INL/CON-23-75810-Revision-0

MOOSE: A Modular Platform for Fission and Fusion Multiphysics

November 2023

Changing the World's Energy Future

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Idaho National Laboratory

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http://www.inl.gov

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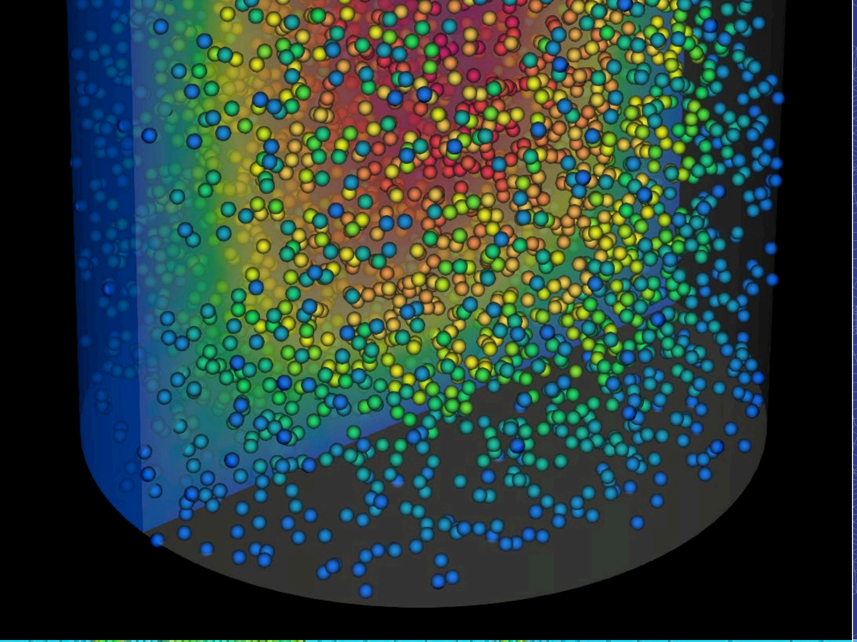

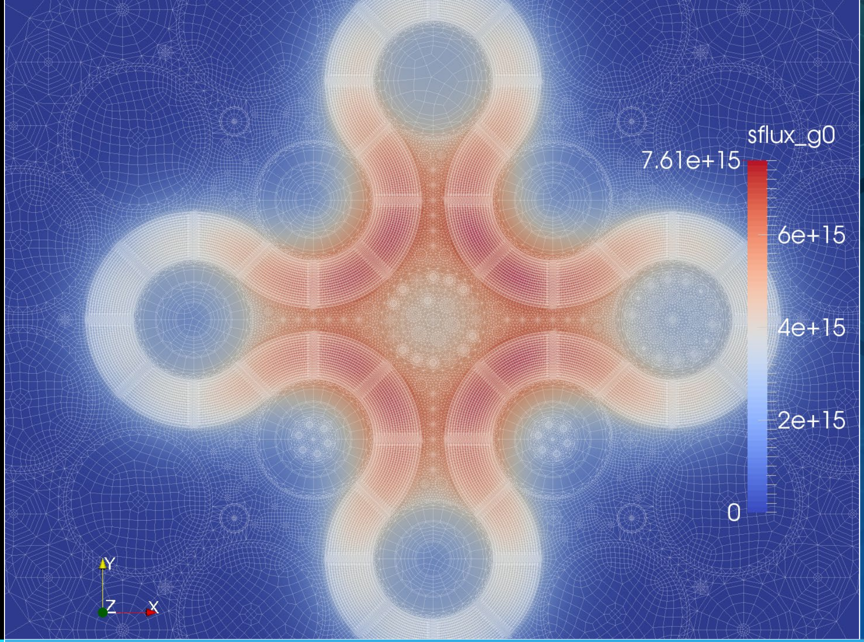

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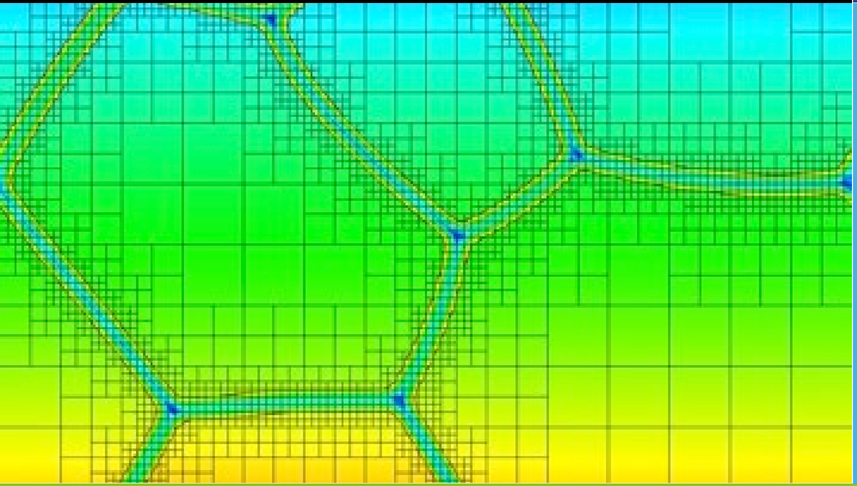
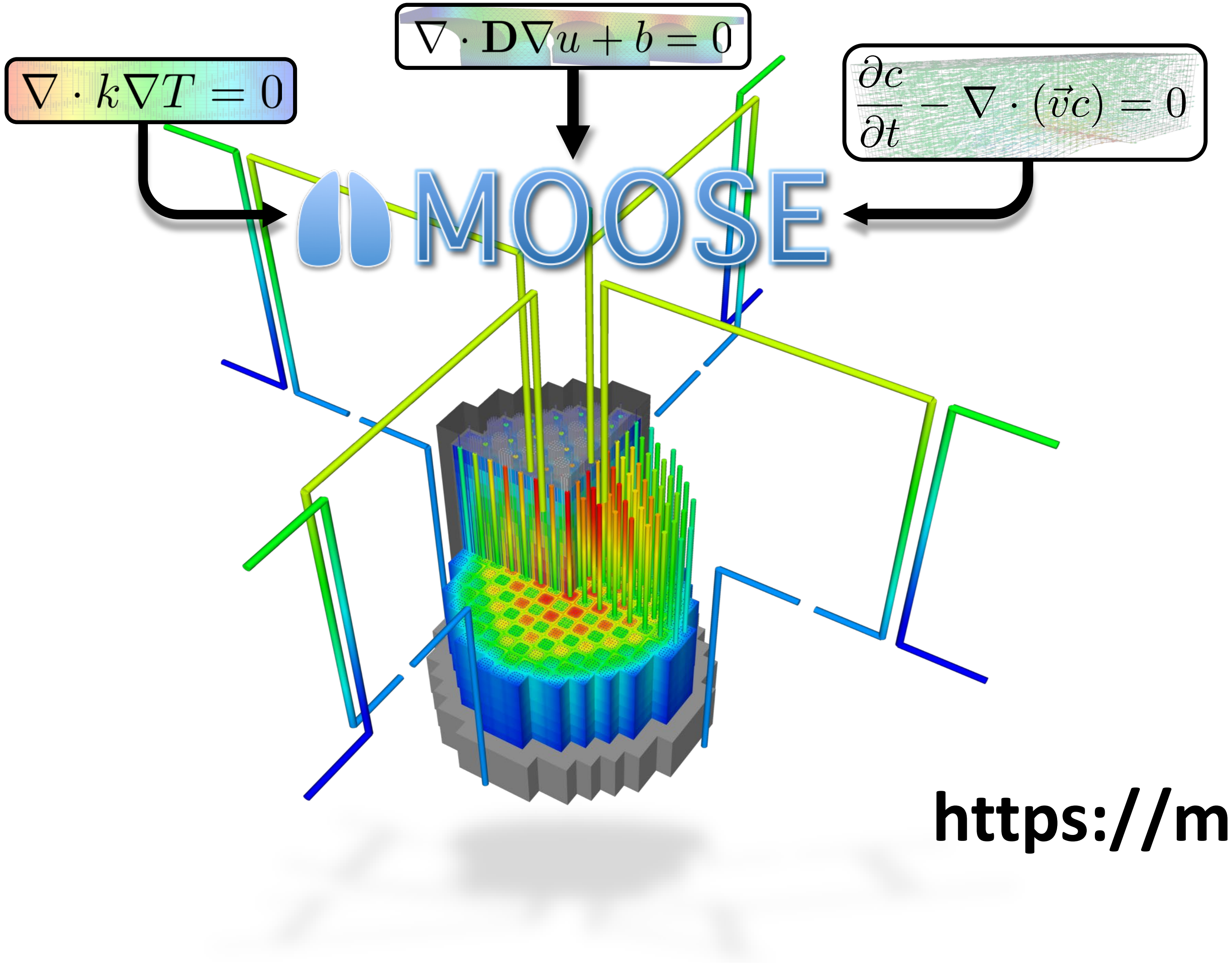


MOOSE: A Modular Platform for Fission and Fusion Multiphysics

Idaho National Laboratory

MOOSE Accelerates Development of High-Fidelity Modeling and Simulation Tools



What is MOOSE?

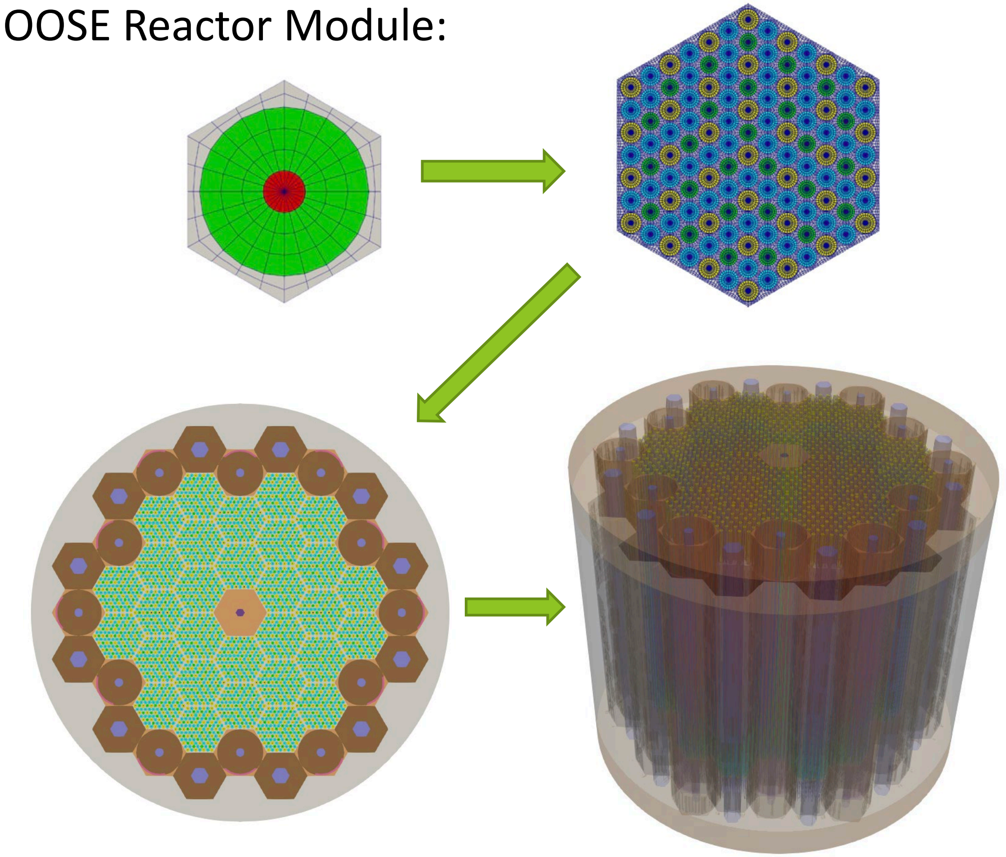
- Multiphysics
- Complete Platform
- Open-source
  - Equity, Inclusion
- Massively Parallel
- Flexible
- NQA-1 Software Quality Assurance

https://mooseframework.inl.gov

MOOSE Physics Modules – All Open Source!

- Chemical Reactions
- Contact
- **Electromagnetics**
- Fluid Properties
- Fluid Structure Interaction (FSI)
- Function Expansion Tools
- Geochemistry
- **Heat Conduction**
- Level Set
- **Navier Stokes**
- Peridynamics
- **Phase Field**
- **Porous Flow**
- **Ray Tracing/Particle Tracking**
- rDG
- Reactor
- Stochastic Tools
- **Tensor (solid) Mechanics**
- **Thermal Hydraulics**
- XFEM

MOOSE Reactor Module:

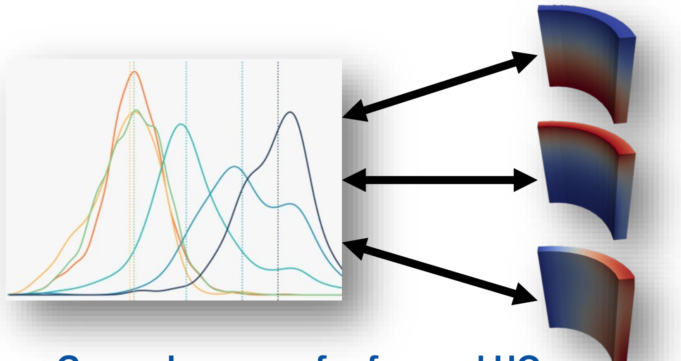


Building a mesh with the Reactor module [1]

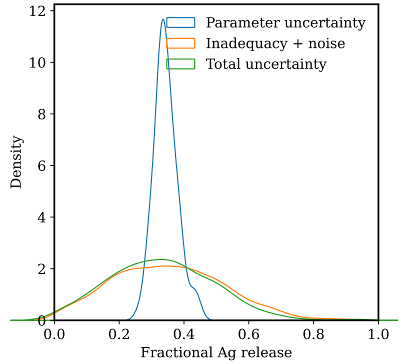
1. Shemon, Emily, Yinbin Miao, Shikhar Kumar, Kun Mo, Yeon Sang Jung, Aaron Oaks, Scott Richards, Guillaume Giudicelli, Logan Harbour, and Roy Stogner. "MOOSE Reactor Module: An Open-Source Capability for Meshing Nuclear Reactor Geometries." *Nuclear Science and Engineering* (2023): 1-25.

The MOOSE Stochastic Tools Module: Cutting Edge AI/ML For Multiphysics

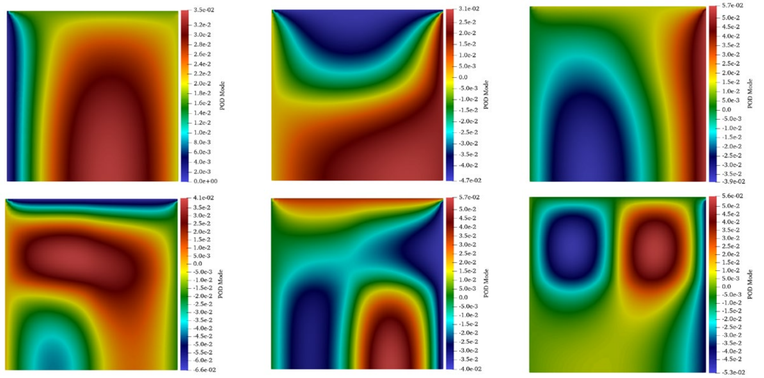
- Provide a **MOOSE interface** for performing stochastic analysis on MOOSE-based models.
- Sample parameters, run applications, and gather data that is both **efficient** (memory and runtime) and **scalable**.
- Perform UQ and sensitivity analysis with **distributed data** with **advanced variance reduction** methods
- **Parallel Scalable Inverse Bayesian UQ** for parameter and model error estimation
- Train meta-models to develop fast-evaluating **surrogates** of the high-fidelity multiphysics model
  - Harness advanced machine learning capabilities through the C++ front end of Pytorch [1]
  - Use active learning models for building surrogates
- Provide a **pluggable** interface for these surrogates.
- Use **POD (Proper Orthogonal Decomposition)-based dimensionality reduction** methods to build mappings between solution variables and latent (low-dimensional) spaces



General process for forward UQ



UQ on modeling TRSIO Particle Ag release



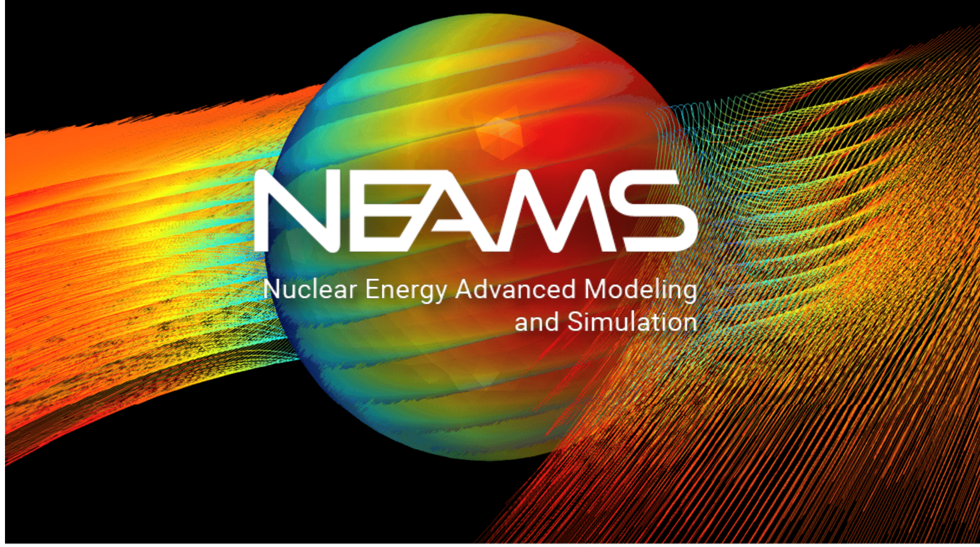
POD modes of a 2D heat conduction problem

[1] Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., ... & Chintala, S. (2019). Pytorch: An imperative style, high-performance deep learning library. *Advances in neural information processing systems*, *32*.

NEAMS Program

www.neams.inl.gov

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



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

INL Idaho National Laboratory

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

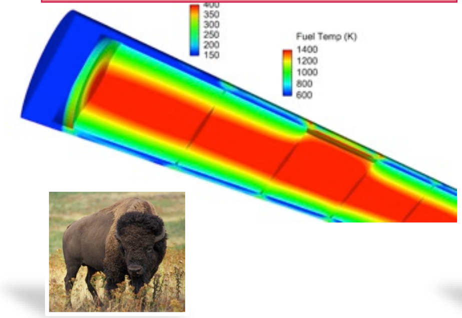
Los Alamos NATIONAL LABORATORY

Accelerating Advanced Reactor Deployment

NEAMS

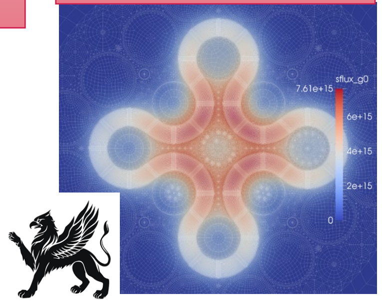
Accelerating Advanced Fission Reactor Deployment

Bison
Nuclear Fuel Performance



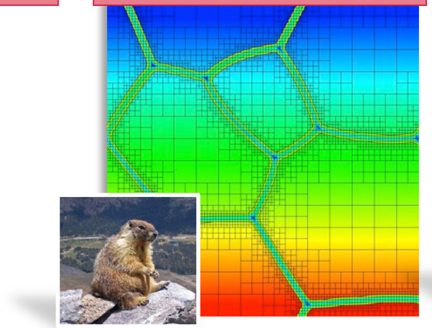
Grizzly
Structural Mechanics for Component Aging

Griffin
Radiation Transport

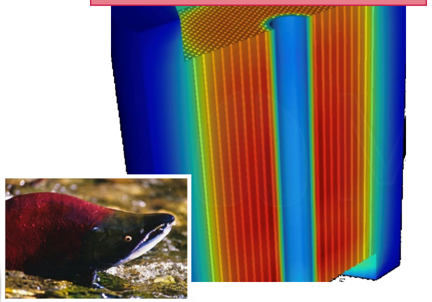


Pronghorn
Medium-fidelity CFD

Marmot
Mesoscale Materials



Sockeye
Heat pipe Simulation



U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Kairos Power

RADIANT

Westinghouse

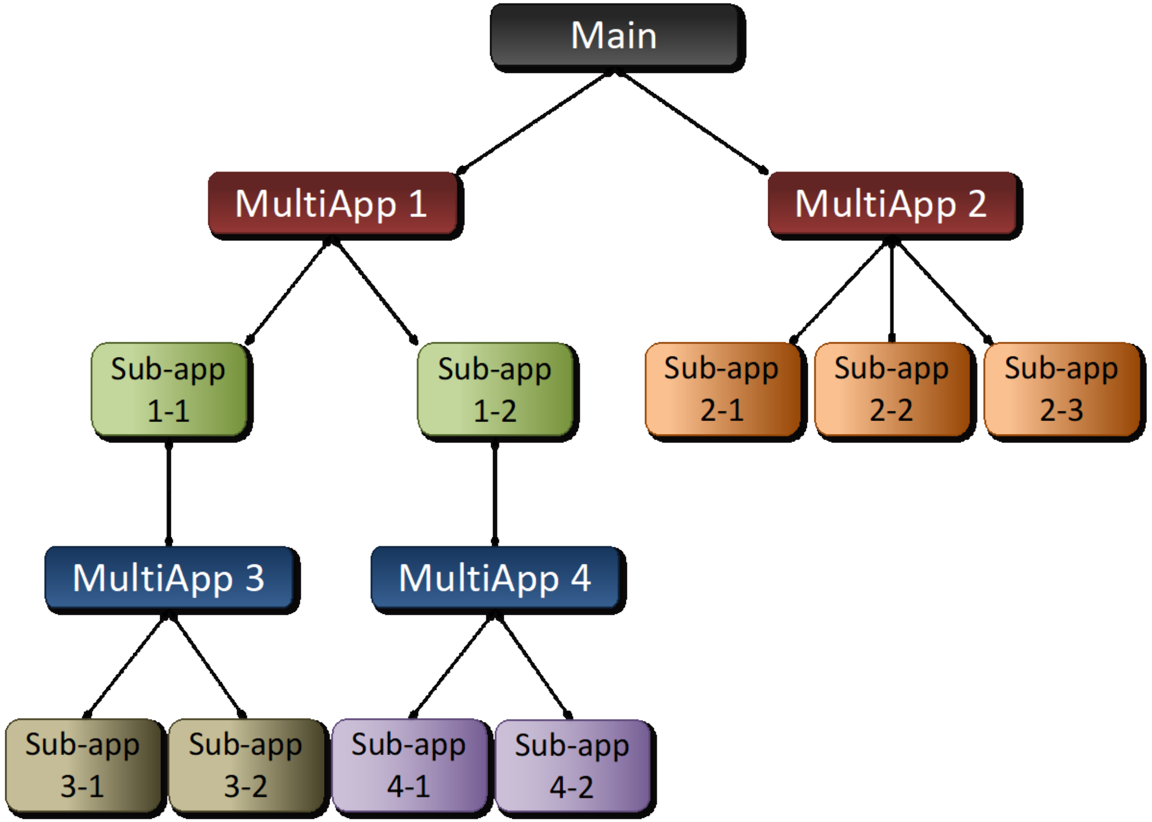
BWXT
Nuclear Energy Canada Inc.

Structural Integrity Associates, Inc.®

EPRI

How it Works: MultiApps and Transfers

- MultiApps:
  - MOOSE-based solves can be nested to achieve Multiscale-Multiphysics simulations
  - Each solve is spread out in parallel to make the most efficient use of computing resources
  - Efficiently ties together multiple team's codes
  - Non-MOOSE-based codes can be "wrapped"
- Transfers
  - Move data between applications
  - MANY types: fields, points, postprocessed values, etc.

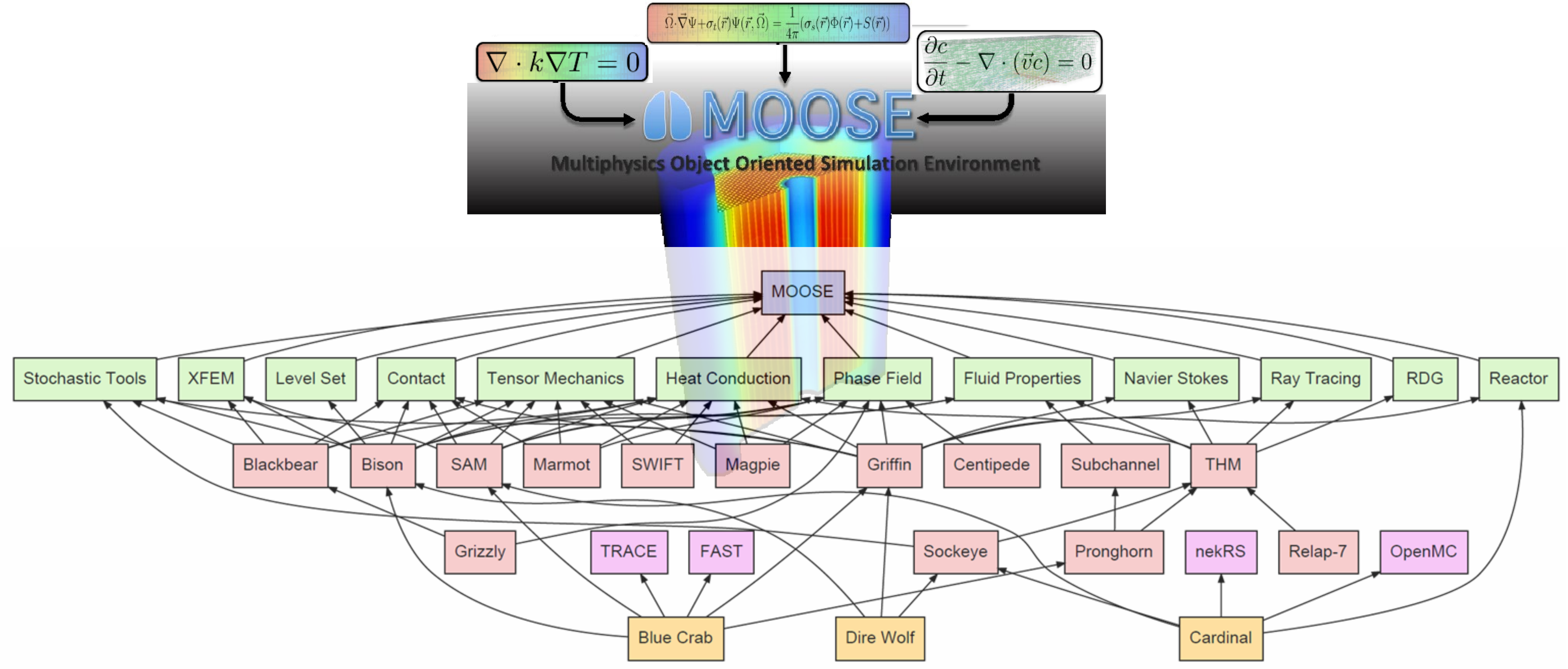


MSR Case Studies

Equilibrium Isotope Transport

- Griffin
- Mole
- NekRS
- Pronghorn
- SAM
- Stochastic Tools
- Phase-field

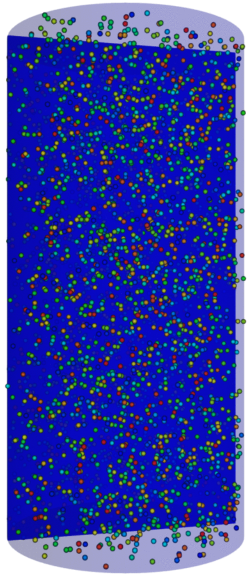
MOOSE Framework Ecosystem for Non-LWR Analysis



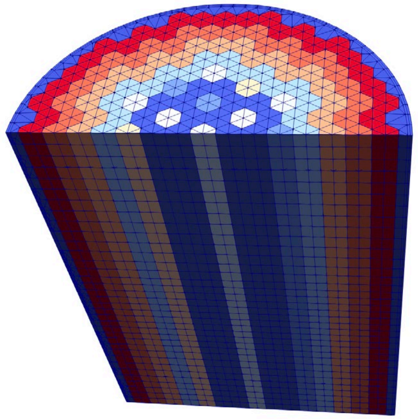
- MOOSE Framework
- MOOSE Modules
- MOOSE-Based Applications
- MOOSE-Wrapped Applications
- MOOSE-Coupling Applications

HTGR | FHR | MSR | Microreactor | LMFR

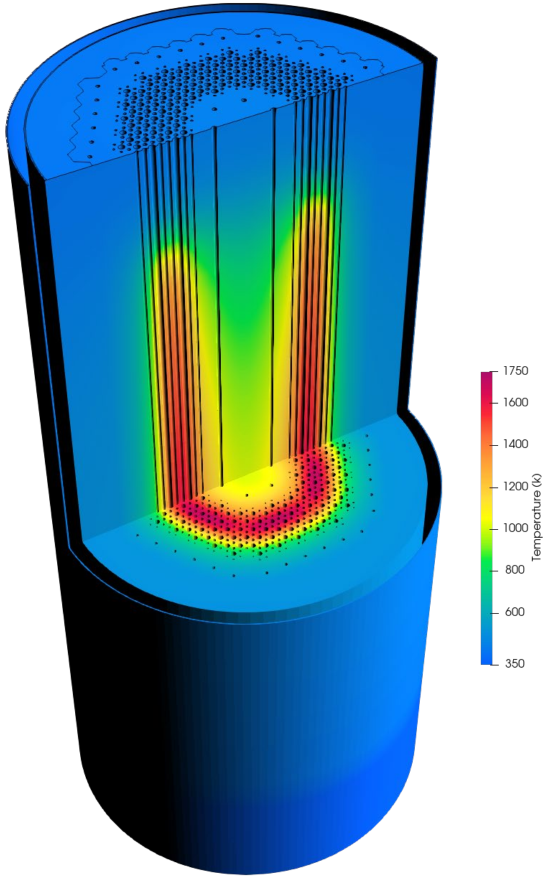
Modular System Enhances Flexibility



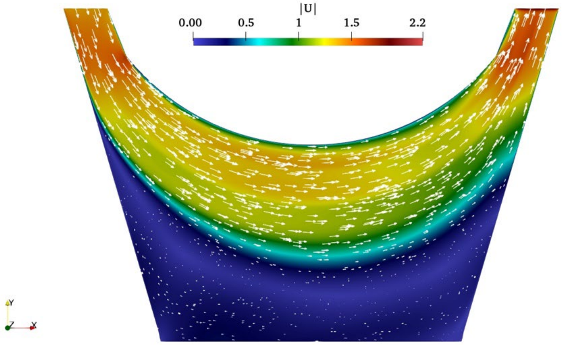
Graphite Compact with 4,000
TRISO particles in BISON
Credit: Jiang



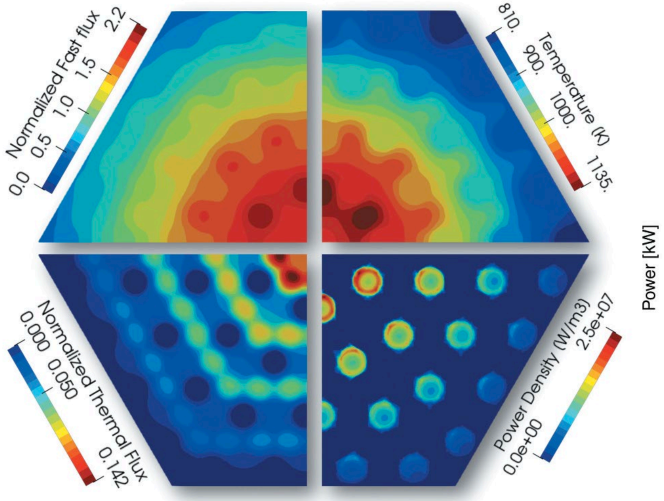
<u>Advanced Burner Test Reactor</u>
Griffin+Thermomechanics
Credit: Ortensi



<u>High-Temperature Test Facility</u>
Heat Conduction+THM
Credit: Charlot



<u>Molten Salt Fast Reactor</u>
Griffin + Pronghorn + SAM
Steady-state and transient simulations
Credit: Tano

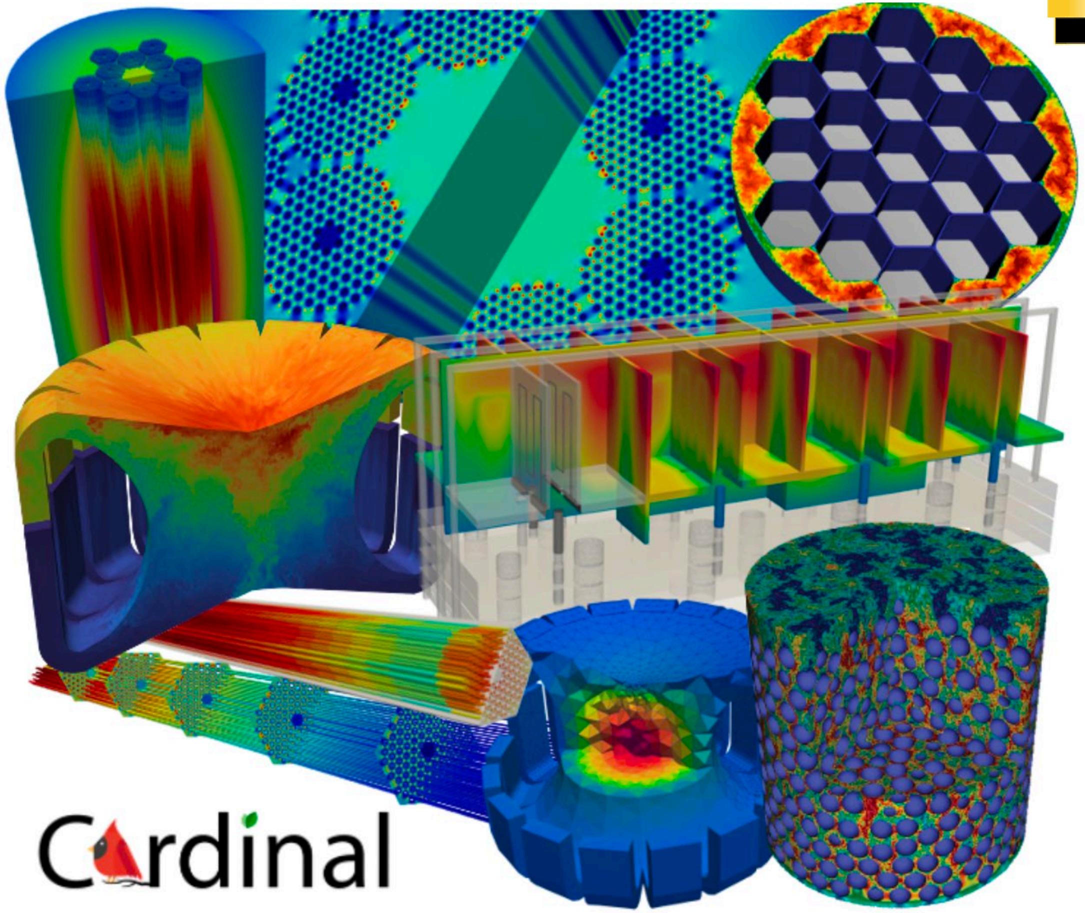


<u>Empire Design</u>
Griffin + Sockeye + Bison
Steady-state and transient simulations
Credit: Ortensi, Stauff

Cardinal: Exascale Fission and Fusion Simulation

2023 R&D 100 WINNER

- Cardinal: MOOSE+OpenMC+NekRS
- Showcase for coupling non-MOOSE-based applications
  - MOOSE physics used as “glue”
- Has simulated: gas-cooled microreactors, sodium fast reactors, molten salt reactors, high-temperature gas reactors, and tritium breeder blankets
- Used 27k GPUs on Summit to simulate a full pebble-bed reactor (350k pebbles)



Cardinal Applications. Top row: neutron transport, fluid flow, and heat transfer in a gas-cooled microreactor; large eddy simulation in the core of a sodium fast reactor. Middle row: neutron transport and large eddy simulation in a molten salt fast reactor; coupled neutron-photon transport and heat conduction in a tritium breeder blanket module from the EU DEMO fusion plant. Bottom row: fluid flow and neutron transport in a high temperature gas reactor; fission heating simulated in a Computer Aided Design (CAD) geometry; large eddy simulation in a pebble bed reactor with 1568 pebbles.

Novak, A. J., D. Andrs, P. Shriwise, J. Fang, H. Yuan, D. Shaver, E. Merzari, P. K. Romano, and R. C. Martineau. "Coupled Monte Carlo and thermal-fluid modeling of high temperature gas reactors using Cardinal." *Annals of Nuclear Energy* 177 (2022): 109310.

NEAMS Nuclear Energy Advanced Modeling and Simulation | Argonne NATIONAL LABORATORY | INL Idaho National Laboratory

Contact: abdalla.aboujaoude@inl.gov

https://mooseframework.inl.gov/virtual_test_bed

Virtual Test Bed (VTB)

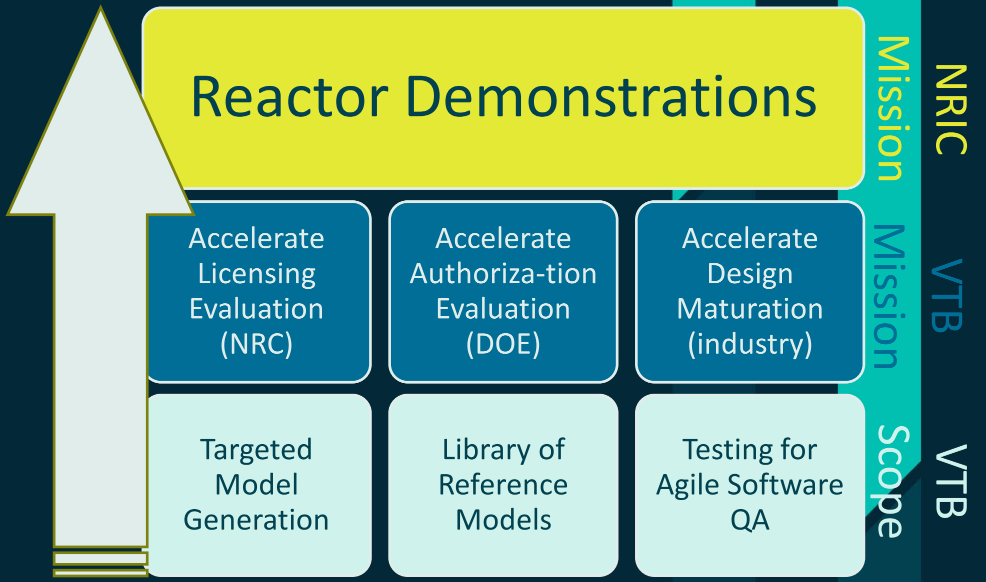
- The VTB supports NRIC's mission of delivering successful demonstration and deployment of advanced nuclear energy

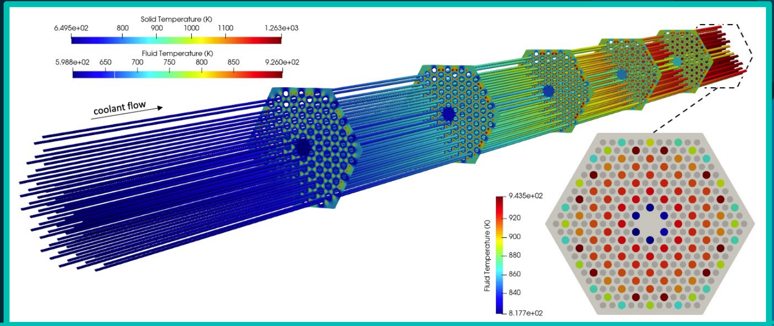
How?

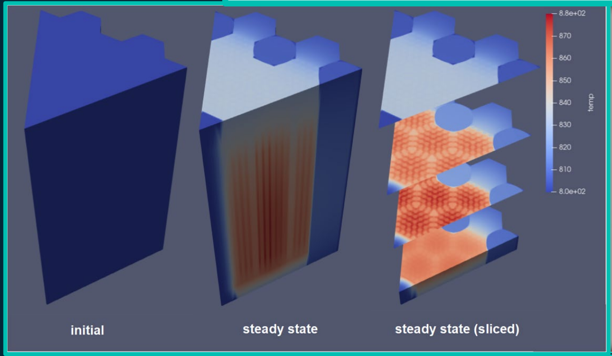
- **Library of Reference Model**: database of advanced multiphysics advanced reactor models that users can download, edit, and re-run
- **Targeted Model Generation**: developing demonstration-relevant models (e.g., candidates for DOME/LOTUS) to accelerate safety evaluations
- **Continuous Software QA**: linking repository to software development to avoid legacy issues while enabling rapid code development

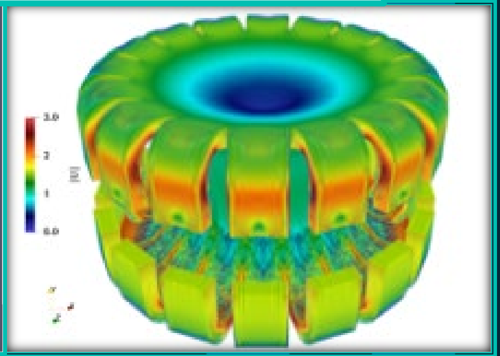
VTB So Far

- 30+ models hosted (and counting): 14 reactor designs, and 7 codes showcased
- Collaboration with NEAMS, industry, NRC, and academia
- Help accelerate timelines for DOE/NRC confirmatory analysis
- Accelerate development cycle for industry and academia









NRIC | INL

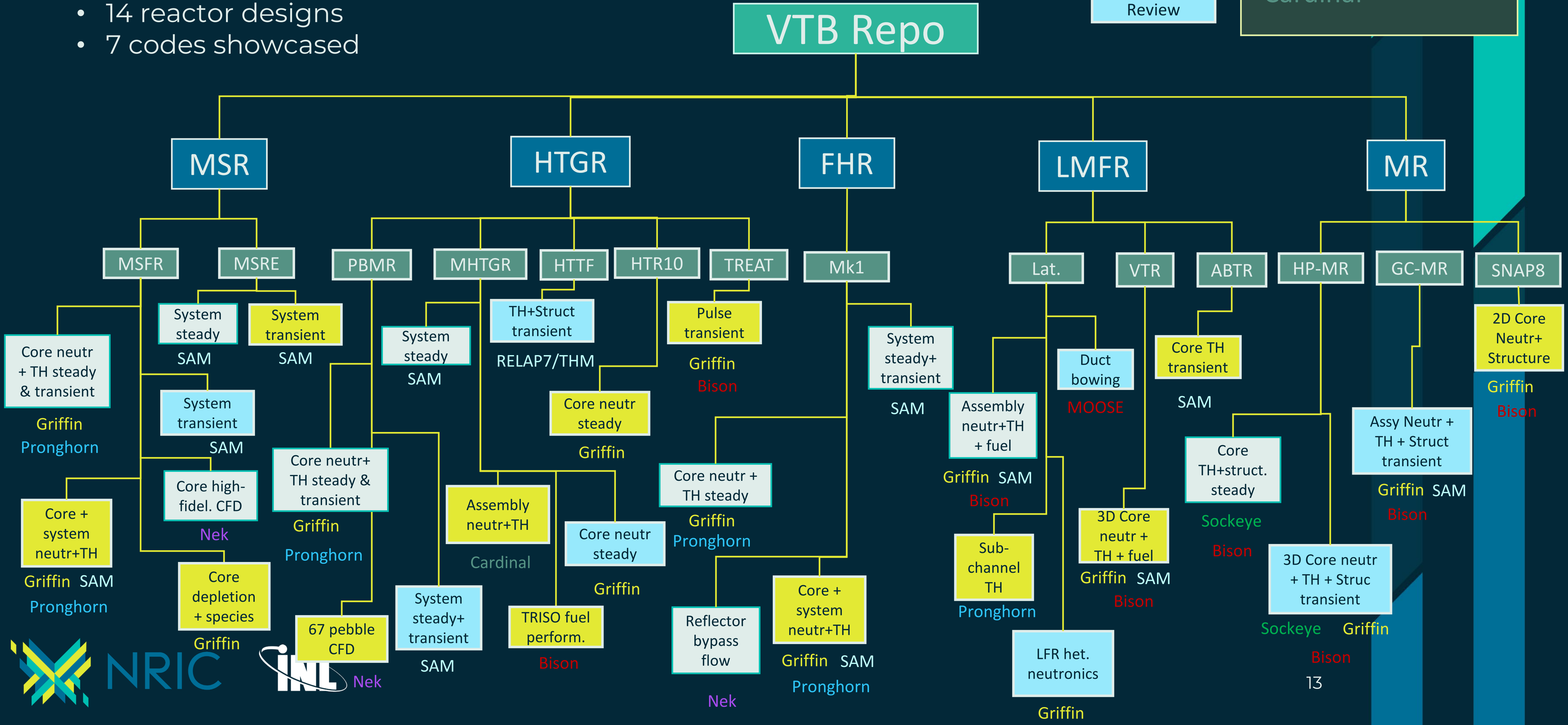
VTB Model Tree

- 30+ distinct simulations
- 14 reactor designs
- 7 codes showcased

Codes Represented:

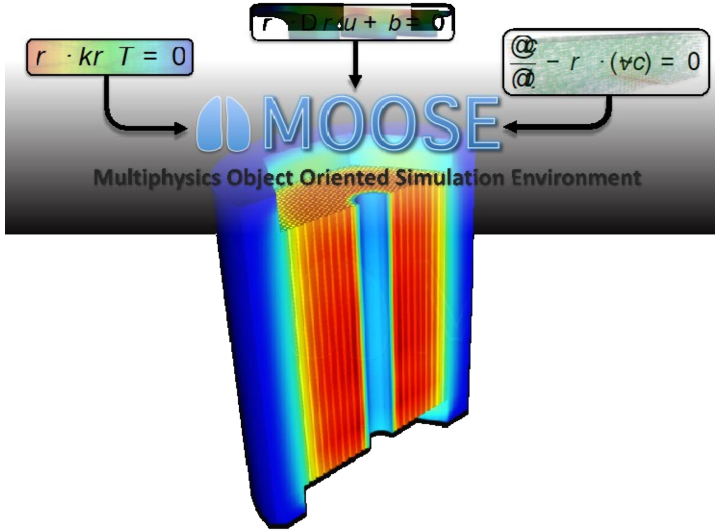
FY21
FY22
FY23 + Under Review

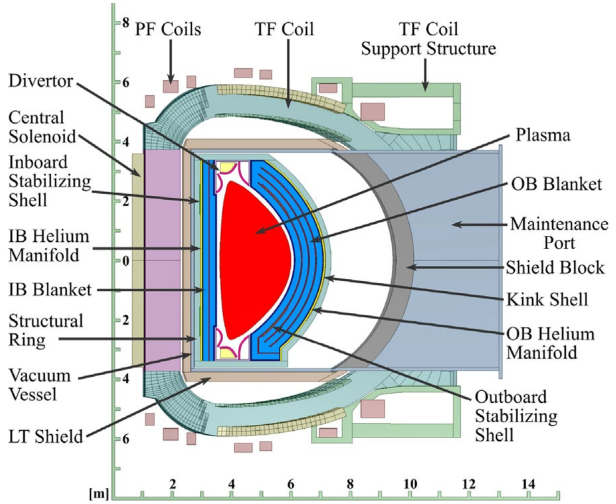
Griffin
Nek
Pronghorn
Sockeye
SAM
Bison
Cardinal



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**.

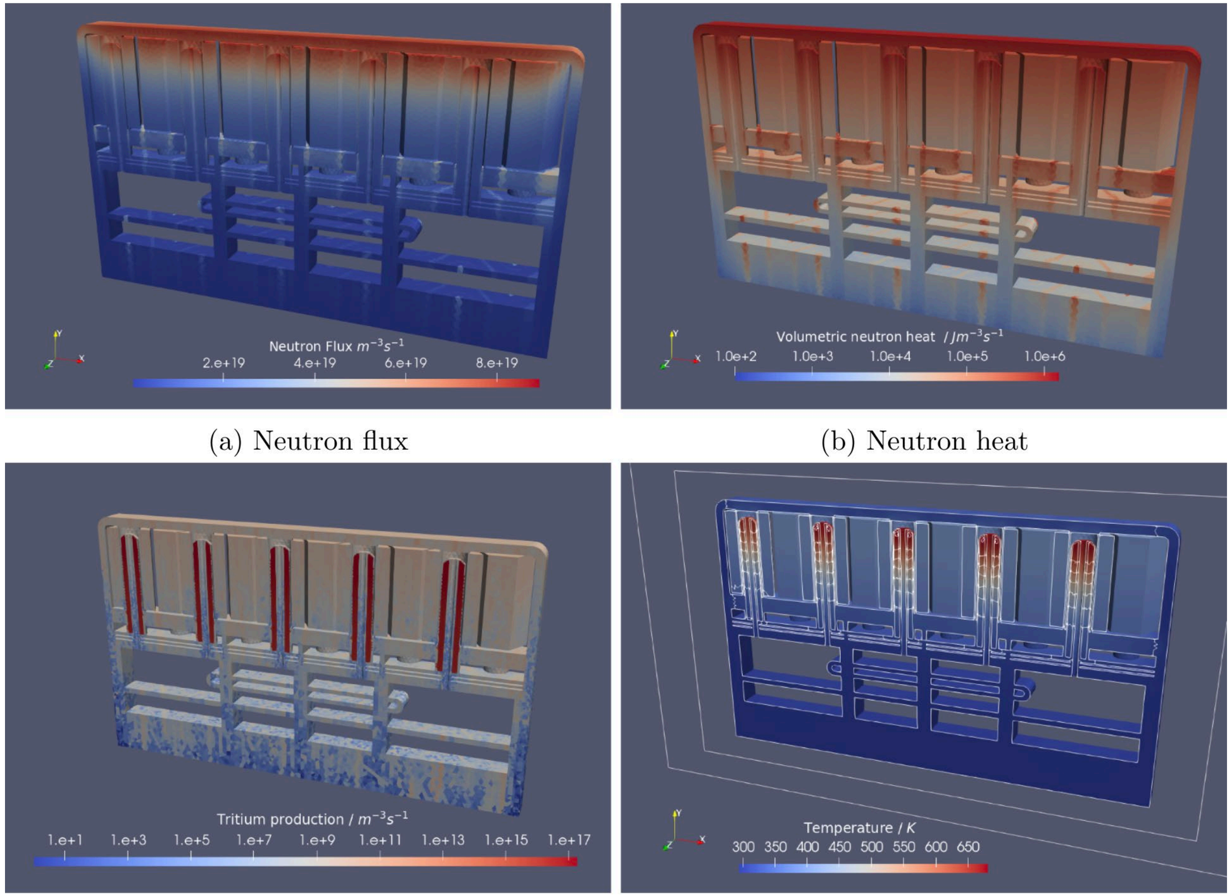




Bottom Image: Huang, Y., Tillack, M. S., Ghoniem, N. M., Blanchard, J. P., El-Guebaly, L. A., & Kessel, C. E. (2018). Multiphysics modeling of the FW/blanket of the US Fusion Nuclear Science Facility (FNSF). Fusion Engineering and Design, 135, 279-289.

MOOSE-based fusion applications under development at UKAEA

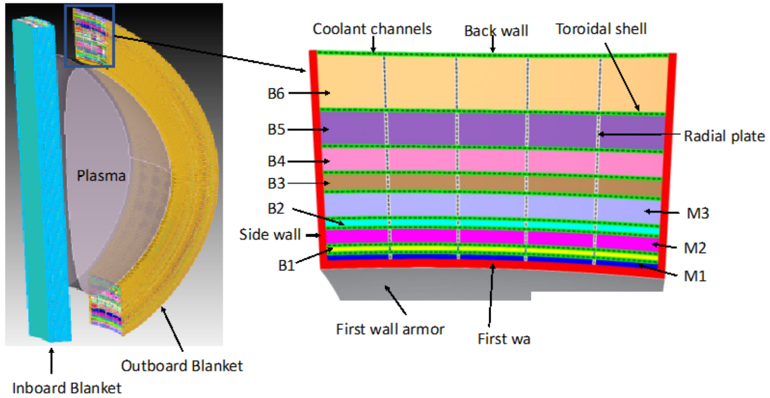
- **Aurora**: Tokamak Multiphysics calculations
  - MOOSE + OpenMC + DAGMC
- **Apollo**: 3D Electromagnetics
  - MFEM+MOOSE
- **Proteus**: Fluid Flow
- **Phaethon**: Fast Ion Heat Flux
  - ASCOT5 + MOOSE



Aurora breeder blanket model. [1]

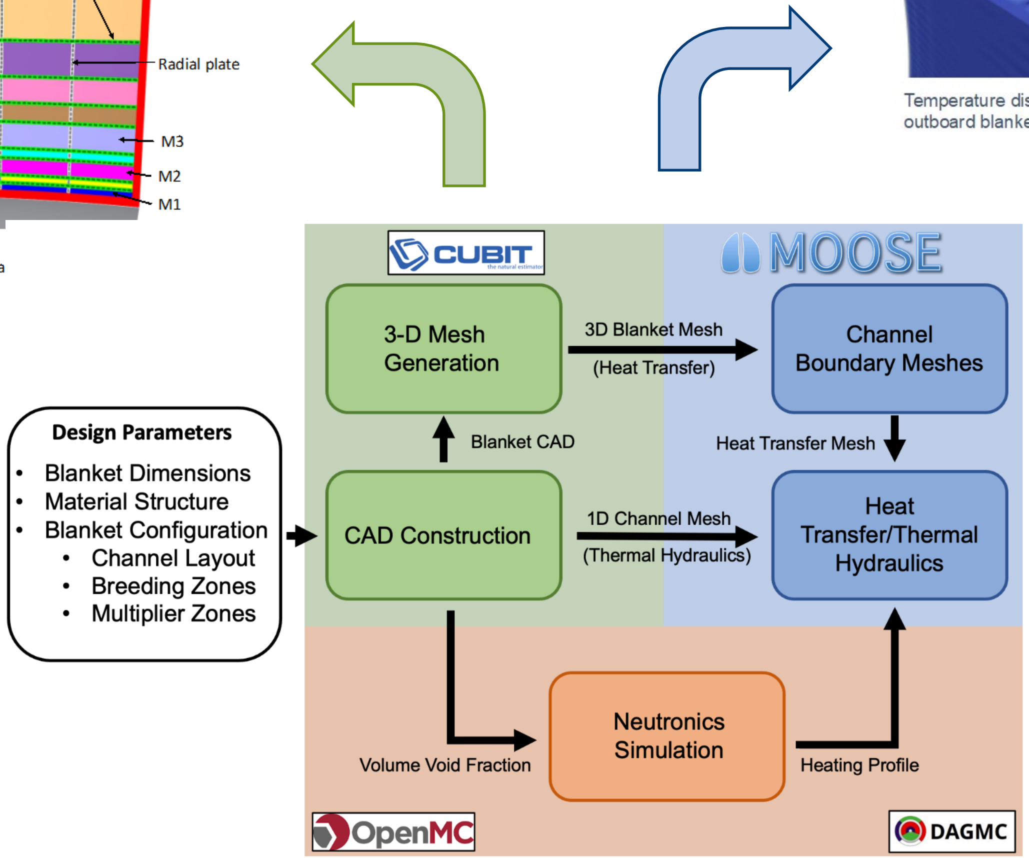
1: Brooks, Helen, and Andrew Davis. "Scalable multi-physics for fusion reactors with AURORA." *Plasma Physics and Controlled Fusion* 65, no. 2 (2022): 024002.

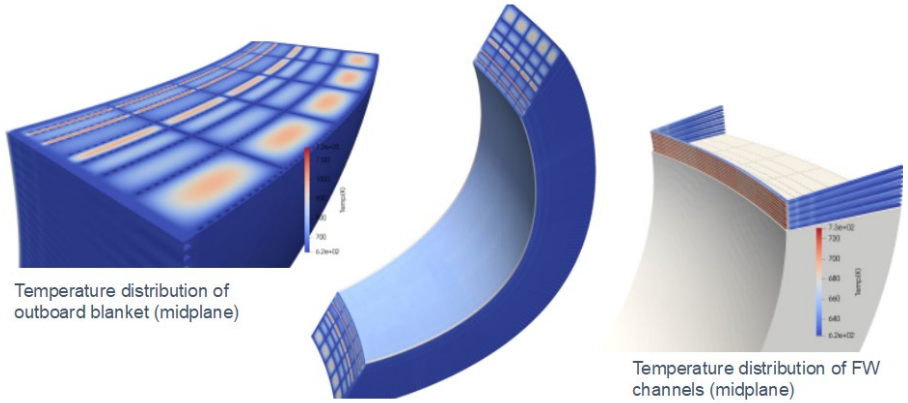
Highlight: Creating iterative design workflows for ceramic breeding blankets using MOOSE (INL, ORNL, VCU)



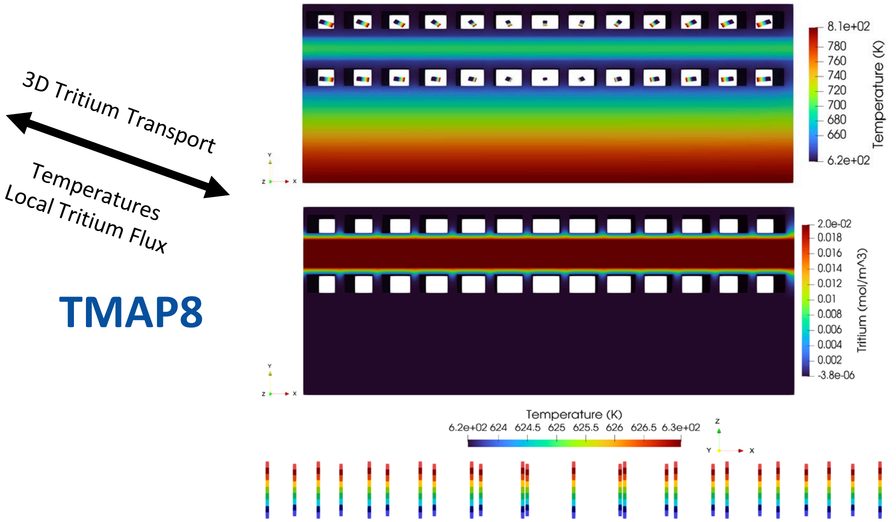
- Three solid multiplier ($Be_{12}Ti$) zones
- Six cellular ceramic breeder (Li_2ZrO_3) zones

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





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)



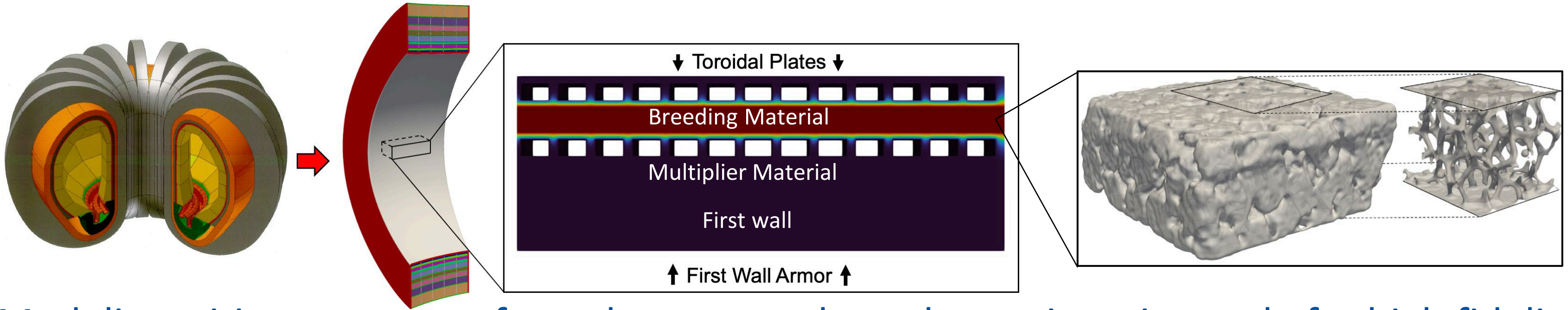
Credit: Fande Kong (former INL), Casey Icenhour (INL), Pierre-Clément Simon (INL), Paul Humrickhouse (ORNL), Trevor Franklin (VCU, advised by Dr. Lane Carasik)

Kong, F. et al., "Toward a Fully Integrated Multiphysics Simulation Framework for Fusion Blanket Design," IEEE Transactions on Plasma Science, 50, 11, 4446–4452 (2022).

Tritium Migration Analysis Program, version 8 (TMAP8)

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.



* TMAP8 simulations of a ceramic breeder material and of a blanket section

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

Tritium Migration Analysis Program, Version 8 (TMAP8) GitHub repository: https://github.com/idaholab/TMAP8. Idaho Falls, Feb. 08, 2023
F. Kong et al., IEEE Transactions on Plasma Science, Nov. 2022, doi: 10.1109/TPS.2022.3173158.
P.-C. A. Simon et al., IEEE Transactions on Plasma Science, pp. 1–7, 2022, doi: 10.1109/TPS.2022.3183525.

LDRD: Understanding multiphysics interactions around plasma facing components (PFC) Fusion ENergy Integrated multiphys-X (FENIX) framework

Scope

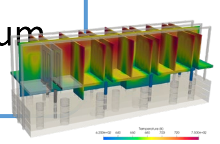
Is coupling plasma physics, neutronics, and thermomechanics necessary to accurately model PFC performances?
To better understand PFC degradation and operational impacts on their performance, this project aims to develop FENIX: an open-source, NQA-1 compliant, fully integrated, multiscale, MOOSE based framework facilitating 3D, high fidelity PFC modeling.

Tasks

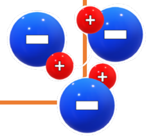
Thermomechanics, thermal-hydraulics, and tritium transport (TMAP8)

FENIX

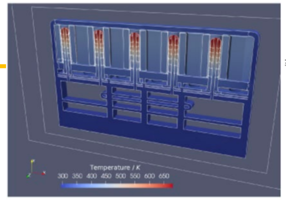
Neutronics (Cardinal) provide heat activation and tritium source terms



Particle in cell for plasma periphery to provide neutron and heat source terms



Proof of concept and benchmarking on DEMO-like and Tritium Plasma Experiment



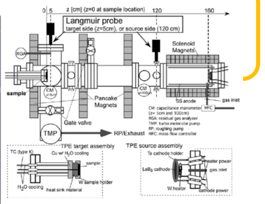


FIG. 1. Schematic of the tritium plasma experiment.

Team

Idaho National Laboratory

NC STATE UNIVERSITY

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

UK Atomic Energy Authority

Impact

FENIX will enable high fidelity, multiphysics simulations of PFCs and will support fundamental research for material design and device design optimization studies.
FENIX will also support uncertainty quantification, identifying key areas where improvements are most impactful.
These capabilities will make FENIX a strategic asset for the fusion community.

Brooks H,et al., *Int. Conf. on Physics of Reactors 2022 (PHYSOR 2022)*
F. Kong et al., IEEE Transactions on Plasma Science, Nov. 2022, doi: 10.1109/TPS.2022.3173158.
A.J. Novak et al., Annals of Nuclear Energy, Vol. 177, 2022 doi: 10.1016/j.anucene.2022.109310
M. Shimada et al., Rev. Sci. Instrum. 82, 083503 (2011), doi: 10.1063/1.3627609

LDRD: Superconducting magnets and surrounding assemblies (INL, UIUC)

- Magnet systems are the principal enabling technology for magnetic confinement fusion reactors, with strong magnetic field strength driving plasma ignition, interaction and efficient operation.
- Coils experience **significant electromagnetic-thermomechanical (EM-TM) stresses** due to plasma pressure, radiative heating, Joule heating of the coil windings, self-generated EM forces, and interactions between coils themselves → **highly-coupled physical system that impacts surrounding structures.**
- Post-ITER devices have projected up to **1.4x higher magnetic field strengths** or more to achieve **over 2x higher fusion power** ($P_F \sim B^2$) → high coil current density requirements (>60 A/mm^2).
- Designing for these systems is and will be difficult – traditional coil materials (Cu) are limiting and costly, so advanced and emerging superconducting materials (LTS, HTS) need to be studied.
- **Codes with tightly coupled EM-TM models are required to design and study emerging magnet systems with novel materials as well as their surrounding structures.**
- **We intend to create an open source EM-TM capability using MOOSE to enable virtual design iteration, safety evaluation, and one component of fusion digital twin development.**

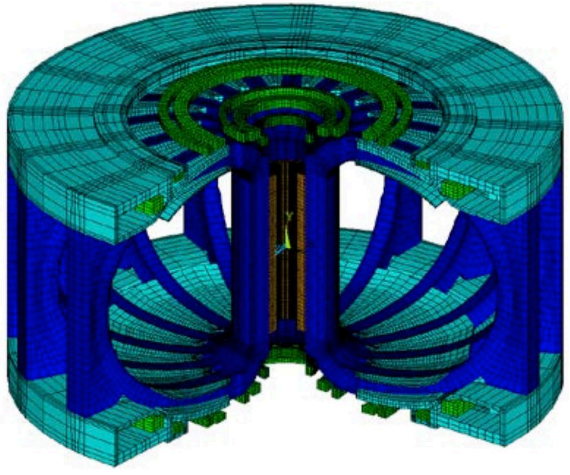
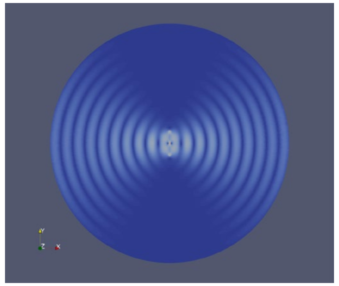
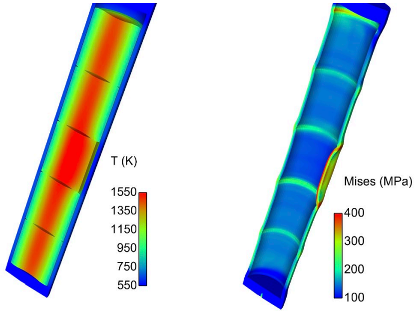


Image: Kessel, et al



MOOSE Electromagnetics

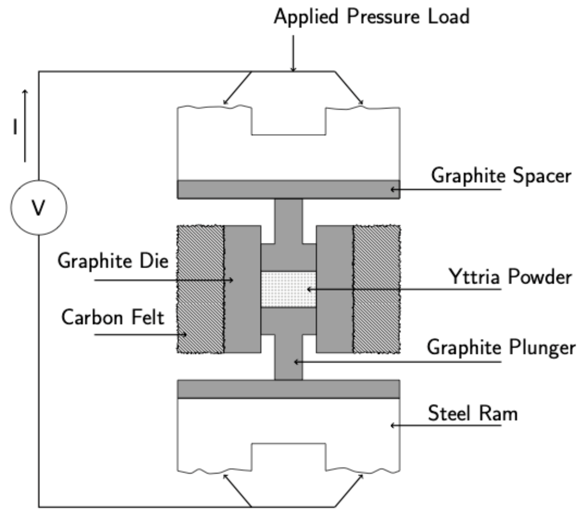
MOOSE Thermo-mechanics

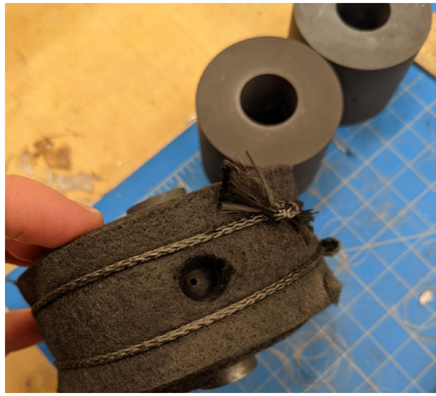


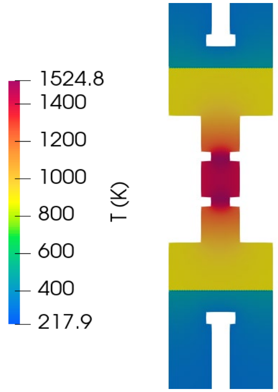
Looking forward: Evaluation and Optimization of Material Manufacturing using MOOSE

- The MOOSE Application Library for Advanced Manufacturing Utilities (MALAMUTE) is a MOOSE-based application for modeling advanced manufacturing (AM) processes.
- Inherits capability from the MOOSE contact, electromagnetics, heat conduction, level set, Navier-Stokes, phase field, and tensor mechanics modules
- Manufacturing methods simulated:
  - Electric field assisted sintering / spark plasma sintering (EFAS / SPS)
  - Direct Energy Deposition (3D printing)
  - Laser Powder Bed Fusion
  - Laser Welding

MALAMUTE







<u>SPS Goal</u>: Production of fine grained parts through efficient heat transfer (DC Joule Heating)

<u>Potential Applications:</u> First wall materials, moderators, breeding materials, etc.

Multiphysics AM simulation enables virtual design iteration; narrows experimental focus to **maximize impact and reduce cost**.

Anselmi-Tamburini and Groze, Materials Science and Technology 22 (2017) 16
Manière et al. J. American Ceramic Society (2018) 16046

Conclusions

- MOOSE is a proven system for complex multiphysics analysis
  - Open-source enables inclusion and diversity
- NEAMS is utilizing the flexibility to address many device designs
- The VTB is enabling community knowledge growth
- Cardinal showcases:
  - Leadership class computing capability
  - Successful coupling of bespoke simulation tools
- UKAEA effort shows this approach works for fusion
- Ongoing INL fusion mod/sim efforts:
  - TMAP8, FENIX, Blanket/Magnet Multiphysics, Advanced Manufacturing
- **MOOSE as an open, flexible framework can create pathways to fully integrated, whole device modeling.**

Idaho National Laboratory

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy. INL is the nation's center for nuclear energy research and development, and also performs research in each of DOE's strategic goal areas: energy, national security, science and the environment.