A Novel Adjoint Based Reduced Order Model for Depletion Calculations in Nuclear Reactor Physics

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Article

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Thibault Sauzedde *, Pascal Archier and Frédéric Nguyen

CEA, DES, IRESNE, DER, SPRC, Cadarache, F-13108 Saint-Paul-lez-Durance, France

* Correspondence: thibault.sauzedde@cea.fr

Abstract: The licensing of new reactors implies the use of verified and validated neutronics codes. Numerical validation can rely on sensitivity and uncertainty studies but they require repeated execution of time-consuming neutron flux and depletion calculations. The computational costs can be shortened by using perturbation theories. However, Depletion Perturbation Theory is restricted to single integral values such as a nuclide density. Relying on reduced basis approaches, which reconstruct the whole nuclide densities at once, is one way to get around this restriction. Furthermore, the adjoint-based reduced-order model uses the direct and adjoint equations for the projection. For diffusion or transport calculations, Exact-to-Precision Generalized Perturbation Theory has been developed. Still, no models for depletion calculations are readily available. Therefore, this paper describes a novel adjoint-based reduced order model for the Bateman equation. It uses a range-finding algorithm to create the basis and the Depletion Perturbation Theory for the reconstruction of the nuclide densities at first order. Our paper shows that for several perturbed cases, the depletion reduced-order model successfully reconstructs the nuclide densities. As a result, this serves as a proof of concept for our adjoint-based reduced order model which can perform sensitivity and uncertainty burn-up analysis in a shorter time.

Keywords: reduced order model; perturbation theory; depletion; burn-up analysis; reactor physics; adjoint methods

1. Introduction

Nuclear power plants are a response to the production of low-carbon electricity and heat in the context of global warming. New reactor designs heavily rely on neutronics codes, which must be verified and validated. For example, one must ensure that these codes correctly evaluate the reactivity and power map of the cores throughout their entire cycle. Sensitivity and uncertainty studies can be used for the numerical validation step but they require repeated execution of time consuming neutron flux and depletion calculations. Hence, reducing the time required for these calculations can result in a significant reduction of the numerical validation studies' cost.

Perturbation theories can be helpful in diminishing the coupled diffusion and depletion calculation time. Indeed, perturbation theories are approximated computational schemes that avoid a direct calculation to obtain the responses of a perturbed problem. Depletion Perturbation Theory [1], Generalized Perturbation Theory [2,3] or Standard Perturbation Theory [4] are widely used in reactor physics. Yet, they are restricted to single integral values perturbations, such as reaction rate ratios, reactivity or nuclide density.

Reduced basis methods are a response to this limitation. They allow the reconstruction of the full-power map or nuclide densities in a shorter time than solving the direct problem. They are usually divided into two steps, an offline step carried out once and an online step for each new calculation. In reactor physics, Proper Orthogonal Decomposition [5,6] or Principal Component Analysis in statistics [7] are commonly used for the creation of the basis. The basis can be constructed using a range-finding algorithm which captures the active subspace of our problem and provides an a posteriori estimator for the precision [8]. Modal expansion could also be used, but it has been proven faulty for interesting perturbed neutron flux reconstruction cases [9]. Concerning the online step, most reduced order

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models are based on projections. For example, Galerkin projection allows solving a reduced order system instead of the full one [10]. Differently, adjoint based reduced order model uses the adjoint equation to calculate the projection coefficients [6]. Hence, one does not solve a reduced order system but simply calculates the projection of the solution on the reduced basis. Because of their computational performance, particularly for first-order formulation, adjoint based reduced order models are highly appealing for sensitivity and uncertainty studies. Furthermore, only one adjoint calculation per vector of the basis is needed rather than one adjoint calculation per isotope, as in Depletion Perturbation Theory.

In reactor physics, Exact-to-Precision Generalized Perturbation Theory has been developed for diffusion or transport calculations [11]. This adjoint based reduced order model relies on a range-finding algorithm for the creation of the basis and Generalized Perturbation Theory for the calculation of the projection coefficients. For the depletion calculations, work has been done on reduced order modelling [12] but no adjoint based reduced order model is readily available.

Therefore, this paper describes a novel adjoint based reduced order model for the Bateman equations. Our model uses the Depletion Perturbation Theory for the reconstruction of the nuclide densities and a range-finding algorithm to create the basis. This reduced order model takes advantage of the correlation between nuclide densities due to the transition matrices and the flux's smooth spatial variation. Indeed, for Pressurized Water Reactors calculations, it is common to have few hundreds of thousands depleting media with up to 50 nuclides. As a proof of concept, this method is tested on an elementary example in Section 4.

2. Materials and Methods

We can define the nuclide densities as $n(t) = (n_0, n_1, \cdots, n_I)^T$ relevant to I isotopes with t the time. This field is then governed by the Bateman equation:

$$\frac{\partial n}{\partial t} = \boldsymbol{M} n(t), \tag{1}$$

with $\boldsymbol{M}$ the burn-up and decay matrix:

$$\boldsymbol{M} = \begin{pmatrix} m_{00} & \dots & m_{0I} \\ \vdots & \ddots & \vdots \\ m_{I0} & \dots & m_{II} \end{pmatrix}.$$

The m_{ij} coefficients often have the following terms:

- λ^i the decay constant of isotope i;
- $\phi\Sigma_a^i$ the absorption reaction rate of isotope i;
- $\phi\Sigma_f^i$ the fission reaction rate of isotope i;
- Y_j^i the fraction of fission product j by the fission of isotope i (fission yield of fissile isotope i to fission product j).

Using the fact that the initial density is $n(t_0)$ and $\boldsymbol{M}$ is time independent, we have:

$$n(t) = n(t_0) e^{\boldsymbol{M}(t-t_0)}. \tag{2}$$

We can also define a perturbed configuration:

$$\frac{\partial n'}{\partial t} = \boldsymbol{M'} n'(t), \tag{3}$$

with $n' = n + \delta n$ and $\boldsymbol{M'} = \boldsymbol{M} + \delta \boldsymbol{M}$.
In this paper, we develop a reduced order model of the nuclide densities at the final time t_f:

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$$\delta n(t_f) = \sum_{i=0}^{R} a_i q_i = \boldsymbol{A}\boldsymbol{Q}. \tag{4}$$

The reduced basis $\boldsymbol{Q} = (q_0, q_1, \ldots, q_R)^T$ of size R is obtained with a range-finding algorithm. It is the offline step. Then, the a_i projection coefficients are calculated in the online step which is based on the Depletion Perturbation Theory. This reduced order model can be then called adjoint based. It can replace the depletion solver for sensitivity and uncertainty burn-up analysis. Since the reduced model works for a given final time, it imposes the use of constant time step during the depletion.

3. Theory

3.1. The Offline Step

The basis $\boldsymbol{Q}$ is created during the offline step by using a range-finding algorithm. This algorithm constructs an active subspace of the nuclide densities. First, one has to calculate R snapshots $\boldsymbol{\delta N} = (\delta n_0(t_f), \ldots, \delta n_R(t_f))^T$ with:

$$\delta n_k(t_f) = n_k(\alpha_k, t_f) - n(\alpha, t_f). \tag{5}$$

Each $n_k(\alpha_k, t_f)$ is the results of the depletion equation (1) for a set of randomized input parameters α_k. α or α_k define the input parameters for the burn-up and decay matrix $\boldsymbol{M}$. The randomization of the input parameters is done on the nuclear data and the neutron flux. These data are sampled according to a normal distribution with their nominal values as mean and a standard deviation given by the user.

Then, after the calculation of R snapshots, we can factorize $\boldsymbol{\delta N}$ using a compact singular value decomposition as :

$$\boldsymbol{\delta N} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{Q}. \tag{6}$$

Since $R < I$, $\boldsymbol{U}$ is a $R \times R$ semi-unitary matrix, $\boldsymbol{\Sigma}$ a $R \times R$ square diagonal matrix and $\boldsymbol{Q}$ a $R \times I$ semi-unitary matrix. $\boldsymbol{Q}$ is then the reduced basis for our reduced order model.

The precision of the basis $\boldsymbol{Q}$ can be estimated using the a posteriori estimator derived in Ref. [8]:

$$\epsilon_{theory} = 10\sqrt{\frac{2}{\pi}} max\left(\|\delta n_j(t_f) - \sum_{l=0}^{R} (q_l^T \delta n_j(t_f)) q_l \|_2 \right), \tag{7}$$

with $j = \{0, 1, ..., s\}$ and s the number of trials for the estimator. With s trials, the following relation:

$$\|\delta n_i(t_f) - \sum_{l=0}^{R} (q_l^T \delta n_i(t_f)) q_l \|_2 \leq \epsilon_{theory}, \tag{8}$$

holds with probability of at least $1 - 10^{-s}$ for every i.

The offline step is summarized in Figure 1.

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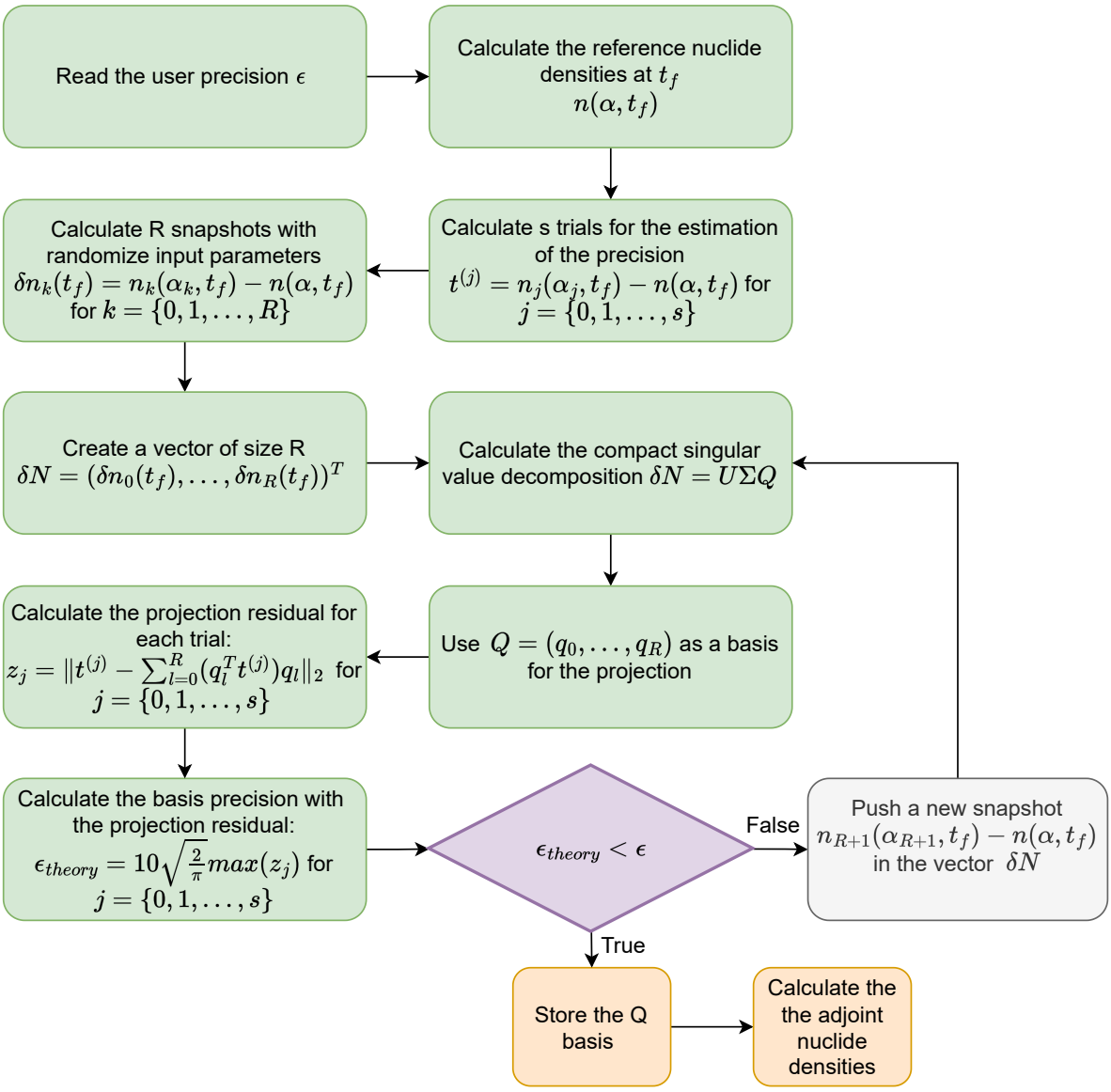

Figure 1. Flow chart of the offline step for the adjoint based reduced order model's offline step.

3.2. The Online Step

Once the basis Q is created, the a_i coefficients have to be calculated. If the nuclide densities map is known at t_f, we have:

$$a_i = \frac{q_i^T \delta n(t_f)}{\|q_i\|_2} = q_i^T \delta n(t_f). \tag{9}$$

Hence, a_i can be calculated with the Depletion Perturbation Theory.

Considering $R_i = q_i^T n(t_f)$, if we want to calculate $\delta R_i = q_i^T \delta n(t_f)$, we can use the method of Lagrange multipliers:

$$K_i(\alpha) = R_i(n) - \int_{t_0}^{t_f} n_i^\dagger(t) \left(\boldsymbol{M(\alpha)} n(t) - \frac{\partial n(t)}{\partial t} \right) dt, \tag{10}$$

with $n_i^\dagger(t)$ the adjoint nuclide densities.

We have for every i, $K_i(\alpha) = R_i(\alpha)$ and $K_i'(\alpha') = R_i'(\alpha')$, hence:

$$\delta K_i = \delta R_i. \tag{11}$$

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By expanding $K_i'(\alpha')$ at first order, we have:

$$K_i' \approx K_i + \frac{\partial K_i}{\partial \alpha}\delta\alpha + \frac{\partial K_i}{\partial n}\delta n + \frac{\partial K_i}{\partial n_i^\dagger}\delta n_i^\dagger. \tag{12}$$

If we try to make $K_i'(\alpha')$ stationary to all the variables except α, we can derive two equations. The first one is the Bateman equation (1):

$$\begin{aligned} &\frac{\partial K_i}{\partial n_i^\dagger}\delta n_i^\dagger = 0, \\ \Leftrightarrow &\frac{\partial}{\partial n_i^\dagger}\int_{t_0}^{t_f} n_i^\dagger(t)\left(\boldsymbol{M}(\boldsymbol{\alpha})n(t) - \frac{\partial n(t)}{\partial t}\right)dt\delta n_i^\dagger = 0, \\ \Leftrightarrow &\left(\boldsymbol{M}(\boldsymbol{\alpha})n(t) - \frac{\partial n(t)}{\partial t}\right) = 0. \end{aligned} \tag{13}$$

The second one is the adjoint Bateman equation:

$$\begin{aligned} &\frac{\partial K_i}{\partial n}\delta n = 0, \\ \Leftrightarrow &\frac{\partial R_i}{\partial n}\delta n + \frac{\partial}{\partial n}\int_{t_0}^{t_f} n_i^\dagger(t)\left(\boldsymbol{M}(\boldsymbol{\alpha})n(t) - \frac{\partial n(t)}{\partial t}\right)dt\delta n = 0, \\ \Leftrightarrow &q_i^T\delta n + \frac{\partial}{\partial n}\int_{t_0}^{t_f}\left(n_i^\dagger(t)\boldsymbol{M}(\boldsymbol{\alpha})n(t) - n_i^\dagger(t)\frac{\partial n(t)}{\partial t}\right)dt\delta n = 0, \\ \Leftrightarrow &q_i^T\delta n + \frac{\partial}{\partial n}\left(\int_{t_0}^{t_f} n(t)\boldsymbol{M}^{\boldsymbol{T}}(\boldsymbol{\alpha})n_i^\dagger(t)dt\right. \\ &\left. -n_i^\dagger(t_f)n(t_f) + n_i^\dagger(t_0)n(t_0) + \int_{t_0}^{t_f} n(t)\frac{\partial n_i^\dagger(t)}{\partial t}dt\right)\delta n = 0, \\ \Leftrightarrow &q_i^T\delta n + \left(\int_{t_0}^{t_f}\boldsymbol{M}^{\boldsymbol{T}}(\boldsymbol{\alpha})n_i^\dagger(t)dt + \int_{t_0}^{t_f}\frac{\partial n_i^\dagger(t)}{\partial t}dt\right)\delta n \\ &- n_i^\dagger(t_f)\delta n(t_f) + n_i^\dagger(t_0)\delta n(t_0) = 0. \end{aligned} \tag{14}$$

By setting $n_i^\dagger(t_f) = q_i^T$, we have:

$$\int_{t_0}^{t_f}\left(\boldsymbol{M}^{\boldsymbol{T}}(\boldsymbol{\alpha})n_i^\dagger(t) + \frac{\partial n_i^\dagger(t)}{\partial t}\right)dt\delta n + n_i^\dagger(t_0)\delta n(t_0) = 0. \tag{15}$$

Enforcing the adjoint nuclides densities to fulfill the adjoint Bateman equation (16):

$$\boldsymbol{M}^{\boldsymbol{T}}(\boldsymbol{\alpha})n_i^\dagger(t) + \frac{\partial n_i^\dagger(t)}{\partial t} = 0, \tag{16}$$

$n_i^\dagger(t_0)\delta n(t_0)$ is the only term remaining in Equation (15).
Thus, we have at first order:

$$\begin{aligned} a_i =&\delta K_i \approx \frac{\partial K_i}{\partial \alpha}\delta\alpha + n_i^\dagger(t_0)\delta n(t_0), \\ a_i \approx &\int_{t_0}^{t_f} n_i^\dagger(t)\boldsymbol{\delta M}n(t)dt + n_i^\dagger(t_0)\delta n(t_0). \end{aligned} \tag{17}$$

Each projection coefficient a_i can be evaluated independently. This allows a trivial parallelization of the online step.

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To evaluate the integral term in Equation (17), one can use a numerical integration algorithm like the trapezoidal rule. This algorithm requires the calculation of several values of $n(t)$ and $n_i^\dagger(t)$ from 0 to t_f. These calculations are done once only in the offline step. It is worth noting that in decay heat calculation context, a robust time discretization is needed because of the short-lived nuclides [13]. An example illustrating the calculation of $\int_{t_0}^{t_f} n_i^\dagger(t)\delta \boldsymbol{M} n(t)dt$ is available in Figure 2. One can see that $n_i^\dagger(t_f)$ is equal to 0 except for the ^{239}Pu. This allows the calculation of $n_{^{239}Pu}$ at t_f using the Depletion Perturbation Theory. Without perturbations in $n(t_0)$, $\delta n_{^{239}Pu}(t_f)$ is equal to the integral $\int_{t_0}^{t_f} n_i^\dagger(t)\delta \boldsymbol{M} n(t)dt$ in blue in Figure 2.

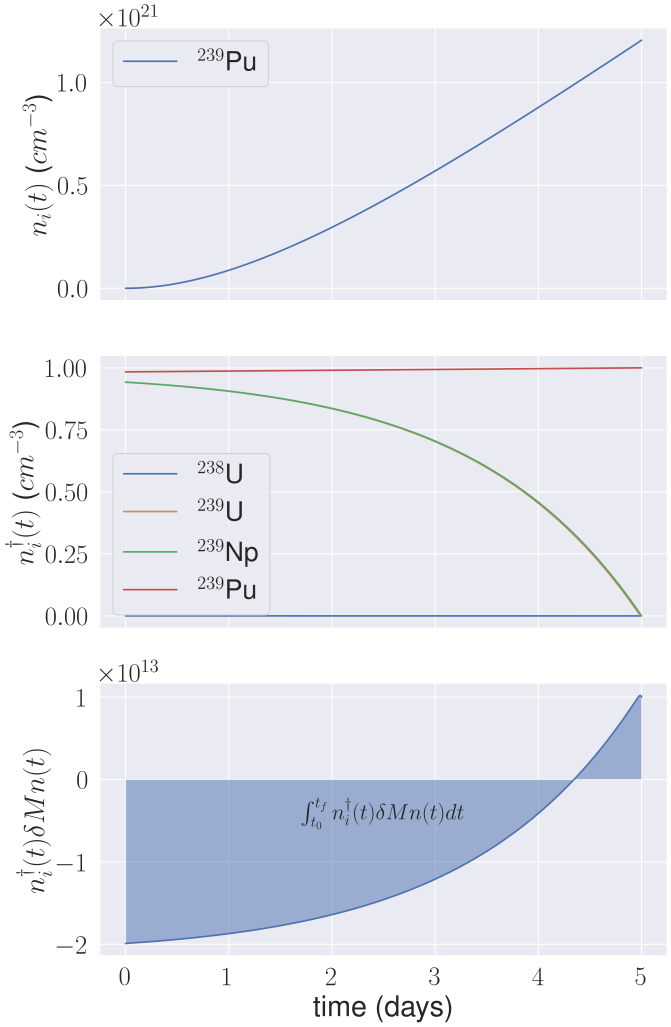

Figure 2. Illustration for the calculation of $\int_{t_0}^{t_f} n_i^\dagger(t)\delta \boldsymbol{M} n(t)dt$ for a vector $n_i^\dagger(t_f)$ equals to 0 except for the ^{239}Pu which is equal to one. $\delta \boldsymbol{M}$ is chosen among the 100 perturbations tested in the results' section.

On the contrary of Exact-to-Precision Generalized Perturbation Theory, we derive only a first order formulation. Indeed, for the exact variation, the coefficient values are:

$$a_i = \int_{t_0}^{t_f} \left(n_i(t)^\intercal(t)\delta \boldsymbol{M} n(t) + n_i^\dagger(t)\delta \boldsymbol{M}\delta n(t) \right) dt + n_i^\dagger(t_0)\delta n(t_0), \tag{18}$$

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and the $\int_{t_0}^{t_f} n_i^\dagger(t)\delta \boldsymbol{M}\delta n(t)dt$ term requires the knowledge of the perturbed densities for every t which cannot be linked to the first order formulation without approximation like in Exact-to-Precision Generalized Perturbation Theory.

4. Results and Discussion

In this section, we apply the adjoint based reduced order model described in Section 3 to the simplified depletion chain of uranium, xenon and samarium with nuclear data using two energy groups. This numerical example is a proof of concept for our novel method. The description of the chains and the nuclear data values are available in Appendix A. The results of the reduced order model are compared to the Depletion Perturbation Theory for each nuclide. The purpose of the reduced order model is the reconstruction of n for a depletion with constant time steps of 5 days. For this numerical example, the vector n has the following definition:

$$\begin{aligned} n = (&n_{^{235}U}, n_{^{238}U}, n_{^{239}U}, n_{^{239}Np}, n_{^{239}Pu}, n_{^{240}Pu}, n_{^{241}Pu}, \\ &n_{^{242}Pu}, n_{^{135}I}, n_{^{135}Xe}, n_{^{149}Nd}, n_{^{149}Pm}, n_{^{149}Sm})^T. \end{aligned} \tag{19}$$

The Depletion Perturbation Theory results use one adjoint nuclide densities calculation for each isotope with the final values equals 0 except for the density of the isotope of interest which is equal to 1. The adjoint based reduced order model relies on the range-finding algorithm described in Section 3.1. Since the dimension of n is small for this simple problem, 13 snapshots are calculated and 10 trials are evaluated to estimate the precision. For each snapshot or trial, the nuclear data and the flux are sampled according to a normal distribution with their nominal values as mean and 1 % as their standard deviation. The a posteriori estimation of the basis's precision is plotted in Figure 3 as a function of the basis's size. Results show that when the basis's size tends towards the range of the depletion problem, the theoretical error ϵ_{theory} tends toward the machine precision.

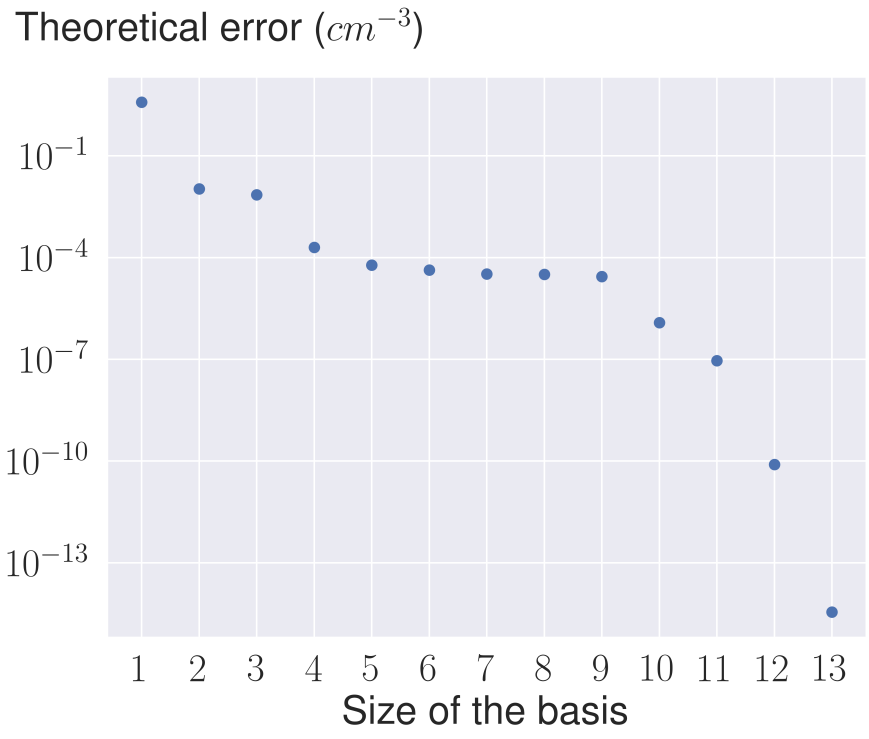

Figure 3. Reduced basis theoretical errors ϵ_{theory} versus the size of the basis.

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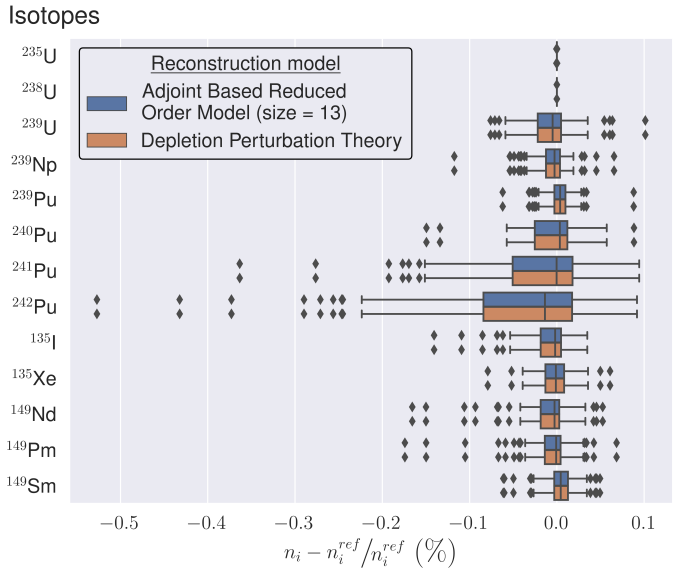
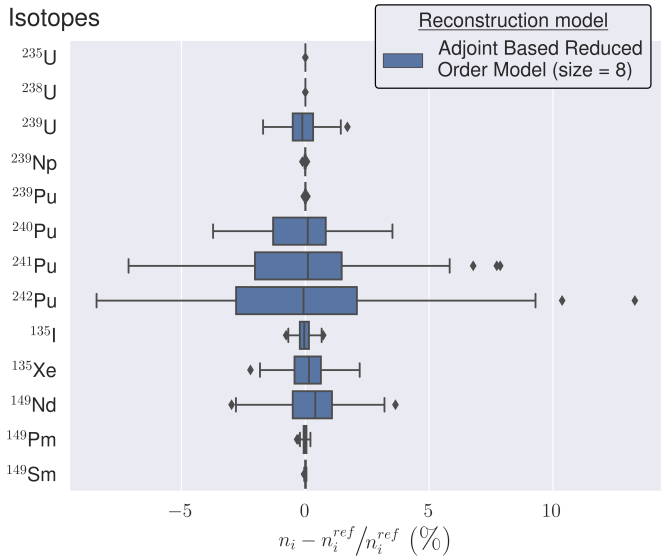
One can see that even for this elementary case, the adjoint based reduced order model can diminish the number of adjoint densities calculations compared to the Depletion Perturbation Theory. Furthermore, the range-finding algorithm will likely be more efficient for real cases where it is common to have few hundreds of thousands depleting media with up to 50 nuclides.

Figure 4 presents the distribution of the reduced order model and Depletion Perturbation Theory errors $\frac{n_i - n_i^{ref}}{n_i^{ref}}$ as box plot [14] for 100 nuclear data and neutron flux random perturbations. The perturbed values are sampled according to a normal distribution with their nominal values as mean and 1 % as their standard deviation. Depletion Perturbation Theory errors are solely related to the first order approximation whereas the reduced order model errors depend on the reduced basis's precision too.



a. Reduced Order Model with size = 13



b. Reduced Order Model with size = 8

Figure 4. Adjoint based reduced order model errors compared to the Depletion Perturbation Theory for 100 input parameters perturbations. The perturbed values are sampled according to a normal distribution with their nominal values as mean and 1 % as their standard deviation.

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Results show that the errors are identical for Depletion Perturbation Theory and the adjoint based reduced order model with a basis of size 13. When the size of the basis is 8, the errors increase for the isotopes with the lowest densities like ^{242}Pu.

The identical errors for Depletion Perturbation Theory and the adjoint based reduced order model suggest that with a basis reaching machine precision, both methods have the same precision. The fact that errors increase when the basis is smaller is consistent with the theoretical precision and is linked to the large range of nuclide densities: 10^{12} for the ^{242}Pu to 10^{24} for the ^{238}U. This could be an issue for isotopes with small densities and large cross sections like ^{135}Xe. One way to take into account the importance of the isotope and not only its concentration is to weigh each nuclide density by its absorption cross section. This has been successfully applied in Ref. [12] with weights equals to the absorption cross section of the isotope divided by the absorption cross section of ^{238}U.

Overall, this serves as a proof of concept for our adjoint based reduced order model which can replace the depletion solver for sensitivity and uncertainty burn-up analysis.

5. Conclusions

Our results serve as a proof of concept for the novel adjoint based reduced order model presented in this paper. This reduced order model can readily replace the depletion solver to perform sensitivity and uncertainty studies in a shorter time.

Future work will focus on employing this methodology on real case applications like full Pressurized Water Reactors or Sodium-cooled Fast Reactors calculations.

Author Contributions: Conceptualization, T.S.; methodology, T.S.; software, T.S.; writing—original draft preparation, T.S.; writing—review and editing, P.A. and F.N.; supervision, P.A. and F.N.; project administration, P.A. and F.N. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data and software used in this study are openly available in https://github.com/ThibaultSauzedde/depletion_adjoint_rom.

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Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A. Description of the Depletion Chains

The depletion chains used in the proof of concept are given in Figures A1, A2 and A3. They have been simplified to fit Pressurized Water Reactors needs. The nuclear data using two energy group are given in Table A1. They are inspired by the one in the example two of Ref. [1] and are not chosen to be particularly realistic. The definitions of the parameters are:

- $\sigma_{a,g}$ the absorption cross section of the group g;
- $\sigma_{f,g}$ the fission cross section of the group g;
- $\sigma_{c,g} = \sigma_{a,g} - \sigma_{f,g}$ the capture cross section of the group g;
- the energy group g with the values 0 (fast neutrons) and 1 (thermal neutrons);
- n_0 the initial concentration;
- Y the fraction of fission products by the fission of all the isotopes (fission yield of all the isotopes);
- λ the decay constant.

The neutron flux $\phi = (\phi_0, \phi_1)$ values are $\phi_0 = 0.6667 \times 10^{14}$ for the fast group and $\phi_1 = 0.2000 \times 10^{15}$ for the thermal one.

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Table A1. Nuclear data values for the numerical example, blank cells correspond to null values.

Isotope	$\sigma_{a,0}$ (barn)	$\sigma_{a,1}$ (barn)	$\sigma_{f,0}$ (barn)	$\sigma_{f,1}$ (barn)	n_0 (cm^{-3})	Y	λ (s^{-1})
^{235}U	1.80	100.0	1.5	55.0	3.50×10^{23}		
^{238}U	0.35	2.000			96.5×10^{23}		
^{239}U							1.02×10^{-3}
^{239}Np							7.11×10^{-6}
^{239}Pu	2.00	190.0	1.8	120.0			
^{240}Pu	0.20	110.0					
^{241}Pu	2.50	180.0	0.5	140.0			2.98×10^{-9}
^{242}Pu	0.70	70.00					
^{135}I						0.0640	6.01×10^{-5}
^{135}Xe		2.0×10^{5}				0.0010	4.29×10^{-5}
^{149}Nd						0.0109	2.28×10^{-4}
^{149}Pm							7.41×10^{-6}
^{149}Sm		1.0×10^{3}					

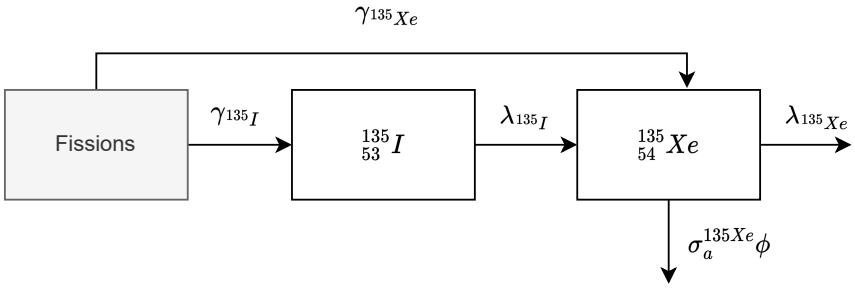

Figure A1. Simplified depletion chain of the $^{135}_{54}$Xe

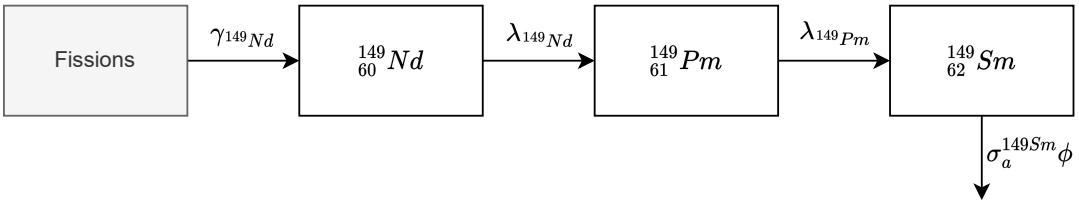

Figure A2. Depletion chain of the $^{149}_{62}$Sm

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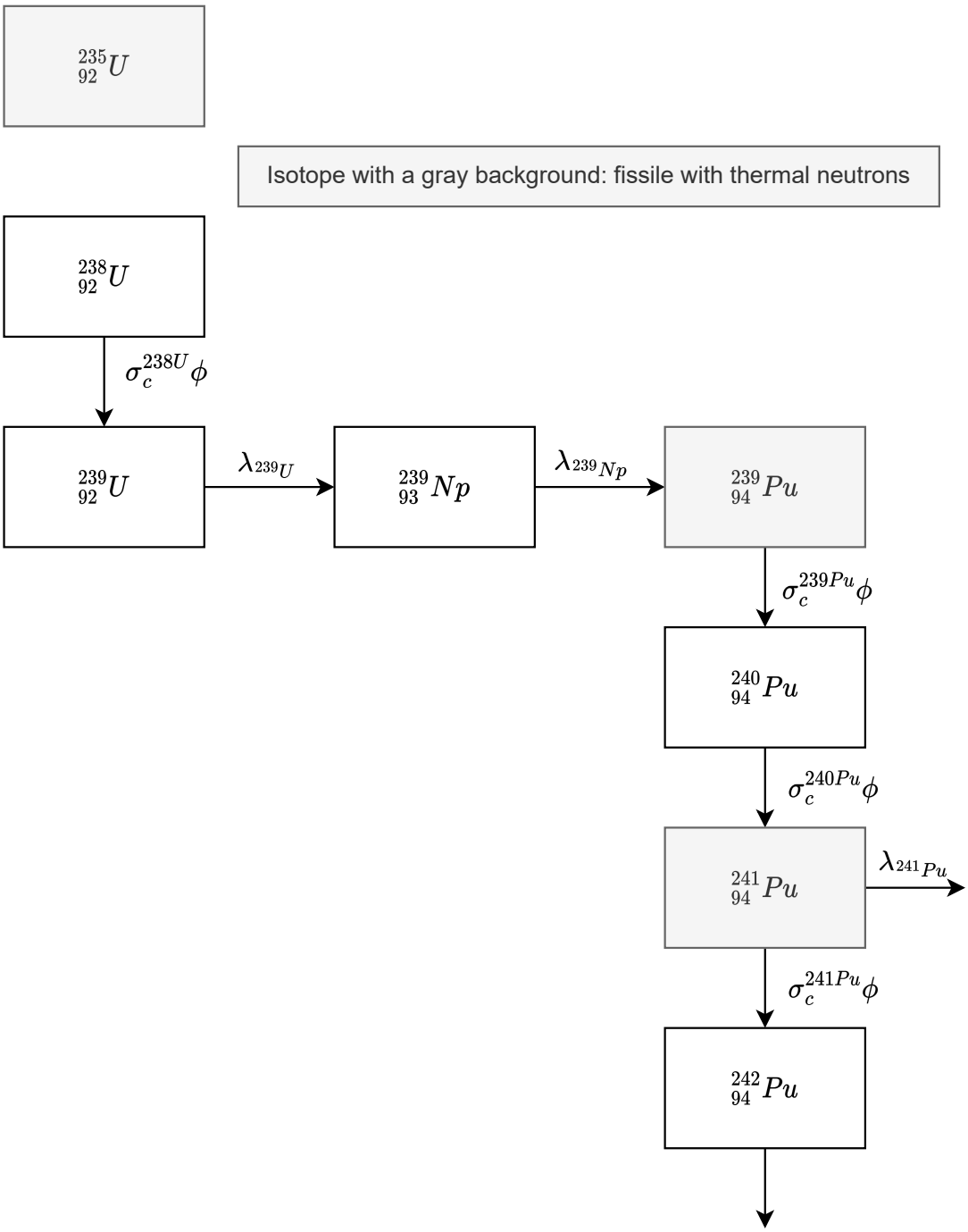

Figure A3. Simplified depletion chain of uranium

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