Applicability Analysis of Reduced-Order Methods for Fluid Dynamics Models of Molten Salt Reactors

Authors: Lin Ming, Maosong Cheng, Dai Zhimin, Cai Xiangzhou, Mao-Song Cheng

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Abstract

For high-fidelity fluid dynamics calculations of full-core molten salt reactors, even with the parallel computing capabilities of supercomputers, enormous efficiency challenges still remain when addressing problems requiring rapid or even real-time solutions. The introduction and adoption of Reduced Order Modeling (ROM) can effectively resolve such issues. Based on Proper Orthogonal Decomposition (POD) and Galerkin projection methods, this work introduces Reduced Order Modeling based on Finite Volume approximation (FV-ROM) and Reduced Order Modeling with supremizer stabilization (SUP-ROM), conducting applicability analysis for laminar and turbulent transient conditions in Liquid Fuel Molten Salt Reactors (LFMSR). The results demonstrate that the FV-ROM method possesses significant advantages in velocity error and computational efficiency, with average L2 relative errors of transient velocity for laminar and turbulent flows below 0.5% and 0.6%, respectively, and speedup ratios per time step of approximately 1500 and 1000 times, respectively. In contrast, the SUP-ROM method exhibits significant advantages in pressure prediction, with average L2 relative errors of transient pressure for laminar and turbulent flows as low as 0.20% and 0.38%, respectively. Therefore, combining the FV-ROM and SUP-ROM methods for predicting velocity and pressure fields in molten salt reactor fluid dynamics can more effectively enhance simulation efficiency and ensure computational reliability and accuracy in transient simulation processes.

Full Text

Preamble

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Applicability Analysis of Reduced Order Modeling Methods for Fluid Dynamics in Molten Salt Reactors

LIN Ming[1], CHENG Maosong[1,2], CAI Xiangzhou[1,2], DAI Zhimin[1,2]
[1] Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China
[2] University of Chinese Academy of Sciences, Beijing 100049, China

Abstract

[**Background**] High-fidelity computational fluid dynamics (CFD) simulations of molten salt reactors, even when leveraging supercomputing parallelization, face significant efficiency challenges for problems requiring rapid or real-time solutions. Reduced Order Modeling (ROM) techniques offer an effective approach to address this limitation while maintaining accuracy. [**Purpose**] This study evaluates the accuracy of ROM methods for reconstructing velocity and pressure fields in molten salt reactor fluid dynamics. [**Methods**] Two ROM methods based on Proper Orthogonal Decomposition (POD) with Galerkin projection—FV-ROM (ROM based on Finite Volume approximation) and SUP-ROM (ROM with supremizer stabilization)—are developed and applied to unsteady laminar and turbulent flow scenarios in a Liquid Fuel Molten Salt Reactor (LFMSR). [**Results**] The FV-ROM method demonstrates notable advantages in velocity prediction and computational efficiency, achieving average L2 relative errors below 0.5% and 0.6% for laminar and turbulent transient velocities, respectively, with acceleration ratios of approximately 1500× and 1000× per time step. Conversely, the SUP-ROM method exhibits significant superiority in pressure prediction, with average L2 relative errors as low as 0.20% and 0.38% for laminar and turbulent scenarios. [**Conclusions**] Combining FV-ROM and SUP-ROM approaches for velocity and pressure field predictions in molten salt reactor fluid dynamics can effectively enhance simulation efficiency while ensuring reliability and accuracy in transient simulations.

Keywords: Reduced Order Modeling, Molten Salt Reactor, FV-ROM, SUP-ROM, Fluid Dynamics

Introduction

High-fidelity thermal-hydraulic calculations for molten salt reactors [1]—including classical finite element methods, finite volume methods, and other high-resolution numerical approaches [2-5]—face substantial efficiency challenges even with supercomputing parallelization when multiple solutions or rapid/real-time responses are required. The solution efficiency must improve by 2–3 orders of magnitude to meet practical demands. Reduced Order Modeling (ROM) is a theoretical and computational framework that can dramatically enhance the efficiency of large-scale engineering calculations while preserving accuracy [6], making its application to molten salt reactor engineering design and analysis (including uncertainty quantification, design optimization, and operational control) highly significant.

ROM has been widely applied in fluid mechanics across aerospace, naval, automotive, and civil engineering [7-10], with recent adoption in nuclear energy systems. Among intrusive ROM approaches for nuclear systems, the POD-Galerkin method is most representative. German, Alberto, and Xiang et al. employed POD-Galerkin to solve neutron diffusion eigenvalue problems with and without temperature feedback [11-14]. Min et al. analyzed flow-induced vibration characteristics of fuel rods in European Pressurized Reactors (EPR) using POD-Galerkin [15]. Sartori et al. developed a single-channel coupled model for lead fast reactors, achieving at least three orders of magnitude speedup [15]. Lorenzi et al. established a reduced-order model for the ALFRED lead-cooled fast reactor and simulated its transient conditions [16]. Tao et al. simulated temperature distribution in the upper plenum of a lead-bismuth fast reactor during accidents, providing an analytical tool for identifying thermal stratification mechanisms [17].

For complex nonlinear systems like molten salt reactors (including pumps and heat exchangers), two primary challenges exist in establishing reduced-order flow dynamics models. First, the reduced basis space obtained through Galerkin projection cannot preserve the original full-order dynamic characteristics [18]. Second, since molten salt is approximated as incompressible, the projected continuity equation inherits divergence-free properties, creating a single-equation multi-variable problem.

To address these issues, Lorenzi et al. [19] proposed the Finite Volume-based ROM (FV-ROM) method, which solves only the momentum equation while neglecting pressure gradient contributions. Ballarin et al. [20] introduced the supremizer stabilization ROM (SUP-ROM) method, which adds extra velocity modes to solve a dual-equation system.

To analyze the applicability of FV-ROM and SUP-ROM for molten salt reactor fluid dynamics, this paper establishes full-order, FV-ROM, and SUP-ROM models within the open-source CFD framework OpenFOAM. Applicability assessment is performed through laminar and turbulent transient scenarios in an LFMSR (Liquid Fuel Molten Salt Reactor) [21].

1. Full Order Model (FOM) for Liquid Fuel Molten Salt Reactor

Assuming molten salt as an incompressible fluid and treating pumps and heat exchangers as porous media, the mass and momentum conservation equations can be derived. The governing equations incorporate porosity effects, where γ represents porosity, μ molecular dynamic viscosity, and μ_t turbulent viscosity. The momentum equation includes a pump volume force term F_{pump} and flow resistance term F_f, with $\mathbf{g}$ representing the gravity vector. When $\gamma = 1$, the equations reduce to standard fluid region formulations.

Based on the definition of Darcy velocity $\mathbf{u}_D$, the equations can be expressed in terms of the Darcy velocity field. The molten salt reactor operates as a closed-loop system, with homogeneous Dirichlet boundary conditions applied to velocity ($\mathbf{u}_D = 0$) and Neumann boundary conditions for pressure ($\nabla p \cdot \mathbf{n} = 0$) at the boundaries.

2. POD-Galerkin Method

2.1 Proper Orthogonal Decomposition (POD)

Constructing a reduced-order model requires basis functions that numerically represent the original system. The velocity field can be decomposed as a linear combination of temporal coefficients $a(t)$ and orthonormal spatial basis functions $\phi(\mathbf{x})$:

$$\mathbf{u}(\mathbf{x}, t) = \sum_{i=1}^{N_u} a_i(t)\phi_i(\mathbf{x})$$

The reduced basis can be obtained through POD, PGD (Proper Generalized Decomposition), or greedy RB (Reduced Basis) methods [22-24]. This work employs POD, which compresses numerical data (in time or parameter space) into fewer modes that capture the most important flow field information. For steady-state snapshots, data are collected across a parameter range, yielding N snapshots. For transient snapshots, K instantaneous flow field datasets are selected at different times, resulting in $N \times K$ total snapshots.

The POD basis is constructed by solving the optimization problem:

$$\arg \min_{\{\phi i\}_{i=1}^{N_u}} \sum_{j=1}^{N_{\text{snap}}} \left\| \mathbf{u}_j - \sum_{i=1}^{N_u} (\mathbf{u}_j, \phi_i)\phi_i \right\|^2$$

subject to orthonormality constraints. This is equivalent to solving the eigenvalue problem:

$$\mathbf{C}_u \mathbf{V}_u = \mathbf{V}_u \Lambda_u$$

where $\mathbf{C}_u$ is the velocity snapshot correlation matrix, $\mathbf{V}_u$ contains eigenvectors, and Λ_u is a diagonal matrix of eigenvalues. POD modes are then formed as:

$$\phi_i = \sum_{j=1}^{N_{\text{snap}}} \mathbf{V}_u(j,i)\mathbf{u}_j$$

Similar procedures derive pressure and turbulent viscosity modes [26]. Superscripts u, p, h denote velocity, pressure, and turbulent viscosity, respectively. By truncating modes based on eigenvalues, the velocity field is approximated as:

$$\mathbf{u}(\mathbf{x},t) \approx \sum_{i=1}^{N_u} a_i(t)\phi_i(\mathbf{x})$$

with analogous expressions for pressure and turbulent viscosity using coefficients $b_i(t)$ and $e_i(t)$. The modal dimensions N_u, N_p, N_h are significantly smaller than the full-order system.

2.2 Galerkin Projection

Projecting the Navier-Stokes equations onto the POD modal space via Galerkin projection transforms the high-dimensional system into a low-dimensional flow model [27-29]. The projected momentum equation becomes:

$$\mathbf{M}\frac{d\mathbf{a}}{dt} + \mathbf{a}^T\mathbf{N}\mathbf{a} + \mathbf{D}\mathbf{a} + \mathbf{B}\mathbf{b} = \mathbf{F}_{\text{pump}} + \mathbf{F}_f + \mathbf{G}$$

where the operators are defined through inner products:

$$M_{ij} = (\phi_i, \phi_j)$$
$$N_{ijk} = (\phi_i, (\phi_j \cdot \nabla)\phi_k)$$
$$D_{ij} = (\nabla\phi_i, \mu\nabla\phi_j)$$
$$B_{ij} = (\phi_i, \nabla\psi_j)$$

Here γ equals 1 in non-porous regions and 0 in porous media zones. A critical issue arises: as linear combinations of divergence-free snapshots, the velocity basis functions remain divergence-free, causing matrix $\mathbf{M}$ to vanish and preventing simultaneous determination of pressure and velocity modal coefficients, thus violating the Ladyzhenskaya-Babuska-Brezzi (LBB) condition [30].

To resolve this, Lorenzi et al. [19] introduced FV-ROM, where pressure and turbulent viscosity fields follow velocity dynamics:

$$\mathbf{u}(\mathbf{x},t) \approx \sum_{i=1}^{N_u} a_i(t)\phi_i^u(\mathbf{x})$$

$$p(\mathbf{x},t) \approx \sum_{i=1}^{N_u} a_i(t)\phi_i^p(\mathbf{x})$$

$$\mu_t(\mathbf{x},t) \approx \sum_{i=1}^{N_u} a_i(t)\phi_i^h(\mathbf{x})$$

Only modal coefficients $a_i(t)$ require solution.

Ballarin et al. [20] proposed SUP-ROM, which adds supremizer modes to the velocity basis, making matrix $\mathbf{M}$ non-zero and enabling separate equations for pressure and velocity coefficients. Supremizer snapshots are computed by solving a Poisson equation:

$$\nabla^2\mathbf{s} = -\nabla p$$

with known pressure snapshots and boundary conditions ($\mathbf{s} = 0$). These snapshots undergo POD to extract dominant modes, which are appended to the velocity basis ϕ_i^u, eliminating the divergence-free property. Flow resistance coefficients c_i and turbulent viscosity coefficients e_i are obtained through Discrete Empirical Interpolation and Radial Basis Function methods [31-32].

2.3 Online Solution and Error Statistics

The ROM computation workflow, illustrated in [Figure 1: see original paper], comprises offline and online phases. The offline phase involves snapshot generation and modal extraction, while the online phase assembles reduced-order operator matrices, solves the algebraic system, and reconstructs fields using modal superposition.

To quantify ROM accuracy, relative global L2 error metrics are employed:

$$\epsilon_u = \frac{\|\mathbf{u}_{\text{ROM}} - \mathbf{u}_{\text{FOM}}\|_{L2}}{\|\mathbf{u}_{\text{FOM}}\|_{L2}}$$

$$\epsilon_p = \frac{\|p_{\text{ROM}} - p_{\text{FOM}}\|_{L2}}{\|p_{\text{FOM}}\|_{L2}}$$

Time-averaged errors are defined as:

$$\bar{\epsilon}_u = \frac{1}{N_t}\sum_{i=1}^{N_t}\epsilon_u(t_i)$$

$$\bar{\epsilon}_p = \frac{1}{N_t}\sum_{i=1}^{N_t}\epsilon_p(t_i)$$

3. LFMSR Fluid Dynamics Reduced-Order Model Analysis

The LFMSR is a liquid-fueled molten salt fast reactor [21] designed for 800 MW thermal power with eight loops. Each loop contains three main components: core, pump, and heat exchanger. The primary loop geometry and mesh structure are shown in [Figure 2: see original paper], with thermophysical properties listed in . The heat exchanger porosity is set to 0.5, with the pump momentum source located at the loop bottom, driving upward fuel flow. The mesh contains 44,770 cells. Full-order simulations run on an Intel® Core™ i5-12500H processor (2.50 GHz) using 8-core parallel computation.

[Figure 3: see original paper] presents pump power variations for transient scenarios: (a) laminar flow (0–350 s) with initial momentum source 10 Pa/m, collecting 70 snapshots at 5 s intervals; (b) turbulent flow (0–5 s) with initial source 20,000 Pa/m, collecting 100 snapshots at 0.05 s intervals. [Figure 4: see original paper] shows normalized modal eigenvalue curves for pressure, velocity, flow resistance, and supremizer modes. In laminar flow, modal energy decays rapidly, with the first 10 modes capturing most flow information. In turbulent flow, turbulent viscosity and velocity modes decay slowly, requiring more modes to represent the flow field accurately.

3.1 Laminar Flow Results

Computational cost typically scales with modal count, but accuracy does not necessarily improve monotonically. [Figure 5: see original paper] compares L2 relative errors for various modal combinations, where N_u, N_{sup}, and N_p denote velocity, supremizer, and pressure modes, respectively. For FV-ROM, five velocity mode counts are tested. Velocity errors converge when $N_u > 8$, while pressure errors decrease modestly but exhibit instability with increasing modes. For SUP-ROM, five modal groups are evaluated. The first group with low cumulative energy shows large velocity errors. Subsequent groups reveal that increasing supremizer modes expands both average and maximum velocity errors, as additional supremizer modes deviate from the original physics, adversely affecting velocity predictions. [Figure 5b: see original paper] shows SUP-ROM maintains pressure errors below 0.78%, with minimal differences among modal groups in terms of average and maximum errors.

quantifies average and maximum L2 relative errors. Based on comprehensive comparison, $N_u = 10$ is selected for FV-ROM, and $N_u = 10$, $N_{\text{sup}} = 8$, $N_p = 6$ for SUP-ROM. For velocity prediction, SUP-ROM' s average error (1.037%) exceeds FV-ROM' s (0.444%), with maximum errors of 3.704% versus 1.110%, respectively. For pressure prediction, SUP-ROM shows clear superiority, maintaining errors below 0.78% while FV-ROM only approaches this accuracy at isolated time points.

Absolute errors at $t = 350$ s are shown in [Figure 6: see original paper]. Both methods exhibit maximum velocity errors near the core outlet with similar distributions, but FV-ROM' s maximum absolute error is substantially smaller.

FV-ROM shows larger pressure errors concentrated near pump and heat exchanger regions, whereas SUP-ROM' s pressure errors are confined to a small region at the core outlet.

[Figure 7: see original paper] presents per-time-step acceleration ratios. FV-ROM maintains a stable ratio around 1500×, consistently outperforming SUP-ROM. SUP-ROM shows larger fluctuations, converging faster during periods of stable pump power but with lower overall acceleration.

3.2 Turbulent Flow Results

[Figure 8: see original paper] evaluates FV-ROM and SUP-ROM performance across five modal groups for turbulent flow. FV-ROM velocity errors remain below 1% when $N_u = 15$, but increase when $N_u > 20$. Pressure predictions deviate significantly after 3.5 s, with errors exceeding 100%. SUP-ROM with modal combination ($N_u = 15$, $N_{\text{sup}} = 3$, $N_p = 3$) yields the most accurate velocity predictions, while pressure errors stay below 1.03% across all groups.

summarizes error statistics. Selected configurations are $N_u = 15$ for FV-ROM and ($N_u = 15$, $N_{\text{sup}} = 3$, $N_p = 3$) for SUP-ROM. FV-ROM achieves lower average velocity error (0.599% vs. 0.914%), while SUP-ROM demonstrates superior pressure prediction (0.387% average error, maximum below 1.1%).

Absolute errors at $t = 5$ s are depicted in [Figure 9: see original paper]. Both methods show concentrated velocity errors below the core with similar patterns. FV-ROM pressure errors appear in pump and heat exchanger regions, while SUP-ROM errors are limited to a minimal region above the core, confirming its pressure prediction accuracy.

[Figure 10: see original paper] shows acceleration ratios for the turbulent transient. FV-ROM achieves approximately 1000× speedup, while SUP-ROM averages around 800× due to larger operator matrix assembly costs. These results demonstrate that even with 8-core parallel full-order simulations, ROM provides substantial acceleration.

Conclusion

This study introduced FV-ROM and SUP-ROM methods to address molten salt reactor fluid dynamics efficiency challenges, evaluating their performance through laminar and turbulent transient test cases in an LFMSR. Numerical results demonstrate that both methods significantly improve computational efficiency. FV-ROM provides more accurate velocity predictions with appropriate modal selection, while SUP-ROM captures pressure field variations more precisely. Combining these approaches ensures reliable, accurate transient simulations with substantially enhanced efficiency, offering an effective theoretical and computational framework for molten salt reactor fluid dynamics analysis.

Author Contributions

LIN Ming developed the full-order and reduced-order models, performed data analysis, and wrote the manuscript. CHENG Maosong conceived the research idea, critically reviewed intellectual content, and revised the manuscript. CAI Xiangzhou supervised research progress and provided funding support. DAI Zhimin guided the research methodology.

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Note: Figure translations are in progress. See original paper for figures.