Feasibility Study on POD-based ROM for Predicting Thermal-Hydraulic Behaviors in Nuclear Systems

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1. Introduction

Physical phenomena in nuclear reactors involve complex three-dimensional thermal-hydraulic behaviors, requiring Computational Fluid Dynamics (CFD) analysis with high-density meshes for precise prediction. However, such high-fidelity simulations entail significant computational costs, posing a challenge for immediate reflection of diverse design or operational variations. To overcome these limitations, data-driven Reduced-Order Modeling (ROM) has recently emerged as an active field of research.

ROM is a technique that extracts key physical behaviors (modes) from Full-Order Model (FOM) data to enable rapid predictions through a low-dimensional model with drastically reduced computational overhead. In particular, Proper Orthogonal Decomposition (POD)-based methods [1,2] are widely utilized in thermal-hydraulic problems because they extract an optimal basis that most efficiently reconstructs the total energy of the flow field. By projecting dominant flow structures from high-dimensional snapshots onto orthogonal bases, POD-ROM reduces the system dimensionality, offering the advantage of near real-time flow field estimation across untrained parameter spaces. In this study, a POD-based ROM is implemented for a fundamental thermal-hydraulic problem to evaluate its applicability and performance.

2. Reduced-Order Modeling Method

This section briefly summarizes the core concepts and implementation procedure of the Proper Orthogonal Decomposition (POD)-based reduced-order modeling (ROM) approach employed in this study. The overall procedure is as follows. First, multiple snapshots are collected from high-fidelity flow simulations and assembled into a snapshot matrix. Subsequently, the dominant flow structures are extracted through Principal Component Analysis (PCA), which is mathematically equivalent to POD. This process yields a set of orthogonal basis vectors that optimally represent the flow field in an energy sense.

Once the reduced basis is obtained, the governing flow variables are projected onto this low-dimensional subspace. The temporal or parametric evolution of the corresponding modal coefficients is then approximated using interpolation, regression, or machine-learning-based surrogate models. Finally, the full flow field is efficiently reconstructed as a linear combination of the POD basis vectors and the predicted coefficients.

2.1 Construction of the Snapshot Matrix and Principal Component Analysis

The flow variables considered in the analysis, such as velocity, pressure, and temperature, are defined on a spatial grid and can be represented as column vectors by stacking the values at all grid points. Let each snapshot vector consist of n grid-based degrees of freedom. By collecting flow solutions obtained under m different operating conditions (e.g., inlet velocity, temperature, or flow rate), a snapshot matrix $Y \in \mathbb{R}^{n\times m}$ is constructed, where each column corresponds to a single snapshot.

To eliminate the mean component and focus on fluctuating features, the ensemble-averaged snapshot vector $\overline{y}$ is computed and subtracted from each snapshot.

The resulting mean-centered snapshot matrix is given by

$$Y_C = \begin{bmatrix} u_{11} - \overline{u_1} & u_{12} - \overline{u_1} & \cdots & u_{1m} - \overline{u_1} \\ u_{21} - \overline{u_2} & u_{22} - \overline{u_2} & \cdots & u_{2m} - \overline{u_2} \\ \vdots & \vdots & \ddots & \vdots \\ u_{n1} - \overline{u_n} & u_{n2} - \overline{u_n} & \cdots & u_{nm} - \overline{u_n} \end{bmatrix} \quad (1)$$

where u_{ij} denotes the value of the i-th grid point in the j-th snapshot, and $\overline{u_i}$ represents the mean value at the same grid location.

Applying Singular Value Decomposition (SVD) directly to Y_C yields a set of orthonormal basis vectors that optimally capture the dominant energetic structures of the flow field. However, in typical CFD applications, the number of spatial degrees of freedom n is significantly larger than the number of snapshots m (i.e., $n \gg m$), making direct SVD of Y_C computationally expensive. To alleviate this issue, the covariance matrix C is introduced.

$$\mathbf{C} = \mathbf{Y_C}^{T}\mathbf{Y_C} \quad (2)$$

The eigenvalue problem associated with C can be solved efficiently due to its reduced dimensionality $m\times$

m, and the resulting eigenvectors are subsequently used to construct the POD basis functions.

2.2 Reduced-Order Model Formulation and Modal Coefficient Prediction

After constructing the POD basis functions, the high-dimensional flow field can be approximated within a low-dimensional subspace spanned by a limited number of dominant modes. Let

$$\mathbf{\Phi} = [\phi_1, \phi_2, \cdots \phi_r] \in \mathbb{R}^{n\times r} \tag{3}$$

denote the matrix of the first r POD modes, where r $\ll \min(n, m)$. Then, The flow field $\mathbf{y} \in \mathbb{R}^n$ can then be approximated as

$$\mathbf{y} \approx \bar{\mathbf{y}} + \sum_{i=1}^{m} a_i \phi_i = \bar{\mathbf{y}} + \mathbf{\Phi a} \tag{4}$$

Where $\bar{\boldsymbol{y}}$ is the mean flow field and $\mathbf{a} = [a_1, a_2, \cdots a_r]^T \in \mathbb{R}^r$ represents the vector of modal coefficients.

For each snapshot $\boldsymbol{y}_j$, the corresponding modal coefficients are obtained through orthogonal projection:

$$\boldsymbol{a}_j = \mathbf{\Phi}^T(\boldsymbol{y}_j - \bar{\boldsymbol{y}}) \tag{5}$$
$$\mathbf{\Phi}^T\mathbf{\Phi} = \mathbf{I} \tag{6}$$

This projection minimizes the reconstruction error in the L_2 sense and ensures that the reduced-order representation retains the maximum possible energy for a given number of modes.

2.3 Modal Truncation and Energy Content

The number of retained modes r is determined based on the cumulative energy captured by the POD modes.

Let λ_i denote the i-th eigenvalue associated with the covariance matrix **C**. The relative energy contribution of the first r modes is defined as

$$E_r = \frac{\sum_{i=1}^{r} \lambda_i}{\sum_{i=1}^{m} \lambda_i} \tag{7}$$

The eigenvalues are typically arranged in descending order $\lambda_1 \geq \lambda_1 \geq \lambda_2 \cdots \geq \lambda_m$. In practice, the truncation level r is selected such that $E_r \geq \eta$, where η is a prescribed energy threshold (e.g., 99% or 99.9%).

In this study, the truncation level is selected such that E_r exceeds a prescribed threshold, ensuring that the dominant flow features are adequately represented while maintaining computational efficiency.

2.4 Surrogate Modeling for Modal Coefficients

To enable rapid prediction of the flow field under new operating conditions, surrogate models are constructed to approximate the relationship between input parameters and modal coefficients. Given a set of input parameters μ (e.g., inlet velocity, temperature, or Reynolds number), the modal coefficients are expressed as $\mathbf{a}(\boldsymbol{\mu}) = F(\boldsymbol{\mu})$, where $F(\cdot)$ denotes a regression or machine-learning-based mapping.

Various modeling strategies can be employed for this purpose, including polynomial regression, radial basis function interpolation, and neural networks. Once the surrogate model is trained using the snapshot data, the modal coefficients corresponding to unseen parameter values can be predicted at negligible computational cost.

2.5 Flow Field Reconstruction

The full-order flow field corresponding to a new parameter set is reconstructed by combining the predicted modal coefficients with the POD basis.

This reconstruction process enables efficient approximation of the high-fidelity solution without performing additional CFD simulations, thereby significantly reducing computational expense.

3. Feasibility Study of POD Method

To analyze nuclear thermal-hydraulic behavior by integrating Proper Orthogonal Decomposition (POD) with Computational Fluid Dynamics (CFD)—which relies on nonlinear Navier-Stokes equations and a turbulence model—it is essential to evaluate both the accuracy of the CFD model and the intrinsic properties of the POD.

In this study, CFD simulations were conducted for the lid-driven cavity flow [3,4], a benchmark case widely used for validating numerical schemes in laminar flow analysis, using the Reynolds number (Re) as a key parameter. The CFD results for various Reynolds numbers were utilized as snapshots for the POD. The values predicted by the POD at a specific Re were then compared with the reference data to evaluate the reliability of the POD-derived results, particularly with respect to the number of snapshots. For the lid-driven cavity flow analysis, the numerical results of Ghia et al., obtained via the stream function-vorticity method, were taken as the reference (ground truth). Simulations were performed at Re = 1000, 3200, 5000, and 7500. These four cases served to validate the CFD results. To expand the snapshot library, additional CFD solutions were obtained for arbitrary Reynolds numbers using the validated grid and appended to the snapshot matrix.

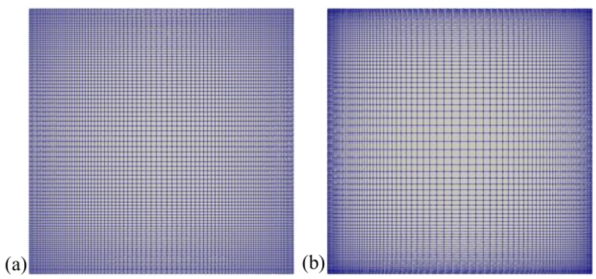


Fig. 1. CFD meshes for lid-driven cavity flow with 100×100 cells, (a) Mesh-1: 1/5 aspect ratio, (b) Mesh-2: 1/20 aspect ratio.

Fig. 1 illustrates the computational meshes used to evaluate the grid dependency of the CFD results for the lid-driven cavity flow. The total number of grid points was fixed at 100×100, while two types of meshes were generated by varying the grid clustering near the walls. Fig. 1(a) shows a mesh with a 1/5 aspect ratio at the wall, while Fig. 1(b) (Mesh-2) presents a more stretched grid near walls with a 1/20 aspect ratio.

Figs. 2 and 3 compare the CFD results for different Reynolds numbers with those of Ghia et al. While Mesh-1 shows good agreement overall, slight discrepancies are observed near the upper moving wall at Re = 7500.

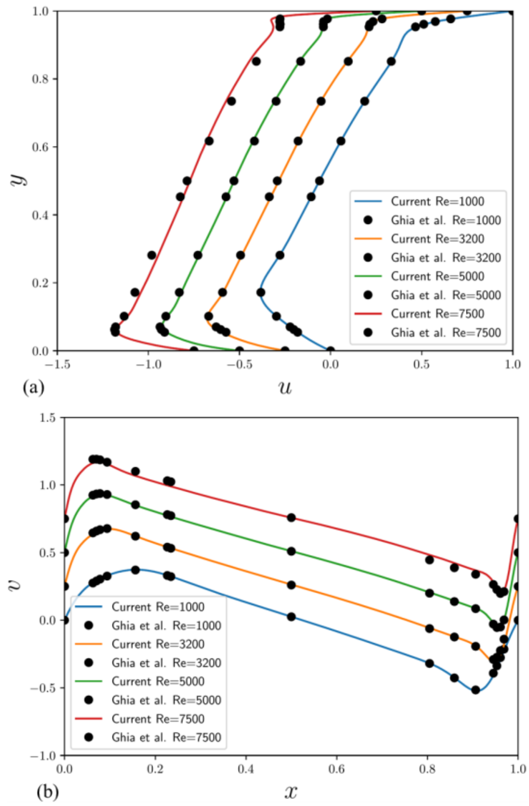
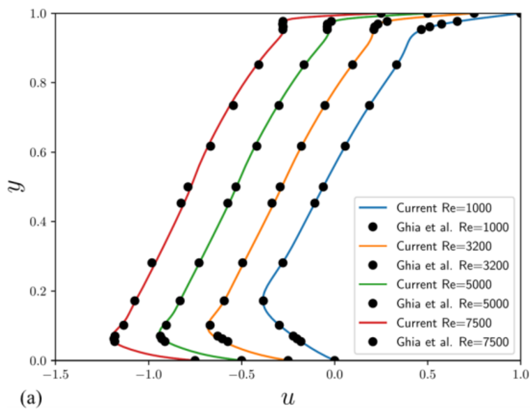


Fig. 2. Comparisons of lid-driven cavity flow between Mesh-1 and Ghia et al.'s data, (a) u-y plot along vertical line, (b) x-v plot along horizontal line.



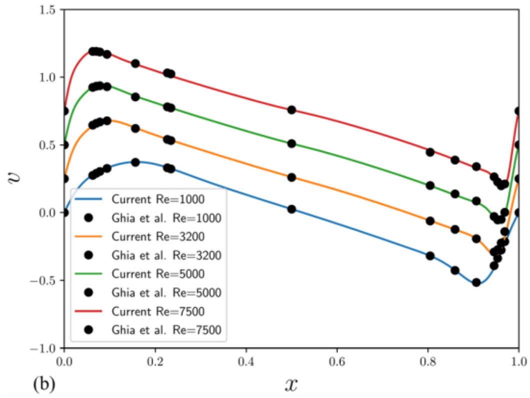


Fig. 3. Comparisons of lid-driven cavity flow between Mesh-2 and Ghia et al.'s data, (a) u-y plot along vertical line, (b) x-v plot along horizontal line.

In contrast, Mesh-2, with its sufficient grid density near the walls, demonstrates excellent agreement with the reference solution. Consequently, Mesh-2 was determined to provide grid-independent solutions across the investigated Reynolds number range.

To evaluate the predictive accuracy of the POD relative to the number of snapshots, the estimation characteristics were compared using cases with three and five snapshots. First, for the 3-snapshot case, the CFD results for Re = 1000, 3200, and 7500 were employed. Using these snapshots, the characteristic vectors and matrices were derived according to the POD methodology described previously. The velocity field was then estimated for the target condition of Re = 5000. As shown in Fig. 4, while the general flow features are captured, noticeable discrepancies in the u-velocity component appear near the upper and lower walls.

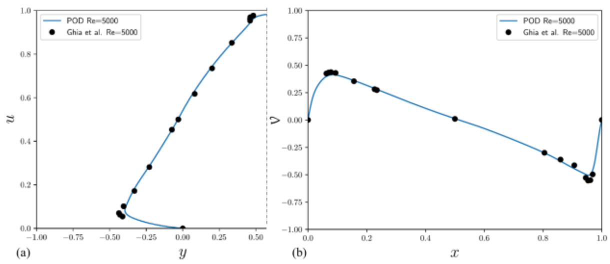


Fig. 4. Comparisons of lid-driven cavity flow between POD using 3 snapshots and Ghia et al.'s data, (a) u-y plot along vertical line, (b) x-v plot along horizontal line.

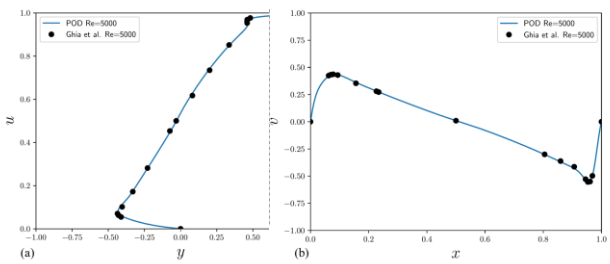


Fig. 5. Comparisons of lid-driven cavity flow between POD using 5 snapshots and Ghia et al.'s data, (a) u-y plot along vertical line, (b) x-v plot along horizontal line.

To improve the model, the number of snapshots was increased to five by including CFD results for Re = 4000 and 6000. Fig. 5 compares the velocity field predicted by the 5-snapshot POD. The results show that the predicted flow field is in excellent agreement with the reference data from Ghia et al., demonstrating that the increased snapshot density significantly enhances the fidelity of the POD reconstruction.

In order to check the flow field reconstructed by POD, the velocity field from the POD method was compared with the CFD results at Re = 5000. Fig. 6. Shows the comparison of velocity fields. Fig. 6(a) is the velocity field from the CFD simulation and Fig. 6(b) is from the POD method. It was confirmed from the comparison of the velocity field that the POD method well predicted the flow field.

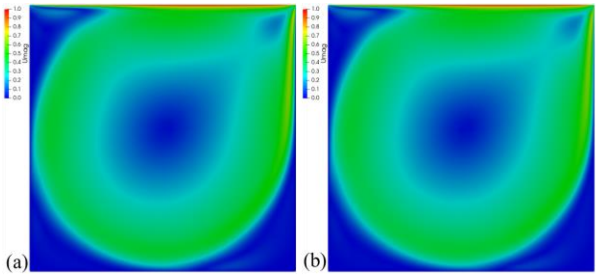


Fig. 6. Comparison of velocity fields for lid-driven cavity flow at Re = 5000, (a) by CFD , (b) by POD.

4. Conclusions

In this study, a Proper Orthogonal Decomposition (POD)-based reduced-order modeling framework was developed to efficiently approximate high-fidelity flow solutions. By extracting dominant flow structures from snapshot data and representing the governing flow variables in a low-dimensional subspace, the proposed approach significantly reduces the computational cost associated with repeated CFD simulations.

Furthermore, the validation under unseen operating conditions confirmed the robustness and predictive capability of the reduced-order model. Although minor discrepancies were observed in regions with strong gradients, the overall agreement between the reduced-order and high-fidelity solutions remained satisfactory, indicating that the proposed method is suitable for practical engineering applications.

The proposed POD-based reduced-order modeling approach is particularly well suited for applications requiring rapid evaluations, such as parametric analysis, design optimization, and real-time flow prediction. Future work will focus on extending the framework to unsteady and multi-physics problems.

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