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

Outlook on the future of Computing Resources for Nuclear Energy Studies - NEAMS

Cody Permann, Ph.D.
Computational Frameworks

NEAMS
Nuclear Energy Advanced Modeling and Simulation

4/17/2024
NSUF Program Review

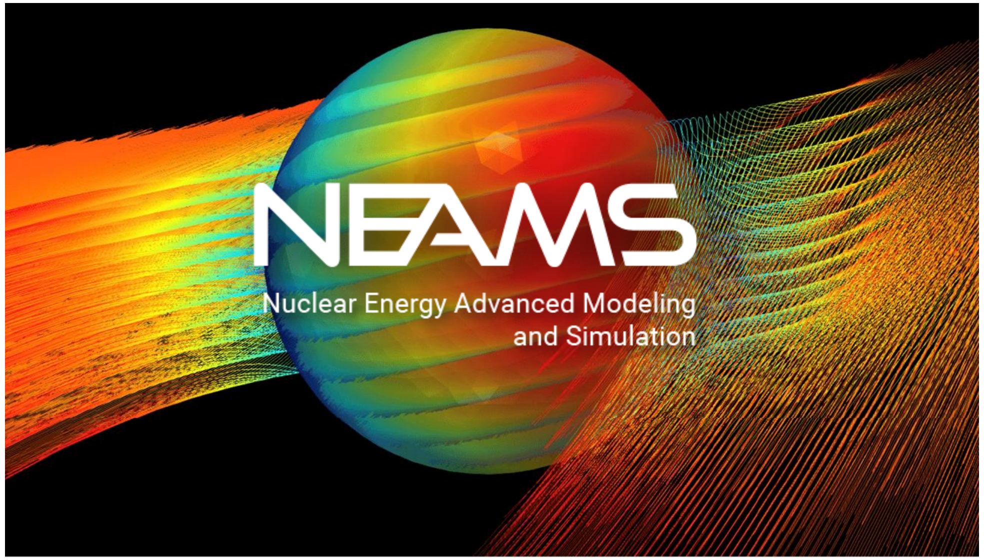
Outline

- NEAMS Program and Software Products Overview
- Multiphysics and Multiapps structure and computing needs
- Flexible Reactor Modeling
- Future Research Directions

- Slide/Image Credits:
  A. Abdelhameed, G. Giudicelli, A. Novak, A. Lindsay, D. Gaston, N. Martin, C. Icenhour, A. Abou Jaoude, Y. Miao, E. Shemon, F. Kong, A. Lindsay, P. Simon, P. Humrickhouse, T. Franklin

NEAMS Program

- Nuclear Energy Advanced Modeling & Simulation
- DOE-NE led program across several national labs: INL, ANL, ORNL, LANL
- Targeting non-LWR advanced reactor designs
- Divided into 5 technical areas:
  - Fuel Performance
  - Reactor Physics
  - Thermal Hydraulics
  - Structural Materials & Chemistry
  - **Multiphysics Applications**
- Primarily leveraging the MOOSE framework for software development



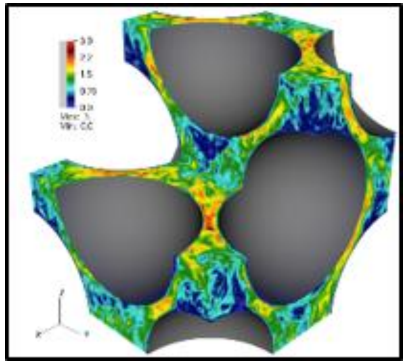
INL Idaho National Laboratory

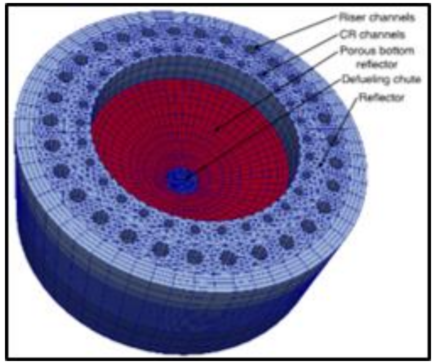
Argonne NATIONAL LABORATORY

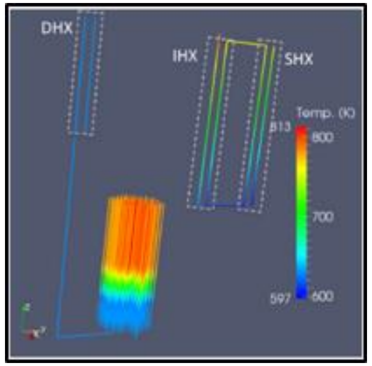
OAK RIDGE National Laboratory

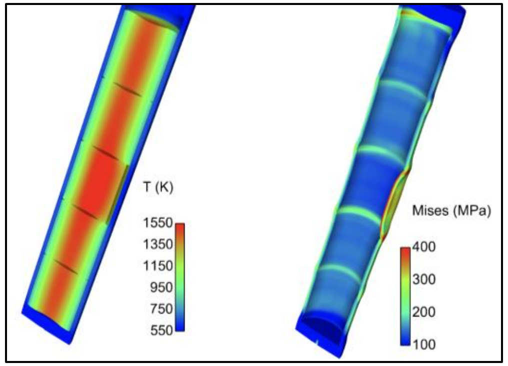
Los Alamos NATIONAL LABORATORY

NEAMS Suite of Tools for Advanced Reactor Simulation









NEK-5000 + **GRIFFIN** + **PRONGHORN** + **SAM** + **Bison/ Yellowjacket**

Fuel Performance/ Thermochemistry

High Fidelity

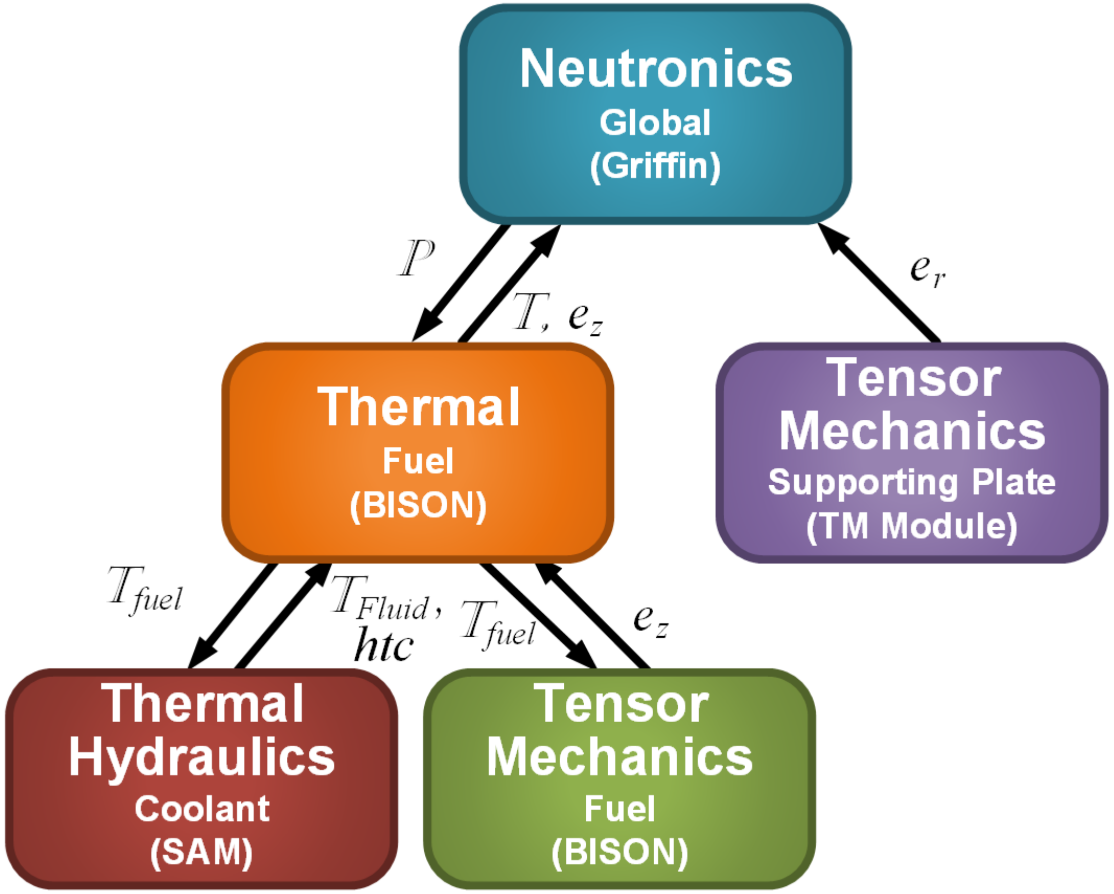
2D/3D Multiphysics Transients

Balance of Plant

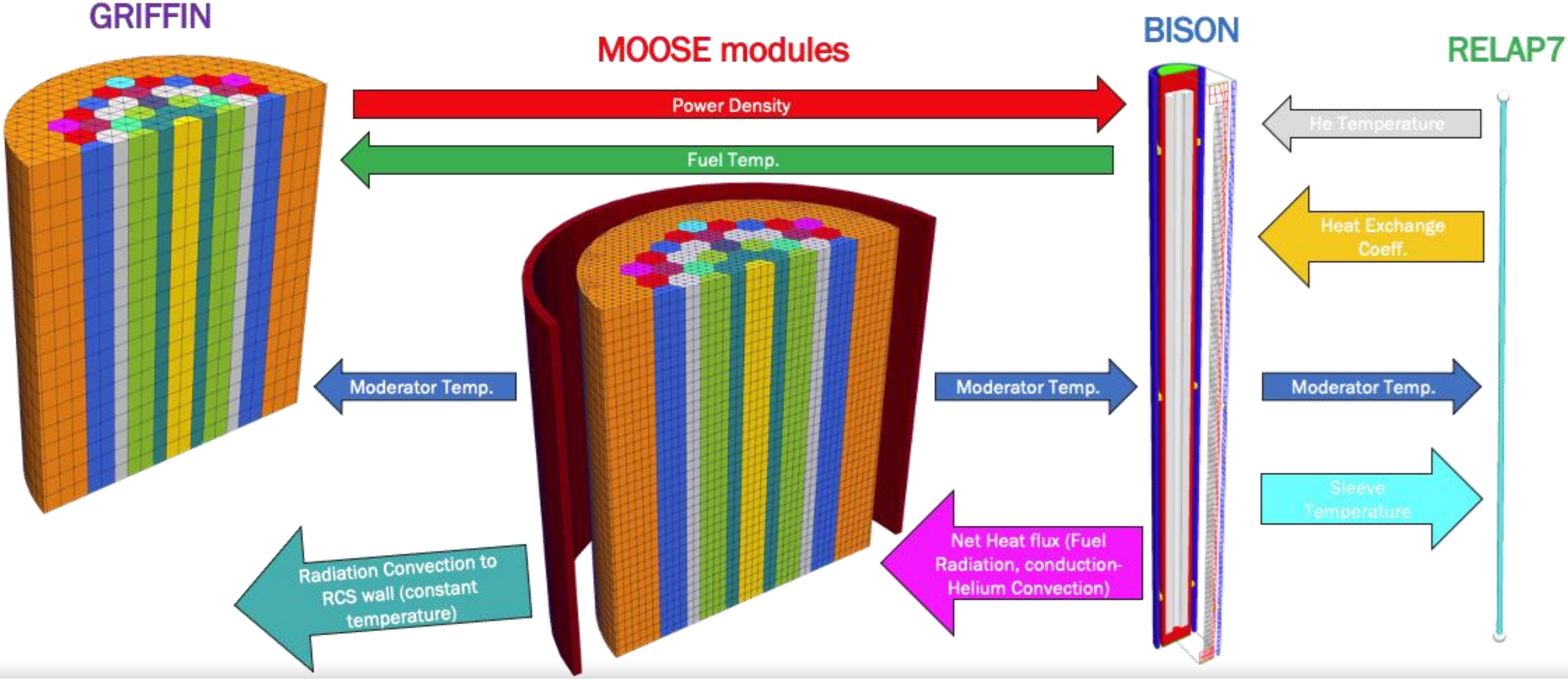
Depletion & Fuel Performance

MultiApps: Enabling Multiscale Simulation

- MOOSE-based solves can be nested to achieve Multiscale-Multiphysics simulations
  - Macroscale simulations can be coupled to embedded microstructure simulations
- Arbitrary levels of solves
- Each solve is spread out in parallel to make the most efficient use of computing resources
- Efficiently ties together multiple team’s codes



Multiapp Coupling Example



GRIFFIN

MOOSE modules

BISON

RELAP7

Power Density

Fuel Temp.

He Temperature

Heat Exchange Coeff.

Moderator Temp.

Moderator Temp.

Moderator Temp.

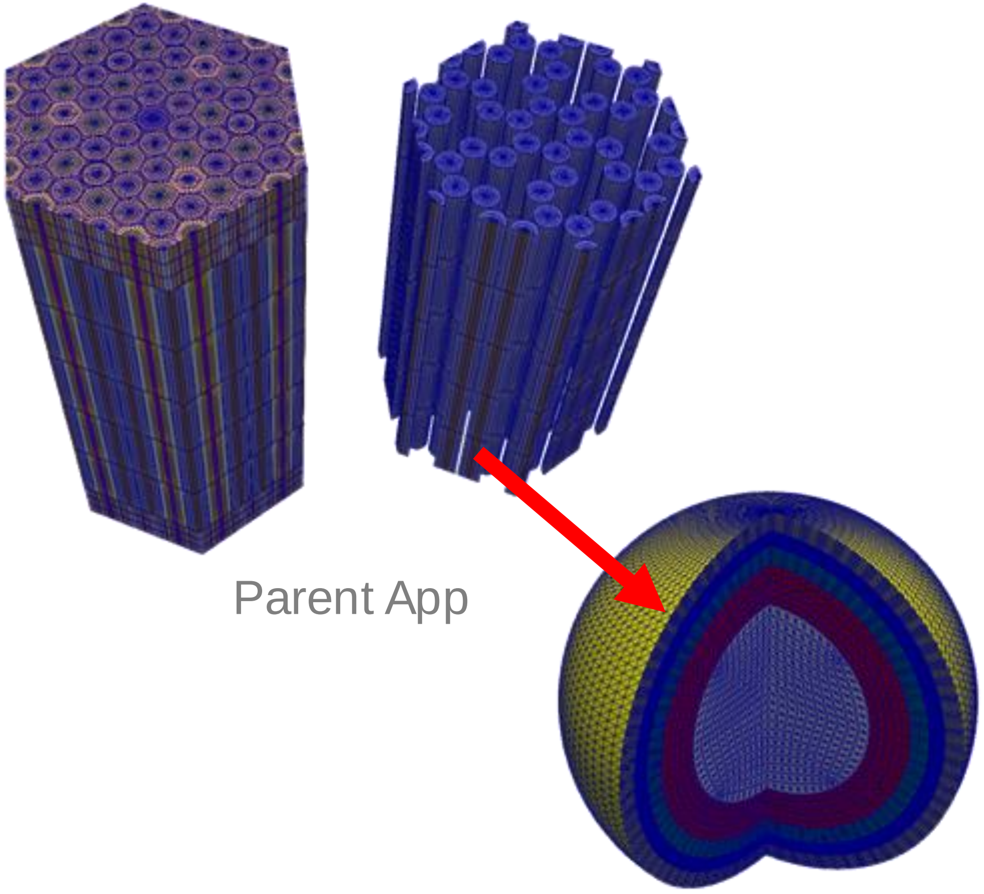
Sleeve Temperature

Net Heat flux (Fuel Radiation, conduction-Helium Convection)

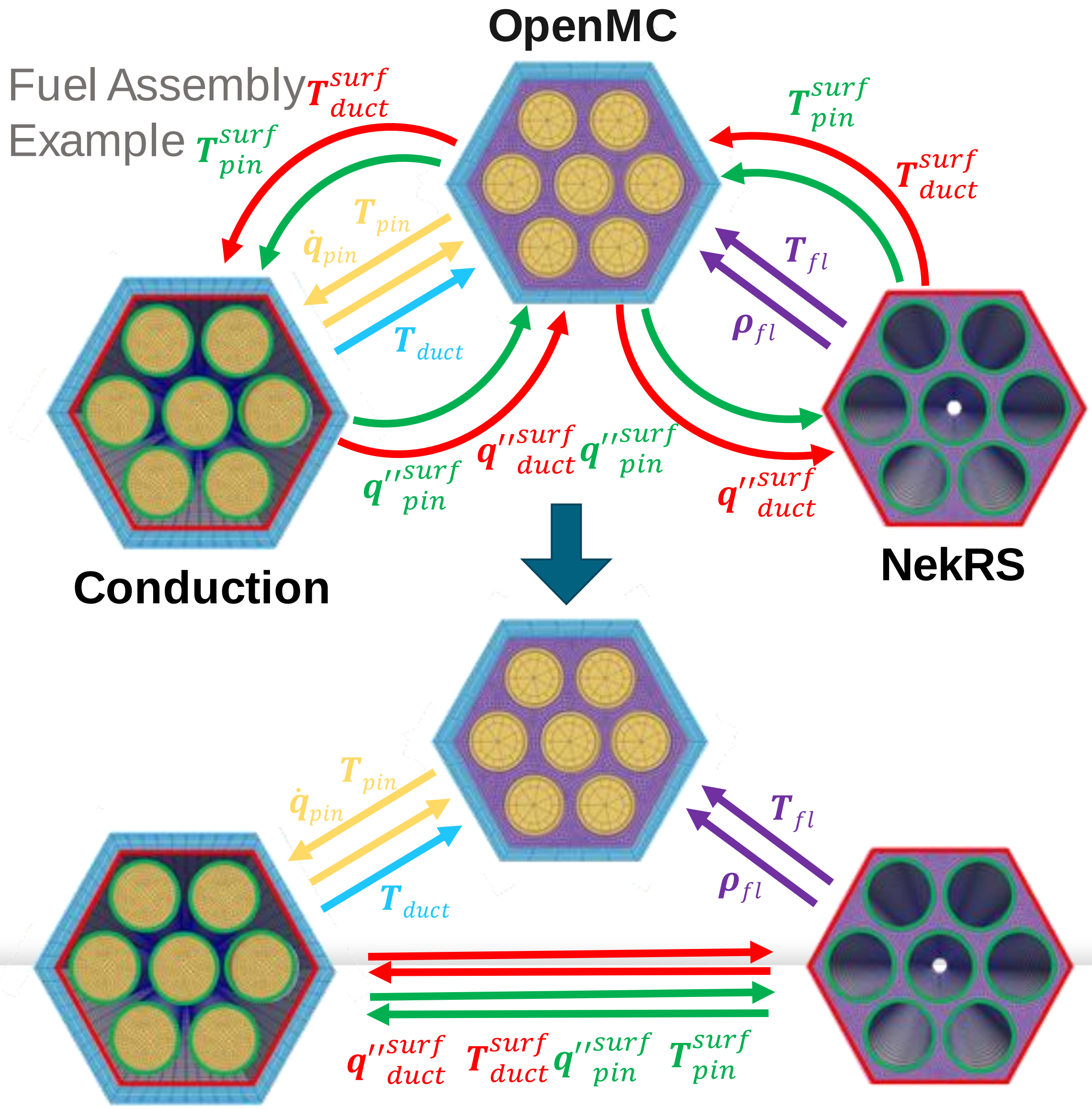
Radiation Convection to RCS wall (constant temperature)

Multiapp Objects Examples

- MultiApps hierarchy/type determines the order/timing of app execution.
- CentroidMultiApp
  - Generates a sub app at every element centroid
  - Useful for multiscale simulations
    - Example TRISO Fuel Compact
    - Parent: Assembly with Fuel compact
      - Homogenized properties
      - Neutronics/Thermomechanics
    - Child: TRISO particle
      - Detailed heterogeneous properties
      - Peal fuel temperature
- Stochastic Related MultiApps
  - Just to statistically control some key parameters in child applications



Additional Complex Multiphysics Models



Fuel Assembly Example

- NekRS – high fidelity CFD (not MOOSE-based)
- OpenMC – high fidelity neutron transport (not MOOSE-based

- Sibling Transfer Illustration

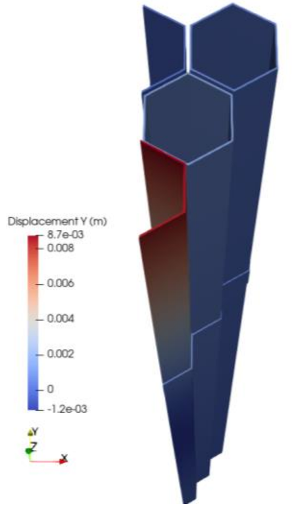
Model Characteristics/Parallelism

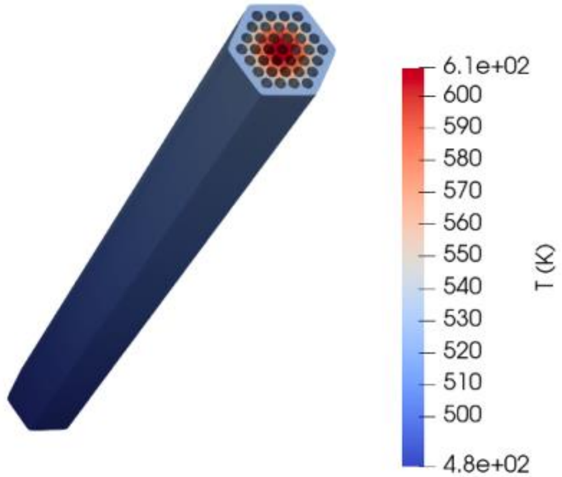
- MOOSE is hybrid parallel following the MPI+thread model
  - OpenMP, pthreads, and C++ threads
- Model sizes can reach billions of DOFs
  - Corresponding processor counts from 1 to tens of thousands of cores
- MultiApp coupling with flexible parallel solution transfer capabilities
  - Multiscale coupling with advanced time stepping options, solution transfer options
- Online mesh generation, can be parallelized
- General distributed mesh capability with customizable ”stencils”

- Currently have limited GPU capabilities:
  - PETSc has some GPU solver capabilities
  - Some algorithms (i.e. transport sweeper) have been ported
  - New funding in FY24+ is being used to explore more GPU usage oppurtunities
  - NekRS runs on GPUs

- **NEAMS/MOOSE usage account for ~250 million core hours per year in the INL HPC Enclave**

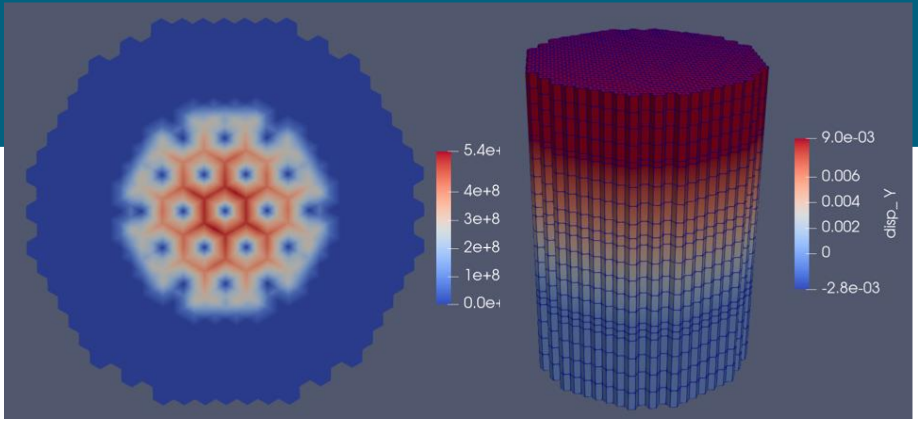
Reactor Use Case: SFR





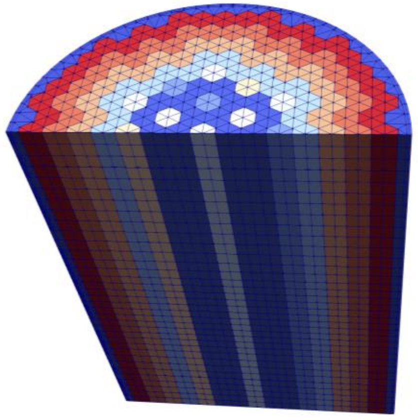
Hexagonal Assembly

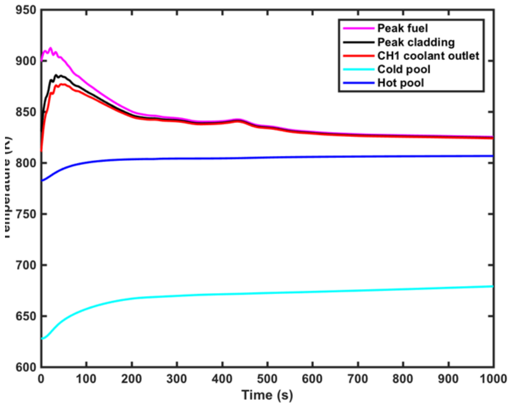
- Duct bowing simulation due to temperature gradient (IAEA benchmark) – POC: Nicolas Wozniak (ANL)
- Subchannel liquid metal flow simulation (Toshiba 37-pin benchmark) – POC: Mauricio Tano (INL)



Versatile Test Reactor (VTR)

- Fully-coupled feedback model between neutronics, conduction, hydraulics, and structural expansion
- Codes coupled: Griffin, Bison, and SAM
- POC: Nicolas Martin (INL)



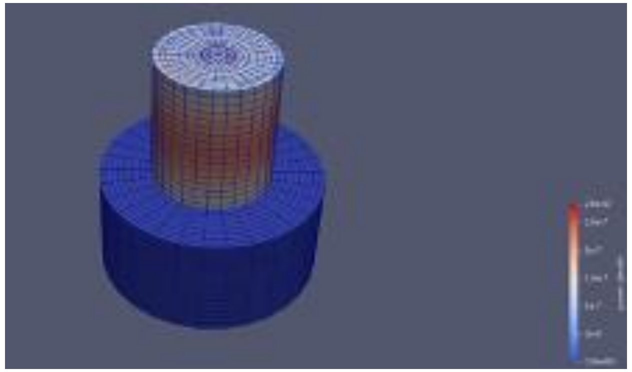


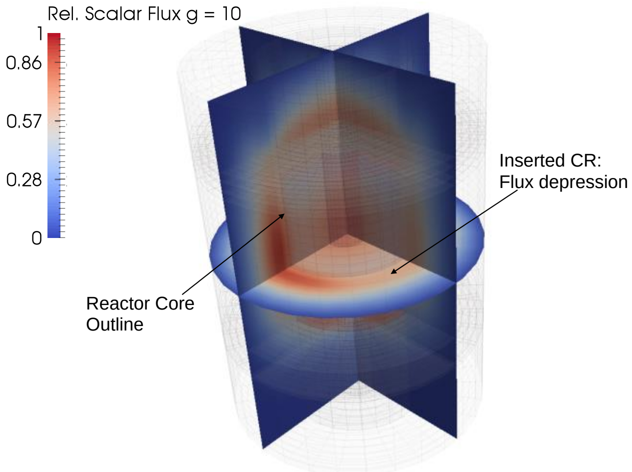
Advanced Burner Test Reactor (ABTR)

- Neutronics (Griffin) coupled with structural thermomechancis – POC: Javier Ortensi (INL)
- System code hydraulic (SAM) simulation coupled with point kinetics model – POC: Rui Hu (ANL)

NRIC National Reactor Innovation Center

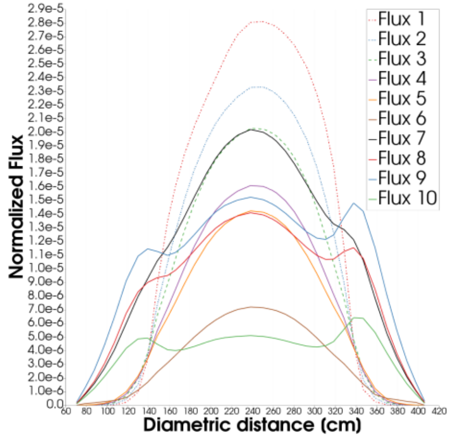
Reactor Use Case: HTGR

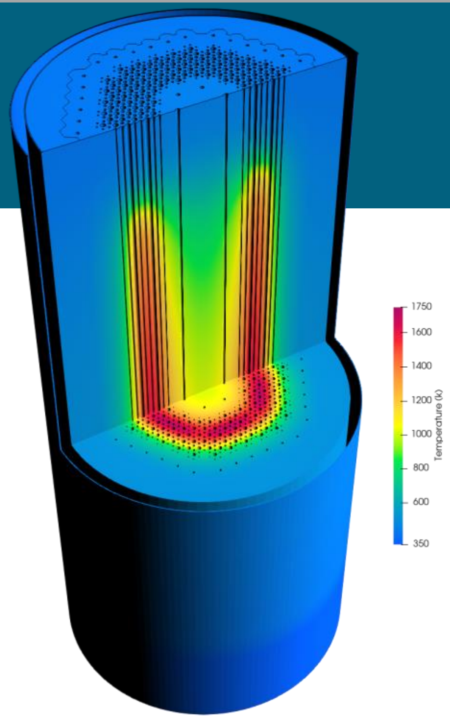




High-Temperature Reactor (HTR-10)

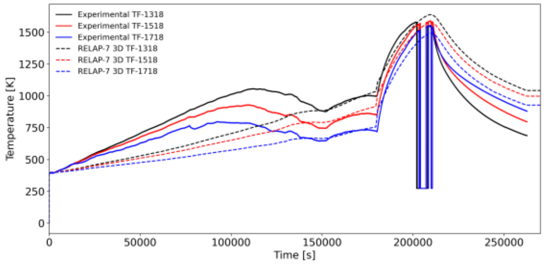
- Steady-state benchmarks with different control rod positions
- Neutronics (Griffin) with heat conduction (MOOSE)
- POC: Javier Ortensi (INL)





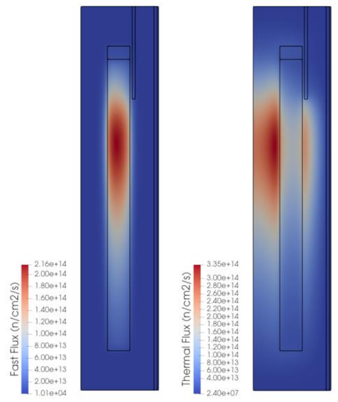
High-Temperature Test Facility (HTTF)

- Coupled heat conduction with system hydraulics
- Steady-state and transient simulations



Pebble-Bed Modular Reactor (PBMR400)

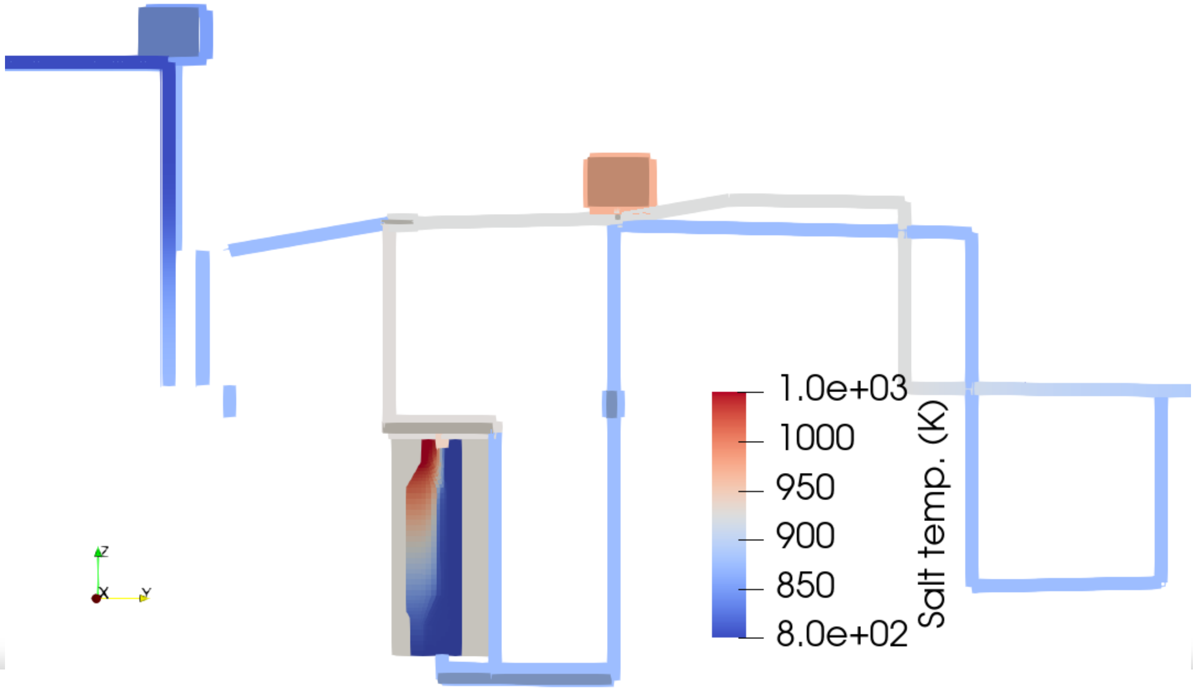
- Coupled neutronics (Griffin) with thermal hydraulics (Pronghorn)
- Multiscale modeling: core-pebble-particle
- Steady-state and transient simulations
- POC: Paolo Balestra (INL)



Reactor Use Case: FHR

Mk-I FHR

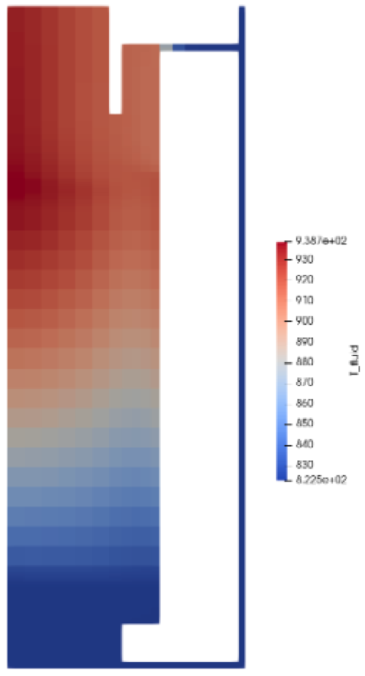
- Coupled core neutronics (Griffin) with core thermal hydraulics (Pronghorn) with plant hydraulics (SAM)
- Steady-state and transient simulations
- POC: Guillaume Giudicelli (INL)



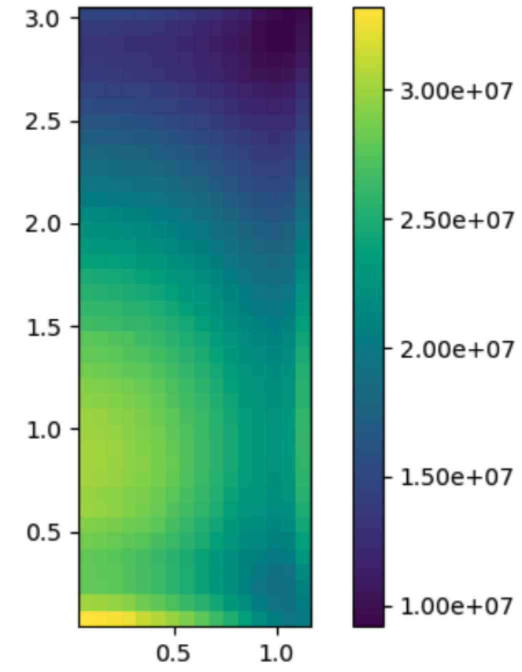
Generic Fluoride High-Temperature Reactor (gFHR)

- Equilibrium core calculation with pebble tracking
- Coupled neutronics (Griffin) with thermal hydraulics (Pronghorn)
- Steady-state and transient simulations
- POC: Sebastien Schunert and Javier Ortensi (INL)

Fluid temperature [K]



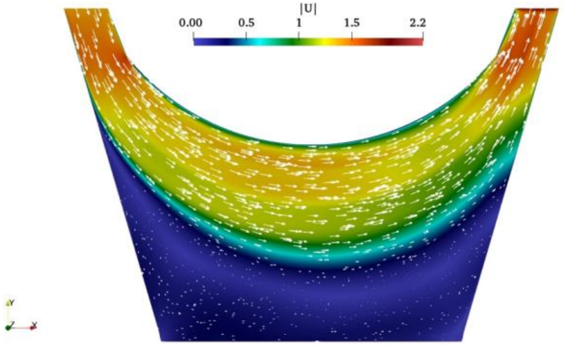
Power density [W/m3]

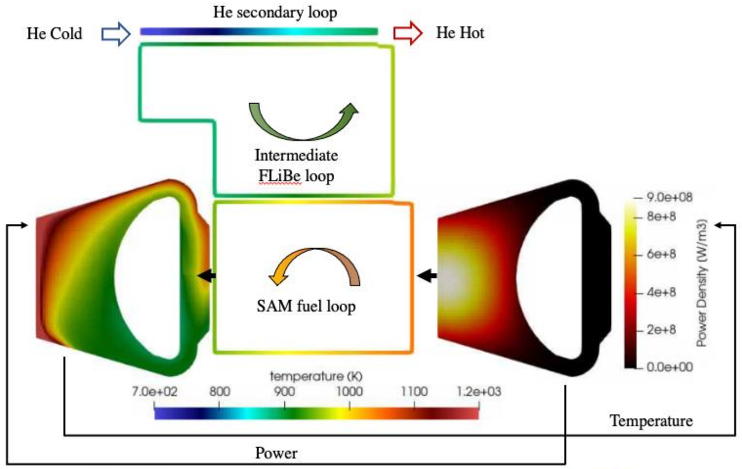


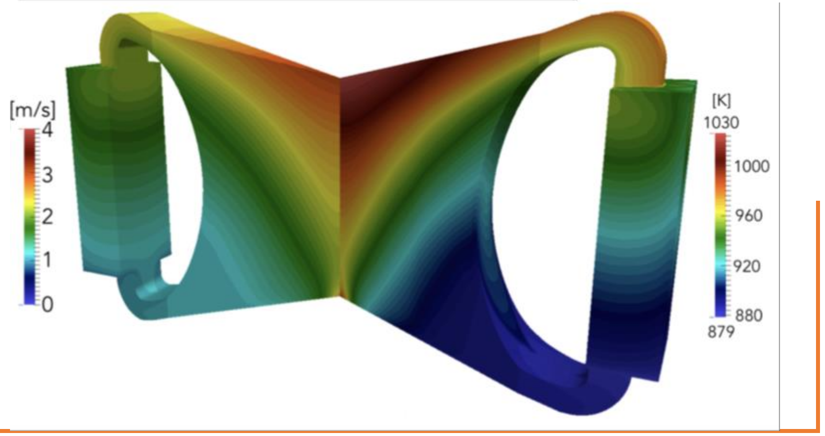
Reactor Use Case: MSR

Molten Salt Fast Reactor (MSFR)

- Coupled core neutronics (Griffin) with core thermal hydraulics (Pronghorn) with plant hydraulics (SAM)
- Steady-state and transient simulations
- POC: Mauricio Tano (INL)

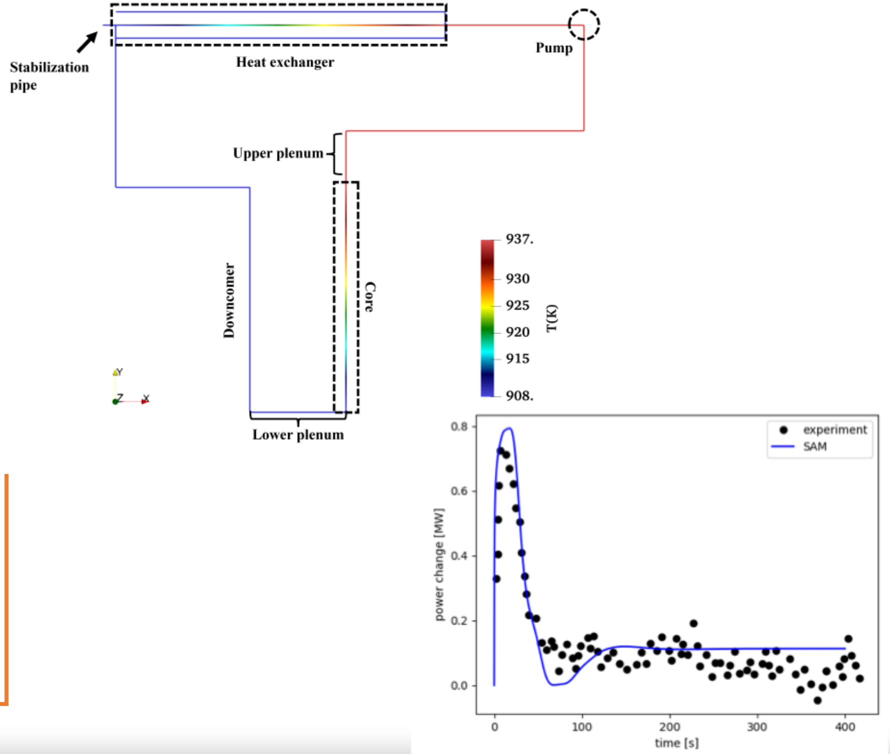






Molten Salt Reactor Experiment (MSRE

- Coupled systems hydraulics with point kinetics model (SAM)
- Steady-state and transient simulations
- Benchmarked against MSRE data
- POC: Rui Hu (INL)



NEAMS

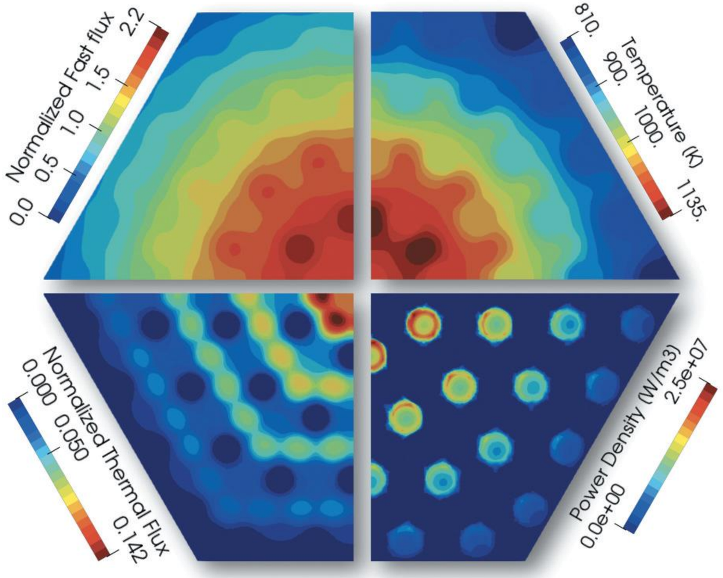
NRIC National Reactor Innovation Center

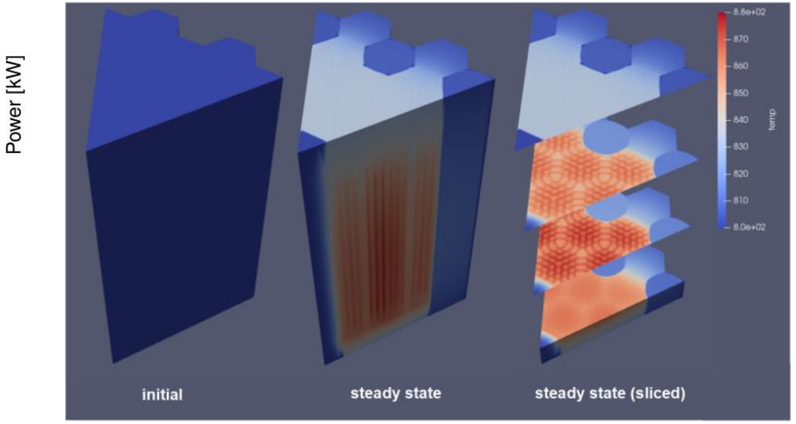
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

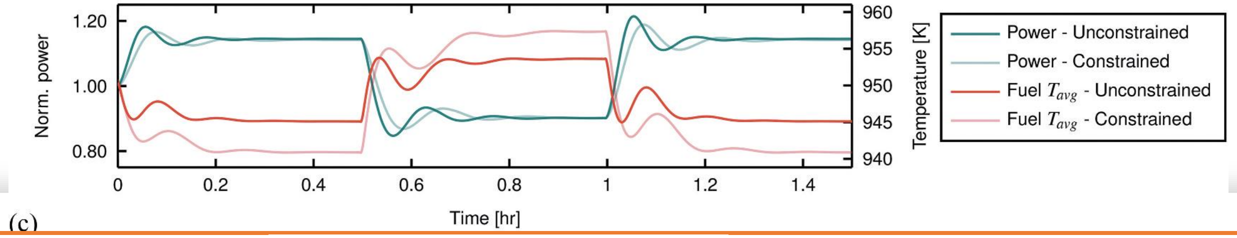
Reactor Use Case: Microreactor

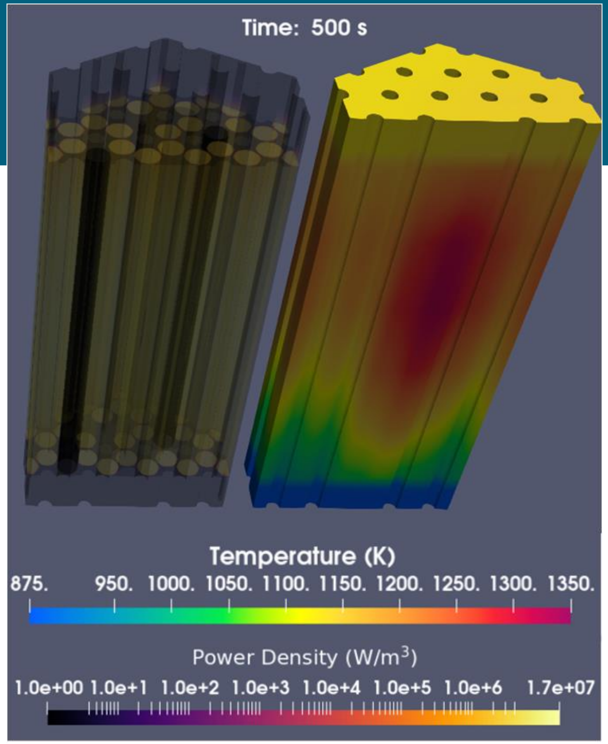
Empire Design

- Coupled core neutronics (Griffin), heat pipe (Sockeye), and thermomechanics (Bison)
- Steady-state and transient simulations
- POC: Javier Ortensi(INL), Nicolast Stauff (ANL)









Generic Gas-cooled Microreactor (GC-MR)

- Neutronics (Griffin) coupled with system hydraulics (SAM) and thermomechanics (Bison)
- Steady state and transient capabilities
- POC: Nicolas Stauff (ANL)

NEAMS Summary

- INL HPC resources are the preferred NEAMS resource for National Labs, Universities, and Industry Collaborators through Nuclear Computational Resource Center.
- INL HPC resources are commonly leveraged for tool training and workshops (e.g. ANL meshing workshop, NRC training, etc.).
- INL HPC is the preferred resource for multi-lab computing projects due to ease of access (e.g. NRIC DOME modeling).
- INL HPC resources are the most flexible for applied multiphysics research

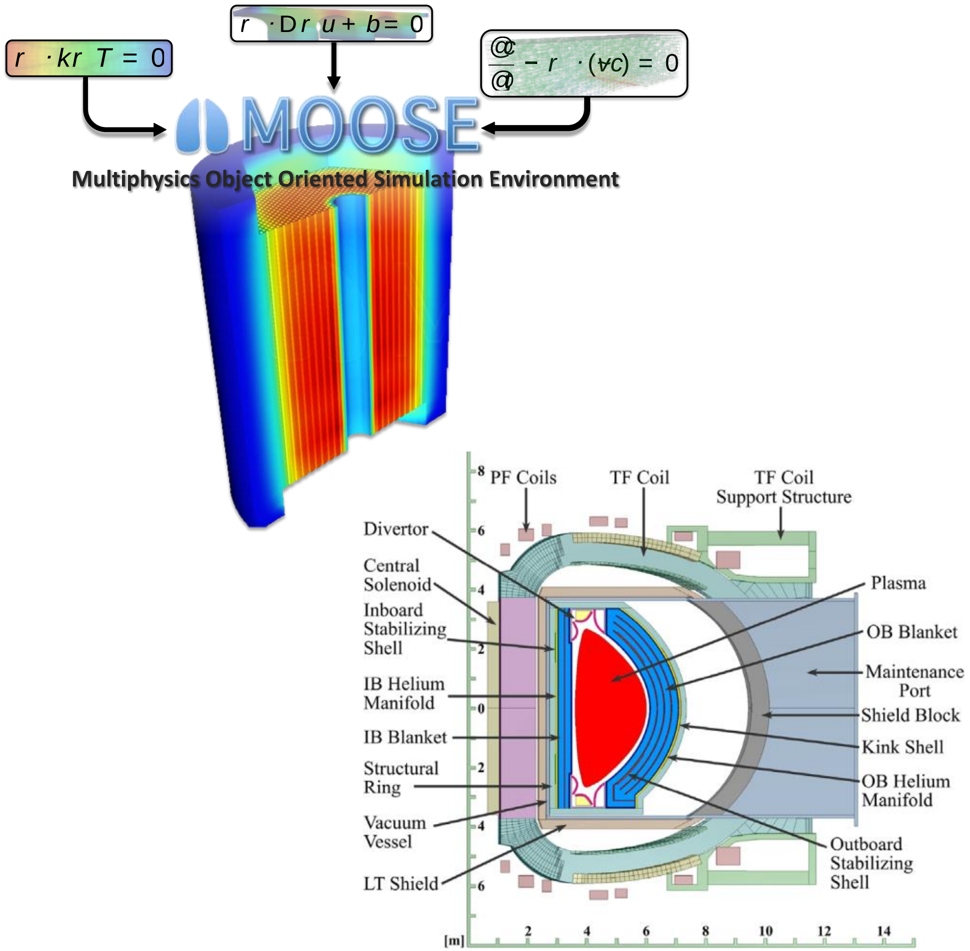
DOE CONNECT Program

- **C**reation of **N**ext-gen **N**uclear **E**nergy **C**omputational **T**echnology
- DOE supported effort to leverage Office of Science (ECP) accelerator technologies deployed in applied programs
- Multilab effort: INL, ANL, ORNL
- Exploring the use of various accelerator libraries in MOOSE

- Kokkos: https://kokkos.org/
- libCEED: https://ceed.exascaleproject.org/libceed/
- MFEM: https://mfem.org/

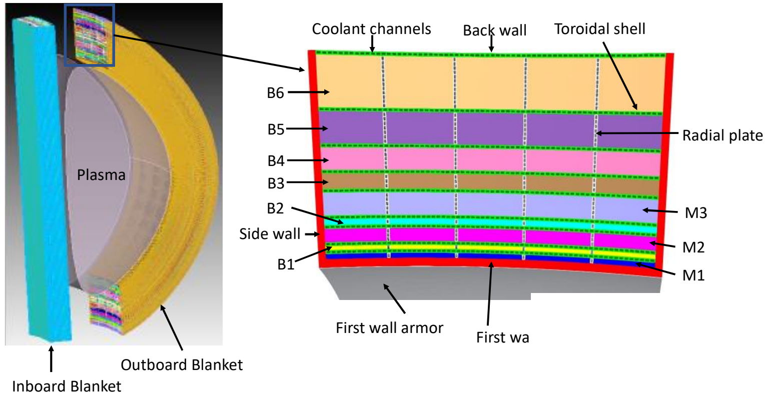
Future Directions: Fusion

- Accelerating Fusion Device Design using MOOSE
- Design iteration and rapid commercialization requires equally rapid evaluations of components and systems, with **tightly coupled physics**:
    - Tritium generation/transport/safety analysis
    - Neutronics, plasma
    - TH / CFD / MHD
    - Mechanical, structural
    - Computational materials
- MOOSE provides a comprehensive solution: a **multiscale, multiphysics** simulation framework with **established track record of success** in nuclear fission reactors with **unified, modular interfaces**.
- Open, flexible frameworks can create pathways to **fully integrated, whole device modeling**.



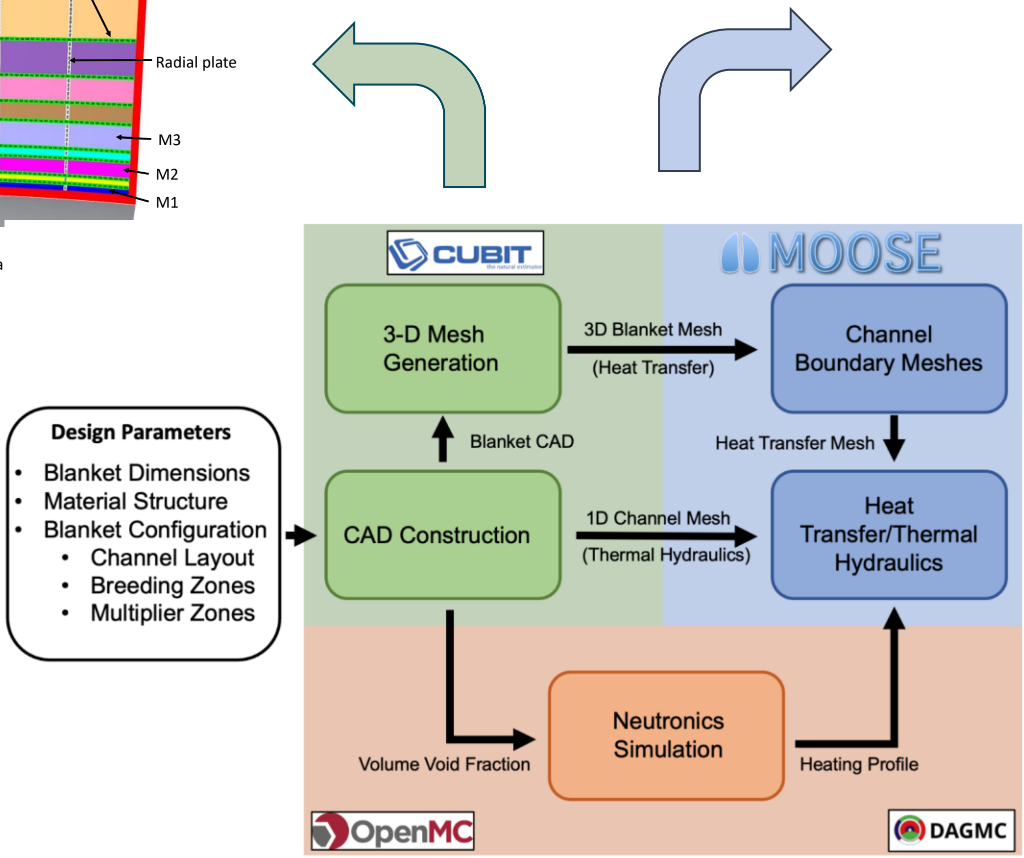
Bottom Image: Huang, Y., Tillack, M. S., Ghoniem, N. M., Blanchard, J. P., El-Guebaly, L. A., & Kessel, C. E. (2018). Multiphysics modeling of the FW/blanket of the US Fusion Nuclear Science Facility (FNSF). Fusion Engineering and Design, 135, 279-289.

Highlight: Creating iterative design workflows for ceramic breeding blankets using MOOSE (INL, ORNL, VCU)



- Three solid multiplier ($Be_{12}Ti$) zones
- Six cellular ceramic breeder (Li_2ZrO_3) zones

- 250 first wall channels
- 152 plate channels
- 594 shell channels
    - **Total: 996 channel simulations**



Design Parameters
- Blanket Dimensions
- Material Structure
- Blanket Configuration
    - Channel Layout
    - Breeding Zones
    - Multiplier Zones

3-D Mesh Generation

3D Blanket Mesh (Heat Transfer)

Channel Boundary Meshes

Blanket CAD

Heat Transfer Mesh

CAD Construction

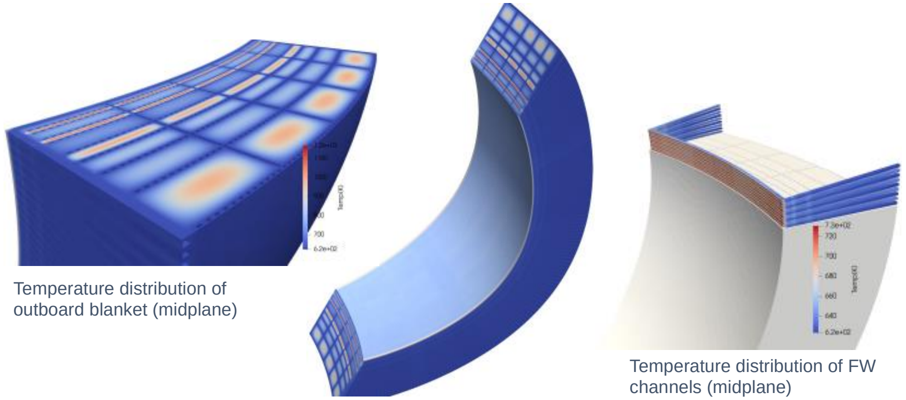
1D Channel Mesh (Thermal Hydraulics)

Heat Transfer/Thermal Hydraulics

Volume Void Fraction

Neutronics Simulation

Heating Profile



Temperature distribution of outboard blanket (midplane)

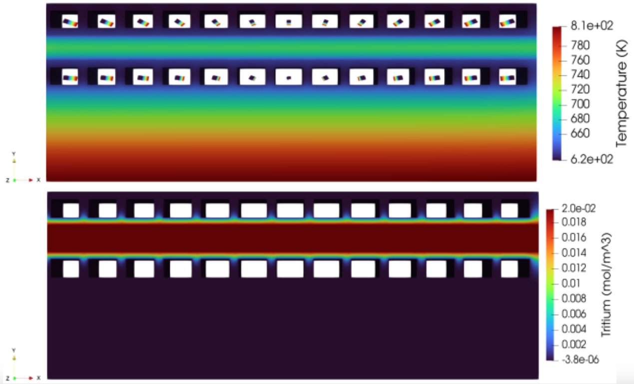
Temperature distribution of FW channels (midplane)

Component	Max temp	Temp limit
Breeder	1200 K (927°C)	1510 K (1237°C)
Multiplier	780 K (506°C)	973 K (700°C)
First wall	960 K (687°C)	823 K (550°C)
Structures	870 K (597°C)	823 K (550°C)

3D Tritium Transport

Temperatures
Local Tritium Flux

TMAP8

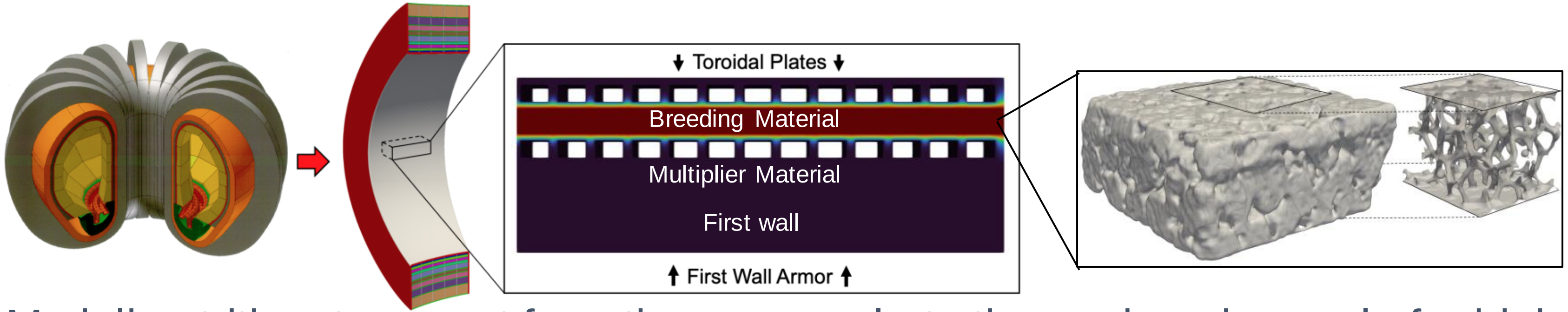


Fusion Energy Science Collaborations

TMAP8

- TMAP4 and TMAP7, although widely used, have significant limitations.
- TMAP8, started in 2019 with INL's PD funds, is a MOOSE-based application.
- TMAP8 enables high fidelity, multi-scale, 3D, multiphysics simulations of tritium transport.
- TMAP8 is open source, NQA-1 compliant, offers user support and massively parallel capabilities.

Model Development and V&V



- Modeling tritium transport from the mesoscale to the engineering scale for high fidelity simulations
- Verification & Validation efforts are demonstrating the robustness of the models and code.

Future Development & Research

- Enable high fidelity modeling of liquid blanket designs by coupling TMAP8 with thermal hydraulics capabilities.
- Keep improving predictive capabilities.
- Demonstrate accelerated material and system design.
- Training and workforce development through internships, seminars, and workshops.

UK Atomic Energy Authority

SAPIENZA
UNIVERSITÀ DI ROMA

VCU

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

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

Questions?

U.S. DEPARTMENT OF
ENERGY

Office of
NUCLEAR ENERGY