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Not peer-reviewed version

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Posted Date: 4 January 2023

doi: 10.20944/preprints202210.0091.v10

Keywords: Duality principles; Generalized method of lines; Ginzburg-Landau type equations



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Article

Dual Variational Formulations for a Large Class of Non-Convex Models in the Calculus of Variations

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Abstract: This article develops dual variational formulations for a large class of models in variational optimization. The results are established through basic tools of functional analysis, convex analysis and duality theory. The main duality principle is developed as an application to a Ginzburg-Landau type system in superconductivity in the absence of a magnetic field. In the first sections, we develop new general dual convex variational formulations, more specifically, dual formulations with a large region of convexity around the critical points which are suitable for the non-convex optimization for a large class of models in physics and engineering. Finally, in the last section we present some numerical results concerning the generalized method of lines applied to a Ginzburg-Landau type equation.

1. Introduction

In this section we establish a dual formulation for a large class of models in non-convex optimization.

The main duality principle is applied to the Ginzburg-Landau system in superconductivity in an absence of a magnetic field.

Such results are based on the works of J.J. Telega and W.R. Bielski [2,3,13,14] and on a D.C. optimization approach developed in Toland [15].

About the other references, details on the Sobolev spaces involved are found in [1]. Related results on convex analysis and duality theory are addressed in [5–7,9,12]. Finally, similar models on the superconductivity physics may be found in [4,11].

Remark 1. It is worth highlighting, we may generically denote

$$\int_{\Omega} [(-\gamma \nabla^2 + KI_d)^{-1} v^*] v^* dx$$

simply by

$$\int_{\Omega} \frac{(v^*)^2}{-\gamma \nabla^2 + K} \, dx,$$

where I_d denotes a concerning identity operator.

Other similar notations may be used along this text as their indicated meaning are sufficiently clear.

Also, ∇^2 denotes the Laplace operator and for real constants $K_2 > 0$ and $K_1 > 0$, the notation $K_2 \gg K_1$ means that $K_2 > 0$ is much larger than $K_1 > 0$.

Finally, 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 (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 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*

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

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

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

Firstly we emphasize that, for the Banach space $Y = Y^* = L^2(\Omega)$, we have

$$\langle v, v^* \rangle_{L^2} = \int_{\Omega} v \ v^* \ dx, \ \forall v, v^* \in L^2(\Omega).$$

For the primal formulation we consider the functional $J: U \to \mathbb{R}$ where

$$J(u) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2}.$$
(3)

Here we assume $\alpha > 0, \beta > 0, \gamma > 0, U = W_0^{1,2}(\Omega), f \in L^2(\Omega)$. Moreover we denote

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

Define also $G_1: U \to \mathbb{R}$ by

$$G_1(u) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx,$$

 $G_2: U \times Y \to \mathbb{R}$ by

$$G_2(u,v) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta + v)^2 dx + \frac{K}{2} \int_{\Omega} u^2 dx,$$

and $F: U \to \mathbb{R}$ by

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

where $K \gg \gamma$.

It is worth highlighting that in such a case

$$J(u) = G_1(u) + G_2(u,0) - F(u) - \langle u, f \rangle_{L^2}, \ \forall u \in U.$$

Furthermore, define the following specific polar functionals specified, namely, $G_1^*:[Y^*]^2 \to \mathbb{R}$ by

$$G_1^*(v_1^* + z^*) = \sup_{u \in U} \{ \langle u, v_1^* + z^* \rangle_{L^2} - G_1(u) \}$$

$$= \frac{1}{2} \int_{\Omega} [(-\gamma \nabla^2)^{-1} (v_1^* + z^*)] (v_1^* + z^*) dx, \tag{4}$$

$$G_2^*: [Y^*]^2 \to \mathbb{R}$$
 by

$$G_{2}^{*}(v_{2}^{*}, v_{0}^{*}) = \sup_{(u,v) \in U \times Y} \{\langle u, v_{2}^{*} \rangle_{L^{2}} + \langle v, v_{0}^{*} \rangle_{L^{2}} - G_{2}(u,v)\}$$

$$= \frac{1}{2} \int_{\Omega} \frac{(v_{2}^{*})^{2}}{2v_{0}^{*} + K} dx$$

$$+ \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} dx + \beta \int_{\Omega} v_{0}^{*} dx, \qquad (5)$$

if $v_0^* \in B^*$ where

$$B^* = \{v_0^* \in Y^* : 2v_0^* + K > K/2 \text{ in } \Omega\}.$$

At this point, we give more details about this calculation.

Observe that

$$G_{2}^{*}(v_{2}^{*}, v_{0}^{*}) = \sup_{(u,v) \in U \times Y} \left\{ \langle u, v_{2}^{*} \rangle_{L^{2}} + \langle v, v_{0}^{*} \rangle_{L^{2}} - G_{2}(u,v) \right\}$$

$$= \sup_{(u,v) \in U \times Y} \left\{ \langle u, v_{2}^{*} \rangle_{L^{2}} + \langle v, v_{0}^{*} \rangle_{L^{2}} - \frac{\alpha}{2} \int_{\Omega} (u^{2} - \beta + v)^{2} dx - \frac{K}{2} \int_{\Omega} u^{2} dx \right\}. \quad (6)$$

Defining $w = u^2 - \beta + v$, we have $v = w - u^2 + \beta$, so that

$$G_{2}^{*}(v_{2}^{*}, v_{0}^{*})$$

$$= \sup_{(u,v)\in U\times Y} \left\{ \langle u, v_{2}^{*} \rangle_{L^{2}} + \langle v, v_{0}^{*} \rangle_{L^{2}} - \frac{\alpha}{2} \int_{\Omega} (u^{2} - \beta + v)^{2} dx - \frac{K}{2} \int_{\Omega} u^{2} dx \right\}$$

$$= \sup_{(u,w)\in U\times Y} \left\{ \langle u, v_{2}^{*} \rangle_{L^{2}} + \langle w - u^{2} + \beta, v_{0}^{*} \rangle_{L^{2}} - \frac{\alpha}{2} \int_{\Omega} (w)^{2} dx - \frac{K}{2} \int_{\Omega} u^{2} dx \right\}$$

$$= \langle \tilde{u}, v_{2}^{*} \rangle_{L^{2}} + \langle \tilde{w} - \tilde{u}^{2} + \beta, v_{0}^{*} \rangle_{L^{2}} - \frac{\alpha}{2} \int_{\Omega} (\tilde{w})^{2} dx - \frac{K}{2} \int_{\Omega} \tilde{u}^{2} dx, \tag{7}$$

where (\tilde{u}, \tilde{w}) are solution of equations (optimality conditions for such a quadratic optimization problem)

$$v_0^* - \alpha \tilde{w} = 0,$$

and

$$v_2^* - (2v_0^* + K)\tilde{u} = 0,$$

and therefore

$$\tilde{w} = \frac{v_0^*}{\alpha}$$
,

and

$$\tilde{u} = \frac{v_2^*}{2v_0^* + K}.$$

Replacing such results into (7) we obtain

$$G^{*}(v_{1}^{*}, v_{0}^{*}) = \frac{1}{2} \int_{\Omega} \frac{(v_{2}^{*})^{2}}{2v_{0}^{*} + K} dx + \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} dx + \beta \int_{\Omega} v_{0}^{*} dx,$$
 (8)

if $v_0^* \in B^*$.

Finally, $F^*: Y^* \to \mathbb{R}$ is defined by

$$F^{*}(z^{*}) = \sup_{u \in U} \{\langle u, z^{*} \rangle_{L^{2}} - F(u) \}$$
$$= \frac{1}{2K} \int_{\Omega} (z^{*})^{2} dx. \tag{9}$$

Define also

$$A^* = \{v^* = (v_1^*, v_2^*, v_0^*) \in [Y^*]^2 \times B^* : v_1^* + v_2^* - f = 0, \text{ in } \Omega\},$$

 $J^*: [Y^*]^4 \to \mathbb{R}$ by

$$J^*(v^*, z^*) = -G_1^*(v_1^* + z^*) - G_2^*(v_2^*, v_0^*) + F^*(z^*)$$

and $J_1^*: [Y^*]^4 \times U \to \mathbb{R}$ by

$$J_1^*(v^*, z^*, u) = J^*(v^*, z^*) + \langle u, v_1^* + v_2^* - f \rangle_{I^2}.$$

2. The Main Duality Principle, a Convex Dual Formulation and the Concerning Proximal Primal Functional

Our main result is summarized by the following theorem.

Theorem 1. Considering the definitions and statements in the last section, suppose also $(\hat{v}^*, \hat{z}^*, u_0) \in [Y^*]^2 \times B^* \times Y^* \times U$ is such that

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

Under such hypotheses, we have

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

$$\hat{v}^* \in A^*$$

and

$$J(u_0) = \inf_{u \in U} \left\{ J(u) + \frac{K}{2} \int_{\Omega} |u - u_0|^2 dx \right\}$$

= $J^*(\hat{v}^*, \hat{z}^*)$
= $\sup_{v^* \in A^*} \left\{ J^*(v^*, \hat{z}^*) \right\}.$ (10)

Proof. Since

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

from the variation in v_1^* we obtain

$$-\frac{(\hat{v}_1^*+\hat{z}^*)}{-\gamma\nabla^2}+u_0=0 \text{ in } \Omega,$$

so that

$$\hat{v}_1^* + \hat{z}^* = -\gamma \nabla^2 u_0.$$

From the variation in v_2^* we obtain

$$-\frac{\hat{v}_2^*}{2\hat{v}_0^* + K} + u_0 = 0$$
, in Ω .

From the variation in v_0^* we also obtain

$$\frac{(\hat{v}_2^*)^2}{(2\hat{v}_0^* + K)^2} - \frac{\hat{v}_0^*}{\alpha} - \beta = 0$$

and therefore,

$$\hat{v}_0^* = \alpha(u_0^2 - \beta).$$

From the variation in u we get

$$\hat{v}_{1}^{*} + \hat{v}_{2}^{*} - f = 0$$
, in Ω

and thus

$$\hat{v}^* \in A^*$$
.

Finally, from the variation in z^* , we obtain

$$-\frac{(\hat{v}_1^*+\hat{z}^*)}{-\gamma\nabla^2}+\frac{\hat{z}^*}{K}=0, \text{ in } \Omega.$$

so that

$$-u_0 + \frac{\hat{z}^*}{K} = 0,$$

that is,

$$\hat{z}^* = Ku_0 \text{ in } \Omega.$$

From such results and $\hat{v}^* \in A^*$ we get

$$0 = \hat{v}_1^* + \hat{v}_2^* - f$$

= $-\gamma \nabla^2 u_0 - \hat{z}^* + 2(v_0^*)u_0 + Ku_0 - f$
= $-\gamma \nabla^2 u_0 + 2\alpha (u_0^2 - \beta)u_0 - f$, (11)

so that

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

Also from this and from the Legendre transform proprieties we have

$$G_1^*(\hat{v}_1^* + \hat{z}^*) = \langle u_0, \hat{v}_1^* + \hat{z}^* \rangle_{L^2} - G_1(u_0),$$

$$G_2^*(\hat{v}_2^*, \hat{v}_0^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} + \langle 0, v_0^* \rangle_{L^2} - G_2(u_0, 0),$$

$$F^*(\hat{z}^*) = \langle u_0, \hat{z}^* \rangle_{L^2} - F(u_0)$$

and thus we obtain

$$J^{*}(\hat{\sigma}^{*}, \hat{z}^{*}) = -G_{1}^{*}(\hat{\sigma}_{1}^{*} + \hat{z}^{*}) - G_{2}^{*}(\hat{\sigma}_{2}^{*}, \hat{\sigma}_{0}^{*}) + F^{*}(\hat{z}^{*})$$

$$= -\langle u_{0}, \hat{\sigma}_{1}^{*} + \hat{\sigma}_{2}^{*} \rangle + G_{1}(u_{0}) + G_{2}(u_{0}, 0) - F(u_{0})$$

$$= -\langle u_{0}, f \rangle_{L^{2}} + G_{1}(u_{0}) + G_{2}(u_{0}, 0) - F(u_{0})$$

$$= J(u_{0}). \tag{12}$$

Summarizing, we have got

$$J^*(\hat{v}^*, \hat{z}^*) = J(u_0). \tag{13}$$

On the other hand

$$J^{*}(\hat{v}^{*}, \hat{z}^{*}) = -G_{1}^{*}(\hat{v}_{1}^{*} + \hat{z}^{*}) - G_{2}^{*}(\hat{v}_{2}^{*}, \hat{v}_{0}^{*}) + F^{*}(\hat{z}^{*})$$

$$\leq -\langle u, \hat{v}_{1}^{*} + \hat{z}^{*} \rangle_{L^{2}} - \langle u, \hat{v}_{2}^{*} \rangle_{L^{2}} - \langle 0, v_{0}^{*} \rangle_{L^{2}} + G_{1}(u) + G_{2}(u, 0) + F^{*}(\hat{z}^{*})$$

$$= -\langle u, f \rangle_{L^{2}} + G_{1}(u) + G_{2}(u, 0) - \langle u, \hat{z}^{*} \rangle_{L^{2}} + F^{*}(\hat{z}^{*})$$

$$= -\langle u, f \rangle_{L^{2}} + G_{1}(u) + G_{2}(u, 0) - F(u) + F(u) - \langle u, \hat{z}^{*} \rangle_{L^{2}} + F^{*}(\hat{z}^{*})$$

$$= J(u) + \frac{K}{2} \int_{\Omega} u^{2} dx - \langle u, \hat{z}^{*} \rangle_{L^{2}} + F^{*}(\hat{z}^{*})$$

$$= J(u) + \frac{K}{2} \int_{\Omega} u^{2} dx - K\langle u, u_{0} \rangle_{L^{2}} + \frac{K}{2} \int_{\Omega} u_{0}^{2} dx$$

$$= J(u) + \frac{K}{2} \int_{\Omega} |u - u_{0}|^{2} dx, \ \forall u \in U.$$

$$(14)$$

Finally by a simple computation we may obtain the Hessian

$$\left\{\frac{\partial^2 J^*(v^*,z^*)}{\partial (v^*)^2}\right\} < \mathbf{0}$$

in $[Y^*]^2 \times B^* \times Y^*$, so that we may infer that J^* is concave in v^* in $[Y^*]^2 \times B^* \times Y^*$.

Therefore, from this, (13) and (14), we have

$$J(u_0) = \inf_{u \in U} \left\{ J(u) + \frac{K}{2} \int_{\Omega} |u - u_0|^2 dx \right\}$$

$$= J^*(\hat{v}^*, \hat{z}^*)$$

$$= \sup_{v^* \in A^*} \left\{ J^*(v^*, \hat{z}^*) \right\}.$$
 (15)

The proof is complete. \Box

3. A Primal Dual Variational Formulation

In this section we develop a more general primal dual variational formulation suitable for a large class of models in non-convex optimization.

Consider again $U=W_0^{1,2}(\Omega)$ and let $G:U\to\mathbb{R}$ and $F:U\to\mathbb{R}$ be three times Fréchet differentiable functionals. Let $J:U\to\mathbb{R}$ be defined by

$$J(u) = G(u) - F(u), \ \forall u \in U.$$

Assume $u_0 \in U$ is such that

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

and

$$\delta^2 I(u_0) > 0$$
.

Denoting $v^* = (v_1^*, v_2^*)$, define $J^* : U \times Y^* \times Y^* \to \mathbb{R}$ by

$$J^*(u, v^*) = \frac{1}{2} \|v_1^* - G'(u)\|_2^2 + \frac{1}{2} \|v_2^* - F'(u)\|_2^2 + \frac{1}{2} \|v_1^* - v_2^*\|_2^2$$
(16)

Denoting $L_1^*(u, v^*) = v_1^* - G'(u)$ and $L_2^*(u, v^*) = v_2^* - F'(u)$, define also

$$C^* = \left\{ (u, v^*) \in U \times Y^* \times Y^* : \|L_1^*(u, v_1^*)\|_{\infty} \le \frac{1}{K} \text{ and } \|L_2^*(u, v_1^*)\|_{\infty} \le \frac{1}{K} \right\},$$

for an appropriate K > 0 to be specified.

Observe that in C^* the Hessian of J^* is given by

$$\{\delta^{2}J^{*}(u,v^{*})\} = \left\{ \begin{array}{ccc} G''(u)^{2} + F''(u)^{2} + \mathcal{O}(1/K) & -G''(u) & -F''(u) \\ -G''(u) & 2 & -1 \\ -F''(u) & -1 & 2 \end{array} \right\}, \tag{17}$$

Observe also that

$$\det\left\{\frac{\partial^2 J^*(u,v^*)}{\partial v_1^*\partial v_2^*}\right\} = 3,$$

and

$$\det\{\delta^2 J^*(u,v^*)\} = (G''(u) - F''(u))^2 + \mathcal{O}(1/K) = (\delta^2 J(u))^2 + \mathcal{O}(1/K).$$

Define now

$$\hat{v}_1^* = G'(u_0),$$

 $\hat{v}_2^* = F'(u_0),$

so that

$$\hat{v}_1^* - \hat{v}_2^* = \mathbf{0}.$$

From this we may infer that $(u_0, \hat{v}_1^*, \hat{v}_2^*) \in C^*$ and

$$J^*(u_0, \hat{v}^*) = 0 = \min_{(u, v^*) \in C^*} J^*(u, v^*).$$

Moreover, for K > 0 sufficiently big, J^* is convex in a neighborhood of (u_0, \hat{v}^*) . Therefore, in the last lines, we have proven the following theorem.

Theorem 2. Under the statements and definitions of the last lines, there exist $r_0 > 0$ and $r_1 > 0$ such that

$$J(u_0) = \min_{u \in B_{r_0}(u_0)} J(u)$$

and $(u_0, \hat{v}_1^*, \hat{v}_2^*) \in C^*$ is such that

$$J^*(u_0, \hat{v}^*) = 0 = \min_{(u, v^*) \in U \times [Y^*]^2} J^*(u, v^*).$$

Moreover, J^* is convex in

$$B_{r_1}(u_0, \hat{v}^*).$$

4. One More Duality Principle and a Concerning Primal Dual Variational Formulation

In this section we establish a new duality principle and a related primal dual formulation. The results are based on the approach of Toland, [15].

4.1. Introduction

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

Let $J: V \to \mathbb{R}$ be a functional such that

$$J(u) = G(u) - F(u), \forall u \in V,$$

where $V = W_0^{1,2}(\Omega)$.

Suppose *G*, *F* are both three times Fréchet differentiable convex functionals such that

$$\frac{\partial^2 G(u)}{\partial u^2} > 0$$

and

$$\frac{\partial^2 F(u)}{\partial u^2} > 0$$

 $\forall u \in V$.

Assume also there exists $\alpha_1 \in \mathbb{R}$ such that

$$\alpha_1 = \inf_{u \in V} J(u).$$

Moreover, suppose that if $\{u_n\} \subset V$ is such that

$$||u_n||_V \to \infty$$

then

$$J(u_n) \to +\infty$$
, as $n \to \infty$.

At this point we define $J^{**}: V \to \mathbb{R}$ by

$$J^{**}(u) = \sup_{(v^*,\alpha)\in H^*} \{\langle u,v^*\rangle + \alpha\},\,$$

where

$$H^* = \{ (v^*, \alpha) \in V^* \times \mathbb{R} : \langle v, v^* \rangle_V + \alpha \le F(v), \forall v \in V \}.$$

Observe that $(0, \alpha_1) \in H^*$, so that

$$J^{**}(u) \ge \alpha_1 = \inf_{u \in V} J(u).$$

On the other hand, clearly we have

$$J^{**}(u) \leq J(u), \forall u \in V,$$

so that we have got

$$\alpha_1 = \inf_{u \in V} J(u) = \inf_{u \in V} J^{**}(u).$$

Let $u \in V$.

Since *J* is strongly continuous, there exist $\delta > 0$ and A > 0 such that,

$$\alpha_1 \leq J^{**}(v) \leq J(v) \leq A, \forall v \in B_{\delta}(u).$$

From this, considering that J^{**} is convex on V, we may infer that J^{**} is continuous at u, $\forall u \in V$. Hence J^{**} is strongly lower semi-continuous on V, and since J^{**} is convex we may infer that J^{**} is weakly lower semi-continuous on V.

Let $\{u_n\} \subset V$ be a sequence such that

$$\alpha_1 \leq J(u_n) < \alpha_1 + \frac{1}{n}, \ \forall n \in \mathbb{N}.$$

Hence

$$\alpha_1 = \lim_{n \to \infty} J(u_n) = \inf_{u \in V} J(u) = \inf_{u \in V} J^{**}(u).$$

Suppose there exists a subsequence $\{u_{n_k}\}$ of $\{u_n\}$ such that

$$||u_{n_k}||_V \to \infty$$
, as $k \to \infty$.

From the hypothesis we have

$$J(u_{n_k}) \to +\infty$$
, as $k \to \infty$,

which contradicts

$$\alpha_1 \in \mathbb{R}$$
.

Therefore there exists K > 0 such that

$$||u_n||_V \leq K, \ \forall u \in V.$$

Since V is reflexive, from this and the Katutani Theorem, there exists a subsequence $\{u_{n_k}\}$ of $\{u_n\}$ and $u_0 \in V$ such that

$$u_{n_k} \rightharpoonup u_0$$
, weakly in V .

Consequently, from this and considering that J^{**} is weakly lower semi-continuous, we have got

$$\alpha_1 = \liminf_{k \to \infty} J^{**}(u_{n_k}) \ge J^{**}(u_0),$$

so that

$$J^{**}(u_0) = \min_{u \in V} J^{**}(u).$$

Define $G^*, F^*: V^* \to \mathbb{R}$ by

$$G^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - G(u)\},\,$$

and

$$F^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - F(u)\}.$$

Defining also $J^*: V \to \mathbb{R}$ by

$$I^*(v^*) = F^*(v^*) - G^*(v^*),$$

from the results in [15], we may obtain

$$\inf_{u \in V} J(u) = \inf_{v^* \in V^*} J^*(v^*),$$

so that

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

= $\inf_{u \in V} J(u) = \inf_{v^* \in V^*} J^*(v^*).$ (18)

Suppose now there exists $\hat{u} \in V$ such that

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

From the standard necessary conditions, we have

$$\delta I(\hat{u}) = \mathbf{0},$$

so that

$$\frac{\partial G(\hat{u})}{\partial u} - \frac{\partial F(\hat{u})}{\partial u} = \mathbf{0}.$$

Define now

$$v_0^* = \frac{\partial F(\hat{u})}{\partial u}.$$

From these last two equations we obtain

$$v_0^* = \frac{\partial G(\hat{u})}{\partial u}.$$

From such results and the Legendre transform properties, we have

$$\hat{u} = \frac{\partial F^*(v_0^*)}{\partial v^*},$$

$$\hat{u} = \frac{\partial G^*(v_0^*)}{\partial v^*},$$

so that

$$\delta J^*(v_0^*) = \frac{\partial F^*(v_0^*)}{\partial v^*} - \frac{\partial G^*(v_0^*)}{\partial v^*} = \hat{u} - \hat{u} = \mathbf{0},$$

$$G^*(v_0^*) = \langle \hat{u}, v_0^* \rangle_V - G(\hat{u})$$

and

$$F^*(v_0^*) = \langle \hat{u}, v_0^* \rangle_V - F(\hat{u})$$

so that

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

$$= G(\hat{u}) - F(\hat{u})$$

$$= \inf_{v^* \in V^*} J^*(v^*)$$

$$= F^*(v_0^*) - G^*(v_0^*)$$

$$= J^*(v_0^*). \tag{19}$$

4.2. The Main Duality Principle and a Related Primal Dual Variational Formulation

Considering these last statements and results, we may prove the following theorem.

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

Let $J: V \to \mathbb{R}$ be a functional such that

$$J(u) = G(u) - F(u), \forall u \in V,$$

where $V = W_0^{1,2}(\Omega)$.

Suppose G, F are both three times Fréchet differentiable functionals such that there exists K>0 such that

$$\frac{\partial^2 G(u)}{\partial u^2} + K > 0$$

and

$$\frac{\partial^2 F(u)}{\partial u^2} + K > 0$$

 $\forall u \in V$.

Assume also there exists $u_0 \in V$ and $\alpha_1 \in \mathbb{R}$ such that

$$\alpha_1 = \inf_{u \in V} J(u) = J(u_0).$$

Assume $K_3 > 0$ *is such that*

$$||u_0||_{\infty} < K_3.$$

Define

$$\tilde{V} = \{ u \in V : ||u||_{\infty} \le K_3 \}.$$

Assume $K_1 > 0$ is such that if $u \in \tilde{V}$ then

$$\max \left\{ \|F'(u)\|_{\infty}, \|G'(u)\|_{\infty}, \|F''(u)\|_{\infty}, \|F'''(u)\|_{\infty}, \|F'''(u)\|_{\infty}, \|G''(u)\|_{\infty}, \|G'''(u)\|_{\infty} \right\} \leq K_1.$$

Suppose also

$$K \gg \max\{K_1, K_3\}.$$

Define F_K , $G_K : V \to \mathbb{R}$ *by*

$$F_K(u) = F(u) + \frac{K}{2} \int_{\Omega} u^2 dx,$$

and

$$G_K(u) = G(u) + \frac{K}{2} \int_{\Omega} u^2 dx,$$

 $\forall u \in V.$

Define also G_K^* , $F_K^*: V^* \to \mathbb{R}$ *by*

$$G_K^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - G_K(u)\},\,$$

and

$$F_K^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - F_K(u)\}.$$

Observe that since $u_0 \in V$ *is such that*

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

we have

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

Let $\varepsilon > 0$ *be a small constant.*

Define

$$v_0^* = \frac{\partial F_K(u_0)}{\partial u} \in V^*.$$

Under such hypotheses, defining $J_1^*: V \times V^* \to \mathbb{R}$ *by*

$$J_{1}^{*}(u, v^{*}) = F_{K}^{*}(v^{*}) - G_{K}^{*}(v^{*}) + \frac{1}{2\varepsilon} \left\| \frac{\partial G_{K}^{*}(v^{*})}{\partial v^{*}} - u \right\|_{2}^{2} + \frac{1}{2\varepsilon} \left\| \frac{\partial F_{K}^{*}(v^{*})}{\partial v^{*}} - u \right\|_{2}^{2} + \frac{1}{2\varepsilon} \left\| \frac{\partial G_{K}^{*}(v^{*})}{\partial v^{*}} - \frac{\partial F_{K}^{*}(v^{*})}{\partial v^{*}} \right\|_{2}^{2},$$

$$(20)$$

we have

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

$$= \inf_{(u,v^*) \in V \times V^*} J_1^*(u,v^*)$$

$$= J_1^*(u_0,v_0^*).$$
(21)

Proof. Observe that from the hypotheses and the results and statements of the last subsection

$$J(u_0) = \inf_{u \in V} J(u) = \inf_{v^* \in Y^*} J_K^*(v^*) = J_K^*(v_0^*),$$

where

$$J_K^*(v^*) = F_K^*(v^*) - G_K^*(v^*), \forall v^* \in V^*.$$

Moreover we have

$$J_1^*(u, v^*) \ge J_K^*(v^*), \forall u \in V, v^* \in V^*.$$

Also from hypotheses and the last subsection results,

$$u_0 = \frac{\partial F_K^*(v_0^*)}{\partial v^*} = \frac{\partial G_K^*(v_0^*)}{\partial v^*},$$

so that clearly we have

$$J_1^*(u_0, v_0^*) = J_K^*(v_0^*).$$

From these last results, we may infer that

$$J(u_{0}) = \inf_{u \in V} J(u)$$

$$= \inf_{v^{*} \in V^{*}} J_{K}^{*}(v^{*})$$

$$= J_{K}^{*}(v_{0}^{*})$$

$$= \inf_{(u,v^{*}) \in V \times V^{*}} J_{1}^{*}(u,v^{*})$$

$$= J_{1}^{*}(u_{0},v_{0}^{*}). \tag{22}$$

The proof is complete.

Remark 2. At this point we highlight that J_1^* has a large region of convexity around the optimal point (u_0, v_0^*) , for K > 0 sufficiently large and corresponding $\varepsilon > 0$ sufficiently small.

Indeed, observe that for $v^* \in V^*$,

$$G_K^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - G_K(u)\} = \langle \hat{u}, v^* \rangle_V - G_K(\hat{u})$$

where $\hat{u} \in V$ is such that

$$v^* = \frac{\partial G_K(\hat{u})}{\partial u} = G'(\hat{u}) + K\hat{u}.$$

Taking the variation in v^* in this last equation, we obtain

$$1 = G''(u)\frac{\partial \hat{u}}{\partial v^*} + K\frac{\partial \hat{u}}{\partial v^*},$$

so that

$$\frac{\partial \hat{u}}{\partial v^*} = \frac{1}{G''(u) + K} = \mathcal{O}\left(\frac{1}{K}\right).$$

From this we get

$$\frac{\partial^2 \hat{u}}{\partial (v^*)^2} = -\frac{1}{(G''(u) + K)^2} G'''(u) \frac{\partial \hat{u}}{\partial v^*}$$

$$= -\frac{1}{(G''(u) + K)^3} G'''(u)$$

$$= \mathcal{O}\left(\frac{1}{K^3}\right). \tag{23}$$

On the other hand, from the implicit function theorem

$$\frac{\partial G_K^*(v^*)}{\partial v^*} = u + [v^* - G_K'(\hat{u})] \frac{\partial \hat{u}}{\partial v^*} = u,$$

so that

$$\frac{\partial^2 G_K^*(v^*)}{\partial (v^*)^2} = \frac{\partial \hat{u}}{\partial v^*} = \mathcal{O}\left(\frac{1}{K}\right)$$

and

$$\frac{\partial^3 G_K^*(v^*)}{\partial (v^*)^3} = \frac{\partial^2 \hat{u}}{\partial (v^*)^2} = \mathcal{O}\left(\frac{1}{K^3}\right).$$

Similarly, we may obtain

$$\frac{\partial^2 F_K^*(v^*)}{\partial (v^*)^2} = \mathcal{O}\left(\frac{1}{K}\right)$$

and

$$\frac{\partial^3 F_K^*(v^*)}{\partial (v^*)^3} = \mathcal{O}\left(\frac{1}{K^3}\right).$$

Denoting

$$A = \frac{\partial^2 F_K^*(v_0^*)}{\partial (v^*)^2}$$

and

$$B = \frac{\partial^2 G_K^*(v_0^*)}{\partial (v^*)^2},$$

we have

$$\begin{split} \frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial (v^*)^2} &= A - B + \frac{1}{\varepsilon} \left(2A^2 + 2B^2 - 2AB \right), \\ \frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial u^2} &= \frac{2}{\varepsilon}, \end{split}$$

and

$$\frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial (v^*)\partial u} = -\frac{1}{\varepsilon} (A+B).$$

From this we get

$$\det(\delta^{2}J^{*}(v_{0}^{*},u_{0})) = \frac{\partial^{2}J_{1}^{*}(u_{0},v_{0}^{*})}{\partial(v^{*})^{2}} \frac{\partial^{2}J_{1}^{*}(u_{0},v_{0}^{*})}{\partial u^{2}} - \left[\frac{\partial^{2}J_{1}^{*}(u_{0},v_{0}^{*})}{\partial(v^{*})\partial u}\right]^{2}$$

$$= 2\frac{A-B}{\varepsilon} + 2\frac{(A-B)^{2}}{\varepsilon^{2}}$$

$$= \mathcal{O}\left(\frac{1}{\varepsilon^{2}}\right)$$

$$\gg \mathbf{0}$$
(24)

about the optimal point (u_0, v_0^*) .

5. A Convex Dual Variational Formulation

In this section, again for $\Omega \subset \mathbb{R}^3$ an open, bounded, connected set with a regular (Lipschitzian) boundary $\partial\Omega$, $\gamma>0$, $\alpha>0$, $\beta>0$ and $f\in L^2(\Omega)$, we denote $F_1:V\times Y\to\mathbb{R}$, $F_2:V\to\mathbb{R}$ and $G:V\times Y\to\mathbb{R}$ by

$$F_{1}(u, v_{0}^{*}) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx - \frac{K}{2} \int_{\Omega} u^{2} \, dx + \frac{K_{1}}{2} \int_{\Omega} (-\gamma \nabla^{2} u + 2v_{0}^{*} u - f)^{2} \, dx + \frac{K_{2}}{2} \int_{\Omega} u^{2} \, dx,$$
(25)

$$F_2(u) = \frac{K_2}{2} \int_{\Omega} u^2 dx + \langle u, f \rangle_{L^2},$$

and

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

We define also

$$J_1(u, v_0^*) = F_1(u, v_0^*) - F_2(u) + G(u, 0),$$

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

and $F_1^*:[Y^*]^3\to\mathbb{R}$, $F_2^*:Y^*\to\mathbb{R}$, and $G^*:[Y^*]^2\to\mathbb{R}$, by

$$F_{1}^{*}(v_{2}^{*}, v_{1}^{*}, v_{0}^{*})$$

$$= \sup_{u \in V} \{\langle u, v_{1}^{*} + v_{2}^{*} \rangle_{L^{2}} - F_{1}(u, v_{0}^{*})\}$$

$$= \frac{1}{2} \int_{\Omega} \frac{(v_{1}^{*} + v_{2}^{*} + K_{1}(-\gamma \nabla^{2} + 2v_{0}^{*})f)^{2}}{(-\gamma \nabla^{2} - K + K_{2} + K_{1}(-\gamma \nabla^{2} + 2v_{0}^{*})^{2})} dx$$

$$- \frac{K_{1}}{2} \int_{\Omega} f^{2} dx, \qquad (26)$$

$$F_2^*(v_2^*) = \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \}$$

$$= \frac{1}{2K_2} \int_{\Omega} (v_2^*)^2 dx, \qquad (27)$$

and

$$G^{*}(v_{1}^{*}, v_{0}^{*}) = \sup_{(u,v) \in V \times Y} \{\langle u, v_{1}^{*} \rangle_{L^{2}} - \langle v, v_{0}^{*} \rangle_{L^{2}} - G(u,v)\}$$

$$= \frac{1}{2} \int_{\Omega} \frac{(v_{1}^{*})^{2}}{2v_{0}^{*} + K} dx + \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} dx$$

$$+\beta \int_{\Omega} v_{0}^{*} dx$$
(28)

if $v_0^* \in B^*$ where

$$B^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \le K/2 \text{ and } -\gamma \nabla^2 + 2v_0^* < -\varepsilon I_d\},$$

for some small real parameter $\varepsilon > 0$ and where I_d denotes a concerning identity operator.

Finally, we also define $J_1^*: [Y^*]^2 \times B^* \to \mathbb{R}$,

$$J_1^*(v_2^*, v_1^*, v_0^*) = -F_1^*(v_2^*, v_1^*, v_0^*) + F_2^*(v_2^*) - G^*(v_1^*, v_0^*).$$

Assuming

$$K_2 \gg K_1 \gg K \gg \max\{1/(\varepsilon^2), 1, \gamma, \alpha\}$$

by directly computing $\delta^2 J_1^*(v_2^*, v_1^*, v_0^*)$ we may obtain that for such specified real constants, J_1^* in convex in v_2^* and it is concave in (v_1^*, v_0^*) on $Y^* \times Y^* \times B^*$.

Considering such statements and definitions, we may prove the following theorem.

Theorem 4. Let $(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) \in Y^* \times Y^* \times B^*$ be such that

$$\delta J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}$$

and $u_0 \in V$ be such that

$$u_0 = \frac{\hat{v}_1^* + \hat{v}_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f}{K_2 - K - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2}.$$

Under such hypotheses, we have

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

so that

$$J(u_{0}) = \inf_{u \in V} \left\{ J(u) + \frac{K_{1}}{2} \int_{\Omega} (-\gamma \nabla^{2} u + 2\hat{v}_{0}^{*} u - f)^{2} dx \right\}$$

$$= \inf_{v_{2}^{*} \in Y^{*}} \left\{ \sup_{(v_{1}^{*}, v_{0}^{*}) \in Y^{*} \times B^{*}} J_{1}^{*}(v_{2}^{*}, v_{1}^{*}, v_{0}^{*}) \right\}$$

$$= J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{1}^{*}, \hat{v}_{0}^{*}). \tag{29}$$

Proof. Observe that $\delta J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}$ so that, since J_1^* is convex in v_2^* and concave in (v_1^*, v_0^*) on $Y^* \times Y^* \times B^*$, we obtain

$$J_1^*(\hat{v}_2^*,\hat{v}_1^*,\hat{v}_0^*) = \inf_{v_2^* \in Y^*} \left\{ \sup_{(v_1^*,v_0^*) \in Y^* \times B^*} J_1^*(v_2^*,v_1^*,v_0^*) \right\}.$$

Now we are going to show that

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

From

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*)}{\partial v_2^*} = \mathbf{0},$$

we have

$$-u_0 + \frac{\hat{v}_2^*}{K_2} = 0,$$

and thus

$$\hat{v}_2^* = K_2 u_0.$$

From

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*)}{\partial v_1^*} = \mathbf{0},$$

we obtain

$$-u_0 - \frac{\hat{v}_1^* - f}{2\hat{v}_0^* + K} = 0,$$

and thus

$$\hat{v}_1^* = -2\hat{v}_0^* u_0 - Ku_0 + f.$$

Finally, denoting

$$D = -\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f,$$

from

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*)}{\partial v_0^*} = \mathbf{0},$$

we have

$$-2Du_0 + u_0^2 - \frac{\hat{v}_0^*}{\alpha} - \beta = 0,$$

so that

$$\hat{v}_0^* = \alpha (u_0^2 - \beta - 2Du_0). \tag{30}$$

Observe now that

$$\hat{v}_1^* + \hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f = (K_2 - K - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2)u_0$$

so that

$$K_{2}u_{0} - 2\hat{v}_{0}u_{0} - Ku_{0} + f$$

$$= K_{2}u_{0} - Ku_{0} - \gamma \nabla^{2}u_{0} + K_{1}(-\gamma \nabla^{2} + 2\hat{v}_{0}^{*})(-\gamma \nabla^{2}u_{0} + 2\hat{v}_{0}^{*}u_{0} - f).$$
(31)

The solution for this last system of equations (30) and (31) is obtained through the relations

$$\hat{v}_0^* = \alpha(u_0^2 - \beta)$$

and

$$-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f = D = 0,$$

so that

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha (u_0^2 - \beta)u_0 - f = 0$$

and

$$\delta \left\{ J(u_0) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f)^2 dx \right\} = 0,$$

and hence, from the concerning convexity in u on V,

$$J(u_0) = \min_{u \in V} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\}.$$

Moreover, from the Legendre transform properties

$$F_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \langle u_0, \hat{v}_2^* + \hat{v}_1^* \rangle_{L^2} - F_1(u_0, \hat{v}_0^*),$$

$$F_2^*(\hat{v}_2^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_2(u_0),$$

$$G^*(\hat{v}_1^*, \hat{v}_0^*) = -\langle u_0, \hat{v}_1^* \rangle_{L^2} - \langle 0, \hat{v}_0^* \rangle_{L^2} - G(u_0, 0),$$

so that

$$J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{1}^{*}, \hat{v}_{0}^{*}) = -F_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{1}^{*}, \hat{v}_{0}^{*}) + F_{2}^{*}(\hat{v}_{2}^{*}) - G^{*}(\hat{v}_{1}^{*}, \hat{v}_{0}^{*})$$

$$= F_{1}(u_{0}, \hat{v}_{0}^{*}) - F_{2}(u_{0}) + G(u_{0}, 0)$$

$$= J(u_{0}). \tag{32}$$

Joining the pieces, we have got

$$J(u_{0}) = \inf_{u \in V} \left\{ J(u) + \frac{K_{1}}{2} \int_{\Omega} (-\gamma \nabla^{2} u + 2\hat{v}_{0}^{*} u - f)^{2} dx \right\}$$

$$= \inf_{v_{2}^{*} \in Y^{*}} \left\{ \sup_{(v_{1}^{*}, v_{0}^{*}) \in Y^{*} \times B^{*}} J_{1}^{*}(v_{2}^{*}, v_{1}^{*}, v_{0}^{*}) \right\}$$

$$= J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{1}^{*}, \hat{v}_{0}^{*}). \tag{33}$$

The proof is complete. \Box

Remark 3. We could have also defined

$$B^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \le K/2 \text{ and } -\gamma \nabla^2 + 2v_0^* > \varepsilon I_d\},$$

for some small real parameter $\varepsilon > 0$. In this case, $-\gamma \nabla^2 + 2v_0^*$ is positive definite, whereas in the previous case, $-\gamma \nabla^2 + 2v_0^*$ is negative definite.

6. Another Convex Dual Variational Formulation

In this section, again for $\Omega \subset \mathbb{R}^3$ an open, bounded, connected set with a regular (Lipschitzian) boundary $\partial\Omega$, $\gamma>0$, $\alpha>0$, $\beta>0$ and $f\in L^2(\Omega)$, we denote $F_1:V\times Y\to\mathbb{R}$, $F_2:V\to\mathbb{R}$ and $G:Y\to\mathbb{R}$ by

$$F_{1}(u, v_{0}^{*}) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}}$$

$$+ \frac{K_{1}}{2} \int_{\Omega} (-\gamma \nabla^{2} u + 2v_{0}^{*} u - f)^{2} \, dx + \frac{K_{2}}{2} \int_{\Omega} u^{2} \, dx,$$

$$F_{2}(u) = \frac{K_{2}}{2} \int_{\Omega} u^{2} \, dx + \langle u, f \rangle_{L^{2}},$$

$$G(u^{2}) = \frac{\alpha}{2} \int_{\Omega} (u^{2} - \beta)^{2} \, dx.$$
(34)

and

We define also

$$J_{1}(u, v_{0}^{*}) = F_{1}(u, v_{0}^{*}) - F_{2}(u) - \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} + G(u^{2}),$$

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

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

$$V_{2} = \{ u \in V : ||u||_{\infty} \le K_{3} \},$$

$$V_{1} = A^{+} \cap V_{1},$$

and $F_1^*: [Y^*]^2 \to \mathbb{R}$, $F_2^*: Y^* \to \mathbb{R}$, and $G^*: Y^* \to \mathbb{R}$, by

$$F_{1}^{*}(v_{2}^{*}, v_{0}^{*}) = \sup_{u \in V} \{\langle u, v_{2}^{*} \rangle_{L^{2}} - F_{1}(u, v_{0}^{*}) \}$$

$$= \frac{1}{2} \int_{\Omega} \frac{(v_{2}^{*} + K_{1}(-\gamma \nabla^{2} + 2v_{0}^{*})f)^{2}}{(-\gamma \nabla^{2} + 2v_{0}^{*} + K_{2} + K_{1}(-\gamma \nabla^{2} + 2v_{0}^{*})^{2})} dx$$

$$- \frac{K_{1}}{2} \int_{\Omega} f^{2} dx, \qquad (35)$$

$$F_2^*(v_2^*) = \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \}$$

= $\frac{1}{2K_2} \int_{\Omega} (v_2^* + f)^2 dx$, (36)

and

$$G^{*}(v_{0}^{*}) = \sup_{v \in Y} \{ \langle v, v_{0}^{*} \rangle_{L^{2}} - G(v) \}$$

$$= \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} dx + \beta \int_{\Omega} v_{0}^{*} dx$$
(37)

At this point we define

$$B_1^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \le K/2\},$$

$$B_2^* = \{v_0^* \in Y^* : -\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 > \mathbf{0}\},\$$

$$B_3^* = \{v_0^* \in Y^* : -1/\alpha + 4K_1[u(v_2^*, v_0^*)^2] + 100/K_2 \le \mathbf{0}, \forall v_2^* \in E_1^*\},$$

where

$$u(v_2^*, v_0^*) = \frac{\varphi_1}{\varphi},$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f)$$

and

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

Finally, we also define

$$E_1^* = \{v_2^* \in Y^* : \|v_2^*\|_{\infty} \le (5/4)K_2\}.$$

$$E_2^* = \{v_2^* \in Y^* \ : \ fv_2^* > 0, \text{ a.e. in } \Omega\},$$

$$E^* = E_1^* \cap E_2^*,$$

$$B^* = B_1^* \cap B_3^*$$
,

and $J_1^*: E^* \times B^* \to \mathbb{R}$, by

$$J_1^*(v_2^*, v_0^*) = -F_1^*(v_2^*, v_0^*) + F_2^*(v_2^*) - G^*(v_0^*).$$

Moreover, assume

$$K_2 \gg K_1 \gg K \gg K_3 \gg \max\{1, \gamma, \alpha\}.$$

By directly computing $\delta^2 J_1^*(v_2^*, v_0^*)$ we may obtain that for such specified real constants, J_1^* is concave in v_0^* on $E^* \times B^*$.

Indeed, recalling that

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f),$$

and

$$u=\frac{\varphi_1}{\varphi},$$

we obtain

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_2^*)^2} = 1/K_2 - 1/\varphi > \mathbf{0},$$

in $E^* \times B_3^*$ and

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} = 4u^2 K_1 - 1/\alpha + \mathcal{O}(1/K_2) < \mathbf{0},$$

in $E^* \times B^*$.

Considering such statements and definitions, we may prove the following theorem.

Theorem 5. Let $(\hat{v}_2^*, \hat{v}_0^*) \in E^* \times (B^* \cap B_2^*)$ be such that

$$\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \mathbf{0}$$

and $u_0 \in V_1$ be such that

$$u_0 = \frac{\hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f}{K_2 + 2\hat{v}_0^* - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2}.$$

Under such hypotheses, we have

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

so that

$$J(u_0) = \inf_{u \in V_1} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\}$$

$$= \inf_{v_2^* \in E^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(v_2^*, v_0^*) \right\}$$

$$= J_1^*(\hat{v}_2^*, \hat{v}_0^*). \tag{38}$$

Proof. Observe that $\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \mathbf{0}$ so that, since J_1^* concave in v_0^* on $E^* \times B^*$, $v_0^* \in B_2^*$ and J_1^* is quadratic in v_2^* , we get

$$\sup_{v_0^* \in B^*} J_1^*(\hat{v}_2^*, v_0^*) = J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \inf_{v_2^* \in E^*} J_1^*(v_2^*, \hat{v}_0^*).$$

Consequently, from this and the Min-Max Theorem, we obtain

$$J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \inf_{v_2^* \in E^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(v_2^*, v_0^*) \right\} = \sup_{v_0^* \in B^*} \left\{ \inf_{v_2^* \in E^*} J_1^*(v_2^*, v_0^*) \right\}.$$

Now we are going to show that

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

From

$$\frac{\partial J_1^*(\hat{v}_2^*,\hat{v}_0^*)}{\partial v_2^*}=\mathbf{0},$$

we have

$$-u_0 + \frac{\hat{v}_2^*}{K_2} = 0,$$

and thus

$$\hat{v}_2^* = K_2 u_0.$$

Finally, denoting

$$D = -\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f,$$

from

$$\frac{\partial J_1^*(\hat{v}_2^*,\hat{v}_0^*)}{\partial v_0^*}=\mathbf{0},$$

we have

$$-2Du_0 + u_0^2 - \frac{\hat{v}_0^*}{\alpha} - \beta = 0,$$

so that

$$\hat{v}_0^* = \alpha (u_0^2 - \beta - 2Du_0). \tag{39}$$

Observe now that

$$\hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f = (K_2 - \gamma \nabla^2 + 2\hat{v}_0^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2)u_0$$

so that

$$K_{2}u_{0} - 2\hat{v}_{0}u_{0} - Ku_{0} + f$$

$$= K_{2}u_{0} - Ku_{0} - \gamma \nabla^{2}u_{0} + K_{1}(-\gamma \nabla^{2} + 2\hat{v}_{0}^{*})(-\gamma \nabla^{2}u_{0} + 2\hat{v}_{0}^{*}u_{0} - f). \tag{40}$$

The solution for this last equation is obtained through the relation

$$-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f = D = 0,$$

so that from this and (49), we get

$$\hat{v}_0^* = \alpha (u_0^2 - \beta).$$

Thus,

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha (u_0^2 - \beta)u_0 - f = 0$$

and

$$\delta \left\{ J(u_0) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f)^2 dx \right\} = 0,$$

and hence, from the concerning convexity in u on V,

$$J(u_0) = \min_{u \in V} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\}.$$

Moreover, from the Legendre transform properties

$$F_1^*(\hat{v}_2^*, \hat{v}_0^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_1(u_0, \hat{v}_0^*),$$

$$F_2^*(\hat{v}_2^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_2(u_0),$$

$$G^*(\hat{v}_0^*) = \langle u_0^2, \hat{v}_0^* \rangle_{L^2} - G(u_0^2),$$

so that

$$J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{0}^{*}) = -F_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{0}^{*}) + F_{2}^{*}(\hat{v}_{2}^{*}) - G^{*}(\hat{v}_{0}^{*})$$

$$= F_{1}(u_{0}, \hat{v}_{0}^{*}) - F_{2}(u_{0}) - \langle u_{0}^{2}, \hat{v}_{0}^{*} \rangle_{L^{2}} + G(u_{0}^{2})$$

$$= J(u_{0}). \tag{41}$$

Joining the pieces, we have got

$$J(u_0) = \inf_{u \in V_1} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\}$$

$$= \inf_{v_2^* \in E^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(v_2^*, v_0^*) \right\}$$

$$= J_1^*(\hat{v}_2^*, \hat{v}_0^*). \tag{42}$$

The proof is complete.

7. A Third Duality Principle and Related Convex Dual Variational Formulation

In this section, we assume a finite dimensional version for the model in question, in a finite differences or finite elements context, although the concerning spaces and operators have not been relabeled.

Again, for $\Omega \subset \mathbb{R}^3$ an open, bounded, connected set with a regular (Lipschitzian) boundary $\partial\Omega$, $\gamma < 0$, $\alpha < 0$, $\beta > 0$, $K_2 < 0$ and $f \in L^2(\Omega)$, we denote $F_1 : V \times Y \to \mathbb{R}$, $F_2 : V \to \mathbb{R}$ and $G : Y \to \mathbb{R}$ by

$$F_{1}(u, v_{0}^{*}) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} + \frac{K_{1}}{2} \int_{\Omega} (-\gamma \nabla^{2} u + 2v_{0}^{*} u + f)^{2} \, dx + \frac{K_{2}}{2} \int_{\Omega} u^{2} \, dx,$$

$$(43)$$

$$F_2(u) = \frac{K_2}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

and

$$G(u^2) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx.$$

We define also

$$J_{1}(u, v_{0}^{*}) = F_{1}(u, v_{0}^{*}) - F_{2}(u) - \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} + G(u^{2}),$$

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

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

$$V_{2} = \{ u \in V : ||u||_{\infty} \le K_{3} \},$$

$$V_{1} = A^{-} \cap V_{1},$$

and $F_1^*: [Y^*]^2 \to \mathbb{R}$, $F_2^*: Y^* \to \mathbb{R}$, and $G^*: Y^* \to \mathbb{R}$, by

$$F_{1}^{*}(v_{2}^{*}, v_{0}^{*}) = \inf_{u \in V} \{ \langle u, v_{2}^{*} \rangle_{L^{2}} - F_{1}(u, v_{0}^{*}) \}$$

$$= \frac{1}{2} \int_{\Omega} \frac{(v_{2}^{*} - K_{1}(-\gamma \nabla^{2} + 2v_{0}^{*})f)^{2}}{(-\gamma \nabla^{2} + 2v_{0}^{*} + K_{2} + K_{1}(-\gamma \nabla^{2} + 2v_{0}^{*})^{2})} dx$$

$$- \frac{K_{1}}{2} \int_{\Omega} f^{2} dx, \qquad (44)$$

$$F_2^*(v_2^*) = \inf_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \}$$

= $\frac{1}{2K_2} \int_{\Omega} (v_2^* - f)^2 dx$, (45)

and

$$G^{*}(v_{0}^{*}) = \inf_{v \in Y} \{ \langle v, v_{0}^{*} \rangle_{L^{2}} - G(v) \}$$

$$= \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} dx + \beta \int_{\Omega} v_{0}^{*} dx$$
(46)

At this point we define

$$B_1^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \le K/2\},$$

$$B_2^* = \{v_0^* \in Y^* : -\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 > \mathbf{0}\},$$

$$B_3^* = \{v_0^* \in Y^* : -1/\alpha + 4K_1[u(v_2^*, v_0^*)^2] + 100/|K_2| > \mathbf{0}, \forall v_2^* \in E_1^*\},$$

where

$$u(v_2^*, v_0^*) = \frac{\varphi_1}{\varphi},$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f)$$

and

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

By direct computation we may obtain

$$\frac{\partial^2 [u(v_2^*,v_0^*)^2]}{\partial (v_0^*)^2} \geq \mathbf{0}, \forall v_0^* \in B^*, \forall v_2^* \in E_1^*$$

so that B_3^* is convex.

Finally, we also define

$$B_4^* = \{v_0^* \in Y^* : -[-\gamma \nabla^2 + 2v_0^*] \le -\varepsilon I_d\},$$
 $E_1^* = \{v_2^* \in Y^* : \|v_2^*\|_{\infty} \le (5/4)|K_2|\},$ $E_2^* = \{v_2^* \in Y^* : fv_2^* > 0, \text{ a.e. in } \Omega\},$ $E^* = E_1^* \cap E_2^*,$

And J_1^* by

$$J_1^*(v_2^*, v_0^*) = -F_1^*(v_2^*, v_0^*) + F_2^*(v_2^*) - G^*(v_0^*).$$

We assume $K_2 < 0$, and

$$|K_2| \gg K_1 \gg K \gg K_3 \gg \max\{|\alpha|, |\gamma|, \beta, 1/\epsilon^2\}.$$

Recalling that

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f),$$

and

$$u=\frac{\varphi_1}{\varphi},$$

we obtain

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_2^*)^2} = 1/K_2 - 1/\varphi > \mathbf{0},$$

in $E^* \times B_3^*$ and

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} = 4u^2 K_1 - 1/\alpha + \mathcal{O}(1/|K_2|).$$

Also,

$$\frac{\partial^{2} J_{1}^{*}(v_{2}^{*}, v_{0}^{*})}{\partial (v_{2}^{*})^{2}} \frac{\partial^{2} J_{1}^{*}(v_{2}^{*}, v_{0}^{*})}{\partial (v_{0}^{*})^{2}} - \frac{\partial^{2} J_{1}^{*}(v_{2}^{*}, v_{0}^{*})}{\partial v_{2}^{*} \partial v_{0}^{*}}$$

$$= \mathcal{O}\left(\frac{K_{1}^{2} A_{3} + K_{1} A_{4}}{-\alpha K_{2} \varphi}\right), \tag{47}$$

where

$$A_3 = 8\alpha (f^2 + 4f(-\gamma \nabla^2 + 2v_0^*)u + 3[(-\gamma \nabla^2 + 2v_0^*)u]^2$$

and

$$A_4 = (-\gamma \nabla^2 + 2v_0^*)^2 - 12\alpha[(-\gamma \nabla^2 + 2v_0^*)u]u.$$

Observe that at a critical point $A_3 = \mathbf{0}$ and $A_4 > \mathbf{0}$ so that, for the dual formulation, we set the restrictions $A_3 \ge 0$ and $A_4 \ge \varepsilon I_d$.

Thus, we define

$$B_5^* = \{v_0^* \in Y^* : A_3 \ge \mathbf{0} \text{ and } A_4 \ge \varepsilon I_d\},$$

and

$$B^* = B_1^* \cap B_2^* \cap B_3^* \cap B_4^* \cap B_5^*$$
.

Observe also that

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_1^*)^2} \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} - \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial v_2^* \partial v_0^*} > \mathbf{0},$$

on $B^* \times E^*$, so that J_1^* is convex on $E^* \times B^*$

Considering such statements and definitions, we may prove the following theorem.

Theorem 6. Let $(\hat{v}_2^*, \hat{v}_0^*) \in E^* \times B^*$ be such that

$$\delta J_1^*(\hat{v}_2^*,\hat{v}_0^*) = \mathbf{0}$$

and $u_0 \in V_1$ be such that

$$u_0 = \frac{\hat{v}_2^* - K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f}{K_2 + 2\hat{v}_0^* - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2}.$$

Under such hypotheses, we have

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

so that

$$J(u_0) = \sup_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\}$$

$$= \inf_{(v_2^*, v_0^*) \in E^* \times B^*} J_1^*(v_2^*, v_0^*)$$

$$= J_1^*(\hat{v}_2^*, \hat{v}_0^*). \tag{48}$$

Proof. Observe that $\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \mathbf{0}$ so that, since J_1^* convex on the convex set $E^* \times B^*$, we have that

$$J_1^*(\hat{v}_2^*,\hat{v}_0^*) = \inf_{(v_2^*,v_0^*) \in E^* \times B^*} J_1^*(v_2^*,v_0^*).$$

Now we are going to show that

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

From

$$\frac{\partial J_1^*(\hat{v}_2^*,\hat{v}_0^*)}{\partial v_2^*}=\mathbf{0},$$

we have

$$-u_0 + \frac{\hat{v}_2^*}{K_2} = 0,$$

and thus

$$\hat{v}_2^* = K_2 u_0.$$

Finally, denoting

$$D = -\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f,$$

from

$$\frac{\partial J_1^*(\hat{v}_2^*,\hat{v}_0^*)}{\partial v_0^*}=\mathbf{0},$$

we have

$$-2Du_0 + u_0^2 - \frac{\hat{v}_0^*}{\alpha} - \beta = 0,$$

so that

$$\hat{v}_0^* = \alpha (u_0^2 - \beta - 2Du_0). \tag{49}$$

Observe now that

$$\hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f = (K_2 - \gamma \nabla^2 + 2\hat{v}_0^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2)u_0$$

so that

$$K_2 u_0 - 2\hat{v}_0 u_0 - K u_0 + f$$

$$= K_2 u_0 - K u_0 - \gamma \nabla^2 u_0 + K_1 (-\gamma \nabla^2 + 2\hat{v}_0^*) (-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f).$$
(50)

The solution for this last equation is obtained through the relation

$$-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f = D = 0,$$

so that from this and (49), we get

$$\hat{v}_0^* = \alpha(u_0^2 - \beta).$$

Thus,

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha (u_0^2 - \beta) u_0 - f = 0$$

and

$$\delta \left\{ J(u_0) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\} = 0,$$

and hence, from the concerning cocavity in u on V,

$$J(u_0) = \min_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\}.$$

Moreover, from the Legendre transform properties

$$F_1^*(\hat{v}_2^*, \hat{v}_0^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_1(u_0, \hat{v}_0^*),$$

$$F_2^*(\hat{v}_2^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_2(u_0),$$

$$G^*(\hat{v}_0^*) = \langle u_0^2, \hat{v}_0^* \rangle_{L^2} - G(u_0^2),$$

so that

$$J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{0}^{*}) = -F_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{0}^{*}) + F_{2}^{*}(\hat{v}_{2}^{*}) - G^{*}(\hat{v}_{0}^{*})$$

$$= F_{1}(u_{0}, \hat{v}_{0}^{*}) - F_{2}(u_{0}) - \langle u_{0}^{2}, \hat{v}_{0}^{*} \rangle_{L^{2}} + G(u_{0}^{2})$$

$$= J(u_{0}). \tag{51}$$

Finally, observe that

$$J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{0}^{*}) \geq F_{1}(u, \hat{v}_{0}^{*}) - \langle u, \hat{v}_{2}^{*} \rangle_{L^{2}} + F_{2}^{*}(\hat{v}_{2}^{*}) - G^{*}(\hat{v}_{0}^{*})$$

$$\geq \inf_{v_{0}^{*} \in Y^{*}} \left\{ \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{K_{2}}{2} \int_{\Omega} u^{2} \, dx - \langle u, \hat{v}_{2}^{*} \rangle_{L^{2}} + F_{2}^{*}(\hat{v}_{2}^{*}) + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} - \frac{\alpha}{2} \int_{\Omega} (v_{0}^{*})^{2} \, dx - \beta \int_{\Omega} v_{0}^{*} \, dx \right\}$$

$$= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_{\Omega} (u^{2} - \beta)^{2} \, dx + \langle u, f \rangle_{L^{2}} + \frac{K_{2}}{2} \int_{\Omega} u^{2} \, dx - \langle u, K_{2} u_{0} \rangle_{L^{2}} + \frac{K_{2}}{2} \int_{\Omega} u_{0}^{2} \, dx$$

$$= J(u) + \frac{K_{2}}{2} \int_{\Omega} (u - u_{0})^{2} \, dx, \qquad (52)$$

 $\forall u \in V_1$ where we recall that $K_2 < 0$.

Joining the pieces, we have got

$$J(u_0) = \sup_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\}$$

$$= \inf_{(v_2^*, v_0^*) \in E^* \times B^*} J_1^* (v_2^*, v_0^*)$$

$$= J_1^* (\hat{v}_2^*, \hat{v}_0^*). \tag{53}$$

The proof is complete.

8. Closely Related Primal-Dual Variational Formulations

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

Observe that

$$J(u) = J(u) + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} - \langle u^{2}, v_{0}^{*} \rangle_{L^{2}}$$

$$= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} - \langle u, f \rangle_{L^{2}}$$

$$-\langle u^{2}, v_{0}^{*} \rangle_{L^{2}} + \frac{\alpha}{2} \int_{\Omega} (u^{2} - \beta)^{2} \, dx$$

$$\geq \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} - \langle u, f \rangle_{L^{2}}$$

$$+ \inf_{v \in Y} \left\{ -\langle v, v_{0}^{*} \rangle_{L^{2}} + \frac{\alpha}{2} \int_{\Omega} (v - \beta)^{2} \, dx \right\}$$

$$= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} - \langle u, f \rangle_{L^{2}}$$

$$-\frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} \, dx - \beta \int_{\Omega} v_{0}^{*} \, dx$$

$$= J_{1}(u, v_{0}^{*}). \tag{54}$$

Having obtained $J_1^*(u, v_0^*)$, we propose the following exactly penalized primal-dual formulation $J_2^*(u, v_0^*)$, where

$$J_2^*(u,v_0^*) = J_1^*(u,v_0^*) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2v_0^* u - f)^2 dx,$$

so that

$$J_{2}^{*}(u, v_{0}^{*}) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} - \langle u, f \rangle_{L^{2}}$$

$$- \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} \, dx - \beta \int_{\Omega} v_{0}^{*} \, dx$$

$$+ \frac{K_{1}}{2} \int_{\Omega} (-\gamma \nabla^{2} u + 2v_{0}^{*} u - f)^{2} \, dx,$$
(55)

In particular, if we set

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

and

$$K_1 = 1/(8K_3^2\alpha),$$

we may also define

$$J_3(u) = \sup_{v_0^* \in B^*} J_2^*(u, v_0^*),$$

where

$$B^* = \{ v_0^* \in Y^* : \|v_0^*\|_{\infty} \le K/8 \},$$

for appropriate K, $K_3 > 0$.

Here we highlight that J_2^* is concave in v_0^* on B^* (indeed it is concave on Y^*) and the parameter $K_1 > 0$ multiplying a positive definite quadratic functional in u improves the convexity conditions of J_3 .

9. One More Duality Principle Suitable for the Primal Formulation Global Optimization

In this section we establish one more duality principle and related convex dual formulation suitable for a global optimization of the primal variational formulation.

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

For the primal formulation, we define $V = W_0^{1,2}(\Omega)$ and consider a functional $J: V \to \mathbb{R}$ where

$$J(u) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 \, dx$$
$$-\langle u, f \rangle_{L^2}. \tag{56}$$

Here we assume $f \in L^2(\Omega)$, and define $Y = Y^* = L^2(\Omega)$

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

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

and

$$V_1^* = A^+ \cap V_1$$
,

for an appropriate constant $K_3 > 0$ to be specified.

Define also the functionals $F_1: V \to \mathbb{R}$, $F_2: V \times Y \to \mathbb{R}$ and $G: Y \to \mathbb{R}$ by

$$F_1(u) = \frac{K_2}{2} \int_{\Omega} (\nabla^2 u)^2 dx - \langle u, f \rangle_{L^2},$$

$$F_{2}(u, v_{3}^{*}, v_{0}^{*}) = -\frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx - \langle u^{2}, v_{0}^{*} \rangle_{L^{2}} + \frac{K_{2}}{2} \int_{\Omega} (\nabla^{2} u)^{2} \, dx - \frac{K_{1}}{2} \int_{\Omega} (-\gamma_{1} \nabla^{2} u + 2v_{3}^{*} u - h_{1})^{2} \, dx,$$

$$(57)$$

and

$$G(u^2) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx,$$

for appropriate positive constants K_1 , K_2 , K_3 to be specified.

Moreover, define $F_1^*: Y^* \to \mathbb{R}$, and $F_2^*: [Y^*]^2 \to \mathbb{R}$ and $G^*: Y^* \to \mathbb{R}$, by

$$F_1^*(v_2^*) = \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_1(u) \}$$

$$= \frac{1}{2K_2} \int_{\Omega} \frac{(v_2^* + f)^2}{\nabla^4} dx, \tag{58}$$

and

$$\begin{split} F_2^*(v_2^*, v_3^*, v_0^*) &= \sup_{u \in V} \{\langle u, v_2^* \rangle_{L^2} - F_2(u, v_3^*, v_0^*) \} \\ &= \frac{1}{2} \int_{\Omega} \frac{(v_2^* + K_1(-\gamma_1 \nabla^2 + 2v_3^*)h_1)^2}{K_2 \nabla^4 + \gamma \nabla^2 - 2v_0^* - K_1(-\gamma_1 \nabla^2 + 2v_3^*)^2} \\ &- \frac{K_1}{2} \int_{\Omega} h_1^2 \, dx \end{split}$$

for appropriate $\gamma_1 > 0$ and $H_1 \in L^2(\Omega)$, and

$$G^{*}(v_{0}^{*}) = \sup_{v \in Y} \{\langle v, v_{0}^{*} \rangle_{L^{2}} - G(v)\}$$
$$= \frac{1}{2\alpha} \int_{\Omega} (v_{0}^{*})^{2} dx + \beta \int_{\Omega} v_{0}^{*} dx.$$
 (59)

Furthermore, we define

$$D^* = \{ v_2^* \in Y^* : \|v_2^*\|_{\infty} \le (3/2)K_2 \},$$
$$B^* = \{ v_3^* \in Y^* : \|v_3^*\|_{\infty} \le K_4 \},$$

for an appropriate constant $K_4 > 0$ to be specified.

Define also

$$C_1^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \le K_4\}.$$

and $J_1^*: D^* \times C_1^* \to \mathbb{R}$ by

$$J_1^*(v_2^*, v_3^*, v_0^*) = -F_1^*(v_2^*) + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*).$$

Moreover, assuming $K_2 \gg K_1 \gg K_4 \gg \max\{1, K_3, \alpha, \beta, \gamma, \gamma_1, \|f\|_{\infty}, \|h_1\|_{\infty}\}$. By directly computing $\delta^2 J_1^*(v_2^*, v_3^*, v_0^*)$ denoting

$$A = -2K_1h_1,$$
 $B = 4K_1(-\gamma_1\nabla^2 + 2v_3^*),$
 $\varphi = -K_2\nabla^4 - \gamma\nabla^2 + 2v_0^* + K_1(-\gamma_1\nabla^2 + 2v_3^*)^2),$
 $\varphi_1 = v_2^* - K_1(-\gamma_1\nabla^2 + 2v_3^*)h_1,$
 $u = -\frac{\varphi_1}{\varphi},$

we may obtain, considering that $\varphi < 0$

$$\frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial (v_3^*)^2} = 4K_1u^2 - \frac{(A - uB)^2}{\varphi} > \mathbf{0}$$

on $D^* \times B^*$.

Moreover,

$$\frac{\partial^{2} J_{1}^{*}(v_{2}^{*}, v_{3}^{*}, v_{0}^{*})}{\partial (v_{2}^{*})^{2}} \frac{\partial^{2} J_{1}^{*}(v_{2}^{*}, v_{3}^{*}, v_{0}^{*})}{\partial (v_{3}^{*})^{2}} - \left(\frac{\partial^{2} J_{1}^{*}(v_{2}^{*}, v_{3}^{*}, v_{0}^{*})}{\partial v_{2}^{*} \partial v_{3}^{*}}\right)^{2}$$

$$= \mathcal{O}\left(\frac{K_{1}^{2} H_{1} + K_{1} H_{2}}{K_{2} \varphi}\right), \tag{60}$$

where

$$H_1 = (8(-h_1^2 + 4h_1(-\gamma_1\nabla^2 + 2v_3^*)u - 3[(-\gamma_1\nabla^2 + 2v_3^*)^2u]u),$$

and

$$H_2 = [(-\gamma \nabla^2 + 2v_0^*)u]u.$$

At a critical point we have $H_1 = \mathbf{0}$ and

$$H_2 = f u_0 > 0$$
, a.e in Ω.

With such results, we may define the restrictions

$$C_2^* = \{v_0^* \in Y^* : H_1(v_2^*, v_3^*, v_0^*) \ge 0, \ \forall v_2^* \in D^*, v_3^* \in B^*\}.$$

$$C_3^* = \{v_0^* \in Y^* : H_2(v_2^*, v_3^*, v_0^*) \ge 0, \forall v_2^* \in D^*, v_3^* \in B^*\}.$$

Here, we define $C^* = C_1^* \cap C_2^* \cap C_3^*$.

On the other hand, clearly we have

$$\frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial (v_0^*)^2} < \mathbf{0}$$

From such results, we may obtain that J_1^* in convex in (v_2^*, v_3^*) and it is concave in v_0^* on $D^* \times B^* \times C^*$.

The Main Duality Principle and a Related Convex Dual Formulation

Considering the statements and definitions presented in the previous section, we may prove the following theorem.

Theorem 7. Let $(\hat{v}_2^*, \hat{v}_3^* \hat{v}_0^*) \in D^* \times B^* \times C^*$ be such that

$$\delta J_1^*(\hat{v}_2^*,\hat{v}_3^*,\hat{v}_0^*)=\mathbf{0}$$

and $u_0 \in V_1$ be such that

$$u_0 = \frac{\partial F_1^*(\hat{v}_2^*)}{\partial v_2^*}.$$

Assume also

$$u_0 \neq 0$$
, a.e. in Ω .

Under such hypotheses, we have

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

$$-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1 = \mathbf{0},$$

and

$$J(u_0) = \inf_{u \in V_1} J(u)$$

$$= \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\}$$

$$= J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*). \tag{61}$$

Proof. Observe that $\delta J_1^*(\hat{v}_2^*,\hat{v}_3^*,\hat{v}_0^*)=\mathbf{0}$ so that, since J_1^* is convex in $(v_2^*,v_3^*)\in D^*\times B^*\times C^*$ and

$$\frac{\partial^2 J_1^*(\hat{v}_2^*,\hat{v}_3^*,v_0^*)}{\partial (v_0^*)^2} > \mathbf{0}, \ \forall v_0^* \in C_1^*,$$

we obtain

$$J_1^*(\hat{v}_2^*,\hat{v}_3^*,\hat{v}_0^*) = \inf_{(v_2^*,v_3^*) \in D^* \times B^*} J_1^*(v_2^*,v_3^*,\hat{v}_0^*) \sup_{v_0^* \in C^*} J_1^*(\hat{v}_2^*,\hat{v}_3^*,v_0^*).$$

Consequently, from this and the Saddle Point Theorem, we obtain

$$J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\}.$$

Now we are going to show that

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

From

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_2^*} = \mathbf{0},$$

and

$$\frac{\partial F_1^*(\hat{v}_2^*)}{\partial v_2^*} = u_0$$

we have

$$-\frac{\partial F_2^*(\hat{v}_2^*,\hat{v}_3^*,\hat{v}_0^*)}{\partial v_2^*} - u_0 = \mathbf{0}$$

and

$$\hat{v}_2^* = K_2 \nabla^4 u_0 - f.$$

Observe now that

$$F_2^*(\hat{v}_2^*, \hat{v}_3^*, v_0^*) = \sup_{u \in V} \{ -\langle u, v_2^* \rangle_{L^2} - F_2(u, v_3^*, v_0^*) \}.$$

Denoting

$$H(v_2^*, v_3^*, v_1^*, u) = \langle u, v_2^* \rangle_{L^2} - F_2(u, v_3^*, v_0^*),$$

there exists $\hat{u} \in V$ such that

$$\frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} = \mathbf{0},$$

and

$$F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u}),$$

so that

$$\frac{\partial F_{2}^{*}(\hat{v}_{2}^{*}, \hat{v}_{3}^{*}, \hat{v}_{0}^{*})}{\partial v_{2}^{*}} = \frac{\partial H(\hat{v}_{2}^{*}, \hat{v}_{3}^{*}, \hat{v}_{0}^{*}, \hat{u})}{\partial v_{2}^{*}} + \frac{\partial H(\hat{v}_{2}^{*}, \hat{v}_{3}^{*}, \hat{v}_{0}^{*}, \hat{u})}{\partial u} \frac{\partial \hat{u}}{\partial v_{2}^{*}} = \hat{u}.$$
(62)

Summarizing, we have got

$$u_0 = \frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_2^*} = \hat{u}.$$

From such results and the Legendre tranform proprieties we get

$$v_2^* = \frac{\partial F_1(u_0)}{\partial u}$$

and

$$v_2^* = \frac{\partial F_2(u_0, \hat{v}_3^*, \hat{v}_0^*)}{\partial u}.$$

On the other hand, from the variation of J_1^* in v_3^* , we have

$$\frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_3^*} \\
= -K_1(-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1) 2u_0 + \frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} \frac{\partial \hat{u}}{\partial v_3^*} \\
= -K_1(-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1) 2u_0 \\
= \mathbf{0}. \tag{63}$$

From such results, since

$$u_0 \neq 0$$
, a.e. in Ω ,

we get

$$-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1 = 0$$
, a.e. in Ω .

Finally, from the variation of J_1^* in v_0^* we obtain

$$\frac{\partial F_2^*(\hat{v}_2^*,\hat{v}_3^*,\hat{v}_0^*)}{\partial v_0^*} - \frac{\partial G^*(v_0^*)}{\partial v_0^*} = 0,$$

so that

$$u_0^2 + \frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} \frac{\partial \hat{u}}{\partial v_0^*} - \frac{v_0^*}{\alpha} - \beta = \mathbf{0}.$$

Thus,

$$v_0^* = \alpha(u_0^2 - \beta).$$

Consequently, from such last results, we have

$$\mathbf{0} = \hat{v}_{2}^{*} - \hat{v}_{2}^{*}
= \frac{\partial F_{1}(u_{0})}{\partial u} - \frac{\partial F_{2}(u_{0}, \hat{v}_{3}^{*}, \hat{v}_{0}^{*})}{\partial u}
= K_{2}\nabla^{4}u_{0} - f - K_{2}\nabla^{4}u_{0} - \gamma\nabla^{2}u_{0} + 2v_{0}^{*}u_{0}
= -\gamma\nabla^{2}u_{0} + 2\alpha(u_{0}^{2} - \beta)u_{0} - f
= \delta J(u_{0}).$$
(64)

Summarizing,

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

Furthermore, also from such last results and the Legendre transform properties, we have

$$F_1^*(\hat{v}_2^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_1(u_0),$$

$$F_2^*(\hat{v}_2^*, \hat{v}_3^* \hat{v}_0^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_2(u_0, \hat{v}_3^*, \hat{v}_0^*),$$

$$G^*(\hat{v}_0^*) = \langle u_0^2, v_0^* \rangle_{L^2} - G(u_0^2),$$

so that

$$J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)$$

$$= -F_1^*(\hat{v}_2^*) + F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) - G^*(\hat{v}_0^*)$$

$$= J(u_0). \tag{65}$$

Finally, observe that

$$J_1^*(v_2^*, v_3^*, v_0^*) \le F_1(u) - \langle u, v_2^* \rangle_{L^2} + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*),$$

 $\forall u \in V_1, \ v_2^* \in D^*, \ v_3^* \in B^*, \ v_0^* \in C^*.$

Therefore,

$$\sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \le \sup_{v_0^* \in C_1^*} \{ -\langle u, v_2^* \rangle_{L^2} + F_1(u) + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*) \},$$

so that

$$\inf_{\substack{(v_{2}^{*}, v_{3}^{*}) \in D^{*} \times B^{*} \\ (v_{0}^{*} \in C^{*})}} \left\{ \sup_{\substack{v_{0}^{*} \in C^{*} \\ v_{0}^{*} \in C^{*}}} J_{1}^{*}(v_{2}^{*}, v_{3}^{*}, v_{0}^{*}) \right\} \\
\leq \inf_{\substack{(v_{2}^{*}, v_{3}^{*}) \in D^{*} \times B^{*} \\ (v_{0}^{*} \in C_{1}^{*})}} \left\{ \sup_{\substack{v_{0}^{*} \in C_{1}^{*} \\ v_{0}^{*} \in C_{1}^{*}}} \left\{ -\langle u, v_{2}^{*} \rangle_{L^{2}} + F_{1}(u) + F_{2}^{*}(v_{2}^{*}, v_{3}^{*}, v_{0}^{*}) - G^{*}(v_{0}^{*}) \right\} \right\} \\
= J(u), \forall u \in V_{1}. \tag{66}$$

Summarizing, we have got

$$J_{1}^{*}(\hat{v}_{2}^{*}, \hat{v}_{3}^{*}, \hat{v}_{0}^{*}) = \inf_{\substack{(v_{2}^{*}, v_{3}^{*}) \in D^{*} \times B^{*} \\ u \in V_{1}}} \left\{ \sup_{v_{0}^{*} \in C^{*}} J_{1}^{*}(v_{2}^{*}, v_{3}^{*}, v_{0}^{*}) \right\}$$

$$\leq \inf_{u \in V_{1}} J(u).$$

$$(67)$$

Joining the pieces, we have got

$$J(u_0) = \inf_{u \in V_1} J(u)$$

$$= \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\}$$

$$= J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*). \tag{68}$$

The proof is complete.

10. A Related Numerical Computation through the Generalized Method of Lines

We start by recalling that the generalized method of lines was originally introduced in the book entitled "Topics on Functional Analysis, Calculus of Variations and Duality" [7], published in 2011.

Indeed, the present results are extensions and applications of previous ones which have been published since 2011, in books and articles such as [5,7–9]. About the Sobolev spaces involved we would mention [1]. Concerning the applications, related models in physics are addressed in [4,11].

We also emphasize that, in such a method, the domain of the partial differential equation in question is discretized in lines (or more generally, in curves) and the concerning solution is written on these lines as functions of boundary conditions and the domain boundary shape.

In fact, in its previous format, this method consists of an application of a kind of a partial finite differences procedure combined with the Banach fixed point theorem to obtain the relation between two adjacent lines (or curves).

In the present article, we propose an improvement concerning the way we truncate the series solution obtained through an application of the Banach fixed point theorem to find the relation between two adjacent lines. The results obtained are very good even as a typical parameter $\varepsilon > 0$ is very small.

In the next lines and sections we develop in details such a numerical procedure.

10.1. About a Concerning Improvement for the Generalized Method of Lines

Let $\Omega \subset \mathbb{R}^2$ where

$$\Omega = \{ (r, \theta) \in \mathbb{R}^2 : 1 \le r \le 2, 0 \le \theta \le 2\pi \}.$$

Consider the problem of solving the partial differential equation

$$\begin{cases}
-\varepsilon \left(\frac{\partial^{2} u}{\partial r^{2}} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^{2}} \frac{\partial^{2} u}{\partial \theta^{2}} \right) + \alpha u^{3} - \beta u = f, & \text{in } \Omega, \\
u = u_{0}(\theta), & \text{on } \partial \Omega_{1}, \\
u = u_{f}(\theta), & \text{on } \partial \Omega_{2}.
\end{cases} (69)$$

Here

$$\Omega = \{(r, \theta) \in \mathbb{R}^2 : 1 \le r \le 2, \ 0 \le \theta \le 2\pi\},$$

$$\partial \Omega_1 = \{(1, \theta) \in \mathbb{R}^2 : 0 \le \theta \le 2\pi\},$$

$$\partial \Omega_2 = \{(2, \theta) \in \mathbb{R}^2 : 0 \le \theta \le 2\pi\},$$

 $\varepsilon > 0$, $\alpha > 0$, $\beta > 0$, and $f \equiv 1$, on Ω .

In a partial finite differences scheme, such a system stands for

$$-\varepsilon\left(\frac{u_{n+1}-2u_n+u_{n-1}}{d^2}+\frac{1}{t_n}\frac{u_n-u_{n-1}}{d}+\frac{1}{t_n^2}\frac{\partial^2 u_n}{\partial \theta^2}\right)+\alpha u_n^3-\beta u_n=f_n,$$

 $\forall n \in \{1, \dots, N-1\}$, with the boundary conditions

$$u_0 = 0$$
,

and

$$u_N = 0.$$

Here *N* is the number of lines and d = 1/N.

In particular, for n = 1 we have

$$-\varepsilon \left(\frac{u_2 - 2u_1 + u_0}{d^2} + \frac{1}{t_1} \frac{(u_1 - u_0)}{d} + \frac{1}{t_1^2} \frac{\partial^2 u_1}{\partial \theta^2} \right) + \alpha u_1^3 - \beta u_1 = f_1,$$

so that

$$u_1 = \left(u_2 + u_1 + u_0 + \frac{1}{t_1}(u_1 - u_0) d + \frac{1}{t_1^2} \frac{\partial^2 u_1}{\partial \theta^2} d^2 + (-\alpha u_1^3 + \beta u_1 - f_1) \frac{d^2}{\varepsilon}\right) / 3.0,$$

We solve this last equation through the Banach fixed point theorem, obtaining u_1 as a function of u_2 .

Indeed, we may set

$$u_1^0 = u_2$$

and

$$u_1^{k+1} = \left(u_2 + u_1^k + u_0 + \frac{1}{t_1}(u_1^k - u_0) d + \frac{1}{t_1^2} \frac{\partial^2 u_1^k}{\partial \theta^2} d^2 + (-\alpha(u_1^k)^3 + \beta u_1^k - f_1) \frac{d^2}{\varepsilon}\right) / 3.0,$$
(70)

 $\forall k \in \mathbb{N}$.

Thus, we may obtain

$$u_1 = \lim_{k \to \infty} u_1^k \equiv H_1(u_2, u_0).$$

Similarly, for n = 2, we have

$$u_{2} = \left(u_{3} + u_{2} + H_{1}(u_{2}, u_{0}) + \frac{1}{t_{1}}(u_{2} - H_{1}(u_{2}, u_{0})) d + \frac{1}{t_{1}^{2}} \frac{\partial^{2} u_{2}}{\partial \theta^{2}} d^{2} + (-\alpha u_{2}^{3} + \beta u_{2} - f_{2}) \frac{d^{2}}{\varepsilon}\right) / 3.0,$$

$$(71)$$

We solve this last equation through the Banach fixed point theorem, obtaining u_2 as a function of u_3 and u_0 .

Indeed, we may set

$$u_2^0 = u_3$$

and

$$u_{2}^{k+1} = \left(u_{3} + u_{2}^{k} + H_{1}(u_{2}^{k}, u_{0}) + \frac{1}{t_{2}}(u_{2}^{k} - H_{1}(u_{2}^{k}, u_{0})) d + \frac{1}{t_{2}^{2}} \frac{\partial^{2} u_{2}^{k}}{\partial \theta^{2}} d^{2} + (-\alpha(u_{2}^{k})^{3} + \beta u_{2}^{k} - f_{2}) \frac{d^{2}}{\varepsilon}\right) / 3.0,$$

$$(72)$$

 $\forall k \in \mathbb{N}$.

Thus, we may obtain

$$u_2 = \lim_{k \to \infty} u_2^k \equiv H_2(u_3, u_0).$$

Now reasoning inductively, having

$$u_{n-1} = H_{n-1}(u_n, u_0),$$

we may get

$$u_{n} = \left(u_{n+1} + u_{n} + H_{n-1}(u_{n}, u_{0}) + \frac{1}{t_{n}}(u_{n} - H_{n-1}(u_{n}, u_{0})) d + \frac{1}{t_{n}^{2}} \frac{\partial^{2} u_{n}}{\partial \theta^{2}} d^{2} + (-\alpha u_{n}^{3} + \beta u_{n} - f_{n}) \frac{d^{2}}{\varepsilon}\right) / 3.0,$$

$$(73)$$

We solve this last equation through the Banach fixed point theorem, obtaining u_n as a function of u_{n+1} and u_0 .

Indeed, we may set

$$u_n^0 = u_{n+1}$$

and

$$u_n^{k+1} = \left(u_{n+1} + u_n^k + H_{n-1}(u_n^k, u_0) + \frac{1}{t_n}(u_n^k - H_{n-1}(u_n^k, u_0)) d + \frac{1}{t_n^2} \frac{\partial^2 u_n^k}{\partial \theta^2} d^2 + (-\alpha(u_n^k)^3 + \beta u_n^k - f_n) \frac{d^2}{\varepsilon}\right) / 3.0,$$

$$(74)$$

 $\forall k \in \mathbb{N}$.

Thus, we may obtain

$$u_n = \lim_{k \to \infty} u_n^k \equiv H_n(u_{n+1}, u_0).$$

We have obtained $u_n = H_n(u_{n+1}, u_0), \forall n \in \{1, \dots, N-1\}$. In particular, $u_N = u_f(\theta)$, so that we may obtain

$$u_{N-1} = H_{N-1}(u_N, u_0) = H_{N-1}(0) \equiv F_{N-1}(u_N, u_0) = F_{N-1}(u_f(\theta), u_0(\theta)).$$

Similarly,

$$u_{N-2} = H_{N-2}(u_{N-1}, u_0) = H_{N-2}(H_{N-1}(u_N, u_0)) = F_{N-2}(u_N, u_0) = F_{N-1}(u_f(\theta), u_0(\theta)),$$

an so on, up to obtaining

$$u_1 = H_1(u_2) \equiv F_1(u_N, u_0) = F_1(u_f(\theta), u_0(\theta)).$$

The problem is then approximately solved.

10.2. Software in Mathematica for Solving Such an Equation

We recall that the equation to be solved is a Ginzburg-Landau type one, where

$$\begin{cases}
-\varepsilon \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} \right) + \alpha u^3 - \beta u = f, & \text{in } \Omega, \\
u = 0, & \text{on } \partial \Omega_1, \\
u = u_f(\theta), & \text{on } \partial \Omega_2.
\end{cases} \tag{75}$$

Here

$$\begin{split} \Omega &= \{(r,\theta) \in \mathbb{R}^2 \ : \ 1 \leq r \leq 2, \ 0 \leq \theta \leq 2\pi\}, \\ \partial \Omega_1 &= \{(1,\theta) \in \mathbb{R}^2 \ : \ 0 \leq \theta \leq 2\pi\}, \\ \partial \Omega_2 &= \{(2,\theta) \in \mathbb{R}^2 \ : \ 0 \leq \theta \leq 2\pi\}, \end{split}$$

 $\varepsilon > 0$, $\alpha > 0$, $\beta > 0$, and $\beta = 1$, on Ω . In a partial finite differences scheme, such a system stands for

$$-\varepsilon\left(\frac{u_{n+1}-2u_n+u_{n-1}}{d^2}+\frac{1}{t_n}\frac{u_n-u_{n-1}}{d}+\frac{1}{t_n^2}\frac{\partial^2 u_n}{\partial \theta^2}\right)+\alpha u_n^3-\beta u_n=f_n,$$

 $\forall n \in \{1, \dots, N-1\}$, with the boundary conditions

$$u_0 = 0$$
,

and

$$u_N = u_f[x].$$

Here *N* is the number of lines and d = 1/N.

At this point we present the concerning software for an approximate solution.

Such a software is for N = 10 (10 lines) and $u_0[x] = 0$..

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***********
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```
1. m_8 = 10; (N = 10 lines)
 2. d = 1/m8;
 3. e_1 = 0.1; (\varepsilon = 0.1)
 4. A = 1.0;
 5. B = 1.0;
 6. For[i = 1, i < m8, i + +, f[i] = 1.0]; (f \equiv 1, \text{ on } \Omega)
 7. a = 0.0;
 8. For[i = 1, i < m8, i + +,
    Clear[b, u];
    t[i] = 1 + i * d;
    b[x_{-}] = u[i+1][x];
 9. For[k = 1, k < 30, k + +, \text{ (we have fixed the number of iterations)}]
    z = \left(u[i+1][x] + b[x] + a + \frac{1}{t[i]}(b[x] - a) * d\right)
    +\frac{1}{t[i]^2}D[b[x],\{x,2\}]*d^2+(-A*b[x]^3+B*u[x]+f[i])*\frac{d^2}{e_1} /3.0;
    Series[z, {u[i+1][x], 0,3}, {u[i+1]'[x], 0,1}, {u[i+1]''[x], 0,1},
    {u[i+1]'''[x],0,0}, {u[i+1]''''[x],0,0};
    z = Normal[z],
    z = Expand[z];
    b[x_{-}]=z];
10. a_1[i] = z;
11. Clear[b];
12. u[i+1][x_-] = b[x];
13. a = a_1[i];
14. b[x_{-}] = u_f[x];
15. For[i = 1, i < m8, i + +,
    A_1 = a_1[m8 - i];
    A_1 = Series[A_1, \{u_f[x], 0, 3\}, \{u_f'[x], 0, 1\}, \{u_f''[x], 0, 1\}, \{u_f'''[x], 0, 0\}, \{u_f''''[x], 0, 0\}];
    A_1 = Normal[A_1];
    A_1 = Expand[A_1];
    u[m8 - i][x_{-}] = A_1;
    b[x_{-}] = A_{1};
    Print[u[m8/2][x]];
```

The numerical expressions for the solutions of the concerning N=10 lines are given by

$$u[1][x] = 0.47352 + 0.00691u_f[x] - 0.00459u_f[x]^2 + 0.00265u_f[x]^3 + 0.00039(u_f'')[x] - 0.00058u_f[x](u_f'')[x] + 0.00050u_f[x]^2(u_f'')[x] - 0.000181213u_f[x]^3(u_f'')[x]$$
(76)

$$u[2][x] = 0.76763 + 0.01301u_f[x] - 0.00863u_f[x]^2 + 0.00497u_f[x]^3 + 0.00068(u_f'')[x] - 0.00103u_f[x](u_f'')[x] + 0.00088u_f[x]^2(u_f'')[x] - 0.00034u_f[x]^3(u_f'')[x]$$
(77)

$$u[3][x] = 0.91329 + 0.02034u_f[x] - 0.01342u_f[x]^2 + 0.00768u_f[x]^3 + 0.00095(u_f'')[x] - 0.00144u_f[x](u_f'')[x] + 0.00122u_f[x]^2(u_f'')[x] - 0.00051u_f[x]^3(u_f'')[x]$$
(78)

$$u[4][x] = 0.97125 + 0.03623u_f[x] - 0.02328u_f[x]^2 + 0.01289u_f[x]^3 + 0.00147331(u_f'')[x] - 0.00223u_f[x](u_f'')[x] + 0.00182u_f[x]^2(u_f'')[x] - 0.00074u_f[x]^3(u_f'')[x]$$
(79)

$$u[5][x] = 1.01736 + 0.09242u_f[x] - 0.05110u_f[x]^2 + 0.02387u_f[x]^3 + 0.00211(u_f'')[x] - 0.00378u_f[x](u_f'')[x] + 0.00292u_f[x]^2(u_f'')[x] - 0.00132u_f[x]^3(u_f'')[x]$$
(80)

$$u[6][x] = 1.02549 + 0.21039u_f[x] - 0.09374u_f[x]^2 + 0.03422u_f[x]^3 + 0.00147(u_f'')[x] - 0.00634u_f[x](u_f'')[x] + 0.00467u_f[x]^2(u_f'')[x] - 0.00200u_f[x]^3(u_f'')[x]$$
(81)

$$u[7][x] = 0.93854 + 0.36459u_f[x] - 0.14232u_f[x]^2 + 0.04058u_f[x]^3 + 0.00259(u_f'')[x] - 0.00747373u_f[x](u_f'')[x] + 0.0047969u_f[x]^2(u_f'')[x] - 0.00194u_f[x]^3(u_f'')[x]$$
(82)

$$u[8][x] = 0.74649 + 0.57201u_f[x] - 0.17293u_f[x]^2 + 0.02791u_f[x]^3 + 0.00353(u_f'')[x] - 0.00658u_f[x](u_f'')[x] + 0.00407u_f[x]^2(u_f'')[x] - 0.00172u_f[x]^3(u_f'')[x]$$
(83)

$$u[9][x] = 0.43257 + 0.81004u_f[x] - 0.13080u_f[x]^2 + 0.00042u_f[x]^3 + 0.00294(u_f'')[x] - 0.00398u_f[x](u_f'')[x] + 0.00222u_f[x]^2(u_f'')[x] - 0.00066u_f[x]^3(u_f'')[x]$$
(84)

10.3. Some Plots Concerning the Numerical Results

In this section we present the lines 2, 4, 6, 8 related to results obtained in the last section.

Indeed, we present such mentioned lines, in a first step, for the previous results obtained through the generalized of lines and, in a second step, through a numerical method which is combination of the Newton's one and the generalized method of lines. In a third step, we also present the graphs by considering the expression of the lines as those also obtained through the generalized method of lines, up to the numerical coefficients for each function term, which are obtained by the numerical optimization of the functional J, below specified. We consider the case in which $u_0(x) = 0$ and $u_f(x) = \sin(x)$.

For the procedure mentioned above as the third step, recalling that N = 10 lines, considering that $u''_f(x) = -u_f(x)$, we may approximately assume the following general line expressions:

$$u_n(x) = a(1,n) + a(2,n)u_f(x) + a(3,n)u_f(x)^3 + a(4,n)u_f(x)^3, \ \forall n \in \{1, \dots, N-1\}.$$

Defining

$$W_n = -e_1 \frac{(u_{n+1}(x) - 2u_n(x) + u_{n-1}(x))}{d^2} - \frac{e_1}{t_n} \frac{(u_n(x) - u_{n-1}(x))}{d} - \frac{e_1}{t_n^2} u_n''(x) + u_n(x)^3 - u_n(x) - 1,$$

and

$$J(\{a(j,n)\}) = \sum_{n=1}^{N-1} \int_0^{2\pi} (W_n)^2 dx$$

we obtain $\{a(j, n)\}$ by numerically minimizing J.

Hence, we have obtained the following lines for these cases. For such graphs, we have considered 300 nodes in x, with $2\pi/300$ as units in $x \in [0, 2\pi]$.

For the Lines 2, 4, 6, 8, through the generalized method of lines, please see Figures 1, 4, 7, 10.

For the Lines 2, 4, 6, 8, through a combination of the Newton's and the generalized method of lines, please see Figures 2, 5, 8, 11.

Finally, for the Line 2, 4, 6, 8 obtained through the minimization of the functional *J*, please see Figures 3, 6, 9, 12.

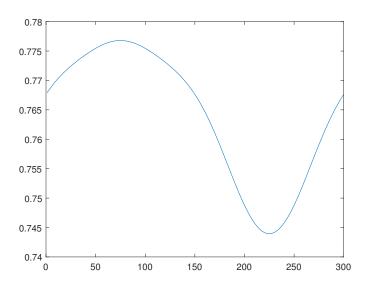


Figure 1. Line 2, solution $u_2(x)$ through the general method of lines

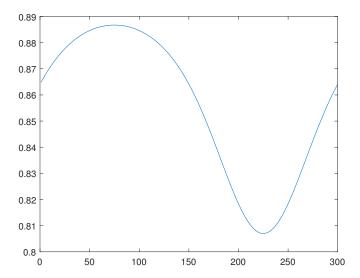


Figure 2. Line 2, solution $u_2(x)$ through the Newton's Method

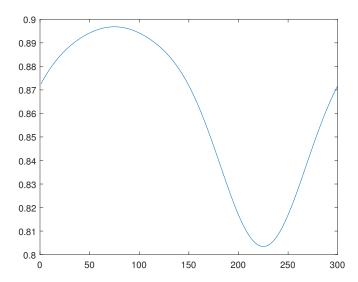


Figure 3. Line 2, solution $u_2(x)$ through the minimization of functional J

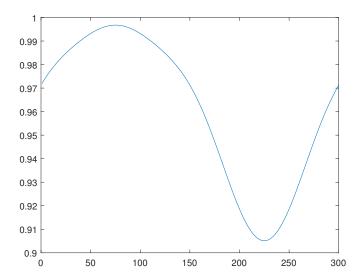


Figure 4. Line 4, solution $u_4(x)$ through the general method of lines

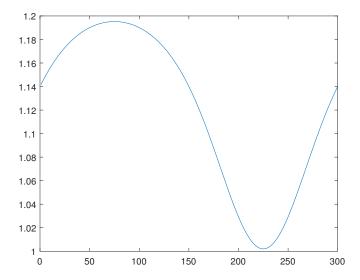


Figure 5. Line 4, solution $u_4(x)$ through the Newton's Method

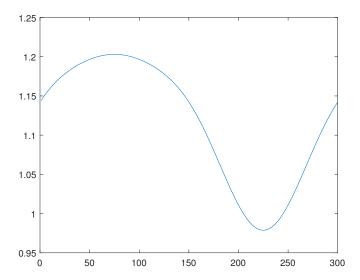


Figure 6. Line 4, solution $u_4(x)$ through the minimization of functional J

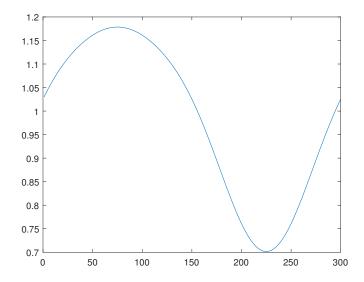


Figure 7. Line 6, solution $u_6(x)$ through the general method of lines

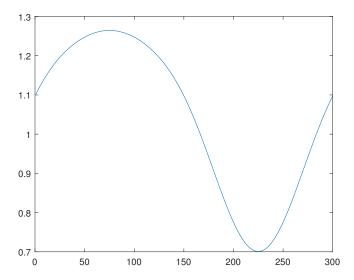


Figure 9. Line 6, solution $u_6(x)$ through the minimization of functional J

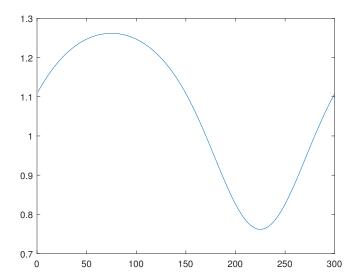


Figure 8. Line 6, solution $u_6(x)$ through the Newton's Method

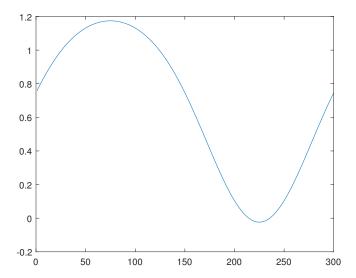


Figure 10. Line 8, solution $u_8(x)$ through the general method of lines

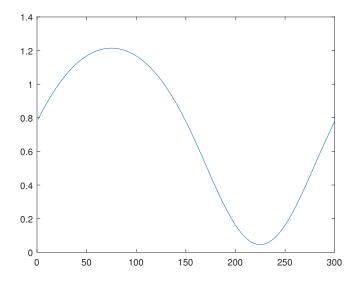


Figure 11. Line 8, solution $u_8(x)$ through the Newton's Method

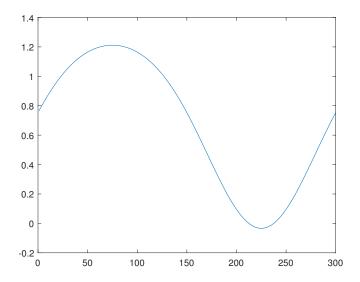


Figure 12. Line 8, solution $u_8(x)$ through the minimization of functional J

11. Conclusions

In the first part of this article we develop duality principles for non-convex variational optimization. In the final concerning sections we propose dual convex formulations suitable for a large class of models in physics and engineering. In the last article section, we present an advance concerning the computation of a solution for a partial differential equation through the generalized method of lines. In particular, in its previous versions, we used to truncate the series in d^2 however, we have realized the results are much better by taking line solutions in series for $u_f[x]$ and its derivatives, as it is indicated in the present software.

This is a little difference concerning the previous procedure, but with a great result improvement as the parameter $\varepsilon > 0$ is small.

Indeed, with a sufficiently large N (number of lines), we may obtain very good qualitative results even as $\varepsilon > 0$ is very small.

References

- 1. R.A. Adams and J.F. Fournier, Sobolev Spaces, 2nd edn. (Elsevier, New York, 2003).
- W.R. Bielski, A. Galka, J.J. Telega, The Complementary Energy Principle and Duality for Geometrically Nonlinear Elastic Shells. I. Simple case of moderate rotations around a tangent to the middle surface. Bulletin of the Polish Academy of Sciences, Technical Sciences, Vol. 38, No. 7-9, 1988.
- 3. W.R. Bielski and J.J. Telega, A Contribution to Contact Problems for a Class of Solids and Structures, Arch. Mech., 37, 4-5, pp. 303-320, Warszawa 1985.
- 4. J.F. Annet, Superconductivity, Superfluids and Condensates, 2nd edn. (Oxford Master Series in Condensed Matter Physics, Oxford University Press, Reprint, 2010)
- 5. F.S. Botelho, Functional Analysis, Calculus of Variations and Numerical Methods in Physics and Engineering, CRC Taylor and Francis, Florida, 2020.
- 6. F.S. Botelho, Variational Convex Analysis, Ph.D. thesis, Virginia Tech, Blacksburg, VA -USA, (2009).
- 7. F. Botelho, *Topics on Functional Analysis, Calculus of Variations and Duality*, Academic Publications, Sofia, (2011).
- 8. F. Botelho, *Existence of solution for the Ginzburg-Landau system, a related optimal control problem and its computation by the generalized method of lines*, Applied Mathematics and Computation, 218, 11976-11989, (2012).
- 9. F. Botelho, Functional Analysis and Applied Optimization in Banach Spaces, Springer Switzerland, 2014.
- 10. J.C. Strikwerda, Finite Difference Schemes and Partial Differential Equations, SIAM, second edition (Philadelphia, 2004).

- 11. L.D. Landau and E.M. Lifschits, Course of Theoretical Physics, Vol. 5- Statistical Physics, part 1. (Butterworth-Heinemann, Elsevier, reprint 2008).
- 12. R.T. Rockafellar, Convex Analysis, Princeton Univ. Press, (1970).
- 13. J.J. Telega, *On the complementary energy principle in non-linear elasticity. Part I: Von Karman plates and three dimensional solids*, C.R. Acad. Sci. Paris, Serie II, 308, 1193-1198; Part II: Linear elastic solid and non-convex boundary condition. Minimax approach, ibid, pp. 1313-1317 (1989)
- 14. A.Galka and J.J.Telega *Duality and the complementary energy principle for a class of geometrically non-linear structures. Part I. Five parameter shell model; Part II. Anomalous dual variational priciples for compressed elastic beams*, Arch. Mech. 47 (1995) 677-698, 699-724.
- 15. J.F. Toland, A duality principle for non-convex optimisation and the calculus of variations, Arch. Rat. Mech. Anal., 71, No. 1 (1979), 41-61.

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