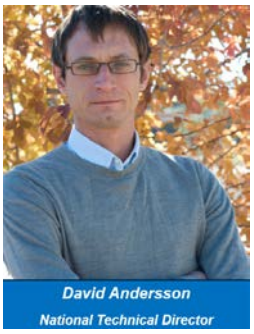
NEAMS

Nuclear Energy Advanced Modeling and Simulation

NEWSLETTER

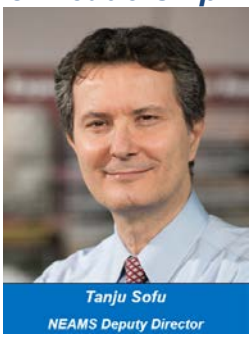
April | 2025

A MESSAGE FROM NEAMS Senior Leadership



David Andersson
National Technical Director

David Henderson
DOE Federal Program Manager



Tanju Sofu
NEAMS Deputy Director

Recently, we have heard exciting news about the role of nuclear energy in supporting increasing demand for electricity driven by the expansion of data centers to advance Artificial Intelligence (AI) technology. This highlights the opportunity to produce more electricity from the current fleet of reactors by uprating the power and extending the lifetime and to deploy new advanced reactors that provide additional opportunities and potential benefits. The NEAMS (Nuclear Energy Advanced Modeling and Simulation) program has an important role to play in making this opportunity a reality. Our vision is that predictive modeling and simulation enable innovation in design, development, licensing, deployment and operation of nuclear reactors. To achieve this vision the program develops advanced methods, models and simulation software for existing Light Water Reactors (LWRs), new LWR designs, and next-generation reactors (High Temperature Gas Reactors, Fluoride Salt-cooled Reactors, Liquid Metal Fast Reactors, Molten Salt Reactors, and Micro-Reactors). The computational tools we develop are intended to support industry stakeholders in their efforts to develop, license, deploy and operate nuclear reactors. They also cater to regulatory applications by the U.S. Nuclear Regulatory Commission (NRC) and research and development performed by other Department of Energy (DOE) programs. The NEAMS program is eager to work with industry and other collaborators to see the benefits of advanced modeling and simulation, including the use of AI/ML (Machine Learning), come to fruition in this critical time for nuclear energy.

The NEAMS program is led by a Senior Leadership Team with a National Technical Director (David Andersson, LANL), Deputy National Technical Director (Tanju Sofu, ANL) and Federal Program Manager (David Henderson, U.S. DOE). The research and development activities are carried out in five Technical Areas (TAs): Fuel Performance, Thermal Fluids, Reactor Physics, Structural Materials & Chemistry, and Multiphysics Applications. In this inaugural NEAMS newsletter we will introduce the TAs and leadership team by providing an overview of work in each TA, the tools that the TAs are developing, and a recent highlight to exemplify ongoing work. The intent is to release a few newsletters throughout the year to feature accomplishments, meetings and upcoming events, such as trainings and review meetings, to program stakeholders and other interested parties.

Fiscal Year 2025 is off to rapid start for NEAMS with several milestones already completed. On January 14-16, the program held an internal planning meeting that brought together almost 100 scientists and engineers to review technical progress, discuss the research plan and identify emerging opportunities. This spring, NEAMS will hold five virtual review meetings to present our work supporting each of the key reactor technologies. The details of the meetings are provided in the upcoming events section of this newsletter. The meetings are open to everyone, and we hope for broad participation from the community and look forward to discussions and feedback on our work. Invitations will be sent out separately.

-David Andersson, David Henderson & Tanju Sofu

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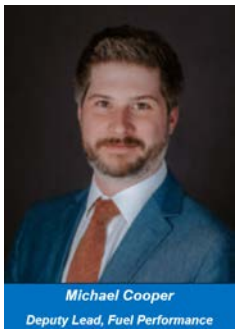
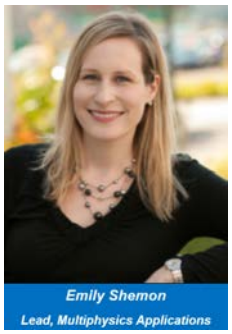
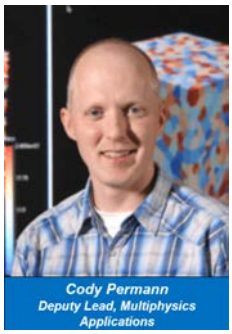
Figure 1 NEAMS Annual Meeting January 14-16, 2025.

NEAMS Extended Leadership Team (Technical Area Leads and Deputies):







NEWSLETTER

TECHNICAL AREAS

FUEL PERFORMANCE:

BISON is the NEAMS engineering-scale fuel performance code. It embeds emerging technology for advanced fuel performance computation in multiple options for dimensions, physics, coupling approaches, and length scale information, depending on application and industry requirements. BISON includes models for metallic, UO_2, Zircaloy, steel, TRISO, UN, U_3Si_2, and MOX fuel and cladding. Industry can use these models in BISON independently, supplement use of existing tools, or consult with NEAMS modeling experts to implement a multi-faceted approach to fuels performance calculations.

A practical hierarchical approach is taken for exchanging information between scales (from atoms to fuel pellets/kernels and cladding), as opposed to concurrent coupling of multi-scale materials models. This multiscale approach is based on the conviction that deriving fuel behavior from an instantaneous knowledge of fuel and cladding chemistry and microstructure, rather than by correlating it to an empirical metric such as "burnup," delivers an unprecedented degree of predictability in nuclear fuel performance. We have recently begun implementing information from lower length scale/mechanistic calculations for fuel and cladding into engineering-scale simulations through the development of reduced order models. An example of this is highlighted in the Lookback section, where a better understanding of fuel response to stress is demonstrated. An example of utilizing the broader BISON capabilities is Kairos Power's use of BISON in the NRC licensing process. The research team that develops BISON received an R&D-100 award in 2021.

MULTIPHYSICS APPLICATIONS:

The Multiphysics Applications Technical Area supports a variety of activities to enable, demonstrate, and deploy the simulation of coupled multiphysics phenomena in nuclear reactors. The NQA-1 compliant, open-source Multiphysics Object Oriented Simulation Environment (MOOSE) provides flexible and robust coupling mechanisms among MOOSE-based (e.g. Griffin, BISON, SAM) and MOOSE-wrapped (e.g. Cardinal) physics applications to simulate a variety of advanced reactor applications as well as support LWR applications. MOOSE's capabilities can be leveraged from beginning to end of analysis, and include reactor geometry-specialized mesh generation, coupling schemes with user-defined space and time scales, convergence monitoring, and efficient output processing. MOOSE also provides uncertainty quantification methods that can be wrapped around multiphysics simulations. The Multiphysics Applications Technical Area supports reactor analysis-driven improvements in MOOSE and in the NEAMS Workbench, the program's open-source, graphical user interface for input validation, workflow management, and output processing. Workbench is readily available on INL's High Performance Computing resources.

A critical component of this Technical Area is the demonstration and assessment of multiphysics capabilities to provide new methods and identify code capability gaps for a wide variety of reactor concepts. LWR activities focus on engagement with the LWR industry, proposing new modeling and simulation functionalities to address relevant LWR challenge problems, and applying these functionalities using the program's LWR tools (including VERA, originally developed by the DOE NE-funded CASL consortium). Non-LWR applications focus on identification and testing of multiphysics functionalities for Fast Reactors, High Temperature Gas Reactors, Micro-Reactors, and Molten Salt Reactors. Challenge problems relevant to reactor design and licensing are prioritized. Software verification and validation activities accompany demonstration activities when possible.

REACTOR PHYSICS:

Reactor physics modeling and simulation quantifies particle-nuclide interactions, nuclide decay transitions, and their respective energy-release and secondary particle release. These reaction rates underpin the calculation of design and safety quantities of interest and detailed design quantities of interest.

Since the inception of the NEAMS and Hub programs, the U.S. Department of Energy has invested in HPC-based codes with higher energy and spatial fidelity than legacy approaches. Griffin is a flexible MOOSE-based reactor physics application for multiphysics simulations of advanced reactor designs jointly developed by Idaho National Laboratory and Argonne National Laboratory. Shift is flexible Monte Carlo tool for reference reactor transport solutions, cross section generation, shielding, and sensitivity/uncertainty analysis. The MPACT code provides 2D/1D full-core transport solutions for LWR simulation through the VERA LWR core simulator.

STRUCTURAL MATERIALS & CHEMISTRY:

Nuclear reactor structural components must safely perform their intended functions under long-term exposure to aggressive environmental conditions. Decisions regarding the safe long-term operation of existing reactors and material selection and designs for proposed reactors, many of which will be operated at temperatures much higher than current LWRs, require understanding the progression of degradation mechanisms and the ability of reactor structures, systems, and components to safely perform in the presence of environmentally induced degradation.

Many of the advanced-concept nuclear reactors currently being developed employ molten salts to serve as their coolant or simultaneously as the coolant and fuel bearing medium. For such a system, it is essential to have salt property databases and simulation tools that, used together, can accurately predict the composition and state of molten salt throughout the coolant system. The interactions between the salt and salt-facing materials, which could potentially result in corrosion and plating out of solid materials, will determine material lifetime and affect operational performance.

The Structural Materials & Chemistry Technical Area is collaborating with other programs (DOE MSR) to develop computational models, tools, and databases to address these challenges, many of which involve complex interactions between multiple physics and length scales. The Grizzly code models the performance of structural components. The LAROMANCE reduced-order models and the NEML2 library provide mechanical constitutive models for high-temperature alloys. The Mole and Pronghorn system-level codes and the MOSCATO high-fidelity code simulate the behavior of chemical species in molten-salt systems. The MSTDB-TP database provides thermophysical properties, and the MSTDB-TC database and Thermochimica Gibbs-energy minimizer provide thermochemical properties used in molten-salt system simulations.

THERMAL FLUIDS:

The Thermal Fluids Technical Area advances the state of the art of thermal-hydraulic simulations through novel solution strategies for historically challenging fluid flow and heat transfer issues in light-water and non-light-water reactors. The Thermal Fluids Technical Area includes the Center of Excellence for Thermal-Fluids Applications in Nuclear Industry, a group formed by laboratory and university counterparts that aims for close collaboration with reactor vendors with consultation from the U.S. Nuclear Regulatory Commission. The mission of the center is to provide a front-end to the advanced reactor industry for thermal-fluids problems,

demonstrate the use of T/H tools for industrial use, and stimulate collaborations.

Our advanced T/H research and development approach synergistically combines three length and time scales in a hierarchal multi-scale approach. At the *System Scale,* analysis for nuclear reactors is composed of one-dimensional fluid flow pipe networks, zero-dimensional system components, and other reduced order model (ROM) approaches. Safety analysis and simulations for licensing purposes are typically conducted at this scale. The Technical Area developed the Systems Analysis module (SAM) based on the MOOSE framework. The *Engineering Length Scale* integrates coarse mesh approaches for homogenized multi-dimensional conjugate heat transfer (CHT), such as those found in gas-cooled pebble-bed reactors. The primary code supported is the Pronghorn code, based on the MOOSE framework. Specialized codes such as CTF for LWR subchannel analysis and the heat-pipe code Sockeye are also supported. Finally, the *Lower Length Scale* focuses on resolving the high-resolution physics associated with single and multi-phase, highly turbulent CHT with highly resolved thermal boundary layers (heat flux). The primary code supported is Nek5000/NekRS/Cardinal, an open-source high-order code that offers complementary capability to commercial CFD options. It is integrated with the MOOSE framework through Cardinal.

Several new features were recently added to the multi-scale T/H simulations toolbox. Pronghorn has been demonstrated for use in several Molten Salt Reactor applications, which includes advanced features such as modeling of gas bubbling and turbulence models for coarse-CFD simulations. Further, Pronghorn and SAM can now run coupled seamlessly through an advanced overlapping domain coupling approach. A new one-dimensional model was developed and implemented in SAM for thermal mixing and stratification effects in large pools and enclosures, which is critical for accurate safety analysis under certain scenarios. At the Lower Length Scale, level-set methods were developed and implemented in NekRS for interface resolved two-phase modeling.

Lookback:

FUEL PERFORMANCE:

Modeling creep of UO_2 pellets using a multiscale approach: While UO_2 has been used extensively for decades in LWRs, fuel vendors are using dopants to modify the UO_2 pellet mechanical properties with the aim of improving pellet-cladding mechanical interactions during operation. By reducing the strain imparted on the cladding by the pellet, it is hoped that cladding performance during accident conditions can be enhanced. Dopants (like chromia) increase the grain size of the fuel during pellet fabrication; therefore, understanding the relationship between microstructure and mechanical deformation of UO_2 is key to supporting operators to claim benefits from doping UO_2.

One aim of the NEAMS program is to develop high-fidelity physics-based advanced modeling and simulation tools to describe fuel performance. Compared to empirical models, mechanistic physics-based models provide benefits, such as fewer data points for fitting and better extrapolation where experimental data is scarce or non-existent. To this end, a mechanistic diffusional creep model informed by lower-length scale simulations was developed for UO_2. A driving factor for developing this model was the lack of consensus for the dominant diffusional creep mechanism, i.e., Nabarro-Herring (bulk) or Coble (grain boundary), which have different grain size dependencies (impacting their application to large-grain doped UO_2). Lower length-scale simulations were used to inform a validated mechanistic creep model, which conclusively showed that Coble creep mechanism is dominant and explained discrepancies between experiments due to very small deviations in sample stoichiometry.

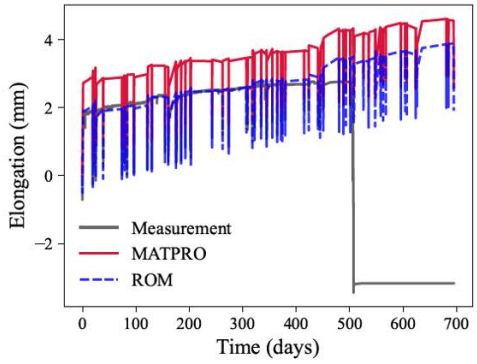


Figure 2 BISON simulations of the IFA-716.1 rod1 test using i) the empirical creep model (MATPRO) and ii) the new reduced order model (ROM). Measurements of rod elongation are shown for comparison.

The mechanistic diffusional creep model was used to train an artificial neural network surrogate model. This was then implemented in BISON to identify how the results differ from those currently implemented using a fully empirical creep model. Figure 2 shows BISON simulations of a Halden Reactor Project experiment. Fuel elongation predictions when using the empirical model (MATPRO) are compared to those when using the mechanistically informed reduced-order model (ROM). Using the ROM, predictions for rod elongation are improved compared to the MATPRO model.

Recently, Bayesian inference techniques have been applied to the mechanistic diffusional UO_2 creep model. This approach was able to confirm quantitively that uncertainty in the experimental conditions and underlying model uncertainty could self-consistently explain UO_2 diffusional creep behavior. The resultant model uncertainties will be propagated to engineering scale BISON simulations in future work.

The detail of this work is described in the following references:

- *C. O. T. Galvin, D. A. Andersson, R. Sweet, L. Capolungo, and M. W. D. Cooper, Diffusional creep model in UO2 informed by lower length scale simulations, Journal of Nuclear Materials, 2024, https://doi.org/10.1016/j.jnucmat.2025.155659*
- *R. Sweet, Y. Che, C. O. T Galvin, M. W. D Cooper, and D. Schwen, A New Reduced Order Model For The Mechanistic Creep Behavior Of UO_2, Technical Report, 2024, 10.2172/2479147*

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MULTIPHYSICS APPLICATIONS:

Enabling access to NEAMS tools using the Workbench and MOOSE Containers on INL HPC: Access to MOOSE framework-based physics applications such as Griffin, BISON, and SAM has recently been streamlined for users with INL High Performance Computing (HPC) Nuclear Computational Resources Center (NCRC) accounts (available upon request). Once logged into an INL HPC session, users can easily activate and interact with containerized binaries through the NEAMS Workbench, a user-friendly desktop application (Figure 3). Starting up a NEAMS Workbench session permits immediate use of NEAMS physics applications and assists the user with input editing, navigation, validation, job submission, and output inspection, removing several barriers to code access and adoption. Ultimately, this synergy between containerized MOOSE applications, INL HPC execution, and the NEAMS Workbench enhances accessibility, reproducibility, and efficiency in multiphysics simulations, while also empowering users—from beginners to experts—to seamlessly navigate and exploit high-performance computing resources.

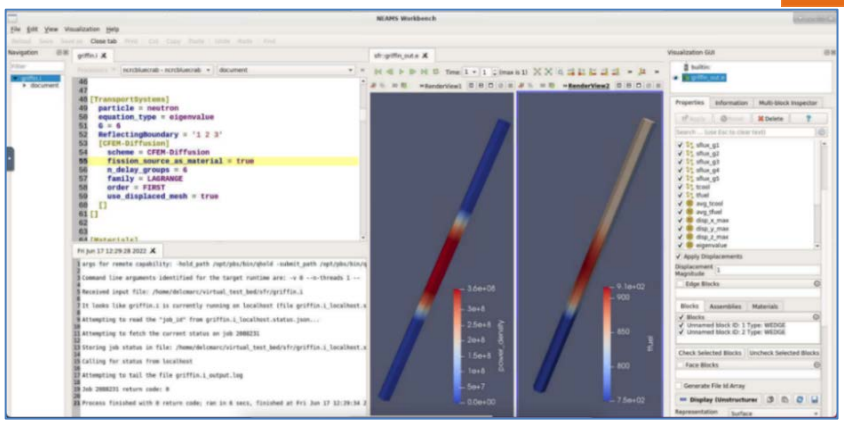

Figure 3 Using the NEAMS Workbench to run multiphysics models on INL HPC.

Detailed information on MOOSE Applications and associated containers is located at https://mooseframework.inl.gov/help/inl/applications.html.

More information about using the NEAMS Workbench on INL HPC with MOOSE Application containers can be found at https://mooseframework.inl.gov/virtual_test_bed/resources/neams-workbench.html.

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Logan Harbour (INL) MOOSE Container POC – logan.harbour@inl.gov

REACTOR PHYSICS:

Griffin training for the U.S. Nuclear Regulatory Commission: The reactor physics technical area is committed to training and equipping our user base. The Griffin development team conducted a three-day workshop at U.S. Nuclear Regulatory Commission headquarters December 18-20, 2024. This was a hybrid workshop attended by members of the U.S. Nuclear Regulatory Commission, Department of Energy, and various national laboratories. The total number of attendees was forty (thirty-one participants), with four instructors from Idaho National Laboratory, three from Argonne National Laboratory, and two from Oak Ridge National Laboratory. The topics covered included neutron transport, neutron cross section preparation, fast and pebble-bed reactor analysis workflows, general reactor physics, and verification of Griffin solutions with the Shift Monte Carlo code.

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STRUCTURAL MATERIALS & CHEMISTRY:

Integration of Pronghorn & Thermochimica to model speciation, thermodynamic equilibrium and corrosion in Molten-Salt Reactors: A key need for Molten Salt Reactor (MSR) operation is the continuous tracking of species—including gas transport, plating, and leaching with structures—and the modeling of corrosion processes. Accurate modeling of these phenomena is essential to ensure reactor operability, minimize long-term material degradation, and optimize reactor efficiency.

An important advance toward an MSR simulation capability was recently made by integrating Pronghorn, a MOOSE (multiphysics object-oriented simulation environment)-based coarse-mesh computational fluid dynamics tool, with Thermochimica, a Gibbs energy minimizer software, the MSTDB-TC (molten salt thermal property database – thermochemical), and Griffin, a reactor-physics code. This work was performed in close collaboration with several Technical Areas with Structural Materials & Chemistry providing the Thermochimica and MSTDB-TC capabilities. Pronghorn handles fluid flow and heat transfer simulations, while Thermochimica calculates the thermodynamic equilibrium and chemical speciation of the molten salt. In this simulation tool, corrosion and fission products are tracked using the Poisson-Nernst-Planck model and Butler-Volmer kinetics, and two-phase flow is modeled to track volatile species and their transport between liquid and gaseous phases. Advanced depletion models provided by Griffin track isotopic evolution, coupled with speciation, and their impact on species transport and corrosion.

This tool provides the foundational capabilities for detailed and accurate simulations of MSR behavior. It was used to demonstrate species tracking and Thermochimica-driven phase equilibrium calculations in full-loop MSRs, with examples of a fluoride system (the molten salt reactor experiment, or MSRE), as shown in Figure 4, and a chloride system (the Lotus MSR).

The details of this work is described in the following reference:

- *Mauricio Tano, Samuel Walker, Parikshit Bajpai, and Daniel Schwen. Integration of Thermochimica into MOOSE-based Molten Salt Reactor Loop Simulations. INL/RPT-24-81124-Rev001. Idaho National Laboratory, Idaho Falls, ID, 2024.*

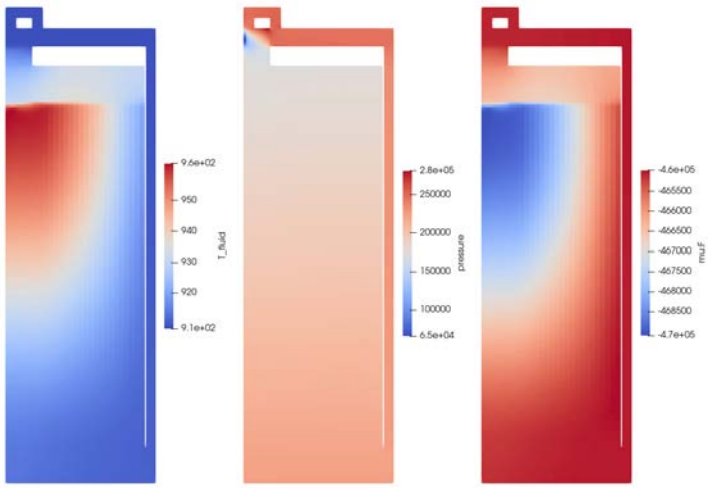

Figure 4 Thermochemically important fields within MSRE at steady-state operation predicted by the coupled MSR simulator: (a) temperature [K], (b) pressure [Pa], (c) chemical potential of fluoride (F−) [J/mol].

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THERMAL FLUIDS:

Stabilization methods for interface problems in Nek5000/RS: A high-fidelity interface-capturing capability is of immense importance to the design of the existing fleet of LWRs and advanced nuclear reactor concepts, including Molten Salt Reactors in particular. Two-phase regimes remain one of the most challenging flow scenarios to model, with large uncertainties in existing models despite their predominance in nuclear reactor thermal hydraulics. This is due to a combination of modeling complexity, the need for complex closures and high computational cost. High resolution and accurate interface modeling in strong scaling codes such as NekRS [1], which can also leverage GPU acceleration offered by state-of-the-art supercomputing systems, is therefore of considerable value to modeling nuclear reactor flow regimes.

High-order methods are typically not well suited for interface-resolving simulations because of sharp gradients across the two phases. In the absence of any numerical stabilization methods, interface transport invariably causes high-frequency oscillations, more commonly referred to as Gibbs phenomena [2], introducing dispersion errors in the solution with time advancement. The development of stabilization methods and their specific application to two-phase interface capturing problems in high-order continuous Galerkin (CG) based spectral element methods, such as Nek5000/NekRS, has not been previously explored. However, recent advancements in the stabilization methods and solvers in Nek5000, specifically tailored for the CG spectral element framework, have enabled the accurate transport of interfaces for two-phase problems. Figure 5 demonstrates the interface-capturing capability implemented in the Nek5000 solver for the Rayleigh-Taylor instability problem. Time evolution of the interface front for meshes with increasing resolution is shown in Figure 6 to show the consistency of the solver. This represents a significant breakthrough and an important addition to Nek5000/NekRS.

References:

1. *P. Fischer, S. Kerkemeier, M. Min, Y.-H. Lan, M. Phillips, T. Rathnayake, E. Merzari, A. Tomboulides, A. Karakus, N. Chalmers, T. Warburton, Nekrs, a gpu-accelerated spectral element navier-stokes solver, Parallel Computing 114. doi:10.1016/j.parco.2022.102982.*
2. *D. Gottlieb, C.-W. Shu, On the gibbs phenomenon and its resolution, SIAM review 39 (4) (1997) 644–668.*
3. *J.-L. Guermond, L. Quartapelle, A projection fem for variable density incompressible flows, Journal of Computational Physics 165 (1) (2000) 167–188.*
4. *P.-H. Chiu, Y.-T. Lin, A conservative phase field method for solving incompressible two-phase flows, Journal of Computational Physics 230 (1) (2011) 185–204.*

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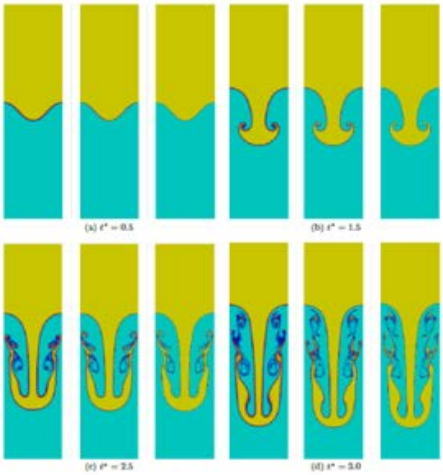

Figure 5 CLS field contour for Rayleigh-Taylor instability problem at different timestamps with meshes {25 × 100, 50 × 200, 100 × 400}, shown from left to right.

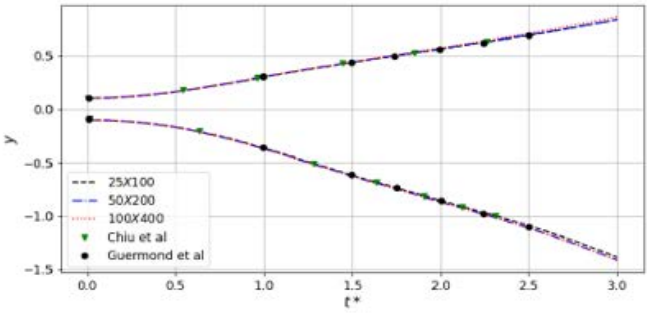

Figure 6 Interface location along the domain center and boundary with different mesh compared with results from Guermond et al [3] and Chiu et al [4]

Lookahead:

Upcoming Meetings:

NEAMS Virtual Review Meetings by reactor type:

- Light Water Reactors: May 7th, 2025
- High Temperature Gas-cooled and Fluoride Salt-cooled Reactors: May 8th, 2025
- Micro-Reactors: May 12th, 2025
- Molten Salt Reactors: May 28th, 2025
- Fast Reactors: May 29th, 2025

Trainings and workshops:

- MOOSE Reactor Module Workshop (Registration: 2025 MOOSE Reactor Module Training): May 5-6, 2025
- MOOSE Summer Workshop: June 3-5, 2025
- The Molten Salts Thermal Properties Working Group is conducting a Workshop on the Effects of Contaminant-Level Oxygen, Hydrogen, and Moisture in Salts: June 3-4, 2025

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is a U.S. Department of Energy-Office of Nuclear Energy (DOE-NE) program developing advanced modeling and simulation tools and capabilities to accelerate the deployment of advanced nuclear energy technologies, including Light Water Reactors (LWRs), non-LWRs, and advanced fuels. We work with DOE-NE, the U.S. Nuclear Regulatory Commission (NRC), and industry to develop, demonstrate, and deploy usable advanced modeling and simulation capabilities across five technical areas: Fuel Performance, Reactor Physics, Structural Materials and Chemistry, Thermal Fluids, and Multiphysics Applications.

The NEAMS program has sites at Argonne National Laboratory, Idaho National Laboratory, Los Alamos National Laboratory, and Oak Ridge National Laboratory.

Learn more about the NEAMS program at neams.inl.gov