INL/MIS-19-55828

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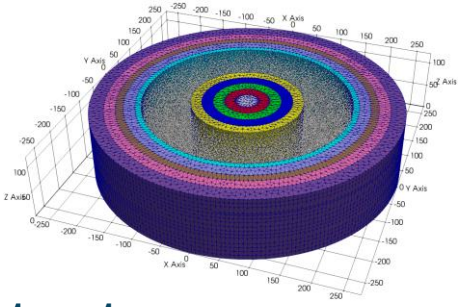
IDAHO NATIONAL LABORATORY 70th Anniversary

Idaho National Laboratory

Multi-Physics Simulation of Advanced Reactor Designs using MOOSE-Based Reactor Physics Methods



Mark D. DeHart, PhD
Deputy Director for Reactor Physics Modeling and Simulation
Nuclear Science and Technology Directorate
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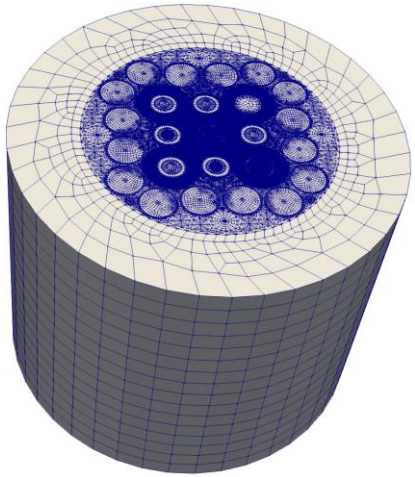

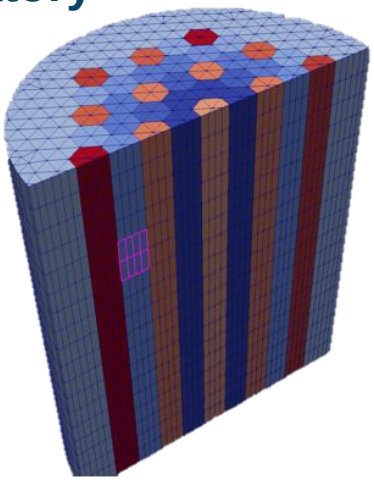

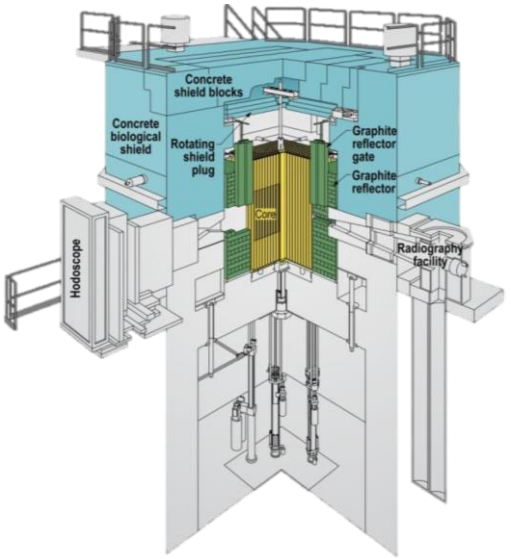

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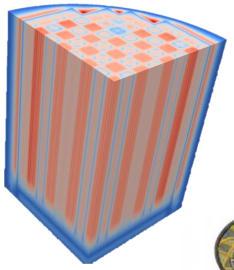
Introduction to MAMMOTH and Rattlesnake Analysis

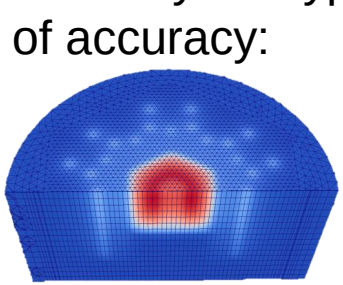
- Modern nuclear reactor core simulations must include all the necessary interlinked physics to enable high fidelity analysis:
  - Radiation transport,
  - Thermal-fluids,
  - Fuel composition changes,
  - Fuel deformation,
  - Clad creep and deformation,
  - Water chemistry changes

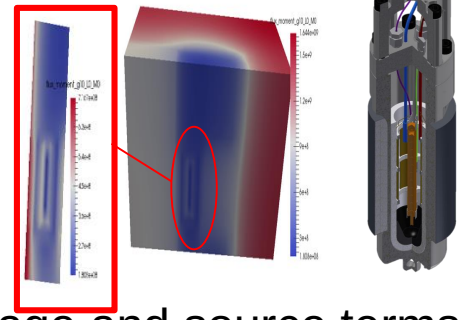


MAMMOTH

RattleSnake

- These also require neutron cross section changes from all relevant feedback effects.
- The number of interlinked physics should be driven by the type of downstream engineering application and its required level of accuracy:
  - Reactor design,
  - Experiment design,
  - Post irradiation examination (PIE),
  - Analysis of aging in vessel internals,
  - Isotopic inventories for spent fuel criticality, long term storage and source terms (decay heat and radiological, etc.)





- There is a general desire to leverage modern methods to provide higher fidelity reactor simulations to resolve global and localized phenomena that affect these engineering applications.

Introduction to MAMMOTH and Rattlesnake Analysis

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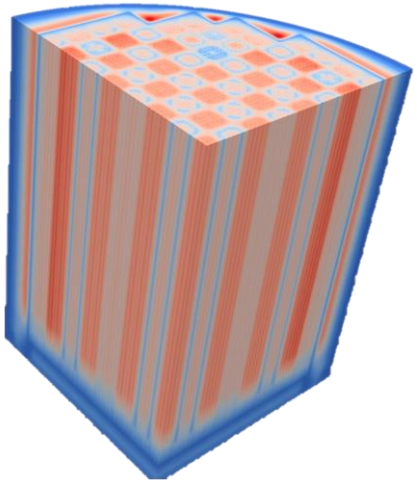

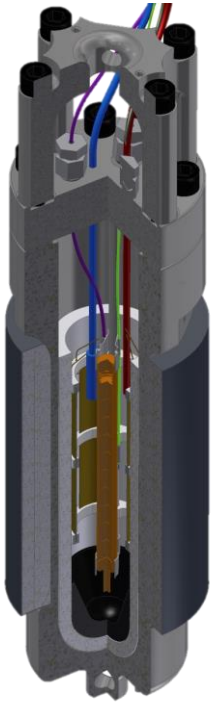

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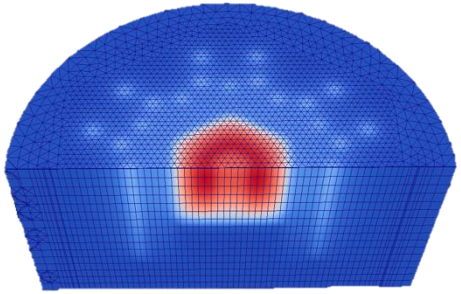
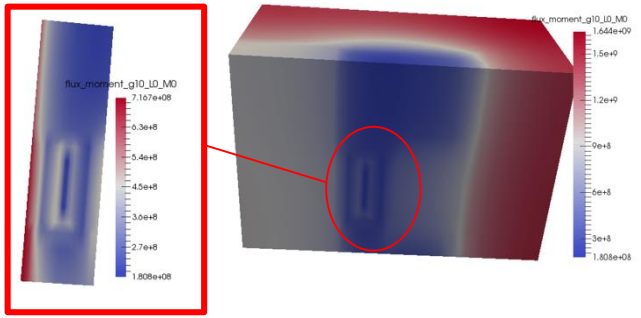




Rattlesnake: A Radiation Transport Application for Multi-Physics Simulations

- Rattlesnake solves the time-dependent Boltzmann transport equation
- Finite-element based solver using both CFEM and DFEM (continuous and discontinuous finite element methods)
- Designed for strongly and tightly coupled nonlinear multi-physics simulations including thermal hydraulics and fuel performance analysis.
- Originally developed for multi-scheme simulation of the INL Advanced Test Reactor (ATR)
  - Multi-scheme methods apply a fine-scale resolution in places where interesting multi-physics phenomena take place.
  - Uses a lower order and/or homogenized solution for less interesting areas
- Lattice, pebble bed and hexagonal fuels, ATR, TRIGA cores, SPERT experiments and the Transient Reactor Test Facility (TREAT)
- Validated for LWR, HTGR, TREAT, TRIGA (NRAD, UWNR) reactor designs
- Used to explore fast reactor, gas reactor (prismatic and pebble) micro-reactor and fast and coupled fast/thermal reactor concepts
- **https://rattlesnake.inl.gov/**

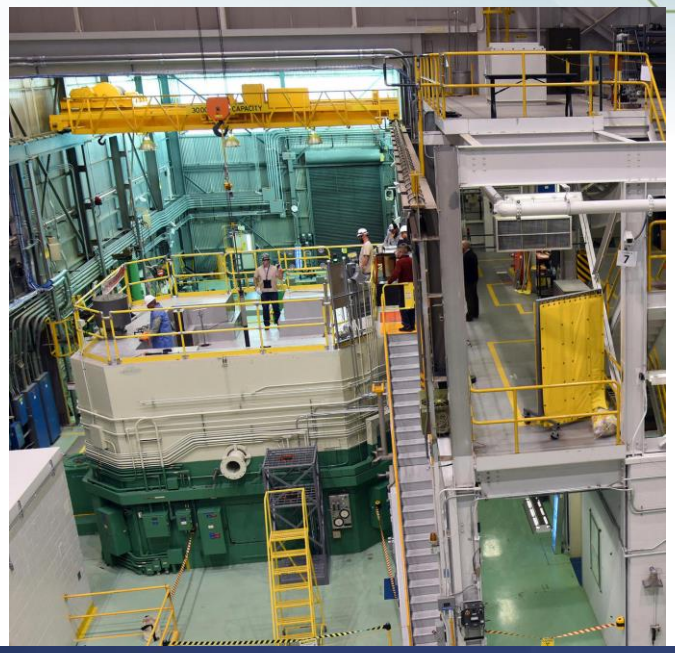
Neutronics V&V

- Completed
  - C5G7 (computational benchmark)
  - LRA BWR kinetics (computational benchmark)
  - BEAVRS (reactor data benchmark)
  - IAEA 3-D PWR (computational benchmark)
  - KAIST-3A reactor quarter core (computational benchmark)
  - OECD 3-D MHTGR-350 Core (computational benchmark)
  - TREAT Minimum Core (reactor data)
  - TREAT M8 Calibration Series (reactor data, steady state and transient)
  - GODIVA neutronic/thermal-mechanical benchmark (reactor data/IRPhE benchmark)
  - HTR-10 (computational benchmark based on reactor data)
  - 2018 TREAT Transient Prescription Measurements (reactor data, steady state and transient)
  - 2019 Transient experiments and measurements
- In Progress
  - ATR 94CIC (reactor data/ IRPhE benchmark)
  - C5G7-TD (time-dependent computational benchmark)
  - TREAT M2/M3 Calibration Measurements (reactor steady state and kinetic data)
  - SPERT 4 transients with MAMMOTH, BISON and RELAP-7 (reactor data)
- Other validation efforts focus on depletion (analytical and measured data)

MAMMOTH

- Like Rattlesnake MAMMOTH has been built using the MOOSE framework (Multi-physics Object Oriented Simulation Environment)
- MOOSE allows implicit, strong, and loose coupling of MOOSE animal solutions
- MAMMOTH is the MOOSE-based multi-physics reactor analysis tool.
- From 2015-2018, MAMMOTH R&D largely focused on support for TREAT transient analysis.
- For early work, TREAT **core** simulation efforts rely on only Rattlesnake (time-dependent neutron transport) within MAMMOTH. Energy deposition conversion to temperature was performed by the heat equation, a kernel in MOOSE.
- Cross sections are 3D in nature and are generated using Serpent 2 for fixed state points (temperatures and control rod position)
- Initial work assumed an adiabatic condition. We have recently coupled to a heat conduction kernel to improve simulation for longer transients (> 10s).
- Once the core modeling capability was “mastered” work began to focus on experiment simulations.
- **There is no other computational tool that can directly model 3D kinetics with spatially resolved temperature feedback.**

TREAT:
The Transient Reactor Test Facility



Advanced Modeling & Simulation

- Early validation efforts were based on data available from M8CAL calibration measurements from early 1990s
- Parallel simulations have been performed to model a number of experiments in support of the accident tolerant fuel campaign at TREAT
  - Transient prescription (wire) measurements (completed in 2018)
  - MARCH-SETH fuel pin tests (completed in 2018)
  - New experiments (calibration/learning/NASA) are rolling in faster than we can model them
  - Multi-SERTTA (next year) will be the first planned extensive fuel performance test series
- At this time, calculations have two phases:
  - Predictive calculations for experiment design support
  - Confirmatory calculations (and fine tuning) to match measured data
- Extension to multi-scale and two-stage simulations
  - Multi-scale solutions allow, for example, a diffusion solution for the core coupled to a high-fidelity solution for an experiment
  - Two stage solutions are used to generate a core-driven transient boundary condition on a subset model (experiment region) to support experiment design.

Advanced Modeling & Simulation

- Most of the fine tuning has focused on development of methods to handle cross section challenges
  - 3D effects – base cross sections generated using *Serpent 2*
  - Strong neutron streaming in hodoscope slot and air channels
  - Strong absorption near control rods
  - Motion of control rods
  - Support for homogenization of most of core (computational efficiency)
    - Superhomogenization (SPH) treatments*
    - Discontinuity factors†
  - Complex experiment configurations.

* J. Ortensi, Y. Wang, A. Laurier, S. Schunert, A. Hébert, M. DeHart, "A Newton solution for the Superhomogenization method: The PJFNK-SPH," *Annals of Nuclear Energy*, **111**, 2018, 579-594

† V. Labouré, Y. Wang, J. Ortensi, S. Schunert, F. Gleicher, M. DeHart, R. Martineau, "Hybrid super homogenization and discontinuity factor method for continuous finite element diffusion," *Annals of Nuclear Energy*, **128**, 2019, 443-454

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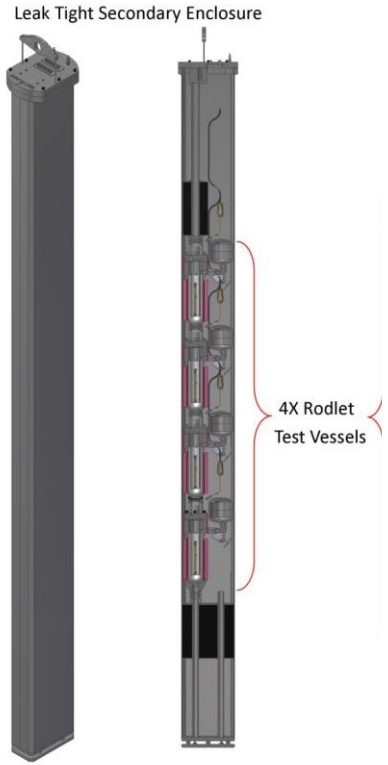
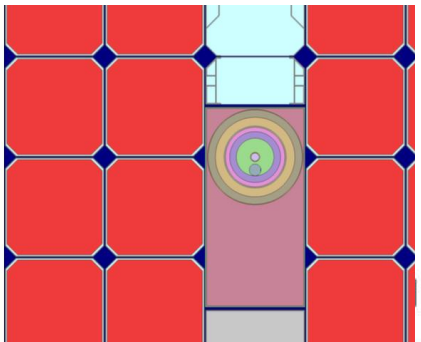
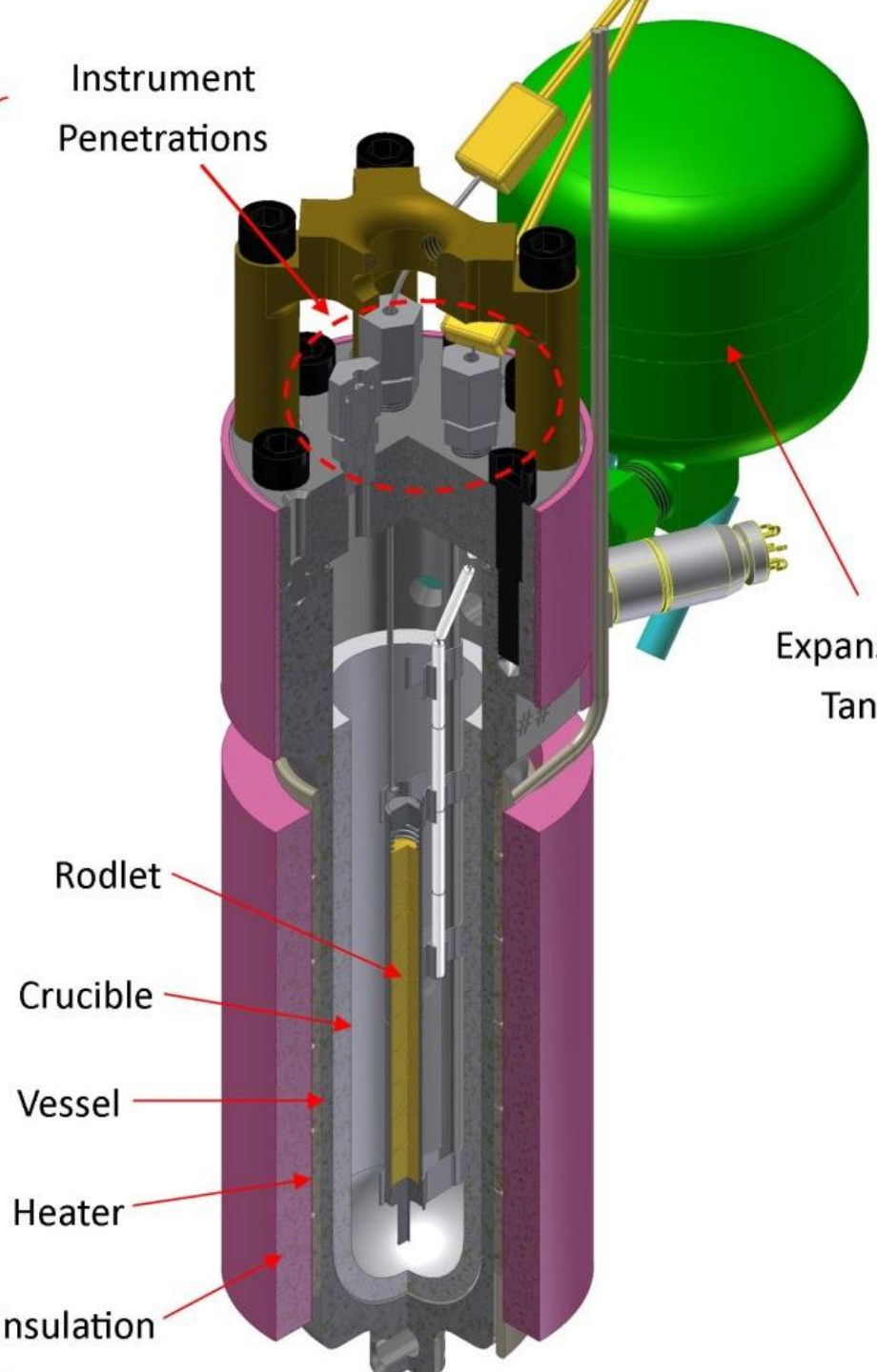
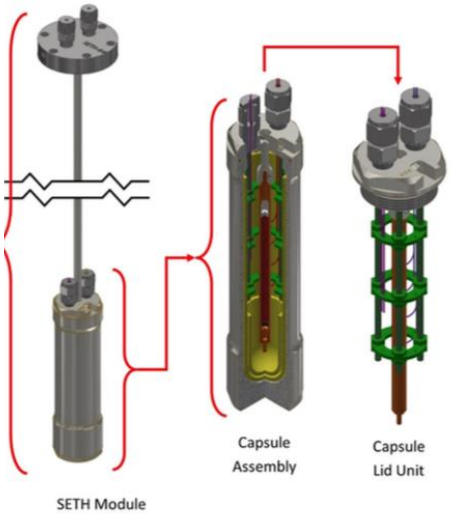
Advanced M… MARCH-SET… …ERTTA and





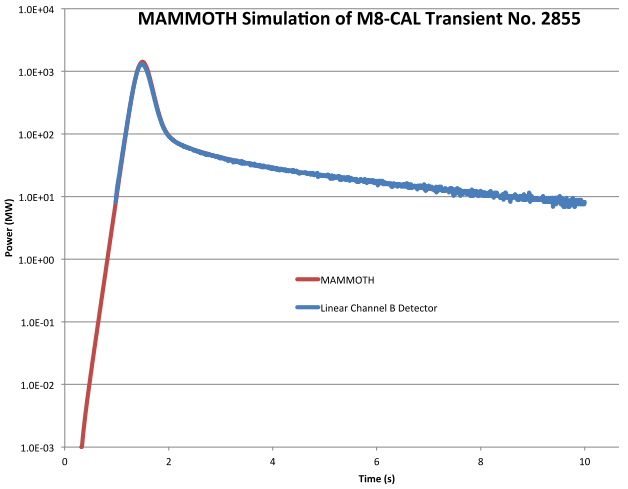


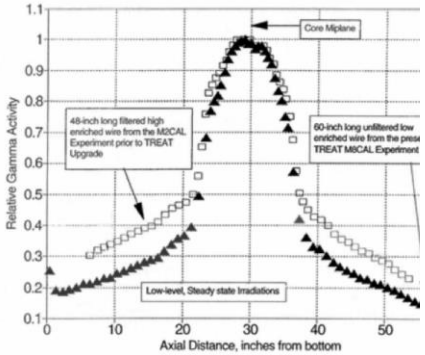


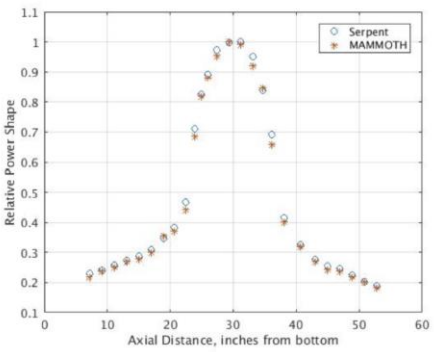
TREAT M8 Calibration: Transient 2855

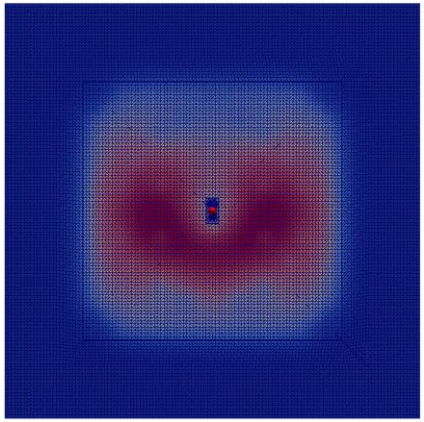
- Peak Power
  - MAMMOTH Value = 1363 MW
  - Detector readings - 1208 to 1303 MW (4.6 to 12.8% error)
    - Average 1258 MW (8.4% error)
  - Listed value = 1245 MW (9.5% error)

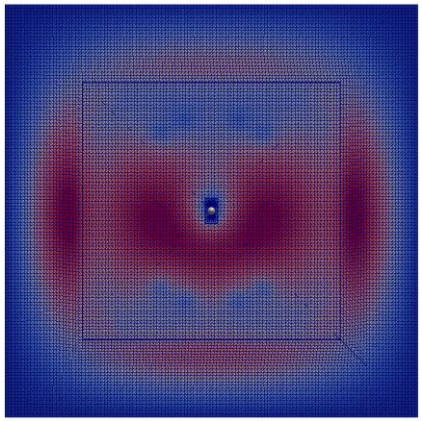
Item	Wire ID	Measured PCF	Correction Type	Revised Prediction of PCF	Error (%)
1	L91-8-10	1.79	Q value, Rod position B, Temperature	1.74	-2.79
2	L91-60-1	1.40	Q value, Temperature	1.39	-0.71
5	H91-7-1	0.503	Q value, Temperature	0.487	-3.02
6	L91-8-6	1.84	Q value, Rod position B, Temperature	1.88	+2.17





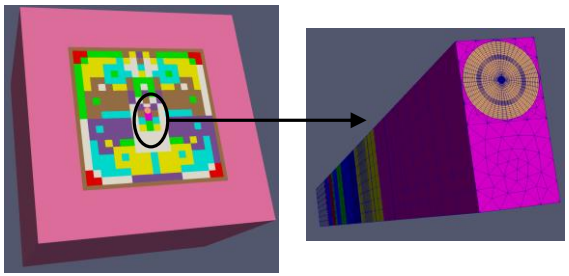


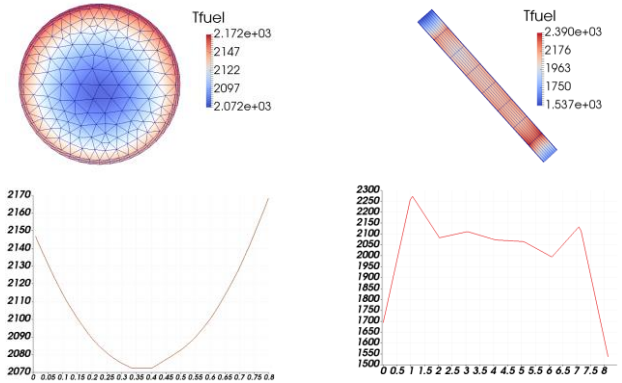


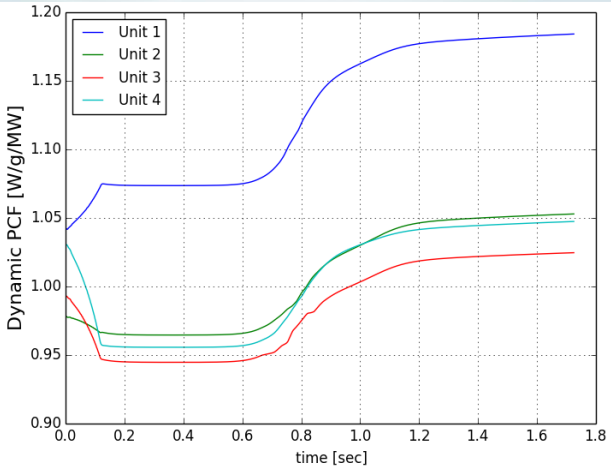


TREAT Experiment Design Support

- The Multi-SERTTA provides a significant challenge and opportunity for advanced modeling and simulation.
- The MAMMOTH reactor multi-physics application is being used to simulate the behavior of fuel stacks within the Multi-SERTTA test rig during a transient.
- Both the energy deposition rates and true fuel temperatures are necessary to accurately predict the performance of the test fuel, and MAMMOTH multi-physics simulations provide the opportunity to model both simultaneously.
- One of the most significant advantages of developing more rigorous 3-D spatial dynamics simulations is in providing the ability to better understand the transient effects on energy deposition in the Multi-SERTTA test fuel samples.



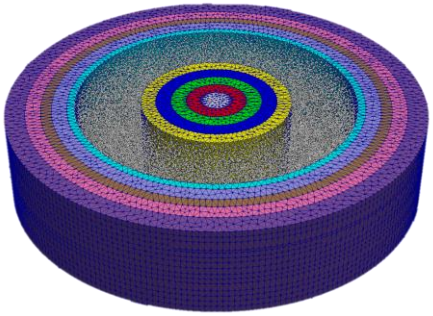




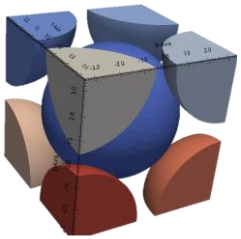
- Novel calculation of a Dynamic Power Coupling Factor (DPCF) for TREAT operations:
  - Shows effects of collar design and CR movement.
- Pellet resolution in each SERTTA unit.
- This work targets improvement of experiment design by providing a time dependent flux boundary condition for the experiment region.

Pebble Tracking Transport Algorithm for Pebble Bed Reactor Analysis (PTT)

- Motivation:
  - To support high resolution multi-physics simulations of pebble bed reactors.
  - To remove the region homogenization of the pebble-bed domain in traditional methods.
  - To enable direct transport calculations with pebble tracking.
- Capabilities
  - Works with DEM (discrete element method), which provides positions of all pebbles, to establish an equilibrium core.
  - Will be able to track motion and burnup of each individual pebble.
- Preliminary Results
  - PTT can converge k_{eff} and reaction rates less than 0.1% for all cases with respect to Serpent reference calculation (simple 9-sphere model, fresh fuel).

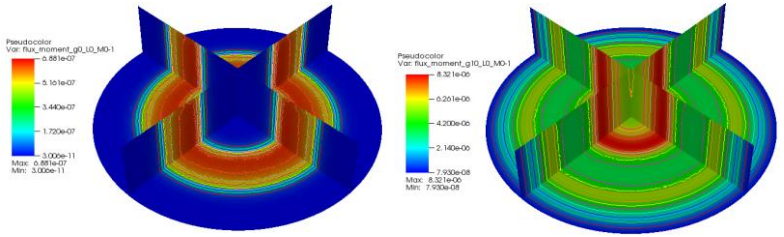


HTR-10 Pebble Bed Mesh: Total 437,735 tetrahedra. 76,869 node points. Pebble packing region has 291,107 tetrahedra, reflection top and bottom.



Error (pcm) in k_{eff} Relative to Reference Model
(Similar error seen in predicted reaction rates)

SN	P				
	1	2	3	4	5
2	43.2377	43.3009	43.3141	43.3378	43.3579
4	43.2400	43.2653	43.2696	43.2783	43.2817
6	43.2406	43.2660	43.2707	43.2794	43.2824
8	43.2411	43.2657	43.2702	43.2796	43.2827



Fast (left) and thermal (right) fluxes in HTR-10 simulation

Pebble Bed Modeling and Simulation

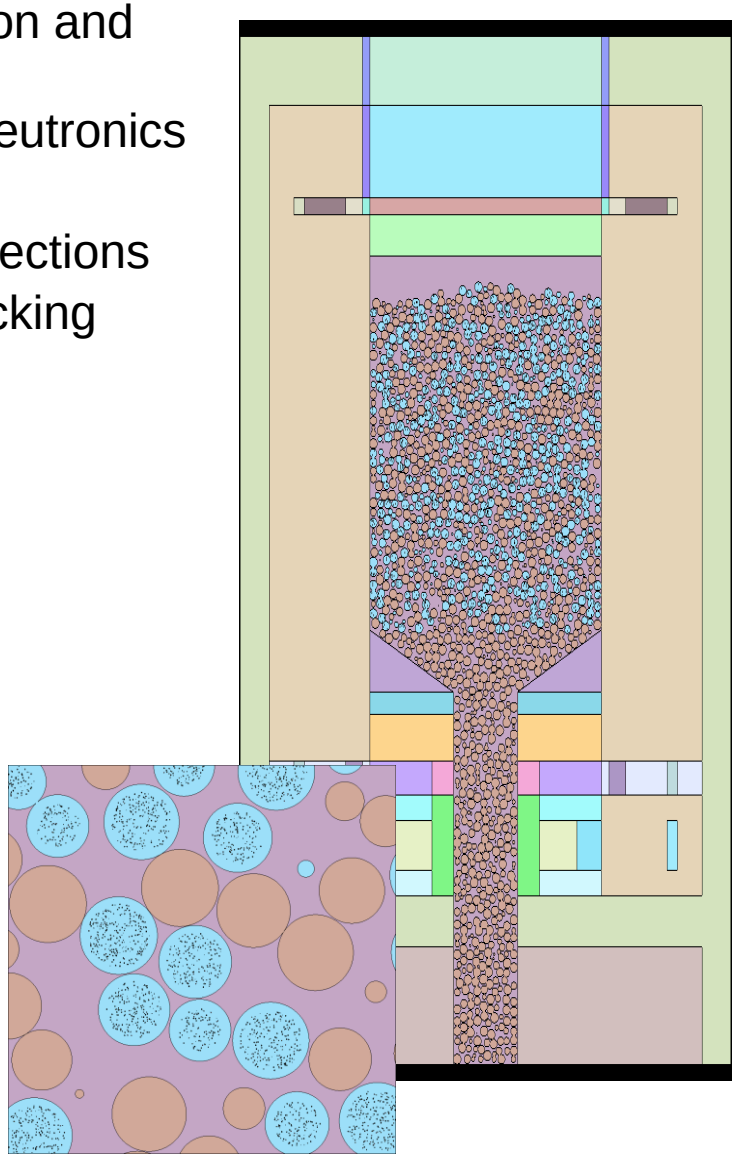
- High resolution model
  - Use LAMMPS for pebble motion and equilibrium.
  - Serpent MC for steady state neutronics
    - Reference solution
    - Generation of MG cross sections
  - Rattlesnake using Pebble Tracking Transport (PTT) methodology
- Low resolution model
  - Homogenized regions

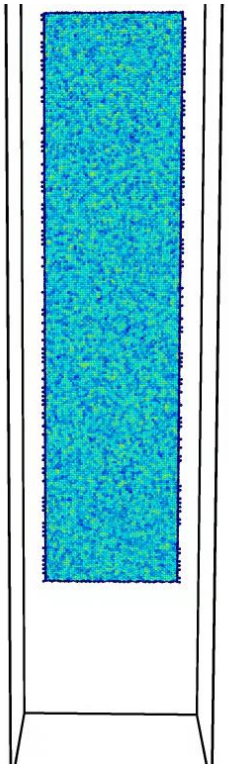
Critical Configuration

Code	keff	uncertainty rel. error [pcm]
MCNP (ENDFB-VI)	1.01190	±21
Serpent (ENDFB-VI)	1.01025	±5.1
Serpent (ENDFB-VII.r1)	1.00023	±2.3
MAMMOTH TDC-SPH-Diffusion	1.00089	67.3

Isothermal Temperature Coefficients

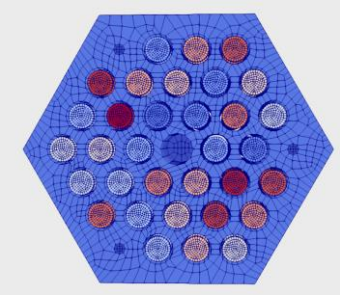
Code	20-120 °C [pcm/°C]	120-250 °C [pcm/°C]
Serpent (INL)	-9.33	-11.28
MAMMOTH (INL)	-10.31	-11.49
VSOP (China)	-7.51	-9.28
VSOP 2-D (Germany)	-10.31	-10.58
VSOP 3-D (Germany)	-10.65	-11.03
VSOP_PBMR (SA)	-7.16	-9.25

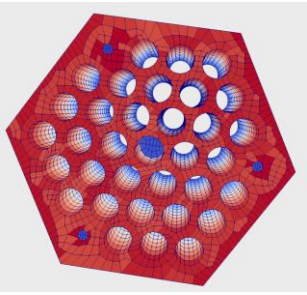




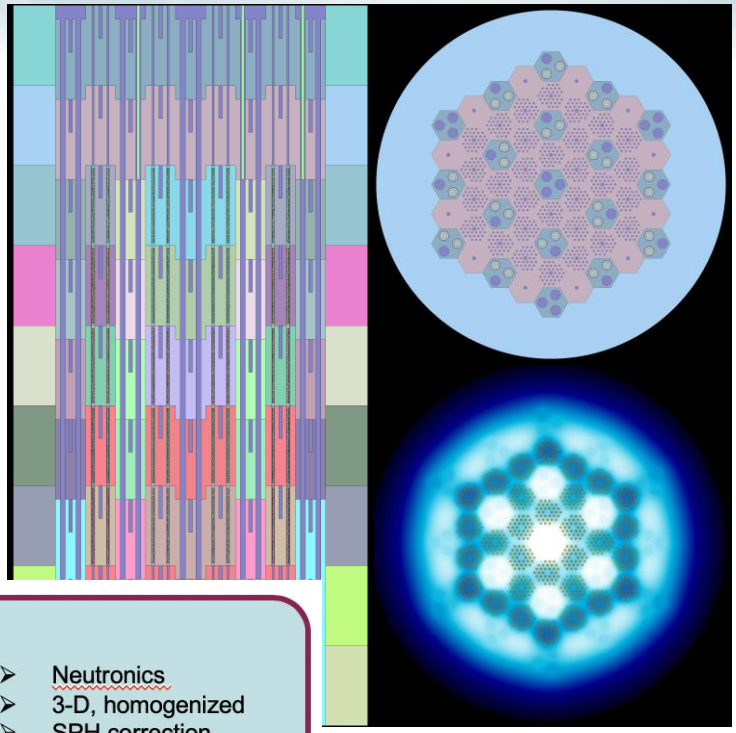
High Temperature Test Reactor

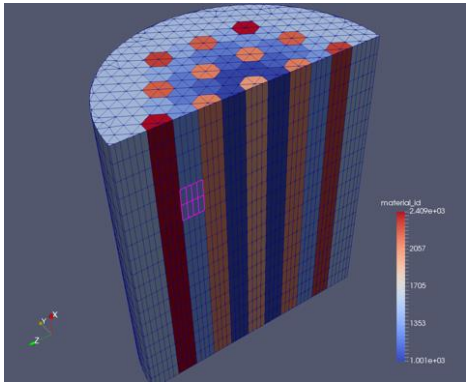
- **Pin-in-Block design**
  - Annular fuel pins
  - Annular flow between pin and block



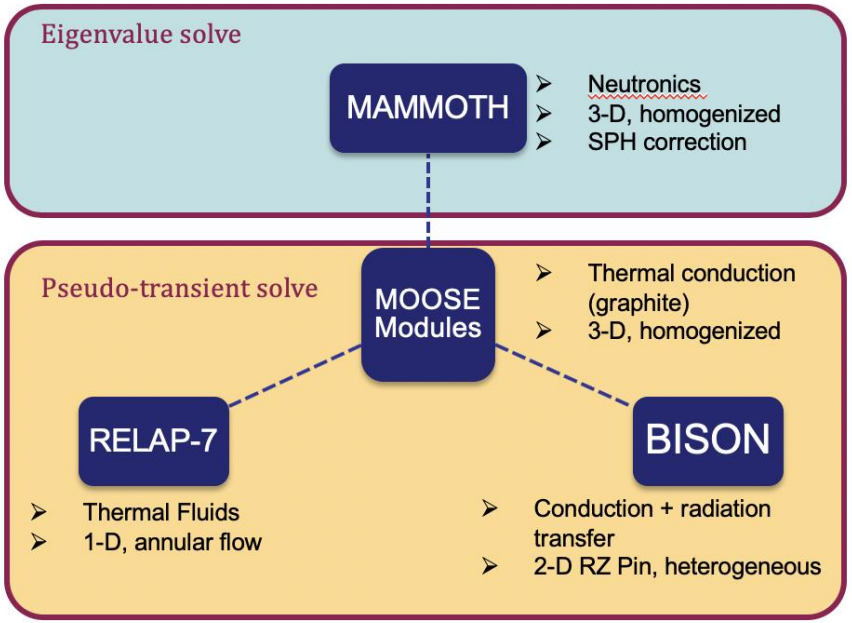


3-D full core Serpent





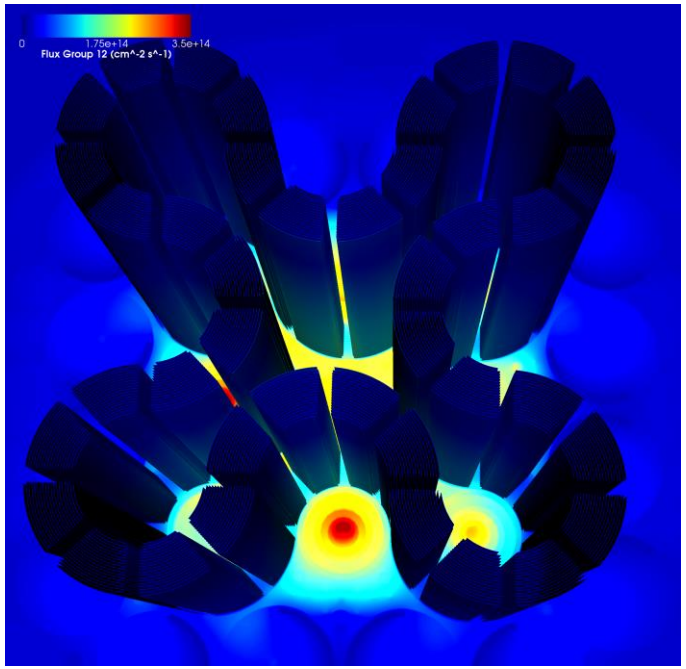
3-D Full core MAMMOTH Block homogenized



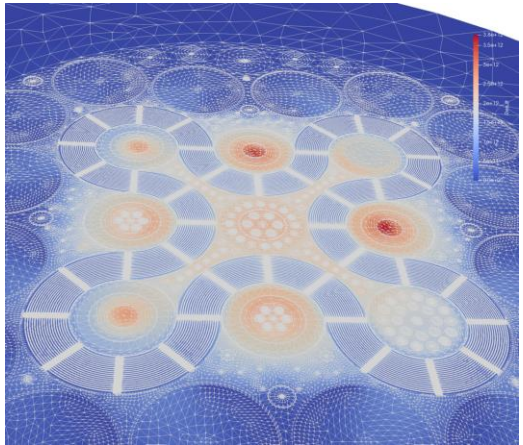
Full Core (3D) ATR Modeling

3D Rattlesnake Heterogeneous Transport Simulation of the ATR Core:

- 3D unstructured mesh with 4,207,728 elements (mixed element types, extruded from a 2D mesh with 16 layers).
- Self Adjoint Angular Flux (SAAF) formulation for transport equation.
- S8 level-symmetric angular quadrature (80 streaming directions).
- 12 energy groups.



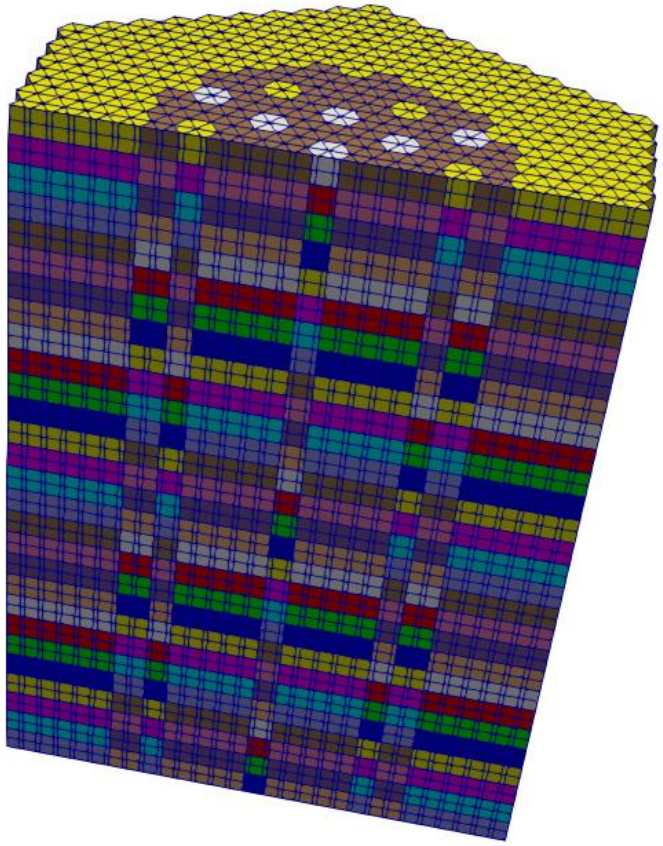
- S8 level-symmetric angular quadrature (80 streaming directions).
- NDOF = 4,178,001,600.
- 2048 cores on INL Falcon cluster.
- Direct transport k-eigenvalue calculation w/ PJFNK.
- Wall time 12,877s about 3.58 hours.

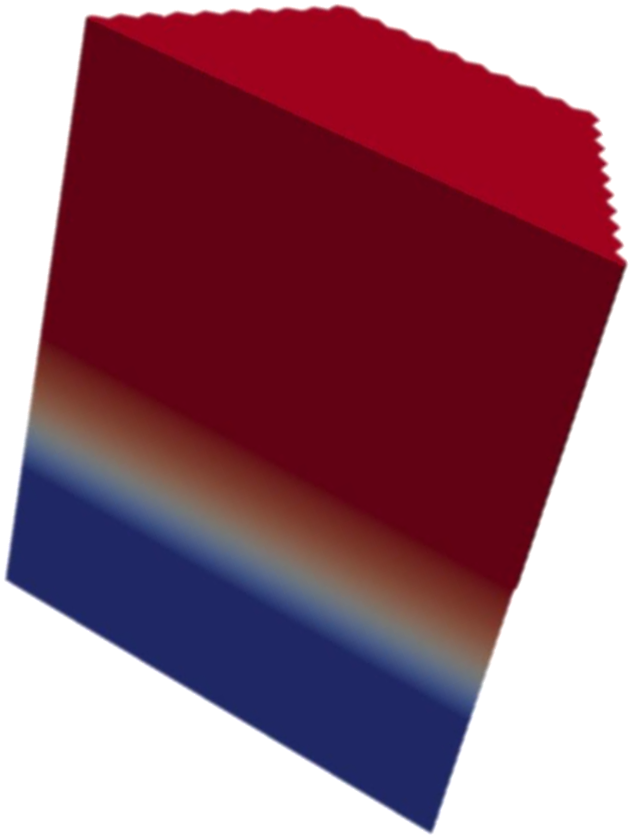


Versatile Test Reactor

MAMMOTH models of the Versatile Test Reactor, a fast reactor concept, have been tightly coupled to BISON and RELAP-7 to study the effect of density feedback.

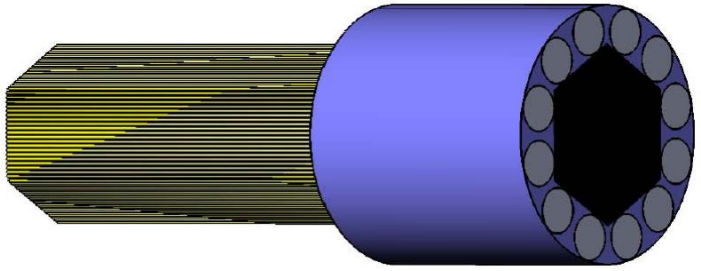
This core is being designed to enable fuels and materials irradiation testing with a new fast spectrum neutron capability.

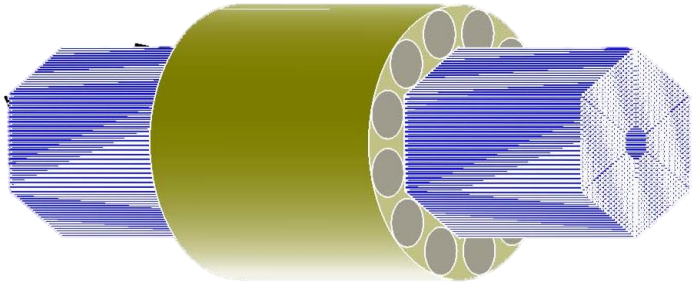




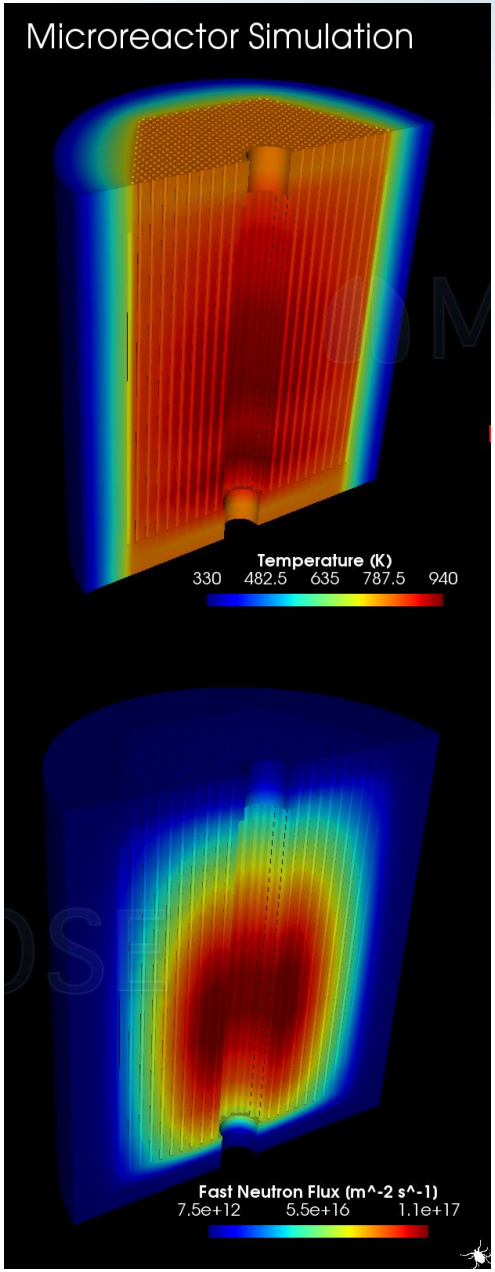
Heat-Pipe-Cooled Micro-Reactor Projects

- Micro-Reactor projects include:
  - MEITNER ARPA-e Solid Core Block (SCB) for an Inherently Safe Heat Pipe Reactor (supporting Westinghouse and LANL)
  - Special Purpose Reactor (SPR) is a small 5 MWt, heat pipe-cooled, fast reactor based on the Los Alamos National Laboratory Mega-Power concept.
  - Oklo fast reactor.





- DireWolf is a new addition to the MOOSE ecosystem for simulation of heat pipe cooled reactor systems
  - *MAMMOTH (reactor physics)*
  - *Rattlesnake* (transient radiation transport)
  - *BISON* (nuclear fuel performance)
  - *Grizzly* (structural mechanics)
  - *Sockeye* (advanced heat pipe technology)
  - *RELAP-7* (Open-air and SC CO2 Brayton cycles)

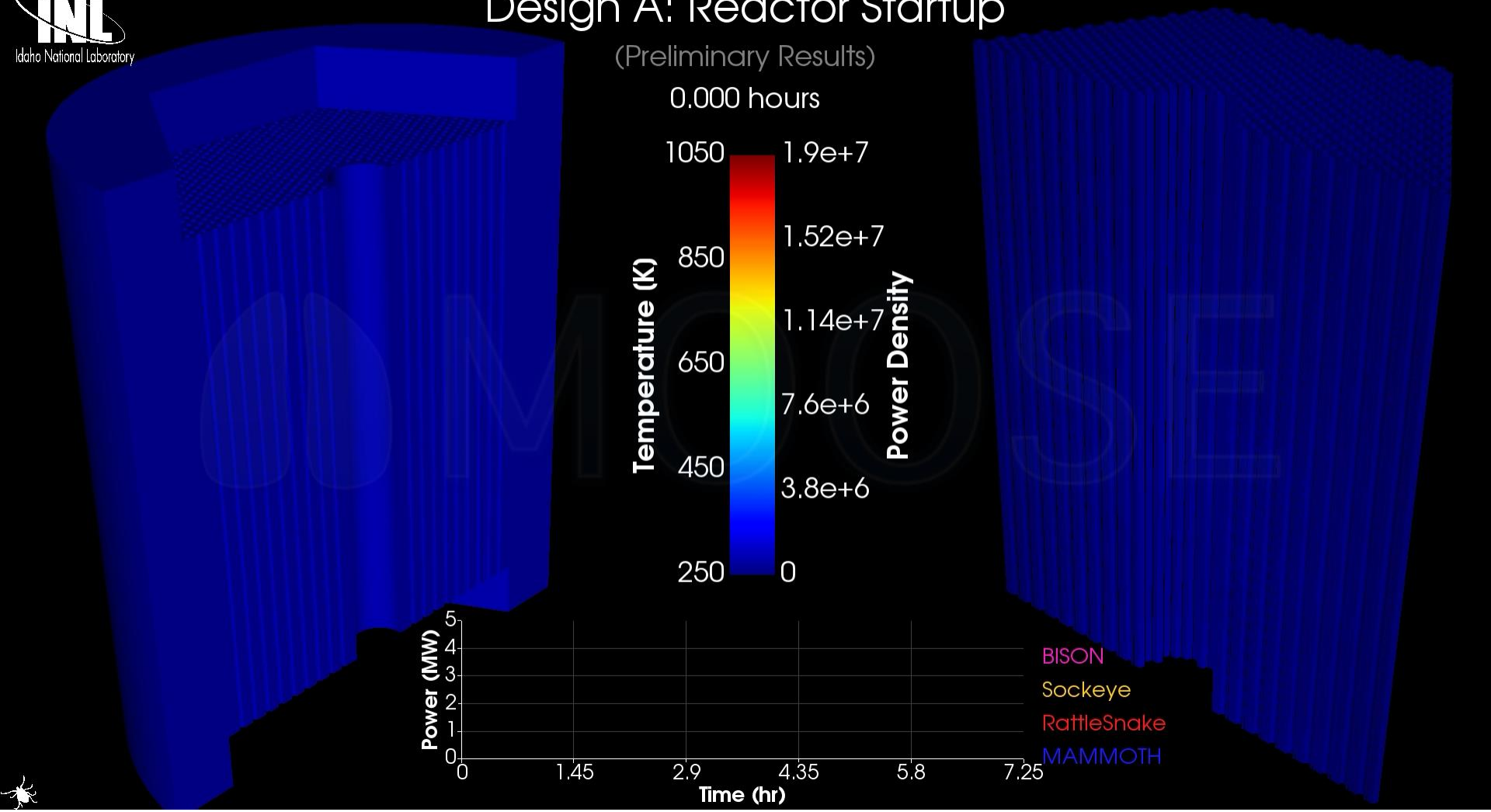


Preliminary Design A Micro-Reactor (Hexagonal Fuel Design) Transient (7.25 hour power up)

- **DireWolf:**
  - MAMMOTH
  - BISON
  - Sockeye
- **Transient Scenario:** 7.25 hr linear ramp to 100% power
- **Number of FEs**:
  - MAMMOTH = 2,287,656 (3D)
  - BISON = 1,506,168 (3D)
  - Sockeye = 732,042 (1D)
- **MPIs** =
  - 256 BISON
  - 1080 MAMMOTH
- **Run time** = ~3 hours

Design A: Reactor Startup

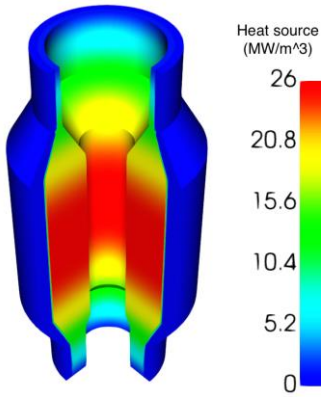
(Preliminary Results)



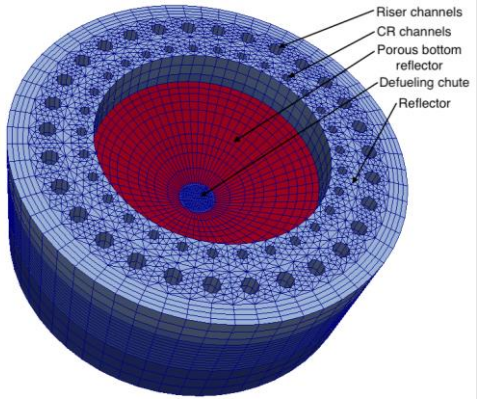
Velociraptor: Advanced Reactor Concepts and the Versatile Test Reactor

Velociraptor is designed to support DOE-NE's Office of Advanced Reactor Technologies (ART), the Advanced Reactor Concepts (ARC) program

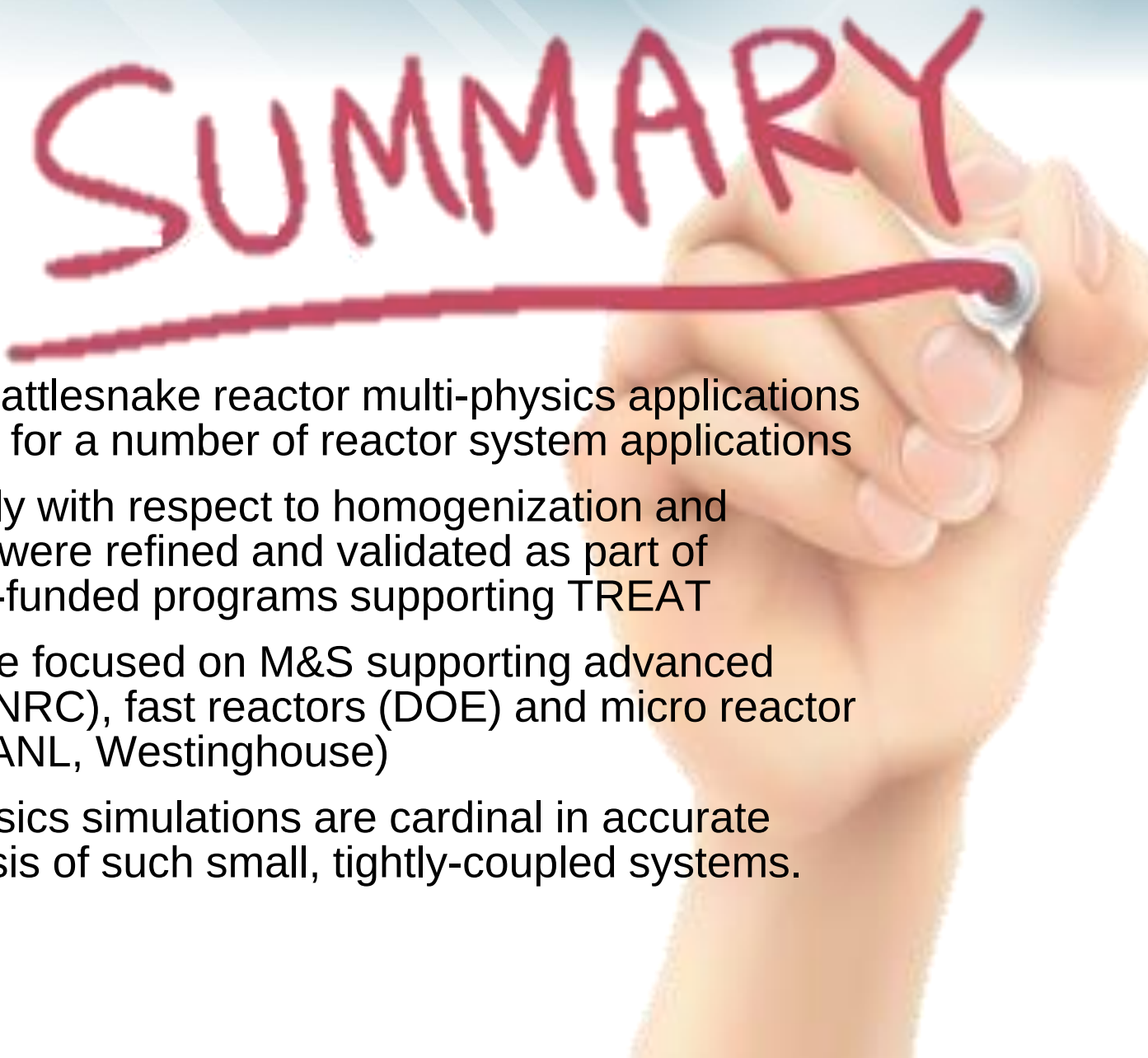
- Leverages NEAMS tools.
- Applicable for VHTR, FHR, MSR, SFR, and VTR
- Full core representation:
  - ***Pronghorn*** – Coarse mesh, multi-dimensional representation for conjugate heat transfer in both 2D (r-z) and 3D. 3D subchannel capability in progress.
  - ***MAMMOTH*** – Reactor physics
  - ***Rattlesnake*** – Radiation transport
  - ***BISON/Marmot*** – Multiscale Nuclear fuels performance for ATF, TRISO, and metal fuel forms.
- Balance of plant and systems analysis:
  - ***RELAP-7*** – Gas-cooled reactor concepts and all power generation cycles.
  - ***SAM*** – RELAP-7 derivative for single-phase liquid coolants.
- Fluid Properties: **Na, He, N_2, H_2, CO_2, 2-θ H_2O**, and **FLiBe**



FHR Power



HTR-10 Lower Reflector



- MAMMOTH and Rattlesnake reactor multi-physics applications have been applied for a number of reactor system applications
- Methods, especially with respect to homogenization and streaming effects, were refined and validated as part of NEAMS- and ATF-funded programs supporting TREAT
- Recent efforts have focused on M&S supporting advanced reactor concepts (NRC), fast reactors (DOE) and micro reactor concepts (DOE, LANL, Westinghouse)
- Coupled multi-physics simulations are cardinal in accurate engineering analysis of such small, tightly-coupled systems.

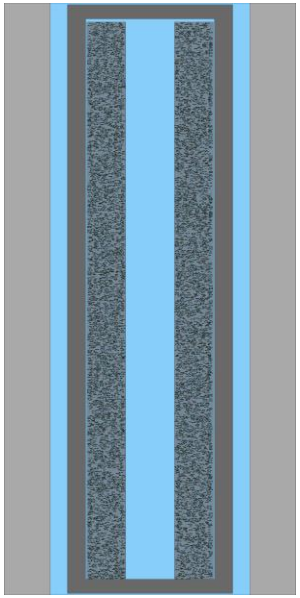
IDAHO NATIONAL LABORATORY
70th
Anniversary
INL
Idaho National Laboratory

Extra Material

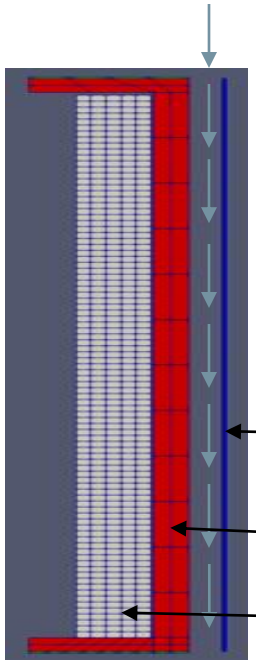
Measurements and Experiments Since Restart

Startup Number	Transient #	Run Type	Purpose
	NA	Initial Critical	
	NA	Critical to 50W	
	NA	Heat Balance	
	NA	Rod Worth	
	NA	Rod Worth	
	NA	Rod Worth	
	NA	Initial Critical	
	NA	50 W power	
	NA	Heat Balance	
	NA	Heat Balance	
	NA	Rod Worths	
	NA	Rod Worths	
17-Jan-18	2886	1.85 Transient	Characterization
24-Jan-18	2887	3.06 Transient	Characterization
30-Jan-18	2888	3.93 Transient	Characterization
14-Feb-18	2889	1.83 Transient	Training
24-Apr-18	NA	SS 80 KW	ATF 3-1
2-May-18	2890	1.48 Transient	ATF 3-1
3-May-18	2891	1.89 Transient	ATF 3-1
10-May-18	2892	2.57 Transient	ATF 3-1
14-May-18	2893	2.57 Transient	ATF 3-1
15-May-18	2894	2.57 Transient	ATF 3-1
16-May-18		SS 80 KW	Radiography
21-May-18		SS 80 KW	Radiography
23-May-18		Aborted SS	Radiography
31-May-18		SS	Radiography
4-Jun-18		SS	Reactivity Computer Test
14-Jun-18	6646	2895 Stepwise	MIT
12-Jun-18		2896 200 KW Flattop	MIT
13-Jun-18		2897 600 KW Flattop	MIT
18-Jun-18	6647	2898 600 KW Flattop	MIT
19-Jun-18	6648	2899 Stepwise	MIT
20-Jun-18	6649	2900 1.8 Transient	MIT
25-Jun-18	6650	2901 3.85 Tranisent	MIT
26-Jun-18	6651	2902 LOCA	
27-Jun-18	6652	2903 LOCA	
28-Jun-18	6653		Radiography
2-Jul-18	6654		Radiography
3-Jul-18	6655	2904 4.2 Transient Clipped at 475 ms	Narrow Pulse Width
9-Jul-18	6656		Failed Rod Drive
11-Jul-18	6656	2905 4.2 Transient Clipped at 500 ms	Narrow Pulse Width
12-Jul-18	6657	2906 4.2 Transient Clipped at 513 ms	Narrow Pulse Width
17-Jul-18	6658	2907 4.2 Transient Clipped at 525 ms	Narrow Pulse Width
18-Jul-18	6659		Failed Rod Drive
19-Jul-18	6660	2908 4.2 Transient Clipped at 450 ms	Narrow Pulse Width
10-Sep-18		2909 1.67 Transient	Characterization
11-Sep-18		2910 2.86 Transient	Characterization
12-Sep-18		2911 3.82 Transient	Characterization
13-Sep-18		2912 0.52 Transient	ATF-SETH Final Trial
18-Sep-18		2913 0.52 Transient	ATF-SETH A
26-Sep-18		2914 0.52 Transient	ATF-SETH B1
17-Oct-18		2915 0.52 Transient	ATF-SETH B1-R2
8-Nov-18		2916	ATF-SETH B2 Trial
20-Nov-18		2917	ATF-SETH B2
28-Nov-18		2918	SETH C Trial
5-Dec-18		2919	SETH C
3-Jan-19		2920	SETH D Trial
7-Jan-19		2921	SETH D Trial 2
10-Jan-19		2922	SETH D
22-Jan-19		2923	SETH E Trial
25-Jan-19		2924	SETH E
3-Apr-19		2925	Extended Mode LOCA
8-Apr-19		2926	Extended Mode LOCA 2
15-Apr-19		2927	Long UTOP
1-May-19		2928	Feedback Flattop
5-Jun-19		2929	NPW 475ms
6-Jun-19		2930	NPW 505ms
10-Jun-19		2931	NPW 535ms
13-Jun-19		2932	SIRIUS Cal Trial
19-Jun-19		2933	SIRIUS Cal
16-Jul-19		2934	1.8 Characterization
17-Jul-19		2935	3.0 Characterization
22-Jul-19		2936	4.0 Characterization
29-Jul-19		2937	1.8 M-SERTTA Trial
31-Jul-19		2938	0.6 SIRIUS-1 Trial
6-Aug-19		2939	SIRIUS-1 Half Power Trial
7-Aug-19		2940	SIRIUS-1 Full Power Trial
19-Aug-19		2941	SETH F0
21-Aug-19		2942	SETH F1
22-Aug-19		2943	SETH F2
28-Aug-19		2944	SETH G
4-Sep-19		2945	0.6 SIRIUS-1
9-Sep-19		2946	SIRIUS-1 Half Power
10-Sep-19		2947	SIRIUS-1 Full Power

HTTR Heat Transfer



3-D Pin

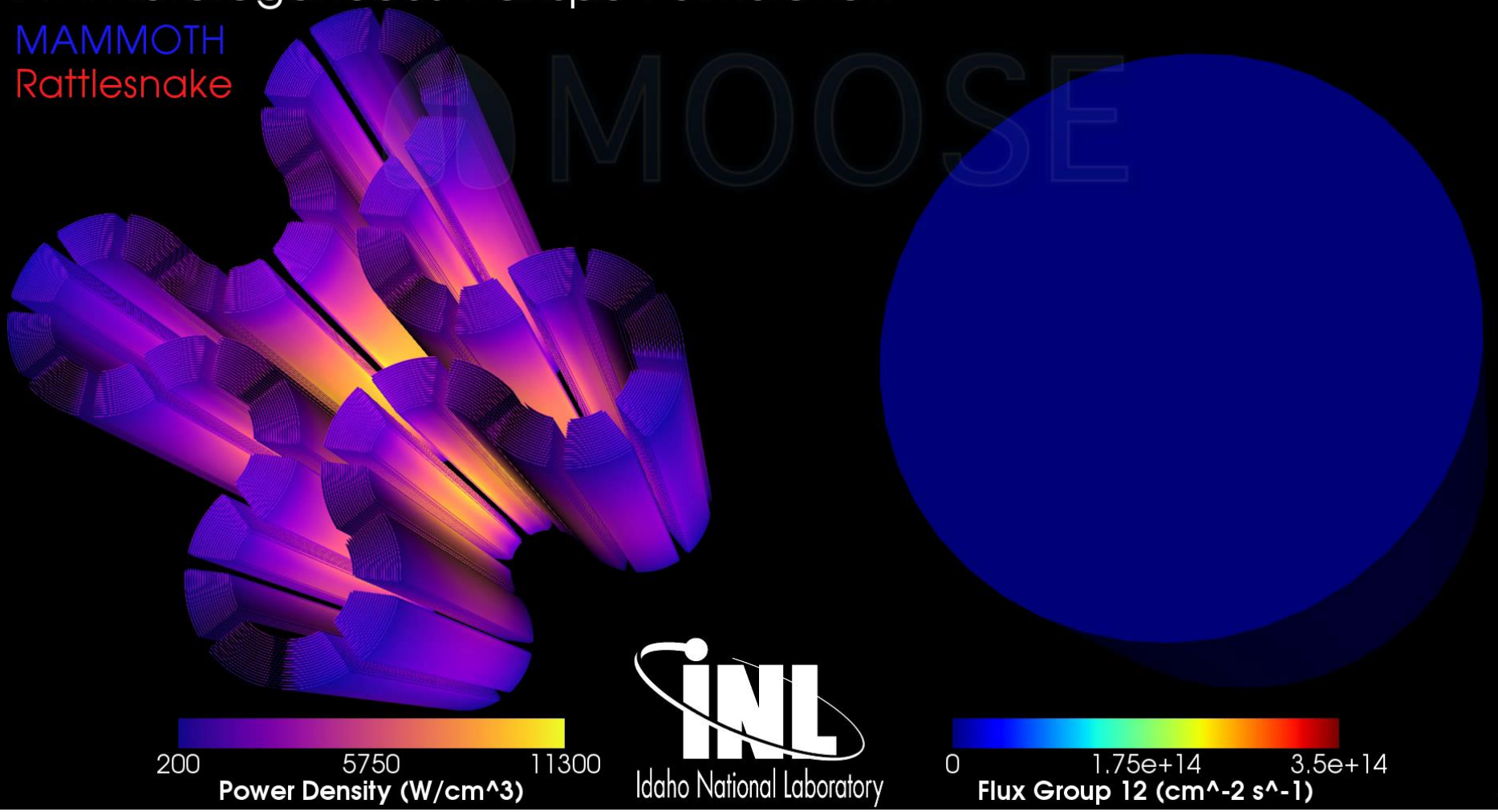


2-D R-Z BISON

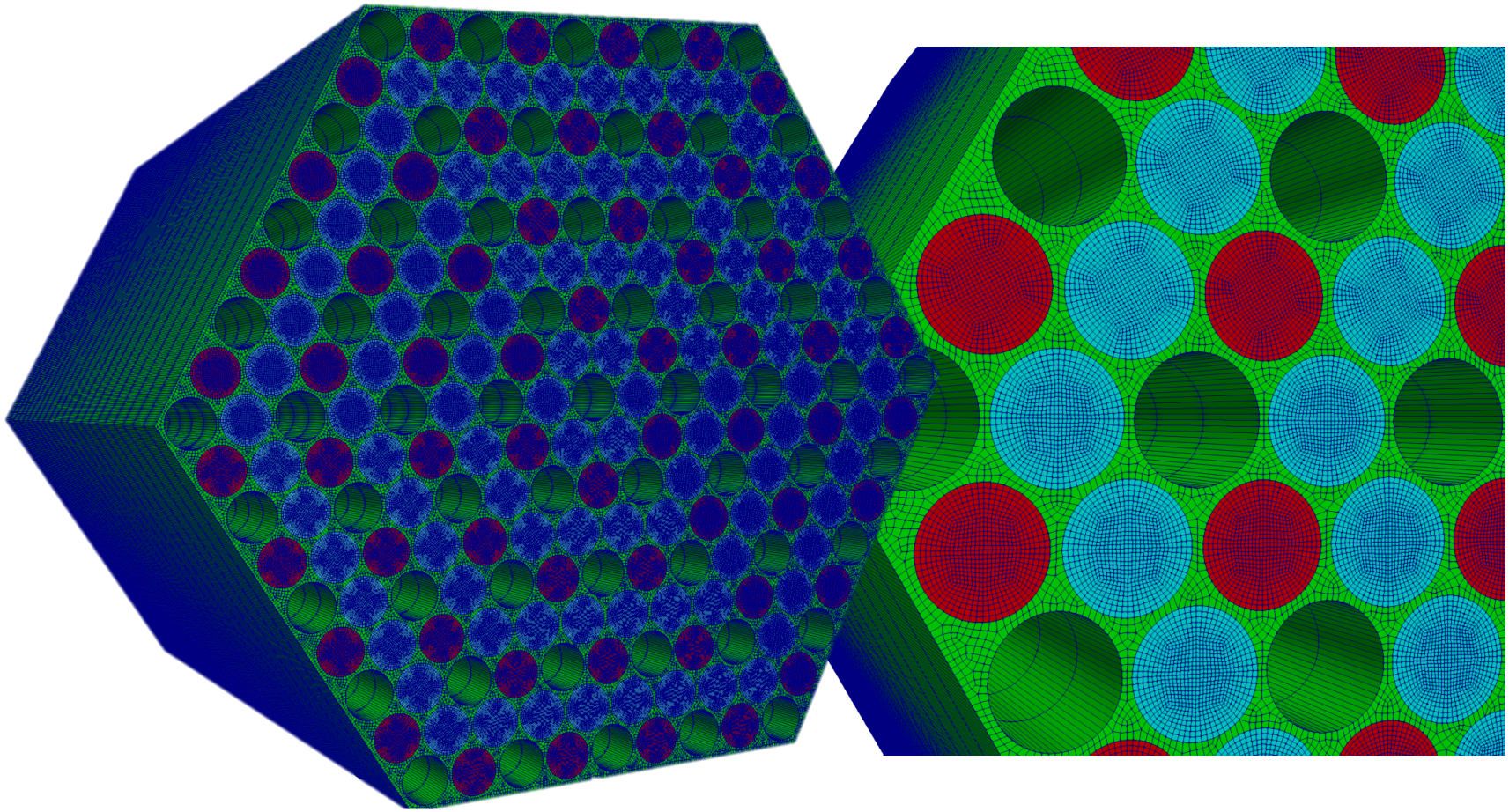
- **Heat flow**
  - Deposited in the fuel compacts
  - Flows to graphite sleeve
    - Conduction through the bottom
    - Convection/radiation through the gap
  - From graphite sleeve to fluid (convection)
  - From fluid to graphite block (convection)
  - From sleeve to graphite block (radiation)
  - Within graphite block (conduction)

ATR Heterogeneous Transport Simulation

MAMMOTH
Rattlesnake

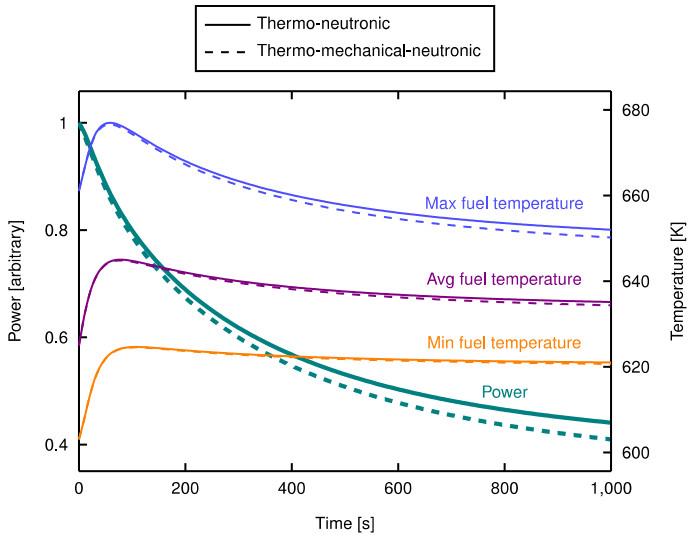


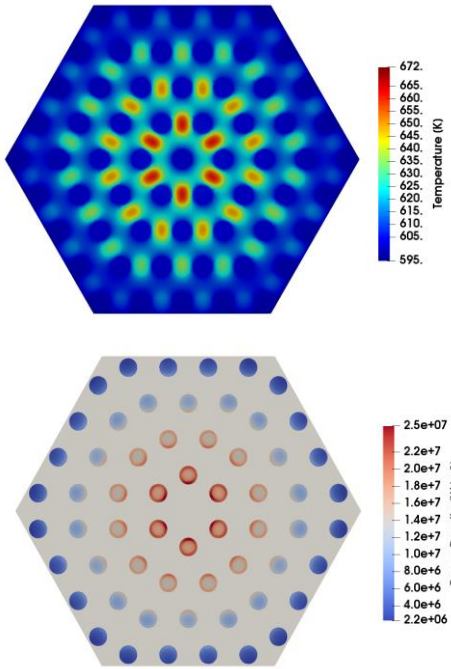
Preliminary Monolithic Micro-Reactor (ARPAe): Mesh

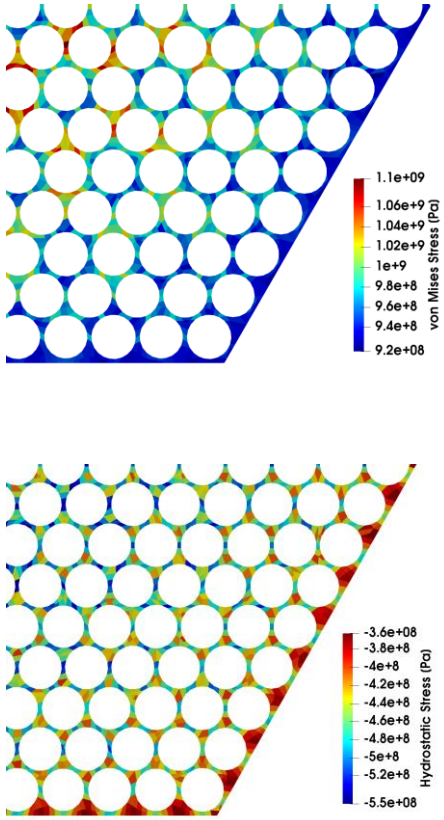


Assessment problem: Unit Assembly
Constant heat pipe temperature BC
(Courtesy Topher Matthews, LANL)

- Steady state: Temperature BC = 600 K
- Transient initiation: Temperature BC = 625 K
- Temperature dependent cross-sections only
- Feedback from cross-section and density



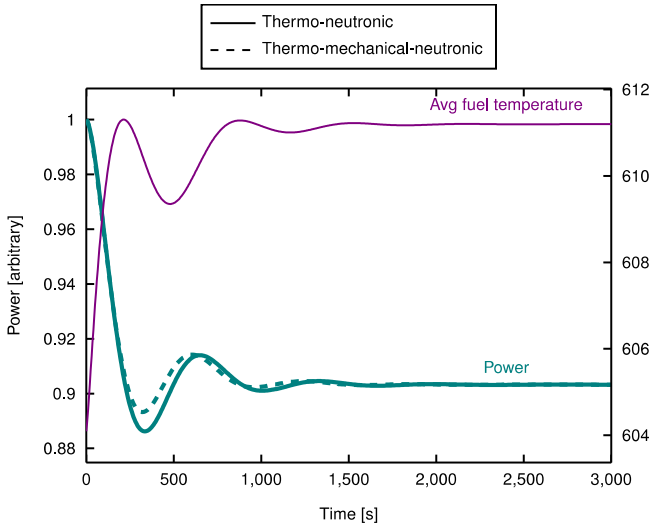


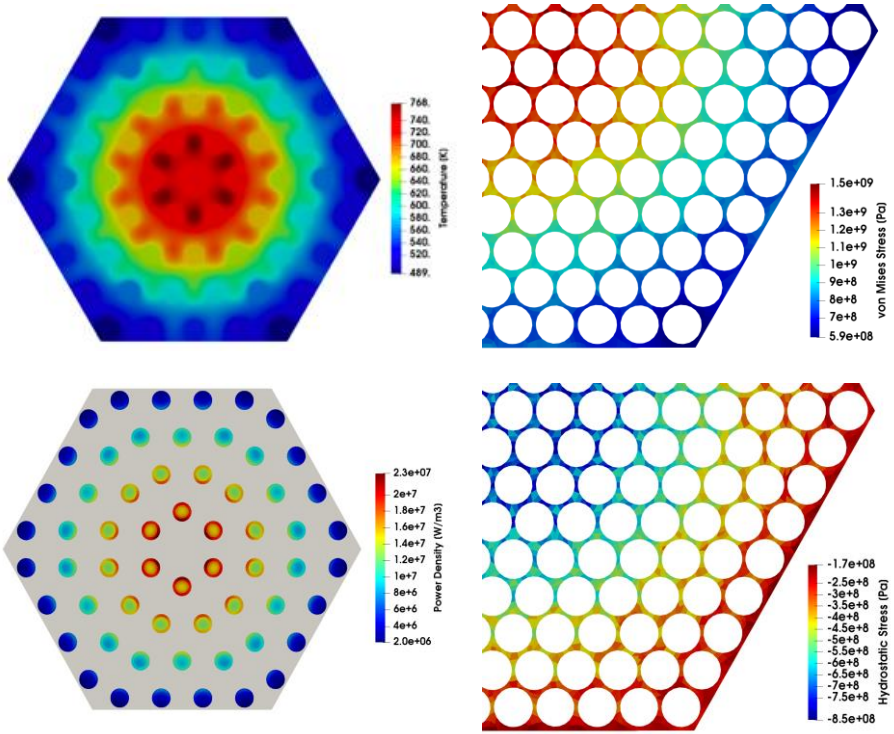


Fuel temperature increase = Power decrease

Assessment problem: Unit Assembly
Constant heat pipe flux BC
(Courtesy Topher Matthews, LANL)

- Steady state: Heat Flux BC = 100% SS power
- Transient initiation: Heat Flux = 90% SS power
- Temperature dependent cross-sections only
- Feedback from cross-section and density





Coupling = Self-regulation