U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Topic Area 4 – Modeling & Simulation

Up to 3 years and up to $1,000,000

M&S-1: Multi-scale Modeling

M&S-2: Verification & Validation/Uncertainty Quantification

M&S-3: Other Modeling & Simulation Topics

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Topic Area 4

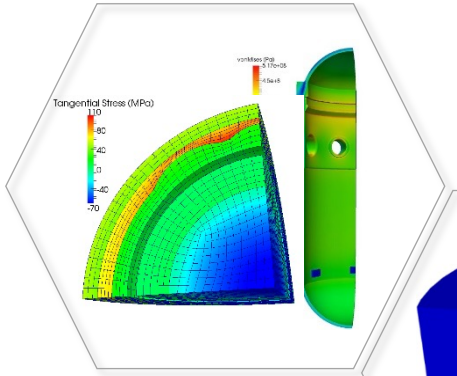
Modeling & Simulation Overview

- Science-based, verified, and validated modeling and simulation capabilities are essential for the design, implementation, and operation of nuclear energy systems.
- This topic areas focuses on nuclear energy related modeling and simulation projects that improve the tools and frameworks for many different modeling and simulation activities including, but not limited to:
  - High fidelity reactor modeling, including neutronics, structural dynamics, and thermal hydraulics;
  - Multi-scale, multi-physics models for characterizing complex neutron kinetics, dynamics, microstructural, and thermomechanical phenomena;
  - Verification and validation;
  - Uncertainty quantification; and
  - Flow modeling, among other relevant areas.

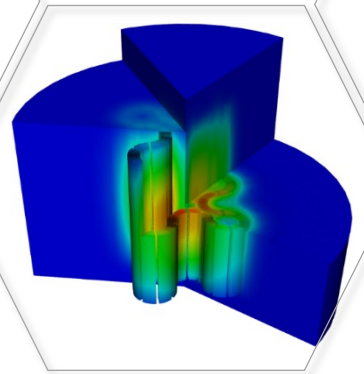
Nuclear Energy Advanced Modeling and Simulation (NEAMS) Overview

NEAMS is the DOE-NE modeling and simulation R&D program that aims to develop and deploy predictive computer methods for the analysis and design of LWRs and non-LWRs.

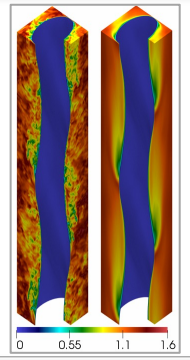
NEAMS core competencies:



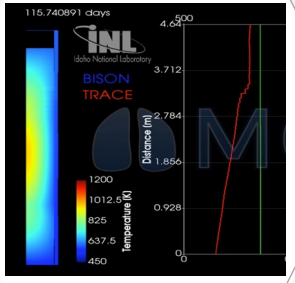
Multiscale fuel performance and structural materials degradation modeling:
BISON, GRIZZLY, YellowJacket



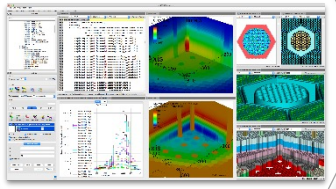
Reactor Physics:
GRIFFIN, MPACT, Shift



Multiscale thermal fluids:
CTF, SAM, PRONGHORN, Sockeye, Nek5000



Multiphysics:
MOOSE, VERA



Workflow Management:
Workbench

NEAMS develops modeling tools for others to use, so coordination and interaction with industry and NE's reactor and fuels R&D programs is critical to NEAMS success. Our work needs to be informed by experimental capabilities and data in order to best support reactor deployment and operation.

Key Success Metric: Use of NEAMS technology (either software or R&D) by stakeholder to improve how they "do business."

Topic Area 4 M&S-1

Multi-Scale Modeling (M&S-1)

Capabilities to accurately model transport phenomena, materials, fuels, and fluid behavior at lower-length scales and reliably translate the effects to the component and/or system level can significantly reduce the amount of experimentation needed to realize new technologies.

This scope is very open within the above description.

Applications should:

- Demonstrate knowledge of existing tools and methods
- Clearly articulate the specific capability to be developed/added and the remaining gap that will exist at completion

Topic Area 4 M&S-1

Relevant Work

The NEAMS program has on-going research through many avenues of funding including directed research, NEUP, SBIR/STTR, SciDAC and Industry FOA.

Previous or on-going research includes the following technologies:

- Frameworks (MOOSE, VERA, Workbench)
- Automated Meshing (NEUP, SBIR)
- Automated optimization approaches
- Multiscale Thermal-hydraulics (2020 IRP)
- Multi-physics TRISO Performance (2020 IRP)
- UO2 fragmentation, relocation, and dispersion
- Fission gas modeling (SciDAC, NEAMS)
- Molten Salt Chemistry/Corrosion (2022 IRP, SciDAC)
- High-fidelity approaches for fast-running transport
- Species transport in system code

The above list of R&D examples is not exhaustive, and it is provided to assist applicants in identifying research that is not duplicative of previous or on-going research.

More information about past/current modeling and simulation R&D can be found on the NEAMS website (neams.inl.gov/technical-areas/), SciDAC Website (scidac.gov/partnerships/nuclear-energy.html), and NEUP website (neup.inl.gov)

Topic Area 4 M&S-1

Non-Relevant Work

Applications should focus on research that support the **DOE-NE mission**

Applications with the following focuses would be considered not relevant to this topic:

- High-performance computing hardware
- Artificial intelligence and machine learning applied to development & operation (see RDO-5 and IC-3)
- Modeling specific to fuel separation processes (see Topic Area 2)
- Nuclear non-proliferation purposes
- Technologies solely for nuclear fusion applications
- Nuclear weapons R&D
- Nuclear medical isotope production
- Nuclear medicine related technologies

Applications on technologies that crosscut any of these areas could be considered responsive if proposal clearly demonstrates the application to nuclear energy.

Topic Area 4 M&S-2

Verification & Validation / Uncertainty Quantification (M&S-2)

Historically, nuclear technology developed has involved continuous prototyping and measurement that has provided the software validation data needed for nuclear regulatory licensing.

This experimental data-heavy approach provides a bounding analysis for regulatory approval but requires substantial conservatism and data to establish uncertainties in predicted safety parameters.

This level of data does not exist for non-light-water reactor types and would inhibit their deployment. Therefore, the use of modeling and simulation with a high focus on uncertainty in predicted safety parameters will be increasingly important and can reduce the need for experimental validation.

Proposals are sought for:

- Development of novel methodologies and approaches for software verification, validation, and establishment of uncertainties for high-fidelity, multiphysics coupled code systems
- Novel approaches for validation and verification of single physics codes and models may also be proposed.

Proposals should address the issue of establishing uncertainties for safety parameters of interest for a given technology within the framework of regulatory licensing.

Topic Area 4 M&S-2

V&V/UQ Relevant Work

The NEAMS program has on-going research through many avenues of funding including directed research, NEUP, SBIR/STTR, and Industry FOA.

Previous or on-going research includes the following advanced control system technologies:

- Visualization and output analytics
- V&V/UQ approaches and workflow (Hub/CASL)
- Benchmarking and code validation (single & multiphysics)

The above list of R&D examples is not exhaustive, and it is provided to assist applicants in identifying research that is not duplicative of previous or on-going research.

More information about past/current V&V/UQ activities can be found on the NEAMS website (neams.inl.gov/technical-areas/), NEUP website (neup.inl.gov), and Nuclear Energy Innovation Hub (casl.gov)

Topic Area 4 M&S-2

Non-Relevant Work

Applications should focus on research that support the **DOE-NE mission**

Applications with the following focuses would be considered not relevant to this topic:

- Nuclear non-proliferation purposes
- Technologies solely for nuclear fusion applications
- Nuclear weapons R&D
- Nuclear medical isotope production

Applications on technologies that crosscut any of these areas could be considered responsive if proposal clearly demonstrates the application to nuclear energy.

Topic Area 4 M&S-3

Other Modeling & Simulation Topics (M&S-3)

Proposals that are relevant to Modeling and Simulation as described in the Topic Area 4 overview but are not covered by the previous topic categories can be submitted to M&S-3 for consideration.

It is important to note that any submission to this category can be crosscutting, but must reinforce the Office of Nuclear Energy's mission and the following supporting goals:

"Advance nuclear energy science and technology to meet U.S. energy, environmental, and economic needs."

1. Enable continued operation of existing U.S. nuclear reactors.
2. Enable deployment of advanced nuclear reactors.
3. Develop advanced nuclear fuel cycles.
4. Maintain U.S. leadership in nuclear energy technology.

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Questions?