Reduced Order Modeling of the Forward Eigenvalue Problem

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INTRODUCTION

The construction of reduced order models for high fidelity models is now considered an important objective in support of all engineering activities which require repeated execution of the simulation. The reduced model must be computationally inexpensive to allow its repeated execution, and must be computationally accurate in order for its predictions to be credible. This summary combines a well-known approach for reduction, the proper orthogonal decomposition [1], with a range finding algorithm from linear algebra to reduce the dimensionality of the state space [2]. This results in reducing the effective size of the model equations which translates in reduced computational cost. Unlike conventional POD algorithms, this approach provides an upper bound on the error resulting from the reduction. This allows the user to define the desired accuracy a priori which controls the maximum allowable reduction. We demonstrate the utility of this approach using an eigenvalue radiation transport model, where the accuracy is selected to match machine precision.

MATHEMATICAL DESCRIPTION

Consider a generalized eigenvalue problem

$$\mathbf{L}(u)\phi = \lambda \mathbf{F}(u)\phi \tag{1}$$

where $\mathbf{L} \in \mathbb{R}^{n\times n}$ and $\mathbf{F} \in \mathbb{R}^{n\times n}$ are matrix operators that describe the numerically-discretized neutron transport loss and production operators, respectively; λ is the largest eigenvalue associated with the eigenvector $\phi \in \mathbb{R}^n$ which denotes the state (i.e. the flux) and sometimes called the fundamental forward flux solution. The $\mathbf{L},\mathbf{F}$ and λ are dependent on the p model parameters described by a vector $u \in \mathbb{R}^p$.

Now, consider a response R that is a linear functional of the flux:

$$R = \Sigma(u)^T \phi \tag{2}$$

with constraints:

$$\Sigma_N{}^T \phi = N \tag{3}$$

where $\Sigma(u)$ is a vector whose elements are dependent on the input parameters. The Σ_N is a vector of weights that determine the normalization condition and N is the normalization constant.

Reactor calculations involve the repeated solution of Eq. 1, each time with different input parameters. A relevant application for this is the repeated execution of lattice physics calculations to functionalize the few-group cross-sections in terms of core neutronics and thermal-hydraulics conditions. Our goal is to transform Eq. 1 using POD techniques into a reduced order system of equations that can be accurately and efficiently solved for the range of input parameters conditions that are of interest to reactor calculations. Earlier work using range finding algorithms (recalled later in the discussion) has shown that all possible flux perturbations belong to a small active subspace of size r [3-4]. This means, using POD language, that instead of solving for the flux in the original space, one can confine the search for the flux to the active subspace only. In doing so, the system of equations to be solved is reduced in size from n to r.

Mathematically, the idea may be described as follows: assume that the perturbed flux varies along a subspace $\mathbb{C}$ which is spanned by a basis or r independent vectors: $\{\theta_1,\theta_2,\cdots,\theta_r\}$. Now consider a general perturbation in the input parameters, the perturbed eigenvalue problem is given by:

$$\tilde{\mathbf{L}}(\tilde{u})\tilde{\phi} = \tilde{\lambda}\tilde{\mathbf{F}}(\tilde{u})\tilde{\phi} \tag{4}$$

where '~' indicates the perturbed terms. The perturbed flux can be rewritten as:

$$\tilde{\phi} = \left(\mathbf{\Theta}\mathbf{\Theta}^T + \mathbf{\Theta}^{\perp}\mathbf{\Theta}^{\perp T}\right)\tilde{\phi} = \mathbf{\Theta}\mathbf{\Theta}^T\tilde{\phi} \tag{5}$$

where $\mathbf{\Theta} = [\theta_1,\theta_2,\cdots,\theta_r]$ and $\mathbf{\Theta}^{\perp} = [\theta_{r+1},\theta_{r+2},\cdots,\theta_n]$ are orthonormal matrices such that $\mathbf{\Theta}\mathbf{\Theta}^T + \mathbf{\Theta}^{\perp}\mathbf{\Theta}^{\perp T} = \mathbf{I}$ is the identity matrix.

To find the active subspace, we employ a range-finding algorithm which is recalled here [2]: consider a matrix $\mathbf{A}$ where one is interested in identifying its effective range spanned by the columns of an orthonormal matrix $\mathbf{\Theta} \in \mathbb{R}^{n\times r}$ such that some user-defined tolerance is satisfied in an upper bound sense, i.e., $\left\| \left(\mathbf{I}\mathbf{\Theta}\mathbf{\Theta}^T \right) \mathbf{A} \right\| \le \varepsilon$. It can be shown that the matrix $\mathbf{\Theta}$ satisfying this inequality can be determined via r+s randomized matrix-vector products of the form $\mathbf{A}p_i$, where r is the rank of the matrix, and s a small number representing few additional random samples, $s = 10$ is conservative for most applications. These matrix-vector products can be calculated by executing the forward model in forward mode with random input parameters perturbations. Details on this may be found in earlier work [4].

The power of this algorithm is that it finds a hard upper-bound on the error. This allows the analyst to decide on the maximum allowable error a priori, i.e., before the reduced system of equations is solved, and employ the algorithm to pick the minimum rank r that satisfies this error criterion. This is the core difference between this approach and traditional snapshots algorithm commonly used in POD techniques [5]. In the snapshot approach, the solution at different times employing reference parameters values is utilized to form the basis for the active subspace. There is however no guarantee that the error resulting from the reduction can be constrained for all possible parameters perturbations.

DETAILS OF IMPLEMENTATION

Now, combining Eq. (4) and Eq. (5) gives

$$\mathbf{P}\tilde{\mathbf{L}}\left(\tilde{u}\right)\mathbf{\Theta}\mathbf{\Theta}^T\tilde{\phi} = \tilde{\lambda}\mathbf{P}\tilde{\mathbf{F}}\left(\tilde{u}\right)\mathbf{\Theta}\mathbf{\Theta}^T\tilde{\phi} \tag{6}$$

where $\mathbf{P} \in \mathbb{R}^{r\times n}$ is a pre-conditioner. For this simple demonstration, we choose $\mathbf{P} = \mathbf{\Theta}^T$, thus Eq. (6) becomes:

$$\mathbf{\Theta}^T\tilde{\mathbf{L}}\left(\tilde{u}\right)\mathbf{\Theta}\mathbf{\Theta}^T\tilde{\phi} = \tilde{\lambda}\mathbf{\Theta}^T\tilde{\mathbf{F}}\left(\tilde{u}\right)\mathbf{\Theta}\mathbf{\Theta}^T\tilde{\phi} \tag{7}$$

Let $\hat{\mathbf{L}} = \mathbf{\Theta}^T\tilde{\mathbf{L}}\mathbf{\Theta}, \hat{\mathbf{F}}\mathbf{\Theta} = \mathbf{F}\tilde{\mathbf{\Theta}}$, and $\hat{\phi}\mathbf{\Theta} = \tilde{\phi}$, therefore, the POD reduced order model becomes:

$$\hat{\mathbf{L}}\hat{\phi} = \hat{\lambda}\hat{\mathbf{F}}\hat{\phi} \tag{8}$$

where $\hat{\mathbf{L}} \in \mathbb{R}^{r\times r}, \hat{\mathbf{F}} \in \mathbb{R}^{r\times r}, \hat{\phi} \in \mathbb{R}^r$ and $\hat{\lambda}$ is the eigenvalue approximated by the reduced order model.

NUMERICAL EXPERIMENT

The case study is based on a two-group diffusion model employing Anistratov's test problem setups in 1-D slab geometry with two fuel assemblies [6]. The state is described by the two-group flux solution. The inputs parameters are represented by the two-group cross sections. The model schematic is shown in Fig. 1. Each assembly contains only one kind of fuel pin cells, with 8 pin cells per assembly, and the associated specification are listed in Table I.

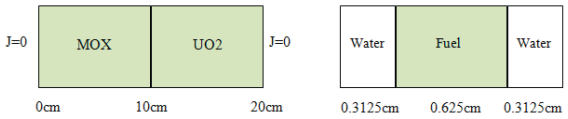

Figure 1. Model Layout

The responses are defined in accordance to Eq. (2):

$$R_i = \Sigma_i^T\phi, \text{ for } i = 1,\cdots,256 \tag{9}$$

with reference values for $\Sigma_i = e_i$, where e_i is the standard basis vector with all its elements equal to zero except the i^{th} element is equal to one; $\phi \in \mathbb{R}^{256\times 1}$, and the first 128 values of ϕ denote the fast group fluxes, the remaining values denote the thermal group fluxes.

The reduced order model is exercised with cross-sections perturbed by 10% of their reference values. For benchmarking the reduced order model's predictions, the exact perturbed responses are calculated using direct forward perturbation which requires a full forward model execution. Fig. 2 shows the discrepancy in the eigenvalue, and Fig. 3 shows the discrepancy in the flux. The x-axis in Fig. 2 and Fig. 3 runs from 1 to 256, which represents the size of the active subspace, and the discrepancy in both figures is defined by:

$$rms = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_{i,\text{ exact}} - x_{i,\text{ approx}}}{x_{i,\text{ exact}}}\right)^2} \tag{10}$$

where N=1 and N=256 for the eigenvalue and flux figures, respectively.

Table I. Cross Section Data *

	Σ_t^1	$\Sigma_{s,0}^{1\to1}$	$\Sigma_{s,0}^{1\to2}$	χ^1	Σ_t^2	$\Sigma_{s,0}^{2\to2}$	Σ_f^2	ν_f^2
MOX	0.2	0.185	0.015	1	1.2	0.9	0.3	1.5
UO2	0.2	0.185	0.015	1	1.0	0.9	0.1	1.5
Water	0.2	0.17	0.03	0	1.1	1.1	0	0

* $\Sigma_f^1, \nu_f^1, \overline{\mu}_0^1, \Sigma_{s,0}^{2\to1}, \chi^2, \overline{\mu}_0^2$ are all zeros .

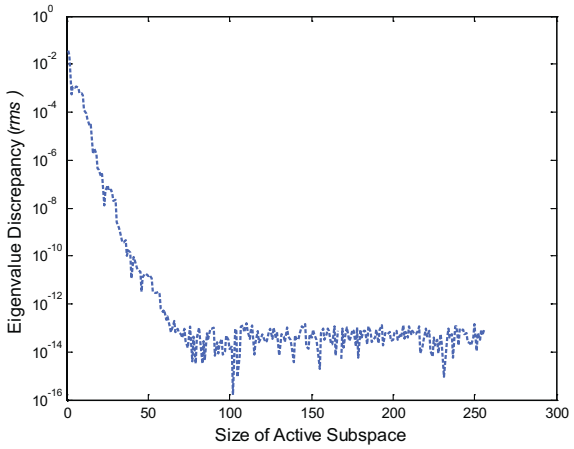

Figure. 2 ROM-predicted Eigenvalue

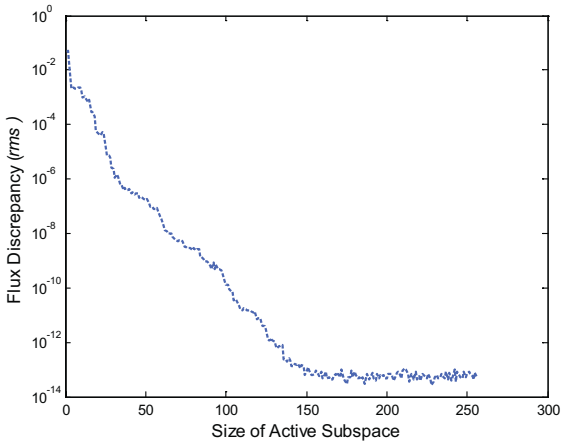

Figure 3. ROM-prediced Flux

CONCLUSIONS

This summary has introduced a reduced order modeling approach that combines advantages of POD techniques and range finding algorithms. POD techniques constrain the state solution to a subspace of size r in order to reduce the computational cost required to solve the model's equations. When r is much smaller than n, the original dimension of the state space, repeated solution of the model's equations for a range of parameters conditions becomes computationally feasible. The range finding algorithm provides a rigorous estimate of the error resulting from the reduction which can be set by the user to meet maximum allowable errors. The bulk of the computational cost lies in the construction of the active subspace which requires the execution of the forward model a number of times proportional to its rank r, which can be done off-line as a pre-computation.

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