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SUBSPACE MULTI -SCALE APPROACH FOR REACTOR ANALYSIS, PART I: ENERGY VARIABLE

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ABSTRACT

This manuscript addresses one of the main challenges facing conventional homogenization theory currently employed in reactor analysis - that is how to capture the effects of unlike assembly neighbors on the assembly-averaged parameters, without having to resort to multi-assembly calculations, often known as color-set calculations. This manuscript presents a proof-of-principle demonstration for a novel approach that employs a mathematical extension operator in a multi-scale framework to update the boundary conditions for single-assembly calculations based on the macroscopic attributes determined by core-wide calculations. This approach is based on the basic hypothesis of homogenization theory as employed in reactor analysis: that is assuming that the exact heterogeneous solution is known a priori and is employed to set the boundary conditions for the single-assembly calculations, then the exact solution would be reproduced by single-assembly calculations, and core-wide calculations would preserve all quantities defined over the regions homogenized by single-assembly calculations. Our approach takes advantage of this property by minimizing a quadratic function that measures the discrepancy between core-wide attributes predicted by core-wide calculations and the same attributes directly collapsed from single-assembly calculations. Unlike existing approaches, our approach can be rigorously shown to eliminate rather than minimize the errors originating from lack of knowledge of the exact boundary conditions for single-assembly calculations, thus leading to an exact estimate of core-wide attributes. The Efficient Subspace Method will be employed to accumulate sensitivity information required to solve the minimization problem.

Key Words: multi-scale algorithms, single-assembly calculations, efficient subspace methods

1. INTRODUCTION

Reactor calculations involve the determination of the ensemble average of the neutron density in a reactor core as a function of space, energy, angle, and time. Mathematically, this can be well described by the Boltzmann transport equation, whose coefficients are the various experimentally-evaluated neutron cross-sections. Obtaining a numerical solution however for the entire reactor core in practical time is not possible in the near future despite the startling growth in computing power. The solution of this equation is difficult because, in addition to the large dimensional phase space, the cross-sections have strong, discontinuous behavior in space on a scale much smaller than the reactor core dimensions due to material heterogeneities, and extreme variations with energy due to resonance phenomena associated with compound nucleus formation. Currently, these difficulties are addressed by homogenization theory via a multi-scale approach, where at the micro-scale the spatial domain is decomposed based upon assumed

boundary conditions, and fine energy, angle and spatial detail are used in solving the transport equation over each sub-domain, with each sub-domain often characterizing a lattice (a 2D radial slice of a fuel assembly). From these sub-domain solutions, appropriately averaged effective cross-sections over angular direction, energy and space are determined so as to preserve neutron reaction rates. At the coarse-scale level (core-wide calculations), a low-order approximation of the transport equation, e.g., the P-1 approximation that is algebraically reduced to the diffusion equation, is solved over the entire spatial domain, where now angular direction dependence has been removed, and energy and spatial detail have been reduced via the few-energy group, spatial homogenization treatment of cross-sections and discontinuity factors as previously noted.

The weakness of the current approach is that the assembly's boundary conditions assumed at the fine-scale are in most cases not refined based upon the coarse-scale solution. Several attempts have been made to address this problem, but without an entirely satisfactory resolution [1, 2]. Our approach provides a mathematically rigorous manner of updating the fine-scale boundary conditions with spatial, angular, and energy details, based on the coarse-scale solution.

This manuscript is organized as follows. Section 2 describes a general multi-scale framework for our approach, and Section 3 implements it for coupling assembly and core-wide calculations. Section 4 presents a case study demonstrating the application of the proposed approach. Concluding remarks and future work are discussed in Section 5.

2. MATHEMATICAL DEVELOPMENT

Although our main interest in this work focuses on coupling assembly and core-wide calculations, we introduce a general multi-scale framework for the proposed approach in order to emphasize its wider applicability to other nuclear models. For example, one can employ the same idea to update the flux profiles used to collapse the point-wise cross-sections to the multi-group format. Other examples include the coupling of Monte Carlo and deterministic models for variance reduction and convergence acceleration.

In general, a multi-scale modeling strategy may be described as follows: let H denote the entire problem domain, and $\vec{T}$ and $\vec{z}$ vector functions defined on H. A domain-wide model at the finest scale reduces to finding a solution $\vec{u}$ such that:

$$\vec{T}(\vec{s},\vec{u}) = \vec{z}(\vec{s}) \text{ on H,} \tag{1}$$

where $\vec{s} = \vec{s}(\vec{v})$ describes fine-scale parameters as a function of domain variables $\vec{v}$, e.g. space, energy, etc[1].

[1] Sometimes model parameters depend on the solution. For example, cross-sections depend on temperature which depends on the power which is determined by the flux. Another example from thermal analysis is temperature-dependent thermal conductivity. In our notation, we assume that such dependence of model parameters on the solution is already included in the operators $\vec{T}$ and $\vec{z}$, such that the parameters $\vec{s}$ represent the solution-independent properties only, e.g. resonance parameters for the neutronics example, and various coefficients that appear in the thermal conductivity correlation for the thermal analysis example.

Our notations assume that the solution comprises the direct solution and any other differential-type quantity derived from it (e.g., $\vec{u}$ represents both the neutron flux distribution and the derived neutron current). This compact notation generalizes boundary conditions description of the sub-domain problems (e.g. a Dirichlet condition specifying the neutron flux, or a Neumann condition specifying the current, or a mixed boundary condition specifying a relationship between the neutron flux and current).

Solving Eq. (1) directly is not computationally feasible due to the large degree of heterogeneity. Hence, one resorts to a multi-scale strategy, in which the fine-scale model is solved only over a smaller region of the problem domain, i.e., sub-domain, which is decoupled from the rest of the domain by assuming some boundary conditions. Denoted mathematically, let $\vec{T}_f^{(i)}$ and $\vec{z}_f^{(i)}$ be functions defined on H_i, the solution $\vec{u}_f^{(i)}$ for the i^{th} sub-domain solves the following equations:

$$\vec{T}_f^{(i)}(\vec{s}_f^{(i)}, \vec{u}_f^{s(i)}, \vec{u}_f^{(i)}) = \vec{z}_f^{(i)}(\vec{s}_f^{(i)}, \vec{u}_f^{s(i)}) \text{ on } \mathrm{H}_i, \tag{2}$$

where both $\vec{z}_f^{(i)}$ and $\vec{T}_f^{(i)}$ are contractions of the functions in Eq. (1) and now also depend on the choice of the sub-domain boundary conditions $\vec{u}_f^{s(i)}$. See Fig. 1 for illustration.

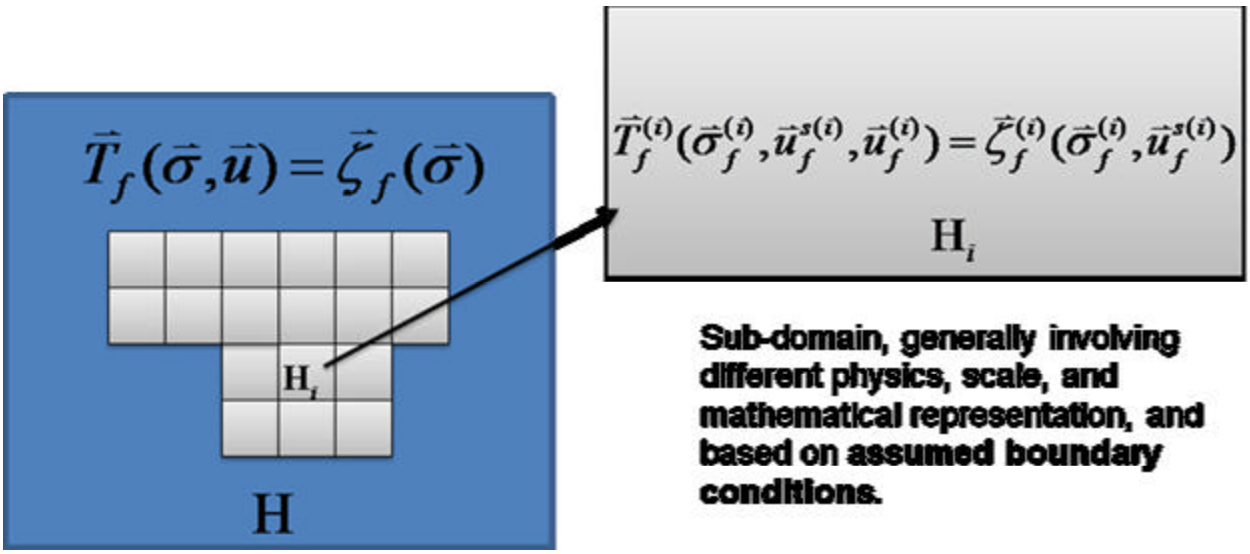

Figure 1. Schematic for General Multi-Scale Framework

It is important to remark that there are several distinctions between the sub-domains as defined here, and the sub-domains defined by the rich work on classical domain-decomposition and multi-grid techniques [4-8]. These techniques are utilized when the computational overheads are overwhelming, and the entire problem model is broken up into different sub-domains, each with the same characteristics, e.g. same physics, scale, and mathematical description.
In a multi-scale model, however, the sub-domains can, in general, be based on: a) different scales, e.g., fine-scales for regions where explicit knowledge of the local conditions must be

accurately represented, and coarse-scales for other regions that can be approximated well enough using coarser models; b) different physics representations (e.g. Boltzmann neutron transport equation for assembly calculations versus coupled neutronics and thermal-hydraulics for core-wide calculations); c) different mathematical models (e.g. integral form of the transport equation for assembly calculations versus nodal expansion method for core-wide calculations); d) different modeling philosophy (e.g. deterministic versus probabilistic models); and e) different discretization schemes (e.g. orthogonal vs. non-orthogonal grids).

Next, the fine-scale solution is integrated over the sub-domains to calculate the coarse-scale parameters:

$$\vec{s}_c^{(i)} = \vec{\Pi}_c^{(i)}(\vec{s}_f^{(i)}, \vec{u}_f^{(i)}), \tag{3}$$

where $\vec{\Pi}_c^{(i)}$ is an averaging (coarsening) operator for the i^{th} sub-domain. The coarse-scale solution for the entire problem domain solves the following equation:

$$\vec{T}_c(\vec{s}_c, \vec{u}_c) = \vec{z}_c(\vec{s}_c), \tag{4}$$

where $\vec{s}_c$ denotes a vector of the coarse-scale parameters for all sub-domains. The coarse-scale solution $\vec{u}_c$ of Eq. (4) is then used to evaluate the macroscopic system attributes according to:

$$\vec{y}_c = \vec{\Gamma}_c(\vec{s}_c, \vec{u}_c), \tag{5}$$

Consider the same attributes but now evaluated directly using the sub-domains solutions of Eq. (2), i.e., without executing the coarse-scale model:

$$\vec{y}_f = \vec{\Gamma}_f(\vec{s}_f, \vec{u}_f), \tag{6}$$

where $\vec{u}_f$ and $\vec{s}_f$ are vectors denoting the sub-domain fine-scale solutions and model parameters, respectively, for all sub-domains.

The consistency condition for the multi-scale approach described above is that the macroscopic system attributes of Eq. (5) and Eq. (6) are determined such that:

$$\vec{y}_c = \vec{\Gamma}_c(\vec{s}_c, \vec{u}_c) = \vec{y}_f(\vec{s}_f, \vec{u}_f = \vec{u}) \quad \text{on H}, \tag{7}$$

implying that the attributes will be preserved only if the exact fine-scale solution $\vec{u}$ is used to define the boundary conditions for the sub-domains solutions. Note that attributes satisfying this condition must be defined as integrals over an entire sub-domain; Eq. (7) will not hold if the attributes are defined over a sub-region of a sub-domain due to the lost degrees of freedom.

Our approach updates the boundary conditions by enforcing this consistency condition. To achieve that, define a function $\vec{\Omega}$:

$$\Delta\vec{y} = \vec{y}_f(\vec{u}_f(\vec{u}_f^s)) - \vec{y}_c(\vec{u}_c(\vec{u}_f(\vec{u}_f^s))) = \vec{\Omega}(\vec{u}_f^s), \tag{8}$$

which quantifies the discrepancy between the macroscopic attributes predictions based on the sub-domains solutions and the coarse-scale solution. Notice the dependence of the attributes on the coarse-scale solution which depends on the sub-domains solution which depends on the sub-domains boundary conditions (as implied by Eq. (2) through Eq. (4)). Our approach updates the sub-domains boundary conditions in order to reach the equality condition assured by Eq. (7).

This can be achieved by minimizing a quadratic function of the form:

$$\min_{\vec{u}_f^s}\left\{\left\|\vec{\Omega}(\vec{u}_f^s)\right\|_{\mathbf{C}_\Omega}^2 + \Psi(\vec{u}_f^s)\right\}, \tag{9}$$

where $\mathbf{C}_\Omega$ and Ψ are appropriately selected to guide and regularize the search, respectively. The first term is denoted by the misfit term, and the second by the regularized term.

First, guiding the search suggests that instead of updating the boundary conditions for all sub-domains, only those that have the largest impact on the attributes of interest will be updated. This follows since in many engineering application, one is often interested in accurately calculating the attributes only in certain regions of the problem domain, such as regions with high temperatures or heat flux for the heat transfer example. In this case, only the sub-domains boundary conditions that affect the attributes in the region of interest will be updated by the search, i.e. implying that the equality in Eq. (7) will not be necessarily achieved for the entire problem domain H, but only for the regions determined by the minimization and any additional constraints imposed by the design. Further, the residual will provide a measure to assess the accuracy of the simulation.

Second, the need to regularize the search reflects the ill-posedness and the high degree of ill-conditioning of the unregularized minimization problem. The ill-posedness follows from the fact that the number of degrees of freedom available at the coarse-scale model will be less than those at the sub-domain fine-scale level (e.g. the neutron flux and current for assembly calculations have many energy groups dependence and are defined over a detailed spatial grid, whereas core-wide calculations often involve a fewer number of energy groups and a coarser spatial grid). The ill-conditioning results from the smoothing behavior of the misfit term and the continuous dimensionality reduction inherent in the multi-scale modeling strategy; that is going from one scale to the next results in a gradual reduction in problem dimensionality which creates large degrees of correlations in the input and output data streams. Earlier work by the second author has demonstrated this fact for typical LWR calculations (see [3] and references within). It was reported that the effective rank of sensitivity matrices relating changes in macroscopic attributes to multi-group cross-sections is of the order of 10^2 despite both data streams numbering in the millions.

Now, assuming that a sensitivity analysis is available to generate the first-order derivatives of the macroscopic system attributes with respect to the sub-domains boundary conditions, this minimization problem can then be readily solved using a Newton-type search approach. Clearly, this sensitivity analysis is expected to be computationally intractable due to the complexity of the sub-domains and coarse-scale models and the large sizes of their input and output data streams.

3. IMPLEMENTATION

This section applies the above framework to a reactor analysis problem, where the goal is to update the boundary conditions for the single-assembly calculations based on the core-wide model. In this context, a problem domain refers to the entire reactor core; a sub-domain refers to a lattice over which the assembly solution is homogenized; fine-scale parameters refer to the multi-group cross-sections input to assembly calculations; and coarse-scale parameters refer to the assembly-averaged few-group parameters that are input to core-wide model. Assembly calculations are often based on an integral form of the transport equation, while core-wide calculations often employ a diffusion type model. Sometimes, transport calculations are done probabilistically using a Monte Carlo model. The macroscopic attributes calculated by the core-wide model include, for example, flux and power distributions. The boundary conditions for the assembly models are defined as Dirichlet, Neumann, or mixed boundary conditions relating flux and current on the various grid segments of the assembly surface.

Expand Eq. (9) around reference conditions using Taylor series, and retain only the first-order terms. Reference conditions refer to the initial estimates for the assembly's boundary conditions (reflective boundary conditions are often assumed for assembly calculations):

$$\min_{\vec{u}_f^s}\left\{\|\vec{y}_f^{(0)}-\vec{y}_c^{(0)}+(\frac{\partial\vec{y}_f}{\partial\vec{u}_f^s}-\frac{\partial\vec{y}_c}{\partial\vec{u}_f^s})(\vec{u}_f^s-\vec{u}_f^{s(0)})\|_{C_\Omega}^2+l^2\|(\vec{u}_f^s-\vec{u}_f^{s(0)})\|^2\right\} \quad (10)$$

where $\mathbf{O}_f=\frac{\partial\vec{y}_f}{\partial\vec{u}_f^s}$ $\mathbf{O}_c=\frac{\partial\vec{y}_c}{\partial\vec{u}_f^s}$ are sensitivity matrices containing the first-order derivatives of the macroscopic attributes with respect to the single assembly boundary conditions, calculated respectively from the sub-domain and coarse-scale models. The (0) superscript denotes the reference conditions. Tikhonov regularization is employed to address the ill-posedness and ill-conditioned nature of the inverse problem [9].

To solve this problem, one needs to determine the above sensitivity matrices. To appreciate the computational overhead required to estimate these matrices, let us recall that the state-of-the-art in sensitivity analysis for a general model comprises two fundamental approaches [10]. The forward approach involves random or systematic perturbations of input data and multiple executions of the model equal to the number of input data. This is appropriate when the size of input data field is small and the number of output responses is large. Alternatively, the adjoint approach is used when the number of output responses is small and the number of input data is large.

Consider a simplified reactor analysis model with *N* fuel assemblies; each containing *L* different fuel lattices. Each fuel assembly is axially discretized into *Z* segments for the core-wide model (each axial segment is often referred to as a fuel node). For single-assembly calculations, each assembly has *S* surface segments where boundary conditions are to be specified. For each fuel node, *P* few-group parameters are collapsed by assembly calculations, and *T* macroscopic attributes are determined by the core-wide model. Typical values for LWR calculations are *N*~200-600 assemblies; *L* ~ 5 lattices per assembly; *Z* ~ 30 axial segments per assembly; *S* ~ 10-100 segments; *P* ~ 10 few-group parameters, including various cross-sections and nu and kappa values for two energy groups[2]; *T* ~ 5, including thermal and fast fluxes, power, and detectors' responses. In this case, the coarse-scale model reads as input *P* few-group homogenized parameters for each of the *Z* fuel nodes for each of the *N* assemblies for a total of $P \times N \times Z$ input data values. Similarly, it calculates a total of $T \times N \times Z$ output data values describing the macroscopic attributes throughout the core.

To estimate the sensitivity matrix $\mathbf{O}_c$ using a forward sensitivity analysis, one would need to run assembly calculations for each lattice *S* extra times, each representing a perturbation of a surface segment boundary condition. Next, the coarse-scale model is to be executed $P \times N \times Z$ times. This follows since in a diffusive medium, any local change in any of the coarse-scale parameters will produce core-wide perturbations in the macroscopic attributes. Alternatively, for an adjoint sensitivity analysis, assembly calculations must be executed *P* extra times in an adjoint mode, each corresponding to a single few-group parameter representing the response function for the adjoint model. Next, the core-wide model is to be executed a total of $N \times T \times Z$ times. Clearly, either of these two approaches will lead to intractable computational burdens.

We elect therefore to use the Efficient Subspace Method to calculate the required sensitivity information. ESM is a set of novel mathematical algorithms that have been demonstrated to outperform conventional forward and adjoint algorithms for performing sensitivity for complex computational models that are associated with large input and output data streams. ESM achieves the computational efficiency by recognizing that the effective ranks of sensitivity matrices that are associated with multi-scale problems are many times much smaller than the matrices' dimensions. This is not a coincidence; the reason is deeply rooted in the multi-scale strategy: going from one scale to the next results in a gradual reduction in problem dimensionality which creates large degrees of correlations in the input and output data streams. Earlier work by the second author has demonstrated this fact for typical LWR calculations (see [1] and references within). It was reported that the effective rank of the sensitivity matrix is of the order of 10^2 despite both input and output data streams numbering in the millions. The implication is that much smaller matrices, obtained via matrix rank revealing decompositions, can be employed to characterize their actions. For example, consider the sensitivity matrix $\mathbf{O}_c \in \mathbb{R}^{m \times n}$; one can re-write it using the decomposition $\mathbf{O}_c = \mathbf{Q}\mathbf{R}\mathbf{G}^T$. The columns of $\mathbf{Q} \in \mathbb{R}^{m \times r}$ and $\mathbf{G} \in \mathbb{R}^{n \times r}$ - *r* is the rank of the matrix - span subspaces of size *r* which is much smaller than the output stream consisting of *m* data, and the input of size *n*, respectively; the $\mathbf{R} \in \mathbb{R}^{r \times r}$ is a full rank square matrix. If $\mathbf{R}$ is selected to be diagonal; and $\mathbf{Q}$ and $\mathbf{G}$ are orthonormal, the resulting

[2] In this simplified model, we ignore thermal-hydraulics and depletion functionalizations of the few-group cross-sections.

decomposition is referred to as the Singular Value Decomposition, and the diagonal elements of $\mathbf{R}$ are referred to as the singular values of the matrix. The rate of decline of the singular values provides a measure on the degree of ill-conditioning of the minimization problem.

The unique aspect of ESM is that the subspaces representing the mathematical ranges of the matrices $\mathbf{Q}$ and $\mathbf{G}$ are obtained without having to first evaluate the full sensitivity matrix being decomposed. This is very important for the sensitivity coefficient matrices, since as noted above, they are intractable to calculate. The decompositions are obtained via r randomized matrix-vector and matrix-transpose-vector products of the form $\mathbf{O}_c\bar{q}$ and $\mathbf{O}_c^T\bar{g}$ where the rank r is assumed unknown a priori and determined as part of the analysis.

4. CASE STUDY

Given the exploratory nature of this work, a multi-phase approach will be adopted in order to gain insight into the mechanics of the proposed approach. In the initial phase, as represented in this manuscript, we will focus on the homogenization errors arising from the energy variable only. To achieve that, the following simplifying assumptions will be made: a) the assembly and core-wide calculations will both be based on the same mathematical model; b) both will use the same spatial grid, i.e., no spatial homogenization; c) no time dependence, i.e., steady state calculations. The following phases will relax each of these assumptions one at a time. This will allow a detailed analysis of the various error sources arising from homogenization.

In this work, the following test problem is analyzed. The reactor core is composed of one 2x2 array of MOX (Mixed Uranium and Plutonium Oxide fuel) and LEU (Low Enriched Uranium) assemblies (see Fig. 2). Zero current boundary conditions are assumed at the core periphery. Single-assembly calculations are based on a two-dimensional (18 nodes per assembly in each direction) four-group model with cross-sections of each group selected to be spatially uniform for simplicity and with zero current boundary conditions. Based on the calculated four-group single-assembly fluxes, the four-group cross-sections are collapsed into two groups for core-wide calculations. The NESTLE code is employed to perform both single-assembly and core-wide calculations.

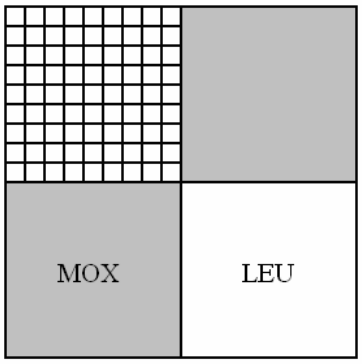

Figure 2. Simplified MOX-LEU Core

Lattice calculations are performed with four groups, representing the multi-group energy structure, and core-wide calculations are performed with two-groups, representing the coarse-energy structure (NESTLE currently can handle only two or four energy groups).

The minimization problem in Eq. (10) is solved, and the resulting current boundary conditions are employed to recalculate the four group single assembly fluxes for both MOX and LEU. The homogenization process is repeated for both assemblies, and core-wide calculations are re-evaluated with the updated few-group cross-sections. The errors in the thermal flux before and after the BC adjustments are compared in Fig. 3 (right axis), labeled as 'Initial Error' and '2G BC Adj', respectively. The exact thermal flux obtained from 4G calculations is displayed for comparison on the left axis of the same figure.

The singular values of the sensitivity matrix $\mathbf{O}_c$ are displayed in Fig. 4 (normalized to a maximum of 1.0); their sharp decline demonstrates the severe ill-conditioning of the minimization problem. The numerical rank is determined as the minimum singular value index that satisfies the following condition:

$$\left| r_i \mathbf{O} \vec{q}_i \right| > e \ ,$$

where e is an error tolerance limit prescribing the minimum acceptable variation in macroscopic attributes.

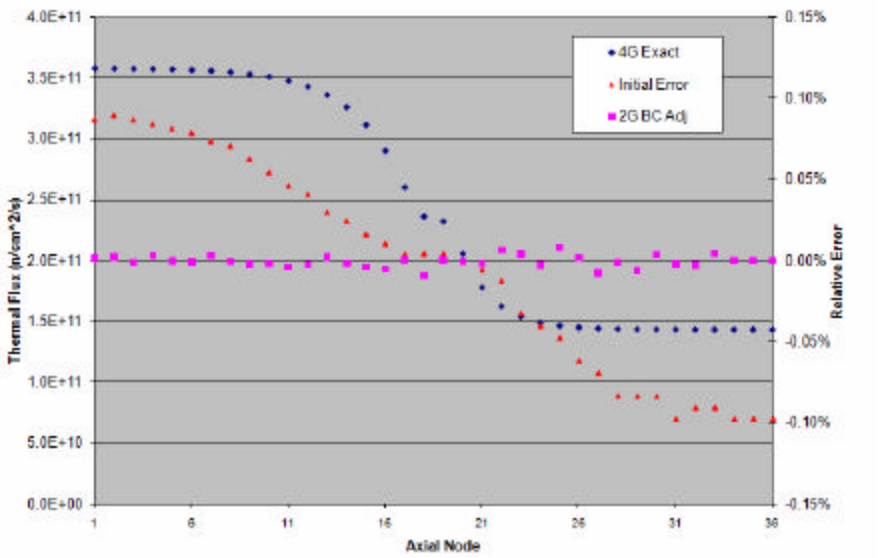

Figure 3. Thermal Flux Gradient across a MOX-LEU Assemblies' Interface

For this problem, the effective rank was found to be ~10 which is much smaller than the matrix dimensions for this problem. Matrix dimensions are determined by the total number of surface currents for single-assembly calculations, and the total number of macroscopic attributes in the core-wide model. There are a total of 4x18x4 boundary conditions (4 group currents specified at

18 different segments per each of the 4 assembly-assembly interfaces). The number of macroscopic attributes is 36x36x2 (36 nodes in each direction and two attributes per node, representing thermal and fast fluxes).

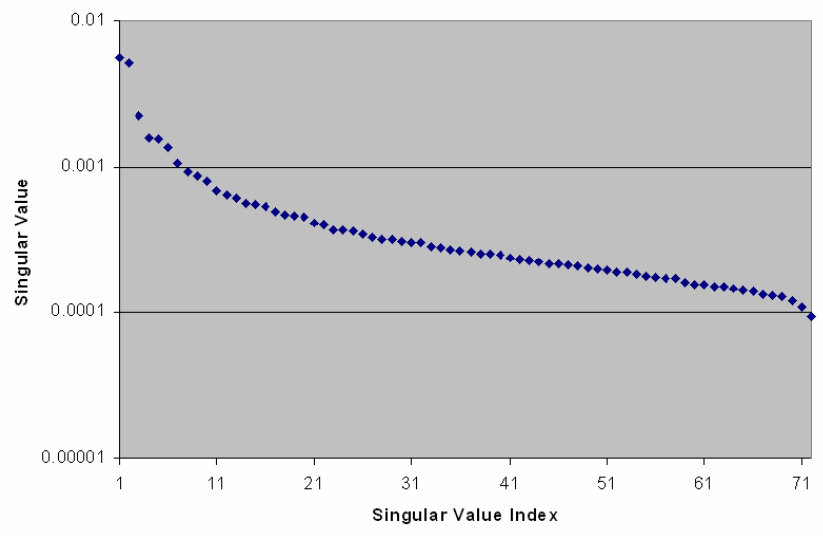

Figure 4. Singular Values Spectrum of $\mathbf{O}_c$

5. Conclusions and Future Work

This work contributes a new computational algorithm to capture the effects of unlike assembly neighbors on the assembly-averaged few-group parameters, without having to resort to color-set calculations. The main objective of this work is to provide a proof-of-principle demonstration for the proposed algorithm. The algorithm is based on the basic hypothesis of homogenization theory - that is if the exact solution is utilized to set boundary conditions for single-assembly calculations, the core-wide model would conserve all assembly's integral properties. We take advantage of this by setting up a minimization problem that measures the discrepancy between macroscopic attributes determined via core-wide and assembly calculations and accordingly updates the single-assembly boundary conditions. The required sensitivity information to solve the minimization problem is obtained via the Efficient Subspace Method. ESM exploits the continuous dimensionality reduction inherent in multi-scale models by finding low rank revealing decompositions to large dense sensitivity matrices, otherwise considered computationally intractable to evaluate using conventional sensitivity analysis techniques.

Given the exploratory nature of this work, a multi-phase approach will be adopted for implementing the proposed algorithm. The first phase, represented by this work, reduced the homogenization errors resulting from collapsing the energy variable only. Both single-assembly and core-wide calculations were modeled using a nodal diffusion code, the NESTLE code. The next phase will focus on removing errors originating from spatial homogenization and a transport model will be employed for single-assembly calculations.

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