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

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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

• 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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  – Source terms (decay heat and radiological),
  – Isotopic inventories for long term storage,

• 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.
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, UWR) 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/](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.
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.


Advanced Modeling and Simulation – Multi-MERTTA and MARCH-SETH experiments.
**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)

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<tr>
<th>Item</th>
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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 $k_{\text{eff}}$ and reaction rates less than 0.1% for all cases with respect to Serpent reference calculation (simple 9-sphere model, fresh fuel).

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

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

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

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Critical Configuration

Isothermal Temperature Coefficients

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<th>120-250 °C [pcm/°C]</th>
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</table>
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

Eigenvalue solve
- Neutronics
- 3-D, homogenized
- SPH correction

Pseudo-transient solve
- Thermal conduction (graphite)
- 3-D, homogenized

MAMMOTH

MOOSE Modules

RELAP-7
- Thermal Fluids
- 1-D, annular flow

BISON
- Conduction + radiation transfer
- 2-D RZ Pin, heterogeneous
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)

Temperature (K)

Power Density

0.000 hours

1050
1.9e+7

1.52e+7

1.14e+7

7.6e+6

3.8e+6

250
0

Power (MW)

5
4
3
2
1
0

Time (hr)

0 1.45 2.9 4.35 5.8 7.25

BISON
Sockeye
RattleSnake
MAMMOTH
**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, N₂, H₂, CO₂, 2-θ H₂O, and FLiBe
- 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.
### Measurements and Experiments Since Restart

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<th>Startup Number</th>
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<td>11-Jul-18</td>
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<td>12-Jul-18</td>
<td>6657</td>
<td>4.2 Transient Clipped at 513 ms</td>
<td>Narrow Pulse Width</td>
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<td>6658</td>
<td>4.2 Transient Clipped at 525 ms</td>
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The table above lists experiments conducted since the restart of operations. Each row represents a specific transient, including the start date, transient number, run type, and purpose. The experiments range from initial critical runs to more complex activities like heat balance and rod worth measurements. The data reflects the progress and safety measures taken to ensure stable and reliable operation.
**HTTR Heat Transfer**

**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

z = 161.92 cm

200 5750 11300

Power Density (W/cm^3)

0 1.75e+14 3.5e+14

Flux Group 12 (cm^-2 s^-1)
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