Reduced Order Modeling for Multi-Physics Problems

Youngsuk Bang and Hany S. Abdel-Khalik

North Carolina State University, Raleigh, North Carolina, USA
ybang@ncsu.edu, adbelkhalik@ncsu.edu

INTRODUCTION

Reduced order modeling (ROM) has been recognized as an indispensable approach when the engineering analysis requires many executions of high fidelity simulation codes. Examples of such engineering analyses in neutronics calculations, representing the main focus of our current work, include the functionalization of few-group cross-sections using lattice physics calculations in terms of the various core conditions, e.g. depletion, temperature, etc. Other examples are sensitivity analysis, design optimization, and uncertainty quantification.

ROM constructs a surrogate model with quantifiable accuracy which can replace the original code for subsequent engineering analysis calculations. Past work [1] has demonstrated the application of a new hybrid approach to constructing a surrogate model for a single physics code with many input parameters. In this summary, we extend the approach to handling codes consisting of serially coupled physics codes. We show that the hybrid approach can be easily extended to render reduction of the data streams transferred between the different physics codes without compromising the overall accuracy of the coupled codes.

The main idea of the ROM approach is reducing the dimensionality of the input parameters, the state, or the responses spaces, by projection onto the so-called *active* subspaces. One can show that parameter perturbations orthogonal to the active parameter subspace produce variations in the state and the responses of interest that can be bounded a priori by a user-defined error tolerance. This is a key requirement to ensure the constructed surrogate model is robust for all possible applications.

Different approaches have been proposed to constructing the active subspace depending on where the reduction is rendered. For example, in the state space, the snapshots algorithm is used [2], wherein the forward model is executed a number of times with random parameter perturbations, and a range finding algorithm is used to find the mathematical range, i.e., the active subspace, of the flux variations. In the parameter space, the first order derivatives of pseudo[1] responses with respect to parameters, sampled at the random points in the parameter space, are employed to construct the active subspace [1].

[1] A pseudo response is a random linear combination of the model's responses. See Ref [1] for more details on its construction.

This summary extends these developments to multi-physics only. Our development is currently limited to serially coupled codes only, where the output of one code is passed as input to the next code in the chain. We take neutronics calculations as an example, whereby resonance and self-shielding calculations represent one physics code, necessary to calculate the effective multi-group cross-sections, before passing them to the next physics code representing transport calculations. The transport code employs the effective cross-sections to solve for he eigenvalue and the state (i.e., flux) and any responses of interest, e.g., pin powers, few-group cross-sections for subsequent downstream core-wide calculations. We show that while each physics code is reducible, by appropriately combining the active subspaces from each code using the idea of subspace intersection, further reduction can be achieved.

DETAILS OF IMPLEMENTATON

Assume that we have Model **A** and Model **B** whereby outputs of Model **A** are passed as inputs to Model **B** and consider the construction of the surrogate model for Model **B** :

Model **A** : $f_{\mathbf{A}}(\vec{x}) = \vec{y}$, where $\vec{x} \in \mathbb{R}^m$, $\vec{y} \in \mathbb{R}^n$

Model **B** : $f_{\mathbf{B}}(\vec{y}) = \vec{z}$, where $\vec{y} \in \mathbb{R}^n$, $\vec{z} \in \mathbb{R}^l$

Note that the **outputs** of Model **A** can be reduced by identifying a subspace determined solely by Model **A**, using the snapshots algorithms described earlier:

$$\vec{y} \simeq \mathbf{Q}_{\mathbf{A}}\mathbf{Q}_{\mathbf{A}}^T\vec{y} = \mathbf{Q}_{\mathbf{A}}\vec{\alpha}, \quad \text{where } \mathbf{Q}_{\mathbf{A}} \in \mathbb{R}^{n\times r_{\mathbf{A}}},\ \vec{\alpha} \in \mathbb{R}^{r_{\mathbf{A}}} \quad (1)$$

Eq. (1) means that the reduced output of Model **A** will be confined to the active subspace spanned by the column vectors of the matrix $\mathbf{Q}_{\mathbf{A}}$, implying that Model **B** will not see any components that are orthogonal to the active subspace generated by Model **A**. Therefore, by a simple transformation, the inputs to model **B** are now effectively reduced to $r_{\mathbf{A}}$ components only. Note that, at this point, Model **B** has not been utilized yet.

Now, considering Model **B** and for now independently of the reduction rendered by Model **A**, the vector $\vec{y}$ represents the **inputs** to Model **B** and therefore can be reduced using an ROM algorithm by sampling the

derivatives of the outputs of Model **B** with respect to its inputs, as mentioned earlier:

$$\vec{y} \simeq \mathbf{Q_B}\mathbf{Q_B}^T\vec{y} = \mathbf{Q_B}\vec{\beta}, \quad \text{where } \mathbf{Q_B} \in \mathbb{R}^{n\times r_B},\ \vec{\beta} \in \mathbb{R}^{r_B} \quad (2)$$

Eq. (2) means that the components of $\vec{y}$ belonging to the active subspace spanned by the column vectors of $\mathbf{Q_B}$ are the most influential to the outputs of Model **B**. The implication is that one need not consider the impact of all $\vec{y}$ components that are orthogonal to the active subspace as determined solely by Model **B**.

Now, in general, one would not expect the active subspace represented by $\mathbf{Q_A}$ to be the same as the $\mathbf{Q_B}$ subspace. In other words, the components of the active subspace belonging to the $\mathbf{Q_A}$ subspace which are also orthogonal to the $\mathbf{Q_B}$ subspace will not be influential to the overall output of the combined model, therefore these components should be discarded, leading to further reduction of the active subspace at the interface between the two models. If the two subspaces determined by Model **A** and **B** happen to be exactly the same, an unlikely situation, then one would not be able to render any further reduction.

Mathematically, this situation may be described as follows: among the r_A components of $\vec{y}$ determined from Model **A**, only the components spanned by $\mathbf{Q_B}$ subspace can contribute to the output response of Model **B**. Therefore, we can define the matrix $\mathbf{Q} \in \mathbb{R}^{n\times r}$ whose range spans the common components (i.e. the intersection between the two subspace) in the $\mathbf{Q_A}$ and $\mathbf{Q_B}$ subspaces. It is natural to expect that the size of the intersection subspace to be smaller than the minimum of the two model-specific subspaces, i.e.,

$$r \le \min\{r_A, r_B\} \quad (3)$$

If r is smaller than either values, one could further reduce the input parameters for Model **B**; thereby leading to a more efficient construction of the surrogate model.

The intersection algorithm is summarized below (See Refs. [1] and [3] for more details) into two steps. Step 1 is a standard snapshots ROM algorithm applied to Model **A**. In Step 2, the derivatives of Model **B**'s outputs are employed to construct an active subspace for its input parameters. The two subspaces are combined using a projection technique which filters out all the components that lie outside the intersection subspace.

Algorithm: Intersection Subspace Construction

Step 1) Construct the active subspace for Model **A**

Generate the random inputs $\left[\vec{x}^{(1)} \quad \cdots \quad \vec{x}^{(k)}\right]$

Compute the outputs $\mathbf{Y} = \left[\vec{y}^{(1)} \quad \cdots \quad \vec{y}^{(k)}\right]$

Determine the rank r_A using a range finding algorithm

Calculate QR decomposition of $\mathbf{Y} = \mathbf{Q_A}\mathbf{R_A}$

Step 2) Construct the intersection subspace:

Generate random inputs $\left[\vec{y}^{(1)} \quad \cdots \quad \vec{y}^{(k)}\right]$

Calculate derivatives of pseudo responses of Model **B**

$$\mathbf{D} = \left[\frac{\partial z_{pseudo}^{(1)}}{\partial \vec{y}^{(1)}} \quad \cdots \quad \frac{\partial z_{pseudo}^{(k)}}{\partial \vec{y}^{(k)}}\right]$$

where $z_{pseudo}^{(j)} = \sum_i \gamma_i^{(j)} z_i^{(j)}$

Project onto the basis of Model **A**

$$\mathbf{U} = \mathbf{Q_A}\mathbf{Q_A}^T\mathbf{D}$$

Using a range finding algorithm, determine the rank r

Calculate QR decomposition of $\mathbf{U} = \mathbf{QR}$

Once determined, the input parameters of Model **B** can be transformed by:

$$\vec{y} \approx \mathbf{Q}\mathbf{Q}^T\vec{y} = \mathbf{Q}\vec{y}_r \quad \text{where } \mathbf{Q} \in \mathbb{R}^{n\times r} \quad (4)$$

NUMIERCAL TESTS AND RESULTS

For the purpose of demonstration, the surrogate model for a pin-cell model is constructed. The TSUNAMI-2D which is a SCALE control module that facilitates the application of sensitivity and uncertainty analysis to criticality safety models [4] is used as a simulation code. The resonance self-shielding calculation (BONAMI/CENTRM) and transport solver (NEWT) are considered as Model **A** and Model **B**, respectively. Nuclide number densities and fuel and moderator temperatures are inputs of Model **A**. Self-shielded Macroscopic reaction cross sections in fuel region, $\vec{\Sigma} \in \mathbb{R}^{18656}$ (44 energy group, 93 nuclides, 7 reaction) are outputs of Model **A** and passed as inputs to Model **B**. The scalar flux (44 energy group, 4 mixture) are considered as output responses of Model **B**.

To determine the size of the basis for $\vec{\Sigma}$, the singular value spectrum of the matrices **Y**, **D** and **U** are calculated. The singular values are measures of the importance of each direction in the active subspace. Fig. 1 shows that the singular values for the intersection subspace decay most rapidly compared to the active subspaces determined by Model **A** and **B**. The size of intersection subspace is determined to be 150 based on a user-defined tolerance of 1.e-6, this represents a reduction from 18656 input values down to 150 values only. Note that the size of the active subspaces for Models **A** and **B** are 4-5 times higher at the same tolerance.

After the subspace is determined, a surrogate model is constructed using a quadratic polynomial regression analysis for the 150 reduced inputs. If the surrogate is constructed properly, it can be used in lieu of BONAMI/-CENTRM-NEWT. As an example of a typical application of TRITON, it is used to generate the homogenized few-group (FG) cross-section as a function of depletion which is needed for downstream calculations. This is done using the BONAMI-CENTRM-NEWT-ORIGEN sequence. ORIGEN is used to perform depletion. In our current work, the ORIGEN code is not reduced yet. TRITON was used to deplete the pin cell model and calculate at each burnup step the few-group cross-sections. The same calculations were repeated using the surrogate model instead to replace the transport solver, i.e. NEWT. Fig. 2 compares these two results for $\nu\Sigma_f$ in the fast region. The results indicate that the discrepancies over the entire range of depletion are negligible, which is a good assessment of the robustness of the surrogate model.

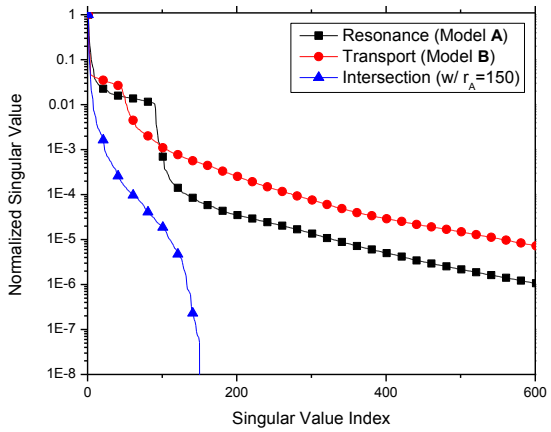

Fig. 1 Singular Value Spectra

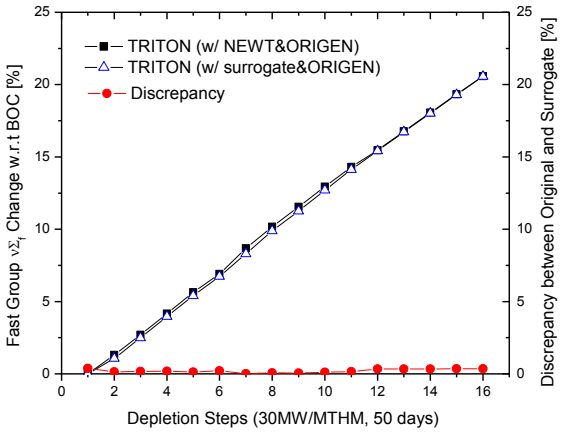

Fig. 2 Robustness of the Surrogate Model

CONCLUSIONS

This summary presented a new extension of the hybrid subspace methodology introduced previously for single physics models [1], to multi-physics models. Given that multi-physics models interface a huge volume of information between each two physics models, the developed algorithm finds an intersection between the subspaces calculated by each physics model to render further reduction. Results indicate that significant reduction is possible which reduces the computational cost to generate the surrogate. Based on previous experience with subspace methods, we expect that similar gains will be achieved with full assembly models. Ultimately, the objective of this work is to generate a surrogate model that can be used to perform lattice physics calculations on the fly for down-stream core calculations. We believe this is possible since existing lattice physics calculations take anywhere from few-minutes (e.g. commercial lattice physics codes) to several hours. With the surrogate however, these calculations can be done in fractions of a sec, since one needs only evaluate a simple polynomial expression to calculate the few-group cross-section. Another objective is to extend the surrogate to enable the propagation of multi-group cross-sections uncertainties, a task that is currently intractable with existing lattice physics capabilities.

REFERENCES

1. Y. BANG, H. ABDEL-KHALIK, J. HITE, "Hybrid Reduced Order Modeling Applied to Nonlinear Models," *International Journal for Numerical Methods in Engineering*, DOI:10.1002/nme.4298, (2012).
2. P. HOMES, J. LUMLEY, G. BERKOOZ, *Turbulence Coherent Structures, Dynamical Systems and Symmetry*, Cambridge University, Cambridge, (1996).
3. N. HALKO, P. MARTINSSON, J. TROPP, "Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions." *SIAM Review*, 53(2), (2011).
4. SCALE 6.1, "A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations", ORNL, June, (2011).