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Semi-Intrusive Reduced Order Modeling for Complex Thermal hydraulic System Code

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1. Introduction

Reduced Order Modeling (ROM) is a mathematical Method for reducing computational cost in simulation, i.e., construct a compact model with less dimensionality and use it for subsequent calculations (especially, many query problems, e.g., design optimization and uncertainty quantification). The most well-known method is a projection-based method, in which the influential subspaces are extracted and the system of equations is projected into the active subspace to reduce the dimensionality. It has been demonstrated that a basis function can be readily constructed by random sampling, and the sampling based ROM is suitable for the calculation of reactor physics problems [1~2].

Basic formulation of ROM can be described as follows. Let a full-order model which is nonlinear dynamic equation as follow:

$$\begin{cases} \dfrac{d\vec{x}(t)}{dt} = \mathbf{A}(\vec{p})\vec{x}(t) + \mathbf{B}(\vec{p})u(t) + \vec{f}\left(\vec{p},\vec{x}(t),\vec{u}(t)\right) \\ \vec{y}(t) = \mathbf{C}(\vec{p})\vec{x}(t) \end{cases}$$

where,

$$\vec{x}(t) \in \mathbb{R}^{n},\quad \vec{u}(t) \in \mathbb{R}^{m},\quad \vec{y}(t) \in \mathbb{R}^{q},$$
$$\mathbf{A}(\vec{p}) \in \mathbb{R}^{n \times n}, \mathbf{B}(\vec{p}) \in \mathbb{R}^{n \times m}, \mathbf{C}(\vec{p}) \in \mathbb{R}^{q \times n}$$

With a reduced basis which captures the most of dynamic behaviors of the state variables $\vec{x}(t)$, the system of equations can be transformed into reduced subspace by projection as:

$$\begin{cases} \dfrac{d\vec{x}_r(t)}{dt} = \mathbf{A}_r(\vec{p})\vec{x}_r(t) + \mathbf{B}_r(\vec{p})u(t) + \mathbf{Q}^T \vec{f}\left(\vec{p},\vec{x}(t),u(t)\right) \\ \vec{y}(t) = \mathbf{C}_r(\vec{p})\vec{x}_r(t) \end{cases}$$

where,

$$\vec{x} \approx \mathbf{Q}\vec{x}_r, \mathbf{Q} \in \mathbb{R}^{n \times r},$$
$$\vec{x}_r(t) \in \mathbb{R}^{r},\quad \vec{u}(t) \in \mathbb{R}^{m},\quad \vec{y}(t) \in \mathbb{R}^{q},$$
$$\mathbf{A}_r(\vec{p}) = \mathbf{Q}^T\mathbf{A}(\vec{p})\mathbf{Q} \in \mathbb{R}^{r \times r}, \mathbf{B}_r(\vec{p}) = \mathbf{Q}^T\mathbf{B}(\vec{p})\mathbf{Q} \in \mathbb{R}^{r \times m},$$
$$\mathbf{C}_r(\vec{p}) = \mathbf{C}(\vec{p})\mathbf{Q} \in \mathbb{R}^{q \times r}$$

The ROM has been examined for various large-scale engineering simulations and proved its applicability in uncertainty quantification, design optimization and optimal control [3]. Though the mathematically well-developed, the implementation into the existing computation tools would not be straightforward. It is important to note that the current real-engineering simulation tools has been developed by many authors over the long period of times and included a number of correlations and functionalized modules, which makes the complex inter-module dependency and requires iterative numerical procedures. Considering the overall efforts for development and verification/validation, the modification of the simulation code system would be very difficult for reduced order modeling and developing new code system would not be practical. Therefore, the non-intrusive approach would be preferred for legacy codes or complexly coupled code systems.

In this study, a hybrid reduced order surrogate modeling approach has been investigated and implementing into the existing engineering thermal hydraulic system code for nuclear power plant accident simulations, i.e. SPACE has been examined [4]. Note that the code consists of a large number of sub-modules and functions and adopts several numerical methods including iterative approach. The reduced order modeling methods has been applied to a module having most of computational cost, i.e., pressure difference calculation. Reduced basis has been constructed by using snapshot samples and applicability of reduced order modeling approach has been examined with a simple problem and complex problem.

2. Mathematical Formulations

2.1 Pressure Difference Calculation

A numerical solution method has been applied to the three field balance equations discretized spatially on a staggered grid and solved employing a semi-implicit time advancement method. The finite difference form of the momentum conservation equations is first of all, rearranged into a summation and difference form, and solved by inverting the coefficient matrix to obtain the linear expressions of velocities as functions of neighboring cell pressures. Once the explicit face velocity and pressure coefficients are determined from the momentum conservation equations, the mass and internal energy balance at scalar cells can be developed by substituting the new time face velocities into mass and internal energy conservation equations. The new time pressure equation at each scalar cell as functions of neighboring cells can be then developed from the solution of the mass and internal energy conservation equations.

2.2 Reduced Order Surrogate Modeling

Assume that the output vector can be represented as a linear combination of basis vectors [5]:

$$\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_t \\ \vdots \\ x_T \end{bmatrix} = a_1(\vec{p})\vec{q}_1 + \cdots + a_i(\vec{p})\vec{q}_i + \cdots + a_r(\vec{p})\vec{q}_r = \mathbf{Q}\vec{a}$$

where,

$\vec{p} = \begin{bmatrix} p_1 \\ \vdots \\ p_i \\ \vdots \\ p_m \end{bmatrix}$ and $\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_t \\ \vdots \\ x_T \end{bmatrix}$ are vectors of input parameters and output responses, respectively. $a_i(\vec{p})$ is a coefficient which is a function of $\vec{p}$. $\mathbf{Q} = [\vec{q}_1 \ \cdots \ \vec{q}_r]$ is a matrix with reduced order basis. To construct a reduced order surrogate model, matrix $\mathbf{Q}$ and vector $\vec{a}$ should be determined.

The basis can be constructed by random sampling and matrix decomposition methods [2]. As the number of basis increased, the size of the subspace that the basis represents would be extended, i.e., the more variations can be captured and reconstructed. The sufficiency of the basis can be examined by calculating the in-active component with additional samples.

The reduced order surrogate can be constructed by approximating the relation between input parameters and coefficients, i.e., $\vec{p}$ and $\vec{a}$. Firstly, the training set should be prepared, i.e., pairs of $\vec{p}^{(i)}$ and $\vec{a}^{(i)}$ for *i*th sample. Using those samples, the surrogate model can be constructed with various methods. In this study, the linear regression method and artificial neural network method have been applied.

Algorithm 1: Randomized Basis Construction

(1) Define a range of input parameter variations.
(2) Prepare an input parameter set by random sampling: $\vec{p}^{(i)}$, *i=1, ..., r*.
(3) Run a simulation code with a set of perturbed input parameters.
(4) Prepare the output response sets $\vec{x}^{(i)}$, *i=1, ..., r*.
(5) Perform QR decomposition: $\mathbf{QR} = \begin{bmatrix} \vec{x}^{(1)} & \cdots & \vec{x}^{(r)} \end{bmatrix}$.
(6) Check the inactive subspace with additional sample: $\vec{x}^{inact} = \left\| \left(\mathbf{I} - \mathbf{QQ}^T\right)\vec{x} \right\|_2$.
(7) If $\varepsilon < \vec{x}^{inact}$, increase *r* and repeat from (1).

Algorithm 2: Building a Training Set for Surrogate Modeling

Assume a surrogate model $\vec{x} = \mathbf{Q}\vec{a}$.
(1) Define a range of input parameter variations.
(2) Prepare an input parameter set by random sampling: $\vec{p}^{(i)}$, *i=1, ..., r*.
(3) Run a simulation code with a set of perturbed input parameters.
(4) Prepare the training data pairs: $\vec{a}^{(i)}$ and $\vec{x}^{(i)}$, *i=1, ..., r*.
(5) Determine $\vec{a}^{(i)} = \mathbf{Q}^{\mathrm{T}}\vec{x}^{(i)}$.

For Linear Regression with a Least Square Method,

Assume a linear relationship $\vec{a} = \mathbf{C}\vec{p} + \vec{\beta}$ where, $\vec{a} \in \mathbb{R}^{r\times 1}$, $\vec{p} \in \mathbb{R}^{m\times 1}$, $\vec{\beta} \in \mathbb{R}^{r\times 1}$ and $\mathbf{C} \in \mathbb{R}^{r\times m}$.
(6) Prepare the training data pairs: $\vec{p}^{(i)}$ and $\vec{a}^{(i)}$, *i=1, ..., r*.

For Artificial Neural Network (ANN),

Assume a relationship $\vec{a} = ANN(\vec{p})$.
(6) Prepare the training data pairs: $\vec{p}^{(i)}$ and $\vec{a}^{(i)}$, *i=1, ..., n*.
(7) Construct the ANN.
(8) Calculate the prediction error with a test data set.

3. Numerical Demonstration

3.1 FLECHET-SEASET Boil-Off Experiment

The boiloff test procedure is similar to that for a reflood test, except that no bundle flooding rate is used. Once the bundle had been filled with saturated water at the test pressure, the rod power was turned on and the bundle was allowed to boil.

In **Figure 1**, the distribution of PCT predicted by random perturbations of input parameters have been presented.

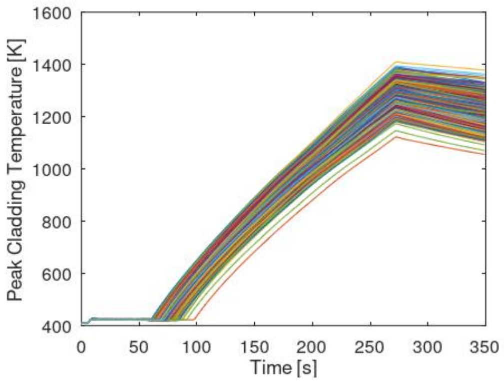

Figure 1. Distribution of PCT Predicted by Random Sampling of Input Parameters

The **Algorithm 1** has been applied for constructing the basis. As can be seen in Figure 2, the inactive components which are not captured by the basis would be decreased rapidly as the number of basis increased. Note that the normalized 2-norm of inactive components would decrease slowly with more than 20 bases. This may be because there are a lot of small fluctuations in output responses which are different with the overall patterns of output response changes.

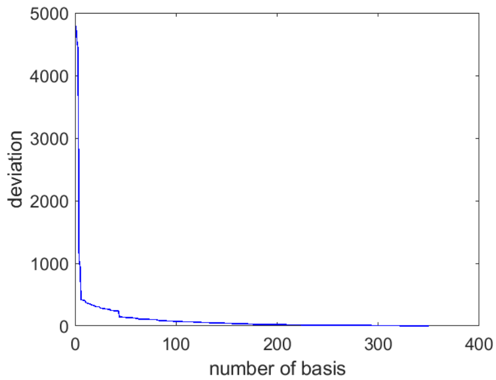

Figure 2. Normalized 2-Norm of Inactive Component (i.e., $\varepsilon^{inact} = \left\| \left(\mathbf{I} - \mathbf{Q}\mathbf{Q}^T \right) \vec{x} \right\|_2$)

In this study, as a preliminary test, the size of the basis has been determined as 20 and **Algorithm 2** has been applied to build a training set for constructing surrogates. Firstly, a linear regression model has been employed to identify the relationship between the input parameters, $\vec{p}$ and the coefficients, $\vec{a}$. After the linear regression is completed the state variable is estimated by

$$\vec{x} = \mathbf{Q}\vec{a}^r \tag{1}$$

where, $\vec{a}^r$ a function of the input parameters, indicates the active degree of freedom obtained by the linear regression. **Figure 3** compares the PCT calculated by SPACE and the reduced order surrogate model.

Secondly, a nonlinear surrogate has been constructed by representing the relationship between input parameters $\vec{p}$ and the coefficients of the surrogate $\vec{a}$ as a neural network. For demonstration, 4 hidden layers with 10, 250, 500 and 20 neurons are used to build a neural network. The python and scikit-learn package have been used for artificial neural network modeling [6]. **Figure 4** presents the peak cladding temperature calculated by SPACE along with the PCT estimated by ROM. Depending on the number of layers, neurons and perturbations, the accuracy has been varied with average 8.23% and standard deviation 3.04% of relative errors.

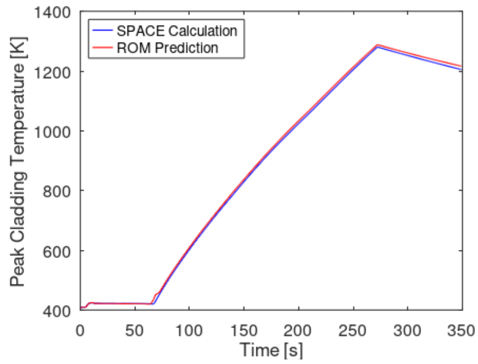

Figure 3. SPACE Calculation vs. Linear Regression based ROM-Surrogate Prediction

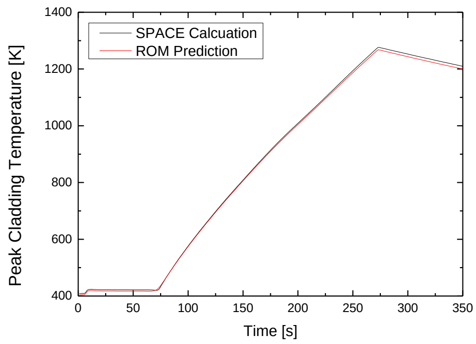

Figure 4. SPACE Calculation vs. Neural Network based ROM-Surrogate Prediction

3.2 Implementation onto SPACE (MIT)

The objective of MIT Pressurizer Test is to investigate heat transfer process occurring in pressurizer. Subcooled liquid is injected into a pressurizer partially full of saturated water. Injection is terminated at 40 s. A balance between interfacial and wall condensation and steam compression determines pressure in test section. The

The **Algorithm 3** below has been applied to MIT Pressurizer Test. The time interval during the SPACE calculation is often less than 0.01 seconds. Therefore, not all solution vectors during the SPACE calculation are included in the training set.

As can be seen in **Figure 5**, the results of calculating the SPACE original matrix system and the reduced order matrix system are different. This difference is resulted because the reduced order matrix system does not include data for all time steps, but only data for specific time steps (i.e., 1s, 2s, …).

Algorithm 3: Constructing ROM in SPACE using Training Basis by building a training set

(1) Construct the training set by perturbation of input parameter.: $X = \left[X_{p=p_1} \quad X_{p=p_2} \quad L \quad X_{p=p_m} \right]$

Here , $X_{p=p_1} = \left[x^{t=t_0} \quad x^{t=t_1} \quad L \quad x^{t=t_n} \right]_{p=p_1}$,

$X_{p=p_2} = \left[x^{t=t_0} \quad x^{t=t_1} \quad L \quad x^{t=t_n} \right]_{p=p_2}$,

$X_{p=p_m} = \left[x^{t=t_0} \quad x^{t=t_1} \quad L \quad x^{t=t_n} \right]_{p=p_m}$ and the time interval is 1 second.

(2) Perform QR decomposition and determine the basis matrix.

(3) Calculate the rom in SPACE using the basis matrix from (2): $\mathbf{A}_r\mathbf{x}_r = \mathbf{y}_r$

(4) Calculate the pressure difference in SPACE

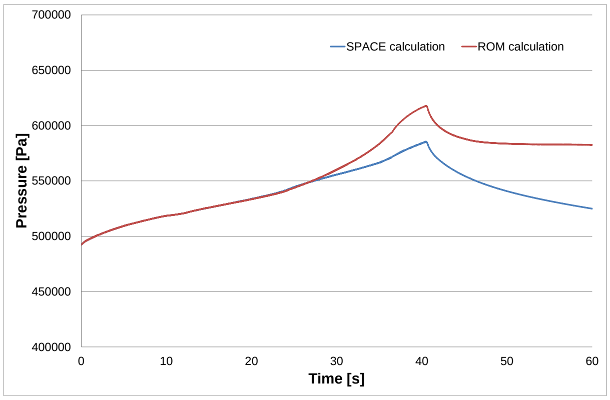

Figure 5. SPACE Calculation vs. ROM calculation

4. Conclusion

Reduced order surrogate model was developed employing a basis search algorithm together with multiple regression methods that fit the active degree of freedom as a function of input parameters. The linear regression and neural network models were applied for the validation of the FLECHET-SEASET Boil-Off Experiment to evaluate the reliability of ROM with particular interest in evaluating PCT. And the SPACE calculation about MIT Pressurizer Test was conducted using basis matrix obtained by ROM. The overall results present promising for application to time-dependent thermal hydraulic accident analysis.

Further research would be conducted to develop a more suitable intrusive ROM applying method on the SPACE considering the time steps under 1 second.

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