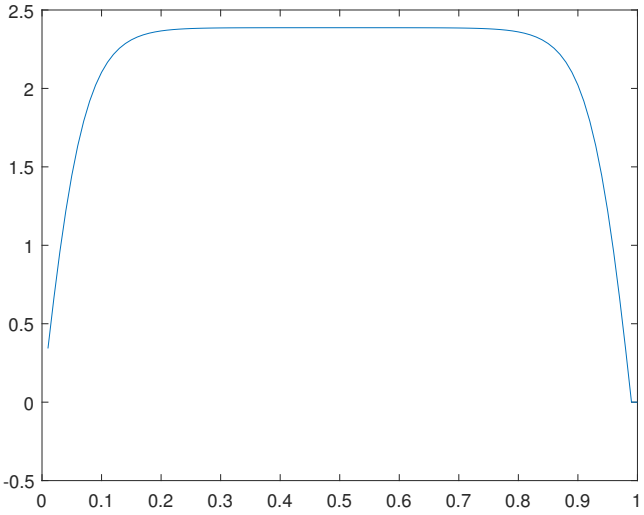

Figure 36. Optimal solution $u(x)$ for the case A.

Here we present the software in MATLAB through which we have obtained such results.
****

1. clear all
   global m8 d yo z1 K e1 dv1 dv2 v3 v4 v1 v2 A A3 B L u
   m8=100;
   d=1/m8;
   A3=0.1;
   A=3.0;
   B=5.0;
   K=120;
   e1=0.0007;
   for i=1:m8
   yo(i,1)=10.0;
   z1(i,1)=0.0;
   end;
   L=1/2;
   for i=1:2*m8
   xo(i,1)=3.0;
   end;
   for k1=1:30
   k1
   k=1;
   b12=1.0;
   while $(b12 > 10^{-4})$ && $(k < 15)$
   k

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```
k=k+1;
X=fminunc('funMarch24LGA7',xo);
b12=max(abs(X-xo))
xo=X;
u(m8/2,1)
end;
for i=1:m8-1
z1(i,1)=K*(dv1(i,1)+z1(i,1)+yo(i,1))/(2*v2(i,1)+K);
end;
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u);
```

****

With the auxiliary function "funMarch24LGA7"

****

1.
```
function S=funMarch24LGA7(x)
global m8 d yo z1 z2 K e1 dv1 dv2 v3 v4 v1 v2 A A3 B L u
for i=1:m8
v1(i,1)=x(i,1);
v2(i,1)=x(i+m8,1);
end;
for i=1:m8-1
dv1(i,1)=(v1(i+1,1)-v1(i,1))/d;
end;
S=0;
for i=1:m8-1
S=S+v1(i,1)^2/2/A3+1/2*(dv1(i,1)+z1(i,1)+yo(i,1))^2/(2*v2(i,1)+K);
S=S+v2(i,1)*B+v2(i,1)^2/2/A;
end;
for i=1:m8-1
u(i,1)=(dv1(i,1)+z1(i,1)+yo(i,1))/(2*v2(i,1)+K);
end;
u(m8,1)=0;
```

****

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48. A Convex Dual Variational Formulation for a Relaxed Non-Convex Primal One

Let $\Omega = [0,1] \subset \mathbb{R}$ and consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = \frac{1}{2}\int_\Omega ((u')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega (u-f)^2\, dx,$$

where

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 0 \text{ and } u(1) = 1/2\}.$$

Denoting $V_0 = W_0^{1,2}(\Omega)$, we define $J_1 : V \times V_0 \times [0,1] \to \mathbb{R}$ where

$$\begin{aligned} J_1(u,\phi,\lambda) &= \frac{\lambda}{2}\int_\Omega ((u' - (1-\lambda)\phi')^2 - 1)^2\, dx \\ &\quad + \frac{(1-\lambda)}{2}\int_\Omega ((u' + \lambda\phi')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega (u-f)^2\, dx. \end{aligned} \tag{284}$$

Observe that

$$\begin{aligned} J_1(u,\phi,\lambda) &= -\langle (u' - (1-\lambda)\phi')^2 - 1, v_3^*\rangle_{L^2} + \frac{\lambda}{2}\int_\Omega ((u' - (1-\lambda)\phi')^2 - 1)^2\, dx \\ &\quad -\langle (u' + \lambda\phi')^2 - 1, v_4^*\rangle_{L^2} + \frac{(1-\lambda)}{2}\int_\Omega ((u' + \lambda\phi')^2 - 1)^2\, dx \\ &\quad +\langle (u' - (1-\lambda)\phi')^2 - 1, v_3^*\rangle_{L^2} - \langle u' - (1-\lambda)\phi', v_1^*\rangle_{L^2} \\ &\quad +\langle (u' + \lambda\phi')^2 - 1, v_4^*\rangle_{L^2} - \langle u' + \lambda\phi', v_2^*\rangle_{L^2} \\ &\quad +\langle u' - (1-\lambda)\phi', v_1^*\rangle_{L^2} + \langle u' + \lambda\phi', v_2^*\rangle_{L^2} \\ &\quad +\frac{1}{2}\int_\Omega (u-f)^2\, dx. \end{aligned} \tag{285}$$

Therefore

$$\begin{aligned} J_1(u,\phi,\lambda) &\geq \inf_{v_3 \in Y}\left\{ -\langle v_3, v_3^*\rangle_{L^2} + \frac{\lambda}{2}\int_\Omega (v_3)^2\, dx \right\} \\ &\quad + \inf_{v_4 \in Y}\left\{ -\langle v_4, v_4^*\rangle_{L^2} + \frac{(1-\lambda)}{2}\int_\Omega (v_4)^2\, dx \right\} \\ &\quad + \inf_{\tilde{v}_3 \in Y}\{ -\langle \tilde{v}_3, v_1^*\rangle_{L^2} + \langle \tilde{v}_3^2 - 1, v_3^*\rangle_{L^2} \\ &\quad + \inf_{\tilde{v}_4 \in Y}\{ -\langle \tilde{v}_4, v_1^*\rangle_{L^2} + \langle \tilde{v}_4^2 - 1, v_3^*\rangle_{L^2} \\ &\quad + \inf_{(u,\phi) \in V \times V_0}\{ -\langle u - (1-\lambda)\phi, (v_1^*)'\rangle_{L^2} - \langle u + \lambda\phi, (v_2^*)'\rangle_{L^2} \\ &\quad + \frac{1}{2}\int_\Omega (u-f)^2\, dx + v_1^*(1)u(1) + v_2^*(1)u(1) \Big\} \\ &= -\frac{1}{2\lambda}\int_\Omega (v_3^*)^2\, dx - \frac{1}{2(1-\lambda)}\int_\Omega (v_4^*)^2\, dx \\ &\quad - \int_\Omega v_3^*\, dx - \int_\Omega v_4^*\, dx \\ &\quad - \int_\Omega \frac{(v_1^*)^2}{4v_3^*}\, dx - \int_\Omega \frac{(v_2^*)^2}{4v_4^*}\, dx \\ &\quad - \frac{1}{2}\int_\Omega ((v_1^*)' + \lambda f)^2\, dx - \frac{1}{2}\int_\Omega ((v_2^*)' + (1-\lambda)f)^2\, dx \\ &\equiv J^*(v_1^*, v_2^*, v_3^*, v_4^*, \lambda), \end{aligned} \tag{286}$$

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$\forall (u,\phi,\lambda) \in V \times V_0 \times [0,1]$, $\forall (v_1^*, v_2^*, v_3^*, v_4^*) \in [Y^*]^2 \times B^*$, where

$$B^* = \{(v_3^*, v_4^*) \in Y^* \times Y^* \ : \ v_3^* > 0 \text{ and } v_4^* > 0, \text{ in } \Omega\},$$

and

$$\begin{aligned} J^*(v_1^*, v_2^*, v_3^*, v_4^*, \lambda) \ = \ & -\frac{1}{2\lambda}\int_\Omega (v_3^*)^2\,dx - \frac{1}{2(1-\lambda)}\int_\Omega (v_4^*)^2\,dx \\ & -\int_\Omega v_3^*\,dx - \int_\Omega v_4^*\,dx \\ & -\int_\Omega \frac{(v_1^*)^2}{4v_3^*}\,dx - \int_\Omega \frac{(v_2^*)^2}{4v_4^*}\,dx \\ & -\frac{1}{2}\int_\Omega ((v_1^*)' + \lambda f)^2\,dx - \frac{1}{2}\int_\Omega ((v_2^*)' + (1-\lambda) f)^2\,dx. \end{aligned} \tag{287}$$

From such results, we may infer that

$$\inf_{(u,\phi,\lambda)\in V\times V_0\times[0,1]} J_1(u,\phi,\lambda) \geq \inf_{\lambda\in[0,1]} \left\{ \sup_{(v_1^*,v_2^*,v_3^*,v_4^*)\in[Y^*]\times B^*} J^*(v_1^*, v_2^*, v_3^*, v_4^*, \lambda) \right\}.$$

We have developed numerical results for the cases $f(x) = \sin(\pi x)/2$ and $f(x) = 0$
For the corresponding optimal solution $u(x)$ for the case $f(x) = \sin(\pi x)/2$, please see Figure 37.
For the corresponding optimal solution $u(x)$ for the case $f(x) = 0$, please see Figure 38.

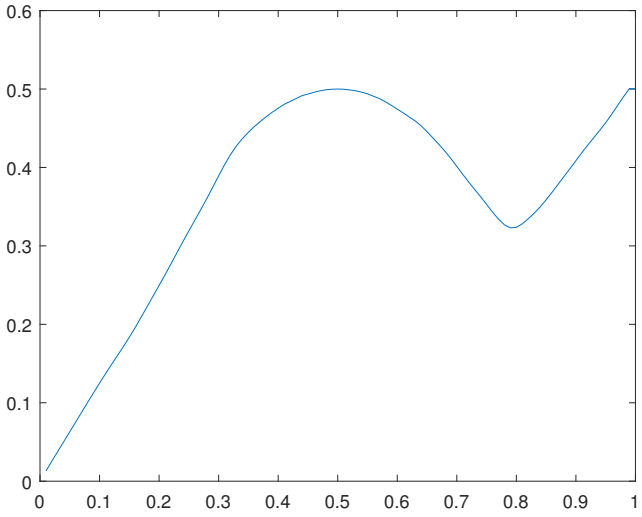

Figure 37. Optimal solution $u(x)$ for the case $f(x) = \sin(\pi x)/2$.

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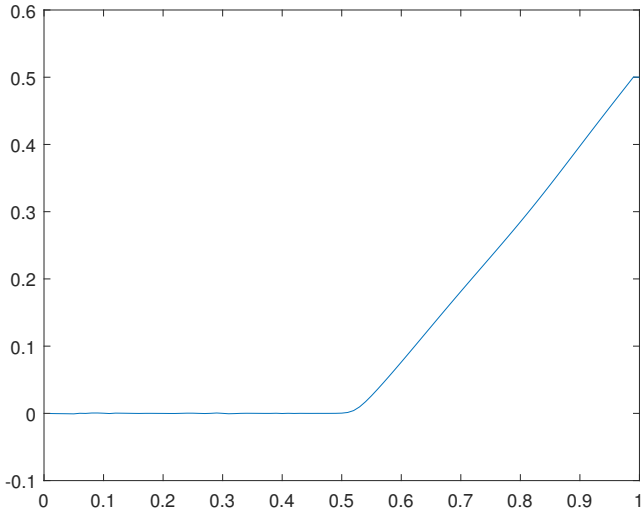

Figure 38. Optimal solution $u(x)$ for the case $f(x) = 0$.

Here we present the software in MATLAB through which we have obtained such numerical results.

****

1. clear all

global m8 d yo u L v1 v2 v3 v4 dv1 dv2 K dz1 z1 e1

m8=100;

d=1/m8;

K=1.0;

e1=0.0007;

L=1/2;

for i=1:m8

yo(i,1)=0.0*sin(pi*i*d)/2;

end;

for i=1:4*m8

xo(i,1)=0.8;

end;

x1(1,1)=1/2;

for k1=1:12

k1

k=1;

b12=1.0;

while $(b12 > 10^{-4})$ && $(k < 15)$

k

k=k+1;

X=fminunc('funMarch24A18',xo);

b12=max(abs(X-xo))

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u(m8/2,1)
xo=X;
end;
X1=fminunc('funMarch24A19',x1);
x1=X1;
u(m8/2,1)
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u);

****

With the auxiliary functions "funMarch24A18" and "funMarch24A19":

****

1. function S=funMarch24A18(x)
global m8 d yo u e1 v1 v2 v3 v4 dv1 dv2 L
for i=1:m8
v1(i,1)=x(i,1);
v2(i,1)=x(i+m8,1);
v3(i,1)=x(i+2*m8,1);
v4(i,1)=x(i+3*m8,1);
end;
for i=1:m8-1
dv1(i,1)=(v1(i+1,1)-v1(i,1))/d;
dv2(i,1)=(v2(i+1,1)-v2(i,1))/d;
end;
S=0;
for i=1:m8-1
S=S+$(v1(i,1))^2/(2*v3(i,1)^2)/2+v3(i,1)^4/2/(L+e1)+v3(i,1)^2+(dv1(i,1)+L*yo(i,1))^2/2+v1(i,1)^2/2/(L+e1)$;
S=S+$(v2(i,1))^2/(2*v4(i,1)^2)/2+v4(i,1)^4/2/((1-L)+e1)+v4(i,1)^2$;
S=S+$(dv2(i,1)+(1-L)*yo(i,1))^2/2+v2(i,1)^2/2/((1-L)+e1)$;
end;
S=S-v1(m8,1)/2/d-v2(m8,1)/2/d;
for i=1:m8-1
u(i,1)=L*(dv1(i,1)+L*yo(i,1))+(1-L)*(dv2(i,1)+(1-L)*yo(i,1));
end;
u(m8,1)=1/2;

****

****

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```
1.  function S1=funMarch24A19(x)
    global m8 d yo e1 v1 v2 v3 v4 dv1 dv2 L u
    L=(sin(x(1,1))+1)/2;
    S=0;
    for i=1:m8-1
    S=S+(v1(i,1))^2/(2*v3(i,1)^2)/2+v3(i,1)^4/2/(L+e1)+v3(i,1)^2+(dv1(i,1)+L*yo(i,1))^2/2+
    v1(i,1)^2/2/(L+e1);
    S=S+(v2(i,1))^2/(2*v4(i,1)^2)/2+v4(i,1)^4/2/((1-L)+e1)+v4(i,1)^2
    S=S+ (dv2(i,1)+(1-L)*yo(i,1))^2/2+v2(i,1)^2/2/((1-L)+e1);
    end;
    S=S-v1(m8,1)/2/d-v2(m8,1)/2/d;
    S1=-S;
```

****

49. A Dual Variational Formulation for the Shape Optimization of a Beam Model

Let $\Omega \subset [0,1] \subset \mathbb{R}$ be the horizontal axis of a straight beam with a variable thickness $H(x)$. Consider the problem of minimizing a relaxed functional $J : V \times [0,1] \times B \to \mathbb{R}$, where

$$\begin{aligned} J(w,\lambda,L_1,L_2) &= \frac{\lambda E_0}{2}\int_\Omega \frac{b}{12}(H(L_1)-(1-\lambda)H_1(L_2))^3 w_{xx}^2\,dx \\ &\quad + \frac{(1-\lambda)E_0}{2}\int_\Omega \frac{b}{12}(H(L_1)+\lambda H_1(L_2))^3 w_{xx}^2\,dx, \end{aligned} \tag{288}$$

subject to

$$\begin{aligned} &\left(\lambda E_0 \frac{b}{12}(H(L_1)-(1-\lambda)H_1(L_2))^3 w_{xx}\right)_{xx} \\ &+\left((1-\lambda)E_0\frac{b}{12}(H(L_1)+\lambda H_1(L_2))^3 w_{xx}\right)_{xx} - P \\ &= 0, \ \text{ in } \Omega. \end{aligned} \tag{289}$$

Here

$$H(x) = L_1(x)h_0,$$
$$H_1(x) = L_2(x)h_0,$$

$h_0 = 0.2m$, $b = 0.15m$, $E_0 = 10^7$ Pa, $P = 400N$.

Also, for a simply supported beam,

$$V = \{w \in W^{2,2}(\Omega) \ : \ w(0) = w_{xx}(0) = w(1) = w_{xx}(1) = 0\},$$

$$\begin{aligned} B &= \Big\{(L_1,L_2) : \Omega \to \mathbb{R}^2 \text{ measurable } : 0.3 \le L_1 \le 1, \\ &\quad -0.7 \le L_2 \le 0.7, \text{ in } \Omega, \int_\Omega L_1(x)\,dx = 0.61 \text{ and } \int_\Omega L_2(x)\,dx = 0\Big\}. \end{aligned} \tag{290}$$

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Moreover, we define $Y = Y^* = L^2(\Omega)$, and

$$\begin{aligned} A &= \{(w,\lambda,L_1,L_2) \in V \times [0,1] \times B \ : \\ &\quad \left(\lambda E_0 \frac{b}{12}(H(L_1) - (1-\lambda)H_1(L_2))^3 w_{xx}\right)_{xx} \\ &\quad + \left((1-\lambda)E_0 \frac{b}{12}(H(L_1) + \lambda H_1(L_2))^3 w_{xx}\right)_{xx} - P \\ &\quad = 0, \quad \text{in } \Omega\}. \end{aligned} \tag{291}$$

Observe that

$$\begin{aligned} &\inf_{(w,\lambda,L_1,L_2)\in A} J(w,\lambda,L_1,L_2) \\ = &\inf_{(\lambda,L_1,L_2)\in[0,1]\times B} \left\{ \sup_{\hat{w}\in V} \left\{ \inf_{w\in V} \{J(w,\lambda,L_1,L_2) \right.\right. \\ &- \left\langle \hat{w}, \left(\lambda E_0 \frac{b}{12}(H(L_1) - (1-\lambda)H_1(L_2))^3 w_{xx}\right)_{xx} \right. \\ &\left.\left.\left. + \left((1-\lambda)E_0 \frac{b}{12}(H(L_1) + \lambda H_1(L_2))^3 w_{xx}\right)_{xx} - P \right\rangle_{L^2} \right\} \right\} \\ = &\inf_{(\lambda,L_1,L_2)\in[0,1]\times B} \left\{ \sup_{\hat{w}\in V} \left\{ \inf_{w\in V} \left\{ \frac{\lambda E_0}{2} \int_\Omega \frac{b}{12}(H(L_1) - (1-\lambda)H_1(L_2))^3 w_{xx}^2 \, dx \right.\right. \right. \\ &+ \frac{(1-\lambda)E_0}{2} \int_\Omega \frac{b}{12}(H(L_1) + \lambda H_1(L_2))^3 w_{xx}^2 \, dx \\ &- \left\langle \hat{w}, \left(\lambda E_0 \frac{b}{12}(H(L_1) - (1-\lambda)H_1(L_2))^3 w_{xx}\right)_{xx} \right. \\ &\left.\left.\left. + \left((1-\lambda)E_0 \frac{b}{12}(H(L_1) + \lambda H_1(L_2))^3 w_{xx}\right)_{xx} - P \right\rangle_{L^2} \right\} \right\} \\ = &\inf_{(\lambda,L_1,L_2)\in[0,1]\times B} \left\{ \sup_{\hat{w}\in V} \left\{ -\frac{\lambda E_0}{2} \int_\Omega \frac{b}{12}(H(L_1) - (1-\lambda)H_1(L_2))^3 \hat{w}_{xx}^2 \, dx \right.\right. \\ &\left.\left. - \frac{(1-\lambda)E_0}{2} \int_\Omega \frac{b}{12}(H(L_1) + \lambda H_1(L_2))^3 \hat{w}_{xx}^2 \, dx + \langle \hat{w}, P \rangle_{L^2} \right\} \right\} \\ = &\inf_{(\lambda,L_1,L_2)\in[0,1]\times B} \left\{ \inf_{(M_1,M_2)\in C^*} \left\{ \frac{1}{2\lambda E_0 b/12} \int_\Omega \frac{(M_1)^2}{(H(L_1) - (1-\lambda)H_1(L_2))^3} \, dx \right.\right. \\ &\left.\left. + \frac{1}{2(1-\lambda)E_0 b/12} \int_\Omega \frac{(M_1)^2}{(H(L_1) + \lambda H_1(L_2))^3} \, dx \right\} \right\}, \end{aligned} \tag{292}$$

where

$$C^* = \{(M_1,M_2) \in Y^* \times Y^* \ : \ (M_1)_{xx} + (M_2)_{xx} + P = 0, \text{ in } \Omega\}.$$

We have obtained numerical results through the following algorithm. It is worth highlighting the convergence criterion in this software slightly differs from the one in the algorithm.

1. Set $n = 1$, $\varepsilon = 10^{-4}$ and $(L_1)_n \equiv 1/2$, $(L_2)_n \equiv 0.1$, $\lambda_n = 1/2$.
2. Calculate $w_n \in V$ such that

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$$\left(\lambda_n E_0 \frac{b}{12}(H((L_1)_n) - (1-\lambda)H_1((L_2)_n))^3 (w_n)_{xx}\right)_{xx}$$
$$+\left((1-\lambda_n)E_0 \frac{b}{12}(H((L_1)_n) + \lambda H_1((L_2)_n))^3 (w_n)_{xx}\right)_{xx} - P$$
$$= 0, \quad \text{in } \Omega, \tag{293}$$

3. Calculate $\lambda_{n+1} \in [0,1]$ such that

$$J(w_n, \lambda_{n+1}, (L_1)_n, (L_2)_n) = \inf_{\lambda \in [0,1]} J((w_n, \lambda, (L_1)_n, (L_2)_n).$$

4. Calculate $((L_1)_{n+1}, (L_2)_{n+1}) \in B$ such that

$$J^*((M_1)_n, (M_2)_n, \lambda_{n+1}, (L_1)_{n+1}, (L_2)_{n+1}) = \inf_{(L_1,L_2)\in B} J^*((M_1)_n, (M_2)_n, \lambda_{n+1}, L_1, L_2),$$

where

$$(M_1)_n = -\lambda_{n+1} E_0 \frac{b}{12}(H((L_1)_n) - (1-\lambda_{n+1})(L_2)_n)^3 (w_n)_{xx},$$

$$(M_2)_n = -(1-\lambda_{n+1}) E_0 \frac{b}{12}(H((L_1)_n) + \lambda_{n+1}(L_2)_n)^3 (w_n)_{xx},$$

and

$$J^*(M_1, M_2) = \frac{1}{2\lambda E_0 b/12} \int_\Omega \frac{(M_1)^2}{(H(L_1) - (1-\lambda)H_1(L_2))^3}\, dx$$
$$+ \frac{1}{2(1-\lambda)E_0 b/12} \int_\Omega \frac{(M_2)^2}{(H(L_1) + \lambda H_1(L_2))^3}\, dx. \tag{294}$$

5. If

$$\|((L_1)_{n+1}, (L_2)_{n+1}) - ((L_1)_n, (L_2)_n\|_\infty < \varepsilon,$$

then stop, otherwise $n := n+1$ and go to item 2.

We have obtained numerical results for a case A with the constant values above specified. For the optimal solution $L_1(x)$, please see Figure 39.

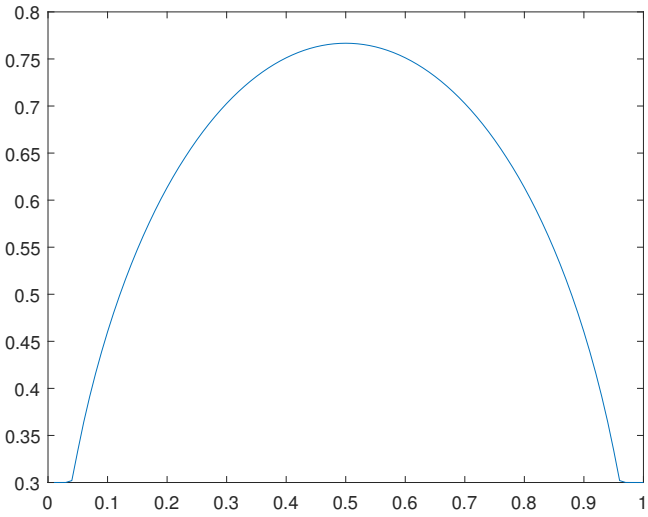

Figure 39. Optimal solution $L_1(x)$ for the case A.

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Here we present the software in MATLAB through which we have obtained such results.

****

1.
```
clear all
global m8 d yo u L1 L2 ho Eo B L H H1 Ho Ho1
m8=100;
d=1/m8;
P=400;
Eo=10^7;
for i=1:m8 yo(i,1)=P; end;
ho=0.20;
B=0.15;
for i=1:m8
L1(i,1)=1/2;
L2(i,1)=0.3;
uo(i,1)=0.1;
Ho(i,1)=L1(i,1)*ho;
Ho1(i,1)=0.1*L2(i,1)*ho;
end;
L=1/2;
for i=1:m8
H(i,1)=L1(i,1)*ho;
H1(i,1)=L2(i,1)*ho;
end;
for i=1:2*m8
xo(i,1)=0.3;
end;
x1(1,1)=1/2;
A=zeros(2*m8,2*m8);
for i=1:m8
A(1,i)=1.0;
A(2,i+m8)=1.0;
end;
b=zeros(2*m8,1);
b(1,1)=m8*0.61;
for i=1:m8
lb(i,1)=0.3;
lb(i+m8,1)=-0.7;
end;
for i=1:m8
```

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ub(i,1)=1;

ub(i+m8,1)=0.7;

end;

i=1;

m12=2;

m50(i)=1/m12;

z(i)=$m50(i)*(-yo(i,1)*d^2)$;

for i=2:m8-1

m12=2-m50(i-1);

m50(i)=1/m12;

z(i)=$m50(i)*(-yo(i,1)*d^2+z(i-1))$;

end;

v(m8,1)=0;

for i=1:m8-1

v(m8-i,1)=m50(m8-i)*v(m8-i+1,1)+z(m8-i);

end;

k1=1;

b14=1.0;

while $(b14>10^{-4})$ && $(k1<15)$

k1

k1=k1+1;

for i=1:m8

y1(i,1)=$v(i,1)/(Eo*L*B/12*(H(i,1)-(1-L)*H1(i,1))^3+Eo*(1-L)*B/12*(H(i,1)+L*H1(i,1))^3)$;

end;

i=1;

m12=2;

m60(i)=1/m12;

z1(i)=$m60(i)*(-y1(i,1)*d^2)$;

for i=2:m8-1

m12=2-m60(i-1);

m60(i)=1/m12;

z1(i)=$m60(i)*(-y1(i,1)*d^2+z1(i-1))$;

end;

u(m8,1)=0;

for i=1:m8-1

u(m8-i,1)=m60(m8-i)*u(m8-i+1)+z1(m8-i);

end;

k=1;

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b12=1.0;

while $(b12 > 10^{-4})$ && $(k < 100)$

k

k=k+1;

X=fmincon('funMarch2024Beam1',xo,[ ],[ ],A,b,lb,ub);

b12=abs(max(xo-X))

xo=X;

L1(m8/2,1)

end;

Ho=H;

Ho1=H1;

X1=fminunc('funMarch2024Beam2',x1);

x1=X1;

b14=max(abs(u-uo))

uo=u;

end;

for i=1:m8

x(i,1)=i*d;

end;

plot(x,L1);

****

With the auxiliary function "funMarch2024Beam1"

****

1. function S1=funMarch2024Beam1(x)

global m8 d yo u L1 L2 ho Eo B L Ho Ho1

for i=1:m8

L1(i,1)=x(i,1);

L2(i,1)=x(i+m8,1);

end;

d2u(1,1)=$(-2 * u(1,1) + u(2,1))/d^2$;

for i=2:m8-1

d2u(i,1)=$(u(i+1,1) - 2 * u(i,1) + u(i-1,1))/d^2$;

end;

for i=1:m8

H(i,1)=L1(i,1)*ho;

H1(i,1)=L2(i,1)*ho;

end;

S=0;

for i=1:m8-1

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S=S+$L*(Eo*B/12*(Ho(i,1)-(1-L)*Ho1(i,1))^3*d2u(i,1))^2/(Eo*B/12*(H(i,1)-(1-L)*H1(i,1))^3)$;

S=S+$(1-L)*(Eo*B/12*(Ho(i,1)+L*Ho1(i,1))^3*d2u(i,1))^2/(Eo*B/12*(H(i,1)+L*H1(i,1))^3)$;

end;

S1=S;

****

And the auxiliary function "funMarch2024Beam2"

****

1. function S=funMarch2024Beam2(x)

global m8 d yo u L1 L2 ho Eo B L Ho Ho1

L=(sin(x(1,1))+1)/2;

d2u(1,1)=$(-2*u(1,1)+u(2,1))/d^2$;

for i=2:m8-1

d2u(i,1)=$(u(i+1,1)-2*u(i,1)+u(i-1,1))/d^2$;

end; for i=1:m8

H(i,1)=L1(i,1)*ho;

H1(i,1)=L2(i,1)*ho;

end;

S=0;

for i=1:m8-1

S=S+$L*Eo*B/12*(H(i,1)-(1-L)*H1(i,1))^3*d2u(i,1)^2$;

S=S +$(1-L)*Eo*B/12*(H(i,1)+L*H1(i,1))^3*d2u(i,1)^2$;

end;

****

50. A Dual Variational Formulation for a Relaxed Primal Formulation Related to a Shape Optimization Model in Elasticity

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the problem of minimizing a relaxed functional $J : V \times [0,1] \times B \to \mathbb{R}$ where

$$J(u,\lambda,\lambda_1,\lambda_2) = \frac{1}{2}\int_\Omega H_{ijkl}(\lambda,\lambda_1(x),\lambda_2(x))e_{ij}(\mathbf{u})e_{kl}(\mathbf{u})\,dx,$$

subject to

$$(H_{ijkl}(\lambda,\lambda_1(x),\lambda_2(x))e_{kl}(\mathbf{u}))_{,j} + f_i = 0, \text{ in } \Omega, \ \forall i\{1,2,3\}.$$

Here for simplicity $V = W_0^{1,2}(\Omega;\mathbb{R}^3)$, $Y = Y^* = L^2(\Omega;\mathbb{R}^3)$, $Y_1 = Y_1^* = L^2(\Omega;\mathbb{R}^{3\times3})$, and $f \in L^2(\Omega;\mathbb{R}^3)$.

Also, $\mathbf{u} = (u_1,u_2,u_3) \in V$ denotes the field of displacements resulting from the action of f,

$$\{e_{ij}(\mathbf{u})\} = \left\{\frac{1}{2}(u_{i,j}+u_{j,i})\right\}, \ \forall i,j \in \{1,2,3\},$$

and $E_b \le E(\lambda,\lambda_1,\lambda_2) \le E_a$, $E_a \gg E_b > 0$, where $\lambda_1(x) = 1$ corresponds to the presence of a stronger material with Young modulus E_a at the point $x \in \Omega$. Moreover, $\lambda_1(x) = 0$ corresponds to the presence

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of a much weaker material with elasticity model E_b, simulating a void space at the point $x \in \Omega$. On the other hand, λ and $\lambda_2(x)$ are a real parameter and a function related to the relaxation process for the minimization of J in λ_1.

Furthermore,

$$\begin{aligned} E(\lambda,\lambda_1(x),\lambda_2(x)) &= \lambda[(\lambda_1(x)-(1-\lambda)\lambda_2(x))^3E_a+(1-(\lambda_1(x)-(1-\lambda)\lambda_2(x)))^3E_b] \\ &\quad +(1-\lambda)[(\lambda_1(x)+\lambda\lambda_2(x))^3E_a+(1-(\lambda_1(x)+\lambda\lambda_2(x)))^3E_b], \end{aligned} \tag{295}$$

$$H_{ijkl}(\lambda,\lambda_1(x),\lambda_2(x)) = E(\lambda,\lambda_1(x),\lambda_2(x))\mathcal{A}_{ijkl},$$

where

$$\mathcal{A}_{ijkl} = \tilde{\lambda}\delta_{ij}\delta_{kl}+\tilde{\mu}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}),$$

$\forall i,j,k,l \in \{1,2,3\}$.

Here $\{\delta_{ij}\}$ is the Kronecker delta and $\tilde{\lambda} > 0$, $\tilde{\mu} > 0$ are appropriate real constants.

At this point we define

$$\begin{aligned} B &= \Big\{(\lambda_1,\lambda_2) : \Omega \to \mathbb{R}^2 \text{ measurable } : 0 \le \lambda_1(x) \le 1, \\ &\quad -0.8 \le \lambda_2(x) \le 0.8, \text{ in } \Omega, \int_\Omega \lambda_1(x)\,dx = c_0 Vol(\Omega), \int_\Omega \lambda_2(x)\,dx = 0\Big\}, \end{aligned} \tag{296}$$

and

$$\begin{aligned} A &= \{(u,\lambda,\lambda_1,\lambda_2) \in V\times[0,1]\times B : \\ &\quad (H_{ijkl}(\lambda,\lambda_1,\lambda_2)e_{kl}(\mathbf{u}))_{,j}+f_i = 0, \text{ in } \Omega, \ \forall i \in \{1,2,3\}\}. \end{aligned} \tag{297}$$

Observe that

$$\begin{aligned} &\inf_{(u,\lambda,\lambda_1,\lambda_2)\in A} J(u,\lambda,\lambda_1,\lambda_2) \\ &= \inf_{(\lambda,\lambda_1,\lambda_2)\in[0,1]\times B}\left\{\sup_{\hat{u}\in V}\left\{\inf_{u\in V}\left\{J(u,\lambda,\lambda_1,\lambda_2)+\langle\hat{u}_i,(H_{ijkl}(\lambda,\lambda_1,\lambda_2)e_{kl}(\mathbf{u}))_j+f_i\rangle_{L^2}\right\}\right\}\right\} \\ &= \inf_{(\lambda,\lambda_1,\lambda_2)\in[0,1]\times B}\left\{\sup_{\hat{u}\in V}\left\{\inf_{u\in V}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(\lambda,\lambda_1,\lambda_2)e_{ij}(\mathbf{u})e_{kl}(\mathbf{u})\,dx\right.\right.\right. \\ &\quad \left.\left.\left.+\langle\hat{u}_i,(H_{ijkl}(\lambda,\lambda_1,\lambda_2)e_{kl}(\mathbf{u}))_j+f_i\rangle_{L^2}\right\}\right\}\right\} \\ &= \inf_{(\lambda,\lambda_1,\lambda_2)\in[0,1]\times B}\left\{\sup_{\hat{u}\in V}\left\{-\frac{1}{2}\int_\Omega H_{ijkl}(\lambda,\lambda_1,\lambda_2)e_{ij}(\hat{\mathbf{u}})e_{kl}(\hat{\mathbf{u}})\,dx+\langle\hat{u}_i,f_i\rangle_{L^2}\right\}\right\} \\ &= \inf_{(\lambda,\lambda_1,\lambda_2)\in[0,1]\times B}\left\{\inf_{\sigma\in C^*}\left\{\frac{1}{2}\int_\Omega \overline{H_{ijkl}(\lambda,\lambda_1,\lambda_2)}\sigma_{ij}\sigma_{kl}\,dx\right\}\right\}, \end{aligned} \tag{298}$$

where

$$\{\overline{H_{ijkl}(\lambda,\lambda_1,\lambda_2)}\} = \{H_{ijkl}(\lambda,\lambda_1,\lambda_2)\}^{-1}$$

in an appropriate tensor sense and

$$C^* = \{\sigma=\{\sigma_{ij}\} \in Y_1^* \ : \ \sigma_{ij,j}+f_i = 0, \text{ in } \Omega, \ \forall i \in \{1,2,3\}\}.$$

We have obtained numerical results concerning the optimal shape of a two-dimensional beam though the following algorithm:

1. Set $n = 1$, $\varepsilon = 10^{-4}$, $\lambda_n = 1/2$, $(\lambda_1)_n(x) \equiv 1/2$, $(\lambda_2)_n(x) \equiv 0$.

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2. Calculate $\mathbf{u}_n \in V$ such that

$$(H_{ijkl}(\lambda_n, (\lambda_1)_n, (\lambda_2)_n)e_{kl}(\mathbf{u}_n))_{,j} + f_i = 0, \text{ in } \Omega, \ \forall i \in \{1,2,3\}.$$

3. Calculate $\lambda_{n+1} \in [0,1]$ such that

$$J(\mathbf{u}_n, \lambda_{n+1}, (\lambda_1)_n, 0) = \inf_{\lambda \in [0,1]} \{J(\mathbf{u}_n, \lambda, (\lambda_1)_n, 0)\}.$$

4. Calculate $((\lambda_1)_{n+1}, (\lambda_2)_{n+1}) \in B$ such that

$$-J(\mathbf{u}_n, \lambda_{n+1}, (\lambda_1)_{n+1}, (\lambda_2)_{n+2}) = \inf_{(\lambda_1,\lambda_2)\in B} \{-J(\mathbf{u}_n, \lambda_{n+1}, \lambda_1, \lambda_2)\}.$$

5. Set $(\lambda_2)_{n+1} \equiv 0$.
6. If $\|(\lambda_1)_{n+1} - (\lambda_1)_n\|_\infty \leq \varepsilon$, then stop. Otherwise $n := n+1$ and go to item 2.

We developed numerical results for a two-dimensional beam, in a two-dimensional elasticity context for two cases, namely, case A and case B.

For the case A we consider a two-dimensional beam of dimensions $1m \times 0.5m$, clamped at $x = 0$ and with a vertical load of $P = -42000000\ (4)\ 500\mathbf{j}$ applied to the point $(x_0, y_0) = (1,\ 0.25)$.

For the case B, we consider a a two-dimensional beam of dimensions $1m \times 0.5m$, simply supported at $(x, y) = (0,0)$ and $(x, y) = (1,0)$, with a vertical load $P = -42000000\ 500\mathbf{j}$ applied to the point $(x_0, y_0) = (1/3,\ 0.5)$.

Denoting $\mathbf{u} = (u, v)$, for both cases we define the strain tensor as

$$e(\mathbf{u}) = (e_x(\mathbf{u}), e_y(\mathbf{u}), e_{xy}(\mathbf{u}))^T,$$

where $e_x(\mathbf{u}) = u_x$, $e_y(\mathbf{u}) = v_y$, and

$$e_{xy}(\mathbf{u}) = \frac{1}{2}(u_y + v_x).$$

We also set $E_a = 205\ 10^9\ P_a$ and $E_b = 300\ P_a$, $\nu = 0.33$ and $c_0 = 0.6091$ for both the cases.

Moreover the stress tensor σ is given by

$$\sigma = H(e(\mathbf{u})),$$

where

$$H = \frac{E(\lambda, \lambda_1(x), \lambda_2(x))}{1-\nu^2} \begin{Bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1}{2}(1-\nu) \end{Bmatrix}. \tag{299}$$

For the optimal shape obtained through λ_1 for the case A, please see Figure 40.

For the optimal shape obtained through λ_1 for the case B, please see Figure 41.

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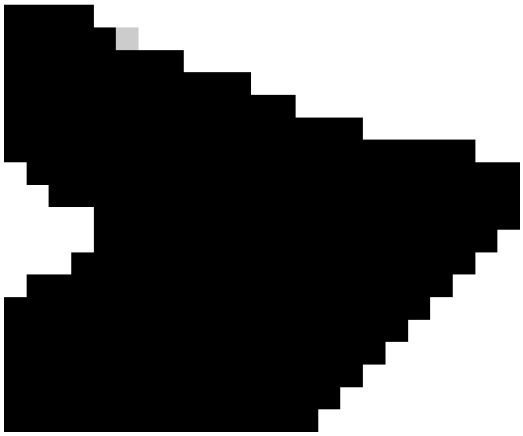

Figure 40. Optimal shape $\lambda_1(x,y)$ for the beam of case A.

Figure 41. Optimal shape $\lambda_1(x,y)$ for the beam of case B.

Here we present the software through which we have obtained such results, in a finite differences context for the case B.

We highlight the convergence criterion in the software is a little different from the one in the algorithm above described.

****

1. clear all

   global P m8 d w Ea Eb Lo d1 z1 m9 du1 du2 dv1 dv2 c3 Lo1 L u v

   m8=24;

   m9=22;

   c3=0.95;

   d=1.0/m8;

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```
d1=0.50/m9;
Ea=410 * 10^6 * 500;
Eb=300;
w=0.30;
P=-42000000*500;
z1=(m8-1)*(m9-1);
A3=zeros(2*z1,2*z1);
for i=1:z1
A3(1,i)=1.0;
A3(2,i+z1)=1.0;
end;
L=1/2;
b=zeros(2*z1,1);
b(1,1)=c3*z1;
for i=1:z1
uo(i,1)=0.0;
uo(i+z1,1)=-0.80;
end;
for i=1:z1
u1(i,1)=1.0;
u1(i+z1,1)=0.80;
end;
for i=1:m9-1
for j=1:m8-1
Lo(i,j)=c3;
Lo1(i,j)=0.1*c3;
end;
end;
for i=1:z1*2
x1(i,1)=c3*z1;
end;
x3(1,1)=1/2;
for i=1:4*m8*m9
xo(i,1)=0.000;
end;
xw=xo;
xv=Lo;
for k2=1:22
c3=0.98*c3;
```

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b(1,1)=c3*z1;

k2

b14=1.0;

k3=0;

while $(b14 > 10^{-3.5})$ && $(k3 < 5)$

k3=k3+1;

b12=1.0;

k=0;

while $(b12 > 10^{-4.0})$ && $(k < 120)$

k=k+1;

k2

k3

k

X=fminunc('funbeamMarch24',xo); xo=X;

b12=max(abs(xw-xo))

xw=X;

end;

X1=fminunc('funbeamMarch24A1',x3);

x3=X1;

for i=1:m9-1

for j=1:m8-1

E1=$3 * L * ((Lo(i,j) - (1 - L) * Lo1(i,j))^2 * Ea - (1 - (Lo(i,j) - (1 - L) * Lo1(i,j)))^2 * Eb);$

E1=E1+$3 * (1 - L) * ((Lo(i,j) + L * Lo1(i,j))^2 * Ea - (1 - (Lo(i,j) + L * Lo1(i,j)))^2 * Eb);$

E2=$3 * L * (Lo(i,j) - (1 - L) * Lo1(i,j))^2 * Ea * (-(1 - L)) - (1 - (Lo(i,j) - (1 - L) * Lo1(i,j)))^2 * Eb * (-(1 - L));$

E2=E2+$3 * (1 - L) * ((Lo(i,j) + L * Lo1(i,j))^2 * Ea * L - (1 - (Lo(i,j) + L * Lo1(i,j)))^2 * Eb * L);$

ex=du1(i,j);

ey=dv2(i,j);

exy=1/2*(dv1(i,j)+du2(i,j));

Sx1=$E1 * (ex + w * ey)/(1 - w^2);$

Sy1=$E1 * (w * ex + ey)/(1 - w^2);$

Sxy1=$E1/(2 * (1 + w)) * exy;$

Sx2=$E2 * (ex + w * ey)/(1 - w^2);$

Sy2=$E2 * (w * ex + ey)/(1 - w^2);$

Sxy2=$E2/(2 * (1 + w)) * exy;$

dc31(i,j)=-(Sx1*ex+Sy1*ey+2*Sxy1*exy);

dc32(i,j)=-(Sx2*ex+Sy2*ey+2*Sxy2*exy);

end;

end;

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```
for i=1:m9-1
for j=1:m8-1
f(j+(i-1)*(m8-1))=dc31(i,j);
f((m9-1)*(m8-1)+j+(i-1)*(m8-1))=dc32(i,j);
end;
end;
for k1=1:1
k1
X1=linprog(f,[ ],[ ],A3,b,uo,u1,x1);
x1=X1;
end;
for i=1:z1
x1(i+z1,1)=0;
end;
for i=1:m9-1
for j=1:m8-1
Lo(i,j)=X1(j+(m8-1)*(i-1));
Lo1(i,j)=X1((m8-1)*(m9-1)+j+(m8-1)*(i-1))*0.0;
end;
end;
b14=max(max(abs(Lo-xv)))
xv=Lo;
colormap(gray); imagesc(-Lo); axis equal; axis tight; axis off;pause(1e-6)
end;
end;
```

****

With the auxiliary function "funbeamMarch24"

****

1.
```
function S=funbeamMarch24(x)
global P m8 d w u v Ea Eb Lo d1 m9 du1 du2 dv1 dv2 Lo1 L
for i=1:m9
for j=1:m8
u(i,j)=x(j+(m8)*(i-1));
v(i,j)=x(m8*m9+(i-1)*m8+j);
end;
end;
u(m9-1,1)=0; v(m9-1,1)=0; u(m9-1,m8-1)=0; v(m9-1,m8-1)=0;
for i=1:m9-1
for j=1:m8-1
```

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du1(i,j)=(u(i,j+1)-u(i,j))/d;
du2(i,j)=(u(i+1,j)-u(i,j))/d1;
dv1(i,j)=(v(i,j+1)-v(i,j))/d;
dv2(i,j)=(v(i+1,j)-v(i,j))/d1;
end;
end;
S=0;
for i=1:m9-1
for j=1:m8-1
E1=$L*((Lo(i,j)-(1-L)*Lo1(i,j))^3*Ea+(1-(Lo(i,j)-(1-L)*Lo1(i,j)))^3*Eb)$;
E2=$(1-L)*((Lo(i,j)+L*Lo1(i,j))^3*Ea+(1-(Lo(i,j)+L*Lo1(i,j)))^3*Eb)$;
ex=du1(i,j);
ey=dv2(i,j);
exy=1/2*(dv1(i,j)+du2(i,j));
Sx=$(E1+E2)*(ex+w*ey)/(1-w^2)$;
Sy=$(E1+E2)*(w*ex+ey)/(1-w^2)$;
Sxy=$(E1+E2)/(2*(1+w))*exy$;
S=S+1/2*(Sx*ex+Sy*ey+2*Sxy*exy);
end;
end;
S=S*d*d1-P*v(2,(m8)/3)*d*d1;
****
And the auxiliary function "funbeamMarch24A1"

****

1. function S1=funbeamMarch24A1(x)
global P m8 d w u v Ea Eb Lo d1 m9 du1 du2 dv1 dv2 L Lo1
L=(sin(x(1,1))+1)/2;
for i=1:m9-1
for j=1:m8-1
du1(i,j)=(u(i,j+1)-u(i,j))/d;
du2(i,j)=(u(i+1,j)-u(i,j))/d1;
dv1(i,j)=(v(i,j+1)-v(i,j))/d;
dv2(i,j)=(v(i+1,j)-v(i,j))/d1;
end;
end;
S=0;
for i=1:m9-1
for j=1:m8-1
E1=$L*((Lo(i,j)-(1-L)*Lo1(i,j))^3*Ea+(1-(Lo(i,j)-(1-L)*Lo1(i,j)))^3*Eb)$;

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E2=$(1-L)*((Lo(i,j)+L*Lo1(i,j))^3*Ea+(1-(Lo(i,j)+L*Lo1(i,j)))^3*Eb)$;

ex=du1(i,j);

ey=dv2(i,j);

exy=1/2*(dv1(i,j)+du2(i,j));

Sx=$(E1+E2)*(ex+w*ey)/(1-w^2)$;

Sy=$(E1+E2)*(w*ex+ey)/(1-w^2)$;

Sxy=$(E1+E2)/(2*(1+w))*exy$;

S=S+1/2*(Sx*ex+Sy*ey+2*Sxy*exy);

end;

end;

S1=S;

****

51. An Existence Result for a General Parabolic Non-Linear Equation

Let $\Omega \subset \mathbb{R}^m$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the parabolic non-linear equation

$$\begin{cases} \frac{\partial u}{\partial t} = \varepsilon\nabla^2 u + g(u) + \sum_{j=1}^m g_j(u)\frac{\partial u}{\partial x_j} + f, \quad \text{in } \Omega\times(0,T), \\ u(x,0) = \hat{u}_0, \text{ in } \Omega, \\ u = 0, \text{ on } \partial\Omega\times[0,T]. \end{cases} \tag{300}$$

Here $\varepsilon > 0$, $f \in L^2([0,T], W^{1,2}(\Omega)) \cap L^\infty(\Omega\times[0,T])$, $\hat{u}_0 \in H_0^1(\Omega)\cap L^\infty(\Omega)$, where t denotes time and $[0,T]$ is a time interval.

Also $g : \mathbb{R} \to \mathbb{R}$ and $g_j : \mathbb{R} \to \mathbb{R}$ are continuous functions neither necessarily linear nor convex, $\forall j \in \{1,\cdots,m\}$.

We assume there exist $K_{33} > 0$ and $K_1 > 0$ such that

$$\|g\|_\infty \leq \frac{K_{33}}{m(\Omega)^{1/2}},$$

$$\|g_j\|_\infty \leq \frac{K_1}{m},$$

$\forall j \in \{1,\cdots,n\}$.

At this point, we recall that fixing $\gamma > 0$,

$$(I_d - \gamma\nabla^2)^{-1} : L^2(\Omega) \to H_0^1(\Omega)$$

is a bounded and linear operator, so that for each $h \in L^2(\Omega)$ there exists a unique $u \in H_0^1(\Omega)$ such that

$$(I_d - \gamma\nabla^2)u = h.$$

In such a case we denote

$$u = (I_d - \gamma\nabla^2)^{-1}h,$$

so that

$$\|u\|_{1,2,\Omega} \leq \|(I_d - \gamma\nabla^2)^{-1}\|\|h\|_{0,2,\Omega}.$$

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Moreover, fixing $N \in \mathbb{N}$ and defining

$$\Delta t_N = \frac{T}{N},$$

in a partial finite differences context, discretizing in t consider the approximate equation system

$$\frac{u_{n+1} - u_n}{\Delta t_N} = \varepsilon \nabla^2 u_{n+1} + g(u_n) + \sum_{j=1}^{m} g_j(u_n)(u_n)_{x_j} + f_n, \text{ in } \Omega,$$

$\forall n \in \{0, 1, \cdots, N-1\}$.

From such a system, for $n = 0$, we obtain

$$u_1 - \hat{u}_0 = \varepsilon \nabla^2 (u_1) \Delta t_N + g(\hat{u}_0) \Delta t_N + \sum_{j=1}^{m} g_j(\hat{u}_0)(\hat{u}_0)_{x_j} \Delta t_N + f_0 \Delta t_N.$$

Hence

$$u_1 = (I_d - \varepsilon(\nabla^2)\Delta t_N)^{-1} \left(\hat{u}_0 + g(\hat{u}_0)\Delta t_N + \sum_{j=1}^{m} g_j(\hat{u}_0)(\hat{u}_0)_{x_j} \Delta t_N + f_0 \Delta t_N \right),$$

so that

$$\begin{aligned} & \|u_1\|_{1,2,\Omega} \\ \leq \; & \|(I_d - \varepsilon(\nabla^2)\Delta t_N)^{-1}\| \\ & \times \left(\|\hat{u}_0\|_{0,2,\Omega} + \|g(\hat{u}_0)\|_{0,2,\Omega} \Delta t_N + \sum_{j=1}^{m} \|g_j(\hat{u}_0)(\hat{u}_0)_{x_j}\|_{0,2,\Omega} \, \Delta t_N + \|f_0\|_{0,2,\Omega} \Delta t_N \right). \end{aligned} \tag{301}$$

Observe that there exists $K_2 > 0$ such that $\|f\|_{\infty,\Omega\times[0,T]} \leq K_2$ so that

$$\|f_n\|_{1,2,\Omega} \leq K_{36}, \; \forall n \in \{0, 1, \cdots, N-1\},$$

for some appropriate $K_{36} > 0$.

From such results and the hypotheses, we may infer that

$$\begin{aligned} & \|u_1\|_{1,2,\Omega} \leq \|(I_d - \varepsilon(\nabla^2)\Delta t_N)^{-1}\| (\|\hat{u}_0\|_{1,2,\Omega} + K_{33}\Delta t_N + K_1 \|\hat{u}_0\|_{1,2,\Omega} \Delta t_N + K_{36}\Delta t_N) \\ \leq \; & \|(I_d - \varepsilon(\nabla^2)\Delta t_N)^{-1}\| (\|\hat{u}_0\|_{1,2,\Omega} + K_1 \|\hat{u}_0\|_{1,2,\Omega} \Delta t_N + K_3 \Delta t_N), \end{aligned} \tag{302}$$

where

$$K_3 = K_{33} + K_{36},$$

so that

$$\|u_1\|_{1,2,\Omega} \leq \alpha_1 \|\hat{u}_0\|_{1,2,\Omega} + \alpha_2,$$

where

$$\alpha_1 = \|(I_d - \varepsilon(\nabla^2)\Delta t_N)^{-1}\| (1 + K_1 \Delta t_N),$$

and

$$\alpha_2 = \|(I_d - \varepsilon(\nabla^2)\Delta t_N)^{-1}\| K_3 \Delta t_N.$$

In fact, generically we may similarly obtain

$$\|u_{n+1}\|_{1,2,\Omega} \leq \alpha_1 \|u_n\|_{1,2,\Omega} + \alpha_2,$$

$\forall n \in \{0, 1, \cdots, N-1\}$.

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From such a result, inductively we may obtain

$$\|u_j\|_{1,2,\Omega} \leq (\alpha_1)^j \|\hat{u}_0\|_{1,2,\Omega} + \sum_{k=0}^{j-1} \alpha_1^k \alpha_2.$$

In particular for $j = N$, we get

$$\begin{aligned} & \|u_N\|_{1,2,\Omega} \\ \leq\ & (\alpha_1)^N \|\hat{u}_0\|_{1,2,\Omega} + \sum_{k=0}^{N-1} \alpha_1^k \alpha_2 \\ =\ & (\alpha_1)^N \|\hat{u}_0\|_{1,2,\Omega} + \frac{1-\alpha_1^N}{1-\alpha_1}\alpha_2 \\ =\ & \left\| \left(I_d - \varepsilon(\nabla^2)\frac{T}{N} \right)^{-1} \right\|^N \left(1 + K_1 \frac{T}{N} \right)^N \|\hat{u}_0\|_{1,2,\Omega} \\ & + \frac{1-\alpha_1^N}{1-\alpha_1}\alpha_2. \end{aligned} \tag{303}$$

Observe that

$$\begin{aligned} & \left\| \left(I_d - \varepsilon(\nabla^2)\frac{T}{N} \right)^{-1} \right\|^N \left(1 + K_1 \frac{T}{N} \right)^N \\ \leq\ & \left(1 + K_1 \frac{T}{N} \right)^N \\ \to\ & e^{K_1 T}, \text{ as } N \to \infty. \end{aligned} \tag{304}$$

Also,

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$$
\begin{aligned}
& \left|\frac{\alpha_2}{1-\alpha_1}\right| \\
= & \frac{\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\| K_3\frac{T}{N}}{|1-\alpha_1|} \\
\leq & \frac{K_3\frac{T}{N}}{|1-\alpha_1|} \\
= & \frac{K_3\frac{T}{N}}{\left|1-\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|\left(1+K_1\frac{T}{N}\right)\right|} \\
= & \frac{K_3}{\frac{N}{T}\left|1-\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|\left(1+K_1\frac{T}{N}\right)\right|} \\
= & \frac{K_3}{\left|\frac{N}{T}-\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1+1\right)\left(\frac{N}{T}+K_1\right)\right|} \\
= & \frac{K_3}{\left|\frac{N}{T}-\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)\left(\frac{N}{T}+K_1\right)-\frac{N}{T}-K_1\right|} \\
= & \\
= & \frac{K_3}{\left|-\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)\left(\frac{N}{T}\right)-K_1-\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
= & \\
= & \frac{K_3}{\left|-\left(\left\|I_d+\sum_{j=1}^{\infty}\left(\varepsilon(\nabla^2)\frac{T}{N}\right)^j\right\|-1\right)\left(\frac{N}{T}\right)-K_1-\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
= & \frac{K_3}{\left|K_1+\left(\left\|I_d+\sum_{j=1}^{\infty}\left(\varepsilon(\nabla^2)\frac{T}{N}\right)^j\right\|-1\right)\left(\frac{N}{T}\right)+\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
\leq & \frac{K_3}{\left|K_1+\left(\|I_d\|-\left\|\sum_{j=1}^{\infty}\left(\varepsilon(\nabla^2)\frac{T}{N}\right)^j\right\|-1\right)\left(\frac{N}{T}\right)+\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
\leq & \frac{K_3}{\left|K_1+\left(\|I_d\|-\sum_{j=1}^{\infty}\left\|\varepsilon(\nabla^2)\frac{T}{N}\right\|^j-1\right)\left(\frac{N}{T}\right)+\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
\leq & \frac{K_3}{\left|K_1-\left(\sum_{j=1}^{\infty}\left\|\varepsilon(\nabla^2)\frac{T}{N}\right\|^j\right)\left(\frac{N}{T}\right)+\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
\leq & \frac{K_3}{\left|K_1-\frac{\|\varepsilon(\nabla^2)\|}{1-\|\varepsilon\nabla^2\|\frac{T}{N}}+\left(\left\|\left(I_d-\varepsilon(\nabla^2)\frac{T}{N}\right)^{-1}\right\|-1\right)K_1\right|} \\
\to & \frac{K_3}{|K_1-\|\varepsilon(\nabla^2)\||}, \text{ as } N\to\infty. \qquad (305)
\end{aligned}
$$

From such results we may infer that

$$
\left|\frac{(1-\alpha_1^N)\alpha_2}{1-\alpha_1}\right| \leq (1+\alpha_1^N)\left|\frac{\alpha_2}{1-\alpha_1}\right|,
$$

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so that

$$\limsup_{N\to\infty}\left|\frac{(1-\alpha_1^N)\alpha_2}{1-\alpha_1}\right| \leq \frac{(1+e^{K_1T})K_3}{|K_1-\|\varepsilon\nabla^2\||}.$$

From these results, denoting now more generically $u_n \equiv u_n^N$ joining the pieces, we have got

$$\limsup_{N\to\infty}\|u_N^N\|_{1,2,\Omega} \leq e^{K_1T}\|\hat{u}_0\|_{1,2,\Omega} + \frac{(1+e^{K_1T})K_3}{|K_1-\|\varepsilon\nabla^2\||}.$$

Consequently, we may infer that there exists $K_4 > 0$ such that

$$\|u_j^N\|_{1,2,\Omega} \leq K_4,\ \forall j \in \{0,1,\cdots,N\}, \forall N \in \mathbb{N}.$$

Define now

$$u_0^N(x,t) = u_n^N(x)\left(n+1-\frac{t}{\Delta t_N}\right) + u_{n+1}^N(x)\left(\frac{t}{\Delta t_N}-n\right),$$

if $t \in [n\Delta t_N, (n+1)\Delta t_N],\ \forall (x,t) \in \Omega\times[0,T]$.

Observe that

$$u_0^N(x,t) = u_n^N(x),\ \text{if } t = n\Delta t_N,\ \forall n \in \{0,1,\cdots,N\},$$

and

$$\begin{aligned}\frac{\partial u_0^N(x,t)}{\partial t} &= \frac{u_{n+1}^N - u_n^N}{\Delta t_N}\\ &= \varepsilon\nabla^2 u_{n+1}^N + g(u_n^N) + \sum_{j=1}^m g_j(u_n^N)(u_n^N)_{x_j} + f_n, \end{aligned} \tag{306}$$

if $t \in [n\Delta t_N, (n+1)\Delta t_N],\ \forall (x,t) \in \Omega\times[0,T]$.

Fix $\varphi \in C_c^\infty(\Omega)$.

Thus, fixing $t \in [n\Delta t_N, (n+1)\Delta t_N]$, we have

$$\begin{aligned}\left|\left\langle\frac{\partial u_0^N}{\partial t},\varphi\right\rangle_{L^2}\right| &\leq \varepsilon|\langle\nabla u_{n+1}^N,\nabla\varphi\rangle_{L^2}| + |\langle g(u_n^N),\varphi\rangle_{L^2}|\\ &\quad + \int_\Omega\left|\sum_{j=1}^m g_j(u_n^N)(u_n^N)_{x_j}\varphi\right|dx + |\langle\varphi,f_n\rangle_{L^2}|\\ &\leq \varepsilon\|u_{n+1}^N\|_{1,2,\Omega}\|\varphi\|_{1,2,\Omega} + K_1\|u_n^N\|_{1,2,\Omega}\|\varphi\|_{1,2,\Omega} + K_3\|\varphi\|_{1,2,\Omega}\\ &\leq K_5\|\varphi\|_{1,2,\Omega}, \forall\varphi\in C_c^\infty(\Omega), \end{aligned} \tag{307}$$

for some appropriate $K_5 > 0$.

Since $\varphi \in C_c^\infty(\Omega)$ is arbitrary, we may conclude that

$$\left\|\frac{\partial u_0^N}{\partial t}\right\|_{H^{-1}(\Omega)} \leq K_6, \forall N \in \mathbb{N},$$

uniformly in t on $[0,T]$, for some appropriate constant $K_6 > 0$.

Also, from the definition of u_0^N we have that there exists $K_7 > 0$ such that

$$\|u_0^N\|_{1,2,\Omega} \leq K_7,\ \forall N \in \mathbb{N}$$

also uniformly in t on $[0,T]$.

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From such results, there exist $u_0 \in L^2([0,T], H_0^1(\Omega))$ and $v_0 \in L^2([0,T]; H^{-1}(\Omega))$ such that

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2((0,T); W^{1,2}(\Omega)),$$

and

$$\frac{\partial u_0^N}{\partial t} \rightharpoonup v_0, \text{ weakly-star in } L^2([0,T], H^{-1}(\Omega)),$$

so that we may easily obtain

$$v_0 = \frac{\partial u_0}{\partial t}$$

in a distributional sense.

At this point, we provide more details about this last result.

Fix $t \in (0,T)$. Thus, there exists $n \in \{0,1,\cdots,N-1\}$ such that $t \in [n\Delta t_N, (n+1)\Delta t_N]$.

Let $\varphi \in C_c^\infty(\Omega \times (0,T))$.

From this, we may infer that

$$\begin{aligned}
& \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi(x,t)\, dx \\
= & \int_\Omega \frac{u_{n+1}^N - u_n^N}{\Delta t_N} \varphi(x,t)\, dx \\
\leq & \ \varepsilon \int_\Omega |\nabla u_{n+1}^N \cdot \nabla \varphi|\, dx \\
& + \int_\Omega |g(u_n^N)\ \varphi(x,t)|\, dx + \int_\Omega \left| \sum_{j=1}^m g_j(u_n^N)(u_n^N)_{x_j} \varphi \right| dx \\
& + \int_\Omega |f_n \varphi|\, dx \\
\leq & \ (K_8 \|u_n^N\|_{1,2,\Omega} + K_{20}) \|\varphi\|_{1,2,\Omega} \\
\leq & \ K_9 \|\varphi\|_{1,2,\Omega}, \qquad (308)
\end{aligned}$$

for some appropriate constants $K_8 > 0,\ K_9 > 0, K_{20} > 0$.

Hence,

$$\begin{aligned}
& \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi(x,t)\, dx\, dx \\
\leq & \ K_9 \int_\Omega \|\varphi\|_{1,2,\Omega}\, dt \\
\leq & \ K_{19} \|\varphi\|_{1,2,\Omega\times(0,T)}, \qquad (309)
\end{aligned}$$

for some appropriate $K_{19} > 0$.

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T))$ is arbitrary, we may infer that

$$\left\| \frac{\partial u_0^N}{\partial t} \right\|_{H^{-1}(\Omega\times(0,T))} \leq K_{15},$$

for $N \in \mathbb{N}$, for some $K_{15} > 0$.

From such a result and from the Banach-Alaoglu Theorem, there exists $v_0 \in H^{-1}(\Omega \times (0,T))$ such that, up to a not relabeled subsequence

$$\frac{\partial u_0^N}{\partial t} \rightharpoonup v_0, \text{ weakly-star in } H^{-1}(\Omega \times (0,T)).$$

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Therefore,

$$\int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \to \int_0^T \int_\Omega v_0 \, \varphi \, dx \, dt,$$

as $N \to \infty$, $\forall \varphi \in H_0^1(\Omega \times (0,T))$.

On the other hand

$$\|u_0^N\|_{0,2,\Omega\times(0,T)} \leq K_{16},$$

$\forall N \in \mathbb{N}$, for some $K_{16} > 0$.

From this and the Kakutani Theorem, there exists $u_0 \in L^2(\Omega \times (0,T))$ such that, up to a not relabeled subsequence,

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2(\Omega \times (0,T)).$$

Now fix again $\varphi \in C_c^\infty(\Omega \times (0,T))$.

Observe that

$$\begin{aligned} \int_0^T \int_\Omega u_0 \varphi_t \, dx \, dt &= \lim_{N\to\infty} \int_0^T \int_\Omega u_0^N \varphi_t \, dx \, dt \\ &= -\lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \\ &= -\int_0^T \int_\Omega v_0 \varphi \, dx \, dt, \end{aligned} \tag{310}$$

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T))$ is arbitrary, we may infer that

$$v_0 = \frac{\partial u_0}{\partial t}$$

in a distributional sense.

Moreover, from such results we may also obtain, again up to a subsequence,

$$\lim_{N\to\infty} \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx = \int_\Omega \frac{\partial u_0}{\partial t} \varphi \, dx,$$

$\forall \varphi \in H_0^1(\Omega)$.

Observe also that, as a consequence of the Rellich-Kondrashov theorem, through appropriate subsequences, we have

$$u_0^{N_k(t)} \to u_0(x,t), \text{ strongly in } L^2(\Omega), \text{ for almost all } t \in [0,T].$$

so that, up to subsequences,

$$u_0^{N_k(t)}(x,t) \to u_0(x,t), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Here we emphasise the sequence $\{N_k(t)\} \subset \mathbb{N}$ may depends on t.

Since g is continuous we have that

$$g(u_0^{N_k(t)}(x,t)) \to g(u_0(x,t)), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Fix $t \in (0,T)$.

Let $\varepsilon > 0$. From the Egorov Theorem, there exists a closed set F such that $m(\Omega \setminus F) \leq \varepsilon$ and $k_0 \in \mathbb{N}$ such that if $k > k_0$, then

$$|g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \leq \varepsilon, \text{ for almost all } x \in F.$$

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Let $\varphi \in C_c^\infty(\Omega)$. Observe now that

$$\begin{aligned}
&\left|\int_\Omega (g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t)))\varphi\, dx\right| \\
\leq\ & \int_\Omega |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\, dx \\
=\ & \int_F |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\, dx + \int_{\Omega\setminus F} |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\, dx \\
\leq\ & \int_F \varepsilon\|\varphi\|_\infty\, dx + \int_\Omega |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\chi_{\Omega\setminus F}\, dx \\
\leq\ & \varepsilon\|\varphi\|_\infty m(\Omega) + (\|g(u_0^{N_k(t)})\|_{0,2,\Omega} + \|g(u_0)\|_{0,2,\Omega})\|\varphi\|_{0,4,\Omega}\|\chi_{\Omega\setminus F}\|_{0,4,\Omega} \\
\leq\ & \varepsilon\|\varphi\|_\infty m(\Omega) + K_{21}\|\varphi\|_{0,4,\Omega} m(\Omega\setminus F)^{1/4} \\
\leq\ & \varepsilon\ \|\varphi\|_\infty\ m(\Omega) + K_{21}\|\varphi\|_{0,4,\Omega}\ \varepsilon^{1/4}, \forall k > k_0, \qquad (311)
\end{aligned}$$

for some appropriate constant $K_{21} > 0$ which does not depend on t.

Since such a $\varepsilon > 0$ is arbitrary, we may infer that

$$\int_\Omega g(u_0^{N_k(t)})\varphi\, dx \to \int_\Omega g(u_0)\varphi\, dx, \ \text{ as } k \to \infty,$$

$\forall \varphi \in C_c^\infty(\Omega)$.

Similarly, fixing $j \in \{1, \cdots, n\}$, since g_j is continuous we have that

$$g_j(u_0^{N_k(t)}(x,t)) \to g_j(u_0(x,t)), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Fix again $t \in (0,T)$

Let $\varepsilon > 0$ (a new value). From the Egorov Theorem, there exists a closed set F_1 such that $m(\Omega \setminus F_1) \leq \varepsilon$ and $k_0 \in \mathbb{N}$ such that if $k > k_0$, then

$$|g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))| \leq \varepsilon, \text{ for almost all } x \in F_1.$$

Observe now that

$$\begin{aligned}
&\int_\Omega |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))|^2\, dx \\
\leq\ & \int_{F_1} |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))|^2\, dx + \int_{\Omega\setminus F_1} |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))|^2\, dx \\
\leq\ & \int_{F_1} \varepsilon^2\, dx + \int_\Omega |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))|^2\chi_{\Omega\setminus F_1}\, dx \\
\leq\ & \varepsilon^2 m(\Omega) + 2K_1^2 \int_\Omega \chi_{\Omega\setminus F_1}\, dx \\
\leq\ & \varepsilon^2 m(\Omega) + 2K_1^2\varepsilon, \ \forall k > k_0. \qquad (312)
\end{aligned}$$

Since such a $\varepsilon > 0$ is arbitrary, we may infer that

$$\int_\Omega |g_j(u_0^{N_k(t)}) - g_j(u_0)|^2\, dx \to 0, \text{ as } k \to \infty,$$

$\forall j \in \{1, \cdots, n\}$.

Select again $\varphi \in C_c^\infty(\Omega)$. Since

$$\|g_j(u_0^{N_k(t)}) - g_j(u_0)\|_{0,2,\Omega} \to 0, \text{ as } k \to \infty$$

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and

$$\nabla u_0^{N_k(t)} \rightharpoonup \nabla u_0, \text{ weakly in } L^2(\Omega;\mathbb{R}^m),$$

we obtain,

$$\begin{aligned}
& \left|\int_\Omega g_j(u_0^{N_k(t)})(u_0^{N_k(t)})_{x_j}\ \varphi\ dx - \int_\Omega g_j(u_0)(u_0)_{x_j}\ \varphi\ dx\right| \\
\leq\ & \left|\int_\Omega g_j(u_0^{N_k(t)})(u_0^{N_k(t)})_{x_j}\ \varphi\ dx - \int_\Omega g_j(u_0)(u_0^{N_k(t)})_{x_j}\ \varphi\ dx\right| \\
& + \left|\int_\Omega g_j(u_0)(u_0^{N_k(t)})_{x_j}\ \varphi\ dx - \int_\Omega g_j(u_0)(u_0)_{x_j}\ \varphi\ dx\right| \\
\leq\ & \|g_j(u_0^{N_k(t)}) - g_j(u_0)\|_{0,2,\Omega} K_7 \|\varphi\|_\infty \\
& + \left|\int_\Omega g_j(u_0)(u_0^{N_k(t)})_{x_j}\ \varphi\ dx - \int_\Omega g_j(u_0)(u_0)_{x_j}\ \varphi\ dx\right| \\
\to\ & 0, \text{ as } k \to \infty, \qquad (313)
\end{aligned}$$

$\forall j \in \{1, \cdots, n\}$.

From such results, we have

$$\begin{aligned}
0 \ =\ & \lim_{k\to\infty}\left(\int_\Omega \frac{\partial u_0^{N_k(t)}}{\partial t}\ \varphi\ dx + \varepsilon\int_\Omega \nabla u_0^{N_k(t)} \cdot \nabla\varphi\ dx\right. \\
& - \int_\Omega g(u_0^{N_k(t)})\varphi\ dx - \sum_{j=1}^m \int_\Omega g_j(u_0^{N_k(t)})(u_0^{N_k(t)})_{x_j}\varphi\ dx \\
& \left. - \int_\Omega f^{N_k(t)}\varphi\ dx\right) \\
=\ & \int_\Omega \frac{\partial u_0}{\partial t}\ \varphi\ dx + \varepsilon\int_\Omega \nabla u_0 \cdot \nabla\varphi\ dx \\
& - \int_\Omega g(u_0)\varphi\ dx - \sum_{j=1}^m \int_\Omega g_j(u_0)(u_0)_{x_j}\varphi\ dx \\
& - \int_\Omega f\varphi\ dx. \qquad (314)
\end{aligned}$$

so that, from this and by the density of $C_c^\infty(\Omega)$ in $H_0^1(\Omega)$, we have got

$$\begin{aligned}
& \int_\Omega \frac{\partial u_0}{\partial t}\ \varphi\ dx + \varepsilon\int_\Omega \nabla u_0 \cdot \nabla\varphi\ dx \\
& - \int_\Omega g(u_0)\varphi\ dx - \sum_{j=1}^m \int_\Omega g_j(u_0)(u_0)_{x_j}\varphi\ dx \\
& - \int_\Omega f\varphi\ dx = 0,\ \forall\varphi \in H_0^1(\Omega), \qquad (315)
\end{aligned}$$

a.e. on $[0,T]$.

Observe now that

$$\partial(\Omega\times(0,T)) = (\partial\Omega\times[0,T]) \cup (\partial[0,T]\times\overline{\Omega}).$$

Let $\varphi \in C_c^\infty(\Omega\times(0,T))$.

Hence

$$\lim_{N\to\infty}\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\ dx\ dt = \int_0^T\int_\Omega \frac{\partial u_0}{\partial t}\varphi\ dx\ dt.$$

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From this, since $C_c^\infty(\Omega \times (0,T))$ is dense $L^2(\Omega \times (0,T))$ we may infer that

$$\lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt = \int_0^T \int_\Omega \frac{\partial u_0}{\partial t} \varphi \, dx \, dt,$$

$\forall \varphi \in L^2(\Omega \times (0,T))$.

Let $\varphi \in C^\infty(\Omega \times [0,T])$ such that

$$\varphi(x,T) = 0, \text{ in } \Omega.$$

From such results, we may obtain

$$\begin{aligned} & \lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \\ = & \lim_{N\to\infty} \left(- \int_0^T \int_\Omega u_0^N \frac{\partial \varphi}{\partial t} \, dx \, dt - \int_\Omega u_0^N(x,0) \varphi(x,0) \, dx \right) \\ = & - \int_0^T \int_\Omega u_0 \frac{\partial \varphi}{\partial t} \, dx \, dt - \int_\Omega u_0(x,0) \varphi(x,0) \, dx. \end{aligned} \tag{316}$$

However, since $u_0^N \rightharpoonup u_0$, weakly in $L^2(\Omega \times (0,T))$, we obtain

$$\lim_{N\to\infty} \int_0^T \int_\Omega u_0^N \, \frac{\partial \varphi}{\partial t} \, dx \, dt = \int_0^T \int_\Omega u_0 \, \frac{\partial \varphi}{\partial t} \, dx \, dt.$$

From these last results, we may infer that

$$\begin{aligned} \int_\Omega \hat{u}_0 \, \varphi(x,0) \, dx &= \lim_{N\to\infty} \int_\Omega u_0^N(x,0) \varphi(x,0) \, dx \\ &= \int_\Omega u_0(x,0) \, \varphi(x,0) \, dx, \end{aligned} \tag{317}$$

so that

$$\int_\Omega \hat{u}_0(x) \varphi(x,0) \, dx = \int_\Omega u_0(x,0) \varphi(x,0) \, dx,$$

$\forall \varphi \in C^\infty(\Omega \times [0,T])$ such that $\varphi(x,T) = 0, \text{ in } \Omega$.

Therefore, we may infer that $u_0(x,0) = \hat{u}_0(x)$ in this specified weak sense.

Similarly, it may be proven that

$$u_0 = 0, \text{ on } \partial\Omega \times [0,T],$$

in an appropriate weak sense.

Hence, we have obtained that u_0 is a solution, in a weak sense, of the parabolic non-linear equation in question.

52. An Existence Result for a General Hyperbolic Non-Linear Equation

Let $\Omega \subset \mathbb{R}^m$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the hyperbolic non-linear equation

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} = \varepsilon \nabla^2 u + g(u) + f, & \text{in } \Omega \times (0,T), \\ u(x,0) = \hat{u}_0, \text{ in } \Omega, \\ u(x,T) = u_f, \text{ in } \Omega, \\ u = 0, \text{ on } \partial\Omega \times [0,T]. \end{cases} \tag{318}$$

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Here $\varepsilon > 0$, $f \in L^2([0,T], W^{1,2}(\Omega)) \cap L^\infty(\Omega \times [0,T])$, $\hat{u}_0, u_f \in H_0^1(\Omega) \cap L^\infty(\Omega)$, where t denotes time and $[0,T]$ is a time interval.

Also $g : \mathbb{R} \to \mathbb{R}$ is a continuous function neither necessarily linear nor convex.

We assume there exists $K_{33} > 0$ such that

$$\|g\|_\infty \leq \frac{K_{33}}{m(\Omega)^{1/2}},$$

Fixing $N \in \mathbb{N}$ and defining

$$\Delta t_N = \frac{T}{N},$$

in a partial finite differences context, discretizing in t consider the approximate equation system

$$\frac{u_{n+1} - 2u_n + u_{n-1}}{\Delta t_N^2} = \varepsilon \nabla^2 u_n + g(u_n) + f_n, \text{ in } \Omega,$$

$\forall n \in \{1, \cdots, N-1\}$.

From such a system, for $n = 1$, we obtain

$$u_2 - 2u_1 + \hat{u}_0 = \varepsilon \nabla^2(u_1)\Delta t_N^2 + g(u_1)\Delta t_N^2 + f_1 \Delta t_N^2.$$

Hence

$$(2I_d u + \varepsilon \nabla^2 \Delta t_N^2) u_1 = \left(u_2 + \hat{u}_0 - g(u_1)\Delta t_N^2 - f_1 \Delta t_N^2\right),$$

so that

$$\begin{aligned} & \|u_1\|_{1,2,\Omega} \\ \leq \; & \|(2I_d + \varepsilon(\nabla^2)\Delta t_N^2)^{-1}\| \\ & \times \left(\|u_2\|_{0,2,\Omega} + \|\hat{u}_0\|_{0,2,\Omega} + \|g(u_1)\|_{0,2,\Omega}\Delta t_N^2 + \|f_1\|_{0,2,\Omega}\Delta t_N^2\right). \end{aligned} \tag{319}$$

Observe that there exists $K_2 > 0$ such that $\|f\|_{\infty,\Omega\times[0,T]} \leq K_2$ so that

$$\|f_n\|_{1,2,\Omega} \leq K_3, \; \forall n \in \{0, 1, \cdots, N-1\},$$

for some appropriate $K_3 > 0$.

From such results and the hypotheses, we may infer that

$$\begin{aligned} & \|u_1\|_{1,2,\Omega} \leq \|(2I_d + \varepsilon(\nabla^2)\Delta t_N^2)^{-1}\|(\|u_2\|_{1,2,\Omega} + K_{33}\Delta t_N^2 + \|\hat{u}_0\|_{1,2,\Omega} + K_3 \Delta t_N^2) \\ \leq \; & \|(2I_d + \varepsilon(\nabla^2)\Delta t_N^2)^{-1}\|(\|u_2\|_{1,2,\Omega} + \|\hat{u}_0\|_{1,2,\Omega} + K_{85}\Delta t_N^2), \end{aligned} \tag{320}$$

where $K_{85} = K_{33} + K_3$.

On the other hand, through a symbolic auxiliary notation, we have

$$\begin{aligned} (2I_d + \varepsilon(\nabla^2)\Delta t_N)^{-1} &= \frac{1}{(2I_d + \varepsilon(\nabla^2)\Delta t_N^2)} \\ &= \frac{1}{2(I_d + \varepsilon(\nabla^2)\Delta t_N^2/2)} \\ &= \frac{1}{2}\left(I_d - \frac{\varepsilon(\nabla^2)\Delta t_N^2/2}{I_d + \varepsilon(\nabla^2)\Delta t_N^2/2}\right), \end{aligned} \tag{321}$$

so that

$$\|(2I_d + \varepsilon(\nabla^2)\Delta t_N)^{-1}\| \leq \frac{1}{2} + \left\| \frac{\varepsilon(\nabla^2)\Delta t_N^2/4}{(I_d + \varepsilon(\nabla^2)\Delta t_N^2/2)} \right\|.$$

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Now denote

$$\theta_N = \left\| \frac{\varepsilon(\nabla^2)}{(I_d + \varepsilon(\nabla^2)\Delta t_N^2/2)} \right\|.$$

Thus,

$$\|(2I_d + \varepsilon(\nabla^2)\Delta t_N)^{-1}\| \leq \frac{1}{2} + \frac{\theta_N \Delta t_N^2}{4},$$

so that

$$\|u_1\|_{1,2,\Omega} \leq \left(\frac{1}{2} + \frac{\theta_N \Delta t_N^2}{4}\right)(\|u_2\|_{1,2,\Omega} + \|\hat{u}_0\|_{1,2,\Omega} + K_{85}\Delta t_N^2).$$

Consequently, from such results, we may infer that

$$\left(\frac{1}{2} + \frac{\theta_N \Delta t_N^2}{4}\right)^{-1} \|u_1\|_{1,2,\Omega} \leq (\|u_2\|_{1,2,\Omega} + \|\hat{u}_0\|_{1,2,\Omega} + K_{85}\Delta t_N^2),$$

so that

$$2\left(1 - \frac{\theta_N \Delta t_N^2/2}{(1 + \theta_N \Delta t_N^2/2)}\right)\|u_1\|_{1,2,\Omega} \leq (\|u_2\|_{1,2,\Omega} + \|\hat{u}_0\|_{1,2,\Omega} + K_{85}\Delta t_N^2).$$

Therefore,

$$\left(2 - \frac{\theta_N \Delta t_N^2}{(1 + \theta_N \Delta t_N^2/2)}\right)\|u_1\|_{1,2,\Omega} \leq (\|u_2\|_{1,2,\Omega} + \|\hat{u}_0\|_{1,2,\Omega} + K_{85}\Delta t_N^2).$$

Let $\varepsilon_1 \in \mathbb{R}$ be such that

$$0 < \varepsilon_1 \ll \max\{\varepsilon, 1\}.$$

Define $\hat{\alpha} = \varepsilon\|\nabla^2\|$ and observe that

$$\frac{\theta_N}{(1 + \theta_N \Delta t_N^2/2)} \to \hat{\alpha}, \text{ as } N \to \infty.$$

Hence, there exists $N_0 \in \mathbb{N}$ such that if $N > N_0$, then

$$\left| \frac{\theta_N}{(1 + \theta_N \Delta t_N^2/2)} - \hat{\alpha} \right| < \varepsilon_1.$$

From these results, if $N > N_0$, we have

$$\left(2 - \frac{\theta_N \Delta t_N^2}{(1 + \theta_N \Delta t_N^2/2)}\right) \geq (2 - (\hat{\alpha} + \varepsilon_1)\Delta t_N^2) > 0.$$

Therefore, defining $\alpha = \hat{\alpha} + \varepsilon_1$, we have got,

$$\left(2 - \alpha \Delta t_N^2\right)\|u_1\|_{1,2,\Omega} \leq (\|u_2\|_{1,2,\Omega} + \|\hat{u}_0\|_{1,2,\Omega} + K_{85}\Delta t_N^2).$$

so that

$$\|u_1\|_{1,2,\Omega} \leq \alpha_1\|u_2\|_{1,2,\Omega} + \beta_1\|\hat{u}_0\|_{1,2,\Omega} + \gamma_1,$$

where

$$\alpha_1 = (2 - \alpha \Delta t_N^2)^{-1},$$

$$\beta_1 = \alpha_1$$

and $\gamma_1 = \alpha_1 K_{85}\Delta t_N^2$.

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Reasoning inductively, for $n \geq 2$ having

$$\|u_{n-1}\|_{1,2,\Omega} \leq \alpha_{n-1}\|u_n\|_{1,2,\Omega} + \beta_{n-1}\|\hat{u}_0\|_{1,2,\Omega} + \gamma_{n-1},$$

we are going to obtain α_n, β_n and γ_n.

Similarly as above, we may obtain

$$\begin{aligned} & (2 - \alpha\Delta t_N^2)\|u_n\|_{1,2,\Omega} \\ \leq\ & \|u_{n+1}\|_{1,2,\Omega} + \|u_{n-1}\|_{1,2,\Omega} + K_{85}\Delta t_n^2, \\ \leq\ & \|u_{n+1}\|_{1,2,\Omega} + \alpha_{n-1}\|u_n\|_{1,2,\Omega} + \beta_{n-1}\|\hat{u}_0\|_{1,2,\Omega} + \gamma_{n-1} + K_{85}\Delta t_n^2. \end{aligned} \tag{322}$$

Thus,

$$\begin{aligned} & (2 - \alpha\Delta t_N^2 - \alpha_{n-1})\|u_n\|_{1,2,\Omega} \\ \leq\ & \|u_{n+1}\|_{1,2,\Omega} + \beta_{n-1}\|\hat{u}_0\|_{1,2,\Omega} + \gamma_{n-1} + K_{85}\Delta t_N^2. \end{aligned} \tag{323}$$

Consequently,

$$\|u_n\|_{1,2,\Omega} \leq \alpha_n\|u_{n+1}\|_{1,2,\Omega} + \beta_n\|\hat{u}_0\|_{1,2,\Omega} + \gamma_n,$$

where

$$\alpha_n = \frac{1}{2 - \alpha\Delta t_N^2 - \alpha_{n-1}},$$
$$\beta_n = \alpha_n\beta_{n-1},$$

and

$$\gamma_n = \alpha_n(\gamma_{n-1} + K_{85}\Delta t_N^2).$$

We recall that $\alpha = \varepsilon\|\nabla^2\| + \varepsilon_1$. Here we assume $T \geq 1$ and

$$\alpha T^2 \leq \frac{1}{2}.$$

Consider the sequence $\{b_n\} \subset \mathbb{R}$ such that

$$b_1 = 1/2,$$

and

$$b_{n+1} = \frac{1}{2 - b_n},\ \forall n \in \mathbb{N}.$$

We may easily obtain by induction that

$$b_n = \frac{n}{n+1}.$$

Define

$$a_n = b_{n-1} = \frac{n-1}{n}, \forall n \geq 2.$$

Observe that

$$\begin{aligned} a_n + \frac{2\alpha T^2}{N} &\leq \frac{N-1}{N} + \frac{2\alpha T^2}{N} \\ &\leq \frac{N-1}{N} + \frac{1}{N} \\ &= 1,\ \forall n \in \{1, \cdots, N-1\}. \end{aligned} \tag{324}$$

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Observe that

$$\begin{aligned}\alpha_1 &\leq \frac{1}{2-\alpha\frac{T^2}{N^2}}\\ &= \frac{1}{2}+\left(\frac{1}{2-\alpha\frac{T^2}{N^2}}-\frac{1}{2}\right)\\ &\leq \frac{1}{2}+\frac{\alpha T^2}{N^2}\\ &\leq a_1+\frac{\alpha T}{N}+\frac{\alpha T^2}{N^2}.\end{aligned} \tag{325}$$

At this point we shall prove by induction that

$$\alpha_n \leq a_n+\frac{\alpha T}{N}+n\frac{\alpha T^2}{N^2},\ \forall n\in\{1,\cdots,N-1\}.$$

For $n=1$ we have already proved it above.
Suppose now that for $n\geq 1$, we have

$$\alpha_n \leq a_n+\frac{\alpha T}{N}+n\frac{\alpha T^2}{N^2}.$$

Observe that

$$\begin{aligned}\alpha_{n+1} &= \frac{1}{2-\alpha\frac{T^2}{N^2}-\alpha_{n-1}}\\ &= \frac{1}{2-a_n}+\left(\frac{1}{2-\alpha\frac{T^2}{N^2}-\alpha_{n-1}}-\frac{1}{2-a_n}\right)\\ &= a_{n+1}+\left(\frac{1}{2-\alpha\frac{T^2}{N^2}-\alpha_n}-\frac{1}{2-a_n}\right)\\ &\leq a_{n+1}+\left(-a_n+\alpha_n+\alpha\frac{T^2}{N^2}\right)\\ &\leq a_{n+1}+\frac{\alpha T}{N}+n\frac{\alpha T^2}{N^2}+\alpha\frac{T^2}{N^2}\\ &= a_{n+1}+\frac{\alpha T}{N}+(n+1)\frac{\alpha T^2}{N^2}.\end{aligned} \tag{326}$$

The induction is complete, indeed we have proven that

$$\alpha_n \leq a_n+\frac{\alpha T}{N}+n\frac{\alpha T^2}{N^2},\ \forall n\in\{1,\cdots,N-1\}.$$

Thus, we have obtained

$$\begin{aligned}\alpha_n &\leq a_n+\frac{\alpha T}{N}+n\frac{\alpha T^2}{N^2}\\ &\leq a_n+\frac{\alpha T^2}{N}+\frac{\alpha T^2}{N}\\ &\leq a_n+\frac{2\alpha T^2}{N}\\ &\leq 1,\ \forall n\in\{1,\cdots N-1\}.\end{aligned} \tag{327}$$

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Summarizing,

$$0 \leq \alpha_n \leq 1,\ \forall n \in \{1, \cdots, N-1\}.$$

Now denoting more generically $\alpha_n^N = \alpha_n$ we may infer that

$$0 \leq \alpha_n^N \leq 1,\ \forall n \in \{1, \cdots, N-1\},\ \forall N > N_0.$$

From such results we may also obtain that there exist $K_{15} > 0$ and $K_{16} > 0$ such that

$$|\beta_n^N| \leq K_{15},$$

and

$$|\gamma_n^N| \leq K_{16},$$

$\forall n \in \{1, \cdots N-1\},\ \forall N > N_0$.

We recall that

$$u_N^N = u_f,$$

so that since

$$\|u_{N-1}^N\|_{1,2,\Omega} \leq \alpha_{N-1}^N \|u_N\|_{1,2,\Omega} + \beta_{N-1}^N \|\hat{u}_0\|_{1,2,\Omega} + \gamma_{N-1}^N,$$

from this and these last results we may infer that

$$\|u_n^N\|_{1,2,\Omega} \leq K_{18},$$

$\forall n \in \{0, \cdots, N-1\},\ \forall N > N_0$, for some appropriate real constant $K_{18} > 0$.

Define now

$$W^N(x,t) = \frac{u_{n+1}^N - 2u_n^N + u_{n-1}^N}{\Delta t_N^2},$$

if $(x,t) \in \Omega \times (n\Delta t_N, (n+1)\Delta t_N],\ \forall (x,t) \in \Omega \times [0,T]$, and

$$u_0^N(x,t) = \hat{u}_0(x) + (u_1^N)'(x)\ t + \int_0^t \int_0^\tau W^N(x,\tau_1)\ d\tau_1\ d\tau,$$

where $(u_1^N)'(x)$ is such that

$$u_0^N(x,T) = u_f(x).$$

Here we highlight that

$$\begin{aligned} \frac{\partial^2 u_0^N(x,t)}{\partial t^2} &= W^N(x,t) \\ &= \frac{u_{n+1}^N - 2u_n^N + u_{n-1}^N}{\Delta t_N^2}, \end{aligned} \tag{328}$$

if $(x,t) \in \Omega \times (n\Delta t_N, (n+1)\Delta t_N],\ \forall (x,t) \in \Omega \times [0,T]$.

Observe that

$$\begin{aligned} \frac{\partial^2 u_0^N(x,t)}{\partial t^2} &= \frac{u_{n+1}^N - 2u_n^N + u_{n-1}^N}{\Delta t_N^2} \\ &= \varepsilon \nabla^2 u_n^N + g(u_n^N) + f_n, \end{aligned} \tag{329}$$

if $t \in (n\Delta t_N, (n+1)\Delta t_N],\ \forall (x,t) \in \Omega \times [0,T]$.

Fix $\varphi \in C_c^\infty(\Omega)$.

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Thus, fixing $t \in (n\Delta t_N, (n+1)\Delta t_N]$, we have

$$\begin{aligned}\left|\left\langle \frac{\partial^2 u_0^N}{\partial t^2}, \varphi \right\rangle_{L^2}\right| &\leq \varepsilon |\langle \nabla u_n^N, \nabla \varphi \rangle_{L^2}| + |\langle g(u_n^N), \varphi \rangle_{L^2}| \\ &\quad + |\langle \varphi, f_n \rangle_{L^2}| \\ &\leq \varepsilon \|u_n^N\|_{1,2,\Omega} \|\varphi\|_{1,2,\Omega} + K_{19} \|u_n^N\|_{1,2,\Omega} \|\varphi\|_{1,2,\Omega} \\ &\quad + K_{25} \|\varphi\|_{1,2,\Omega} \\ &\leq K_{26} \|\varphi\|_{1,2,\Omega}, \forall \varphi \in C_c^\infty(\Omega), \end{aligned} \tag{330}$$

for some appropriate $K_{26} > 0$.

Since $\varphi \in C_c^\infty(\Omega)$ is arbitrary, we may conclude that

$$\left\| \frac{\partial^2 u_0^N}{\partial t^2} \right\|_{H^{-1}(\Omega)} \leq K_6, \forall N > N_0,$$

uniformly in t on $[0, T]$, for some appropriate constant $K_6 > 0$.

Also, from the definition of u_0^N we have that there exists $K_7 > 0$ such that

$$\|u_0^N\|_{1,2,\Omega} \leq K_7, \ \forall N > N_0$$

also uniformly in t on $[0, T]$.

From such results, there exist $u_0 \in L^2([0, T], H_0^1(\Omega))$ and $v_0 \in L^2([0, T]; H^{-1}(\Omega))$ such that

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2((0, T); W^{1,2}(\Omega)),$$

and

$$\frac{\partial^2 u_0^N}{\partial t^2} \rightharpoonup v_0, \text{ weakly-star in } L^2([0, T], H^{-1}(\Omega)),$$

so that we may easily obtain

$$v_0 = \frac{\partial^2 u_0}{\partial t^2}$$

in a distributional sense.

At this point, we provide more details about this last result.

Fix $t \in (0, T)$. Thus, there exists $n \in \{0, 1, \cdots, N-1\}$ such that $t \in (n\Delta t_N, (n+1)\Delta t_N]$.

Let $\varphi \in C_c^\infty(\Omega \times (0, T))$.

From this, we may infer that

$$\begin{aligned} &\int_\Omega \frac{\partial^2 u_0^N}{\partial t^2} \varphi(x, t) \, dx \\ = &\int_\Omega \left(\frac{u_{n+1}^N - 2u_n^N + u_{n-1}^N}{\Delta t_N^2} \right) \varphi(x, t) \, dx \\ \leq &\ \varepsilon \int_\Omega |\nabla u_n^N \cdot \nabla \varphi| \, dx \\ &+ \int_\Omega |g(u_n^N) \ \varphi(x, t)| \, dx \\ &+ \int_\Omega |f_n \varphi| \, dx \\ \leq &\ (K_8(\|u_n^N\|_{1,2,\Omega} + K_{20}) \|\varphi\|_{1,2,\Omega} \\ \leq &\ K_9 \|\varphi\|_{1,2,\Omega}, \end{aligned} \tag{331}$$

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for some appropriate constants $K_8 > 0,\ K_9 > 0, K_{20} > 0$.

Hence,

$$\begin{aligned} & \int_0^T \int_\Omega \frac{\partial^2 u_0^N}{\partial t^2} \varphi(x,t)\, dx\, dx \\ \leq\ & K_9 \int_\Omega \|\varphi\|_{1,2,\Omega}\, dt \\ \leq\ & K_{19} \|\varphi\|_{1,2,\Omega\times(0,T)}, \end{aligned} \tag{332}$$

for some appropriate $K_{19} > 0$.

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T))$ is arbitrary, we may infer that

$$\left\| \frac{\partial^2 u_0^N}{\partial t^2} \right\|_{H^{-1}(\Omega\times(0,T))} \leq K_{15},$$

for $N > N_0$, for some $K_{15} > 0$.

From such a result and from the Banach-Alaoglu Theorem, there exists $v_0 \in H^{-1}(\Omega \times (0,T))$ such that, up to a not relabeled subsequence

$$\frac{\partial^2 u_0^N}{\partial t^2} \rightharpoonup v_0, \text{ weakly-star in } H^{-1}(\Omega \times (0,T)).$$

Therefore,

$$\int_0^T \int_\Omega \frac{\partial^2 u_0^N}{\partial t^2} \varphi\, dx\, dt \to \int_0^T \int_\Omega v_0\ \varphi\, dx\, dt,$$

as $N \to \infty$, $\forall \varphi \in H_0^1(\Omega \times (0,T))$.

On the other hand

$$\|u_0^N\|_{0,2,\Omega\times(0,T)} \leq K_{16},$$

$\forall N > N_0$, for some $K_{16} > 0$.

From this and the Kakutani Theorem, there exists $u_0 \in L^2(\Omega \times (0,T))$ such that, up to a not relabeled subsequence,

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2(\Omega \times (0,T)).$$

Now fix again $\varphi \in C_c^\infty(\Omega \times (0,T))$.

Observe that

$$\begin{aligned} \int_0^T \int_\Omega u_0 \varphi_{tt}\, dx\, dt &= \lim_{N\to\infty} \int_0^T \int_\Omega u_0^N \varphi_{tt}\, dx\, dt \\ &= \lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial^2 u_0^N}{\partial t^2} \varphi\, dx\, dt \\ &= \int_0^T \int_\Omega v_0 \varphi\, dx\, dt, \end{aligned} \tag{333}$$

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T))$ is arbitrary, we may infer that

$$v_0 = \frac{\partial^2 u_0}{\partial t^2}$$

in a distributional sense.

Moreover, from such results we may also obtain, again up to a subsequence,

$$\lim_{N\to\infty} \int_\Omega \frac{\partial^2 u_0^N}{\partial t^2} \varphi\, dx = \int_\Omega \frac{\partial^2 u_0}{\partial t^2} \varphi\, dx,$$

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$\forall \varphi \in H_0^1(\Omega)$.

Observe also that, as a consequence of the Rellich-Kondrashov theorem, through appropriate subsequences, we have

$$u_0^{N_k(t)} \to u_0(x,t), \text{ strongly in } L^2(\Omega), \text{ for almost all } t \in [0,T].$$

so that, up to subsequences,

$$u_0^{N_k(t)}(x,t) \to u_0(x,t), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Here we emphasise the sequence $\{N_k(t)\} \subset \mathbb{N}$ may depends on t.

Since g is continuous we have that

$$g(u_0^{N_k(t)}(x,t)) \to g(u_0(x,t)), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Fix $t \in (0,T)$.

Let $\varepsilon > 0$. From the Egorov Theorem, there exists a closed set F such that $m(\Omega \setminus F) \leq \varepsilon$ and $k_0 \in \mathbb{N}$ such that if $k > k_0$, then

$$|g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \leq \varepsilon, \text{ for almost all } x \in F.$$

Let $\varphi \in C_c^\infty(\Omega)$. Observe now that

$$\begin{aligned}
&\left| \int_\Omega (g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t)))\varphi \, dx \right| \\
\leq\ & \int_\Omega |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \, |\varphi| \, dx \\
=\ & \int_F |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \, |\varphi| \, dx + \int_{\Omega\setminus F} |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \, |\varphi| \, dx \\
\leq\ & \int_F \varepsilon \|\varphi\|_\infty \, dx + \int_\Omega |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \, |\varphi| \chi_{\Omega\setminus F} \, dx \\
\leq\ & \varepsilon \|\varphi\|_\infty m(\Omega) + (\|g(u_0^{N_k(t)})\|_{0,2,\Omega} + \|g(u_0)\|_{0,2,\Omega}) \|\varphi\|_{0,4,\Omega} \|\chi_{\Omega\setminus F}\|_{0,4,\Omega} \\
\leq\ & \varepsilon \|\varphi\|_\infty m(\Omega) + K_{21} \|\varphi\|_{0,4,\Omega} m(\Omega \setminus F)^{1/4} \\
\leq\ & \varepsilon \, \|\varphi\|_\infty \, m(\Omega) + K_{21} \|\varphi\|_{0,4,\Omega} \, \varepsilon^{1/4}, \forall k > k_0,
\end{aligned} \tag{334}$$

for some appropriate constant $K_{21} > 0$ which does not depend on t.

Since such a $\varepsilon > 0$ is arbitrary, we may infer that

$$\int_\Omega g(u_0^{N_k(t)})\varphi \, dx \to \int_\Omega g(u_0)\varphi \, dx, \text{ as } k \to \infty,$$

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$\forall \varphi \in C_c^\infty(\Omega)$. From such results, we have

$$\begin{aligned} 0 &= \lim_{k\to\infty}\left(\int_\Omega \frac{\partial^2 u_0^{N_k(t)}}{\partial t^2}\,\varphi\,dx + \varepsilon\int_\Omega \nabla u_0^{N_k(t)}\cdot\nabla\varphi\,dx\right. \\ &\quad -\int_\Omega g(u_0^{N_k(t)})\varphi\,dx \\ &\quad \left.-\int_\Omega f^{N_k(t)}\varphi\,dx\right) \\ &= \int_\Omega \frac{\partial^2 u_0}{\partial t^2}\,\varphi\,dx + \varepsilon\int_\Omega \nabla u_0\cdot\nabla\varphi\,dx \\ &\quad -\int_\Omega g(u_0)\varphi\,dx \\ &\quad -\int_\Omega f\varphi\,dx. \end{aligned} \tag{335}$$

so that, from this and by the density of $C_c^\infty(\Omega)$ in $H_0^1(\Omega)$, we have got

$$\begin{aligned} &\int_\Omega \frac{\partial^2 u_0}{\partial t^2}\,\varphi\,dx + \varepsilon\int_\Omega \nabla u_0\cdot\nabla\varphi\,dx \\ &-\int_\Omega g(u_0)\varphi\,dx \\ &-\int_\Omega f\varphi\,dx = 0,\ \forall\varphi\in H_0^1(\Omega), \end{aligned} \tag{336}$$

a.e. on $[0,T]$.

Hence, we have obtained that u_0 is a solution, in a weak sense, of the hyperbolic non-linear equation in question.

53. A Numerical Procedure Combining the Euler Method and the Hyper-Finite Differences Approach

Let $\Omega = [0,1] \subset \mathbb{R}$ and consider the equation

$$\begin{cases} \varepsilon u''(x) - Au^3(x) + Bu(x) + 1 = 0, \quad \text{in } \Omega, \\ u(0) = 0,\ u(1) = 0. \end{cases} \tag{337}$$

Here $A > 0$, $B > 0$ and $u \in W_0^{1,2}(\Omega)$.

We may represent such an equation, as a first order system

$$\begin{cases} v' - Au^3/\varepsilon + Bu)/\varepsilon + 1/\varepsilon = 0, \quad \text{in } \Omega, \\ u' = v, \ \text{ in } \Omega, \\ u(0) = 0,\ u(1) = 0. \end{cases} \tag{338}$$

Consider now such a system with generical unknown boundary conditions $\hat{u}_0$ and $\hat{v}_0$, that is,

$$\begin{cases} v' - Au^3/\varepsilon + Bu/\varepsilon + 1/\varepsilon = 0, \quad \text{in } \Omega, \\ u' = v, \ \text{ in } \Omega, \\ u(0) = \hat{u}_0,\ v(0) = \hat{v}_0. \end{cases} \tag{339}$$

Defining $d = 1/m_8$, where m_8 is total number of nodes, in finite differences we have

$$\begin{cases} \frac{v_n - v_{n-1}}{d} - Au_{n-1}^3/\varepsilon + Bu_{n-1}/\varepsilon + 1/\varepsilon = 0, \\ \frac{u_n - u_{n-1}}{d} = v_{n-1} \\ u_0 = \hat{u}_0,\ v_0 = \hat{v}_0. \end{cases} \tag{340}$$

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This is simply the explicit Euler method. We may symbolically obtain $\{u_n\}$ and $\{v_n\}$ as functions of $\hat{u}_0$ and $\hat{v}_0$ (by using the MATHEMATICA or MAPLE software and by truncating the concerning polynomial solutions), through the iterations

$$\begin{cases} v_n = v_{n-1} + Au_{n-1}^3 \frac{d}{\varepsilon} - Bu_{n-1} \frac{d}{\varepsilon} - \frac{d}{\varepsilon}, \\ u_n = u_{n-1} + v_{n-1} d \\ u_0 = \hat{u}_0, \ v_0 = \hat{v}_0. \end{cases} \tag{341}$$

However, it is well known the error in this process could be big. In order to minimize such an error, we use the hyper-finite differences approach for the one-dimensional analogous of the generalized method of lines. More specifically, we will subdivide the interval $[0.1]$ into N_1 sub-interval of same measure, and redefine a not relabeled d as

$$d = \frac{1}{m_8 N_1}.$$

Hence, on each sub-interval $\left[\frac{k-1}{N_1}, \frac{k}{N_1}\right]$, using the MATHEMATICA or MAPLE software we may obtain an approximate solution

$$\{u_{i,k}, \ v_{i,k}\}$$

as functions of the initial conditions

$$\{u_{0,k}, v_{0,k}\}$$

where $i \in \{0, \cdots, m_8\}$, $\forall k \in \{1 \cdots, N_1\}$.

In order to obtain such a solution,

$$\{u_{i,k}, \ v_{i,k}\}$$

we use following interactions

$$\begin{cases} v_{n,k} = v_{n-1,k} + Au_{n-1,k}^3 \frac{d}{\varepsilon} - Bu_{n-1,k} \frac{d}{\varepsilon} - \frac{d}{\varepsilon}, \\ u_{n,k} = u_{n-1,k} + v_{n-1,k} d \\ u_{0,k} = \hat{u}_{0,k}, \ v_{0,k} = \hat{v}_{0,k}. \end{cases} \tag{342}$$

Observe that for obtaining an approximate solution for the original equation in question, we must calculate $\{\hat{u}_{0,k}, \hat{v}_{0,k}\}$ though the solution of the system:

For the boundary conditions:

$$u_{0,1} = 0, \ \ u_{m_8,N_1} = 0.$$

For the solution and its derivative continuity on the nodes related to the N_1 sub-intervals,

$$u_{m8,k} = u_{0,k+1}, \ \ v_{m8,k} = v_{0,k+1}, \ \forall k \in \{1, \cdots N_1\}.$$

Having obtained $\{\hat{u}_{0,k}, \hat{v}_{0,k}\}$, $\forall k \in \{1, \cdots, N_1\}$ we may obtain

$$\{u_{n,k}, v_{n,k}\} \ \forall n \in \{0, \cdots, m_8\}, \ \forall k \in \{1, \cdots, N_1\}.$$

Here we present the software in Mathematica through which we have obtained the numerical results, for the case $\varepsilon = 0.01$, $A = B = 1$ and $N_1 = 16$ subintervals.

****

1. m8 = 100;

   N1 = 16;

   d = 1.0/m8/N1;

   e1 = 0.01;

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A = 1.0;

B = 1.0;

For[k = 1, k < N1 + 1, k++,

Print[k];

u[0, k] = uo[k];

v[0, k] = vo[k];

For[i = 1, i < m8 + 1, i++,

z1 = $(v[i-1,k] + A * d/e1 * u[i-1,k]^3 - B * u[i-1,k] * d/e1 - 1.0 * d/e1)$;

z2 = u[i - 1, k] + v[i - 1, k]*d;

z1 = Series[z1, { uo[k], 0, 8}, { vo[k], 0, 8 }];

z2 = Series[z2, { uo[k], 0, 8 }, {vo[k], 0, 8 }];

z1 = Normal[z1];

z2 = Normal[z2];

v[i, k] = Expand[z1];

u[i, k] = Expand[z2]]];

S = $u[0,1]^2 + u[m8, N1]^2$;

For[k = 1, k < N1, k++,

S = S + $(u[m8,k] - u[0,k+1])^2$;

S = S + $(v[m8,k] - v[0,k+1])^2$];

sol = FindMinimum[

S, {uo[1], uo[2], uo[3], uo[4], uo[5], uo[6], uo[7], uo[8], uo[9],

uo[10], uo[11], uo[12], uo[13], uo[14], uo[15], uo[16], vo[1],

vo[2], vo[3], vo[4], vo[5], vo[6], vo[7], vo[8], vo[9], vo[10],

vo[11], vo[12], vo[13], vo[14], vo[15], vo[16]}]

Clear[U];

For [k = 1, k < N1 + 1, k++,

w[k] = uo[k] /. sol[[2, k]]]

For[i = 1, i < N1 + 1, i++,

U[i - 1] = w[i]]

U[N1] = u[m8,N1];

For[i = 0, i < N1 + 1, i++,

Print["uo[", i + 1, "]=", U[i]]]

uo[1]=1.14453*10^{-25}, in fact $u(0) = 0$

uo[2]=0.817448

uo[3]=1.17018

uo[4]=1.28552

uo[5]=1.32107

uo[6]=1.33205

uo[7]=1.33546

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uo[8]=1.3365

uo[9]=1.33677

uo[10]=1.33667

uo[11]=1.33596

uo[12]=1.33331

uo[13]=1.32382

uo[14]=1.2902

uo[15]=1.175

uo[16]=0.820243

uo[17]=0, in fact $u(1) = 0$.

****

Remark 53.1. *Observe that along the domain the solution is approximately* 1.33 *which is close to* 1.3247, *which is an approximate solution of equation* $u^3 - u - 1 = 0$. *This is expected since* $\varepsilon = 0.01$ *is a relatively small value.*

54. A Proximal Numerical Procedure Combined with the Euler Method

Let $\Omega = [0,1] \subset \mathbb{R}$ and consider the Ginzburg-Landau type equation

$$\begin{cases} \varepsilon u''(x) - Au^3(x) + Bu(x) + 1 = 0, \quad \text{in } \Omega, \\ u(0) = 0,\ u(1) = 0. \end{cases} \tag{343}$$

Here $A > 0$, $B > 0$ and $u \in W_0^{1,2}(\Omega)$.
We may represent such an equation, as a first order system

$$\begin{cases} v' - Au^3/\varepsilon + Bu/\varepsilon + 1/\varepsilon = 0, \quad \text{in } \Omega, \\ u' = v, \ \text{in } \Omega, \\ u(0) = 0,\ u(1) = 0. \end{cases} \tag{344}$$

Consider now such a system with generical unknown boundary conditions $\hat{u}_0$ and $\hat{v}_0$, that is,

$$\begin{cases} v' - Au^3/\varepsilon + Bu/\varepsilon + 1/\varepsilon = 0, \quad \text{in } \Omega, \\ u' = v, \ \text{in } \Omega, \\ u(0) = \hat{u}_0,\ v(0) = \hat{v}_0. \end{cases} \tag{345}$$

Defining $d = 1/m_8$, where m_8 is total number of nodes, in finite differences we have

$$\begin{cases} \frac{v_n - v_{n-1}}{d} - Au_{n-1}^3/\varepsilon + Bu_{n-1}/\varepsilon + 1/\varepsilon = 0, \\ \frac{u_n - u_{n-1}}{d} = v_{n-1} \\ u_0 = \hat{u}_0,\ v_0 = \hat{v}_0. \end{cases} \tag{346}$$

This is simply the explicit Euler method. Setting $u_0 = 0$, we may symbolically obtain $\{u_n\}$ and $\{v_n\}$ as functions of $v_0 = \hat{v}_0$ (by using the MATHEMATICA or MAPLE software and by truncating the concerning polynomial solutions), through the following iterations, which already include a proximal formulation about an initial fixed solution $\{(U_0)_n\}$.

$$\begin{cases} v_n = v_{n-1} + Au_{n-1}^3 \frac{d}{\varepsilon} - Bu_{n-1} \frac{d}{\varepsilon} - \frac{d}{\varepsilon}, \\ u_n = u_{n-1} + v_{n-1} d - \frac{K}{\varepsilon}(u_n - (U_0)_n)d \\ u_0 = 0,\ v_0 = \hat{v}_0. \end{cases} \tag{347}$$

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$\forall n \in \{1, \cdots, m_8\}$.

Indeed, in such a case we have

$$\begin{cases} v_n = v_{n-1} + Au_{n-1}^3 \frac{d}{\varepsilon} - Bu_{n-1}\frac{d}{\varepsilon} - \frac{d}{\varepsilon}, \\ u_n = \left(u_{n-1} + v_{n-1}d + \frac{Kd}{\varepsilon}(U_0)_n\right) / \left(1 + \frac{K\,d}{\varepsilon}\right) \\ u_0 = 0,\ v_0 = \hat{v}_0. \end{cases} \tag{348}$$

$\forall n \in \{1, \cdots, m_8\}$.

We emphasize such a procedure may make the error in the explicit Euler method very small, in fact proportional to $\frac{\varepsilon}{K}$.

Thus, having obtained $u_n = u_n(v_0)$, we may obtain v_0 through the boundary condition $u(1) = 0$, that is, through a solution of equation $u_{m8}(v_0) = 0$.

With such an v_0 calculated, we may obtain explicitly $u_n = u_n(v_0)$, $\forall n \in \{1, \cdots m_8\}$. The next step is to replace $\{(U_0)_n\}$ by $\{u_n\}$ and then to repeat the process until an appropriate convergence criterion is satisfied.

We have obtained numerical results for $\varepsilon = 0.01$, $A = B = 1$, $m8 = 100$ and $K = 10$.

Here we present the software through which we have obtained such results.

We highlight in this software we have fixed a total number of 800 iterations.

****

```
1.  m8 = 100;
    Clear[z1, z2, u, v, vo];
    d = 1.0/m8;
    e1 = 0.01;
    A = 1.0;
    B = 1.0;
    K = 10.0;
    For[i = 0, i < m8 + 1, i++,
    uo[i] = 0.01];
    For[k = 1, k < 800, k++,   (here we have fixed the number of iterations)
    Print[k];
    Clear[vo];
    u[0] = 0.0;
    v[0] = vo;
    For[i = 1, i < m8 + 1, i++,
    z1 = (v[i - 1] + A*d/e1*u[i − 1]^3 - B*u[i - 1]*d/e1 - 1.0*d/e1);
    z2 = (u[i - 1] + v[i - 1]*d + K*uo[i]*d/e1)/(K*d/e1 + 1.0);
    z1 = Series[z1, {vo, 0, 9}];
    z2 = Series[z2, {vo, 0, 9}];
    z1 = Normal[z1];
    z2 = Normal[z2];
    v[i] = Expand[z1];
    u[i] = Expand[z2]];
```

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```
S = (u[m8])^2;
sol = FindMinimum[S, vo];
w = vo /. sol[[2, 1]];
vo = w;
For[i = 0, i < m8 + 1, i++,
uo[i] = u[i]];
Print[u[m8/2]]];
For[i = 0, i < m8/10 + 1, i++,
Print["u[", 10*i, "]=", u[10*i]]]
```

```
u[0]=0.
u[10]=1.09119
u[20]=1.29955
u[30]=1.32239
u[40]=1.32427
u[50]=1.3245
u[60]=1.32386
u[70]=1.31754
u[80]=1.27924
u[90]=1.04636
u[100]=7.31252 * 10^-18
```

****

Remark 54.1. *Observe that along the domain the solution is close to* 1.3247*, which is an approximate solution of equation* $u^3 - u - 1 = 0$*. This is expected since* $\varepsilon = 0.01$ *is a relatively small value.*

55. A Proximal Numerical Procedure Combined with the Euler Method for Solving Partial Differential Equations

Let $\Omega = [0,1] \times [0,1] \subset \mathbb{R}$ and consider the Ginzburg-Landau type equation

$$\begin{cases} \varepsilon \nabla^2 u - Au^3 + Bu + f = 0, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega. \end{cases} \tag{349}$$

Here $A > 0$, $B > 0$, $f \in L^2(\Omega)$ and $u \in W_0^{1,2}(\Omega)$.
We may represent such an equation, as a partially first order system

$$\begin{cases} v_x + u_{yy} - Au^3/\varepsilon + Bu/\varepsilon + f/\varepsilon = 0, & \text{in } \Omega, \\ u_x = v, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega \end{cases} \tag{350}$$

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Defining $d = 1/m_8$, $d_1 = 1/m_9$ and denoting

$$m_2 = \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & \cdots & \cdots & 1 & -2 \end{bmatrix}, \tag{351}$$

where m_8 is total number of nodes in x, and m_9 is the number of nodes in y, in a finite differences context, we may have

$$\begin{cases} \frac{v_n - v_{n-1}}{d} + \frac{m_2}{d_1^2} u_{n-1} - A u_{n-1}^3/\varepsilon + B u_{n-1}/\varepsilon + f_n/\varepsilon = 0, \\ \frac{u_n - u_{n-1}}{d} = v_{n-1} \\ u_0 = 0,\ v_0 = \hat{v}_0. \end{cases} \tag{352}$$

This is simply an adaptation of the explicit Euler method. Observe that we may obtain $\{u_n\}$ and $\{v_n\}$ as functions of $v_0 = \hat{v}_0$ through the following iterations, which already include a proximal formulation about an initial fixed solution $\{(U_0)_n\}$.

$$\begin{cases} v_n = v_{n-1} - \frac{m_2}{d_1^2} u_{n-1} d + A u_{n-1}^3 \frac{d}{\varepsilon} - B u_{n-1} \frac{d}{\varepsilon} - \frac{f_n d}{\varepsilon}, \\ u_n = u_{n-1} + v_{n-1} d - \frac{K}{\varepsilon}(u_n - (U_0)_n) d \\ u_0 = 0,\ v_0 = \hat{v}_0. \end{cases} \tag{353}$$

$\forall n \in \{1, \cdots, m_8\}$.

Indeed, in such a case we have, through a concerning linearization,

$$\begin{cases} v_n = v_{n-1} - \frac{m_2}{d_1^2} u_{n-1} + 3\ A\ (u_0)_{n-1}^2 u_{n-1} \frac{d}{\varepsilon} - 2\ A\ (u_0)_{n-1}^3 \frac{d}{\varepsilon} - B u_{n-1} \frac{d}{\varepsilon} - \frac{f_n\, d}{\varepsilon}, \\ u_n = \left(u_{n-1} + v_{n-1} d + \frac{Kd}{\varepsilon} (U_0)_n \right) / \left(1 + \frac{K\, d}{\varepsilon} \right) \\ u_0 = 0,\ v_0 = \hat{v}_0. \end{cases} \tag{354}$$

$\forall n \in \{1, \cdots, m_8\}$.

We emphasize such a procedure may make the error in the explicit Euler method very small, in fact proportional to $\frac{\varepsilon}{K}$.

Observe now that in particular for $n = 1$, we have

$$\begin{aligned} v_1 &= v_0 - f_1 \frac{d}{\varepsilon} \\ &\equiv (M_1)_1 v_0 + (y_1)_1, \end{aligned} \tag{355}$$

where

$$(M_1)_1 = I_d \text{ identity matrix } (m_9 - 1) \times (m_9 - 1),$$

and

$$(y_1)_1 = -f_1 \frac{d}{\varepsilon}.$$

Also,

$$\begin{aligned} u_1 &= \left(v_0\, d + K (u_0)_1 \frac{d}{\varepsilon} \right) / \left(1 + K \frac{d}{\varepsilon} \right) \\ &\equiv (M_2)_1 v_0 + (y_2)_1, \end{aligned} \tag{356}$$

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where

$$(M_2)_1 = \frac{I_d\ d}{\left(1 + K\frac{d}{\varepsilon}\right)},$$

and

$$(y_2)_1 = \left(\frac{K(u_0)_1\ d}{\varepsilon}\right) / \left(1 + K\frac{d}{\varepsilon}\right).$$

Reasoning inductively, having

$$v_{n-1} = (M_1)_{n-1}v_0 + (y_1)_{n-1},$$

and

$$u_{n-1} = (M_2)_{n-1}v_0 + (y_2)_{n-1},$$

and replacing such relations into the concerning system (364), we obtain

$$\begin{aligned} v_n &= (M_1)_{n-1} + (y_1)_{n-1} - \frac{m_2}{d_1^2}((M_2)_{n-1} + (y_2)_{n-1})d \\ &\quad +3\ A(u_0)_{n-1}^2((M_2)_{n-1} + (y_2)_{n-1})\frac{d}{\varepsilon} - 2A(u_0)_{n-1}^3\frac{d}{\varepsilon} \\ &\quad -B((M_2)_{n-1} + (y_2)_{n-1})\frac{d}{\varepsilon} - f_n\frac{d}{\varepsilon} \\ &= (M_1)_n + (y_1)_n, \end{aligned} \tag{357}$$

where

$$(M_1)_n = (M_1)_{n-1} - \frac{m_2}{d_1^2}((M_2)_{n-1})d + 3\ A(u_0)_{n-1}^2((M_2)_{n-1})\frac{d}{\varepsilon} - B((M_2)_{n-1})\frac{d}{\varepsilon},$$

and

$$\begin{aligned} (y_1)_n &= (y_1)_{n-1} - \frac{m_2}{d_1^2}((y_2)_{n-1})d + 3\ A(u_0)_{n-1}^2((y_2)_{n-1})\frac{d}{\varepsilon} \\ &\quad -2A(u_0)_{n-1}^3\frac{d}{\varepsilon} - B((y_2)_{n-1})\frac{d}{\varepsilon} - f_n\frac{d}{\varepsilon}. \end{aligned} \tag{358}$$

Moreover,

$$\begin{aligned} u_n &= \left((M_2)_{n-1}v_0 + (y_2)_{n-1} + (M_1)_{n-1}v_0d + (y_1)_{n-1}d + K(u_0)_{n-1}\frac{d}{\varepsilon}\right) / \left(1 + K\frac{d}{\varepsilon}\right) \\ &= (M_2)_nv_0 + (y_2)_n, \end{aligned} \tag{359}$$

where

$$(M_2)_n = \frac{(M_2)_{n-1} + (M_1)_{n-1}d}{\left(1 + K\frac{d}{\varepsilon}\right)},$$

and

$$(y_2)_n = \left((y_2)_{n-1} + (y_1)_{n-1}d + K(u_0)_{n-1}\frac{d}{\varepsilon}\right) / \left(1 + K\frac{d}{\varepsilon}\right).$$

Summarizing, we have obtained

$$v_n = (M_1)_nv_0 + (y_1)_n,$$

and

$$u_n = (M_2)_nv_0 + (y_2)_n,$$

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$\forall n \in \{1, \cdots, m_8\}$.

Consequently, from this and the boundary condition $u_{m_8} = 0$, we may have

$$u_{m_8} = 0 = (M_2)_{m_8} v_0 + (y_2)_{m_8}$$

so that

$$v_0 = -[(M_2)_{m_8}]^{-1} (y_2)_{m_8}.$$

From such results we have obtained $\{u_n\}$ and $\{v_n\}, \forall n \in \{1, \cdots, m_8\}$.

The next step is to replace $\{(u_0)_n\}$ by $\{u_n\}$ and then to repeat the process until an appropriate convergence criterion is satisfied.

We have obtained numerical results for $\varepsilon = 0.01$, $A = B = 1$, $f \equiv 1$, in Ω, $m8 = 100$ and $K = 100$.

For the solution $u = u(x, y)$ obtained, please see Figure 42.

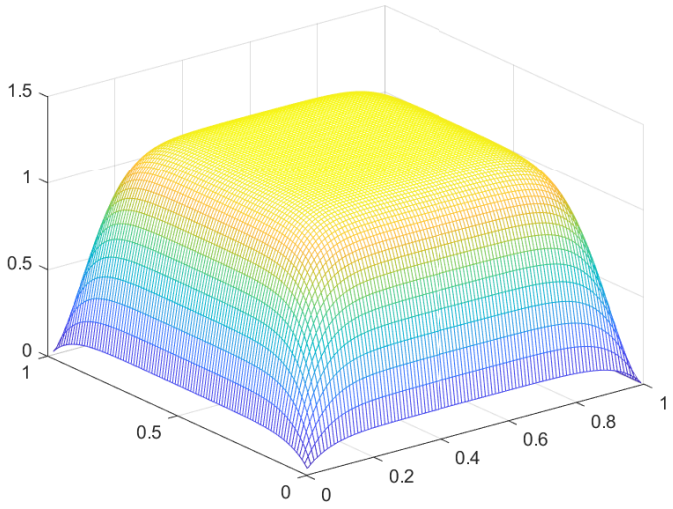

Figure 42. Solution $u(x, y)$ for $\varepsilon = 0.01$

Here we present the software in MAT-LAB through which we have obtained such results.

****

1. clear all

m8=100;

m9=100;

d=1/m8;

d1=1/m9;

e1=0.01;

A=1;

B=1;

K=100;

f=ones(m9-1,1);

for i=1:m8

uo(:,i)=1.4*ones(m9-1,1);

Yo(:,i)=f;

end;

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```
m2=zeros(m9-1,m9-1);
for i=2:m9-2
m2(i,i)=-2.0;
m2(i,i+1)=1.0;
m2(i,i-1)=1.0;
end;
m2(1,1)=-2.0;
m2(1,2)=1.0;
m2(m9-1,m9-1)=-2.0;
m2(m9-1,m9-2)=1.0;
Id=eye(m9-1);
b12=1.0;
k=1;
while (b12 > 10^-10) && (k < 9010)
k
k=k+1;
M1(:,:,1)=Id;
y1(:,1)=-Yo(:,1)*d/e1;
M2(:,:,1)=Id*d/(K*d/e1+1);
y2(:,1)=K*uo(:,1)*(d/e1)/(K*d/e1+1);
for i=2:m8
M1(:,:,i)=M1(:,:,i-1)-m2/d1^2*d*M2(:,:,i-1)+3*A*diag(uo(:,i-1).*uo(:,i-1))*M2(:,:,i-1)*d/e1;
M1(:,:,i)=M1(:,:,i)-B*M2(:,:,i-1)*d/e1;
y1(:,i)=y1(:,i-1)-m2/d1^2*d*y2(:,i-1)+3*A*(uo(:,i-1).*uo(:,i-1)).*y2(:,i-1)*d/e1;
y1(:,i)=y1(:,i)-2*A*(uo(:,i-1).*uo(:,i-1).*uo(:,i-1))*d/e1-B*y2(:,i-1)*d/e1-Yo(:,i-1)*d/e1;
M2(:,:,i)=(M2(:,:,i-1)+d*M1(:,:,i-1))/(K*d/e1+1);
y2(:,i)=(y2(:,i-1)+d*y1(:,i-1)+K*uo(:,i)*d/e1)/(K*d/e1+1);
end;
vo(:,1)=-inv(M2(:,:,m8))*y2(:,m8);
for i=1:m8
u(:,i)=M2(:,:,i)*vo(:,1)+y2(:,i);
end;
u(m9/2,m8/2)
b12=max(max(abs(u-uo)));
uo=u;
end;
for i=1:m8
x1(i,1)=i*d;
end;
```

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```
for j=1:m9-1
y3(j,1)=j*d1;
end;
mesh(x1,y3,u)
*******************************
```

Remark 55.1. *Observe that along the domain the solution is close to* 1.3247*, which is an approximate solution of equation* $u^3 - u - 1 = 0$*. This is expected since* $\varepsilon = 0.01$ *is a relatively small value.*

56. A Proximal Numerical Procedure Combined with the Euler Method for First Order Systems Applied to a Flight Mechanics Model

Let $\Omega = [0, t_f]$ be a time interval.

Consider the first order system of ordinary differential equations given by

$$\begin{cases} \frac{du_j}{dt} = f_j(\{u_l\}), \text{ on } [0, t_f], \ \forall j \in \{1, \cdots, 4\}, \\ u_1(0) = 0, \ u_2(0) = 0.12, \ u_4(0) = 0, \ u_1(t_f) = 11000. \end{cases} \tag{360}$$

Here $f_j : D_j \subset \mathbb{R}^4 \to \mathbb{R}$ is a smooth function on its domain D_j, $\forall j \in \{1, \cdots, 4\}$.

In finite differences, such a system stands for

$$\begin{cases} \frac{(u_j)_n - (u_j)_{n-1}}{d} = f_j(\{u_{n-1}\}), \ \forall j \in \{1, \cdots, 4\}, \\ (u_1)_0 = 0, \ (u_2)_0 = 0.12, \ (u_4)_0 = 0, \ (u_1)_{m8} = 11000. \end{cases} \tag{361}$$

$\forall n \in \{1, \cdots, m_8\}$, where m_8 is number of nodes and $d = t_f / m_8$. This is just the explicit Euler method. It is well known, at first the error in this procedure may be big.

However, such an error may be made very small by introducing a proximal formulation and related linearization about a fixed initial solution $\{(u_0)_n\}$, in a Newton type approach context.

In such a case the approximate system stands for

$$\begin{cases} \frac{(u_1)_n - (u_1)_{n-1}}{d} = f_1(\{(u_0)_{n-1}\}) \\ + \sum_{k=1}^{4} \frac{\partial f_1(\{(u_0)_{n-1}\})}{\partial u_k}((u_k)_{n-1} - (u_{0_k})_{n-1}) - K_5((u_1)_n - ((u_{0_1})_n), \\ \\ \frac{(u_j)_n - (u_j)_{n-1}}{d} = f_j(\{(u_0)_{n-1}\}) + \sum_{k=1}^{4} \frac{\partial f_j(\{(u_0)_{n-1}\})}{\partial u_k}((u_k)_{n-1} - (u_{0_k})_{n-1}), \\ \forall j \in \{2, 3, 4\}, \\ \\ (u_1)_0 = 0, \ (u_2)_0 = 0.12, \ (u_4)_0 = 0, \ (u_1)_{m8} = 11000. \end{cases} \tag{362}$$

Indeed, setting the boundary conditions

$$(u_1)_0 = 0, \ (u_2)_0 = 0.12, \ (u_3)_0 = v_0, \ (u_4)_0 = 0$$

we will calculate

$$\{(u_j)_n(v_0)\}$$

through the following iterations

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$$\begin{cases} (u_1)_n = ((u_1)_{n-1} + f_1(\{(u_0)_{n-1}\})d + \\ \sum_{k=1}^{4} \frac{\partial f_1(\{(u_0)_{n-1}\})}{\partial u_k}((u_k)_{n-1} - (u_{0_k})_{n-1})d + K_5\, d\, ((u_{0_1})_n)\Big)/(1 + K_5\, d), \\ \\ (u_j)_n = (u_j)_{n-1} + f_j(\{(u_0)_{n-1}\})d + \sum_{k=1}^{4} \frac{\partial f_j(\{(u_0)_{n-1}\})}{\partial u_k}((u_k)_{n-1} - (u_{0_k})_{n-1})d, \\ \forall j \in \{2,3,4\}, \\ \\ (u_1)_0 = 0,\ (u_2)_0 = 0.12,\ (u_3)_0 = v_0,\ (u_4)_0 = 0. \end{cases} \tag{363}$$

Observe that the boundary condition $u_1(t_f) = 11000$ corresponds to $(u_1)_{m_8}(v_0) = 11000$ so that, through this last equation we may obtain v_0. Having obtained v_0, we may obtain $\{(u_j)_n\} = \{(u_j)_n(v_0)\}, \forall n \in \{1, \cdots, m_8\}, \forall j \in \{1, \cdots, 4\}$.

The next step is to replace $\{(u_{0_j})_n\})$ by $\{(u_j)_n\}$ and then to repeat the process until an appropriate convergence criterion is satisfied.

We have obtained numerical results for a model in flight mechanics.

More specifically, we model an in-plan climbing motion of an airplane AIR BUS 320, through the variables h, γ, V, x where h denotes the airplane altitude, γ is the angle between its velocity and the axis x, V is the airplane speed and x corresponds to its horizontal coordinate.

The concerning system of equations is given by

$$\begin{cases} \dot{h} = V\sin(\gamma) \\ \\ \dot{\gamma} = \frac{1}{m_f V}(F\sin(a + a_F) + L) - \frac{g}{V}\cos(\gamma) \\ \\ \dot{V} = \frac{1}{m_f}(F\cos(a + a_F) - D) - g\sin(\gamma) \\ \\ \dot{x} = V\cos(\gamma),\ \text{on } [0, t_f], \\ \\ h(0) = 0,\ \gamma(0) = 0.12,\ x(0) = 0,\ h(t_f) = 11000. \end{cases} \tag{364}$$

Here $t_f = 515s$, $F = 240000N$, $m_f = 120000K_g$, $S_f = 260\ m^2$, $a = 0.138$, $g = 9.8m/s^2$,

$$\rho(h) = 1.225\left(1 - \frac{0.0065\, h}{288.15}\right)^{4.225} K_g/m^3,$$

$a_F = 0.0175$, $(C_L)_0 = 0$, $(C_L)_a = 5.0$, $(C_D)_0 = 0.0175$, $K_1 = 0$, $K_2 = 0.06$,

$$C_L = (C_L)_0 + (C_L)_a\, a,$$

$$C_D = (C_D)_0 + K_1 C_L + K_2 C_L^2,$$

$$L = \frac{1}{2}\rho(h)V^2 C_L S_f,$$

$$D = \frac{1}{2}\rho(h)V^2 C_D S_f.$$

For numerical purposes, we define

$$u_1 = h,\ u_2 = \gamma(= b),\ u_3 = V,\ u_4 = x.$$

Here we present the software in MATHEMATICA through which we have obtained the numerical results.

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****

1. m8 = 20000;
   tf = 515.0;
   d = tf/m8;
   K5 = 10.0/d;
   h1 = 11000.0;
   Clear[h, b, V, x, u, a, c];
   h = u[1];
   b = u[2];
   V = u[3];
   x = u[4];
   mf = 120000.0;
   g = 9.8;
   Sf = 260.0;
   a = 0.138;
   af = 0.0175;
   CLo = 0.0;
   CLa = 5.0;
   CDo = 0.0175;
   K1 = 0.0;
   K2 = 0.06;
   CL = CLo + CLa*a;
   CD = CDo + K1*CL + K2*CL^2;
   F = 240000.0;
   r = $1.225 * (1.0 - 0.0065 * h/288.15)^{4.225}$;
   L = $1/2 * r * V^2 * CL * Sf$;
   D1 = $1/2 * r * V^2 * CD * Sf$;
   f[1] = V*Sin[b];
   f[2] = 1/mf/V*(F*Sin[a + af] + L) - g/V*Cos[b];
   f[3] = 1/mf*(F*Cos[a + af] - D1) - g*Sin[b];
   f[4] = V*Cos[b];
   For[i = 0, i < m8 + 1, i++,
   uo[i, 1] = 11000*i/m8;
   uo[i, 2] = 0.15;
   uo[i, 3] = 120;
   uo[i, 4] = 50000*i/m8];
   Clear[u];
   For[i = 1, i < 5, i++,
   For[j = 1, j < 5, j++,

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```
c[i, j] = D[f[i], u[j]]]];
uo[0, 1] = 0.0;
uo[0, 2] = 0.12;
uo[0, 3] = 120;
uo[0, 4] = 0.0;
For[k3 = 1, k3 < 30, k3++,    (Here we have fixed a total of 30 iterations)
Print[k3];
Clear[vo, U];
U[0, 1] = 0.0;
U[0, 2] = 0.12;
U[0, 3] = vo;
U[0, 4] = 0.0;
For[i = 1, i < m8 + 1, i++,
Clear[u];
u[1] = uo[i - 1, 1];
u[2] = uo[i - 1, 2];
u[3] = uo[i - 1, 3];
u[4] = uo[i - 1, 4];
z1 = Expand[U[i - 1, 1] + K5*(uo[i, 1])*d + f[1]*d];
z2 = Expand[U[i - 1, 2] + 0.0*K5*(uo[i, 2])*d + f[2]*d];
z3 = Expand[U[i - 1, 3] + 0.0*K5*(uo[i, 3])*d + f[3]*d];
z4 = Expand[U[i - 1, 4] + 0.0*K5*(uo[i, 4])*d + f[4]*d];
For[k = 1, k < 5, k++,
z1 = z1 + c[1, k]*(U[i - 1, k] - uo[i - 1, k])*d;
z2 = z2 + c[2, k]*(U[i - 1, k] - uo[i - 1, k])*d;
z3 = z3 + c[3, k]*(U[i - 1, k] - uo[i - 1, k])*d;
z4 = z4 + c[4, k]*(U[i - 1, k] - uo[i - 1, k])*d;];
U[i, 1] = Expand[z1/(1.0 + K5*d)];
U[i, 2] = Expand[z2/(1.0 + 0.0*K5*d)];
U[i, 3] = Expand[z3/(1.0 + 0.0*K5*d)];
U[i, 4] = Expand[z4/(1.0 + 0.0*K5*d)]];
Print[U[m8, 1]];
S = (U[m8, 1] - h1);
sol = NSolve[S == 0, vo];
vo = vo  /.  sol[[1, 1]];
Print[vo];
Print[U[m8, 2]];
Print[U[m8, 3]];
Print[U[m8, 4]];
```

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```
For[i = 0, i < m8 + 1, i++,
For[k = 1, k < 5, k++,
uo[i, k] = U[i, k]]];
Print[U[m8/2, 1]]];
**************************
```

1.
```
For[i = 1, i < 11, i++,
Print["h(", 2000*i*d, "s)=U[", 2000*i, ",1]=", U[2000*i, 1]]]
```

```
h(51.5s)=U[2000,1]=1099.37
h(103.s)=U[4000,1]=2199.41
h(154.5s)=U[6000,1]=3299.45
h(206.s)=U[8000,1]=4399.5
h(257.5s)=U[10000,1]=5499.6
h(309.s)=U[12000,1]=6599.74
h(360.5s)=U[14000,1]=7699.8
h(412.s)=U[16000,1]=8799.76
h(463.5s)=U[18000,1]=9899.89
h(515.s)=U[20000,1]=11000.
```

2.
```
For[i = 1, i < 11, i++,
Print["gamma(", 2000*i*d, "s)=U[", 2000*i, ",2]=", U[2000*i, 2]]]
```

```
gamma(51.5s)=U[2000,2]=0.120754
gamma(103.s)=U[4000,2]=0.120085
gamma(154.5s)=U[6000,2]=0.117905
gamma(206.s)=U[8000,2]=0.116329
gamma(257.5s)=U[10000,2]=0.119054
gamma(309.s)=U[12000,2]=0.125181
gamma(360.5s)=U[14000,2]=0.122861
gamma(412.s)=U[16000,2]=0.111435
gamma(463.5s)=U[18000,2]=0.115118
gamma(515.s)=U[20000,2]=0.115257
```

3.
```
For[i = 1, i < 11, i++,
Print["V(", 2000*i*d, "s)=U[", 2000*i, ",3]=", U[2000*i, 3]]]
```

```
V(51.5s)=U[2000,3]=107.325
V(103.s)=U[4000,3]=113.338
V(154.5s)=U[6000,3]=119.7
V(206.s)=U[8000,3]=126.381
```

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V(257.5s)=U[10000,3]=133.568

V(309.s)=U[12000,3]=142.044

V(360.5s)=U[14000,3]=152.19

V(412.s)=U[16000,3]=162.209

V(463.5s)=U[18000,3]=172.269

V(515.s)=U[20000,3]=185.79

4. For[i = 1, i < 11, i++,
Print["x(", 2000*i*d, "s)=U[", 2000*i, ",4]=", U[2000*i, 4]]]

x(51.5s)=U[2000,4]=5318.63

x(103.s)=U[4000,4]=10930.8

x(154.5s)=U[6000,4]=16860.9

x(206.s)=U[8000,4]=23137.6

x(257.5s)=U[10000,4]=29795.8

x(309.s)=U[12000,4]=36872.5

x(360.5s)=U[14000,4]=44395.

x(412.s)=U[16000,4]=52396.6

x(463.5s)=U[18000,4]=60960.3

x(515.s)=U[20000,4]=70129.5

****

57. A Review of the Convergence of Newton's Method Combined with a Proximal Approach

Firstly we highlight similar results to those presented in this section have been presented in my book entitled "Functional Analysis, Calculus of Variations and Numerical Methods for Models in Physics and Engineering", reference [8], in Chapter 25, page 488.

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a C^2 class function and consider the problem of finding a critical point of f, there is, to find a point $\hat{x}_0 \in \mathbb{R}^n$ such that

$$f'(\hat{x}_0) = \mathbf{0}.$$

Fix $k \in \mathbb{N}$ and let $x_k \in \mathbb{R}^n$.
Define $F : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ by

$$\begin{aligned} F(x, x_k) &= f(x_k) + f'(x_k) \cdot (x - x_k) + \frac{1}{2}[f''(x_k)(x - x_k)] \cdot (x - x_k) \\ &\quad + \frac{K}{2}\|x - x_k\|^2, \end{aligned} \tag{365}$$

for some $K > 0$ to be specified.

Let $x_{k+1} \in \mathbb{R}^n$ be such that

$$\left[\frac{\partial F(x, x_k)}{\partial x}\right]_{x=x_{k+1}} = \mathbf{0},$$

so that

$$f'(x_k) + f''(x_k)(x_{k+1} - x_k) + K(x_{k+1} - x_k) = \mathbf{0},$$

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that is

$$x_{k+1} = x_k - (f''(x_k) + KI_d)^{-1} f'(x_k).$$

Now, assume $x_0 \in \mathbb{R}^n$ is such that

$$\|f''(x)\| \leq \hat{K}_1, \ \forall x \in B_r(x_0)$$

for some $r > 0$.

Assume $\hat{K}_1 > 0$ is such that

$$K - \hat{K}_1 > 0.$$

Suppose also $0 < \alpha_1 < 1$ is such that

$$f''(x) \geq \alpha_1(\hat{K}_1 + K)I_d$$

and

$$\left(1 - \frac{\alpha_1}{4}\right) I_d \leq (f''(x) + KI_d)^{-1}(f''(y) + KI_d) \equiv H(x,y) \leq \left(1 + \frac{\alpha_1}{4}\right) I_d,$$

$\forall x, y \in B_r(x_0)$.

We recall that

$$\|f''(x)\| \leq \hat{K}_1,$$

so that

$$(K - \hat{K}_1)I_d \leq KI_d + f''(x),$$

and therefore

$$(f''(x) + KI_d)^{-1} \leq \frac{I_d}{K - \hat{k}_1},$$

$\forall x \in B_r(x_0)$.

Suppose also

$$f'(x) - f'(y) = H_5(x,y) \cdot (x - y),$$

where $H_5(x,y)$ is a symmetric matrix such that

$$0 \leq \frac{H_5(x,y)}{K - \hat{K}_1} \leq \left(1 - \frac{\alpha_1}{2}\right) I_d,$$

and

$$H_5(x,y) \geq \alpha_1(K + \hat{K}_1)I_d,$$

$\forall x, y \in B_r(x_0)$.

Assume also $K > 0$ is such that

$$x_1 \in B_{r(1-\alpha_0)}(x_0),$$

where

$$\alpha_0 = \left(1 - \frac{3}{4}\alpha_1\right).$$

Reasoning inductively, suppose

$$x_0, x_1, \cdots, x_{k+1} \in B_r(x_0).$$

Observe that

$$x_{k+2} - x_{k+1} = -(f''(x_{k+1}) + KI_d)^{-1} f'(x_{k+1}),$$

and

$$x_{k+1} - x_k = -(f''(x_k) + KI_d)^{-1} f'(x_k),$$

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so that

$$(f''(x_{k+1}) + KI_d)(x_{k+2} - x_{k+1}) = -f'(x_{k+1}),$$

and

$$(f''(x_k) + KI_d)(x_{k+1} - x_k) = -f'(x_k).$$

Hence,

$$(f''(x_{k+1}) + KI_d)(x_{k+2} - x_{k+1}) = (f''(x_{k+1}) + KI_d)(x_{k+1} - x_k) - f'(x_{k+1}) + f'(x_k),$$

so that

$$\begin{aligned}
(x_{k+2} - x_{k+1}) &= (f''(x_{k+1}) + KI_d)^{-1}[(f''(x_{k+1}) + KI_d)(x_{k+1} - x_k) - f'(x_{k+1}) + f'(x_k)] \\
&= (f''(x_{k+1}) + KI_d)^{-1}[(f''(x_{k+1}) + KI_d)(x_{k+1} - x_k) \\
&\quad -H_5(x_{k+1}, x_k)(x_{k+1} - x_k)] \\
&= (f''(x_{k+1}) + KI_d)^{-1}[(f''(x_{k+1}) + KI_d)(x_{k+1} - x_k)] \\
&\quad -(f''(x_{k+1}) + KI_d)^{-1}H_5(x_{k+1}, x_k)(x_{k+1} - x_k) \\
&= [H(x_{k+1}, x_k) - (f''(x_{k+1}) + KI_d)^{-1}H_5(x_{k+1}, x_k)](x_{k+1} - x_k). \qquad (366)
\end{aligned}$$

Observe that

$$\begin{aligned}
H_5(x_{k+1}, x_k) &\geq \alpha_1(\hat{K}_1 + K)I_d \\
&\geq \alpha_1(f''(x_{k+1}) + KI_d), \qquad (367)
\end{aligned}$$

so that

$$(f''(x_{k+1}) + KI_d)^{-1}H_5(x_{k+1}, x_k) \geq \alpha_1 I_d.$$

Consequently, from such results we may infer that

$$\begin{aligned}
& I_d\left(1 - \frac{3}{4}\alpha_1\right) \\
= \; & I_d\left(1 + \frac{\alpha_1}{4}\right) - \alpha_1 I_d \\
\geq \; & H(x_{k+1}, x_k) - (f''(x_{k+1}) + KI_d)^{-1}H_5(x_{k+1}, x_k) \\
\geq \; & I_d\left(1 - \frac{\alpha_1}{4}\right) - (K - \hat{K}_1)^{-1}I_d \; H_5(x_{k+1}, x_k) \\
\geq \; & I_d\left(1 - \frac{\alpha_1}{4}\right) - I_d\left(1 - \frac{\alpha_1}{2}\right) \\
= \; & \frac{I_d\alpha_1}{4} \\
\geq \; & 0. \qquad (368)
\end{aligned}$$

from such results we may infer that

$$\|H(x_{k+1}, x_k) - (f''(x_{k+1}) + KI_d)^{-1}H_5(x_{k+1}, x_k)\| \leq \left(1 - \frac{3\alpha_1}{4}\right).$$

Defining

$$\alpha_0 = \left(1 - \frac{3\alpha_1}{4}\right)$$

we have got

$$\|x_{j+2} - x_{j+1}\| \leq \alpha_0\|x_{j+1} - x_j\|, \; \forall j \in \{1, \cdots, k\}.$$

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Therefore

$$\begin{aligned} \|x_{j+2} - x_{j+1}\| &\leq \alpha_0 \|x_{j+1} - x_j\| \\ &\leq \alpha_0^2 \|x_j - x_{j-1}\| \\ &\vdots \\ &\leq \alpha_0^{j+1} \|x_1 - x_0\|. \end{aligned} \tag{369}$$

Thus,

$$\begin{aligned} \|x_{k+2} - x_1\| &= \|x_{k+2} - x_{k+1} + x_{k+1} - \cdots - x_2 + x_2 - x_1\| \\ &\leq \|x_{k+2} - x_{k+1}\| + \|x_{k+1} - x_k\| + \cdots + \|x_2 - x_1\| \\ &\leq \sum_{j=1}^{k+1} \alpha_0^j \|x_1 - x_0\| \\ &\leq \sum_{j=1}^{\infty} \alpha_0^j \|x_1 - x_0\| \\ &= \frac{\alpha_0}{1-\alpha_0} \|x_1 - x_0\|. \end{aligned} \tag{370}$$

Therefore

$$\begin{aligned} \|x_{k+2} - x_0\| &\leq \|x_{k+2} - x_1 + x_1 - x_0\| \\ &\leq \|x_{k+2} - x_1\| + \|x_1 - x_0\| \\ &\leq \frac{\alpha_0}{1-\alpha_0} \|x_1 - x_0\| + \|x_1 - x_0\| \\ &= \frac{1}{1-\alpha_0} \|x_1 - x_0\| \\ &\leq \frac{1}{1-\alpha_0} (1-\alpha_0) r \\ &= r. \end{aligned} \tag{371}$$

Summarizing,

$$\|x_{k+2} - x_0\| < r,$$

so that

$$x_{k+2} \in B_r(x_0).$$

The induction is complete, so that

$$x_k \in B_r(x_0), \ \forall k \in \mathbb{N}.$$

From such results we have also obtained

$$\|x_{k+2} - x_{k+1}\| \leq \alpha_0 \|x_{k+1} - x_k\|, \ \forall k \in \mathbb{N}.$$

Thus, from these results and the Banach fixed point theorem, there exists $\hat{x}_0 \in \overline{B_r}(x_0)$ such that

$$\lim_{k \to \infty} x_k = \hat{x}_0.$$

Hence,

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$$\begin{aligned}\mathbf{0} &= \lim_{k\to\infty} x_{k+1} - x_k \\ &= \lim_{k\to\infty} (-f''(x_k) + KI_d)^{-1} f'(x_k) \\ &= -(f''(\hat{x}_0) + KI_d)^{-1} f'(\hat{x}_0). \end{aligned} \tag{372}$$

Since $\det(f''(\hat{x}_0) + KI_d)^{-1} \neq 0$, from this last equation we obtain

$$f'(\hat{x}_0) = \mathbf{0}.$$

The objective of this section is complete.

57.1. Applications to a Ginzburg-Landau Type Equation

Let $\Omega = [0,1]^2 \subset \mathbb{R}^3$ and consider a functional $F : V \to \mathbb{R}$ where

$$\begin{aligned} F(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad -\frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{373}$$

where $V = H_0^1(\Omega)$, $f \in L^2(\Omega)$, $\alpha > 0,\ \beta > 0$ and $\gamma > 0$.

Let $u \in H_0^1(\Omega)$ and $\varphi \in H_0^1(\Omega)$.

Observe that

$$\begin{aligned} \delta F(u;\varphi) &= \gamma\int_\Omega \nabla u \cdot \nabla \varphi \, dx \\ &\quad \alpha\int_\Omega u^3 \, \varphi \, dx - \beta\int_\Omega u \, \varphi \, dx \\ &\quad -\langle \varphi, f\rangle_{L^2}. \end{aligned} \tag{374}$$

Consider the problem of finding $u_0 \in H_0^1(\Omega)$ such that

$$\delta F(u_0;\varphi) = 0,\ \forall \varphi \in H_0^1(\Omega).$$

Fixing $N \in \mathbb{N}$, consider now a mesh in finite differences for Ω, where we define $d = 1/N$ and the related grid

$$\Omega_N = \{(j/N, k/N)\ \forall j,k \in \{0,1,\cdots,N\}.$$

Denoting by V_N the finite-dimensional space in a finite diferences context corresponding to V and considering the functional F, we assume there exist $u_0 \in V$, the corresponding $u_0^N \in V_N$ and $r > 0$ such that the hypotheses indicated in the last section also for the corresponding function $F_N : V_N \to \mathbb{R}$ are satisfied so that, as developed in such a previous section, we may obtain a solution $u_N : \Omega \to \mathbb{R}$ such that

$$F_N'(u_N) = \mathbf{0}$$

that is,

$$-\gamma\nabla_N^2 u_N + \alpha u_N^3 - \beta u_N - f_N = \mathbf{0},$$

where ∇_N^2 is the finite dimensional operator corresponding to the Laplace operator ∇^2.

Also,

$$F_N''(u) = -\gamma\nabla_N^2 + 3\alpha \ \text{diag}\ (u^2) - \beta I_d,$$

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so that

$$\begin{aligned} F_N'(u_1) - F_N'(u_2) &= -\gamma\nabla_N^2 u_1 + \alpha u_1^3 - \beta u_1 - f_N \\ &\quad -\Big(-\gamma\nabla_N^2 u_2 + \alpha u_2^3 - \beta u_2 - f_N\Big) \\ &= -\gamma\nabla_N^2(u_1-u_2) + \alpha(u_1^3 - u_2^3) - \beta(u_1-u_2) \\ &= -\gamma\nabla_N^2(u_1-u_2) + 3\alpha\ (\tilde{u}^2)\ (u_2-u_1) - \beta(u_1-u_2) \\ &= \Big(-\gamma\nabla_N^2 + 3\alpha\ \text{diag}\ \tilde{u}^2 - \beta I_d\Big)(u_2-u_1) \\ &= F_N''(\tilde{u})(u_2-u_1) \end{aligned} \tag{375}$$

where $(u_1)_j \leq \tilde{u}_j \leq (u_2)_j, \forall u_1, u_2 \in B_r(u_0)$.

From such results, concerning the notation of the last section, we may infer that

$$\begin{aligned} H_5(u_1,u_2) &= F_N''(\tilde{u}(u_1,u_2)) \\ &= -\gamma\nabla_N^2 + 3\alpha\ \text{diag}\ \{[(\tilde{u})(u_1,u_2)]^2\} - \beta I_d. \end{aligned} \tag{376}$$

Now fix $M, N \in \mathbb{N}$.

Observe that

$$-\gamma\nabla_N^2 u_N + \alpha u_N^3 - \beta u_N - f_N = \mathbf{0},$$

and

$$-\gamma\nabla_M^2 u_M + \alpha u_M^3 - \beta u_M - f_M = \mathbf{0}.$$

At this point, denoting $u^N = \{u_{j,k}^N\}$, we define

$$\tilde{u}_0^N(x,y) = \begin{cases} u_{j,k}^N, \text{ if } (x,y) \in ((j-1)\ d, j\ d] \times ((k-1)\ d, k\ d], \\ \forall j,k \in \{1,\cdots,N\}. \end{cases} \tag{377}$$

We also denote for a not relabeled operator ∇_N^2,

$$\nabla_N^2(\tilde{u}_0^N(x,y)) = \begin{cases} \frac{u_{j+1,k}^N - 2u_{j,k}^N + u_{j-1,k}^N}{d^2} + \frac{u_{j,k+1}^N - 2u_{j,k}^N + u_{j,k-1}^N}{d^2}, \\ \text{if } (x,y) \in ((j-1)\ d, j\ d] \times ((k-1)\ d, k\ d], \\ \forall j,k \in \{1,\cdots,N\}. \end{cases} \tag{378}$$

and

$$\nabla_N^2(\tilde{u}_0^N(x,y)) = [\nabla^2 \tilde{u}_0^N](x-d, y-d), \text{ if } x \in (1-d,1] \text{ or } y \in (1-d,1].$$

Moreover, we define

$$u_0^N(x,y) = (\nabla^2)^{-1}(\nabla_N^2(\tilde{u}_0^N(x,y))), \text{ in } \Omega.$$

Observe that

$$\begin{aligned} -\gamma\nabla^2 u_0^N &= -\gamma\nabla_N^2 \tilde{u}_0^N \\ &= -\alpha(\tilde{u}_0^N)^3 + \beta\tilde{u}_0^N + f_N \\ &= -\alpha(u_0^N)^3 + \beta u_0^N + f_N \\ &\quad -\alpha[(\tilde{u}_0^N)^3 - (u_0^N)^3] + \beta(\tilde{u}_0^N - u_0^N), \end{aligned} \tag{379}$$

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Similarly, we may obtain

$$\begin{aligned} -\gamma\nabla^2 u_0^M &= -\gamma\nabla_M^2 \tilde{u}_0^N \\ &= -\alpha(u_0^M)^3 + \beta u_0^M + f_M \\ &\quad -\alpha[(\tilde{u}_0^M)^3 - (u_0^M)^3] + \beta(\tilde{u}_0^M - u_0^M). \end{aligned} \tag{380}$$

Consequently, from such results, we have

$$\begin{aligned} & u_0^N - u_0^M \\ = \; & (-\gamma\nabla^2 + 3\alpha(\hat{u}^{N,M})^2 - \beta I_d)^{-1} \\ & \times\Big[f_N - f_M - 3\alpha(\hat{u}^N)^2(u_0^N - \tilde{u}_0^N) + 3\alpha(\hat{u}^M)^2(u_0^M - \tilde{u}_0^M) \\ & +\beta(u_0^N - \tilde{u}_0^N) - \beta(u_0^M - \tilde{u}_0^M)\Big] \end{aligned} \tag{381}$$

where $\hat{u}^N$ is on the line connecting u_0^N, $\tilde{u}_0^N$ and $\hat{u}^M$ is on the line connecting u_0^M and $\tilde{u}_0^M$ and $\hat{u}^{N,M}$ is on the line connecting u_0^N and u_0^M.

From these results, we obtain

$$\begin{aligned} & \|u_0^N - u_0^M\|_{1,2,\Omega} \\ = \; & \|(-\gamma\nabla^2 + 3\alpha(\hat{u}^{N,M})^2 - \beta I_d)^{-1}\| \\ & \times\Big[\|f_N - f_M\|_{0,2,\Omega} + 3\alpha\|(\hat{u}^N)\|_{0,4,\Omega}^2\|(u_0^N - \tilde{u}_0^N)\|_{0,2,\Omega} + 3\alpha\|(\hat{u}^M)\|_{0,4,\Omega}^2\|(u_0^M - \tilde{u}_0^M)\|_{0,2,\Omega} \\ & +\beta\|(u_0^N - \tilde{u}_0^N)\|_{0,2,\Omega} + \beta\|(u_0^M - \tilde{u}_0^M)\|_{0,2,\Omega}\Big] \\ \leq \; & \Big[K_8\|f_N - f_M\|_{0,2,\Omega} + K_9\|(u_0^N - \tilde{u}_0^N)\|_{0,2,\Omega} + K_9\|(u_0^M - \tilde{u}_0^M)\|_{0,2,\Omega}\Big] \end{aligned} \tag{382}$$

for some appropriate constants $K_8 > 0,\ K_9 > 0$.

Let $\varepsilon > 0$.

Observe that there exists $N_0 \in \mathbb{N}$ such that if $M, N > N_0$, then

$$\|f_N - f_M\|_{0,2,\Omega} < \frac{\varepsilon}{3K_8},$$

$$\|(u_0^N - \tilde{u}_0^N)\|_{0,2,\Omega} \leq \frac{\varepsilon}{3K_9},$$

and

$$\|(u_0^M - \tilde{u}_0^M)\|_{0,2,\Omega} \leq \frac{\varepsilon}{3K_9},$$

so that,

$$\|u_0^N - u_0^M\|_{1,2,\Omega} < \varepsilon.$$

Therefore, $\{u_0^N\}$ is a Cauchy sequence in $H_0^1(\Omega)$ so that there exists $\hat{u}_0 \in H_0^1(\Omega)$ such that

$$u_0^N \to \hat{u}_0, \text{ strongly in } H_0^1(\Omega).$$

Let $\varphi \in H_0^1(\Omega)$.

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From such results and from the Sobolev Imbedding theorem, we may infer that

$$\begin{aligned} 0 &= \lim_{N\to\infty}\Big(\gamma\langle\nabla u_0^N,\nabla\varphi\rangle_{L^2} \\ &\quad +\alpha\langle(u_0^N)^3,\varphi\rangle_{L^2}-\beta\langle u_0^N,\varphi\rangle_{L^2} \\ &\quad -\langle f_N,\varphi\rangle_{L^2}\Big) \\ &= (\gamma\langle\nabla\hat{u}_0,\nabla\varphi\rangle_{L^2} \\ &\quad +\alpha\langle\hat{u}_0^3,\varphi\rangle_{L^2}-\beta\langle\hat{u}_0,\varphi\rangle_{L^2} \\ &\quad -\langle f,\varphi\rangle_{L^2}). \end{aligned} \tag{383}$$

Thus,

$$\gamma\langle\nabla\hat{u}_0,\nabla\varphi\rangle_{L^2}+\alpha\langle\hat{u}_0^3,\varphi\rangle_{L^2}-\beta\langle\hat{u}_0,\varphi\rangle_{L^2}-\langle f,\varphi\rangle_{L^2}=0,$$

$\forall\varphi\in H_0^1(\Omega)$.

From this result we may infer that $\hat{u}_0$ is a weak solution of equation $F'(\hat{u}_0)=\mathbf{0}$.

58. On the Convergence of the Newton's Method Combined with a Proximal Formulation for a General Parabolic Equation

Let $\Omega\subset\mathbb{R}^m$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the parabolic non-linear equation

$$\begin{cases} \frac{\partial u}{\partial t}=\varepsilon\nabla^2u+g(u)+f, & \text{in } \Omega\times(0,T), \\ u(x,0)=\hat{u}_0, \text{ in } \Omega, \\ u=0, \text{ on } \partial\Omega\times[0,T]. \end{cases} \tag{384}$$

Here $\varepsilon>0$, $f\in L^2([0,T],W^{1,2}(\Omega))\cap L^\infty(\Omega\times[0,T])$, $\hat{u}_0\in H_0^1(\Omega)\cap L^\infty(\Omega)$, where t denotes time and $[0,T]$ is a time interval.

Also $g:\mathbb{R}\to\mathbb{R}$ is a continuous function neither necessarily linear nor convex.

We assume there exists $r>0$ such that

$$\|g'(u)\|_\infty\leq K_2,$$

and

$$\|g(u)\|_\infty\leq\hat{K}_7$$

$\forall u\in B_r(\hat{u}_0)$, for some $K_2>0$ and $\hat{K}_7>0$.

Here

$$B_r(\hat{u}_0)=\{u\in H_0^1(\Omega)\ :\ \|u-\hat{u}_0\|_{1,2,\Omega}<r\}.$$

We assume also there exists $K_1>0$ such that

$$-K_1I_d\leq-\varepsilon\nabla^2-g'(u)\leq K_1I_d,\ \forall u\in B_r(\hat{u}_0).$$

Moreover, fixing $N\in\mathbb{N}$ and defining

$$\Delta t_N=\frac{T}{N},$$

in a partial finite differences context, discretizing in t consider the approximate equation system

$$\frac{u_{n+1}-u_n}{\Delta t_N}=\varepsilon\nabla^2u_{n+1}+g(u_{n+1})+f_n, \text{ in } \Omega,$$

$\forall n\in\{0,1,\cdots,N-1\}$.

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Fix $M \in \mathbb{N}$. In a finite elements context for the variable $x \in \mathbb{R}^n$, denoting $h_M = L_0/M$, for an appropriate fixed $L_0 > 0$ consider a mesh with a concerning thickness h_M and a related solution u_n^M of the following system

$$\frac{u_{n+1}^M - u_n^M}{\Delta t_N} = \varepsilon \nabla_M^2 u_{n+1}^M + g(u_{n+1}^M) + f_n^M, \text{ in } \Omega,$$

$\forall n \in \{0, 1, \cdots, N-1\}$.

Here ∇_M^2 is the operator in a finite elements context corresponding to the Laplace operator ∇^2.

We highlight in the next lines, as the meaning is clear, we may denote simply $\nabla_M^2 = \nabla^2$.

Observe that there exists a not relabeled $r > 0$, $K_1 > 0$ and $K_2 > 0$ such that

$$\|g'(u^M)\| \leq K_2,$$

and

$$-K_1 I_d \leq -\varepsilon \nabla_M^2 - g'(u^M) \leq K_1 I_d,$$

$\forall u^M \in B_r(\hat{u}_0^M)$, $\forall M \in \mathbb{N}$.

Observe also that there exists $N_0 \in \mathbb{N}$ such that if $N > N_0$, then

$$0 < \frac{K + 2K_2 \Delta t_N}{K + 1 - K_1 \Delta t_N} < 1.$$

Indeed, we may find $\alpha_0 \in \mathbb{R}$ such that

$$0 < \frac{K + 2K_2 \Delta t_N}{K + 1 - K_1 \Delta t_N} < \alpha_0 < 1, \ \forall N > N_0.$$

Let $M_N \subset \mathbb{N}$ be a sequence such that $M_N < M_{N+1}$, $\forall N \in \mathbb{N}$.

Fix $N > N_0$.

For $n = 0$, we are going to calculate $u_1 = u_1^{M_n, N}$ though the following iterations, which already include a proximal formulation and concerning linearization.

Set $u_1^0 = \hat{u}_0 = \hat{u}_0^{M_N, N}$,

Having u_1^k, let u_1^{k+1} be such that

$$\begin{aligned} u_1^{k+1} - \hat{u}_0 &= \varepsilon \nabla^2 u_1^{k+1} \Delta t_N + g(u_1^k)) \Delta t_N \\ &\quad + g'(u_1^k)(u_1^{k+1} - u_1^k) \Delta t_N + f_1 \Delta t_N - K(u_1^{k+1} - u_1^k), \end{aligned} \tag{385}$$

Here we suppose $K \equiv K_n^N > 0$ is large enough so that

$$u_1^1 \in B_{\frac{r(1-\alpha_0)}{N}}(u_0).$$

Reasoning inductively, suppose $u_1^0, u_1^1, \cdots, u_1^{k+1} \in B_{\frac{r}{N}}(u_0)$, and observe that

$$\begin{aligned} & u_1^{k+1} - \hat{u}_0 - \varepsilon \nabla^2 u_1^{k+1} \Delta t_N - g(u_1^k)) \Delta t_N \\ & - g'(u_1^k)(u_1^{k+1} - u_1^k) \Delta t_N - f_1 \Delta t_N + K(u_1^{k+1} - u_1^k) \\ = \ & 0, \end{aligned} \tag{386}$$

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and

$$\begin{aligned} & u_1^{k+2} - \hat{u}_0 - \varepsilon\nabla^2 u_1^{k+2}\Delta t_N - g(u_1^{k+1}))\Delta t_N \\ & -g'(u_1^{k+1})(u_1^{k+2} - u_1^{k+1})\Delta t_N - f_1\Delta t_N + K(u_1^{k+2} - u_1^{k+1}) \\ = \; & 0, \end{aligned} \tag{387}$$

so that for an appropriate $\tilde{u}_1^k$,

$$\begin{aligned} & \Big(I_d - \varepsilon\nabla_N^2\Delta t_N - g'(u_1^{k+1})\Delta t_N + KI_d\Big)(u_1^{k+2} - u_1^{k+1}) \\ = \; & \Big((-g'(\tilde{u}_1^k) + g'(u_1^{k+1}))\Delta t_N + KI_d\Big)\Big(u_1^{k+1} - u_1^k\Big). \end{aligned} \tag{388}$$

Hence,

$$\begin{aligned} & \|u_1^{k+2} - u_1^{k+1}\| \\ \leq \; & \left\|\Big(I_d - \varepsilon\nabla_N^2\Delta t_N - g'(u_1^{k+1})\Delta t_N + KI_d\Big)^{-1}\Big((-g'(\tilde{u}_1^k) + g'(u_1^{k+1}))\Delta t_N + KI_d\Big)\right\| \\ & \times\left\|u_1^{k+1} - u_1^k\right\| \\ \leq \; & \frac{K + 2K_2\Delta t_N}{K + 1 - K_1\Delta t_N}\left\|u_1^{k+1} - u_1^k\right\| \\ \leq \; & \alpha_0\left\|u_1^{k+1} - u_1^k\right\|. \end{aligned} \tag{389}$$

Thus, we have got

$$\|u_1^{j+2} - u_1^{j+1}\| \leq \alpha_0\|u_1^{j+1} - u_1^j\|, \; \forall j \in \{1, \cdots, k\}.$$

Therefore

$$\begin{aligned} \|u_1^{j+2} - u_1^{j+1}\| & \leq \alpha_0\|u_1^{j+1} - u_1^j\| \\ & \leq \alpha_0^2\|u_1^j - u_1^{j-1}\| \\ & \vdots \\ & \leq \alpha_0^{j+1}\|u_1^1 - u_1^0\|. \end{aligned} \tag{390}$$

Thus,

$$\begin{aligned} \|u_1^{k+2} - u_1^1\| & = \|u_1^{k+2} - u_1^{k+1} + u_1^{k+1} - \cdots - u_1^2 + u_1^2 - u_1^1\| \\ & \leq \|u_1^{k+2} - u_1^{k+1}\| + \|u_1^{k+1} - u_1^k\| + \cdots + \|u_1^2 - u_1^1\| \\ & \leq \sum_{j=1}^{k+1}\alpha_0^j\|u_1^1 - u_1^0\| \\ & \leq \sum_{j=1}^{\infty}\alpha_0^j\|u_1^1 - u_1^0\| \\ & = \frac{\alpha_0}{1 - \alpha_0}\|u_1^1 - u_1^0\|. \end{aligned} \tag{391}$$

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Therefore

$$\begin{aligned}\|u_1^{k+2}-u_1^0\| &\leq \|u_1^{k+2}-u_1^1+u_1^1-u_1^0\|\\ &\leq \|u_1^{k+2}-u_1^1\|+\|u_1^1-u_1^0\|\\ &\leq \frac{\alpha_0}{1-\alpha_0}\|u_1^1-u_1^0\|+\|u_1^1-u_1^0\|\\ &= \frac{1}{1-\alpha_0}\|u_1^1-u_1^0\|\\ &< \frac{1}{1-\alpha_0}(1-\alpha_0)\frac{r}{N}\\ &= \frac{r}{N}.\end{aligned} \tag{392}$$

Summarizing,

$$\|u_1^{k+2}-u_1^0\|<\frac{r}{N},$$

so that

$$u_1^{k+2}\in B_{\frac{r}{N}}(u_0^1).$$

The induction is complete, so that

$$u_1^k\in B_{\frac{r}{N}}(u_0^1),\ \forall k\in\mathbb{N}.$$

From such results we have also obtained

$$\|u_1^{k+2}-u_1^{k+1}\|\leq\alpha_0\|u_1^{k+1}-u_1^k\|,\ \forall k\in\mathbb{N}.$$

Thus, from these results and the Banach fixed point theorem, there exists $u_1=u_1^{M_N,N}\in B_{\frac{r}{N}}(u_0^1)$ such that

$$\lim_{k\to\infty}u_1^k=u_1=u_1^{M_N,N}.$$

$$\begin{aligned}\mathbf{0} &= \lim_{k\to\infty}\Big(u_1^{k+1}-\hat{u}_0\\ &\quad -\varepsilon\nabla^2u_1^{k+1}\Delta t_N-g(u_1^k))\Delta t_N\\ &\quad -g'(u_1^k)(u_1^{k+1}-u_1^k)\Delta t_N-f_1\Delta t_N+K(u_1^{k+1}-u_1^k)\Big)\\ &= u_1-\hat{u}_0-\varepsilon\nabla^2u_1\Delta t_N-g(u_1)\Delta t_N-f_1\Delta t_N,\end{aligned} \tag{393}$$

so that

$$\frac{u_1-\hat{u}_0}{\Delta t_N}=\varepsilon\nabla^2u_1+g(u_1)+f_1,\ \text{in }\Omega,$$

Reasoning inductively again having $u_1\in B_{\frac{r}{N}}(\hat{u}_0)$ and $u_j\in B_{\frac{r}{N}}(u_{j-1}),\ \forall j\in\{2,\cdots,n\}$ similarly as we have obtained u_1 in the last lines, we may obtain

$$u_{n+1}=u_{n+1}^{M_N,N}\in B_{\frac{r}{N}}(u_n),$$

such that

$$\frac{u_{n+1}-u_n}{\Delta t_N}=\varepsilon\nabla^2u_{n+1}+g(u_{n+1})+f_n,\ \text{in }\Omega.$$

The induction on n is also complete.

Fix $n\in\{1,\cdots,N-1\}$.

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Observe that

$$\begin{aligned}\|u_n-\hat{u}_0\| &= \|u_n-u_{n-1}+u_{n-1}-u_{n-2}+\cdots-u_1+u_1-u_0\|\\ &\leq \|u_n-u_{n-1}\|+\cdots+\|u_1-\hat{u}_0\|\\ &\leq \frac{n}{N}r\\ &< r\end{aligned} \tag{394}$$

Summarizing $u_n\in B_r(\hat{u}_0)$, $\forall n\in\{0,1,\cdots,N-1\}$.

From these results, denoting now more generically $u_n\equiv u_n^{M_N,N}=u_n^N$, we may infer that there exists $K_4>0$ such that

$$\|u_j^N\|\leq K_4,\ \forall j\in\{0,1,\cdots,N\},\forall N\in\mathbb{N}.$$

With a completely analogous reasoning, we may obtain that

$$\|u_j^N\|_{1,2,\Omega}\leq \hat{K}_4,\ \forall j\in\{0,1,\cdots,N\},\forall N\in\mathbb{N},$$

for some $\hat{K}_4>0$.

Define now

$$u_0^N(x,t)=u_n^N(x)\left(n+1-\frac{t}{\Delta t_N}\right)+u_{n+1}^N(x)\left(\frac{t}{\Delta t_N}-n\right),$$

if $t\in[n\Delta t_N,(n+1)\Delta t_N]$, $\forall(x,t)\in\Omega\times[0,T]$.

Observe that

$$u_0^N(x,t)=u_n^N(x),\ \text{if } t=n\Delta t_N,\ \forall n\in\{0,1,\cdots,N\},$$

and

$$\begin{aligned}\frac{\partial u_0^N(x,t)}{\partial t} &= \frac{u_{n+1}^N-u_n^N}{\Delta t_N}\\ &= \varepsilon\nabla^2u_{n+1}^N+g(u_{n+1}^N)+f_n,\end{aligned} \tag{395}$$

if $t\in[n\Delta t_N,(n+1)\Delta t_N]$, $\forall(x,t)\in\Omega\times[0,T]$.

Fix $\varphi\in C_c^\infty(\Omega)$.

Thus, fixing $t\in[n\Delta t_N,(n+1)\Delta t_N]$, we have

$$\begin{aligned}\left|\left\langle\frac{\partial u_0^N}{\partial t},\varphi\right\rangle_{L^2}\right| &\leq \varepsilon|\langle\nabla u_{n+1}^N,\nabla\varphi\rangle_{L^2}|+|\langle g(u_{n+1}^N),\varphi\rangle_{L^2}|\\ &\quad+|\langle\varphi,f_n\rangle_{L^2}|\\ &\leq \varepsilon\|u_{n+1}^N\|_{1,2,\Omega}\|\varphi\|_{1,2,\Omega}+K_{18}\|u_{n+1}^N\|_{1,2,\Omega}\|\varphi\|_{1,2,\Omega}+K_3\|\varphi\|_{1,2,\Omega}\\ &\leq K_5\|\varphi\|_{1,2,\Omega},\forall\varphi\in C_c^\infty(\Omega),\end{aligned} \tag{396}$$

for some appropriate $K_5>0$.

Since $\varphi\in C_c^\infty(\Omega)$ is arbitrary, we may conclude that

$$\left\|\frac{\partial u_0^N}{\partial t}\right\|_{H^{-1}(\Omega)}\leq K_6,\forall N>N_0,$$

uniformly in t on $[0,T]$, for some appropriate constant $K_6>0$.

Also, from the definition of u_0^N we have that there exists $K_7>0$ such that

$$\|u_0^N\|_{1,2,\Omega}\leq K_7,\ \forall N\in\mathbb{N}$$

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also uniformly in t on $[0,T]$.

From such results, there exist $u_0 \in L^2([0,T],H_0^1(\Omega))$ and $v_0 \in L^2([0,T];H^{-1}(\Omega))$ such that

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2((0,T);W^{1,2}(\Omega)),$$

and

$$\frac{\partial u_0^N}{\partial t} \rightharpoonup v_0, \text{ weakly-star in } L^2([0,T],H^{-1}(\Omega)),$$

so that we may easily obtain

$$v_0 = \frac{\partial u_0}{\partial t}$$

in a distributional sense.

At this point, we provide more details about this last result.

Fix $t \in (0,T)$. Thus, there exists $n \in \{0,1,\cdots,N-1\}$ such that $t \in [n\Delta t_N,(n+1)\Delta t_N]$.

Let $\varphi \in C_c^\infty(\Omega\times(0,T))$.

From this, we may infer that

$$\begin{aligned}
& \int_\Omega \frac{\partial u_0^N}{\partial t}\varphi(x,t)\,dx \\
= & \int_\Omega \frac{u_{n+1}^N - u_n^N}{\Delta t_N}\varphi(x,t)\,dx \\
\leq & \ \varepsilon\int_\Omega |\nabla u_{n+1}^N\cdot\nabla\varphi|\,dx \\
& + \int_\Omega |g(u_{n+1}^N)\,\varphi(x,t)|\,dx + \int_\Omega |f_n\varphi|\,dx \\
\leq & \ (K_8\|u_{n+1}^N\|_{1,2,\Omega}+K_{20})\|\varphi\|_{1,2,\Omega} \\
\leq & \ K_9\|\varphi\|_{1,2,\Omega}, \qquad (397)
\end{aligned}$$

for some appropriate constants $K_8>0,\ K_9>0, K_{20}>0$.

Hence,

$$\begin{aligned}
& \int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi(x,t)\,dx\,dx \\
\leq & \ K_9\int_\Omega \|\varphi\|_{1,2,\Omega}\,dt \\
\leq & \ K_{19}\|\varphi\|_{1,2,\Omega\times(0,T)}, \qquad (398)
\end{aligned}$$

for some appropriate $K_{19}>0$.

Since such a $\varphi \in C_c^\infty(\Omega\times(0,T))$ is arbitrary, we may infer that

$$\left\|\frac{\partial u_0^N}{\partial t}\right\|_{H^{-1}(\Omega\times(0,T))} \leq K_{15},$$

for $N\in\mathbb{N}$, for some $K_{15}>0$.

From such a result and from the Banach-Alaoglu Theorem, there exists $v_0 \in H^{-1}(\Omega\times(0,T))$ such that, up to a not relabeled subsequence

$$\frac{\partial u_0^N}{\partial t} \rightharpoonup v_0, \text{ weakly-star in } H^{-1}(\Omega\times(0,T)).$$

Therefore,

$$\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\,dx\,dt \to \int_0^T\int_\Omega v_0\,\varphi\,dx\,dt,$$

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as $N \to \infty$, $\forall \varphi \in H_0^1(\Omega \times (0,T))$.

On the other hand

$$\|u_0^N\|_{0,2,\Omega\times(0,T)} \leq K_{16},$$

$\forall N \in \mathbb{N}$, for some $K_{16} > 0$.

From this and the Kakutani Theorem, there exists $u_0 \in L^2(\Omega \times (0,T))$ such that, up to a not relabeled subsequence,

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2(\Omega \times (0,T)).$$

Now fix again $\varphi \in C_c^\infty(\Omega \times (0,T))$.

Observe that

$$\begin{aligned} \int_0^T \int_\Omega u_0 \varphi_t \, dx \, dt &= \lim_{N\to\infty} \int_0^T \int_\Omega u_0^N \varphi_t \, dx \, dt \\ &= -\lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \\ &= -\int_0^T \int_\Omega v_0 \varphi \, dx \, dt, \end{aligned} \tag{399}$$

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T))$ is arbitrary, we may infer that

$$v_0 = \frac{\partial u_0}{\partial t}$$

in a distributional sense.

Moreover, from such results we may also obtain, again up to a subsequence,

$$\lim_{N\to\infty} \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx = \int_\Omega \frac{\partial u_0}{\partial t} \varphi \, dx,$$

$\forall \varphi \in H_0^1(\Omega)$.

Observe also that, as a consequence of the Rellich-Kondrashov theorem, through appropriate subsequences, we have

$$u_0^{N_k(t)} \to u_0(x,t), \text{ strongly in } L^2(\Omega), \text{ for almost all } t \in [0,T].$$

so that, up to subsequences,

$$u_0^{N_k(t)}(x,t) \to u_0(x,t), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Here we emphasise the sequence $\{N_k(t)\} \subset \mathbb{N}$ may depends on t.

Since g is continuous we have that

$$g(u_0^{N_k(t)}(x,t)) \to g(u_0(x,t)), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Fix $t \in (0,T)$.

Let $\varepsilon > 0$. From the Egorov Theorem, there exists a closed set F such that $m(\Omega \setminus F) \leq \varepsilon$ and $k_0 \in \mathbb{N}$ such that if $k > k_0$, then

$$|g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))| \leq \varepsilon, \text{ for almost all } x \in F.$$

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Let $\varphi \in C_c^\infty(\Omega)$. Observe now that

$$\begin{aligned}
&\left|\int_\Omega (g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t)))\varphi\, dx\right| \\
\leq\ & \int_\Omega |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\, dx \\
=\ & \int_F |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\, dx + \int_{\Omega\setminus F} |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\, dx \\
\leq\ & \int_F \varepsilon\|\varphi\|_\infty\, dx + \int_\Omega |g(u_0^{N_k(t)}(x,t)) - g(u_0(x,t))|\ |\varphi|\chi_{\Omega\setminus F}\, dx \\
\leq\ & \varepsilon\|\varphi\|_\infty m(\Omega) + (\|g(u_0^{N_k(t)})\|_{0,2,\Omega} + \|g(u_0)\|_{0,2,\Omega})\|\varphi\|_{0,4,\Omega}\|\chi_{\Omega\setminus F}\|_{0,4,\Omega} \\
\leq\ & \varepsilon\|\varphi\|_\infty m(\Omega) + K_{21}\|\varphi\|_{0,4,\Omega} m(\Omega\setminus F)^{1/4} \\
\leq\ & \varepsilon\ \|\varphi\|_\infty\ m(\Omega) + K_{21}\|\varphi\|_{0,4,\Omega}\ \varepsilon^{1/4}, \forall k > k_0, \qquad (400)
\end{aligned}$$

for some appropriate constant $K_{21} > 0$ which does not depend on t.

Since such a $\varepsilon > 0$ is arbitrary, we may infer that

$$\int_\Omega g(u_0^{N_k(t)})\varphi\, dx \to \int_\Omega g(u_0)\varphi\, dx, \ \text{ as } k \to \infty,$$

$\forall \varphi \in C_c^\infty(\Omega)$.

From such results, we have

$$\begin{aligned}
0 \ =\ & \lim_{k\to\infty}\left(\int_\Omega \frac{\partial u_0^{N_k(t)}}{\partial t}\ \varphi\, dx + \varepsilon\int_\Omega \nabla u_0^{N_k(t)}\cdot\nabla\varphi\, dx\right. \\
& \left. - \int_\Omega g(u_0^{N_k(t)})\varphi\, dx - \int_\Omega f^{N_k(t)}\varphi\, dx\right) \\
=\ & \int_\Omega \frac{\partial u_0}{\partial t}\ \varphi\, dx + \varepsilon\int_\Omega \nabla u_0\cdot\nabla\varphi\, dx \\
& - \int_\Omega g(u_0)\varphi\, dx - \int_\Omega f\varphi\, dx. \qquad (401)
\end{aligned}$$

so that, from this and by the density of $C_c^\infty(\Omega)$ in $H_0^1(\Omega)$, we have got

$$\begin{aligned}
&\int_\Omega \frac{\partial u_0}{\partial t}\ \varphi\, dx + \varepsilon\int_\Omega \nabla u_0\cdot\nabla\varphi\, dx \\
&- \int_\Omega g(u_0)\varphi\, dx - \int_\Omega f\varphi\, dx = 0,\ \forall\varphi \in H_0^1(\Omega), \qquad (402)
\end{aligned}$$

a.e. on $[0,T]$.

Observe now that

$$\partial(\Omega\times(0,T)) = (\partial\Omega\times[0,T]) \cup \left(\partial[0,T]\times\overline{\Omega}\right).$$

Let $\varphi \in C_c^\infty(\Omega\times(0,T))$.

Hence

$$\lim_{N\to\infty}\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\, dx\, dt = \int_0^T\int_\Omega \frac{\partial u_0}{\partial t}\varphi\, dx\, dt.$$

From this, since $C_c^\infty(\Omega\times(0,T))$ is dense $L^2(\Omega\times(0,T))$ we may infer that

$$\lim_{N\to\infty}\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\, dx\, dt = \int_0^T\int_\Omega \frac{\partial u_0}{\partial t}\varphi\, dx\, dt,$$

$\forall \varphi \in L^2(\Omega\times(0,T))$.

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Let $\varphi \in C^{\infty}(\Omega \times [0,T])$ such that

$$\varphi(x,T) = 0, \text{ in } \Omega.$$

From such results, we may obtain

$$\begin{aligned} & \lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \\ = & \lim_{N\to\infty} \left(- \int_0^T \int_\Omega u_0^N \frac{\partial \varphi}{\partial t} \, dx \, dt - \int_\Omega u_0^N(x,0)\varphi(x,0) \, dx \right) \\ = & - \int_0^T \int_\Omega u_0 \frac{\partial \varphi}{\partial t} \, dx \, dt - \int_\Omega u_0(x,0)\varphi(x,0) \, dx. \end{aligned} \tag{403}$$

However, since $u_0^N \rightharpoonup u_0$, weakly in $L^2(\Omega \times (0,T))$, we obtain

$$\lim_{N\to\infty} \int_0^T \int_\Omega u_0^N \, \frac{\partial \varphi}{\partial t} \, dx \, dt = \int_0^T \int_\Omega u_0 \, \frac{\partial \varphi}{\partial t} \, dx \, dt.$$

From these last results, we may infer that

$$\begin{aligned} \int_\Omega \hat{u}_0 \, \varphi(x,0) \, dx &= \lim_{N\to\infty} \int_\Omega u_0^N(x,0)\varphi(x,0) \, dx \\ &= \int_\Omega u_0(x,0) \, \varphi(x,0) \, dx, \end{aligned} \tag{404}$$

so that

$$\int_\Omega \hat{u}_0(x)\varphi(x,0) \, dx = \int_\Omega u_0(x,0)\varphi(x,0) \, dx,$$

$\forall \varphi \in C^{\infty}(\Omega \times [0,T])$ such that $\varphi(x,T) = 0, \text{ in } \Omega$.

Therefore, we may infer that $u_0(x,0) = \hat{u}_0(x)$ in this specified weak sense.

Similarly, it may be proven that

$$u_0 = 0, \text{ on } \partial\Omega \times [0,T],$$

in an appropriate weak sense.

Hence, we have obtained that u_0 is a solution, in a weak sense, of the parabolic non-linear equation in question.

59. On the Convergence of Newton's Method Combined with a Proximal Approach for an Eigenvalue Problem

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the eigenvalue problem of finding $u \in V$ and $\lambda \in \mathbb{R}$ such that

$$\begin{cases} -\varepsilon\nabla^2 u + g(u) - \lambda u = 0, & \text{in } \Omega, \\ u = 0, \text{ on } \partial\Omega, \\ \int_\Omega u^2 \, dx = \|u\|_{0,2,\Omega}^2 = 1. \end{cases} \tag{405}$$

Here $\varepsilon > 0$, $V = H_0^1(\Omega)$, and $g : \mathbb{R} \to \mathbb{R}$ is a C^1 class function, such that either g is linear or such that

$$g(tu) = tg(u), \forall t > 0, \ \forall u \in \mathbb{R}$$

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In a finite differences or finite elements context, already including a proximal formulation, we shall look for a sequence $\{u_n\} \subset \mathbb{R}^N$ for an appropriate $N \in \mathbb{N}$ such that

$$-\varepsilon\nabla^2 u_{n+1} + g(u_{n+1}) - \frac{u_n}{\|u_n\|} + K(u_{n+1} - u_n) = \mathbf{0},$$

$\forall n \in \mathbb{N} \cup \{0\}$.

Now considering a concerning linearization of g, such an equation approximately stands for

$$-\varepsilon\nabla^2 u_{n+1} + g(u_n) + g'(u_n)(u_{n+1} - u_n) - \frac{u_n}{\|u_n\|} + K(u_{n+1} - u_n) = \mathbf{0},$$

$\forall n \in \mathbb{N} \cup \{0\}$.

Assume $u_0 \in \mathbb{R}^N$ is such that there exists $r > 0$ such that

$$K_1 I_d \leq g'(u) \leq K_2 I_d,$$

$\forall u \in B_r(u_0)$, for some $K_1, K_2 > 0$.

Suppose there exists a symmetric matrix $H_6(u, v)$ such that

$$\frac{u}{\|u\|} - \frac{v}{\|v\|} = H_6(u, v)(u - v),$$

and

$$-K_3 I_d \leq H_6(u, v) \leq K_3 I_d,$$

$\forall u, v \in B_r(u_0)$, for some $K_3 > 0$

And also there exists a symmetric matrix $H_5(u, v)$ such that

$$g(u) - g(v) = H_5(u, v)(u - v),$$

and

$$K_4 I_d \leq H_5(u, v) \leq K_5 I_d,$$

$\forall u, v \in B_r(u_0)$, for some $K_4,\ K_5 > 0$. Moreover, we assume that these last constants, $K > 0$ and $0 < \alpha_1 < 1$ are such that

$$(1 - \alpha_1)(-\varepsilon\nabla^2 + K_1 I_d) + K_4 I_d - K_3 I_d - K_2 I_d) \geq \alpha_1 K I_d = K\ I_d - (1 - \alpha_1) K\ I_d,$$

so that

$$(-\varepsilon\nabla^2 + K_1 I_d + K I_d)^{-1}(-K_4 I_d + K_2 I_d + K_3 I_d + K I_d) \leq (1 - \alpha_1) I_d.$$

Observe that

$$\varepsilon\nabla^2 + g'(u) + K\ I_d \geq -\varepsilon\nabla^2 + K_1 I_d + K\ I_d \geq 0$$

and

$$0 \leq -H_5(u, v) + H_6(u, v) + g'(v) + K\ I_d \leq -K_4 I_d + K_2 I_d + K_3 I_d + K I_d,$$

$\forall u, v \in B_r(u_0)$ so that

$$\begin{aligned} & (\varepsilon\nabla^2 + g'(u) + K\ I_d)^{-1}(-H_5(u, v) + H_6(u, v) + g'(v) + K\ I_d) \\ \leq\ & (-\varepsilon\nabla^2 + K_1 I_d + K I_d)^{-1}(-K_4 I_d + K_2 I_d + K_3 I_d + K I_d) \\ \leq\ & (1 - \alpha_1) I_d, \end{aligned} \tag{406}$$

$\forall u, v \in B_r(u_0)$.

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Summarizing, defining $\alpha_0 = 1 - \alpha_1$ we have got

$$\|(\varepsilon\nabla^2 + g'(u) + K\ I_d)^{-1}(-H_5(u,v) + H_6(u,v) + g'(v) + K\ I_d)\| \leq \alpha_0 < 1,$$

$\forall u, v \in B_r(u_0)$.

Suppose $K > 0$ and $\alpha_1 > 0$ are such that $u_1 \in B_{r(1-\alpha_0)}(u_0)$.

Reasoning inductively, suppose also

$$u_0, u_1, \cdots, u_{n+1} \in B_r(u_0).$$

From the results above we have

$$-\varepsilon\nabla^2 u_{n+2} + g(u_{n+1}) + g'(u_{n+1})(u_{n+2} - u_{n+1}) - \frac{u_{n+1}}{\|u_{n+1}\|} + K(u_{n+2} - u_{n+1}) = \mathbf{0},$$

and

$$-\varepsilon\nabla^2 u_{n+1} + g(u_n) + g'(u_n)(u_{n+1} - u_n) - \frac{u_n}{\|u_n\|} + K(u_{n+1} - u_n) = \mathbf{0},$$

so that

$$\begin{aligned} & -\varepsilon(\nabla^2 u_{n+2} - \nabla^2 u_{n+1}) + g'(u_{n+1})(u_{n+2} - u_{n+1}) + K(u_{n+2} - u_{n+1}) \\ = \ & -g(u_{n+1}) + g(u_n) + \frac{u_{n+1}}{\|u_{n+1}\|} - \frac{u_n}{\|u_n\|} + g'(u_n)(u_{n+1} - u_n) + K(u_{n+1} - u_n) \\ = \ & (-H_5(u_{n+1}, u_n) + H_6(u_{n+1}, u_n) + g'(u_n) + KI_d)(u_{n+1} - u_n). \end{aligned} \tag{407}$$

Therefore

$$\begin{aligned} & u_{n+2} - u_{n+1} \\ = \ & ((-\varepsilon\nabla^2 + g'(u_{n+1}) + KI_d)^{-1}(-H_5(u_{n+1}, u_n) + H_6(u_{n+1}, u_n) + g'(u_n) + KI_d) \\ & \times(u_{n+1} - u_n), \end{aligned} \tag{408}$$

so that

$$\begin{aligned} & \|u_{n+2} - u_{n+1}\| \\ \leq \ & \|((-\varepsilon\nabla^2 + g'(u_{n+1}) + KI_d)^{-1}(-H_5(u_{n+1}, u_n) + H_6(u_{n+1}, u_n) + g'(u_n) + KI_d)\| \\ & \times\|u_{n+1} - u_n\| \\ \leq \ & \alpha_0\|u_{n+1} - u_n\|. \end{aligned} \tag{409}$$

Summarizing, we have got

$$\|u_{j+2} - u_{j+1}\| \leq \alpha_0\|u_{j+1} - u_j\|,\ \forall j \in \{1, \cdots, n\}.$$

Therefore

$$\begin{aligned} \|u_{j+2} - u_{j+1}\| & \leq \alpha_0\|u_{j+1} - u_j\| \\ & \leq \alpha_0^2\|u_j - u_{j-1}\| \\ & \vdots \\ & \leq \alpha_0^{j+1}\|u_1 - u_0\|. \end{aligned} \tag{410}$$

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Thus,

$$\begin{aligned}\|u_{n+2}-u_1\| &= \|u_{n+2}-u_{n+1}+u_{n+1}-\cdots-u_2+u_2-u_1\| \\ &\leq \|u_{n+2}-u_{n+1}\|+\|u_{n+1}-u_n\|+\cdots+\|u_2-u_1\| \\ &\leq \sum_{j=1}^{n+1}\alpha_0^j\|u_1-u_0\| \\ &\leq \sum_{j=1}^{\infty}\alpha_0^j\|u_1-u_0\| \\ &= \frac{\alpha_0}{1-\alpha_0}\|u_1-u_0\|. \end{aligned} \tag{411}$$

Therefore

$$\begin{aligned}\|u_{n+2}-u_0\| &\leq \|u_{n+2}-u_1+u_1-u_0\| \\ &\leq \|u_{n+2}-u_1\|+\|u_1-u_0\| \\ &\leq \frac{\alpha_0}{1-\alpha_0}\|u_1-u_0\|+\|u_1-u_0\| \\ &= \frac{1}{1-\alpha_0}\|u_1-u_0\| \\ &< \frac{1}{1-\alpha_0}(1-\alpha_0)r \\ &= r. \end{aligned} \tag{412}$$

Summarizing,

$$\|u_{n+2}-u_0\|<r,$$

so that

$$u_{n+2}\in B_r(u_0).$$

The induction is complete, so that

$$u_n\in B_r(u_0),\ \forall n\in\mathbb{N}.$$

From such results we have also obtained

$$\|u_{n+2}-u_{n+1}\|\leq\alpha_0\|u_{n+1}-u_n\|,\ \forall n\in\mathbb{N}.$$

Thus, from these results and the Banach fixed point theorem, there exists $\hat{u}_0\in\overline{B}_r(u_0)$ such that

$$\lim_{n\to\infty}u_n=\hat{u}_0.$$

From such results we obtain

$$\begin{aligned}\mathbf{0} &= \lim_{n\to\infty}\Big(-\varepsilon\nabla^2u_{n+1}+g(u_n)+g'(u_n)(u_{n+1}-u_n) \\ &\quad -\frac{u_n}{\|u_n\|}+K(u_{n+1}-u_n)\Big) \\ &= -\varepsilon\nabla^2\hat{u}_0+g(\hat{u}_0)-\frac{\hat{u}_0}{\|\hat{u}_0\|}. \end{aligned} \tag{413}$$

Summarizing, we have got

$$-\varepsilon\nabla^2\hat{u}_0+g(\hat{u}_0)-\frac{\hat{u}_0}{\|\hat{u}_0\|}=\mathbf{0}.$$

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Consequently, defining

$$\tilde{u}_0 = \frac{\hat{u}_0}{\|\hat{u}_0\|_{0,2,\Omega}},$$

$$\lambda = \frac{1}{\|\hat{u}_0\|}$$

and recalling that

$$g(t\hat{u}_0) = tg(\hat{u}_0),\ \forall t > 0,$$

we have obtained

$$-\varepsilon\nabla^2\tilde{u}_0 + g(\tilde{u}_0) - \lambda\tilde{u}_0 = \mathbf{0},$$

and

$$\|\tilde{u}_0\|_{0,2,\Omega} = 1.$$

The objective of this section is complete.

Remark 59.1. *For the general case we may drop the hypotheses of g being linear or $g(tu) = tg(u),\ \forall t > 0,\ \forall u \in \mathbb{R}$, by defining the following iterations:*

$$-\varepsilon\nabla^2 u_{n+1} + \|u_n\|\, g\left(\frac{u_n}{\|u_n\|}\right) - \frac{u_n}{\|u_n\|} + K(u_{n+1} - u_n) = \mathbf{0},\ \forall n \in \mathbb{N}\cup\{0\}.$$

However in such a case some changes on the hypotheses are necessary in order to obtain the related theoretical results.

59.1. A Numerical Example

For $\Omega = [0,1] \subset \mathbb{R}$, we have obtained numerical results for the following eigenvalue equation

$$\begin{cases} -\varepsilon u'' + Au^3 - \lambda u = 0, & \text{in } \Omega, \\ u = 0, \text{ on } \partial\Omega, \\ \int_\Omega u^2\, dx = \|u\|^2_{0,2,\Omega} = 1, \end{cases} \tag{414}$$

where $\varepsilon = 0.01$, and $A = 1.0$

Observe that for a fixed $K > 0$ we may obtain for this last equation

$$-\varepsilon u'' + Au^3 + K\, u - K\, u - \lambda u = 0, \text{ in } \Omega,$$

so that

$$-\varepsilon u'' + Au^3 + K\, u - \lambda_1 u = 0, \text{ in } \Omega,$$

where $\lambda_1 = K + \lambda$. In this example we have fixed $K = 500$.

In order to obtain such numerical results we have used the following algorithm:

1. Choose $u_1 \in W_0^{1,2}$, set $n = 1$, $b_{12} = 10^{-4}$ and $n_{max} = 100$.
2. Calculate $u_{n+1} \in W_0^{1,2}$ solution of equation

$$-\varepsilon u''_{n+1} + A\frac{u_n^3}{\|u_n\|^2_{0,2,\Omega}} + K\, u_{n+1} - \frac{u_n}{\|u_n\|_{0,2,\Omega}} = 0, \text{ in } \Omega,$$

3. If $\|u_{n+1} - u_n\|_\infty \leq b_{12}$ or $n > n_{max}$, then stop. Otherwise $n := n + 1$ and go to item 2.

For the optimal solution u obtained, please see Figure 43.

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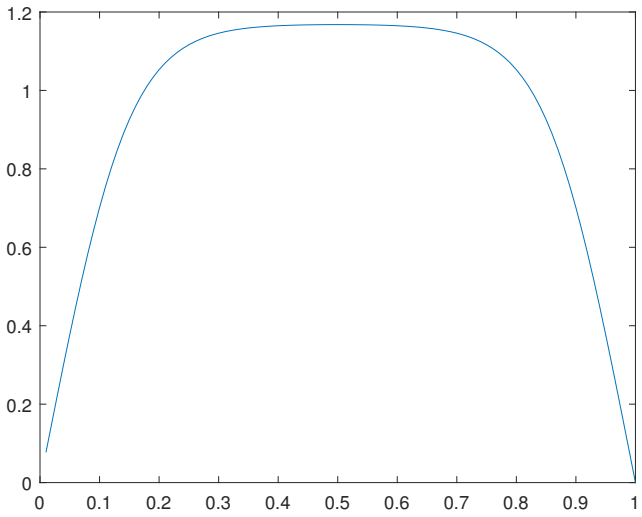

Figure 43. Solution $u(x)$ for $\varepsilon = 0.01$

Here we present the software in MAT-LAB through which we have obtained such numerical results.

****

1. clear all
   m8=100;
   d=1/m8;
   K=500;
   A=1;
   e1=0.01;
   for i=1:m8
   uo(i,1)=0.1;
   end;
   b12=1.0;
   k=1;
   while $(b12 > 10^{-4})$ && $(k < 100)$
   k
   k=k+1;
   S=0;
   for i=1:m8-1
   S=S+$uo(i,1)^2 * d$;
   end;
   S=sqrt(S);
   m12=2+K*d^2;
   m50(1)=1/m12;
   z(1)=m50(1)*($uo(i,1)/S * d^2$-A*$uo(i,1)^3/S^2 * d^2/e1$);
   for i=2:m8-1

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m12=2+K*d^2-m50(i-1);

m50(i)=1/m12;

z(i)=m50(i)*$(uo(i,1)/S*d^2 - A*uo(i,1)^3/S^2*d^2/e1 + z(i-1))$;

end;

u(m8,1)=0;

for i=1:m8-1

u(m8-i,1)=m50(m8-i)*u(m8-i+1)+z(m8-i);

end;

b12=max(abs(uo-u));

uo=u;

end;

end;

for i=1:m8

x(i,1)=i*d;

end;

plot(x,uo/S)

****

Remark 59.2. *With the high value $K = 500$ we have obtained the following eigenvalue for this problem:*

$$\lambda = \left(\frac{1}{S} - K\right) \varepsilon = 133.8090\, \varepsilon = 1.338.$$

60. On the Convergence of Newton's Method Combined with a Proximal Approach for a General Parabolic Non-Linear System

Let $\Omega \subset \mathbb{R}^m$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider the parabolic non-linear system

$$\begin{cases} \frac{\partial u_j}{\partial t} = \varepsilon_j \nabla^2 u_j + g_j(u) + \sum_{k=1}^{r} \sum_{l=1}^{m} g_{jkl}(u) \frac{\partial u_k}{\partial x_l} + f_j, \quad \text{in } \Omega \times (0,T), \\ u_j(x,0) = (\hat{u}_0)_j, \text{ in } \Omega, \\ u_j = 0, \text{ on } \partial\Omega \times [0,T], \ \forall j \in \{1, \cdots, r\}. \end{cases} \tag{415}$$

Here

$$u = (u_1, \cdots, u_r) = \{u_j\} \in H_0^1(\Omega; \mathbb{R}^r),$$

$\varepsilon_j > 0$, $f = \{f_j\} \in L^2([0,T], W^{1,2}(\Omega; \mathbb{R}^r)) \cap L^\infty(\Omega \times [0,T]; \mathbb{R}^r)$, $\hat{u}_0 = \{(\hat{u}_0)_j\} \in H_0^1(\Omega; \mathbb{R}^r) \cap L^\infty(\Omega; \mathbb{R}^r)$, where t denotes time and $[0,T]$ is a time interval.

Also $g_j : \mathbb{R} \to \mathbb{R}$ and $g_{jkl} : \mathbb{R} \to \mathbb{R}$ are C^1 class functions neither necessarily linear nor convex, $\forall j,k \in \{1, \cdots, r\}$, $l \in \{1, \cdots, m\}$.

We define

$$F_j(u) = \varepsilon_j \nabla^2 u_j + g_j(u) + \sum_{k=1}^{r} \sum_{l=1}^{m} g_{jkl}(u) \frac{\partial u_k}{\partial x_l} + f_j,$$

$\forall j \in \{1, \cdots, r\}$, so that the system in question stands for

$$\frac{\partial u_j}{dt} = F_j(u), \ \forall j \in \{1, \cdots, r\}.$$

Fixing $N \in \mathbb{N}$ and defining $\Delta t_N = T/N$, in a finite differences context we may define the following approximate system

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$$\frac{u_{n+1}-u_n}{\Delta t_N} = F_j(u_{n+1}),\ \forall j \in \{1,\cdots,r\},\ \forall n \in \{0,\cdots,N-1\}.$$

Fix $n=0$. In a Newton's method context combined with a proximal approach, we shall obtain u_1 through the following iterations,

Define $u_1^0 = \hat{u}_0$ and having u_1^k let u_1^{k+1} be such that

$$u_1^{k+1} - u_1^0 = F_j(u_1^k)\Delta t_N + \Delta t_N \left\{ \frac{\partial F_j(u_1^k)}{\partial u_l} \right\} (u_1^{k+1} - u_1^k) - K(u_1^{k+1} - u_1^k).$$

At this point we assume there exist $r > 0$ and $K_1 > 0$, such that

$$-K_1 I_d \leq \left\{ \frac{\partial F_j(u)}{\partial u_l} \right\} \leq K_1 I_d,$$

$\forall u \in B_r(\hat{u}_0)$.

Moreover, generically denoting $F(u) = \{F_j(u)\}$, we assume there exists a matrix operator $H_5(u,v)$, such that

$$F(u) - F(v) = H_5(u,v)(u-v),$$

and

$$-K_3 I_d \leq H_5(u,v) \leq K_3 I_d,$$

$\forall u, v \in B_r(\hat{u}_0)$, for some appropriate real constant $K_3 > 0$.

Now suppose $K > 0$ and $0 < \alpha_1 < 1$ are such that there exists $N_0 \in \mathbb{N}$ such that if $N > N_0$, then

$$(1-\alpha_1)(I_d - K_1 I_d \Delta t_N) - K_1 I_d \Delta t_N - K_3 I_d \Delta t_N) \geq \alpha_1 K\ I_d = K\ I_d - (1-\alpha_1) K\ I_d,$$

so that

$$(I_d - K_1 I_d \Delta t_N + K I_d)^{-1}(K_1 I_d \Delta t_N + K_3 I_d \Delta t_N + K\ I_d) \leq (1-\alpha_1) K\ I_d.$$

Observe that such an N_0 may be such that

$$I_d - \left\{ \frac{\partial F_j(u)}{\partial u_l} \right\} \Delta t_N + K I_d \geq I_d - K_1 I_d \Delta t_N + K I_d > 0\ I_d,$$

and

$$0 \leq H_5(u,v)\Delta t_N - \left\{ \frac{\partial F_j(v)}{\partial u_l} \right\} \Delta t_N + K I_d \leq K_1 I_d \Delta t_N + K_3 I_d \Delta t_N + K\ I_d,$$

so that

$$\begin{aligned} & \left(I_d - \left\{ \frac{\partial F_j(u)}{\partial u_l} \right\} \Delta t_N + K I_d \right)^{-1} \left(H_5(u,v)\Delta t_N - \left\{ \frac{\partial F_j(v)}{\partial u_l} \right\} \Delta t_N + K I_d \right) \\ \leq\ & (I_d - K_1 I_d \Delta t_N + K I_d)^{-1}(K_1\ I_d\ \Delta t_N + K_3\ I_d\ \Delta t_N + K\ I_d) \\ \leq\ & (1-\alpha_1) I_d, \end{aligned} \tag{416}$$

$\forall u, v \in B_r(\hat{u}_0),\ \forall N > N_0$.

Hence, denoting $\alpha_0 = (1-\alpha_1)$, we have got

$$\begin{aligned} & \left\| \left(I_d - \left\{ \frac{\partial F_j(u)}{\partial u_l} \right\} \Delta t_N + K I_d \right)^{-1} \left(H_5(u,v)\Delta t_N - \left\{ \frac{\partial F_j(v)}{\partial u_l} \right\} \Delta t_N + K I_d \right) \right\| \\ \leq\ & \left\| (I_d - K_1 I_d \Delta t_N + K I_d)^{-1}(K_1 I_d \Delta t_N + K_3 I_d \Delta t_N + K\ I_d) \right\| \\ \leq\ & \alpha_0. \end{aligned} \tag{417}$$

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$\forall u, v \in B_r(\hat{u}_0), \forall N > N_0$.

Fix now a new $N > N_0$.

Suppose now $K = K_n^N > 0$ and $0 < \alpha_1 = (\alpha_1)_n^N < 1$ are such that

$$u_1^1 \in B_{\frac{r}{N}(1-\alpha_0)}(\hat{u}_0).$$

Reasoning inductively, suppose $u_1^0, u_1^1, \cdots, u_1^{k+1} \in B_{\frac{r}{N}}(u_0)$, and observe that

$$u_1^{k+1} - u_0^1 = F_j(u_1^k)\Delta t_N + \Delta t_N \left\{ \frac{\partial F_j(u_1^k)}{\partial u_l} \right\} (u_1^{k+1} - u_1^k) - K(u_1^{k+1} - u_1^k).$$

and

$$u_1^{k+2} - u_0^1 = F_j(u_1^{k+1})\Delta t_N + \Delta t_N \left\{ \frac{\partial F_j(u_1^{k+1})}{\partial u_l} \right\} (u_1^{k+2} - u_1^{k+1}) - K(u_1^{k+2} - u_1^{k+1}),$$

so that

$$\begin{aligned} & \left(I_d - \left\{ \frac{\partial F_j(u_1^{k+1})}{\partial u_l} \right\} \Delta t_N + KI_d \right) (u_1^{k+2} - u_1^{k+1}) \\ = & \left((F(u_1^{k+1}) - F(u_1^k))\Delta t_N - \left\{ \frac{\partial F_j(u_1^k)}{\partial u_l} \right\} \Delta t_N + KI_d \right) (u_1^{k+1} - u_1^k) \\ = & \left(H_5(u_1^{k+1}, u_1^k)\Delta t_N - \left\{ \frac{\partial F_j(u_1^k)}{\partial u_l} \right\} \Delta t_N + KI_d \right) (u_1^{k+1} - u_1^k). \end{aligned} \tag{418}$$

Thus,

$$\begin{aligned} & u_1^{k+2} - u_1^{k+1} \\ = & \left(I_d - \left\{ \frac{\partial F_j(u_1^{k+1})}{\partial u_l} \right\} \Delta t_N + KI_d \right)^{-1} \left(H_5(u_1^{k+1}, u_1^k)\Delta t_N - \left\{ \frac{\partial F_j(u_1^k)}{\partial u_l} \right\} \Delta t_N + KI_d \right) \\ & \times (u_1^{k+1} - u_1^k). \end{aligned} \tag{419}$$

Summarizing, we have got

$$\begin{aligned} & \left\| u_1^{k+2} - u_1^{k+1} \right\| \\ = & \left\| \left(I_d - \left\{ \frac{\partial F_j(u_1^{k+1})}{\partial u_l} \right\} \Delta t_N + KI_d \right)^{-1} \left(H_5(u_1^{k+1}, u_1^k)\Delta t_N - \left\{ \frac{\partial F_j(u_1^k)}{\partial u_l} \right\} \Delta t_N + KI_d \right) \right\| \\ & \times \|u_1^{k+1} - u_1^k\| \\ \leq & \alpha_0 \|u_1^{k+1} - u_1^k\|. \end{aligned} \tag{420}$$

Thus, we have got

$$\|u_1^{j+2} - u_1^{j+1}\| \leq \alpha_0 \|u_1^{j+1} - u_1^j\|, \ \forall j \in \{1, \cdots, k\}.$$

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Therefore

$$\begin{aligned} \|u_1^{j+2} - u_1^{j+1}\| &\leq \alpha_0 \|u_1^{j+1} - u_1^j\| \\ &\leq \alpha_0^2 \|u_1^j - u_1^{j-1}\| \\ &\vdots \\ &\leq \alpha_0^{j+1} \|u_1^1 - u_1^0\|. \end{aligned} \tag{421}$$

Thus,

$$\begin{aligned} \|u_1^{k+2} - u_1^1\| &= \|u_1^{k+2} - u_1^{k+1} + u_1^{k+1} - \cdots - u_1^2 + u_1^2 - u_1^1\| \\ &\leq \|u_1^{k+2} - u_1^{k+1}\| + \|u_1^{k+1} - u_1^k\| + \cdots + \|u_1^2 - u_1^1\| \\ &\leq \sum_{j=1}^{k+1} \alpha_0^j \|u_1^1 - u_1^0\| \\ &\leq \sum_{j=1}^{\infty} \alpha_0^j \|u_1^1 - u_1^0\| \\ &= \frac{\alpha_0}{1-\alpha_0} \|u_1^1 - u_1^0\|. \end{aligned} \tag{422}$$

Therefore

$$\begin{aligned} \|u_1^{k+2} - u_1^0\| &\leq \|u_1^{k+2} - u_1^1 + u_1^1 - u_1^0\| \\ &\leq \|u_1^{k+2} - u_1^1\| + \|u_1^1 - u_1^0\| \\ &\leq \frac{\alpha_0}{1-\alpha_0} \|u_1^1 - u_1^0\| + \|u_1^1 - u_1^0\| \\ &= \frac{1}{1-\alpha_0} \|u_1^1 - u_1^0\| \\ &< \frac{1}{1-\alpha_0} (1-\alpha_0) \frac{r}{N} \\ &= \frac{r}{N}. \end{aligned} \tag{423}$$

Summarizing,

$$\|u_1^{k+2} - u_1^0\| < \frac{r}{N},$$

so that

$$u_1^{k+2} \in B_{\frac{r}{N}}(u_0^1).$$

The induction is complete, so that

$$u_1^k \in B_{\frac{r}{N}}(u_0^1), \ \forall k \in \mathbb{N}.$$

From such results we have also obtained

$$\|u_1^{k+2} - u_1^{k+1}\| \leq \alpha_0 \|u_1^{k+1} - u_1^k\|, \ \forall k \in \mathbb{N}.$$

Thus, from these results and the Banach fixed point theorem, there exists $u_1 \in B_{\frac{r}{N}}(u_0^1)$ such that

$$\lim_{k \to \infty} u_1^k = u_1.$$

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$$\begin{aligned}\mathbf{0} &= \lim_{k\to\infty}\Big(u_1^{k+1}-\hat{u}_0\\ &\quad -F(u_1^k)\Delta t_N-\Delta t_N\left\{\frac{\partial F_j(u_1^k)}{\partial u_l}\right\}(u_1^{k+1}-u_1^k)\\ &\quad +K(u_1^{k+1}-u_1^k)\Big)\\ &= u_1-\hat{u}_0-F(u_1)\Delta t_N \end{aligned} \tag{424}$$

so that

$$\frac{u_1-\hat{u}_0}{\Delta t_N}=F(u_1) \text{ in } \Omega,$$

Reasoning inductively again having $u_1\in B_{\frac{r}{N}}(\hat{u}_0)$ and $u_j\in B_{\frac{r}{N}}(u_{j-1})$, $\forall j\in\{2,\cdots,n\}$ similarly as we have obtained u_1 in the last lines, we may obtain

$$u_{n+1}\in B_{\frac{r}{N}}(u_n),$$

such that

$$\frac{u_{n+1}-u_n}{\Delta t_N}=F(u_{n+1}), \text{ in } \Omega.$$

The induction on n is also complete.

Fix $n\in\{1,\cdots,N-1\}$.

Observe that

$$\begin{aligned}\|u_n-u_0\| &= \|u_n-u_{n-1}+u_{n-1}-u_{n-2}+\cdots-u_1+u_1-u_0\|\\ &\leq \|u_n-u_{n-1}\|+\cdots+\|u_1-u_0\|\\ &\leq \frac{n}{N}r\\ &< r. \end{aligned} \tag{425}$$

Summarizing $u_n\in B_r(\hat{u}_0)$, $\forall n\in\{0,1,\cdots,N-1\}$.

From these results, denoting now more generically $u_n\equiv u_n^N$, we may infer that there exists $\hat{K}_4>0$ such that

$$\|u_j^N\|_{1,2,\Omega}\leq\hat{K}_4,\ \forall j\in\{0,1,\cdots,N\},\forall N\in\mathbb{N}.$$

Define now

$$u_0^N(x,t)=u_n^N(x)\left(n+1-\frac{t}{\Delta t_N}\right)+u_{n+1}^N(x)\left(\frac{t}{\Delta t_N}-n\right),$$

if $t\in[n\Delta t_N,(n+1)\Delta t_N]$, $\forall(x,t)\in\Omega\times[0,T]$.

Observe that

$$u_0^N(x,t)=u_n^N(x),\ \text{if } t=n\Delta t_N,\ \forall n\in\{0,1,\cdots,N\},$$

and

$$\begin{aligned}\frac{\partial u_0^N(x,t)}{\partial t} &= \frac{u_{n+1}^N-u_n^N}{\Delta t_N}\\ &= F(u_{n+1}^N), \end{aligned} \tag{426}$$

if $t\in[n\Delta t_N,(n+1)\Delta t_N]$, $\forall(x,t)\in\Omega\times[0,T]$.

Fix $\varphi\in C_c^\infty(\Omega;\mathbb{R}^r)$.

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Thus, fixing $t \in [n\Delta t_N, (n+1)\Delta t_N]$, we have

$$\begin{aligned} \left| \left\langle \frac{\partial u_0^N}{\partial t}, \varphi \right\rangle_{L^2} \right| &\leq \left| \langle F(u_{n+1}^N), \varphi \rangle_{L^2} \right| \\ &\leq K_5 \|\varphi\|_{1,2,\Omega}, \forall \varphi \in C_c^\infty(\Omega; \mathbb{R}^r), \end{aligned} \tag{427}$$

for some appropriate $K_5 > 0$.

Since $\varphi \in C_c^\infty(\Omega; \mathbb{R}^r)$ is arbitrary, we may conclude that

$$\left\| \frac{\partial u_0^N}{\partial t} \right\|_{H^{-1}(\Omega;\mathbb{R}^r)} \leq K_6, \forall N > N_0,$$

uniformly in t on $[0, T]$, for some appropriate constant $K_6 > 0$.

Also, from the definition of u_0^N we have that there exists $K_7 > 0$ such that

$$\|u_0^N\|_{1,2,\Omega} \leq K_7, \ \forall N \in \mathbb{N}$$

also uniformly in t on $[0, T]$.

From such results, there exist $u_0 \in L^2([0,T], H_0^1(\Omega; \mathbb{R}^r))$ and $v_0 \in L^2([0,T]; H^{-1}(\Omega; \mathbb{R}^r))$ such that

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2((0,T); W^{1,2}(\Omega; \mathbb{R}^r)),$$

and

$$\frac{\partial u_0^N}{\partial t} \rightharpoonup v_0, \text{ weakly-star in } L^2([0,T], H^{-1}(\Omega; \mathbb{R}^r)),$$

so that we may easily obtain

$$v_0 = \frac{\partial u_0}{\partial t}$$

in a distributional sense. At this point, we provide more details about this last result.

Fix $t \in (0, T)$. Thus, there exists $n \in \{0, 1, \cdots, N-1\}$ such that $t \in [n\Delta t_N, (n+1)\Delta t_N]$.

Let $\varphi \in C_c^\infty(\Omega \times (0,T); \mathbb{R}^r)$.

From this, we may infer that

$$\begin{aligned} & \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi(x,t) \, dx \\ = & \int_\Omega \frac{u_{n+1}^N - u_n^N}{\Delta t_N} \varphi(x,t) \, dx \\ \leq & \langle F(u_{n+1}^N), \varphi \rangle_{L^2} \\ \leq & K_9 \|\varphi\|_{1,2,\Omega}, \end{aligned} \tag{428}$$

for some appropriate constant $K_9 > 0$.

Hence,

$$\begin{aligned} & \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi(x,t) \, dx \, dt \\ \leq & K_9 \int_\Omega \|\varphi\|_{1,2,\Omega} \, dt \\ \leq & K_{19} \|\varphi\|_{1,2,\Omega \times (0,T)}, \end{aligned} \tag{429}$$

for some appropriate $K_{19} > 0$.

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T); \mathbb{R}^r)$ is arbitrary, we may infer that

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$$\left\| \frac{\partial u_0^N}{\partial t} \right\|_{H^{-1}(\Omega\times(0,T);\mathbb{R}^r)} \leq K_{15},$$

for $N \in \mathbb{N}$, for some $K_{15} > 0$.

From such a result and from the Banach-Alaoglu Theorem, there exists $v_0 \in H^{-1}(\Omega \times (0,T);\mathbb{R}^r)$ such that, up to a not relabeled subsequence

$$\frac{\partial u_0^N}{\partial t} \rightharpoonup v_0, \text{ weakly-star in } H^{-1}(\Omega \times (0,T);\mathbb{R}^r).$$

Therefore,

$$\int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \to \int_0^T \int_\Omega v_0 \, \varphi \, dx \, dt,$$

as $N \to \infty$, $\forall \varphi \in H_0^1(\Omega \times (0,T);\mathbb{R}^r)$.

On the other hand

$$\|u_0^N\|_{0,2,\Omega\times(0,T)} \leq K_{16},$$

$\forall N > N_0$, for some $K_{16} > 0$.

From this and the Kakutani Theorem, there exists $u_0 \in L^2(\Omega \times (0,T);\mathbb{R}^r)$ such that, up to a not relabeled subsequence,

$$u_0^N \rightharpoonup u_0, \text{ weakly in } L^2(\Omega \times (0,T);\mathbb{R}^r).$$

Now fix again $\varphi \in C_c^\infty(\Omega \times (0,T);\mathbb{R}^r)$.

Observe that

$$\begin{aligned} \int_0^T \int_\Omega u_0 \varphi_t \, dx \, dt &= \lim_{N\to\infty} \int_0^T \int_\Omega u_0^N \varphi_t \, dx \, dt \\ &= -\lim_{N\to\infty} \int_0^T \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx \, dt \\ &= -\int_0^T \int_\Omega v_0 \varphi \, dx \, dt, \end{aligned} \tag{430}$$

Since such a $\varphi \in C_c^\infty(\Omega \times (0,T);\mathbb{R}^r)$ is arbitrary, we may infer that

$$v_0 = \frac{\partial u_0}{\partial t}$$

in a distributional sense.

Moreover, from such results we may also obtain, again up to a subsequence,

$$\lim_{N\to\infty} \int_\Omega \frac{\partial u_0^N}{\partial t} \varphi \, dx = \int_\Omega \frac{\partial u_0}{\partial t} \varphi \, dx,$$

$\forall \varphi \in H_0^1(\Omega;\mathbb{R}^r)$.

Observe also that, as a consequence of the Rellich-Kondrashov theorem, through appropriate subsequences, we have

$$u_0^{N_k(t)} \to u_0(x,t), \text{ strongly in } L^2(\Omega;\mathbb{R}^r), \text{ for almost all } t \in [0,T].$$

so that, up to subsequences,

$$u_0^{N_k(t)}(x,t) \to u_0(x,t), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Here we emphasise the sequence $\{N_k(t)\} \subset \mathbb{N}$ may depends on t.

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Fix $j \in \{1, \cdots, r\}$.

Since g_j is continuous we have that

$$g_j(u_0^{N_k(t)}(x,t)) \to g_j(u_0(x,t)), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Fix $t \in (0,T)$.

Let $\varepsilon > 0$. From the Egorov Theorem, there exists a closed set F such that $m(\Omega \setminus F) \leq \varepsilon$ and $k_0 \in \mathbb{N}$ such that if $k > k_0$, then

$$|g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))| \leq \varepsilon, \text{ for almost all } x \in F.$$

Let $\varphi \in C_c^\infty(\Omega)$. Observe now that

$$\begin{aligned}
& \left| \int_\Omega (g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t)))\varphi \, dx \right| \\
\leq & \int_\Omega |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))| \, |\varphi| \, dx \\
= & \int_F |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))| \, |\varphi| \, dx + \int_{\Omega\setminus F} |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))| \, |\varphi| \, dx \\
\leq & \int_F \varepsilon \|\varphi\|_\infty \, dx + \int_\Omega |g_j(u_0^{N_k(t)}(x,t)) - g_j(u_0(x,t))| \, |\varphi| \chi_{\Omega\setminus F} \, dx \\
\leq & \varepsilon \|\varphi\|_\infty m(\Omega) + (\|g_j(u_0^{N_k(t)})\|_{0,2,\Omega} + \|g_j(u_0)\|_{0,2,\Omega}) \|\varphi\|_{0,4,\Omega} \|\chi_{\Omega\setminus F}\|_{0,4,\Omega} \\
\leq & \varepsilon \|\varphi\|_\infty m(\Omega) + K_{21} \|\varphi\|_{0,4,\Omega} m(\Omega \setminus F)^{1/4} \\
\leq & \varepsilon \, \|\varphi\|_\infty \, m(\Omega) + K_{21} \|\varphi\|_{0,4,\Omega} \, \varepsilon^{1/4}, \forall k > k_0,
\end{aligned} \tag{431}$$

for some appropriate constant $K_{21} > 0$ which does not depend on t.

Since such a $\varepsilon > 0$ is arbitrary, we may infer that

$$\int_\Omega g_j(u_0^{N_k(t)})\varphi \, dx \to \int_\Omega g_j(u_0)\varphi \, dx, \text{ as } k \to \infty,$$

$\forall \varphi \in C_c^\infty(\Omega), \forall j \in \{1, \cdots, r\}$.

Similarly, fixing $j, p \in \{1, \cdots, n\}$, and $l \in \{1, \cdots, m\}$, since g_{jpl} is continuous we have that

$$g_{jpl}(u_0^{N_k(t)}(x,t)) \to g_{jpl}(u_0(x,t)), \text{ a.e. in } \Omega, \text{ for almost all } t \in [0,T].$$

Fix again $t \in (0,T)$

Let $\varepsilon > 0$ (a new value). From the Egorov Theorem, there exists a closed set F_1 such that $m(\Omega \setminus F_1) \leq \varepsilon$ and $k_0 \in \mathbb{N}$ such that if $k > k_0$, then

$$|g_{jpl}(u_0^{N_k(t)}(x,t)) - g_{jpl}(u_0(x,t))| \leq \varepsilon, \text{ for almost all } x \in F_1.$$

Observe now that

$$\begin{aligned}
& \int_\Omega |g_{jpl}(u_0^{N_k(t)}(x,t)) - g_{jpl}(u_0(x,t))|^2 \, dx \\
\leq & \int_{F_1} |g_{jpl}(u_0^{N_k(t)}(x,t)) - g_{jpl}(u_0(x,t))|^2 \, dx + \int_{\Omega\setminus F_1} |g_{jpl}(u_0^{N_k(t)}(x,t)) - g_{jpl}(u_0(x,t))|^2 \, dx \\
\leq & \int_{F_1} \varepsilon^2 \, dx + \int_\Omega |g_{jpl}(u_0^{N_k(t)}(x,t)) - g_{jpl}(u_0(x,t))|^2 \chi_{\Omega\setminus F_1} \, dx \\
\leq & \varepsilon^2 m(\Omega) + 2K_1^2 \int_\Omega \chi_{\Omega\setminus F_1} \, dx \\
\leq & \varepsilon^2 m(\Omega) + 2K_1^2 \varepsilon, \ \forall k > k_0.
\end{aligned} \tag{432}$$

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Since such a $\varepsilon > 0$ is arbitrary, we may infer that

$$\int_\Omega |g_{jpl}(u_0^{N_k(t)}) - g_{jpl}(u_0)|^2 \, dx \to 0, \text{ as } k \to \infty,$$

$\forall j, p \in \{1, \cdots, r\}, l \in \{1, \cdots, m\}$.

Select again $\varphi \in C_c^\infty(\Omega)$. Since

$$\|g_{jpl}(u_0^{N_k(t)}) - g_{jpl}(u_0)\|_{0,2,\Omega} \to 0, \text{ as } k \to \infty$$

and

$$\nabla u_0^{N_k(t)} \rightharpoonup \nabla u_0, \text{ weakly in } L^2(\Omega; \mathbb{R}^{r\times m}),$$

we obtain,

$$\begin{aligned}
& \left| \int_\Omega g_{jpl}(u_0^{N_k(t)})((u_0)_p^{N_k(t)})_{x_l} \, \varphi \, dx - \int_\Omega g_{jpl}(u_0)((u_0)_p)_{x_l} \, \varphi \, dx \right| \\
\leq & \left| \int_\Omega g_{jpl}(u_0^{N_k(t)})((u_0)_p^{N_k(t)})_{x_l} \, \varphi \, dx - \int_\Omega g_{jpl}(u_0)((u_0)_p^{N_k(t)})_{x_l} \, \varphi \, dx \right| \\
& + \left| \int_\Omega g_{jpl}(u_0)((u_0)_p^{N_k(t)})_{x_l} \, \varphi \, dx - \int_\Omega g_{jpl}(u_0)((u_0)_p)_{x_l} \, \varphi \, dx \right| \\
\leq & \|g_{jpl}(u_0^{N_k(t)}) - g_{jpl}(u_0)\|_{0,2,\Omega} K_7 \|\varphi\|_\infty \\
& + \left| \int_\Omega g_{jpl}(u_0)((u_0)_p^{N_k(t)})_{x_l} \, \varphi \, dx - \int_\Omega g_{jpl}(u_0)((u_0)_p)_{x_l} \, \varphi \, dx \right| \\
\to & \ 0, \text{ as } k \to \infty,
\end{aligned} \tag{433}$$

$\forall j, p \in \{1, \cdots, r\}$, $l \in \{1, \cdots, m\}$.

From such results, for an arbitrary $\varphi \in C_c^\infty(\Omega; \mathbb{R}^r)$, we have

$$\begin{aligned}
0 &= \lim_{k\to\infty} \left(\int_\Omega \frac{\partial (u_0)_j^{N_k(t)}}{\partial t} \, \varphi_j \, dx - \langle F_j(u_0^{N_k(t)}), \varphi_j \rangle_{L^2} \right) \\
&= \int_\Omega \frac{\partial (u_0)_j}{\partial t} \, \varphi_j \, dx + \varepsilon_j \langle \nabla (u_0)_j, \nabla \varphi_j \rangle_{L^2} - \langle g_j(u_0), \varphi_j \rangle_{L^2} \\
&\quad - \sum_{p=1}^r \sum_{l=1}^m \langle g_{jpl}(u_0)((u_0)_p)_{x_l}, \varphi_j \rangle_{L^2} - \langle f_j, \varphi_j \rangle_{L^2}
\end{aligned} \tag{434}$$

so that, from this and by the density of $C_c^\infty(\Omega;;\mathbb{R}^r)$ in $H_0^1(\Omega; \mathbb{R}^r)$, we have got

$$\begin{aligned}
& \int_\Omega \frac{\partial (u_0)_j}{\partial t} \, \varphi_j \, dx \\
= & -\varepsilon_j \langle \nabla (u_0)_j, \nabla \varphi_j \rangle_{L^2} + \langle g_j(u_0), \varphi_j \rangle_{L^2} \\
& + \sum_{p=1}^r \sum_{l=1}^m \langle g_{jpl}(u_0)((u_0)_p)_{x_l}, \varphi_j \rangle_{L^2} + \langle f_j, \varphi_j \rangle_{L^2},
\end{aligned} \tag{435}$$

$\forall j \in \{1, \cdots, r\}$, $\forall \varphi \in H_0^1(\Omega; \mathbb{R}^r)$, a.e. on $[0, T]$,

Observe now that

$$\partial(\Omega \times (0, T)) = (\partial\Omega \times [0, T]) \cup (\partial[0, T] \times \overline{\Omega}).$$

Let $\varphi \in C_c^\infty(\Omega \times (0, T); \mathbb{R}^r)$.

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Hence

$$\lim_{N\to\infty}\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\ dx\ dt = \int_0^T\int_\Omega \frac{\partial u_0}{\partial t}\varphi\ dx\ dt.$$

From this, since $C_c^\infty(\Omega\times(0,T);\mathbb{R}^r)$ is dense $L^2(\Omega\times(0,T);\mathbb{R}^r)$ we may infer that

$$\lim_{N\to\infty}\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\ dx\ dt = \int_0^T\int_\Omega \frac{\partial u_0}{\partial t}\varphi\ dx\ dt,$$

$\forall \varphi\in L^2(\Omega\times(0,T);\mathbb{R}^r)$.

Let $\varphi\in C^\infty(\Omega\times[0,T];\mathbb{R}^r)$ such that

$$\varphi(x,T)=0,\ \text{in}\ \Omega.$$

From such results, we may obtain

$$\begin{aligned}
&\lim_{N\to\infty}\int_0^T\int_\Omega \frac{\partial u_0^N}{\partial t}\varphi\ dx\ dt\\
=\ &\lim_{N\to\infty}\left(-\int_0^T\int_\Omega u_0^N\frac{\partial\varphi}{\partial t}\ dx\ dt-\int_\Omega u_0^N(x,0)\varphi(x,0)\ dx\right)\\
=\ &-\int_0^T\int_\Omega u_0\frac{\partial\varphi}{\partial t}\ dx\ dt-\int_\Omega u_0(x,0)\varphi(x,0)\ dx. \qquad (436)
\end{aligned}$$

However, since $u_0^N\rightharpoonup u_0,$ weakly in $L^2(\Omega\times(0,T);\mathbb{R}^r)$, we obtain

$$\lim_{N\to\infty}\int_0^T\int_\Omega u_0^N\ \frac{\partial\varphi}{\partial t}\ dx\ dt=\int_0^T\int_\Omega u_0\ \frac{\partial\varphi}{\partial t}\ dx\ dt.$$

From these last results, we may infer that

$$\begin{aligned}
\int_\Omega \hat{u}_0\ \varphi(x,0)\ dx &= \lim_{N\to\infty}\int_\Omega u_0^N(x,0)\varphi(x,0)\ dx\\
&= \int_\Omega u_0(x,0)\ \varphi(x,0)\ dx, \qquad (437)
\end{aligned}$$

so that

$$\int_\Omega \hat{u}_0(x)\varphi(x,0)\ dx=\int_\Omega u_0(x,0)\varphi(x,0)\ dx,$$

$\forall\varphi\in C^\infty(\Omega\times[0,T];\mathbb{R}^r)$ such that $\varphi(x,T)=0,\ \text{in}\ \Omega.$

Therefore, we may infer that $u_0(x,0)=\hat{u}_0(x)$ in this specified weak sense.

Similarly, it may be proven that

$$u_0=0,\ \text{on}\ \partial\Omega\times[0,T],$$

in an appropriate weak sense.

Hence, we have obtained that u_0 is a solution, in a weak sense, of the parabolic non-linear system in question.

61. A Note on the Convergence of the Finite Elements Method

In this section we develop some remarks on the convergence of the finite elements method.

This section is based on reference [18], Chapter 7.

For the proofs not presented here and for more details please see reference [18], Chapter 7.

We start by recalling the following classical result.

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Theorem 61.1 (Lax-Milgram). *Let V be a separable Hilbert space with a inner product*

$$\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R},$$

and related norm

$$\| \cdot \| : V \to \mathbb{R}^+$$

where

$$\|u\| = \sqrt{\langle u, u \rangle}, \ \forall u \in V.$$

Let $a : V \times V \to \mathbb{R}$ be a bilinear form such that

1. *a is continuous, that is, there exists $M > 0$ such that*

$$|a(u, v)| \leq M \|u\| \ \|v\|, \ \forall u, v \in V,$$

2. *a is coercive, that is, there exists $\alpha > 0$ such that*

$$a(v, v) \geq \alpha \|v\|^2, \ \forall u \in V.$$

Moreover, let $L : V \to \mathbb{R}$ be a linear and continuous functional.
Under such hypotheses, there exists a unique $u \in V$ such that

$$a(u, v) = L(v), \ \forall v \in V.$$

Definition 61.2. *Let V be a Banach space. We say that a sequence $\{V_n\}$ of finite dimensional subspaces of V is a Galerkin scheme for V if for each $v \in V$, there exists a sequence $\{v_k\} \subset \cup_{n=1}^{\infty} V_n$ where $v_k \in V_k$, $\forall k \in \mathbb{N}$, such that*

$$v_k \to v, \text{ strongly in norm, as } k \to \infty.$$

Remark 61.3. *Let $\Omega \subset \mathbb{R}^2$ be a polygonal set. A triangulation T of Ω is a finite union of subsets of $\overline{\Omega}$, such that*

1.

$$\overline{\Omega} = \cup_{K \in T} K,$$

2. *Each set $K \in T$ is a triangle,*
3. *For each pair $K_1, K_2 \in T$, such sets are quasi-disjoints, that is, their interiors are disjoint.*

We define

$$h(T) = \max_{K \in T} diam(K) \equiv h,$$

where

$$diam(K) = \sup\{|x, y| \ : \ x, y \in K\}.$$

In such a case we also denote $T = T_h$.
Moreover, we define

$$V_h = \{v \in C(\overline{\Omega}) \ : \ v \text{ is affine on each } K \in T_h \text{ and } v = 0, \text{ on } \partial\Omega\}.$$

We denote by a_j the vertices in the triangulation T_h, where

$$j \in \{1, \cdots, I(h)\}.$$

Let $\{\varphi_j\} \subset V_h$ be such that

$$\varphi_j(a_k) = \delta_{jk}, \ \forall 1 \leq j, k \leq I(h).$$

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Here

$$\delta_{jk} = \begin{cases} 1, & \text{if } j = k, \\ 0, & \text{if } j \neq k. \end{cases} \tag{438}$$

Observe that $\{\varphi_1, \cdots, \varphi_{I(h)}\}$ *is a basis for* V_h.
At this point we define

$$P_h(v) = \sum_{j=1}^{I(h)} v(a_j)\varphi_j, \ \forall v \in V.$$

Here we assume $\{T_h\}_{h>0}$ *be a regular family of triangulations of* Ω.
Let $\{h_n\} \subset \mathbb{R}^+$ *be a sequence such that*

$$0 < h_{n+1} < h_n, \ \forall n \in \mathbb{N},$$

and

$$\lim_{n\to\infty} h_n = 0.$$

We denote $V_n = V_{h_n}$ *and* $P_n = P_{h_n}$, $\forall n \in \mathbb{N}$.
Consider the Ginzburg-Landau type equation

$$\begin{cases} -\gamma\nabla^2 u + \alpha u^3 - \beta u - f = 0, & \text{in } \Omega, \\ u = 0, \text{ on } \partial\Omega. \end{cases} \tag{439}$$

Here $\gamma > 0, \alpha > 0, \beta > 0$ *and* $f \in L^2(\Omega)$.
Assume $u_n \in V_n$ *is a weak solution of this last equation, in the following sense,*

$$\begin{aligned} & \gamma\langle\nabla u_n, \nabla\varphi\rangle_{L^2} + \alpha\langle u_n^3, \varphi\rangle_{L^2} \\ & -\beta\langle u_n, \varphi\rangle_{L^2} - \langle f, \varphi\rangle_{L^2}, \\ = \ & 0, \ \forall\varphi \in V_n. \end{aligned} \tag{440}$$

We assume there exist $u_0 \in H_0^1 \cap W^{1,\infty}(\Omega)$, $r > 0$, $\alpha_1 > 0$ *and* $M > 0$ *such that*

$$\begin{aligned} & \alpha_1\|u - v\|_{1,2,\Omega}^2 \\ \leq \ & \gamma\langle\nabla(u-v), \nabla(u-v)\rangle_{L^2} + \alpha\langle 3\tilde{u}^2(u,v)(u-v), (u-v)\rangle_{L^2} - \beta\langle(u-v), (u-v)\rangle_{L^2}, \end{aligned}$$

and

$$\begin{aligned} & \left|\gamma\langle\nabla(u-v), \nabla(u-w)\rangle_{L^2} + \alpha\langle 3\tilde{u}^2(u,v)(u-v), (u-w)\rangle_{L^2} - \beta\langle(u-v), (u-w)\rangle_{L^2}\right| \\ \leq \ & M\|u-v\|_{1,2,\Omega}\|u-w\|_{1,2,\Omega}, \end{aligned} \tag{441}$$

$\forall u, v, w \in B_r(u_0)$.
Here $\tilde{u}(u,v)$ *is on the line connecting* u *and* v *so that*

$$u^3 - v^3 = 3\tilde{u}^2(u-v).$$

Similarly as we have done in previous sections, we assume u_0 *and* $r > 0$ *are such that we may obtain* $u_n \in B_r(u_0)$, $\forall n \in \mathbb{N}$.

Also similarly as in the previous section, we may consider such a ball either related to the $H_0^1(\Omega)$ *norm or the* $W^{1,\infty}(\Omega)$ *one.*

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Let $m, n \in \mathbb{N}$ be such that $m > n$.
Observe that $u_n, u_m \in V_m$ so that

$$\begin{aligned} & \gamma\langle\nabla u_m, \nabla(u_n - u_m)\rangle_{L^2} + \alpha\langle u_m^3, (u_n - u_m)\rangle_{L^2} \\ & -\beta\langle u_m, (u_n - u_m)\rangle_{L^2} - \langle f, (u_n - u_m)\rangle_{L^2} \\ = \; & 0, \end{aligned} \tag{442}$$

so that, for $\varphi \in V_n$, we obtain

$$\begin{aligned} & \gamma\langle\nabla(u_n - u_m), \nabla(u_n - u_m)\rangle_{L^2} + \alpha\langle(u_n^3 - u_m^3), (u_n - u_m)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (u_n - u_m)\rangle_{L^2} \\ = \; & \gamma\langle\nabla(u_n - u_m), \nabla(u_n - \varphi)\rangle_{L^2} + \alpha\langle(u_n^3 - u_m^3), (u_n - \varphi)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (u_n - \varphi)\rangle_{L^2} \\ & +\gamma\langle\nabla(u_n - u_m), \nabla(\varphi - u_m)\rangle_{L^2} + \alpha\langle(u_n^3 - u_m^3), (\varphi - u_n)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (\varphi - u_m)\rangle_{L^2} \\ = \; & \gamma\langle\nabla(u_n - u_m), \nabla(\varphi - u_m)\rangle_{L^2} + \alpha\langle(u_n^3 - u_m^3), (\varphi - u_m)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (\varphi - u_m)\rangle_{L^2}. \end{aligned} \tag{443}$$

Summarizing, we have got

$$\begin{aligned} & \gamma\langle\nabla(u_n - u_m), \nabla(u_n - u_m)\rangle_{L^2} + \alpha\langle 3\tilde{u}_n^2(u_n - u_m), (u_n - u_m)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (u_n - u_m)\rangle_{L^2} \\ = \; & \gamma\langle\nabla(u_n - u_m), \nabla(\varphi - u_m)\rangle_{L^2} + \alpha\langle 3\tilde{u}_n^2(u_n - u_m), (\varphi - u_m)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (\varphi - u_m)\rangle_{L^2} \end{aligned} \tag{444}$$

$\forall \varphi \in V_n$, where $\tilde{u}_n$ is on the line connecting u_m and u_n.
Here we recall that $\alpha_1 > 0$ and $M > 0$ are such that

$$\begin{aligned} & \gamma\langle\nabla(u_n - u_m), \nabla(u_n - u_m)\rangle_{L^2} + \alpha\langle 3\tilde{u}_n^2(u_n - u_m), (u_n - u_m)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (u_n - u_m)\rangle_{L^2} \\ \geq \; & \alpha_1\|u_n - u_m\|_{1,2,\Omega}^2 \end{aligned} \tag{445}$$

and

$$\begin{aligned} & \gamma\langle\nabla(u_n - u_m), \nabla(\varphi - u_m)\rangle_{L^2} + \alpha\langle 3\tilde{u}_n^2(u_n - u_m), (\varphi - u_m)\rangle_{L^2} \\ & -\beta\langle(u_n - u_m), (u_n - \varphi)\rangle_{L^2} \\ \leq \; & M\|u_m - u_n\|_{1,2,\Omega}\|\varphi - u_m\|_{1,2,\Omega}, \end{aligned} \tag{446}$$

where α_1 and M does not depend on m, n.
From such results, we may infer that

$$\|u_m - u_n\|_{1,2,\Omega} \leq \frac{M}{\alpha_1}\|u_m - \varphi\|_{1,2,\Omega}, \; \forall \varphi \in V_n$$

so that

$$\|u_m - u_n\|_{1,2,\Omega} \leq \frac{M}{\alpha_1}\|u_m - P_n(u_m)\|_{1,2,\Omega}, \; \forall m > n.$$

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Moreover, since $u_m \in H_0^1(\Omega)$, *there exists a sequence* $\{v_k = v_k^m\} \subset C_c^\infty(\Omega)$ *such that*

$$\|v_k^m - u_m\|_{1,2,\Omega} \to 0, \text{ as } k \to \infty.$$

From such results, for a not relabeled subsequence we have

$$v_k^m \to u_m, \text{ a.e. in } \Omega,$$
$$\nabla v_k^m \to \nabla u_m, \text{ a.e. in } \Omega.$$

Let $\varepsilon > 0$.
From the Egorov theorem, for each $m \in \mathbb{N}$ *there exists a closed set* $F_m \subset \Omega$ *such that* $m(F_m) < \varepsilon/2^m$ *and*

$$v_k^m \to u_m, \text{ uniformly in } \Omega \setminus F_m,$$

$$\nabla v_k^m \to \nabla u_m, \text{ uniformly in } \Omega \setminus F_m.$$

Define $F = \cup_{m=1}^\infty F_m$ *so that*

$$m(F) \leq \sum_{m=1}^\infty (F_m) \leq \sum_{m=1}^\infty \varepsilon/2^m \leq \varepsilon.$$

Observe that there exists $k_0 = k_0^m \in \mathbb{N}$ *such that if* $k > k_0 = k_0^m$, *then*

$$\|v_k^m - u_m\|_{1,2,\Omega} < \varepsilon,$$

and

$$\|v_k^m - u_m\|_{\infty,\Omega\setminus F_m} < \varepsilon,$$

and

$$\|\nabla v_k^m - \nabla u_m\|_{\infty,\Omega\setminus F_m} < \varepsilon.$$

Fixing $m \in \mathbb{N}$ *we may find* $j_0 \in \mathbb{N}$ *(which does not depend on m) and* $l_m \in \mathbb{N}$

$$\|P_j(v_k^l) - P_j(u_l)\|_{0,2,\Omega\setminus F_l} < K_1\varepsilon,$$

and

$$\|\nabla P_j(v_k^l) - \nabla P_j(u_l)\|_{0,2,\Omega\setminus F_l} < K_5\varepsilon, \ \forall j > j_0, \ \forall l > l_m \in \mathbb{N}, \ \forall k > k_0^l,$$

for some appropriate real constants $K_1 > 0, \ K_5 > 0$.

At this point we highlight that concerning the finite elements method $\|u_m\|_{1,\infty}$ *is uniformly bounded in m so that*

$$\{\|v_k^m\|_{1,\infty}, \ k > k_0^m, \ m \in \mathbb{N}\}$$

is also uniformly bounded in m and $k > k_0^m$.

With such results in mind, fix $n > j_0$ *and select* $m_n > \max\{n, k_0^n, l_n\}$ *so that for* $\forall m > m_n$ *and* $k > k_0^m$, *we have*

$$\begin{aligned} & \|\nabla u_m - \nabla P_n(v_k^m)\|_{0,2,\Omega/F_m} \\ \leq \ & \|\nabla u_m - \nabla v_k^m + \nabla v_k^m - \nabla P_n(v_k^m)\|_{0,2,\Omega/F_m} \\ \leq \ & \|\nabla u_m - \nabla v_k^m\|_{0,2,\Omega} + \|\nabla v_k^m - \nabla P_n(v_k^m)\|_{0,2,\Omega/F_m} \\ \leq \ & \varepsilon + K_7/n, \end{aligned} \tag{447}$$

for some appropriate $K_7 > 0$.

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From such results, we may infer that

$$\begin{aligned} & \| u_m - P_n(u_m))\|_{1,2,\Omega} \\ \leq\ & \|u_m - P_n(v_k^m) + P_n(v_k^m) - P_n(u_m)))\|_{1,2,\Omega} \\ \leq\ & \|u_m - P_n(v_k^m)\|_{1,2,\Omega} + \|P_n(v_k^m) - P_n(u_m)\|_{1,2,\Omega/F_m} + \|P_n(v_k^m) - P_n(u_m)\|_{1,2,F_m} \\ \leq\ & K_9(\varepsilon + K_7/n + \varepsilon^{1/2}), \end{aligned} \tag{448}$$

for some appropriate $K_9 > 0$, so that

$$\begin{aligned} \|u_m - u_n\|_{1,2,\Omega} &\leq \frac{M}{\alpha_1}\|u_m - P_n(u_m)\|_{1,2,\Omega} \\ &\leq K_{10}(\varepsilon + K_7/n + \varepsilon^{1/2}),\ \forall m > m_n, \end{aligned} \tag{449}$$

where

$$K_{10} = K_9\frac{M}{\alpha_1}.$$

Therefore, if $p, l > m_n$, then

$$\begin{aligned} \|u_l - u_n\|_{1,2,\Omega} &\leq \frac{M}{\alpha_1}\|u_l - P_n(u_l)\|_{1,2,\Omega} \\ &\leq K_{10}(\varepsilon + K_7/n + \varepsilon^{1/2}) \end{aligned} \tag{450}$$

and

$$\begin{aligned} \|u_p - u_n\|_{1,2,\Omega} &\leq \frac{M}{\alpha_1}\|u_p - P_n(u_p)\|_{1,2,\Omega} \\ &\leq K_{10}(\varepsilon + K_7/n + \varepsilon^{1/2}), \end{aligned} \tag{451}$$

so that

$$\begin{aligned} \|u_l - u_p\|_{1,2,,\Omega} &= \|u_l - u_n + u_n - u_p\|_{1,2,\Omega} \\ &\leq \|u_l - u_n\|_{1,2,\Omega} + \|u_p - u_n\|_{1,2,\Omega} \\ &\leq 2K_{10}(\varepsilon + K_7/n + \varepsilon^{1/2}). \end{aligned} \tag{452}$$

Consequently, from such results we may infer that $\{u_n\}$ is a Cauchy sequence in $H_0^1(\Omega)$ so that there exists $u_0 \in H_0^1(\Omega)$ such that

$$u_n \to u_0,\ \textit{strongly in}\ H_0^1(\Omega).$$

Let $\varphi \in \cup_{n\in\mathbb{N}} V_n$.
Indeed, we have got

$$\begin{aligned} 0 &= \lim_{n\to\infty}\Big(\gamma\langle\nabla u_n, \nabla\varphi\rangle_{L^2} + \alpha\langle u_n^3, \varphi\rangle_{L^2} \\ &\quad -\beta\langle u_n, \varphi\rangle_{L^2} - \langle f, \varphi\rangle_{L^2}) \\ &= \gamma\langle\nabla u_0, \nabla\varphi\rangle_{L^2} + \alpha\langle u_0^3, \varphi\rangle_{L^2} \\ &\quad -\beta\langle u_n, \varphi\rangle_{L^2} - \langle f, \varphi\rangle_{L^2}. \end{aligned} \tag{453}$$

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Summarizing, we may infer that

$$\begin{aligned} & \gamma\langle\nabla u_0, \nabla\varphi\rangle_{L^2} + \alpha\langle u_0^3, \varphi\rangle_{L^2} \\ & -\beta\langle u_n, \varphi\rangle_{L^2} - \langle f, \varphi\rangle_{L^2} \\ = \;& 0, \; \forall\varphi \in H_0^1(\Omega). \end{aligned} \tag{454}$$

Therefore $u_0 \in H_0^1(\Omega)$ is a weak solution of the equation in question so that, under the indicated hypotheses, the finite element method is convergent.

62. A Dual Functional for a General Weak Primal Variational Formulation Combined with the Newton's Method

Let $\Omega = [0,1] \subset \mathbb{R}$ and consider a weak variational formulation for a Ginzburg-Landau type equation corresponding to a functional $J : V \times V \to \mathbb{R}$, where

$$J(u, v_1^*) = \int_\Omega v_1^*(-\varepsilon u'' + Au^3 - B\,u - f)\,dx,$$

where $\varepsilon > 0$, $A > 0$, $B > 0$ and $f \in Y = Y^* = L^2(\Omega)$.

Moreover $u \in V = W_0^{1,2}(\Omega)$.

Observe that the variation in v_1^* of J, which stands for

$$\frac{\partial J(u, v_1^*)}{\partial v_1^*} = \mathbf{0},$$

corresponds to the following Ginzburg-Landau type equation

$$-\varepsilon u'' + Au^3 - B\,u - f = 0, \text{ in } \Omega.$$

In a Newton type approach context, we linearize such an equation about a initial solution $u_0 \in V$, obtaining,

$$-\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - B\,u - f = 0, \text{ in } \Omega.$$

With such results in mind, we define the functional $J_1 : [V]^3 \to \mathbb{R}$, where

$$J_1(u, u_0, v_1^*) = \int_\Omega v_1^*(-\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - B\,u - f)\,dx.$$

We also define the functionals $F_1 : [V]^3 \to \mathbb{R}$ and $F_2 : V \to \mathbb{R}$, where

$$F_1(u, u_0, v_1^*) = J_1(u, u_0, v_1^*) + \frac{K}{2}\int_\Omega u^2\,dx,$$

and

$$F_2(u) = \frac{K}{2}\int_\Omega u^2\,dx.$$

Moreover, we define the polar functionals $F_1^* : [V]^2 \times Y^* \to \mathbb{R}$ and $F_2^* : Y^* \to \mathbb{R}$ as

$$F_1^*(u_0, v_1^*, z^*) = \sup_{u \in V}\{\langle u, z^*\rangle_{L^2} - F_1(u, u_0, v_1^*)\},$$

and

$$\begin{aligned} F_2^*(z^*) &= \sup_{v \in Y}\{\langle v, z^*\rangle_{L^2} - F_2(v)\} \\ &= \frac{1}{2K}\int_\Omega (z^*)^2\,dx. \end{aligned} \tag{455}$$

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Finally, we define the dual functional $J^* : [V]^2 \times Y^* \to \mathbb{R}$ by

$$J^*(u_0, v_1^*, z^*) = -F_1^*(u_0, v_1^*, z^*) + F_2^*(z^*).$$

Remark 62.1. *Observe that*

$$F_1^*(u_0, v_1^*, z^*) = \sup_{u \in V}\{\langle u, z^*\rangle_{L^2} - F_1(u, u_0, v_1^*)\},$$

and such a supremum is attained through the equation

$$\frac{\partial}{\partial u}(\langle u, z^*\rangle_{L^2} - F_1(u, u_0, v_1^*)) = 0,$$

which stands for

$$z^* - (-\varepsilon(v_1^*)'' + 3Au_0^2 v_1^* - Bv_1^*) - Ku = 0,$$

so that

$$u = \frac{\varepsilon(v_1^*)'' - 3Au_0^2 v_1^* + Bv_1^* + z^*}{K}.$$

Consequently, we may obtain

$$\begin{aligned} F_1^*(u_0, v_1^*, z^*) &= \frac{1}{2K}\int_\Omega (\varepsilon(v_1^*)'' - 3Au_0^2 v_1^* + Bv_1^* + z^*)^2\, dx \\ &\quad + \int_\Omega (2Au_0^3 + f)v_1^*\, dx. \end{aligned} \tag{456}$$

Hence, the variation in v_1^* of J^*,

$$\frac{\partial J^*}{\partial v_1^*} = -\frac{\partial F_1^*(v_1^*)}{\partial v_1^*} = \mathbf{0},$$

stands for

$$-\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - Bu - f = 0, \text{ in } \Omega,$$

where, as above indicated,

$$u = \frac{\varepsilon(v_1^*)'' - 3Au_0^2 v_1^* + Bv_1^* + z^*}{K}.$$

We have obtained a critical of J^* through the following algorithm.

1. Set $n = 1$, $b_{12} = 10^{-4}$, $n_{max} = 100$, $z_1^* = 0$ and choose $(u_0)_1 \in V$.
2. Calculate $(v_1^*)_n \in V$ such that
$$\frac{\partial J^*((u_0)_n, (v_1^*)_n, z_n^*)}{\partial v_1^*} = \mathbf{0},$$
3. Calculate $u_n \in V$ such that
$$\frac{\partial H(u_n, (u_0)_n, (v_1^*)_n, z_n^*)}{\partial u} = \mathbf{0},$$
where
$$H(u, (u_0), v_1^*, z^*) = \langle u, z^*\rangle - F_1(u, u_0, v_1^*),$$
so that
$$u_n = \frac{\varepsilon(v_1^*)_n'' - 3A(u_0)_n^2(v_1^*)_n + B(v_1^*)_n + z_n^*}{K}.$$
4. Set $(u_0)_{n+1} = u_n$ and $z_{n+1}^* = Ku_n$.
5. If $\|(u_0)_{n+1} - (u_0)_n\|_\infty < b_{12}$ or $n > n_{max}$, then stop. Otherwise, $n := n + 1$, and go to item 2.

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Here we highlight that if $\hat{u}_0 = \lim_{n\to\infty} u_n$ with corresponding limits $\hat{v}_1^*$ and $\hat{z}^* = K\hat{u}_0$, the solution of equation indicated in the item 2, given by

$$\frac{\partial J^*(\hat{u}_0, \hat{v}_1^*, \hat{z}^*)}{\partial v_1^*} = \mathbf{0},$$

will stand for

$$-\varepsilon \hat{u}_0'' + A\hat{u}_0^3 - B\hat{u}_0 - f = 0, \text{ in } \Omega.$$

We have obtained numerical results for $\varepsilon = 0.1$, $A = B = 1$ and $f \equiv 1$, in Ω.
For such an optimal solution $\hat{u}_0$ obtained please see Figure 44.

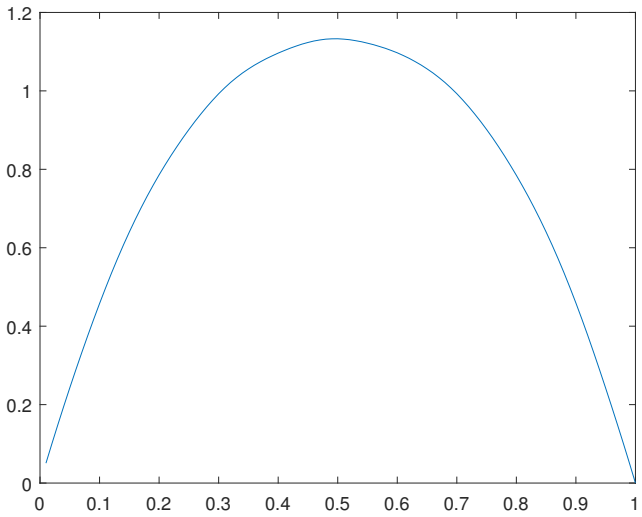

Figure 44. Solution $\hat{u}_0(x)$ through the dual functional for $\varepsilon = 0.1$.

Here we present the software in MAT-LAB through which we have obtained such numerical results.

****

1. clear all

   global m8 d yo K uo u z A B e1 v1

   m8=100;

   d=1/m8;

   K=10;

   A=1;

   B=1;

   e1=0.1;

   z(:,1)=0.1*ones(m8,1);

   yo(:,1)=ones(m8,1);

   uo(:,1)=1.2*ones(m8,1);

   for i=1:m8

   xo(i,1)=1.2;

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end
b12=1.0;
k=1;
while $(b12 > 10^{-4})$ && $(k < 100)$
k
k=k+1;
b14=1.0;
k1=1;
while $(b14 > 10^{-4})$ && $(k1 < 35)$
k1
k1=k1+1;
X=fminunc('funJune2024C10',xo);
b14=max(abs(X-xo));
xo=X;
u(m8/2,1)
end;
b12=max(abs(u-uo));
uo=u;
z=K*u;
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u);
****

With the auxiliary function "funJune2024C10", where

****

1. function S=funJune2024C10(x)
   global m8 d yo K uo u z A B e1 v1
   for i=1:m8
   v1(i,1)=x(i,1);
   end;
   v1(m8,1)=0;
   d2v1(1,1)=(-2*v1(1,1)+v1(2,1))/d^2;
   for i=2:m8-1
   d2v1(i,1)=(v1(i+1,1)-2*v1(i,1)+v1(i-1,1))/d^2;
   end;
   for i=1:m8-1

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u(i,1)=$(e1 * d2v1(i,1) + z(i,1) - 3 * A * uo(i,1)^2 * v1(i,1) + B * v1(i,1))/K$;

end;

u(m8,1)=0;

S=0;

for i=1:m8-1

S=S+$(-e1 * d2v1(i,1) * u(i,1)) + v1(i,1) * 3 * A * uo(i,1)^2 * u(i,1)$

$-B * v1(i,1) * u(i,1) + K * u(i,1)^2/2 - yo(i,1) * v1(i,1) - 2 * A * uo(i,1)^3 * v1(i,1)$;

S=S $-z(i,1) * u(i,1) - v1(i,1)^2/2$;

end;

S=-S;

****

63. A New Convex Dual Variational Formulation for a Galerkin Type Non-Convex Primal One

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \times [Y]^2 \to \mathbb{R}$ where

$$\begin{aligned} J(u, v_0, v_1) &= \frac{1}{2}\int_\Omega \left(-\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}\right)^2 dx \\ &+ \frac{1}{2}\int_\Omega \left(v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}\right)^2 dx \\ &+ \frac{1}{2}\int_\Omega (v_0 - A(u^2 - B))^2\, dx. \end{aligned} \tag{457}$$

Here $\varepsilon > 0,\ A > 0,\ B > 0,\ K > 0, f \in L^2(\Omega) \cap L^\infty(\Omega), u \in V = W_0^{1,2}(\Omega), v_0, v_1 \in Y = Y^* = L^2(\Omega)$.

Observe that the minimization of J corresponds to the solution of the following system of equations:

$$-\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2} = 0, \text{ in } \Omega,$$

$$v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2} = 0, \text{ in } \Omega,$$

and

$$v_0 - A(u^2 - B) = 0, \text{ in } \Omega.$$

From such a solution we may obtain the solution of the following Ginzburg-Landau type equation:

$$-\varepsilon\nabla^2 u + A(u^2 - B)\, u - f = 0, \text{ in } \Omega,$$

which is our final objective in this section.

Define the approximate relaxed functional $J_1 : V \times [Y]^2 \to \mathbb{R}$ where

$$J_1(u, v_0, v_1) = J(u_0, v_0, v_1) + \frac{\varepsilon_1}{2}\int_\Omega v_1^2\, dx,$$

where $\varepsilon_1 > 0$ is a small real constant.

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Observe that

$$
\begin{aligned}
J_1(u,v_0,v_1) &= -\left\langle -\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_1^* \right\rangle_{L^2} \\
&\quad + \frac{1}{2}\int_\Omega \left(-\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2} \right)^2 dx \\
&\quad - \left\langle v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_2^* \right\rangle_{L^2} \\
&\quad + \frac{1}{2}\int_\Omega \left(v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2} \right)^2 dx \\
&\quad - \left\langle v_0 - A(u^2 - B), v_3^* \right\rangle_{L^2} + \frac{1}{2}\int_\Omega (v_0 - A(u^2-B))^2\, dx \\
&\quad + \left\langle -\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_1^* \right\rangle_{L^2} \\
&\quad + \left\langle v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_2^* \right\rangle_{L^2} \\
&\quad + \left\langle v_0 - A(u^2 - B), v_3^* \right\rangle_{L^2} + \frac{\varepsilon_1}{2}\int_\Omega v_1^2\, dx \\
&\geq \inf_{w_1 \in Y} \left\{ -\langle w_1, v_1^* \rangle_{L^2} + \frac{1}{2}\int_\Omega w_1^2\, dx \right\} \\
&\quad + \inf_{w_2 \in Y} \left\{ -\langle w_2, v_2^* \rangle_{L^2} + \frac{1}{2}\int_\Omega w_2^2\, dx \right\} \\
&\quad + \inf_{w_3 \in Y} \left\{ -\langle w_3, v_3^* \rangle_{L^2} + \frac{1}{2}\int_\Omega w_3^2\, dx \right\} \\
&\quad + \inf_{(u,v_0,v_1)\in V\times Y^2} \left\{ \left\langle -\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_1^* \right\rangle_{L^2} \right. \\
&\quad + \left\langle v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_2^* \right\rangle_{L^2} \\
&\quad \left. + \left\langle v_0 - A(u^2 - B), v_3^* \right\rangle_{L^2} + \frac{\varepsilon_1}{2}\int_\Omega v_1^2\, dx \right\} \\
&= -\frac{1}{2}\int_\Omega (v_1^*)^2\, dx - \frac{1}{2}\int_\Omega (v_2^*)^2\, dx - \frac{1}{2}\int_\Omega (v_3^*)^2\, dx \\
&\quad - F^*(v_1^*, v_2^*, v_3^*),\ \forall v^* = (v_1^*, v_2^*, v_3^*) \in A^*,
\end{aligned} \tag{458}
$$

where

$$
A^* = \{ v^* \in [Y^*]^3 \ :\ v_1^* + v_2^* \geq 0 \text{ and } v_3^* \leq 0,\ \text{in } \Omega,\ v_1^* = 0,\ \text{on } \partial\Omega \}.
$$

Also

$$
\begin{aligned}
& F^*(v^*) = F^*(v_1^*, v_2^*, v_3^*) \\
&= \sup_{(u,v_0,v_1)\in V\times Y^2} \left\{ -\left\langle -\varepsilon\nabla^2 u + v_0 u - f + v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_1^* \right\rangle_{L^2} \right. \\
&\quad - \left\langle v_1 + K\frac{u^2}{2} + K\frac{v_0^2}{2}, v_2^* \right\rangle_{L^2} \\
&\quad \left. - \left\langle v_0 - A(u^2 - B), v_3^* \right\rangle_{L^2} - \frac{\varepsilon_1}{2}\int_\Omega v_1^2\, dx \right\}.
\end{aligned} \tag{459}
$$

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Hence, defining $J_1^* : A^* \to \mathbb{R}$ by

$$J_1^*(v^*) = -\frac{1}{2}\int_\Omega (v_1^*)^2\,dx - \frac{1}{2}\int_\Omega (v_2^*)^2\,dx - \frac{1}{2}\int_\Omega (v_3^*)^2\,dx - F^*(v^*),$$

we have obtained

$$\inf_{(u,v_0,v_1)\in V\times[Y]^2} J_1(u,v_0,v_1) \geq \sup_{v^*\in A^*} J_1^*(v^*).$$

Remark 63.1. *We highlight that for $K > 0$ sufficiently large, J_1^* is concave on the convex set A^*. Moreover, this last inequality is in fact an equality so that there is no duality gap between such approximate primal and dual formulations.*

63.1. A Numerical Example for a Related Similar Functional

In order to obtain numerical results we proceed in following fashion.

Firstly we define $\Omega = [0,1] \subset \mathbb{R}$ and in a Newton's method context, we linearize the Ginzburg-Landau equation in question namely,

$$-\varepsilon u'' + Au^3 - Bu - f = 0, \text{ in } \Omega$$

about an initial solution u_0, obtaining the following approximate equation

$$-\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - Bu - f = 0, \text{ in } \Omega.$$

Now we define the functional $J_1^* : [V]^2 \times [Y^*]^3 \to \mathbb{R}$, where

$$\begin{aligned} J_1^*(u,u_0,w_1,v_1^*,v_2^*) &= \left\langle -\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - Bu - f + w_1 + \frac{K}{2}u^2, v_1^* \right\rangle_{L^2} \\ &+ \left\langle w_1 + \frac{K}{2}u^2, v_2^* \right\rangle_{L^2} - \frac{1}{2}\int_\Omega (v_1^*)^2\,dx - \frac{1}{2}\int_\Omega (v_2^*)^2\,dx. \end{aligned} \tag{460}$$

Again, similarly as in the Newton's method approach, we obtain a quadratic approximation for the non-quadratic terms

$$\frac{K}{2}u^2(v_1^* + v_2^*),$$

expressed by

$$Ku^2((v_1^*)_0 + (v_2^*)_0) - \frac{K}{2}u_0^2(v_1^* + v_2^*).$$

With replacements in mind, we define the functional $J_2^* : [V]^2 \times [Y^*]^5 \to \mathbb{R}$, where

$$\begin{aligned} J_2^*(u,u_0,w_1,v_1^*,v_2^*,(v_1^*)_0,(v_2^*)_0) &= \left\langle -\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - Bu - f,\ v_1^* \right\rangle_{L^2} \\ &+ \left\langle Ku^2, (v_1^*)_0 + (v_2^*)_0 \right\rangle_{L^2} - \left\langle \frac{K}{2}u_0^2, v_1^* + v_2^* \right\rangle_{L^2} \\ &+ \langle w_1, v_1^* + v_2^* \rangle_{L^2} - \frac{1}{2}\int_\Omega (v_1^*)^2\,dx - \frac{1}{2}\int_\Omega (v_2^*)^2\,dx. \end{aligned} \tag{461}$$

Let $\hat{u} \in V$ be such that

$$\left.\frac{\partial J_2^*(u,u_0,w_1,v_1^*,v_2^*,(v_1^*)_0,(v_2^*)_0)}{\partial u}\right|_{u=\hat{u}} = \mathbf{0},$$

so that we define the functional $J_3^* : V \times [Y^*]^5 \to \mathbb{R}$ by

$$J_3^*(u_0,w_1,v_1^*,v_2^*,(v_1^*)_0,(v_2^*)_0) = J_2^*(\hat{u},u_0,w_1,v_1^*,v_2^*,(v_1^*)_0,(v_2^*)_0).$$

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The variation in v_1^* of J_3^* stands for

$$\begin{aligned}\frac{\partial J_3^*(u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_1^*} &= \frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial u}\frac{\partial \hat{u}}{\partial v_1^*} \\ &+ \frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_1^*} \\ &= \frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_1^*}. \end{aligned} \tag{462}$$

Similarly, the variation of J_3^* in v_2^*, stands for

$$\begin{aligned}\frac{\partial J_3^*(u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_2^*} &= \frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial u}\frac{\partial \hat{u}}{\partial v_2^*} \\ &+ \frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_2^*} \\ &= \frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_2^*}. \end{aligned} \tag{463}$$

Summarizing, a critical point of J_3^* must satisfy the following equations:

$$\frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial u} = \mathbf{0},$$

which stands for

$$-\varepsilon(v_1^*)'' + 3Au_0^2 v_1^* - Bv_1^* + 2Ku((v_1^*)_0 + (v_2^*)_0) = \mathbf{0},$$

$$\frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_1^*} = \mathbf{0},$$

which stands for

$$-\varepsilon u'' + 3Au_0^2 u - 2Au_0^3 - Bu - f + w_1 - \frac{K}{2}u_0^2 - v_1^* = \mathbf{0},$$

$$\frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial v_2^*} = \mathbf{0},$$

which stands for

$$w_1 - \frac{K}{2}u_0^2 - v_2^* = \mathbf{0},$$

and

$$\frac{\partial J_2^*(\hat{u}, u_0, w_1, v_1^*, v_2^*, (v_1^*)_0, (v_2^*)_0)}{\partial w_1} = \mathbf{0},$$

which stands for

$$v_1^* + v_2^* = \mathbf{0}.$$

It is worth highlighting such a system is linear in (u, w_1, v_1^*, v_2^*) so that we have obtained numerical results, in a Newton's method context, through the following algorithm.

1. Set $n = 1$, $b_{12} = 10^{-4}$, $n_{max} = 100$, $(v_1^*)_0 \equiv 0.4$, $(v_2^*)_0 \equiv 0.4$ and $(u_0) \equiv 1.2$.
2. Calculate $(u_n, (w_1)_n, (v_1^*)_n, (v_2^*)_n)$ such that the following linear system of equations is satisfied

   (a)
   $$\frac{\partial J_2^*(u_n, (u_0)_n, (w_1)_n, (v_1^*)_n, (v_2^*)_n, ((v_1^*)_0)_n, ((v_2^*)_0)_n)}{\partial u} = \mathbf{0},$$

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(b)

$$\frac{\partial J_2^*(u_n,(u_0)_n,(w_1)_n,(v_1^*)_n,(v_2^*)_n,((v_1^*)_0)_n,((v_2^*)_0)_n)}{\partial v_1^*}=\mathbf{0},$$

(c)

$$\frac{\partial J_2^*(u_n,(u_0)_n,(w_1)_n,(v_1^*)_n,(v_2^*)_n,((v_1^*)_0)_n,((v_2^*)_0)_n)}{\partial v_2^*}=\mathbf{0},$$

(d)

$$\frac{\partial J_2^*(u_n,(u_0)_n,(w_1)_n,(v_1^*)_n,(v_2^*)_n,((v_1^*)_0)_n,((v_2^*)_0)_n)}{\partial w_1}=\mathbf{0}.$$

3. Set $(u_0)_{n+1}=u_n$, $((v_1^*)_0)_{n+1}=(v_1^*)_n$, and $((v_2^*)_0)_{n+1}=(v_2^*)_n$.
4. If $\|(u_0)_{n+1}-(u_0)_n\|_\infty < b_{12}$ or $n > n_{max}$, then stop.

   Otherwise $n := n+1$ and go to item 2.

We have obtained numerical results for $\varepsilon = 0.01$, $A = B = 1$ and $f \equiv 1$, in Ω.

For such an optimal solution $\hat{u}_0$ obtained please see Figure 45.

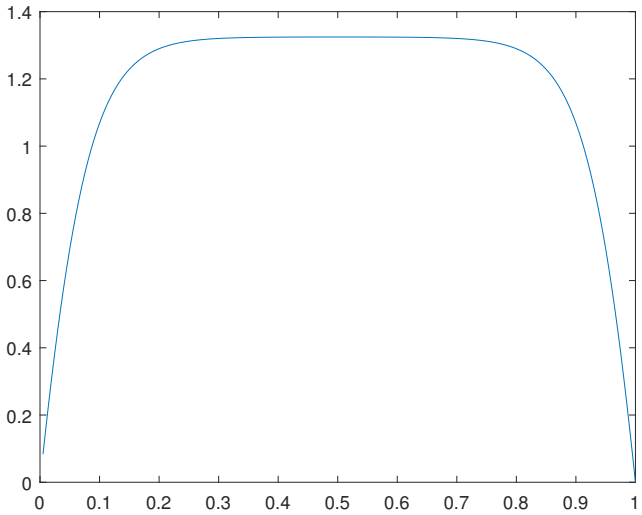

Figure 45. Solution $\hat{u}_0(x)$ through the dual functional for $\varepsilon = 0.01$.

Here we present the software in MAT-LAB through which we have obtained such numerical results.

****

1. clear all

   global m8 d yo u K e1 A B v1 v2 uo vo1 vo2 K1

   m8=200;

   d=1/m8;

   K=10;

   K1=38;

   e1=0.01;

   A=1;

   B=1;

   uo(:,1)=1.2*ones(m8,1);

   yo(:,1)=ones(m8,1);

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vo1(:,1)=0.4*ones(m8,1);
vo2(:,1)=0.4*ones(m8,1);
xo=1.2*ones(4*m8,1);
b14=1;
k1=1;
while $(b14 > 10^{-4})$ && $(k1 < 100)$
k1
k1=k1+1;
b12=1;
k=1;
while $(b12 > 10^{-4})$ && $(k < 25)$
k
k=k+1;
X=lsqnonlin('funJune2024DC25',xo);
b12=max(abs(X-xo));
xo=X;
u(m8/2,1)
end;
b14=max(abs(u-uo));
uo=u;
vo1=v1;
vo2=v2;
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u);
****

With the auxiliary function "funJune2024DC25",

****

1. function W=funJune2024DC25(x)
   global m8 d yo u K e1 A B v1 v2 vo1 vo2 uo
   for i=1:m8
   u(i,1)=x(i,1);
   v1(i,1)=x(i+m8,1);
   v2(i,1)=x(i+2*m8,1);
   w(i,1)=x(i+3*m8,1);
   end;

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v1(m8,1)=0;

u(m8,1)=0;

d2v(1,1)=$(-2*v1(1,1)+v1(2,1))/d^2$;

d2u(1,1)=$(-2*u(1,1)+u(2,1))/d^2$;

for i=2:m8-1

d2v1(i,1)=$(v1(i+1,1)-2*v1(i,1)+v1(i-1,1))/d^2$;

d2u(i,1)=$(u(i+1,1)-2*u(i,1)+u(i-1,1))/d^2$;

end;

for i=1:m8-1

$W(i,1) = -e1*d2v1(i,1)+3*A*uo(i,1)^2*v1(i,1)-B*v1(i,1)+2*K*vo1(i,1)*u(i,1)+2*K*vo2(i,1)*u(i,1)$;

$W(i+m8,1) = -e1*d2u(i,1)+3*A*uo(i,1)^2*u(i,1)-2*uo(i,1)^3*A-B*u(i,1)-yo(i,1)+w(i,1)-K*uo(i,1)^2/2-v1(i,1)$;

$W(i+2*m8,1) = w(i,1)-K*uo(i,1)^2/2-v2(i,1)$;

$W(i+3*m8,1) = v1(i,1)+v2(i,1)$;

end;

****

64. A Convex Dual Variational Formulation for a Burger's Type Equation

Let $\Omega = [0,1] \subset \mathbb{R}$.

Consider the Burger's type equation

$$\begin{cases} \nu u_{xx} - u\ u_x = 0, & \text{in } \Omega, \\ u(0) = 1, & u(1) = 0. \end{cases} \tag{464}$$

Here $\nu > 0$ is a real constant.

Define the Galerkin type functional $J : V \to \mathbb{R}$ where

$$J(u) = \frac{1}{2}\int_\Omega (\nu u_{xx} - u\ u_x)^2\, dx,$$

and

$$V = \{u \in W^{1,2}(\Omega)\ :\ u(0) = 1,\ \text{and}\ u(1) = 0\}.$$

Denoting $Y = Y^* = L^2(\Omega)$, define $F_1 : V \times Y^* \to \mathbb{R}$ and $F_2 : V \times Y^* \to \mathbb{R}$ by

$$F_1(u, v_1^*) = \frac{1}{2}\int_\Omega (\nu u_{xx} - u\ u_x + v_1^* + Ku^2 + Ku_x^2)^2\, dx,$$

and

$$F_2(u, v_1^*) = \frac{1}{2}\int_\Omega (v_1^* + Ku^2 + Ku_x^2)^2\, dx,$$

respectively. Here $K > 0$ is an appropriate large real constant.

Define also $J_1 : V \times Y^* \to \mathbb{R}$ by

$$J_1(u, v_1^*) = F_1(u, v_1^*) + F_2(u, v_1^*),$$

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Observe that

$$\begin{aligned}
J_1(u,v_1^*) &= F_1(u,v_1^*)+F_2(u,v_1^*)\\
&= -\langle v_1^*+\nu u_{xx},v_4^*\rangle_{L^2}-\langle u,v_2^*\rangle_{L^2}-\langle u_x,v_3^*\rangle_{L^2}+F_1(u,v_1^*)\\
&\quad -\langle v_1^*,v_7^*\rangle_{L^2}-\langle u,v_5^*\rangle_{L^2}-\langle u_x,v_6^*\rangle_{L^2}+F_2(u,v_1^*)\\
&\quad +\langle v_1^*+\nu u_{xx},v_4^*\rangle_{L^2}+\langle u,v_2^*\rangle_{L^2}+\langle u_x,v_3^*\rangle_{L^2}\\
&\quad +\langle v_1^*,v_7^*\rangle_{L^2}+\langle u,v_5^*\rangle_{L^2}+\langle u_x,v_6^*\rangle_{L^2}\\
&\geq \inf_{(v_1,v_2,v_3)\in[Y]^3}\left\{-\langle v_1,v_4^*\rangle_{L^2}-\langle v_2,v_2^*\rangle_{L^2}-\langle v_3,v_3^*\rangle_{L^2}+\tilde{F}_1(v_1,v_2,v_3)\right\}\\
&\quad +\inf_{(v_1,v_2,v_3)\in[Y]^3}\left\{-\langle v_1,v_7^*\rangle_{L^2}-\langle v_2,v_2^*\rangle_{L^2}-\langle v_3,v_3^*\rangle_{L^2}+\tilde{F}_2(v_1,v_2,v_3)\right\}\\
&\quad +\inf_{(u,v_1^*)\in V\times Y^*}\{\langle v_1^*+\nu u_{xx},v_4^*\rangle_{L^2}+\langle u,v_2^*\rangle_{L^2}+\langle u_x,v_3^*\rangle_{L^2}\\
&\quad +\langle v_1^*,v_7^*\rangle_{L^2}+\langle u,v_5^*\rangle_{L^2}+\langle u_x,v_6^*\rangle_{L^2}\}\\
&= -\tilde{F}_1^*(v_4^*,v_2^*,v_3^*)-\tilde{F}_2^*(v_7^*,v_5^*,v_6^*)\\
&\quad +\nu(v_4^*)_x(0)u_0(0),\forall(u,v_1^*)\in V\times Y^*,\ \forall v^*\in A^*\cap B^*,
\end{aligned}\tag{465}$$

where

$$A^*=\{v^*=(v_4^*,v_2^*,v_3^*,v_5^*,v_6^*,v_7^*)\in[Y^*]^6\ :\ \nu(v_4^*)_{xx}+v_2^*-(v_3^*)_x=0,\ \text{in }\Omega\},$$

$$B^*=\{v^*\in[Y^*]^6\ :\ v_4^*\geq 0,\ v_7^*\geq 0,\ v_4^*+v_7^*=0,\ \text{in }\Omega\text{ and }v_4^*(0)=v_4^*(1)=0\}.$$

Moreover, denoting

$$\tilde{F}_1(v_1,v_2,v_3)=\frac{1}{2}\int_\Omega(v_1-v_2v_3+Kv_2^2+Kv_3^2)^2\,dx,$$

and

$$\tilde{F}_1(v_1,v_2,v_3)=\frac{1}{2}\int_\Omega(v_1+Kv_2^2+Kv_3^2)^2\,dx,$$

for $v^*\in B^*$, we have

$$\begin{aligned}
&\tilde{F}_1^*(v_4^*,v_2^*,v_3^*)\\
&= \sup_{(v_1,v_2,v_3)\in[Y]^3}\left\{\langle v_1,v_4^*\rangle_{L^2}+\langle v_2,v_2^*\rangle_{L^2}+\langle v_3,v_3^*\rangle_{L^2}-\tilde{F}_1(v_1,v_2,v_3)\right\}\\
&= \frac{1}{2(K^2-1)}\int_\Omega\frac{(2v_2^*v_3^*+2K((v_2^*)^2+(v_3^*)^2))}{v_4^*}\,dx+\frac{1}{2}\int_\Omega(v_4^*)^2\,dx,
\end{aligned}\tag{466}$$

$$\begin{aligned}
&\tilde{F}_2^*(v_7^*,v_5^*,v_6^*)\\
&= \sup_{(v_1,v_2,v_3)\in[Y]^3}\left\{\langle v_1,v_7^*\rangle_{L^2}+\langle v_2,v_5^*\rangle_{L^2}+\langle v_3,v_6^*\rangle_{L^2}-\tilde{F}_2(v_1,v_2,v_3)\right\}\\
&= \frac{1}{4K}\int_\Omega\frac{(v_5^*)^2}{v_7^*}\,dx+\frac{1}{4K}\int_\Omega\frac{(v_6^*)^2}{v_7^*}\,dx+\frac{1}{2}\int_\Omega(v_7^*)^2\,dx.
\end{aligned}\tag{467}$$

Here we define $J^*:[Y^*]^6\to\mathbb{R}$ by

$$J^*(v^*)=-\tilde{F}_1^*(v_4^*,v_2^*,v_3^*)-\tilde{F}_2^*(v_7^*,v_5^*,v_6^*)+\nu(v_4^*)_x(0)u_0(0).$$

It is worth highlighting we have got

$$\inf_{(u,v_1^*)\in V\times Y^*}J_1(u,v_1^*)\geq\sup_{v^*\in A^*\cap B^*}J^*(v^*).$$

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Finally, we also emphasize that J^* is convex (in fact concave) in the convex set $A^* \cap B^*$ so that we have obtained a convex dual formulation for an originally non-convex primal dual one.

Remark 64.1. *The conditions which define B^* must be replaced by those concerning the regularized set*

$$B^*_\varepsilon = \{v^* \in [Y^*]^6 \ : \ v^*_4 \geq \varepsilon, \ v^*_7 \geq \varepsilon, \ v^*_4 + v^*_7 = 3\varepsilon, \ \textit{in } \Omega \textit{ and } v^*_4(0) = v^*_4(1) = \varepsilon\}$$

for an appropriate real constant $0 < \varepsilon \ll 1$. Therefore, through B^*_ε, we may define an approximate dual formulation so that will be particularly interested in the system behaviour as

$$\varepsilon \to 0^+.$$

65. A Convex Dual Variational Formulation for an Approximate Navier-Stokes System

Let $\Omega \subset \mathbb{R}^2$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega = S$.

Consider the approximate incompressible and time independent Navier-Stokes system, where

$$\begin{cases} \nu\nabla^2 u - u\, u_x - v\, u_y - P_x = 0, \\ \nu\nabla^2 v - u\, v_x - v\, v_y - P_y = 0, \\ \nabla^2 P + u_x^2 + v_y^2 + 2u_y v_x = 0, \qquad \text{in } \Omega, \\ u = u_0, \ v = v_0, \ P = P_0, \qquad \text{on } \partial\Omega = S. \end{cases} \tag{468}$$

Here $\nu > 0$ is a real constant. Moreover, $\mathbf{n}$ denotes the outward normal field to $\partial\Omega = S$.

Define the Galerkin type functional $J : V \to \mathbb{R}$, where

$$\begin{aligned} J(u,v,P) \ &= \ \frac{1}{2}\int_\Omega (\nu\nabla^2 u - u\, u_x - v\, u_y - P_x)^2\, dx \\ &+ \frac{1}{2}\int_\Omega (\nu\nabla^2 v - u\, v_x - v\, v_y - P_y)^2\, dx \\ &+ \frac{1}{2}\int_\Omega (\nabla^2 P + u_x^2 + v_y^2 + 2u_y v_x)^2\, dx, \end{aligned} \tag{469}$$

and

$$V = \{\mathbf{u} = (u,v,P) \in W^{1,2}(\Omega;\mathbb{R}^3) \ : \ u = u_0, \ v = v_0 \text{ and } P = P_0 \text{ on } \partial\Omega\}.$$

Denoting $Y = Y^* = L^2(\Omega)$, define $F_1 : V \times Y^* \to \mathbb{R}$, $F_2 : V \times Y^* \to \mathbb{R}$, $F_3 : V \times Y^* \to \mathbb{R}$, $F_4 : V \times Y^* \to \mathbb{R}$, $F_5 : V \times Y^* \to \mathbb{R}$ and $F_6 : V \times Y^* \to \mathbb{R}$ by

$$F_1(\mathbf{u}, v^*_{50}) = \frac{1}{2}\int_\Omega (\nu\nabla^2 u - u\, u_x - v\, u_y - P_x + Ku^2 + Ku_x^2 + Kv^2 + Ku_y^2 + v^*_{50})^2\, dx,$$

$$F_2(\mathbf{u}, v^*_{60}) = \frac{1}{2}\int_\Omega (\nu\nabla^2 v - u\, v_x - v\, v_y - P_y + Ku^2 + Kv_x^2 + Kv^2 + Kv_y^2 + v^*_{60})^2\, dx,$$

$$F_3(\mathbf{u}, v^*_{70}) = \frac{1}{2}\int_\Omega (\nabla^2 P + u_x^2 + v_y^2 + 2u_y v_x + Ku_x^2 + Kv_y^2 + Kv_x^2 + Ku_y^2 + v^*_{70})^2\, dx,$$

$$F_4(\mathbf{u}, v^*_{50}) = \frac{1}{2}\int_\Omega (Ku^2 + Ku_x^2 + Kv^2 + Ku_y^2 + v^*_{50})^2\, dx,$$

$$F_5(\mathbf{u}, v^*_{60}) = \frac{1}{2}\int_\Omega (Ku^2 + Kv_x^2 + Kv^2 + Kv_y^2 + v^*_{60})^2\, dx,$$

and

$$F_6(\mathbf{u}, v^*_{70}) = \frac{1}{2}\int_\Omega (Ku_x^2 + Kv_y^2 + Kv_x^2 + Ku_y^2 + v^*_{70})^2\, dx,$$

respectively. Here $K > 0$ is an appropriate large real constant.

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Define also $J_1 : V \times [Y^*]^3 \to \mathbb{R}$ by

$$\begin{aligned} J_1(\mathbf{u}, v_{50}^*, v_{60}^*, v_{70}^*) &= F_1(\mathbf{u}, v_{50}^*) + F_2(\mathbf{u}, v_{60}^*) \\ &\quad + F_3(\mathbf{u}, v_{70}^*) + F_4(\mathbf{u}, v_{50}^*) \\ &\quad + F_5(\mathbf{u}, v_{60}^*) + F_6(\mathbf{u}, v_{70}^*). \end{aligned} \tag{470}$$

Observe that

$$\begin{aligned} J_1(\mathbf{u}, v_{50}^*, v_{60}^*, v_{70}^*) &= F_1(\mathbf{u}, v_{50}^*) + F_2(\mathbf{u}, v_{60}^*) \\ &\quad + F_3(\mathbf{u}, v_{70}^*) + F_4(\mathbf{u}, v_{50}^*) \\ &\quad + F_5(\mathbf{u}, v_{60}^*) + F_6(\mathbf{u}, v_{70}^*) \\ &= -\langle v_{50}^* + \nu\nabla^2 u - P_x, v_1^*\rangle_{L^2} - \langle u, v_2^*\rangle_{L^2} - \langle u_x, v_3^*\rangle_{L^2} \\ &\quad - \langle v, v_4^*\rangle_{L^2} - \langle u_y, v_5^*\rangle_{L^2} + F_1(\mathbf{u}, v_{50}^*) \\ &\quad - \langle v_{60}^* + \nu\nabla^2 v - P_y, v_6^*\rangle_{L^2} - \langle u, v_7^*\rangle_{L^2} - \langle v_x, v_8^*\rangle_{L^2} \\ &\quad - \langle v, v_9^*\rangle_{L^2} - \langle v_y, v_{10}^*\rangle_{L^2} + F_2(\mathbf{u}, v_{60}^*) \\ &\quad - \langle v_{70}^* + \nabla^2 P, v_{11}^*\rangle_{L^2} - \langle u_x, v_{12}^*\rangle_{L^2} - \langle v_y, v_{13}^*\rangle_{L^2} \\ &\quad - \langle v_x, v_{14}^*\rangle_{L^2} - \langle u_y, v_{15}^*\rangle_{L^2} + F_3(\mathbf{u}, v_{70}^*) \\ &\quad - \langle v_{50}^*, v_{16}^*\rangle_{L^2} - \langle u, v_{17}^*\rangle_{L^2} - \langle u_x, v_{18}^*\rangle_{L^2} \\ &\quad - \langle v, v_{19}^*\rangle_{L^2} - \langle u_y, v_{20}^*\rangle_{L^2} + F_4(\mathbf{u}, v_{50}^*) \\ &\quad - \langle v_{60}^*, v_{21}^*\rangle_{L^2} - \langle u, v_{22}^*\rangle_{L^2} - \langle v_x, v_{23}^*\rangle_{L^2} \\ &\quad - \langle v, v_{24}^*\rangle_{L^2} - \langle v_y, v_{25}^*\rangle_{L^2} + F_5(\mathbf{u}, v_{60}^*) \\ &\quad - \langle v_{70}^*, v_{26}^*\rangle_{L^2} - \langle u_x, v_{27}^*\rangle_{L^2} - \langle v_y, v_{28}^*\rangle_{L^2} \\ &\quad - \langle v_x, v_{29}^*\rangle_{L^2} - \langle u_y, v_{30}^*\rangle_{L^2} + F_6(\mathbf{u}, v_{70}^*) \\ &\quad + \langle v_{50}^* + \nu\nabla^2 u - P_x, v_1^*\rangle_{L^2} + \langle u, v_2^*\rangle_{L^2} + \langle u_x, v_3^*\rangle_{L^2} \\ &\quad + \langle v, v_4^*\rangle_{L^2} + \langle u_y, v_5^*\rangle_{L^2} \\ &\quad + \langle v_{60}^* + \nu\nabla^2 v - P_y, v_6^*\rangle_{L^2} + \langle u, v_7^*\rangle_{L^2} + \langle v_x, v_8^*\rangle_{L^2} \\ &\quad + \langle v, v_9^*\rangle_{L^2} + \langle v_y, v_{10}^*\rangle_{L^2} \\ &\quad + \langle v_{70}^* + \nabla^2 P, v_{11}^*\rangle_{L^2} - \langle u_x, v_{12}^*\rangle_{L^2} - \langle v_y, v_{13}^*\rangle_{L^2} \\ &\quad + \langle v_x, v_{14}^*\rangle_{L^2} + \langle u_y, v_{15}^*\rangle_{L^2} \\ &\quad + \langle v_{50}^*, v_{16}^*\rangle_{L^2} + \langle u, v_{17}^*\rangle_{L^2} + \langle u_x, v_{18}^*\rangle_{L^2} \\ &\quad + \langle v, v_{19}^*\rangle_{L^2} + \langle u_y, v_{20}^*\rangle_{L^2} \\ &\quad + \langle v_{60}^*, v_{21}^*\rangle_{L^2} + \langle u, v_{22}^*\rangle_{L^2} + \langle v_x, v_{23}^*\rangle_{L^2} \\ &\quad + \langle v, v_{24}^*\rangle_{L^2} + \langle v_y, v_{25}^*\rangle_{L^2} \\ &\quad + \langle v_{70}^*, v_{26}^*\rangle_{L^2} + \langle u_x, v_{27}^*\rangle_{L^2} + \langle v_y, v_{28}^*\rangle_{L^2} \\ &\quad + \langle v_x, v_{29}^*\rangle_{L^2} + \langle u_y, v_{30}^*\rangle_{L^2}. \end{aligned} \tag{471}$$

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From such a result, we obtain

$$
\begin{aligned}
& J_1(\mathbf{u}, v_{50}^*, v_{60}^*, v_{70}^*) \\
\geq & \inf_{(v_1,\cdots,v_5)\in[Y]^5}\{-\langle v_1, v_1^*\rangle_{L^2} - \langle v_2, v_2^*\rangle_{L^2} - \langle v_3, v_3^*\rangle_{L^2} \\
& -\langle v_4, v_4^*\rangle_{L^2} - \langle v_5, v_5^*\rangle_{L^2} + \tilde{F}_1(v_1,\cdots,v_5)\} \\
& \inf_{(v_6,\cdots,v_{10})\in[Y]^5}\{-\langle v_6, v_6^*\rangle_{L^2} - \langle v_7, v_7^*\rangle_{L^2} - \langle v_8, v_8^*\rangle_{L^2} \\
& -\langle v_9, v_9^*\rangle_{L^2} - \langle v_{10}, v_{10}^*\rangle_{L^2} + \tilde{F}_2(v_6,\cdots,v_{10})\} \\
& \inf_{(v_{11},\cdots,v_{15})\in[Y]^5}\{-\langle v_{11}, v_{11}^*\rangle_{L^2} - \langle v_{12}, v_{12}^*\rangle_{L^2} - \langle v_{13}, v_{13}^*\rangle_{L^2} \\
& -\langle v_{14}, v_{14}^*\rangle_{L^2} - \langle v_{15}, v_{15}^*\rangle_{L^2} + \tilde{F}_3(v_{11},\cdots,v_{15})\} \\
& \inf_{(v_{16},\cdots,v_{20})\in[Y]^5}\{-\langle v_{16}, v_{16}^*\rangle_{L^2} - \langle v_{17}, v_{17}^*\rangle_{L^2} - \langle v_{18}, v_{18}^*\rangle_{L^2} \\
& -\langle v_{19}, v_{19}^*\rangle_{L^2} - \langle v_{20}, v_{20}^*\rangle_{L^2} + \tilde{F}_4(v_{16},\cdots,v_{20})\} \\
& \inf_{(v_{21},\cdots,v_{25})\in[Y]^5}\{-\langle v_{21}, v_{21}^*\rangle_{L^2} - \langle v_{22}, v_{22}^*\rangle_{L^2} - \langle v_{23}, v_{23}^*\rangle_{L^2} \\
& -\langle v_{24}, v_{24}^*\rangle_{L^2} - \langle v_{25}, v_{25}^*\rangle_{L^2} + \tilde{F}_5(v_{21},\cdots,v_{25})\} \\
& \inf_{(v_{26},\cdots,v_{30})\in[Y]^5}\{-\langle v_{26}, v_{26}^*\rangle_{L^2} - \langle v_{27}, v_{27}^*\rangle_{L^2} - \langle v_{28}, v_{28}^*\rangle_{L^2} \\
& -\langle v_{29}, v_{29}^*\rangle_{L^2} - \langle v_{30}, v_{30}^*\rangle_{L^2} + \tilde{F}_6(v_{26},\cdots,v_{30})\} \\
& + \inf_{(\mathbf{u},v_{50}^*,v_{60}^*,v_{70}^*)\in V\times[Y]^3}\{\langle v_{50}^* + \nu\nabla^2 u - P_x, v_1^*\rangle_{L^2} + \langle u, v_2^*\rangle_{L^2} + \langle u_x, v_3^*\rangle_{L^2} \\
& +\langle v, v_4^*\rangle_{L^2} + \langle u_y, v_5^*\rangle_{L^2} \\
& -\langle v_{60}^* + \nu\nabla^2 v - P_y, v_6^*\rangle_{L^2} + \langle u, v_7^*\rangle_{L^2} + \langle v_x, v_8^*\rangle_{L^2} \\
& +\langle v, v_9^*\rangle_{L^2} + \langle v_y, v_{10}^*\rangle_{L^2} \\
& +\langle v_{70}^* + \nabla^2 P, v_{11}^*\rangle_{L^2} + \langle u_x, v_{12}^*\rangle_{L^2} + \langle v_y, v_{13}^*\rangle_{L^2} \\
& +\langle v_x, v_{14}^*\rangle_{L^2} + \langle u_y, v_{15}^*\rangle_{L^2} \\
& +\langle v_{50}^*, v_{16}^*\rangle_{L^2} + \langle u, v_{17}^*\rangle_{L^2} + \langle u_x, v_{18}^*\rangle_{L^2} \\
& +\langle v, v_{19}^*\rangle_{L^2} + \langle u_y, v_{20}^*\rangle_{L^2} \\
& +\langle v_{60}^*, v_{21}^*\rangle_{L^2} + \langle u, v_{22}^*\rangle_{L^2} + \langle v_x, v_{23}^*\rangle_{L^2} \\
& +\langle v, v_{24}^*\rangle_{L^2} + \langle v_y, v_{25}^*\rangle_{L^2} \\
& +\langle v_{70}^*, v_{26}^*\rangle_{L^2} + \langle u_x, v_{27}^*\rangle_{L^2} + \langle v_y, v_{28}^*\rangle_{L^2} \\
& +\langle v_x, v_{29}^*\rangle_{L^2} + \langle u_y, v_{30}^*\rangle_{L^2}\} \\
= & -\tilde{F}_1^*(v_1^*,\cdots,v_5^*) - \tilde{F}_2^*(v_6^*,\cdots,v_{10}^*) - \tilde{F}_3^*(v_{11}^*,\cdots,v_{15}^*) \\
& -\tilde{F}_4^*(v_{16}^*,\cdots,v_{20}^*) - \tilde{F}_5^*(v_{21}^*,\cdots,v_{25}^*) - \tilde{F}_6^*(v_{26}^*,\cdots,v_{30}^*) \\
& +\nu\int_{\partial\Omega} u_0(\nabla v_1^*\cdot\mathbf{n})\,dS + \nu\int_{\partial\Omega} v_0(\nabla v_6^*\cdot\mathbf{n})\,dS + \int_{\partial\Omega} P_0(\nabla v_{11}^*\cdot\mathbf{n})\,dS, \qquad (472)
\end{aligned}
$$

if $v^* = (v_1^*,\cdots,v_{30}^*) \in A^*\cap B^*$, where $A^* = A_1^*\cap A_2^*\cap A_3^*$,

$$
\begin{aligned}
A_1^* = & \{v^*\in[Y^*]^{30} \ : \ \nu\nabla^2 v_1^* + v_2^* - (v_3^*)_x - (v_5^*)_y \\
& v_7^* - (v_{12}^*)_x - (v_{14}^*)_y + v_{17}^* \\
& -(v_{18}^*)_x - (v_{20}^*)_y - v_{22}^* - (v_{30}^*)_y = 0, \text{ in } \Omega\}, \qquad (473)
\end{aligned}
$$

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$$\begin{aligned} A_2^* &= \{v^* \in [Y^*]^{30} \,:\, v_4^* + \nu\nabla^2 v_6^* - (v_8^*)_x - v_9^* \\ &\quad -(v_{10}^*)_y - (v_{15}^*)_x + v_{19}^* - (v_{23}^*)_x \\ &\quad +v_{24}^* - (v_{25}^*)_y - (v_{28}^*)_y - (v_{29}^*)_x = 0, \text{ in } \Omega\}, \end{aligned} \tag{474}$$

$$A_3^* = \{v^* \in [Y^*]^{30} \,:\, (v_1^*)_x + (v_6^*)_y + \nabla^2 v_{11}^* = 0, \text{ in } \Omega\}, \tag{475}$$

$$\begin{aligned} B^* &= \{v^* \in [Y^*]^{30} \,:\, v_1^* + v_{16}^* = 0,\ v_6^* + v_{21}^* = 0,\ v_{11}^* + v_{26}^* = 0, \\ &\quad v_1^* \geq 0,\ v_6^* \geq 0,\ v_{11}^* \geq 0, \\ &\quad v_{16}^* \geq 0,\ v_{21}^* \geq 0,\ v_{26}^* \geq 0, \text{ in } \Omega, \\ &\quad v_1^* = v_6^* = v_{11}^* = 0, \text{ on } \partial\Omega\} \end{aligned} \tag{476}$$

Moreover, denoting

$$\tilde{F}_1(v_1, \cdots, v_5) = \frac{1}{2}\int_\Omega (v_1 - v_2v_3 - v_4v_5 + Kv_2^2 + Kv_3^2 + Kv_4^2 + Kv_5^2)^2\, dx,$$

$$\tilde{F}_2(v_6, \cdots, v_{10}) = \frac{1}{2}\int_\Omega (v_6 - v_7v_8 - v_9v_{10} + Kv_7^2 + Kv_8^2 + Kv_9^2 + Kv_{10}^2)^2\, dx,$$

$$\tilde{F}_3(v_{11}, \cdots, v_{15}) = \frac{1}{2}\int_\Omega (v_{11} + v_{12}^2 + v_{13}^2 + 2v_{14}v_{15} + Kv_{12}^2 + Kv_{13}^2 + Kv_{14}^2 + Kv_{15}^2)^2\, dx,$$

$$\tilde{F}_4(v_{16}, \cdots, v_{20}) = \frac{1}{2}\int_\Omega (v_{16} + Kv_{17}^2 + Kv_{18}^2 + Kv_{19}^2 + Kv_{20}^2)^2\, dx,$$

$$\tilde{F}_5(v_{21}, \cdots, v_{25}) = \frac{1}{2}\int_\Omega (v_{21} + Kv_{22}^2 + Kv_{23}^2 + Kv_{24}^2 + Kv_{25}^2)^2\, dx,$$

$$\tilde{F}_6(v_{26}, \cdots, v_{30}) = \frac{1}{2}\int_\Omega (v_{26} + Kv_{27}^2 + Kv_{28}^2 + Kv_{29}^2 + Kv_{30}^2)^2\, dx,$$

we have

$$\begin{aligned} &\tilde{F}_1^*(v_1^*, \cdots, v_5^*) \\ &= \sup_{(v_1,\cdots,v_5)\in[Y]^5} \{\langle v_1, v_1^*\rangle_{L^2} + \langle v_2, v_2^*\rangle_{L^2} + \langle v_3, v_3^*\rangle_{L^2} \\ &\quad \langle v_4, v_4^*\rangle_{L^2} + \langle v_5, v_5^*\rangle_{L^2} - \tilde{F}_1(v_1, \cdots, v_5)\} \\ &= \frac{1}{2(4K^2-1)}\int_\Omega \frac{2v_2^*v_3^* + 2v_4^*v_5^* + 2K((v_2^*)^2 + (v_3^*)^2 + (v_4^*)^2 + (v_5^*)^2)}{v_1^*}\, dx \\ &\quad +\frac{1}{2}\int_\Omega (v_1^*)^2\, dx, \end{aligned} \tag{477}$$

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$$\begin{aligned}
&\tilde{F}_2^*(v_6^*,\cdots,v_{10}^*)\\
=&\sup_{(v_6,\cdots,v_{10})\in[Y]^5}\{\langle v_6,v_6^*\rangle_{L^2}+\langle v_7,v_7^*\rangle_{L^2}+\langle v_8,v_8^*\rangle_{L^2}\\
&\langle v_9,v_9^*\rangle_{L^2}+\langle v_{10},v_{10}^*\rangle_{L^2}-\tilde{F}_2(v_6,\cdots,v_{10})\}\\
=&\frac{1}{2(4K^2-1)}\int_\Omega\frac{2v_7^*v_8^*+2v_9^*v_{10}^*+2K((v_7^*)^2+(v_8^*)^2+(v_9^*)^2+(v_{10}^*)^2)}{v_6^*}\,dx\\
&+\frac{1}{2}\int_\Omega(v_6^*)^2\,dx,
\end{aligned}\tag{478}$$

$$\begin{aligned}
&\tilde{F}_3^*(v_{11}^*,\cdots,v_{15}^*)\\
=&\sup_{(v_{11},\cdots,v_{15})\in[Y]^5}\{\langle v_{11},v_{11}^*\rangle_{L^2}+\langle v_{12},v_{12}^*\rangle_{L^2}+\langle v_{13},v_{13}^*\rangle_{L^2}\\
&\langle v_{14},v_{14}^*\rangle_{L^2}+\langle v_{15},v_{15}^*\rangle_{L^2}-\tilde{F}_3(v_{11},\cdots,v_{15})\}\\
=&\frac{1}{4(K^2-1)}\int_\Omega\frac{(-1+K)((v_{12}^*)^2+(v_{13}^*)^2)+K(v_{14}^*)^2-2v_{14}^*v_{15}^*+K(v_{15}^*)^2}{v_{11}^*}\,dx\\
&+\frac{1}{2}\int_\Omega(v_{11}^*)^2\,dx,
\end{aligned}\tag{479}$$

$$\begin{aligned}
&\tilde{F}_4^*(v_{16}^*,\cdots,v_{20}^*)\\
=&\sup_{(v_{16},\cdots,v_{20})\in[Y]^5}\{\langle v_{16},v_{16}^*\rangle_{L^2}+\langle v_{17},v_{17}^*\rangle_{L^2}+\langle v_{18},v_{18}^*\rangle_{L^2}\\
&\langle v_{19},v_{19}^*\rangle_{L^2}+\langle v_{20},v_{20}^*\rangle_{L^2}-\tilde{F}_2(v_{15},\cdots,v_{20})\}\\
=&\frac{1}{4K}\int_\Omega\frac{((v_{17}^*)^2+(v_{18}^*)^2+(v_{19}^*)^2+(v_{20}^*)^2)}{v_{16}^*}\,dx\\
&+\frac{1}{2}\int_\Omega(v_{16}^*)^2\,dx,
\end{aligned}\tag{480}$$

$$\begin{aligned}
&\tilde{F}_5^*(v_{21}^*,\cdots,v_{25}^*)\\
=&\sup_{(v_{21},\cdots,v_{25})\in[Y]^5}\{\langle v_{21},v_{21}^*\rangle_{L^2}+\langle v_{22},v_{22}^*\rangle_{L^2}+\langle v_{23},v_{23}^*\rangle_{L^2}\\
&\langle v_{24},v_{24}^*\rangle_{L^2}+\langle v_{25},v_{25}^*\rangle_{L^2}-\tilde{F}_5(v_{21},\cdots,v_{25})\}\\
=&\frac{1}{4K}\int_\Omega\frac{((v_{22}^*)^2+(v_{23}^*)^2+(v_{24}^*)^2+(v_{25}^*)^2)}{v_{21}^*}\,dx\\
&+\frac{1}{2}\int_\Omega(v_{21}^*)^2\,dx,
\end{aligned}\tag{481}$$

$$\begin{aligned}
&\tilde{F}_6^*(v_{26}^*,\cdots,v_{30}^*)\\
=&\sup_{(v_{26},\cdots,v_{30})\in[Y]^5}\{\langle v_{26},v_{26}^*\rangle_{L^2}+\langle v_{27},v_{27}^*\rangle_{L^2}+\langle v_{28},v_{28}^*\rangle_{L^2}\\
&\langle v_{29},v_{29}^*\rangle_{L^2}+\langle v_{30},v_{30}^*\rangle_{L^2}-\tilde{F}_6(v_{25},\cdots,v_{30})\}\\
=&\frac{1}{4K}\int_\Omega\frac{((v_{27}^*)^2+(v_{28}^*)^2+(v_{29}^*)^2+(v_{30}^*)^2)}{v_{26}^*}\,dx\\
&+\frac{1}{2}\int_\Omega(v_{26}^*)^2\,dx.
\end{aligned}\tag{482}$$

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Here we define $J^* : [Y^*]^{30} \to \mathbb{R}$ by

$$\begin{aligned} J^*(v^*) &= -\tilde{F}_1^*(v_1^*, \cdots, v_5^*) - \tilde{F}_2^*(v_6^*, \cdots, v_{10}^*) - \tilde{F}_3^*(v_{11}^*, \cdots, v_{15}^*) \\ &\quad -\tilde{F}_4^*(v_{16}^*, \cdots, v_{20}^*) - \tilde{F}_5^*(v_{21}^*, \cdots, v_{25}^*) - \tilde{F}_6^*(v_{26}^*, \cdots, v_{30}^*) \\ &\quad +\nu \int_{\partial\Omega} u_0(\nabla v_1^* \cdot \mathbf{n})\, dS + \nu \int_{\partial\Omega} v_0(\nabla v_6^* \cdot \mathbf{n})\, dS + \int_{\partial\Omega} P_0(\nabla v_{11}^* \cdot \mathbf{n})\, dS, \end{aligned} \tag{483}$$

It is worth highlighting we have got

$$\inf_{(\mathbf{u}, v_{50}^*, v_{60}^*, v_{70}^*) \in V \times [Y]^3} J_1(\mathbf{u}, v_{50}^*, v_{60}^*, v_{70}^*) \geq \sup_{v^* \in A^* \cap B^*} J^*(v^*).$$

Finally, we also emphasize that J^* is convex (in fact concave) in the convex set $A^* \cap B^*$ so that we have obtained a convex dual formulation for an originally non-convex primal dual one.

Remark 65.1. *Here we highlight the conditions which define B^* must be appropriately regularized through a small parameter*

$$0 < \varepsilon \ll 1,$$

similarly as we have done in the previous section.

66. A D.C. Type Dual Variational Formulation for a Burger's Type Equation

In this section we shall write a primal Galerkin type variational formulation for a Burger's type equation as a difference of two convex functionals (the so called D.C. approach) and establish a related convex dual variational formulation.

Let $\Omega = [0, 1] \subset \mathbb{R}$.

Consider the Burger's type equation

$$\begin{cases} \nu u_{xx} - u\, u_x = 0, & \text{in } \Omega, \\ u(0) = 1, & u(1) = 0. \end{cases} \tag{484}$$

Here $\nu > 0$ is a real constant.

Define a Galerkin type functional $J : V \to \mathbb{R}$, where

$$J(u) = \frac{1}{2} \int_\Omega (\nu u_{xx} - u\, u_x)^2\, dx,$$

and

$$V = \{u \in W^{1,2}(\Omega) \ : \ u(0) = 1, \text{ and } u(1) = 0\}.$$

Denoting $Y = Y^* = L^2(\Omega)$, define $F_1, F_2 : V \times Y^* \to \mathbb{R}$ and $F_3, F_4 : V \to \mathbb{R}$ by

$$F_1(u, v_{50}^*) = \frac{1}{2} \int_\Omega (\nu u_{xx} - u\, u_x + v_{50}^* + Ku^2 + Ku_x^2)^2\, dx + \frac{K_1}{2} \int_\Omega u^2\, dx + \frac{K_1}{2} \int_\Omega u_x^2\, dx,$$

$$F_2(u, v_{50}^*) = \frac{1}{2} \int_\Omega (v_{50}^* + Ku^2 + Ku_x^2)^2\, dx + \frac{K_1}{2} \int_\Omega u^2\, dx + \frac{K_1}{2} \int_\Omega u_x^2\, dx,$$

$$F_3(u) = \frac{K_1}{2} \int_\Omega u^2\, dx + \frac{K_1}{2} \int_\Omega u_x^2\, dx$$

and

$$F_4(u) = \frac{K_1}{2} \int_\Omega u^2\, dx + \frac{K_1}{2} \int_\Omega u_x^2\, dx,$$

respectively.

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Here $K, K_1 > 0$ are appropriate large real constants such that

$$K_1 \gg K.$$

Define also $J_1 : V \times Y^* \to \mathbb{R}$ by

$$J_1(u, v_{50}^*) = F_1(u, v_{50}^*) + F_2(u, v_{50}^*) - F_3(u) - F_4(u),$$

Observe that

$$\inf_{(u,v_{50}^*)\in V\times Y^*} J_1(u, v_{50}^*) = 0,$$

so that, denoting

$$\tilde{F}_1(v_1, v_2, v_3) = \frac{1}{2}\int_\Omega (v_1 - v_2 v_3 + K v_2^2 + K v_3^2)^2\, dx + \frac{K_1}{2}\int_\Omega (v_2)^2\, dx + \frac{K_1}{2}\int_\Omega (v_3)^2\, dx,$$

$$\tilde{F}_2(v_4, v_5, v_6) = \frac{1}{2}\int_\Omega (v_6 + K v_4^2 + K v_5^2)^2\, dx + \frac{K_1}{2}\int_\Omega (v_4)^2\, dx + \frac{K_1}{2}\int_\Omega (v_5)^2\, dx,$$

$$\tilde{F}_3(z_1, z_2) = \frac{K_1}{2}\int_\Omega (z_1)^2\, dx + \frac{K_1}{2}\int_\Omega (z_2)^2\, dx,$$

$$\tilde{F}_4(z_1, z_2) = \frac{K_1}{2}\int_\Omega (z_3)^2\, dx + \frac{K_1}{2}\int_\Omega (z_4)^2\, dx,$$

we have

$$\begin{aligned}
0 \le J_1(u, v_{50}^*) &= F_1(u, v_{50}^*) + F_2(u, v_{50}^*) - F_3(u) - F_4(u)\\
&= -\langle u, z_1^*, \rangle_{L^2} - \langle u_x, z_2^*\rangle_{L^2} + F_1(u, v_{50}^*)\\
&\quad -\langle u, z_3^*\rangle_{L^2} - \langle u_x, z_4^*\rangle_{L^2} + F_2(u, v_{50}^*)\\
&\quad +\langle u, z_1^*\rangle_{L^2} + \langle u_x, z_2^*\rangle_{L^2} - F_3(u)\\
&\quad +\langle u, z_3^*\rangle_{L^2} + \langle u_x, z_4^*\rangle_{L^2} - F_4(u)\\
&\le -\langle z_1^*, u\rangle_{L^2} - \langle u_x, z_2^*\rangle_{L^2} + F_1(u, v_{50}^*)\\
&\quad -\langle u, z_3^*\rangle_{L^2} - \langle u_x, z_4^*\rangle_{L^2} + F_2(u, v_{50}^*)\\
&\quad + \sup_{(z_1,z_2)\in Y} \{\langle z_1, z_1^*\rangle_{L^2} + \langle z_2, z_2^*\rangle_{L^2} - \tilde{F}_3(z_1, z_2)\}\\
&\quad \sup_{(z_3,z_4)\in Y} \{\langle z_3, z_3^*\rangle_{L^2} + \langle z_4, z_4^*\rangle_{L^2} - \tilde{F}_4(z_3, z_4)\}\\
&= -\langle z_1^*, u\rangle_{L^2} - \langle u_x, z_2^*\rangle_{L^2} + F_1(u, v_{50}^*)\\
&\quad -\langle u, z_3^*\rangle_{L^2} - \langle u_x, z_4^*\rangle_{L^2} + F_2(u, v_{50}^*)\\
&\quad +\tilde{F}_3^*(z_1^*, z_2^*) + \tilde{F}_4^*(z_3^*, z_4^*),\ \forall u \in V,\ (z_1^*, \cdots, z_4^*) \in [Y^*]^4. \qquad (485)
\end{aligned}$$

From such results, similarly as obtained in [5], we may infer that

$$\begin{aligned}
0 &= \inf_{(u,v_{50}^*)\in V\times Y} J_1(u, v_{50}^*)\\
&\le \inf_{(u,v_{50}^*)\in V\times Y} \{-\langle u, z_1^*, \rangle_{L^2} - \langle u_x, z_2^*\rangle_{L^2} + F_1(u, v_{50}^*)\\
&\quad -\langle u, z_3^*\rangle_{L^2} - \langle u_x, z_4^*\rangle_{L^2} + F_2(u, v_{50}^*)\}\\
&\quad +\tilde{F}_3^*(z_1^*, z_2^*) + F_4^*(z_3^*, z_4^*),\ \forall z^* = (z_1^*, \cdots, z_4^*) \in [Y^*]^4. \qquad (486)
\end{aligned}$$

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On the other hand, observe that

$$\begin{aligned}
& -\langle u, z_1^*, \rangle_{L^2} - \langle u_x, z_2^* \rangle_{L^2} \\
& -\langle \nu u_{xx} + v_{50}^*, v_1^* \rangle_{L^2} - \langle u, v_2^* \rangle_{L^2} - \langle u_x, v_3^* \rangle_{L^2} + F_1(u, v_{50}^*) \\
& -\langle u, z_3^* \rangle_{L^2} - \langle u_x, z_4^* \rangle_{L^2} \\
& -\langle v_{50}^*, v_6^* \rangle_{L^2} - \langle u, v_4^* \rangle_{L^2} - \langle u_x, v_5^* \rangle_{L^2} + F_2(u, v_{50}^*) \\
& +\langle \nu u_{xx} + v_{50}^*, v_1^* \rangle_{L^2} + \langle u, v_2^* \rangle_{L^2} + \langle u_x, v_3^* \rangle_{L^2} \\
& +\langle v_{50}^*, v_6^* \rangle_{L^2} + \langle u, v_4^* \rangle_{L^2} + \langle u_x, v_5^* \rangle_{L^2} \\
\geq\ & \inf_{(v_1,v_2,v_3)\in[Y]^3} \{ -\langle v_2, z_1^* \rangle_{L^2} - \langle v_3, z_2^* \rangle_{L^2} \\
& -\langle v_1, v_1^* \rangle_{L^2} - \langle v_2, v_2^* \rangle_{L^2} - \langle v_3, v_3^* \rangle_{L^2} + \tilde{F}_1(v_1, v_2, v_3) \} \\
& + \inf_{(v_4,v_5,v_6)\in[Y]^3} \{ -\langle v_4, z_3^* \rangle_{L^2} - \langle v_5, z_4^* \rangle_{L^2} \\
& -\langle v_6, v_6^* \rangle_{L^2} - \langle v_4, v_4^* \rangle_{L^2} - \langle v_5, v_5^* \rangle_{L^2} + \tilde{F}_2(v_4, v_5, v_6) \} \\
& + \inf_{(u,v_{50}^*)\in V\times Y} \{ \langle \nu u_{xx} + v_{50}^*, v_1^* \rangle_{L^2} + \langle u, v_2^* \rangle_{L^2} + \langle u_x, v_3^* \rangle_{L^2} \\
& +\langle v_{50}^*, v_6^* \rangle_{L^2} + \langle u, v_4^* \rangle_{L^2} + \langle u_x, v_5^* \rangle_{L^2} \} \\
=\ & -\tilde{F}_1^*(v_1^*, v_2^*, v_3^*, z_1^*, z_2^*) - \tilde{F}_2^*(v_4^*, v_5^*, v_6^*, z_3^*, z_4^*) - \nu(v_1^*)_x(0)u(0),
\end{aligned} \tag{487}$$

if $v^* = (v_1^*, \cdots, v_6^*) \in A^* \cap B^*$, where

$$A^* = A_1^* \cap A_2^*,$$

$$A_1^* = \{ v^* \in [Y^*]^6 \ : \ \nu(v_1^*)_{xx} + v_2^* - (v_3^*)_x + v_4^* - (v_5^*)_x = 0, \text{ in } \Omega \},$$

$$A_2^* = \{ v^* \in [Y^*]^6 \ : \ v_1^* + v_6^* = 0, \ v_1^* \geq 0, \ v_6^* \geq 0, \text{ in } \Omega \},$$

and

$$B^* = \{ v^* \in [Y^*]^6 \ : \ v_1^*(0) = v_1^*(1) = 0 \}.$$

At this point we recall that

$$\begin{aligned}
& \tilde{F}_1^*(v_1^*, v_2^*, v_3^*, z_1^*, z_2^*) \\
=\ & \sup_{(v_1,v_2,v_3)\in[Y]^3} \{ \langle v_2, z_1^* \rangle_{L^2} + \langle v_3, z_2^* \rangle_{L^2} \\
& +\langle v_1, v_1^* \rangle_{L^2} + \langle v_2, v_2^* \rangle_{L^2} + \langle v_3, v_3^* \rangle_{L^2} - \tilde{F}_1(v_1, v_2, v_3) \} \\
=\ & \frac{K_1}{2} \int_\Omega \frac{(v_2^* + z_1^*)^2 + (v_3^* + z_2^*)^2}{(2Kv_1^* + K_1)^2 - (v_1^*)^2} \, dx \\
& + \int_\Omega \frac{(v_1^*)^2((v_2^* + z_1^*)(v_3^* + z_2^*) + K(v_2^* + z_1^*)^2 + K(v_3^* + z_2^*)^2)}{(2Kv_1^* + K_1)^2 - (v_1^*)^2} \, dx \\
& + \frac{1}{2} \int_\Omega (v_1^*)^2 \, dx,
\end{aligned} \tag{488}$$

$$\begin{aligned}
& \tilde{F}_2^*(v_4^*, v_5^*, v_6^*, z_3^*, z_4^*) \\
=\ & \sup_{(v_4,v_5,v_6)\in[Y]^3} \{ \langle v_4, z_3^* \rangle_{L^2} + \langle v_5, z_4^* \rangle_{L^2} \\
& +\langle v_6, v_6^* \rangle_{L^2} + \langle v_4, v_4^* \rangle_{L^2} + \langle v_5, v_5^* \rangle_{L^2} - \tilde{F}_2(v_4, v_5, v_6) \} \\
=\ & \frac{1}{2} \int_\Omega \frac{(v_4^* + z_3^*)^2 + (v_5^* + z_4^*)^2}{(K_1 + 2Kv_6^*)} \, dx + \frac{1}{2} \int_\Omega (v_6^*)^2 \, dx,
\end{aligned} \tag{489}$$

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$$\begin{aligned}\tilde{F}_3^*(z_1^*,z_2^*) &= \sup_{(z_1,z_2)\in[Y]^2}\{\langle z_1,z_1^*\rangle_{L^2}+\langle z_1,z_1^*\rangle_{L^2}-F_3(z_1,z_2)\}\\ &= \frac{1}{2K_1}\int_\Omega (z_1^*)^2\,dx+\frac{1}{2K_1}\int_\Omega (z_2^*)^2\,dx,\end{aligned}\tag{490}$$

and

$$\begin{aligned}\tilde{F}_4^*(z_3^*,z_4^*) &= \sup_{(z_3,z_4)\in[Y]^2}\{\langle z_3,z_3^*\rangle_{L^2}+\langle z_4,z_4^*\rangle_{L^2}-F_4(z_3,z_4)\}\\ &= \frac{1}{2K_1}\int_\Omega (z_3^*)^2\,dx+\frac{1}{2K_1}\int_\Omega (z_4^*)^2\,dx.\end{aligned}\tag{491}$$

Moreover, for $K_1>0$ sufficiently large, up to a restriction for the dual variables related to a ball of radius proportional to K_1, from the standard results on convex analysis and duality theory, we have

$$\begin{aligned}&\inf_{(u,v_{50}^*)\in V\times Y}\{-\langle u,z_1^*,\rangle_{L^2}-\langle u_x,z_2^*\rangle_{L^2}\\ &-\langle \nu u_{xx}+v_{50}^*,v_1^*\rangle_{L^2}-\langle u,v_2^*,\rangle_{L^2}-\langle u_x,v_3^*\rangle_{L^2}+F_1(u,v_{50}^*)\\ &-\langle u,z_3^*\rangle_{L^2}-\langle u_x,z_4^*\rangle_{L^2}\\ &-\langle v_{50}^*,v_6^*\rangle_{L^2}-\langle u,v_4^*,\rangle_{L^2}-\langle u_x,v_5^*\rangle_{L^2}+F_2(u,v_{50}^*)\}\\ =\ &\sup_{v^*\in A^*\cap B^*}\{-\tilde{F}_1^*(v_1^*,v_2^*,v_3^*,z_1^*,z_2^*)-\tilde{F}_2^*(v_4^*,v_5^*,v_6^*,z_3^*,z_4^*)-\nu(v_1^*)_x(0)u(0)\}.\end{aligned}\tag{492}$$

Consequently, from such results and (486) we have got

$$\begin{aligned}0=&\inf_{(u,v_{50}^*)\in V\times Y}J_1(u,v_{50}^*)\\ \leq\ &\inf_{z^*\in Y^*}\left\{\sup_{v^*\in A^*\cap B^*}\{-\tilde{F}^*(v_1^*,v_2^*,v_3^*,z_1^*,z_2^*)-\tilde{F}^*(v_4^*,v_5^*,v_6^*,z_3^*,z_4^*)-\nu(v_1^*)_x(0)u(0)\}\right.\\ &\left.+\tilde{F}_3^*(z_1^*,z_2^*)+F_4^*(z_3^*,z_4^*)\right\}.\end{aligned}\tag{493}$$

Therefore, defining $J^*:[Y^*]^{10}\to\mathbb{R}$ by

$$\begin{aligned}J^*(v^*,z^*) &= -\tilde{F}^*(v_1^*,v_2^*,v_3^*,z_1^*,z_2^*)-\tilde{F}^*(v_4^*,v_5^*,v_6^*,z_3^*,z_4^*)-\nu(v_1^*)_x(0)u(0)\\ &\quad+\tilde{F}_3^*(z_1^*,z_2^*)+F_4^*(z_3^*,z_4^*),\end{aligned}\tag{494}$$

we have got

$$0=\inf_{(u,v_{50}^*)\in V\times Y}J_1(u,v_{50}^*)\leq\inf_{z\in[Y^*]^4}\left\{\sup_{v^*\in A^*\cap B^*}J^*(v^*,z^*)\right\}.$$

Finally, we also emphasize that J^* is concave in v^* on the convex set $A^*\cap B^*$ and convex in z^*, so that, after the supremum evaluation in v^*, we have obtained a final convex dual formulation in z^* for an originally non-convex primal dual one.

67. A Convex Dual Formulation for the Rank-One Approximation of a Non-Convex Primal One

In this section, we develop a convex dual formulation for an approximate rank-one primal formulation found in some vectorial phase transition models.

Let $\Omega\subset\mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Define a functional $J:V\to\mathbb{R}$ by

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$$J(u)=\frac{1}{2}\int_{\Omega}\left(\alpha_{ijkl}\left(\frac{\partial u_i}{\partial x_j}-\beta_{ij}\right)\left(\frac{\partial u_k}{\partial x_l}-\beta_{kl}\right)\right)^2 dx-\langle u_i,f_i\rangle_{L^2},$$

where $\{\alpha_{ijkl}\}$ is a a fourth order constant positive definite and symmetric tensor, $\{\beta_{ij}\}\in\mathbb{R}^{3N}$, $f=(f_1,f_2,f_3)\in L^2(\Omega;\mathbb{R}^N)$ and

$$V=W_0^{1,2}(\Omega;\mathbb{R}^N).$$

From now and on we denote $Y=Y^*=L^2(\Omega)$ and

$$Y_1=Y_1^*=[Y]^{3N+N+3+1}.$$

Define also $F_1:Y_1\to\mathbb{R}$, $F_2:Y_1\to\mathbb{R}$ and $F_3:[Y]^{N+3+1}\to\mathbb{R}$ by

$$\begin{aligned}&F_1(w,\xi,\eta,v_{50})\\ =\;&\frac{1}{2}\int_{\Omega}\Big(\alpha_{ijkl}(w_{ij}-\beta_{ij})(w_{kl}-\beta_{kl})+K|\xi|^2+K|\eta|^2+v_{50}\Big)^2 dx,\end{aligned}\tag{495}$$

$$F_2(w,\xi,\eta,v_{50})=\sum_{i=1}^{N}\sum_{j=1}^{3}\frac{K_1}{2}\int_{\Omega}\Big(w_{ij}-\xi_i\eta_j+K|\xi|^2+K|\eta|^2+v_{50}\Big)^2 dx,$$

and

$$F_3(\xi,\eta,v_{50})=\frac{K_1}{2}\int_{\Omega}\Big(K|\xi|^2+K|\eta|^2+v_{50}\Big)^2 dx,$$

respectively.

Here $K,K_1>0$ are real constants such that $K_1\gg K\gg 1$.

Moreover, define

$$\begin{aligned}&J_1(u,w,\xi,\eta,v_{50})\\ =\;&-\langle\xi_i\eta_j,(v_1^*)_{ij}\rangle_{L^2}+F_1(w,\xi,\eta,v_{50})\\ &+F_2(w,\xi,\eta,v_{50})+F_3(\xi,\eta,v_{50})\\ &+\left\langle\frac{\partial u_i}{\partial x_j},(v_1^*)_{ij}\right\rangle_{L^2}-\langle u_i,f_i\rangle_{L^2}.\end{aligned}\tag{496}$$

Observe that

$$\begin{aligned}&J_1(u,w,\xi,\eta,v_{50})\\ \geq\;&\inf_{(\xi,\eta)\in[Y]^{3+N}}\{-\langle\xi_i\eta_j,(v_1^*)_{ij}\rangle_{L^2}+F_1(w,\xi,\eta,v_{50})\\ &+F_2(w,\xi,\eta,v_{50})+F_3(\xi,\eta,v_{50})\}\\ &+\inf_{u\in V}\left\{\left\langle\frac{\partial u_i}{\partial x_j},(v_1^*)_{ij}\right\rangle_{L^2}-\langle u_i,f_i\rangle_{L^2}\right\}\\ =\;&-\tilde{F}_{12}^*(v_1^*),\ \forall v_1^*\in A_1^*,\end{aligned}\tag{497}$$

where

$$\tilde{F}_{12}^*(v_1^*)=\sup_{(\xi,\eta)\in[Y]^{3+N}}\{\langle\xi_i\eta_j,(v_1^*)_{ij}\rangle_{L^2}-F_1(w,\xi,\eta,v_{50})-F_2(w,\xi,\eta,v_{50})-F_3(\xi,\eta,v_{50})\}$$

and

$$A_1^*=\{v_1^*\in[Y^*]^{3N}\ :\ (v_1^*)_{ij,j}+f_i=0,\ \forall i\in\{1,\cdots,N\},\ \text{ in }\Omega\}.$$

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On the other hand

$$\begin{aligned}
& \tilde{W} \\
= \; & -\langle \xi_i \eta_j, (v_1^*)_{ij} \rangle_{L^2} + F_1(w, \xi, \eta, v_{50}) \\
& + F_2(w, \xi, \eta, v_{50}) + F_3(\xi, \eta, v_{50}) \\
= \; & -\langle \xi_i \eta_j, (v_1^*)_{ij} \rangle_{L^2} - \langle w_{ij}, (w_1^*)_{ij} \rangle_{L^2} - \langle \xi_i, (v_2^*)_i \rangle_{L^2} \\
& - \langle \eta_j, (v_3^*)_j \rangle_{L^2} - \langle v_{50}, v_4^* \rangle_{L^2} + F_1(w, \xi, \eta, v_{50}) \\
& - \langle w_{ij}, (w_2^*)_{ij} \rangle_{L^2} - \langle \xi_i, (v_5^*)_i \rangle_{L^2} \\
& - \langle \eta_j, (v_6^*)_j \rangle_{L^2} - \langle v_{50}, v_7^* \rangle_{L^2} + F_2(w, \xi, \eta, v_{50}) \\
& - \langle \xi_i, (v_8^*)_i \rangle_{L^2} - \langle \eta_j, (v_9^*)_j \rangle_{L^2} \\
& - \langle v_{50}, v_{10}^* \rangle_{L^2} + F_3(w, \xi, \eta, v_{50}) \\
& + \langle w_{ij}, (w_1^*)_{ij} \rangle_{L^2} + \langle \xi_i, (v_2^*)_i \rangle_{L^2} \\
& + \langle \eta_j, (v_3^*)_j \rangle_{L^2} + \langle v_{50}, v_4^* \rangle_{L^2} \\
& + \langle w_{ij}, (w_2^*)_{ij} \rangle_{L^2} + \langle \xi_i, (v_5^*)_i \rangle_{L^2} \\
& + \langle \eta_j, (v_6^*)_j \rangle_{L^2} + \langle v_{50}, v_7^* \rangle_{L^2} \\
& + \langle \xi_i, (v_8^*)_i \rangle_{L^2} + \langle \eta_j, (v_9^*)_j \rangle_{L^2} + \langle v_{50}, v_{10}^* \rangle_{L^2}
\end{aligned} \tag{498}$$

Thus,

$$\begin{aligned}
& \tilde{W} \\
\geq \; & \inf_{(w,\xi,\eta,v_{50}) \in Y_1} \{ -\langle \xi_i \eta_j, (v_1^*)_{ij} - \langle w_{ij}, (w_1^*)_{ij} \rangle_{L^2} - \langle \xi_i, (v_2^*)_i \rangle_{L^2} \\
& - \langle \eta_j, (v_3^*)_j \rangle_{L^2} - \langle v_{50}, v_4^* \rangle_{L^2} + F_1(w, \xi, \eta, v_{50}) \} \\
& + \inf_{(w,\xi,\eta,v_{50}) \in Y_1} \{ -\langle w_{ij}, (w_2^*)_{ij} \rangle_{L^2} - \langle \xi_i, (v_5^*)_i \rangle_{L^2} \\
& - \langle \eta_j, (v_6^*)_j \rangle_{L^2} - \langle v_{50}, v_7^* \rangle_{L^2} + F_2(w, \xi, \eta, v_{50}) \} \\
& + \inf_{(\xi,\eta,v_{50}) \in [Y]^{3+N+1}} \{ -\langle \xi_i, (v_8^*)_i \rangle_{L^2} - \langle \eta_j, (v_9^*)_j \rangle_{L^2} \\
& - \langle v_{50}, v_{10}^* \rangle_{L^2} + F_3(w, \xi, \eta, v_{50}) \} \\
& + \inf_{(w,\xi,\eta,v_{50}) \in Y_1} \{ \langle w_{ij}, (w_1^*)_{ij} \rangle_{L^2} + \langle \xi_i, (v_2^*)_i \rangle_{L^2} \\
& + \langle \eta_j, (v_3^*)_j \rangle_{L^2} + \langle v_{50}, v_4^* \rangle_{L^2} \\
& + \langle w_{ij}, (w_2^*)_{ij} \rangle_{L^2} + \langle \xi_i, (v_5^*)_i \rangle_{L^2} \\
& + \langle \eta_j, (v_6^*)_j \rangle_{L^2} + \langle v_{50}, v_7^* \rangle_{L^2} \\
& + \langle \xi_i, (v_8^*)_i \rangle_{L^2} + \langle \eta_j, (v_9^*)_j \rangle_{L^2} + \langle v_{50}, v_{10}^* \rangle_{L^2} \} \\
= \; & -\tilde{F}_1^*(w_1^*, v_1^*, v_2^*.v_3^*, v_4^*) - \tilde{F}_2^*(w_2^*, v_5^*, v_6^*, v_7^*) - \tilde{F}_2^*(v_8^*, v_9^*, v_{10}^*), \\
& \forall (w^*, v^*) \in A^*,
\end{aligned} \tag{499}$$

where $w^* = (w_1^*, w_2^*) \in [Y]^{6N} \equiv Y_2^*$,

$$v^* = (v_1^*, v_2^*, v_3^*, v_4^*, v_5^*, v_6^*, v_7^*, v_8^*, v_9^*, v_{10}^*) \in [Y]^{12N+9} \equiv Y_3^*,$$

$$\begin{aligned}
A_2^* \; = \; & \{ (w^*, v^*) \in Y_2^* \times Y_3^* \; : \; (w_1^*)_{ij} + (w_2^*)_{ij} = 0, \; \forall i \in \{1, \cdots, N\}, \; \forall j \in \{1,2,3\}, \text{ in } \Omega, \\
& (v_2^*)_i + (v_5^*)_i + (v_8^*)_i = 0, \; \forall i \in \{1, \cdots, N\}, \text{ in } \Omega, \\
& (v_3^*)_j + (v_6^*)_j + (v_9^*)_j = 0, \; \forall j \in \{1,2,3\}, \text{ in } \Omega, \\
& v_4^* + v_7^* + v_{10}^* = 0, \text{ in } \Omega \},
\end{aligned} \tag{500}$$

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$$A_3^* = \{(w^*, v^*) \in Y_2^* \times Y_3^* \ : \ v_1^* \in A_1^*\},$$

and

$$A^* = A_2^* \cap A_3^*.$$

Furthermore,

$$\begin{aligned} & \tilde{F}_1^*(w_1^*, v_1^*, v_2^*, v_3^*, v_4^*) \\ = & \sup_{(w,\xi,\eta,v_{50})\in Y_1} \{\langle \xi_i \eta_j, (v_1^*)_{ij}\rangle_{L^2} + \langle w_{ij}, (w_1^*)_{ij}\rangle_{L^2} + \langle \xi_i, (v_2^*)_i\rangle_{L^2} \\ & + \langle \eta_j, (v_3^*)_j\rangle_{L^2} + \langle v_{50}, v_4^*\rangle_{L^2} - F_1(w, \xi, \eta, v_{50})\}, \end{aligned} \tag{501}$$

$$\begin{aligned} & \tilde{F}_2^*(w_1^*, v_5^*, v_6^*, v_7^*) \\ = & \sup_{(w,\xi,\eta,v_{50})\in Y_1} \{\langle w_{ij}, (w_2^*)_{ij}\rangle_{L^2} + \langle \xi_i, (v_5^*)_i\rangle_{L^2} \\ & + \langle \eta_j, (v_6^*)_j\rangle_{L^2} + \langle v_{50}, v_7^*\rangle_{L^2} - F_2(w, \xi, \eta, v_{50})\}, \end{aligned} \tag{502}$$

$$\begin{aligned} & \tilde{F}_3^*(v_8^*, v_9^*, v_{10}^*) \\ = & \sup_{(\xi,\eta,v_{50})\in [Y]^{3+N+1}} \{\langle \xi_i, (v_8^*)_i\rangle_{L^2} + \langle \eta_j, (v_9^*)_j\rangle_{L^2} \\ & + \langle v_{50}, v_{10}^*\rangle_{L^2} - F_3(\xi, \eta, v_{50})\}. \end{aligned} \tag{503}$$

Denoting

$$J^*(w^*, v^*) = -\tilde{F}_1^*(w_1^*, v_1^*, v_2^*, v_3^*, v_4^*) - \tilde{F}_2^*(w_1^*, v_5^*, v_6^*, v_7^*) - \tilde{F}_3^*(v_8^*, v_9^*, v_{10}^*),$$

we have got

$$\begin{aligned} \inf_{u\in V} J(u) & \geq \inf_{(u,w,\xi,\eta,v_{50})\in V\times Y_1} J_1(u, w, \xi, \eta, v_{50}) \\ & \geq \sup_{(w^*,v^*)\in A^*} J^*(w^*, v^*). \end{aligned} \tag{504}$$

Finally, we emphasize J^* is a convex (in fact concave) functional.

68. A Dual Variational Formulation for a General Non-Convex Primal One

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) & = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx \\ & + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{505}$$

where $\gamma > 0$, $\alpha > 0$, $\beta > 0$ and $f \in L^2(\Omega)$.

Here $u \in V = W_0^{1,2}(\Omega)$ and we denote $Y = Y^* = L^2(\Omega)$.

At this point, we define the functionals $F_1 : V \to \mathbb{R}$, $F_2 : V \times Y \to \mathbb{R}$ and $F_3 : V \to \mathbb{R}$, where

$$F_1(u) = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx,$$

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$$F_2(u,v) = \frac{\alpha}{2}\int_\Omega (u^2 - \beta + v)^2\,dx + \frac{K}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2};$$

and

$$F_3(u) = \frac{K}{2}\int_\Omega u^2\,dx,$$

for some constant $K > 0$.

Moreover, we define

$$V_1 = \left\{u \in V \ : \ \|u\|_\infty < \frac{3}{2}\right\}$$

and the following polar functionals

$$\begin{aligned} F_1^*(v_1^*, z^*) &= \sup_{u\in V}\{\langle u, v_1^* + z^*\rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^* + z^*)^2}{(-\gamma\nabla^2)}\,dx, \end{aligned} \tag{506}$$

$$\begin{aligned} F_2^*(v_1^*, v_0^*) &= \sup_{(u,v)\in V\times Y^*}\{\langle u, -v_1^*\rangle_{L^2} + \langle v, v_0^*\rangle_{L^2} - F_2(u,v)\} \\ &= \frac{1}{2}\int_\Omega \frac{(-v_1^* + f)^2}{2v_0^* + K}\,dx \\ &\quad + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2\,dx + \beta\int_\Omega v_0^*\,dx, \end{aligned} \tag{507}$$

if $v_0^* \in B^*$, where

$$B^* = \left\{v_0^* \in Y^* \ : \ \|2v_0^*\|_\infty \le \frac{K}{8}\right\}$$

and,

$$\begin{aligned} F_3^*(z^*) &= \sup_{v\in Y}\{\langle v, z^*\rangle_{L^2} - F_3(v)\} \\ &= \frac{1}{2K}\int_\Omega (z^*)^2\,dx. \end{aligned} \tag{508}$$

Finally, denoting

$$D^* = \left\{v_1^* \in Y^* \ : \ \|-v_1^* + f\|_\infty \le \frac{5}{4}K\right\},$$

we also define $J_1^* : D^* \times B^* \times Y^* \to \mathbb{R}$ by

$$\begin{aligned} J_1^*(v_1^*, v_0^*, z^*) &= -F_1^*(v_1^*, z^*) - F_2^*(v_1^*, v_0^*) + F_3^*(z^*) \\ &\quad + \frac{K_1}{2}\left\|\frac{v_1^* + z^*}{-\gamma\nabla^2} - \frac{z^*}{K}\right\|_{0,2}^2 \\ &\quad + \frac{K_1}{2}\left\|\frac{-v_1^* + f}{2v_0^* + K} - \frac{z^*}{K}\right\|_{0,2}^2. \end{aligned} \tag{509}$$

Observe that if $K_1 > 0$ is sufficiently large, then J_1^* is convex in (v_1^*, z^*), $\forall v_0^* \in B^*$.

Let $(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \in D^* \times B^* \times Y^*$ be such that

$$\delta J_1^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) = \mathbf{0}.$$

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From such a concerning convexity of J_1^* in (v_1^*, z^*) we may infer that

$$J_1^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \leq J_1^*(v_1^*, \hat{v}_0, z^*),\ \forall v_1^* \in D^*, z^* \in Y^*.$$

In particular fixing $u \in V_1$, for $v_1^* = (2v_0^* + K)u$ and $z^* = Ku$, we obtain

$$\begin{aligned}
J_1^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) &\leq J_1^*(v_1^*, \hat{v}_0, z^*) \\
&\leq -\langle u, v_1^* + z^* \rangle_{L^2} + \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u\, dx \\
&\quad + \langle u, v_1^* \rangle_{L^2} + \langle u^2, \hat{v}_0^* \rangle_{L^2} + \frac{K}{2}\int_\Omega u^2\, dx \\
&\quad - \langle u, f \rangle_{L^2} + \langle u, z^* \rangle_{L^2} - \frac{K}{2}\int_\Omega u^2\, dx \\
&\quad - \frac{1}{2\alpha}\int_\Omega (\hat{v}_0^*)^2\, dx - \beta\int_\Omega \hat{v}_0^*\, dx \\
&\quad + \frac{K_1}{2}\left\| \frac{-\gamma\nabla^2 u + 2\hat{v}_0^* u - f}{-\gamma\nabla^2} \right\|_{0,2}^2 \\
&\leq \sup_{v_0^* \in Y^*} \left\{ \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u\, dx + \langle u^2, v_0^* \rangle_{L^2} - \langle u, f \rangle_{L^2} \right. \\
&\quad - \frac{1}{2\alpha}\int_\Omega (v_0^*)^2\, dx - \beta\int_\Omega v_0^*\, dx \\
&\quad \left. + \frac{K_1}{2}\left\| \frac{-\gamma\nabla^2 u + 2\hat{v}_0^* u - f}{-\gamma\nabla^2} \right\|_{0,2}^2 \right\} \\
&= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u\, dx + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2\, dx \\
&\quad - \langle u, f \rangle_{L^2} + \frac{K_1}{2}\left\| \frac{-\gamma\nabla^2 u + 2\hat{v}_0^* u - f}{-\gamma\nabla^2} \right\|_{0,2}^2 \\
&= J(u) + \frac{K_1}{2}\left\| \frac{-\gamma\nabla^2 u + 2\hat{v}_0^* u - f}{-\gamma\nabla^2} \right\|_{0,2}^2 .
\end{aligned} \tag{510}$$

Summarizing, we have got

$$J_1^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \leq J(u) + \frac{K_1}{2}\left\| \frac{-\gamma\nabla^2 u + 2\hat{v}_0^* u - f}{-\gamma\nabla^2} \right\|_{0,2}^2,\ \forall u \in V_1.$$

Let $u_0 \in V$ be such that

$$u_0 = \frac{\hat{z}^*}{K}.$$

Assume $u_0 \in V_1$.
Similarly as in the previous sections, we may prove that

$$\hat{v}_0^* = \alpha(u_0^2 - \beta),$$
$$\delta J(u_0) = -\gamma\nabla^2 u_0 + 2\hat{v}_0 u_0 - f = \mathbf{0},$$

and

$$J(u_0) = J_1^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*),$$

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so that

$$\begin{aligned} J(u_0) &= \min_{u\in V_1}\left\{ J(u) + \frac{K_1}{2}\left\| \frac{-\gamma\nabla^2 u + 2\hat{v}_0^* u - f}{-\gamma\nabla^2}\right\|_{0,2}^2 \right\} \\ &= J_1^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \\ &= \inf_{(v_1^*, z^*)\in D^*\times Y^*} J_1^*(v_1^*, \hat{v}_0^*, z^*). \end{aligned} \tag{511}$$

The objective of this section is complete.

69. A D.C. Type Duality Principle Suitable for Non-Convex Variational Optimization

In this section we develop results concerning a D.C. approach inspired by the results of J.J. Telega, W.R. Bielski and co-workers, [1–4] and Toland, [5].

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\varepsilon}{2}\int_\Omega \nabla u\cdot\nabla u\, dx \\ &\quad + \frac{\alpha}{2}\int_\Omega (u^2-\beta)^2\, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{512}$$

where $\varepsilon > 0$, $\alpha > 0$, $\beta > 0$ and $f \in L^2(\Omega)$.

Here $u \in V = W_0^{1,2}(\Omega)$ and we denote $Y = Y^* = L^2(\Omega)$.

At this point, for a large constant $K_1 > 0$, we define the approximate functional $J_1 : V \times Y \to \mathbb{R}$, by

$$\begin{aligned} J_1(u,v) &= \frac{\varepsilon}{2}\int_\Omega \nabla u\cdot\nabla u\, dx + \frac{\alpha}{2}\int_\Omega (v-\beta)^2\, dx \\ &\quad + \frac{K_1}{2}\int_\Omega (v-u^2)\, dx - \langle u, f\rangle_{L^2}. \end{aligned} \tag{513}$$

We define also the functionals $F_1 : V \to \mathbb{R}$, $F_2 : Y \to \mathbb{R}$, $F_3 : V \times Y \to \mathbb{R}$, and $F_4 : V \to \mathbb{R}$, where

$$F_1(u) = \frac{\varepsilon}{2}\int_\Omega \nabla u\cdot\nabla u\, dx - \langle u, f\rangle_{L^2},$$

$$F_2(v) = \frac{\alpha}{2}\int_\Omega (v-\beta)^2\, dx$$

$$F_3(u,v) = \frac{K_1}{2}\int_\Omega (v-u^2)\, dx + \frac{K}{2}\int_\Omega u^2\, dx$$

and

$$F_4(u) = \frac{K}{2}\int_\Omega u^2\, dx,$$

for some appropriate constant $K > 0$.

Moreover, we define the following polar functionals

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u\in V}\{-\langle u, v_1^*\rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(-v_1^*+f)^2}{(-\varepsilon\nabla^2)}\, dx, \end{aligned} \tag{514}$$

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$$\begin{aligned} F_2^*(v_2^*) &= \sup_{v\in Y^*}\{\langle v, v_2^*\rangle_{L^2} - F_2(v)\} \\ &= \frac{1}{2\alpha}\int_\Omega (v_2^*)^2\,dx + \beta\int_\Omega v_2^*\,dx, \end{aligned} \tag{515}$$

$$\begin{aligned} F_3^*(v_1^*, v_2^*, z^*) &= \sup_{(u,v)\in V\times Y}\{\langle u, v_1^* + z^*\rangle_{L^2} - \langle v, v_2^*\rangle_{L^2} - F_3(u,v)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*+z^*)^2}{2v_2^*+K}\,dx + \frac{1}{2K_1}\int_\Omega (v_2^*)^2\,dx, \end{aligned} \tag{516}$$

if $v_2^* \in B^*$, where

$$B^* = \left\{ v_2^* \in Y^* \ : \ \|2v_2^*\|_\infty \leq \frac{K}{2} \right\}$$

and,

$$\begin{aligned} F_4^*(z^*) &= \sup_{w\in Y}\{\langle w, z^*\rangle_{L^2} - F_4(w)\} \\ &= \frac{1}{2K}\int_\Omega (z^*)^2\,dx. \end{aligned} \tag{517}$$

Finally, we define

$$D^* = \left\{ z^* \in Y^* \ : \ \|z^*\|_\infty \leq \frac{5}{4}K \right\},$$

and $J_1^* : D^* \times B^* \times Y^* \to \mathbb{R}$ by

$$J_1^*(v_1^*, v_2^*, z^*) = -F_1^*(v_1^*) - F_2^*(v_2^*) - F_3^*(v_1^*, v_2^*, z^*) + F_4^*(z^*).$$

Let $\alpha_1 \in \mathbb{R}$ be such that

$$\inf_{(u,v)\in V\times Y} J_1(u,v) = \alpha_1.$$

Observe that

$$\begin{aligned} \alpha_1 &\leq J_1(u,v) \\ &= F_1(u) + F_2(v) + F_3(u,v) - F_4(u) \\ &= -\langle u, z^*\rangle_{L^2} + F_1(u) + F_2(v) + F_3(u,v) \\ &\quad + \langle u, z^*\rangle_{L^2} - F_4(u) \\ &\leq -\langle u, z^*\rangle_{L^2} + F_1(u) + F_2(v) + F_3(u,v) \\ &\quad + \sup_{w\in Y}\{\langle w, z^*\rangle_{L^2} - F_4(w)\} \\ &= -\langle u, z^*\rangle_{L^2} + F_1(u) + F_2(v) + F_3(u,v) + F_4^*(z^*),\ \forall u \in V,\ v \in Y,\ z^* \in D^*. \end{aligned} \tag{518}$$

From such results we may infer that

$$\alpha_1 \leq \inf_{(u,v)\in V\times Y}\{-\langle u, z^*\rangle_{L^2} + F_1(u) + F_2(v) + F_3(u,v)\} + F_4^*(z^*).$$

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On the other hand, for an appropriate value of $K > 0$ and $z^* \in D^*$, from standard results in convex analysis, we have

$$\begin{aligned} & \inf_{(u,v)\in V\times Y}\{-\langle u, z^*\rangle_{L^2} + F_1(u) + F_2(v) + F_3(u,v)\} \\ = & \sup_{(v_1^*,v_2^*)\in Y^*\times B^*}\{-F_1^*(v_1^*) - F_2^*(v_2^*) - F_3^*(v_1^*, v_2^*, z^*)\}. \end{aligned} \tag{519}$$

Joining the pieces, we have got

$$\alpha_1 \leq \sup_{(v_1^*,v_2^*)\in Y^*\times B^*}\{-F_1^*(v_1^*) - F_2^*(v_2^*) - F_3^*(v_1^*, v_2^*, z^*)\} + F_4^*(z^*),$$

so that

$$\alpha_1 \leq \inf_{z^*\in D^*}\left\{\sup_{(v_1^*,v_2^*)\in Y^*\times B^*}\{-F_1^*(v_1^*) - F_2^*(v_2^*) - F_3^*(v_1^*, v_2^*, z^*)\} + F_4^*(z^*)\right\},$$

that is,

$$\alpha_1 = \inf_{(u,v)\in V\times Y} J_1(u,v) \leq \inf_{z^*\in D^*}\left\{\sup_{(v_1^*,v_2^*)\in Y^*\times B^*} J_1^*(v_1^*, v_2^*, z^*)\right\}.$$

Let $(\hat{v}_1^*, \hat{v}_2^*, \hat{z}^*) \in D^* \times B^* \times Y^*$ be such that

$$\delta J_1^*(\hat{v}_1^*, \hat{v}_2^*, \hat{z}^*) = \mathbf{0}.$$

Let $(u_0, v_0) \in V \times Y$ be such that

$$u_0 = \frac{\hat{z}^*}{K}$$

and

$$v_0 = \frac{\hat{v}_2^*}{\alpha} + \beta.$$

Similarly as in the previous sections, we may prove that

$$\delta J_1(u_0, v_0) = \mathbf{0},$$

and

$$J_1(u_0, v_0) = J_1^*(\hat{v}_1^*, \hat{v}_2^*, \hat{z}^*),$$

so that

$$\begin{aligned} J_1(u_0, v_0) &= J_1^*(\hat{v}_1^*, \hat{v}_2^*, \hat{z}^*) \\ &= \sup_{(v_1^*,v_2^*)\in Y^*\times B^*} J_1^*(v_1^*, v_2^*, \hat{z}^*). \end{aligned} \tag{520}$$

The main objective of this section is complete.

69.1. A Numerical Example

We have obtained numerical results for an one-dimensional case where, $\Omega = [0,1] \subset \mathbb{R}$, $A = B = 1$, $f \equiv 2$ and

1. Case A: $\varepsilon = 0.1$
2. Case B: $\varepsilon = 0.01$
3. Case C: $\varepsilon = 0.001$.

For the optimal solutions $u_0 \in V$ obtained for the cases A,B and C, please see Figures 46, 47 and 48, respectively.

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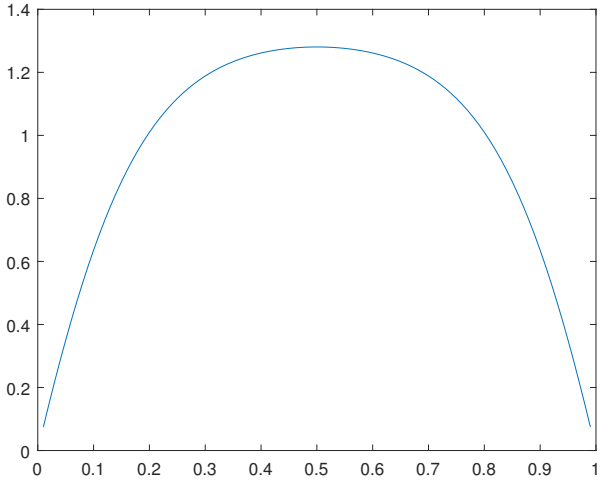

Figure 46. Solution $u_0(x)$ through the dual functional for the case A, $\varepsilon = 0.1$.

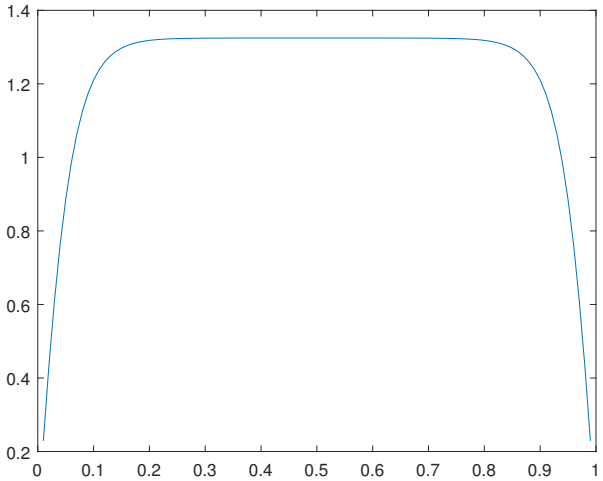

Figure 47. Solution $u_0(x)$ through the dual functional for the case B, $\varepsilon = 0.01$.

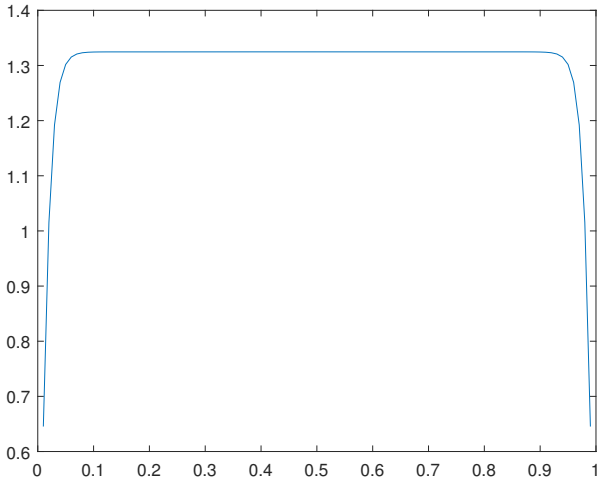

Figure 48. Solution $u_0(x)$ through the dual functional for the case C, $\varepsilon = 0.001$.

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Here we present the software in MAT-LAB through which we have obtained such numerical results.

1. clear all
   global m8 d A B yo e1 K1 e2 u z K v2
   m8=100;
   d=1/m8;
   yo(:,1)=2*ones(m8-1,1);
   z(:,1)=1.2*ones(m8-1,1);
   A=1;
   B=1;
   e1=0.001;
   e2=0.00000001;
   K1=1000000;
   K=30;
   for i=1:2*(m8-1)
   xo(i,1)=0.7;
   x1(i,1)=1.1;
   end;
   b14=1.0;
   k7=1.0;
   while $(b14 > 10^{-4})$ && $(k7 < 70)$
   k7
   k7=k7+1;
   b12=1.0;
   k=1;
   while $(b12 > 10^{-4})$ && $(k < 10)$
   k
   k=k+1;
   X=fminunc('funJuly2024A1',xo);
   b12=max(abs(X-xo));
   xo=X;
   u(m8/2,1)
   end;
   z=K*u;
   b14=max(abs(x1-xo));
   x1=xo;
   end;
   for i=1:m8-1
   x(i,1)=i*d;

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end;

plot(x,u);

****

With the auxiliary function "funJuly2024A1", where

****

1. function S=funJuly2024A1(x)

global m8 d A B yo e1 K1 e2 u z K v2

m2=zeros(m8-1,m8-1);

y1=ones(m8-1,1);

for i=2:m8-2

m2(i,i)=-2.0;

m2(i,i+1)=1.0;

m2(i,i-1)=1.0;

end;

m2(1,1)=-2.0;

m2(1,2)=1.0;

m2(m8-1,m8-1)=-2.0;

m2(m8-1,m8-2)=1.0;

for i=1:m8-1

v1(i,1)=x(i,1);

v2(i,1)=x(i+(m8-1),1);

end;

$S = 1/2 * (-v1 + yo)' * inv(-e1 * m2/d^2) * (-v1 + yo) + v2' * v2/2/A + B * v2' * y1;$

for i=1:m8-1

$S = S + (v1(i,1) + z(i,1))^2/(2 * v2(i,1) + K)/2 + v2(i,1)^2/2/K1;$

end;

$u = inv(-e1 * m2/d^2) * (-v1 + yo);$

****

70. A Concave Dual Variational Formulation for an Originally Non-Convex Primal One

In this section we develop results also inspired by the approach found in the articles of J.J. Telega, W.R. Bielski and co-workers, [1–4] and Toland, [5].

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx \\ &\quad + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{521}$$

where $\gamma > 0$, $\alpha > 0$, $\beta > 0$ and $f \in L^2(\Omega)$.

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Here $u \in V = W_0^{1,2}(\Omega)$ and we denote $Y = Y^* = L^2(\Omega)$.
Consider also the functionals $F_1 : V \times Y \to \mathbb{R}$, $F_2 : V \times Y \to \mathbb{R}$ and $F_3 : V \to \mathbb{R}$, where

$$\begin{aligned} F_1(u, v_0^*) &= \frac{\gamma}{4}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{1}{2}\langle u^2, v_0^*\rangle_{L^2} \\ &\quad + \frac{K}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \\ &\quad - \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx - \beta\int_\Omega v_0^* \, dx, \end{aligned} \tag{522}$$

$$\begin{aligned} F_2(u, v_0^*) &= \frac{\gamma}{4}\int_\Omega \nabla u \cdot \nabla u \, dx \\ &\quad + \frac{1}{2}\langle u^2, v_0^*\rangle_{L^2} + \frac{K}{2}\int_\Omega u^2 \, dx, \end{aligned} \tag{523}$$

$$F_3(u) = K\int_\Omega u^2 \, dx,$$

for some appropriate constant $K > 0$.

Moreover, we define the following polar functionals

$$\begin{aligned} F_1^*(v_1^*, v_0^*, z^*) &= \sup_{u\in V}\left\{\left\langle u, v_1^* + \frac{z^*}{2}\right\rangle_{L^2} - F_1(u, v_0^*)\right\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^* + z^*/2 + f)^2}{(-\gamma\nabla^2 + 2v_0^*)/2 + K} \, dx \\ &\quad + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx + \beta\int_\Omega v_0^* \, dx, \end{aligned} \tag{524}$$

$$\begin{aligned} F_2^*(v_1^*, v_0^*, z^*) &= \sup_{u\in V}\left\{\left\langle u, -v_1^* + \frac{z^*}{2}\right\rangle_{L^2} - F_2(u, v_0^*)\right\} \\ &= \frac{1}{2}\int_\Omega \frac{(-v_1^* + z^*/2)^2}{(-\gamma\nabla^2 + 2v_0^*)/2 + K} \, dx, \end{aligned} \tag{525}$$

if $v_0^* \in B^*$, where

$$B^* = \left\{v_0^* \in Y^* \ : \ \|2v_0^*\|_\infty \le \frac{K}{4}\right\},$$

and,

$$\begin{aligned} F_3^*(z^*) &= \sup_{w\in Y}\{\langle w, z^*\rangle_{L^2} - F_3(w)\} \\ &= \frac{1}{4K}\int_\Omega (z^*)^2 \, dx. \end{aligned} \tag{526}$$

Finally, we define

$$A^+ = \{z^* \in Y^* \ : \ f\, z^* \ge 0, \text{ in } \Omega\},$$

$$D^* = \left\{z^* \in A^+ \ : \ \|z^*\|_\infty \le \frac{5}{2}K\right\},$$

and $J_2^* : Y^* \times B^* \times D^* \to \mathbb{R}$ by

$$J_2^*(v_1^*, v_0^*, z^*) = -F_1^*(v_1^*, v_0^*, z^*) - F_2^*(v_1^*, v_0^*, z^*) + F_3^*(z^*).$$

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Observe that the variation of J_2^* in v_1^* stands for

$$-\frac{v_1^*+z^*/2+f}{(-\gamma\nabla^2+2v_0^*)/2+K}+\frac{-v_1^*+z^*/2}{(-\gamma\nabla^2+2v_0^*)/2+K}=\mathbf{0},$$

so that

$$2v_1^*+f=\mathbf{0}.$$

The variation of J_2^* in z^* stands for

$$-\frac{1}{2}\frac{v_1^*+z^*/2+f}{(-\gamma\nabla^2+2v_0^*)/2+K}-\frac{1}{2}\frac{-v_1^*+z^*/2}{(-\gamma\nabla^2+2v_0^*)/2+K}+\frac{z^*}{2K}=\mathbf{0}.$$

Finally, the variation of J_2^* in v_0^* stands for,

$$\frac{1}{2}\left(\frac{v_1^*+z^*/2+f}{(-\gamma\nabla^2+2v_0^*)/2+K}\right)^2+\frac{1}{2}\left(\frac{-v_1^*+z^*/2}{(-\gamma\nabla^2+2v_0^*)/2+K}\right)^2-\frac{v_0^*}{\alpha}-\beta=\mathbf{0}.$$

With such results in mind, we define the functional $J_3^*:Y^*\times B^*\times D^*\to\mathbb{R}$, by

$$\begin{aligned}
&J_3^*(v_1^*,v_0^*,z^*)\\
=\;&J_2^*(v_1^*,v_0^*,z^*)-\frac{K_2}{2}\|2v_1^*+f\|_{0,2}^2\\
&+\frac{\sqrt[8]{K_2}}{2}\left\|-\frac{1}{2}\frac{v_1^*+z^*/2+f}{(-\gamma\nabla^2+2v_0^*)/2+K}-\frac{1}{2}\frac{-v_1^*+z^*/2}{(-\gamma\nabla^2+2v_0^*)/2+K}+\frac{z^*}{2K}\right\|_{0,2}^2\\
&+\frac{\sqrt[8]{K_2}}{2}\left\|\frac{1}{2}\left(\frac{v_1^*+z^*/2+f}{(-\gamma\nabla^2+2v_0^*)/2+K}\right)^2+\frac{1}{2}\left(\frac{-v_1^*+z^*/2}{(-\gamma\nabla^2+2v_0^*)/2+K}\right)^2-\frac{v_0^*}{\alpha}-\beta\right\|_{0,2}^2. \qquad (527)
\end{aligned}$$

Observe that for $K_2>0$ sufficiently large $J_5^*:E^*\to\mathbb{R}$ is concave in v_1^* on E^*, where

$$J_5^*(v_1^*)=\text{ sta }_{(v_0^*,z^*)\in B^*\times D^*}J_3^*(v_1^*,v_0^*,z^*),$$

and

$$E^*=\{v_1^*\in Y^*\;:\;\|2v_1^*+f\|_\infty\leq 5\}.$$

Let $(\hat{v}_1^*,\hat{v}_0^*,\hat{z}^*)\in E^*\times B^*\times D^*$ be such that

$$\delta J_3^*(\hat{v}_1^*,\hat{v}_0^*,\hat{z}^*)=\mathbf{0}.$$

Let $u_0\in V$ be such that

$$u_0=\frac{\hat{z}^*}{2K}$$

Similarly as in the previous sections, we may prove that

$$\delta J(u_0)=\mathbf{0},$$

and

$$J(u_0)=J_3^*(\hat{v}_1^*,\hat{v}_0^*,\hat{z}^*),$$

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so that

$$\begin{aligned} J(u_0) &= J_3^*(\hat{v}_1^*, \hat{v}_0^*, \hat{z}^*) \\ &= \sup_{v_1^* \in E^*} J_3^*(v_1^*, \hat{v}_0^*, \hat{z}^*) \\ &= \sup_{v_1^* \in E^*} J_5^*(v_1^*) \\ &= J_5^*(\hat{v}_1^*). \end{aligned} \tag{528}$$

The main objective of this section is complete.

71. A Dual Variational Formulation for an Originally Non-Convex Primal One

In this section we develop results also inspired by the approach found in the articles of J.J. Telega, W.R. Bielski and co-workers, [1–4] and Toland, [5].

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx \\ &+ \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{529}$$

where $\gamma > 0$, $\alpha > 0$, $\beta > 0$ and $f \in L^2(\Omega)$.

Here $u \in V = W_0^{1,2}(\Omega)$ and we denote $Y = Y^* = L^2(\Omega)$.

Consider also the functionals $F_1 : V \to \mathbb{R}$ and $F_2 : V \times Y \to \mathbb{R}$ where,

$$F_1(u) = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{K}{2}\int_\Omega u^2 \, dx, \tag{530}$$

$$\begin{aligned} F_2(u, v_0^*) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \langle u^2, v_0^*\rangle_{L^2} \\ &- \langle u, f\rangle_{L^2} - \frac{K}{2}\int_\Omega u^2 \, dx \\ &- \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx - \beta\int_\Omega v_0^* \, dx \end{aligned} \tag{531}$$

for some appropriate constant $K > 0$.

Moreover, we define the following polar functionals

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u \in V}\{\langle u, v_1^*\rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{-\gamma\nabla^2 + K} \, dx \end{aligned} \tag{532}$$

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and

$$\begin{aligned} F_2^*(v_1^*, v_0^*) &= \inf_{u\in V}\{\langle u, v_1^*\rangle_{L^2} - F_2(u, v_0^*)\} \\ &= \frac{1}{2}\int_\Omega \frac{(-v_1^*+f)^2}{2v_0^*-K}\,dx \\ &\quad + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2\,dx + \beta\int_\Omega v_0^*\,dx, \end{aligned} \tag{533}$$

if $v_0^* \in B^*$, where

$$B^* = \left\{ v_0^* \in Y^* \ : \ \|2v_0^*\|_\infty \le \frac{K}{2} \right\}.$$

Finally, we define

$$A^+ = \{u \in V \ : \ f\ u \ge 0, \text{ in } \Omega\},$$

$$V_1 = \left\{ u \in A^+ \ : \ \|u\|_\infty \le \frac{3}{2} \right\},$$

$$D^* = \left\{ v^* \in Y^* \ : \ \left\| \frac{v_1^*}{-\gamma\nabla^2 + K} \right\|_\infty \le \frac{3}{2} \right\}$$

and $J_2^* : D^* \times B^* \to \mathbb{R}$ by

$$J_2^*(v_1^*, v_0^*) = -F_1^*(v_1^*) - F_2^*(v_1^*, v_0^*).$$

Observe that the variation of J_2^* in v_1^* stands for

$$\varphi_1 = -\frac{v_1^*}{-\gamma\nabla^2 + K} + \frac{-v_1^*+f}{2v_0^*-K} = \mathbf{0}.$$

On the other hand, the variation of J_2^* in v_0^* stands for

$$\varphi_2 = \left(\frac{-v_1^*+f}{2v_0^*-K}\right)^2 - \frac{v_0^*}{\alpha} - \beta = \mathbf{0},$$

so that

$$\varphi_3 = \left(\frac{v_1^*}{-\gamma\nabla^2 + K}\right)^2 - \frac{v_0^*}{\alpha} - \beta = \mathbf{0}.$$

With such results in mind, we define the functional $J_3^* : D^* \times B^* \to \mathbb{R}$, by

$$\begin{aligned} & J_3^*(v_1^*, v_0^*) \\ = \ & J_2^*(v_1^*, v_0^*) \\ & + \frac{K_2}{2}\left\| -\frac{v_1^*}{-\gamma\nabla^2 + K} + \frac{-v_1^*+f}{2v_0^*-K} \right\|_{0,2}^2 \\ & + \frac{K_2}{2}\left\| \left(\frac{-v_1^*+f}{2v_0^*-K}\right)^2 - \frac{v_0^*}{\alpha} - \beta \right\|_{0,2}^2 \end{aligned} \tag{534}$$

Here we assume $K_2 \gg K \gg \max\{1, \alpha, \beta, \gamma, 1/\alpha, 1/\gamma\}$.

Let $(\hat{v}_1^*, \hat{v}_0^*) \in D^* \times B^*$ be such that

$$\delta J_3^*(\hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}.$$

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Let $u_0 \in V_1$ be such that

$$u_0 = \frac{\hat{v}_1^*}{-\gamma\nabla^2 + K}$$

Similarly as in the previous sections, we may prove that

$$\delta J(u_0) = \mathbf{0},$$

and

$$J(u_0) = J_3^*(\hat{v}_1^*, \hat{v}_0^*).$$

Moreover, at a critical point of J_3^* we have $\varphi_1 = \varphi_2 = \varphi_3 = \mathbf{0}$ so that,

$$\frac{\partial^2 J_3^*(v_1^*, v_0^*)}{\partial (v_1^*)^2} = \mathcal{O}(K_2^2),$$

$$\frac{\partial^2 J_3^*(v_1^*, v_0^*)}{\partial (v_0^*)^2} = \mathcal{O}(K_2^2),$$

and with the help of software MATHEMATICA, at a critical point, we may obtain

$$\det\left\{\frac{\partial^2 J_3^*(v_1^*, v_0^*)}{\partial v_1^* \partial v_0^*}\right\} = \frac{K_2^2(-\gamma\nabla^2 + 4\alpha u^2 + 2v_0^*)^2}{\alpha^2(-\gamma\nabla^2 + K)^2(K - 2v_0^*)^2} + \mathcal{O}(K_2) > 0.$$

With such results in mind, since

$$\delta J(u_0) = -\gamma\nabla^2 u_0 + 2\alpha(u_0^2 - \beta)u_0 - f = \mathbf{0},$$

joining the pieces, assuming an approximate finite dimensional version for the model in question, if necessary, we may infer that there exist $r, r_1 > 0$ such that

$$\begin{aligned} J(u_0) &= \inf_{u \in B_r(u_0)} \left\{ J(u) + \frac{K_2}{2} \left\| \frac{-\gamma\nabla^2 u + 2\alpha(u^2 - \beta)u - f}{-\gamma\nabla^2 + K} \right\|_{0,2}^2 \right\} \\ &= J_3^*(\hat{v}_1^*, \hat{v}_0^*) \\ &= \inf_{(v_1^*, v_0^*) \in B_{r_1}(\hat{v}_1^*, \hat{v}_0^*)} J_3^*(v_1^*, v_0^*). \end{aligned} \tag{535}$$

The main objective of this section is complete.

72. A Convex Dual Variational Formulation for an Originally Non-Convex Primal One

In this section we develop results again inspired by the approach found in the articles of J.J. Telega, W.R. Bielski and co-workers, [1–4] and Toland, [5].

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx \\ &\quad + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2}, \end{aligned} \tag{536}$$

where $\gamma > 0$, $\alpha > 0$, $\beta > 0$ and $f \in L^2(\Omega)$.

Here $u \in V = W_0^{1,2}(\Omega)$ and we denote $Y = Y^* = L^2(\Omega)$.

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Consider also the functionals $F_1 : V \to \mathbb{R}$ and $F_2 : V \times Y \to \mathbb{R}$ where,

$$F_1(u) = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{K}{2}\int_\Omega u^2 \, dx, \tag{537}$$

$$\begin{aligned} F_2(u, v_0^*) = & \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \langle u^2, v_0^* \rangle_{L^2} \\ & - \langle u, f \rangle_{L^2} - \frac{K}{2}\int_\Omega u^2 \, dx \\ & - \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx - \beta \int_\Omega v_0^* \, dx \end{aligned} \tag{538}$$

for some appropriate constant $K > 0$.

Moreover, we define the following polar functionals $F_1^* : Y^* \to \mathbb{R}$ and $F_2^* : Y^* \times Y^* \to \mathbb{R}$ where,

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u \in V} \{ \langle u, v_1^* \rangle_{L^2} - F_1(u) \} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{-\gamma\nabla^2 + K} \, dx, \end{aligned} \tag{539}$$

$$\begin{aligned} F_2^*(v_1^*, v_0^*) = & \inf_{u \in V} \{ \langle u, v_1^* \rangle_{L^2} - F_2(u, v_0^*) \} \\ = & \frac{1}{2}\int_\Omega \frac{(-v_1^* + f)^2}{2v_0^* - K} \, dx \\ & + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx + \beta \int_\Omega v_0^* \, dx, \end{aligned} \tag{540}$$

if $v_0^* \in B^*$, where

$$B^* = \left\{ v_0^* \in Y^* \ : \ \|2v_0^*\|_\infty \leq \frac{K}{2} \right\}.$$

Finally, we define

$$A^+ = \{ u \in V \ : \ f \, u \geq 0, \text{ in } \Omega \},$$

$$V_1 = \left\{ u \in A^+ \ : \ \|u\|_\infty \leq \frac{3}{2} \right\},$$

$$D^+ = \left\{ v_1^* \in Y^* \ : \ f \, \frac{v_1^*}{-\gamma\nabla^2 + K} \geq 0, \text{ in } \Omega \right\},$$

$$D^* = \left\{ v^* \in D^+ \ : \ \left\| \frac{v_1^*}{-\gamma\nabla^2 + K} \right\|_\infty \leq \frac{3}{2} \right\}$$

and $J_2^* : D^* \times B^* \to \mathbb{R}$ by

$$J_2^*(v_1^*, v_0^*) = -F_1^*(v_1^*) - F_2^*(v_1^*, v_0^*).$$

Observe that the variation of J_2^* in v_1^* stands for

$$-\frac{v_1^*}{-\gamma\nabla^2 + K} + \frac{-v_1^* + f}{2v_0^* - K} = \mathbf{0}.$$

On the other hand, the variation of J_2^* in v_0^* stands for

$$\left(\frac{-v_1^* + f}{2v_0^* - K} \right)^2 - \frac{v_0^*}{\alpha} - \beta = \mathbf{0},$$

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so that

$$\left(\frac{v_1^*}{-\gamma\nabla^2+K}\right)^2-\frac{v_0^*}{\alpha}-\beta=\mathbf{0},$$

With such results in mind, we define the functional $J_3^*:D^*\times B^*\to\mathbb{R}$, by

$$\begin{aligned}&J_3^*(v_1^*,v_0^*)\\ =\;&J_2^*(v_1^*,v_0^*)\\ &+\frac{K_2}{2}\left\|-\frac{v_1^*}{-\gamma\nabla^2+K}+\frac{-v_1^*+f}{2v_0^*-K}\right\|_{0,2}^2\\ &+\frac{K_2}{2}\left\|\left(\frac{-v_1^*+f}{2v_0^*-K}\right)^2-\frac{v_0^*}{\alpha}-\beta\right\|_{0,2}^2\end{aligned}\tag{541}$$

Observe that for $K_2\gg K\gg\max\{1,\alpha,\beta,\gamma,1/\alpha,1/\gamma\}$ we have that J_3^* is convex in (v_1^*,v_0^*) on $D^*\times B^*$.

Let $(\hat{v}_1^*,\hat{v}_0^*)\in D^*\times B^*$ be such that

$$\delta J_3^*(\hat{v}_1^*,\hat{v}_0^*)=\mathbf{0}.$$

Let $u_0\in V$ be such that

$$u_0=\frac{\hat{v}_1^*}{-\gamma\nabla^2+K}$$

Similarly as in the previous sections, we may prove that

$$\delta J(u_0)=\mathbf{0},$$

and

$$J(u_0)=J_3^*(\hat{v}_1^*,\hat{v}_0^*).$$

so that from a concerning convexity,

$$J(u_0)=J_3^*(\hat{v}_1^*,\hat{v}_0^*)=\inf_{(v_1^*,v_0^*)\in D^*\times B^*}J_3^*(v_1^*,v_0^*).$$

Fix $\tilde{v}_1^*\in D^*$. Let $u\in V_1$ be such that

$$u=\frac{-\tilde{v}_1^*+f}{2\tilde{v}_0^*-K}$$

where $\tilde{v}_0^*\in B^*$ is such that

$$\tilde{v}_0^*=\alpha(u^2-\beta).$$

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From these results and definitions we may obtain

$$\begin{aligned}
J(u_0) &= J_3^*(\hat{v}_1^*, \hat{v}_0^*) \\
&= \inf_{(v_1^*, v_0^*) \in D^* \times B^*} J_3^*(v_1^*, v_0^*) \\
&\leq J_3^*(\tilde{v}_1^*, \tilde{v}_0^*) \\
&= -F_1^*(\tilde{v}_1^*) + \langle u, \tilde{v}_1^* \rangle_{L^2} \\
&\quad + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2} - \frac{K}{2} \int_\Omega u^2 \, dx \\
&\quad + \frac{K_2}{2} \left\| \frac{-\gamma \nabla^2 u + 2\tilde{v}_0^* u - f}{-\gamma \nabla^2 + K} \right\|_{0,2}^2 \\
&\leq F_1(u) + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2} - \frac{K}{2} \int_\Omega u^2 \, dx \\
&\quad + \frac{K_2}{2} \left\| \frac{-\gamma \nabla^2 u + 2\tilde{v}_0^* u - f}{-\gamma \nabla^2 + K} \right\|_{0,2}^2 \\
&= \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2} \\
&\quad + \frac{K_2}{2} \left\| \frac{-\gamma \nabla^2 u + 2\tilde{v}_0^* u - f}{-\gamma \nabla^2 + K} \right\|_{0,2}^2 \\
&= J(u) + \frac{K_2}{2} \left\| \frac{-\gamma \nabla^2 u + 2\alpha(u^2 - \beta) u - f}{-\gamma \nabla^2 + K} \right\|_{0,2}^2 .
\end{aligned} \tag{542}$$

Since

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha(u_0^2 - \beta) u_0 - f = \mathbf{0},$$

joining the pieces we have obtained

$$\begin{aligned}
J(u_0) &= \inf_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \left\| \frac{-\gamma \nabla^2 u + 2\alpha(u^2 - \beta) u - f}{-\gamma \nabla^2 + K} \right\|_{0,2}^2 \right\} \\
&= J_3^*(\hat{v}_1^*, \hat{v}_0^*) \\
&= \inf_{(v_1^*, v_0^*) \in D^* \times B^*} J_3^*(v_1^*, v_0^*).
\end{aligned} \tag{543}$$

The main objective of this section is complete.

73. Conclusion

In the first part of this article we have developed a relaxation proposal and duality principles suitable for a large class of models in physics and engineering.

In a second part we develop duality principles for the quasi-convex envelop of some vectorial models in the calculus of variations.

We highlight such dual variational formulations established are in general convex (in fact concave).

Finally, in the last sections, we develop mathematical models for some types of chemical reactions, including the hydrogen nuclear fusion and the water hydrolysis. Among such results, we highlight our proposal of modeling the Ginzburg-Landau theory in super-conductivity as a two-phase eigenvalue approach.

Data Availability: Details on the software for numerical results avaialable upon request.

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