Title of Project: Reduced Order Modeling of Heat and Fluid Flow: Multi-Scale Modeling of Advanced Reactors to Enable Faster Deployment

Technical Workscope Identification: M&S-1

Project Objectives

We propose to leverage ongoing hardware, software, and algorithmic developments to dramatically enhance thermal-hydraulic analysis capabilities. The work will entail combining advanced simulations on DOE's exascale computing platforms with modern data analysis methods based on reduced-order models (ROMs) that effectively compress these first-principle data to provide efficient exploratory tools. These tools have the potential to improve understanding of thermal stratification effects, mixed convection, and other critical phenomena and can lead to margin reduction and better economics. We illustrate the project overview in Fig. 1(left).

Proposed Scope Description

We seek **to develop novel multi-scale algorithmic approaches for the simulation of heat and fluid flow in advanced reactors**. The methods, which leverage recent advances in hardware and in reduced order modeling (ROM) approaches, will enable thermal-hydraulics (TH) simulations of vastly accelerated speed, while maintaining accuracy comparable to high-fidelity methods such Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). These methods will allow designers to perform parameter sweeps to assess uncertainty and develop closures. They will also enable, for the first time, high fidelity simulation of long transients.

Several advanced reactor concepts are currently being pursued in the United States, with dozens of companies proposing unique designs. Crucial for their deployment is the analysis of reactor transients (e.g., a protected loss of flow), which is an essential part of the evaluation of thermal margins and the overall safety case. In most cases, licensing will be pursued with established methods, based on lumped parameter system codes (e.g., SAM [6]). However, these codes require adequate closures that are typically obtained empirically and require extensive validation. Furthermore, these methods are characterized by high level of uncertainty when dealing with complex three-dimensional turbulent flow, especially in the presence of large enclosures, mixed convection, and thermal stratification. High-fidelity simulation on the other hand remains expensive, especially for large parameter sweeps or for the simulation of nuclear transients, and data remains sparse.

Moreover, as the advanced reactor industry matures and moves past demonstration projects, economics will become a larger driver. This pressure will likely push vendors to maximize the economic potential (e.g., higher power output, higher temperature for process heat, reduced capital cost), especially as new materials and fuels are introduced. These goals will benefit from improved methods to assess thermal margins that push toward high fidelity. **This proposal seeks to develop radically novel**

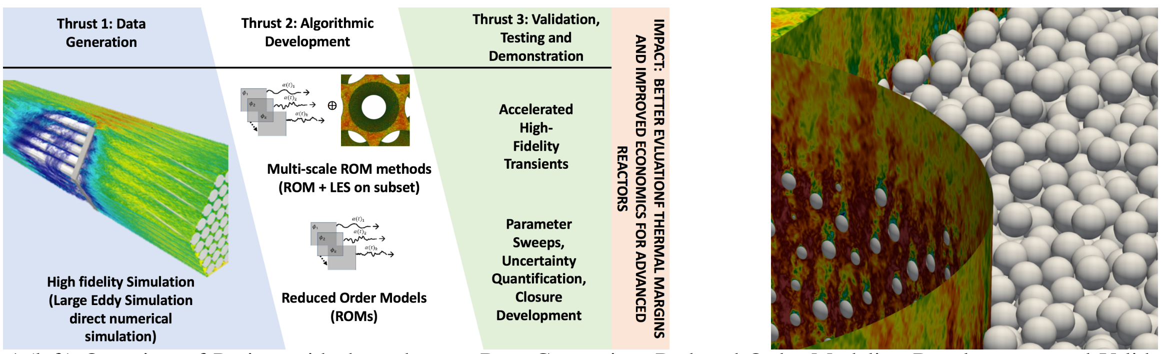

Fig. 1 (left) Overview of Project with three thrusts: Data Generation, Reduced-Order Modeling Development, and Validation/Demonstration. (right) Current capabilities: flow-through of full pebble bed reactor core in 6 hours on Summit (352K pebbles, 51B grid points, 27648 NVIDIA V100s, 0.36 seconds per step).

algorithmic approaches to the simulation of advanced reactors, with an unprecedented level of fidelity, enabling transformative design approaches and improved economics. In particular we aim to:

1. *Enable the simulation of large parameter sweeps using ROMs developed over a subset of the parameter space.* This approach will allow assessment of uncertainties in system-level approaches and to develop closures.

2. *Enable accelerated simulation of transients.* This approach will allow assessment of lower resolution approaches in conjunction with experimental data for the simulation of transients.

As a demonstration application we choose the simulation of Sodium Fast Reactor (SFR) fuel assemblies under steady-state and transient conditions and extend to upper plenum applications as a stretch goal. **We emphasize that the methods developed will apply to a broad range of advanced reactor applications.** To maximize impact, we will integrate the proposed multi-scale approaches in the Cardinal [14] framework thus allowing their usage in SAM [6].

The central component of the work scope is the development of robust low-cost ROMs for reactor thermal design and analysis. ROMs typically comprise a small system of ordinary differential equations (ODEs) that represent the evoluton of $N \approx 100$ basis functions designed to capture the dominant dynamics of the flow field. For this size, the low-dimensional ODE (6) can be advanced extremely fast—**in just a few minutes on a laptop it is possible to evolve tens-of-thousands of convective time units,** much longer than feasible with a high-fidelity simulation, even on an exascale platform, which is one of the reasons that ROMs are interesting for long-time transients. *Parametric model order reduction* (pMOR) is a process through which a ROM or suite of ROMs is constructed to estimate the system behavior over a range of parametric inputs (e.g., inlet flow rates, thermal loading, or Reynolds number) without the need for high-fidelity simulations at every point in the target parameter space. The output of the pMOR will be a small set of coefficients to drive low-rank systems of ODEs that can be directly coupled with either a Systems Analysis Module (SAM) or with detailed, localized, LES or RANS models.

The ROMs are based on data (solution snapshots) from high-fidelity direct numerical (DNS), large-eddy (LES), or unsteady Reynolds-averaged Navier-Stokes (uRANS) simulations of turbulent thermal transport. These *full-order models* (FOMs) will be run on DOE's leadership computing facilities in an *offline* mode using the NEAMS-supported Nek5000/RS code developed by the PIs. (NekRS is the GPU-oriented version of Nek5000, developed under the DOE's Exascale Computing Project.) The ROMs will be used in a real-time *online* mode simulating the governing Navier-Stokes and energy equations as a projection of N basis functions derived from a proper-orthogonal-decomposition (POD) of snapshots generated by the FOMs.

There are three essential categories for the proposed ROM development: *i. The reproduction problem*, in which the ROM is able to adequately reproduce a given quantity of interest (QOI), such as flow rate or Nusselt number, over the same time period and at the same parameter points as the originating FOM data; *ii. The parametric problem*, in which the ROM is used to to predict QOIs at a *different* point in parameter space; and *iii. Long time transients*, in which the ROM is used to predict QOI behavior beyond the sampled time-domain of the FOM. Categories *ii* and *iii* bring their own challenges (e.g., [16]) but they depend crucially on having a stable and accurate ROM for turbulent flows, which is an open research question and a major focus of our Category *i* effort. If the ROM is stable and accurate, then Category *iii* is effectively similar to *ii* since the time window can be viewed as a parameter.

Under NEUP Award 18-15520, we have developed NekROM to provide a pMOR/ROM capability within the Nek5000/RS framework that allows users to build ROMs and perform parameter variation with these models. The analysis process begins with a detailed FOM of size (number of degrees-of-freedom) $\mathcal{N} = 10^7$–10^{11} and $K \approx 10^3$ snapshot files. The NekROM software module then distills the FOM results into a ROM ODE system of size $N \approx 100$, which can be solved with a choice of Fortran, Matlab, or Python drivers in the NekROM suite. An outer driver is provided to iterate between the ROM and Nek5000/RS to pick optimized (error-indicated) anchor (trial) points in the target parameter space, $\mathcal{P}$. The principal focus of this project will be to push the **state-of-the-art** for ROM-based simulations

Case	**Size** (grid points)	**Run time** (CU)	**Snapshots**
Mixed convection (19 pins) [11]	$1 \cdot 10^9$	20,000	5000
Mixed convection (61 pins) [11]	$3 \cdot 10^9$	2000	5000
Parallel Jets [1]	$1 \cdot 10^9$	200,000	10,000
Thermal stratification [12]	$5 \cdot 10^8$	500,000	10,000

Table 1 List of existing cases.

of turbulence, to identify which turbulence problems are tractable, and which are not [16], to integrate the ROM simulator with the RANS and LES capabilities in Nek5000/RS, and to test this multiscale framework within a suite of TH challenge problems described in the next section.

Logical Path to Accomplishing Scope.

Proposed Tasks. We propose the following Tasks to realize a multiscale simulation capability within Nek5000/RS/ROM for reactor analysis.

Task 1: Data Generation. We will perform high fidelity simulations of the flow in SFR fuel assemblies (e.g., Fig. 1, left), including a range of steady-state conditions and a loss-of-flow transient scenario.

i. Define benchmarks for SFR fuel assemblies. These will be used for validation.

ii. Develop data to construct ROMs for SFR fuel assemblies. This task will support Task 2.

iii. Develop data to validate ROMs for both transient and parameter sweeps to support Task 3.

In Task 1, we will leverage several cases developed as benchmarks for mixed convection and thermal striping as part of a recent IRP. The cases are summarized in Table 1. For this project, we will augment these cases by performing simulations for a broader range of parameters and collecting additional snapshots as needed. We remark that using well-defined past benchmarks also allows us to evaluate the performance advantage of ROM-based approaches.

Task 2: Algorithmic Development. This is the core of the project. We seek to develop advanced ROM methods that are seemlessly extended to a multi-scale framework in Nek5000/RS/ROM.

i. Continued development of ROM closure models to increase robustness for high Rayleigh/Reynolds flows. This effort will build on earlier and ongoing work [7–9, 15, 16].

ii. Identify strategies to equip the ROM for long-time transients. Proposed extensions to [9] include employing error indicators developed in [5, 16] for transients and development of LES-based filter-based stabilization methods in the context of ROMs.

iii. Develop multi-scale methods that couple ROMs with LES on a subset of the domain, as illustrated in Fig. 2(right). A principal challenge is to quantify the relaxation distances over which small scale structures will evolve near the ROM-LES interface. The goal will be to combine reactor-scale ROM simulations with localized detailed simulations in regions of interest. This task leverages past work on rod bundles and sub-channels, whose geometric properties have been exploited to maximize the use of small-domain high-fidelity simulation to improve RANS results in a multi-scale fashion [13].

Task 3: Validation and Demonstration. Here we validate and demonstrate the proposed methods.

i. Validate ROM transient calculations with high-fidelity counterparts in an SFR rod-bundle under *low-flow* conditions.

ii. Perform ROM-based parameter sweeps and compare with corresponding FOM data for validation.

iii. Demonstrate accelerated transient capability for cases that are currently not feasible. We will implement the proposed ROM-based and multiscale models within Cardinal [14]. This will enable their usage within the systems analysis code SAM [6]. The co-PI at Penn State has been working extensively on the integration of SAM and NekRS within Cardinal.

Below, we describe subtasks to be addressed in support of the main Tasks outlined above.

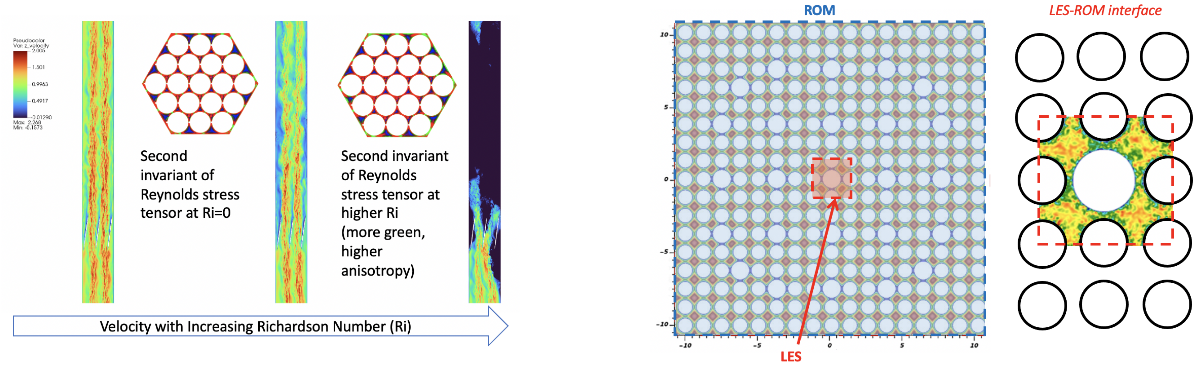

Fig. 2 (left) Velocity distribution in wire-wrapper assembly as a function of the Richardson number at low flow conditions. (right) Example of LES-ROM coupling.

Challenge Problem. (Tasks 1 and 3.) We focus first on mixed convection within fuel assemblies. Fluid flow and heat removal through fuel, shield and reflector assemblies can have major impacts on operation and safety for Sodium Fast Reactors (SFRs). This type of reactor is of great interest in the United States due to the planned deployment of Terrapower's Natrium concept funded partially through the Advanced Reactor Demonstration program (ARDP). These assemblies are formed by bundles from 19 to 217 pins, with a wire wrapped around each pin to maintain the rods in place.

During transients, these assemblies are characterized by a range of conditions that result from reduced flow rates and from large-scale organized flow patterns, including potential *intra-assembly buoyancy-driven circulation.* This in turn affects the temperature of the ducts and the overall thermo-mechanical response of the core, which is a crucial reactivity feedback mechanism.

These low flow cases can provide challenges for experiments due to complications in measuring the flow rates and temperatures with high accuracy in different areas. This consequently also raises the uncertainty of many modeling approaches for these phenomena, where existing correlations and sub-channel methods fail. An example of the complex range of flow patterns is provided in Fig. 2(left), which shows a transition from steady forced convection to mixed convection. Massive circulations are introduced: in a realistic transient the bundle will encounter the full range of conditions. We ultimately seek methods that can provide accurate and *predictive* results. After success in this challenge problem we will tackle thermal striping and thermal stratification as stretch goals.

Fast ROMs for Turbulence. (Tasks 2 and 3.) The goal of this task is to push the state-of-the-art for ROM-based simulation of turbulent flows. The equations of interest are the incompressible Navier-Stokes equations (NSE) with energy transport,

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \frac{1}{Re} \nabla^2 \mathbf{u} + \nabla p = \mathbf{f}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\partial_t T + \mathbf{u} \cdot \nabla T - \frac{1}{Pr\, Re} \nabla^2 T = q, \tag{2}$$

subject to appropriate boundary and initial conditions. Here, Re and Pr are respective Reynolds and Prandtl numbers, q is the volumetric heating, and $\mathbf{f}$ is a body force that may be temperature dependent. To simplify the exposition, we here consider only the NSE (1).

One of the distinguishing features of turbulent flows is that, because of sensitivity to initial conditions, they are repeatable only in a statistical sense. There is no hope of repeating the exact trajectory of the solution in a turbulent flow between two experiments or two simulation algorithms. ROMs, therefore, must target *space-* and/or *time-averaged* QOIs such as velocity profiles, turbulent-kinetic energy distributions, and Nusselt numbers. For the same reason, such quantities are also the currency of engineering design and thus reasonable measures of the success of a ROM as a low-cost analysis tool. Thus, the objective of this project is prediction of engineering QOIs, rather than prediction of precise trajectories. This simplified objective is one of the key features that makes the problem tractable.

While our focus will be on mean engineering quantities, we note that the time-evolving ROMs *also* provide reasonable surrogates for unsteady behavior (or they would not be good predictors of the mean) and therefore can be used to visualize flows, which is often useful for engineering insight (e.g., identifying stagnant and ejected vortices). We will augment qualitative visual analysis of the unsteady behavior with quantitative monitoring of the amplitudes, frequencies, and gradients of QOIs at specified locations in subsets of the domain, which will help assess potential thermal striping, thermal fatigue, and thermal stratification effects. We can also use the ROM evolution to drive LES or RANS boundary conditions, as discussed in the next subtask.

The ROM for the Navier-Stokes equations starts with a collection of K snapshots, $\mathbf{u}^k(\mathbf{x}) := \mathbf{u}(\mathbf{x}, t^k) \in X_0^{\mathcal{N}}$, corresponding to numerical solutions of the Nek5000/RS full-order model (FOM) at well-separated timepoints. For any $\mathbf{u} \in X_0^{\mathcal{N}} \subset \mathcal{H}_0^1$ we have a corresponding vector of basis coefficients $\underline{\mathbf{u}} = [\mathbf{u}_1 \ldots \mathbf{u}_{\mathcal{N}}]^T$ such that $\mathbf{u}(\mathbf{x}) = \sum_{j=1}^{\mathcal{N}} \mathbf{u}_j \phi_j(\mathbf{x})$, with $\phi_j(\mathbf{x})$ the underlying spectral element basis functions spanning the FOM approximation space, $X_0^{\mathcal{N}}$. We collect the snapshots into the a matrix $\boldsymbol{U}_K = [\underline{\mathbf{u}}^1 \ldots \underline{\mathbf{u}}^K]$. From these, one forms the Gramian, $\boldsymbol{U} \in \mathcal{R}^{K \times K}$ with $\boldsymbol{U}_{k,k'} := (\mathbf{u}^k, \mathbf{u}^{k'})_A$, where $(\cdot,\cdot)_A$ is the energy ($\mathcal{H}_0^1$) norm. Following standard POD methodology, the basis functions $\{\underline{\boldsymbol{\zeta}}_n\}$ for the ROM derive from the first N eigenmodes of $\boldsymbol{U}$,

$$\boldsymbol{U} \underline{z}_k \;=\; \lambda_k \underline{z}_k, \quad \underline{z}_k \in \mathbb{R}^K, \quad \lambda_1 \geq \cdots \geq \lambda_K \geq 0 \tag{3}$$

$$\underline{\boldsymbol{\zeta}}_n \;:=\; \boldsymbol{U}_K \underline{z}_n, \quad n = 1, \ldots, N < K. \tag{4}$$

Defining $\zeta_n(\mathbf{x}) := \sum_{j=1}^{\mathcal{N}} (\underline{\boldsymbol{\zeta}}_n)_j \phi_j(\mathbf{x})$, the standard POD Galerkin formulation follows by inserting the reduced-basis expansion

$$\tilde{\boldsymbol{u}}(x,t) \;=\; \sum_{n=1}^{N} \zeta_n(\mathbf{x}) a_n(t)$$

into the Galerkin statement for the NSE, resulting in the following evolution equation for the reduced-order basis coefficients, $a_n(t)$: *For each* $i = 1, \ldots, N$*,*

$$\sum_{j=1}^{N} M_{ij} \frac{da_j}{dt} \;=\; -\sum_{k=1}^{N} \sum_{j=1}^{N} C_{ijk} a_k(t) a_j(t) \;-\; \frac{1}{Re} \sum_{j=1}^{N} A_{ij} a_j(t), \tag{5}$$

where $M_{ij} := \int \zeta_i \cdot \zeta_j \, d\mathbf{x}$ is the mass matrix, $C_{ijk} := \int \zeta_i \cdot (\zeta_k \cdot \nabla \zeta_j) \, d\mathbf{x}$ is the nonlinear interaction term and $A_{ij} := \int \nabla \zeta_i \cdot \nabla \zeta_j \, d\mathbf{x}$ is the viscous term. We note that, in the case of fixed geometries, the divergence and pressure terms drop out of (5) because the underlying basis is already divergence free. A semi-implicit formulation for (5) leads to an $N \times N$ linear system of the form,

$$E(\underline{a}^l, Re)\underline{a}^{l+1} \;=\; \underline{\tilde{f}}(\underline{a}^l, Re), \tag{6}$$

for each timestep t^l (using a larger timestep size than the FOM). It typically takes only minutes on a laptop to run (5) for thousands of convective time-units. Eq. (5) also illustrates how Re is a free parameter in the ROM.

There are, however, several challenges to ensuring that (5) is accurate for turbulent flows, even under the same parametric conditions. A primary issue for turbulence is that energy is dissipated by small-scale structures that are generally absent from POD bases. Several stabilization strategies are possible, such as Leray regularization, in which the advecting field is smoothed [18], or constrained evolution, in which each basis coefficient is constrained to the range observed in the projection of the snapshot space onto the bases [5]. (To the extent that the POD modes are Fourier like, Leray regularization can be implemented simply by truncating the sum over k to $k \leq N' < N$ in (5), although more sophisticated PDE-based filters can also be developed.) Alternatively, one can modify the approximation space. For example, [3] uses a decomposition of modes into distinct sets minimizing the L^2 error (for accuracy) and the $\mathcal{H}^1$ error (for stability). In [10], a basis is derived from Green's functions approximations.

Under prior NEUP support, Kaneko [7, 8] developed an augmented-basis method (ABM) wherein a set of standard POD basis functions, $\{\zeta_i(\mathbf{x})\}$, is augmented with a subset of their nonlinear interaction

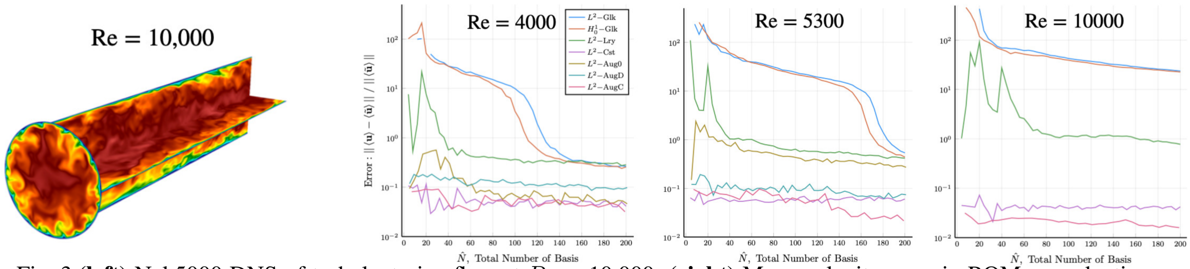

Fig. 3 **(left)** Nek5000 DNS of turbulent pipe flow at Re_D=10,000; **(right)** Mean velocity error in ROM reproduction results for Galerkin POD (L^2-Glk, H^1-Glk), Leray- and constrainted-based regularization (L^2-Lry, H^1-Cst), and ABM with three different subsets of the nonlinear terms (L^2-Aug0=$\zeta_0 \cdot \nabla\zeta_j + \zeta_j \cdot \nabla\zeta_0$, L^2-AugD=$\zeta_j \cdot \nabla\zeta_j$, L^2-AugC=L^2-Aug0 $\bigcup L^2$-AugD) [7, 8].

terms, $\{\zeta_i \cdot \nabla\zeta_j\}$, projected onto a divergence-free space. The success of this method is illustrated in the turbulent pipe flow examples of Fig. 3, which shows that the ABM has much lower error at low N than POD Galerkin and Leray. At lower Reynolds numbers, these standard methods *can* converge for sufficiently large N. The required number of basis functions, however, increases rapidly with Re. Given the $O(N^3)$ costs implied by the rank-3 C_{ijk} tensor in (5), these methods are limited to relatively low Re. The stable ABM and the constrained approaches, however, perform much better, even at $N \approx 20$. Other QOIs, including Nusselt number, show convergence behaviors similar to the plots of Fig. 3, but the ABM can be overly dissipative at higher Re.

Understanding the underlying convergence behavior for ROMs applied to turbulent flows is a major objective of the proposed work. We will explore this question through extensive unit tests such as minimal-channel flows, thermal striping in a T-junction, etc. One possible solution, suggested by Akkari *et al.* [3] is to choose $N = N_P + N_d$ modes with the decomposition of the number of POD modes, N_P, and dissipative modes (here, ABM), N_d based on readily available energy estimates. Kaneko [7, 8] demonstrates that the ABM indeed serves as an energy sink, precisely as required for stability. Following [18], we can also consider filter-based stabilization as is commonly used for LES of turbulent flows. We are pursuing these questions in collaboration with Traian Iliescu at V. Tech. [15].

Stability is a requirement for a successful ROM, but it does not guarantee accuracy of all (or any) of the QOIs. The standard numerical approach to improving accuracy is to increase N, which can be seen to be beneficial for the less performant ROMs of Fig. 3. For $Re = 4000$, there is a significant error reduction for the Galerkin ROMs as N is increased from 100 to 140. For $Re = 5300$, the transition occurs for $N = 140$ to 180. For $N = 10,000$, we cannot observe a transition for $N \leq 200$, but one might speculate that it could be found if we take N large enough. Unfortunately, each step of (6) requires a contraction with the 3rd-order tensor C_{ijk}, which requires $O(N^3)$ operations and dominates the cost of the online (and, potentially, the offline) portion of the ROM. **Mitigation of the $O(N^3)$ cost is of primary importance.** Possible solutions include replacing the nonlinear term with an approximation based on the discrete empirical interpolation method (DEIM) [4] or replacing the rank-3 tensor C_{ijk} with the sum of R rank-1 tensors, which reduces the $O(N^3)$ cost to $O(NR)$. Even if $R = N$, this reduction affords considerable savings, implying that one could enrich the approximation space through substantial increases in N. (An important technical detail is to ensure that the low-rank tensor inherits the skew-symmetry properties that are intrinsic to advection operators in closed systems.)

ROMs generally converge faster on small domains, which suggests using a domain decomposition strategy with (say) $N' = 20$ modes on each of S subdomains such that C_{ijk} is sparse with $O(SN'^3)$ nonzeros, while the number of modes is $N = SN'$. Such an approach would also more readily support convective transport of isolated features than would be possible with an (incomplete) modal basis. We will investigate the feasiblity of such an approach for large-domain test cases.

Coupled Multiscale Simulations (Tasks 2 and 3.) The goal of this task is to reduce computational costs by using ROMs in combination with other computational fluid dynamics and thermal-hydraulic approaches. We note that ROMs can be readily used in the context of systems analysis codes. We will demonstrate this within the context of the recently developed SAM-NekRS coupling in Cardinal.

ROMs can replace the solution of the Navier-Stokes equations with a simplified model, which can greatly reduce computational time. However, some parts of the domain may require additional resolution. Therefore, we will examine hybrid LES-ROM models, which combine a ROM model for the entire system or assembly with a localized, more detailed LES model for specific regions. Fig. 2(right) illustrates a proposed example of an assembly solved using a ROM with four subchannels near a thimble solved using wall-resolved LES for detailed heat transfer. The modal decomposition of the ROM can readily provide the flow boundary conditions for the LES. For small LES domains, a one-way approach where information flows only from the ROM to the LES may be sufficient. If the flow behavior within the LES domain is expected to have a global impact, a two-way coupling approach is needed. We will focus on an overlapping domain approach where the LES behavior is translated into forcing terms for each mode of the ROM.

We will also examine RANS-ROM modeling as a potential interface for ROM methods. This includes using previous work on rod bundles and sub-channels, where high-fidelity simulation was used to improve RANS results [13]. Our aim is to develop a generalized interface between RANS and ROM. For example, ROM results from one assembly can be superposed over a transient RANS model of the entire system to recover unsteady features not modeled correctly by RANS. To this end, it is crucial to ensure that the energy transfer between scales is realistic. We will leverage recent work on the concept of a novel energy-based ROM length scale [15]. We will also explore the potential of an uplifting ROM approach [2] where closure and projection errors are corrected in the prolongation to RANS.

Response to Merit Review Criteria. The proposed project effectively addresses the following merit review criteria for this program.

1. The project will advance the state of knowledge in parametric model order reduction (pMOR) for turbulent flows in general and for SFR applications in particular. Practical deployment of pMOR requires rigorous analysis to develop effective error indicators; a deep understanding of the underlying physics; and careful algorithm development to ensure speed and correctness of the offline and online models. We are particularly focused on challenging large-scale turbulent flows, which remains an open research question, but one that should be tractable given current-day computing resources and novel developments in reduced-order modeling. The work will equip researchers in reactor design and other thermal analysis fields with advanced modeling capabilities.

2. The technical quality of the project is high. It combines rigorous mathematics, practical numerical analysis, and state-of-the-art algorithms to significantly extend the capabilities of the scalable high-order code, Nek5000/RS, on the Nation's leading-edge computing facilities, including DOE's exascale platforms. (NekRS has recently met a critical Figure of Merit milestone as part of the DOE's ExaSMR project, which is one of only three applications to meet the FOM to date.) pMOR/ROM provides a mechanism to leverage these and future computers for effective engineering analysis of challenging problems in reactor thermal hydraulics, with a particular emphasis on mixed convection and long-time transients in SFRs.

3. The applicant team is highly experienced and capable of successfully completing this project. The team comprises experts in reactor thermal-hydraulics, CFD, applied mathematics, numerical algorithms, turbulence, and heat transfer. The PI is the lead developer of Nek5000 and a co-developer of NekRS. Merzari and Shaver lead the integration of Nek5000/RS into the NEAMS tool suite for reactor analysis. As a team, the PIs have co-authored more than 30 articles in reactor thermal-hydraulics, with many of these focused on ROMs. The PI and his students at UIUC continue to push ROM development for turbulent flows, with significant advances realized in augmented basis methods (Fig. 3 [8]) and in feasibility of ROMs for buoyancy-driven flows [9, 16]. Merzari has been a pioneer in exploring POD-based ROMs for TH applications.

Potential risks and mitigation strategies for the project are identified in the Unique Challenges section.

Relevance and Outcomes/Impacts

The methods developed in this proposal aim to deliver a tool for accurate and computationally inexpensive prediction of key thermal-hydraulic phenomena in liquid metal reactors. The operation, safety,

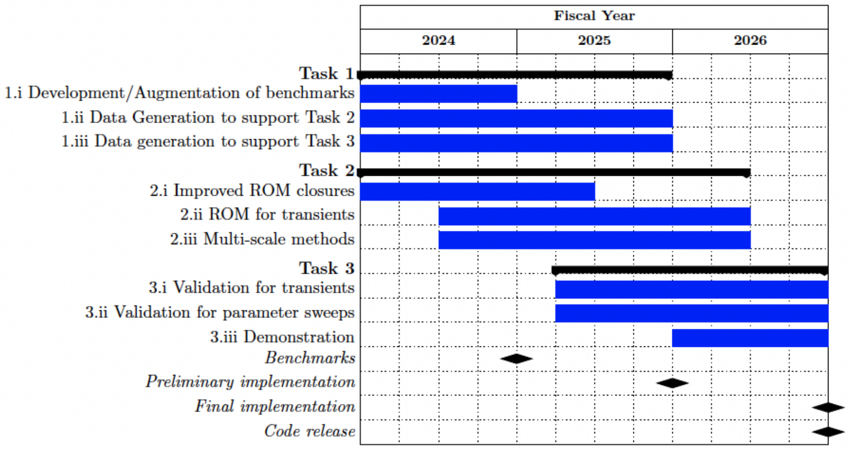

Fig. 4 Timeline of proposal by fiscal year.

and design of Sodium fast reactors are impacted by several critical factors, including thermal stratification, mixing in large enclosures such as liquid metal pools, and mixed convection. The lack of understanding and adequate modeling capability for these phenomena leads to high uncertainty, which limits the reactor's overall performance by requiring excessive margins. The proposed methods have the potential to help reduce these margins, leading to better economics.

During loss of flow incidents, low flow conditions at the periphery of the core, along with steep radial core gradients, can result in mixed convection. This impacts the thermal expansion of assembly ducts and the overall thermo-mechanical behavior of the core, which is a crucial reactivity feedback during these events. Thermal stratification can occur during loss of flow incidents, potentially hindering the establishment of natural circulation, which is crucial during these events. Furthermore, Inadequate mixing in pools contributes to thermal stratification and can result in fluctuating thermal loads (thermal striping) on structural components during normal operation, leading to fatigue and related failures.

These phenomena affect the reactor's thermal limits and margins, with similar considerations applicable to all liquid metal reactors. We note that a lack of cost-effective and accurate prediction methods for these phenomena has long been recognized as a limitation in fast reactor gap analysis studies.

Schedule

The tasks proposed to realize a multiscale simulation capability within Nek5000/RS/ROM for reactor analysis were described in the *Logical Path* section. A schedule for these tasks is provided in Fig. 4.

Milestones and Deliverables

At the end of each year a report will be issued describing progress to date. Four major deliverables are expected out of this project as shown by the diamonds in Fig. 4.

M1: Development of Transient High-resolution Benchmarks (September 2024). We define at least three transient and parametric sweep benchmarks for Sodium Fast Reactors. We also provide initial simulation with LES/DNS using the NEAMS code NekRS. This will be used to support Task 3.
M2: Preliminary Implementation of ROM-based Multiscale algorithms (September 2025). Preliminary implementations are discussed. A comparison against initial benchmark problems is provided. Issues with the methods are highlighted as well as possible solutions.
M2/3: Final Implementation and Demonstration of ROM-based Multiscale Algorithms (September 2026). Culmination of the project. Implementation improvements are discussed, along with recommendations on how to integrate the methods within the NEAMS program.
M4: Code Release. (September 2026). The production code is released in public repositories.

Facilities

The proposed computational work will be performed at various high performance computing facilities, where the PIs already have been awarded allocations.

The PI has access to *Delta* at UIUC, which has 440 NVIDIA A100 GPUs. His lab also has several multi-CPU workstations, including one with two NVIDIA Titan V GPUs for local development work. Through the DOE ECP CEED project, he and his students have access to DOE's pre-exascale and exascale platforms for testing at scale. He also frequently has access to ALCF and OLCF platforms through DOE's standard allocation processes.

The co-PI at Penn State has an allocation at the local ROAR supercomputer that will be leveraged for both testing and optimization simulations. ROAR is Penn States flagship research cluster maintained by ICDS. Roar includes basic, standard, and high memory compute as well as GPU processors. ROAR operates more than 30,000 Basic, Standard and High Memory cores to support Penn State research. The system provides dual 10- or 12-core Xeon E5-2680 processors for Basic and Standard memory configurations and quad 10-core Xeon E7-4830 processors for High Memory configurations. In addition to access to ROAR, request for allocations with DOEs ALCC and INCITE programs will be submitted for access to DOEs supercomputing facilities if needed. Access to INL Sawtooth will also be pursued.

The Nuclear Science and Engineering division at ANL hosts the Nek5k cluster, which is dedicated for high-fidelity CFD simulations using Nek5000/NekRS. This cluster includes 40 nodes, each with dual 20-core Xeon Gold 6230 processors and 92GB of memory connected by a high speed Infiniband network. A planned upgrade will add two additional nodes, each with 8 Nvidia A100 GPUs, expected to be available in early 2023.

Roles/Responsibilities of Partnering Organizations

The project team comprises university partners Fischer (UIUC) and Merzari (PSU) and laboratory partner Shaver (ANL), all working to develop ROM analysis tools that are readily usable by researchers from industry, academia, and national laboratories. PSU and ANL are subcontractors on the UIUC award.

The team will meet every two-weeks to coordinate on different development aspects of the project. Detailed work on specific models will be developed by each co-PI together with the graduate students who will be supported by this project. Each collaborating person/institution contributes a complementary set of expertise, and their responsibilities will be as follows:

- *Paul Fischer* will lead the overall project and ensure a smooth and productive interaction among all areas. He will also lead overall algorithmic development with a focus on order reduction.

- *Elia Merzari* will lead the high fidelity simulation thrust for Large Eddy SImulation (LES) and Direct Numerical Simulation (DNS) datasets in rod bundles as well as the validation, testing and demonstration thrust. He will also support algorithmic development by focusing on the interaction between high fidelity and the reduced order models.

- *Dillon Shaver* will support ongoing efforts by consulting on the relevance to the NEAMS program and the advanced reactor industry. He will also work with Merzari on directing the integration of NekROM with Cardinal/SAM for target cases.

Unique Challenges

Like RANS, one can expect the success of ROMs for turbulent flows to be somewhat sporadic. Unlike elliptic PDEs, for which there is robust and well-established stability and convergence theory, the non-symmetric nonlinear NSE largely defy such analysis ([5, 17], however, make progress in this direction), which makes ROM-for-turbulence development challenging. Like RANS, however, the results can be spectacularly rewarding when ROMs work—thousands of convective time units simulated per minute for small N. Close inspection of the mathematically-driven ROM literature for LES and RANS reveals that many of the examples do not exhibit emergent turbulence. Turbulent cases where ROMs do succeed often feature clear time-scale separation (e.g., 3D flow past a cylinder [18] or a precessing jet [3]), which indicates that succcess is more likely when there is an emergent low-rank dynamical system. If ROMs work only in these cases, we could still consider this a success.

Fortunately, we have a team that is well-versed in multiple numerical methods and their applicability across the broad reactor-TH landscape. The team also understands the benefit/costs of TH analysis in this application space. It is a team that cannot afford to shrink from tackling challenging problems. As such, we expect to push the boundaries of this multiscale approach to turbulent TH applications.

References

[1] J. Acierno and E. Merzari. Large eddy simulation of jet interaction. In *Advances in Thermal-hydraulics '22*, 2022.

[2] S. E. Ahmed, O. San, A. Rasheed, and T. Iliescu. A long short-term memory embedding for hybrid uplifted reduced order models. *Physica D: Nonlinear Phenomena*, 409:132471, 2020.

[3] N. Akkari, F. Casenave, and V. Moureau. Time stable reduced order modeling by an enhanced reduced order basis of the turbulent and incompressible 3d Navier–Stokes equations. *Math. Comp. Appl.*, 24(2), 2019.

[4] S. Chaturantabut and D. C. Sorensen. Nonlinear model reduction via discrete empirical interpolation. *J. Sci. Comput.*, 32(5):2737–2764, 2010.

[5] L. Fick, Y. Maday, A. Patera, and T. Taddei. A stabilized pod model for turbulent flows over a range of Reynolds numbers: Optimal parameter sampling and constrained projection. *J. Comp. Phys.*, 371:214–243, 2018.

[6] R. Hu, L. Zou, G. Hu, D. Nunez, T. Mui, and T. Fei. SAM theory manual. Technical report, Argonne National Lab.(ANL), Argonne, IL (United States), 2021.

[7] K. Kaneko. *An augmented basis method for reduced-order models of turbulent flow*. PhD thesis, Univ. Illinois, Urbana-Champaign, 2022.

[8] K. Kaneko and P. Fischer. Augmented reduced order models for turbulence. *Front. Phys.*, 2022.

[9] K. Kaneko, P.-H. Tsai, and P. Fischer. Towards model order reduction for fluid-thermal analysis. *Nuc. Eng. and Des.*, 370:110866, 2020.

[10] M. Khodkar, P. Hassanzadeh, S. Nabi, and P. Grover. Reduced-order modeling of fully turbulent buoyancy-driven flows using the Green's function method. *Phys. Rev. Fluids*, 4(1):013801, 2019.

[11] A. R. Kraus, E. Merzari, M. Martin, D. Langewisch, and Y. Hassan. High-fidelity simulations of shield assembly mixed convection flows with applications toward reduced-resolution modeling. In *NURETH-19*, 2022.

[12] B. Krohn, A. Manera, and V. Petrov. A novel method to create high density stratification with matching refractive index for optical flow investigations. *Experiments in Fluids*, 59:1–10, 2018.

[13] J. Martinez, Y. Lan, E. Merzari, and M. Min. On the use of LES-based turbulent thermal-stress models for rod bundle simulations. *Int. J. Heat and Mass Trans.*, 142:118399, 2019.

[14] E. Merzari, H. Yuan, M. Min, D. Shaver, R. Rahaman, P. Shriwise, P. Romano, A. Talamo, Y.-H. Lan, D. Gaston, et al. Cardinal: A lower-length-scale multiphysics simulator for pebble-bed reactors. *Nuclear Technology*, 207(7):1118–1141, 2021.

[15] C. Mou, E. Merzari, O. San, and T. Iliescu. A numerical investigation of the lengthscale in the mixing-length reduced order model of the turbulent channel flow. *arXiv preprint arXiv:2108.02254*, 2021.

[16] P. Tsai and P. Fischer. Parametric model-order-reduction development for unsteady convection. *Front. Phys.*, 2022.

[17] K. Veroy and A. Patera. Certified real-time solution of the parametrized steady incompressible Navier-Stokes equations: rigorous reduced-basis a posteriori error bounds. *Int. J. for Num. Meth. in Fluids*, 47 (8–9):773–788, 2005.

[18] D. Wells, Z. Wang, X. Xie, and T. Iliescu. An evolve-then-filter regularized reduced order model for convection-dominated flows. *Int. J. Numer. Methods Fluids*, 84(10):598–615, 2017.