INL/MIS-15-36200

Status Update: TREAT Modeling and Simulation Capability Development

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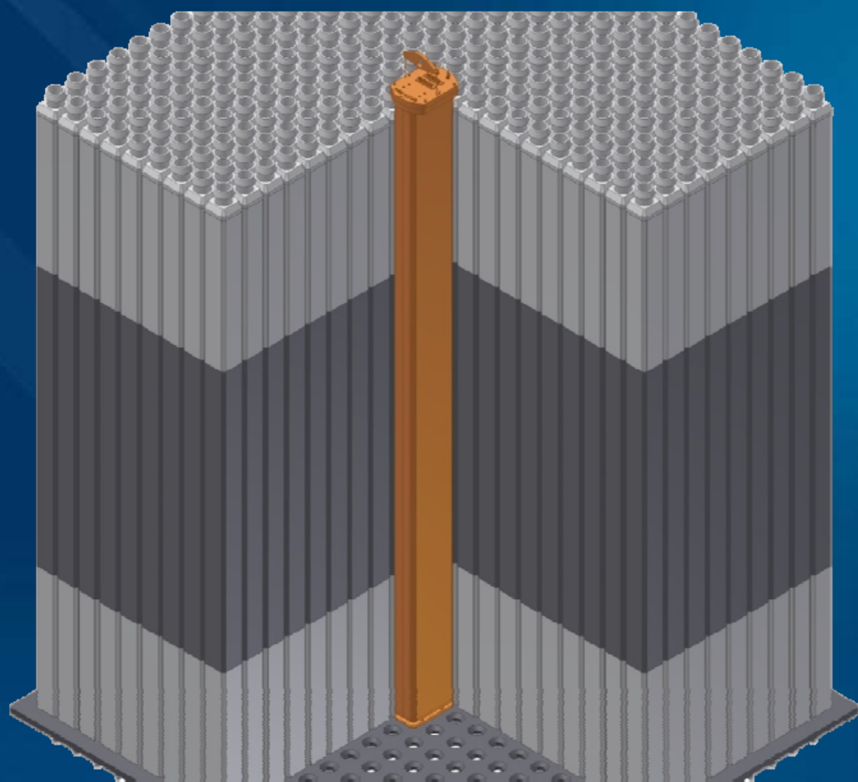
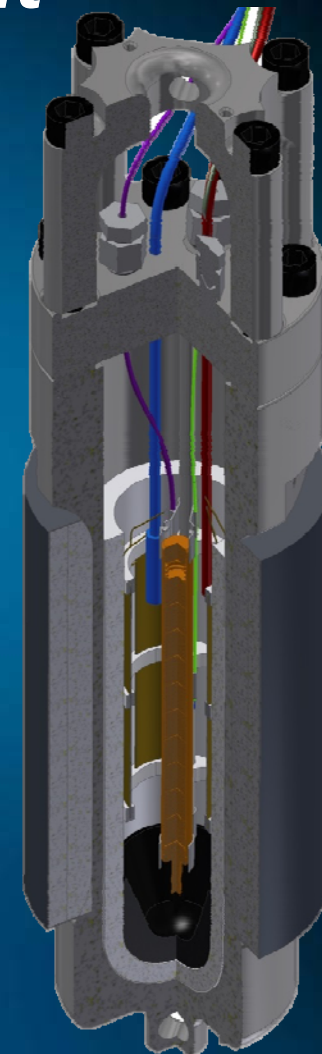




TREAT and Temperature Feedback

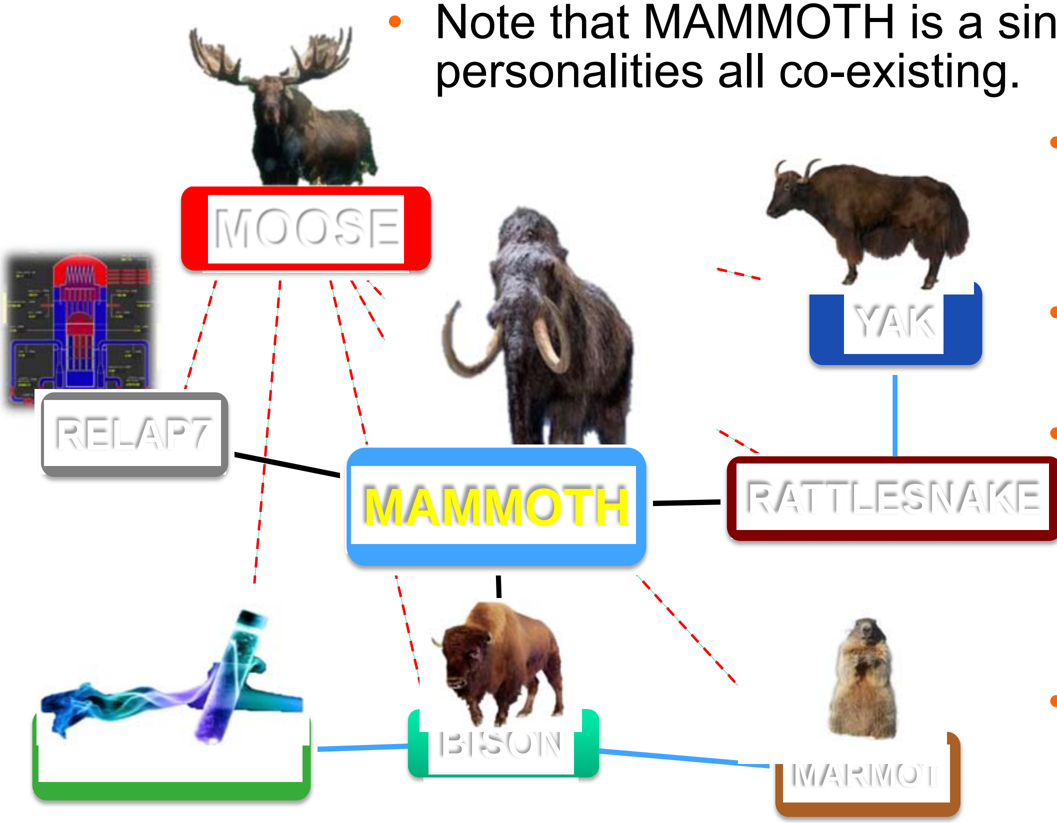
- There is strong nonlinear coupling between the thermal feedback and the neutron radiation field distribution in TREAT.

$$\begin{tikzcd} \phi(r,E,t) \arrow[r] & T(r,\phi,t) \arrow[r] & \sigma(r,E,t) \arrow[ll, bend left] \end{tikzcd}$$

- The best current practice is to apply a split operator approach the radiation transport equations and the heat transport equations. As part of TREAT LEU conversion design, ANL is currently performing TREAT analysis with MCNP and a point kinetics solution with very coarse meshing (9 temperature regions in the core).
- This will result in a reduction of accuracy and is not unlike analysis methods performed in the early 90's. This required numerous calibration transients prior to initiating an experiment series
- Experience to date indicates that the evolution of T as a function of time is a nonlinear function due to temperature dependent thermal properties of graphite.
- Poor characterization of core power transients will lead to the inability to accurately quantify fuel behavior.

Modeling TREAT with MAMMOTH

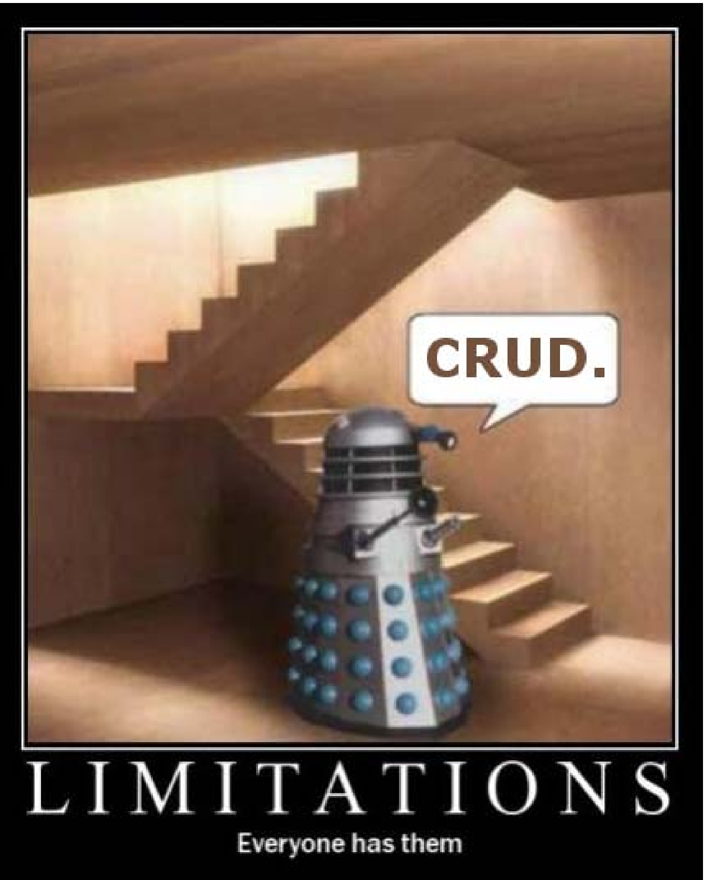
- MAMMOTH has been built using the MOOSE framework (Multi-physics Object Oriented Simulation Environment)
- MOOSE allows implicit, strong, and loose coupling of MOOSE animal solutions
- MAMMOTH is the MOOSE-based multi-physics reactor analysis tool.
  - Note that MAMMOTH is a single executable code with multiple personalities all co-existing.



- All codes are based on FEM – MOOSE routines perform all solutions.
- All data from all codes are available to the solver(s) used.
- At present, TREAT <u>core</u> simulation efforts rely on BISON (fuel performance), Rattlesnake (time-dependent neutron transport) and MAMMOTH.
- LWR-type pin experiments are being evaluated using RELAP-7 as well in a parallel effort.

TREAT Modeling and Simulation (M&S)

- Unfortunately, advanced modeling and simulation isn't.
- Based on an advanced concept, the process to adapt that concept to a complex real-world problem requires time in terms of effort and testing.



- The desired outcome of MAMMOTH M&S will be to simulate the complex interactions occurring in a TREAT experiment, driven by the coupled physics of a temperature-limited or controlled transient.
- The first phase of this approach has been to develop the core transient simulation capability that couples Rattlesnake, BISON, and cross section generation.
- A parallel, independent effort studied burnup of fuel pins during a reactor cycle, followed by a rapid transient.
- For the remainder of this talk I'll focus on the former, **simpler** analysis.

The Simple Form of TREAT Core Transient M&S

$$\nabla\cdot\mathbf{\Omega}\Phi(\mathbf{r},E,\mathbf{\Omega},t)+\Sigma_t(\mathbf{r},E,T)\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$

$$-\iint\Sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega},T)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)dE'd\mathbf{\Omega}'$$

$$-\chi_p(\mathbf{r},E)(1-\beta)\iint\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E',T)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\,dE'\,d\mathbf{\Omega}'$$

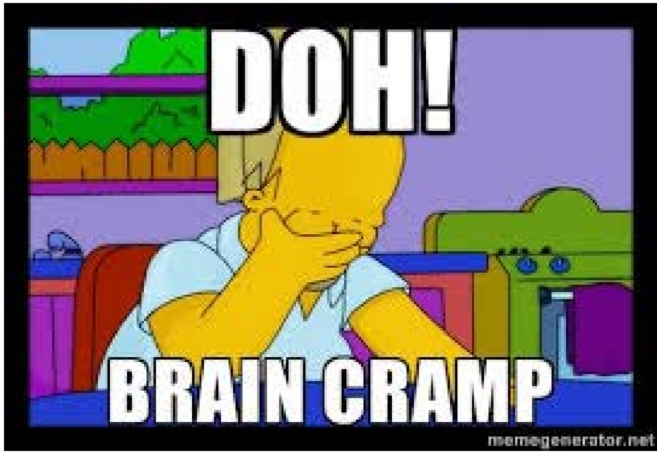
$$-S(\mathbf{r},E,\mathbf{\Omega},t)-\sum_i\lambda_iC_i(\mathbf{r},t)\chi_i(\mathbf{r},E)=-\frac{1}{\upsilon(E)}\frac{\partial}{\partial t}\Phi(\mathbf{r},E,\mathbf{\Omega},t)$$

$$\frac{\partial}{\partial t}C_i(\mathbf{r},t)=\iint\nu(\mathbf{r},E')\beta_i\Sigma_f(\mathbf{r},E',T)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\,dE'\,d\mathbf{\Omega}'$$

$$-\lambda_iC_i(\mathbf{r},t)\qquad i=1,N$$

$$\rho(\mathbf{r},T)c_p(\mathbf{r},T)\frac{\partial T}{\partial t}=\nabla\cdot(k(\mathbf{r},T)\nabla T)$$

$$+E_f\iint\nu(\mathbf{r},E')\Sigma_f(\mathbf{r},E',T)\Phi(\mathbf{r},E',\mathbf{\Omega}',t)\,dE'\,d\mathbf{\Omega}'$$



The Magic of MOOSE

- MOOSE itself "simply" takes these equations and automatically expands them into the corresponding set(s) of finite element equations for user-specified mesh(es).
- These equations are all interdependent and can potentially result in a very large matrix, but but one that will yield a fully implicit solution.
- The Jacobian-free Newton Krylov method is generally used for solving the coupled equations – such matrices are too large to invert.
- Individual "physics" can be solved independently if desired (JFNK or other), then iterations performed between the two solutions until both converge (tight coupling)
- JFNK provides an extremely robust solution method for stiff, highly nonlinear, and tightly coupled problems
  - Provides the convergence of Newton's method without the need to form a Jacobian (saves time and memory)
  - Directly supports advanced preconditioning strategies (physics-based and multilevel)
  - Implicit method is unconditionally stable
- JFNK solvers are readily available in PETSc
- PETSc is incorporated into MOOSE and all of its solution methods are available. In fact, PETSc provides <u>all</u> solvers used in MOOSE

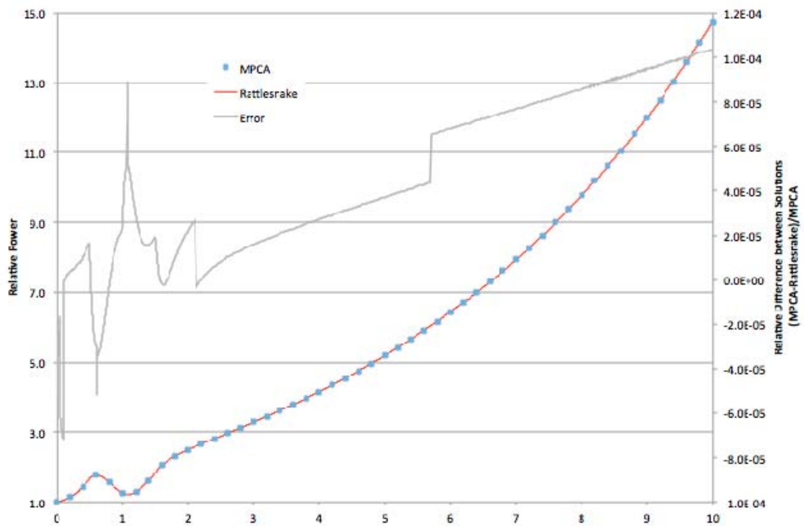
TREAT Research Supporting MAMMOTH M&S

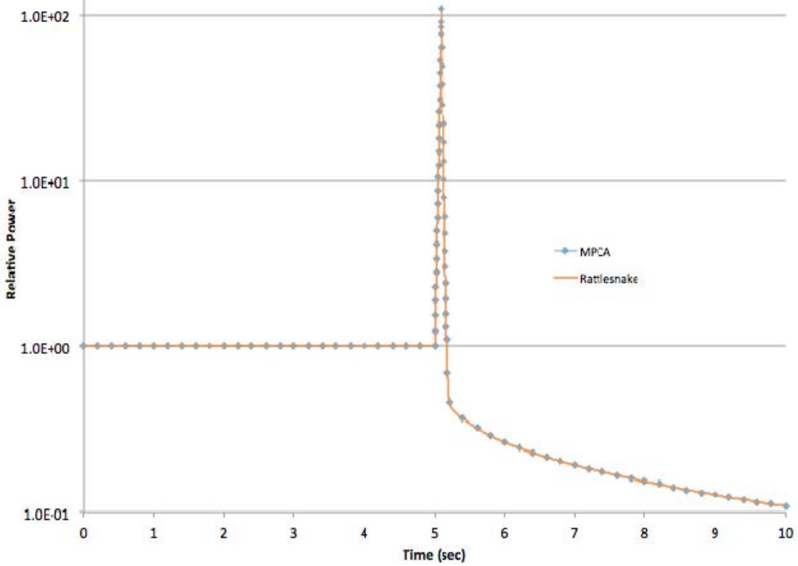
- NEAMS
  - INL (MAMMOTH)
  - MIT (Monte Carl cross sections,)
  - UF (Independent validation using Monte Carlo IQS)
  - TAMU (IQS in Rattlesnake, streaming treatment, transport improvement, cross sections)
  - UAz (Independent validation of Rattlesnake kinetics using PKE)
- INL LDRD (National University Consortium)
  - OrSU (Meshing, validation, depletion methods)
  - UNM (Validation of RELAP-7 for TREAT-type simulations)
  - MIT (Spatial functional expansion tallies)
  - NCSU (Graphite evaluations for mixed graphite/carbon)
- NEUP
  - NCSU (M2/M3 core benchmarks with MAMMOTH)
- TREAT Restart
  - OSU (correction for grain effects in graphite media)
- Regular communication between M&S teams, Restart, Experiment Design and Operations teams is the key to success.

First Steps

- Core data is not located in a single report, repository or set of drawings; some reports/drawings are inconsistent with other available data.
  - INL report "Baseline Assessment of TREAT for Modeling and Analysis Needs," by John Bess and Mark DeHart, INL/EXT-15-35372, was released this month.
  - ~500 pages of measurements, specifications, updated (redrawn) drawings and illustrations
- Cross section evaluations showed that due to the mfp of neutrons in graphite, reflectors regions and control rods must be taken into account in generating fuel cross sections (and vice versa). Cross section generation requires three dimensional flux solutions.
- Infinite media fuel calculations were performed to ensure that S_n, P_n and diffusion cross sections were being generated consistently.
- Development of void treatment for 2nd order S_n, development of 1st order S_n solver.
- Homogenization and streaming effects, SPH treatment
- The space-time transport solution was compared to an equivalent point kinetics solution for simple and increasingly complex transients

Comparison to PKE (MPCA, Ganapol)

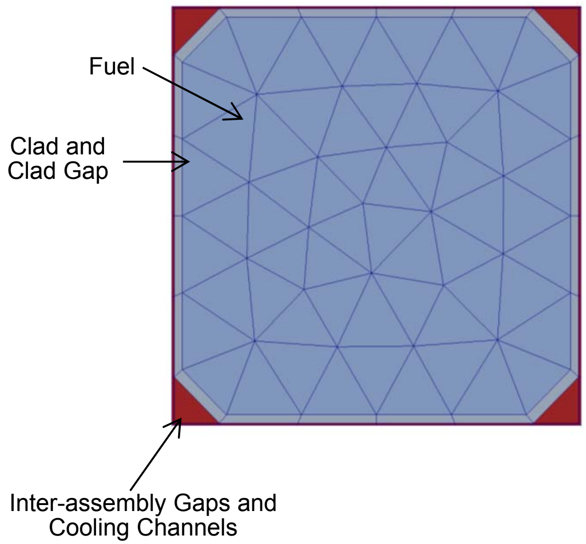




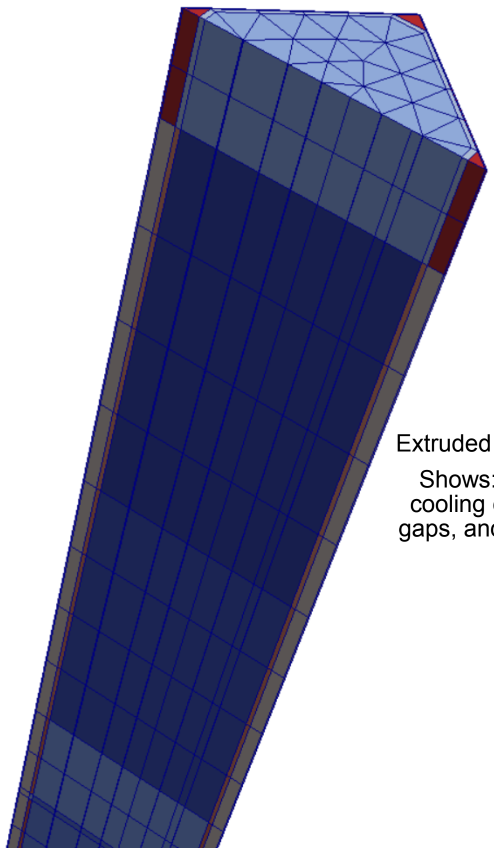
- Zig-zag (alternating reactivity)
  - +$1/s for 0.5s
  - −$1/s for 0.5s
  - +$1/s for 0.5s
  - Then held at $0.5
- Spiked reactivity
  - +$5 at 5.0s
  - −$10 at 5.01s

Model Development

- First developed a rough model of a single element and used for infinite lattice calculations



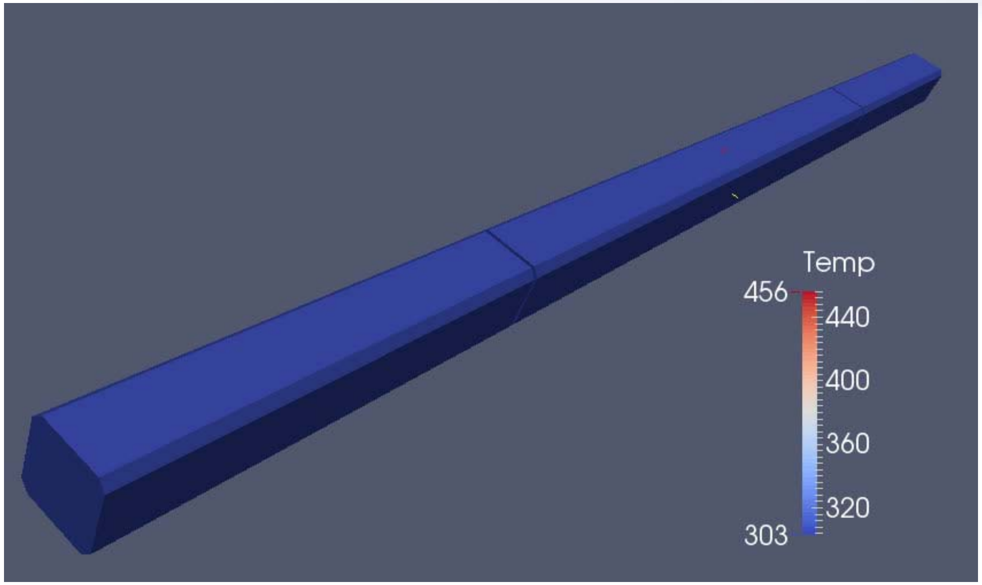
- Used to study modeling parameters
  - Mesh convergence
  - Cross sections
  - Homogenization approaches
  - **Streaming effects**
  - Void treatments
  - Comparison to Monte Carlo solutions
- Also used for first coupled calculations

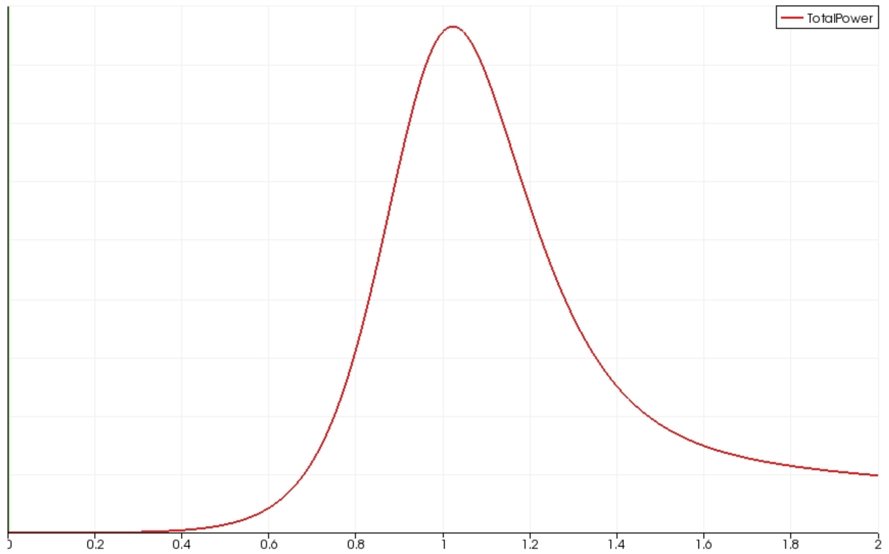


Extruded geometry with 3D mesh:

Shows: - Interassembly gaps, cooling channels, clad and clad gaps, and axial levels of standard assembly

Coupled Physics in MAMMOTH

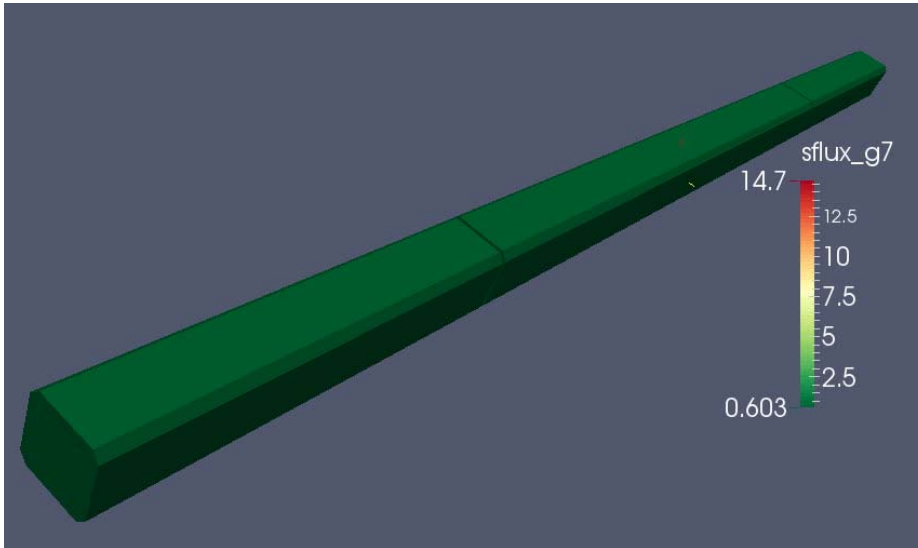




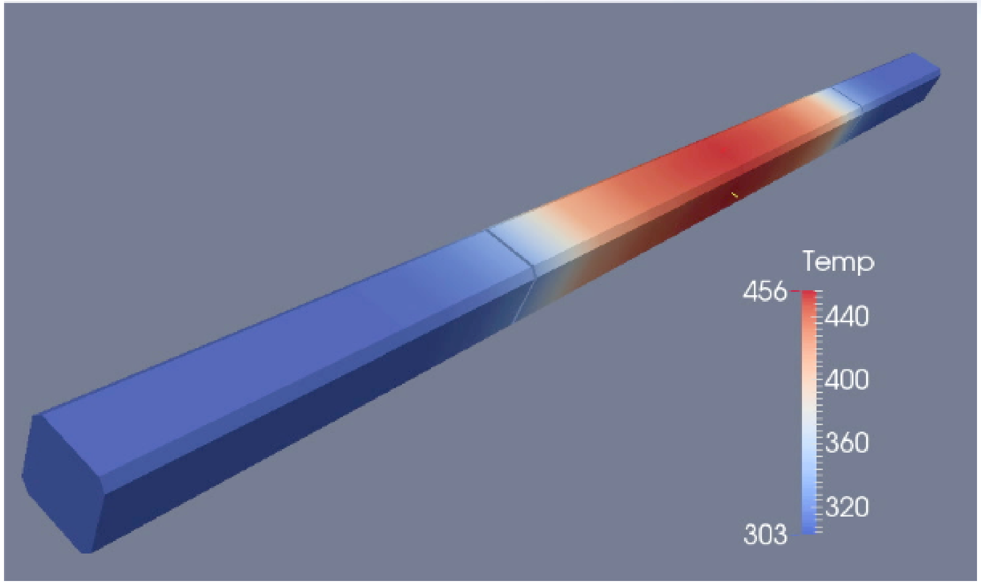
Temperature (K) ↑

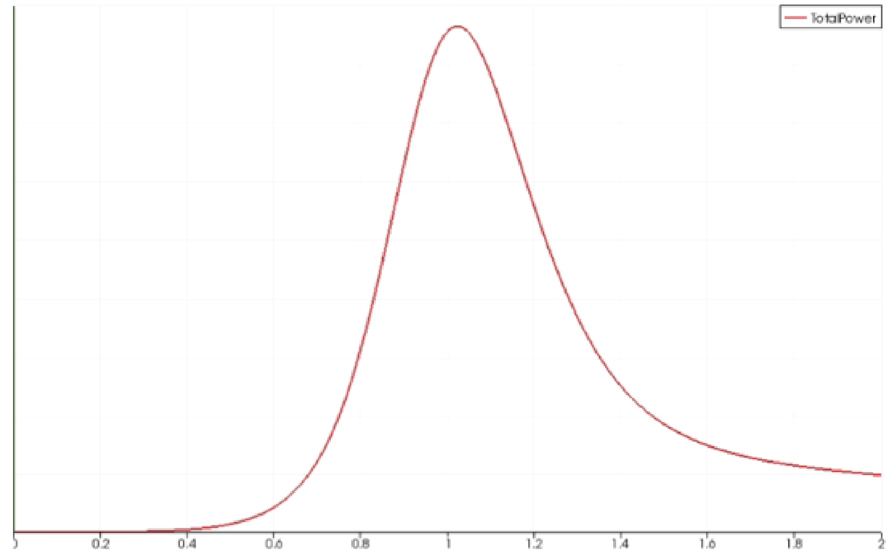
- Reactivity increase (boron removal) between 0.01 and 0.1s
- Reactivity decrease is due to temperature feedback

Thermal Flux ➔



Coupled Physics in MAMMOTH





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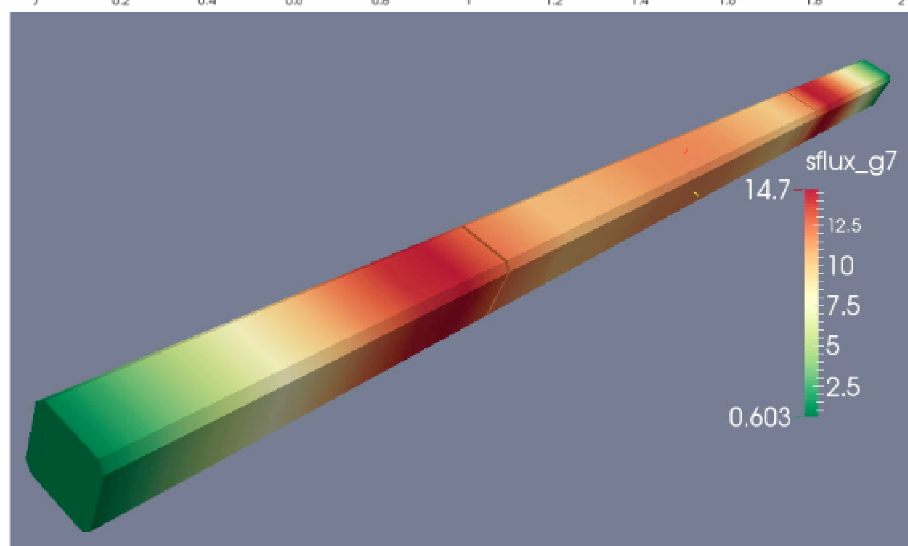


159 Element "Small Core" Configuration

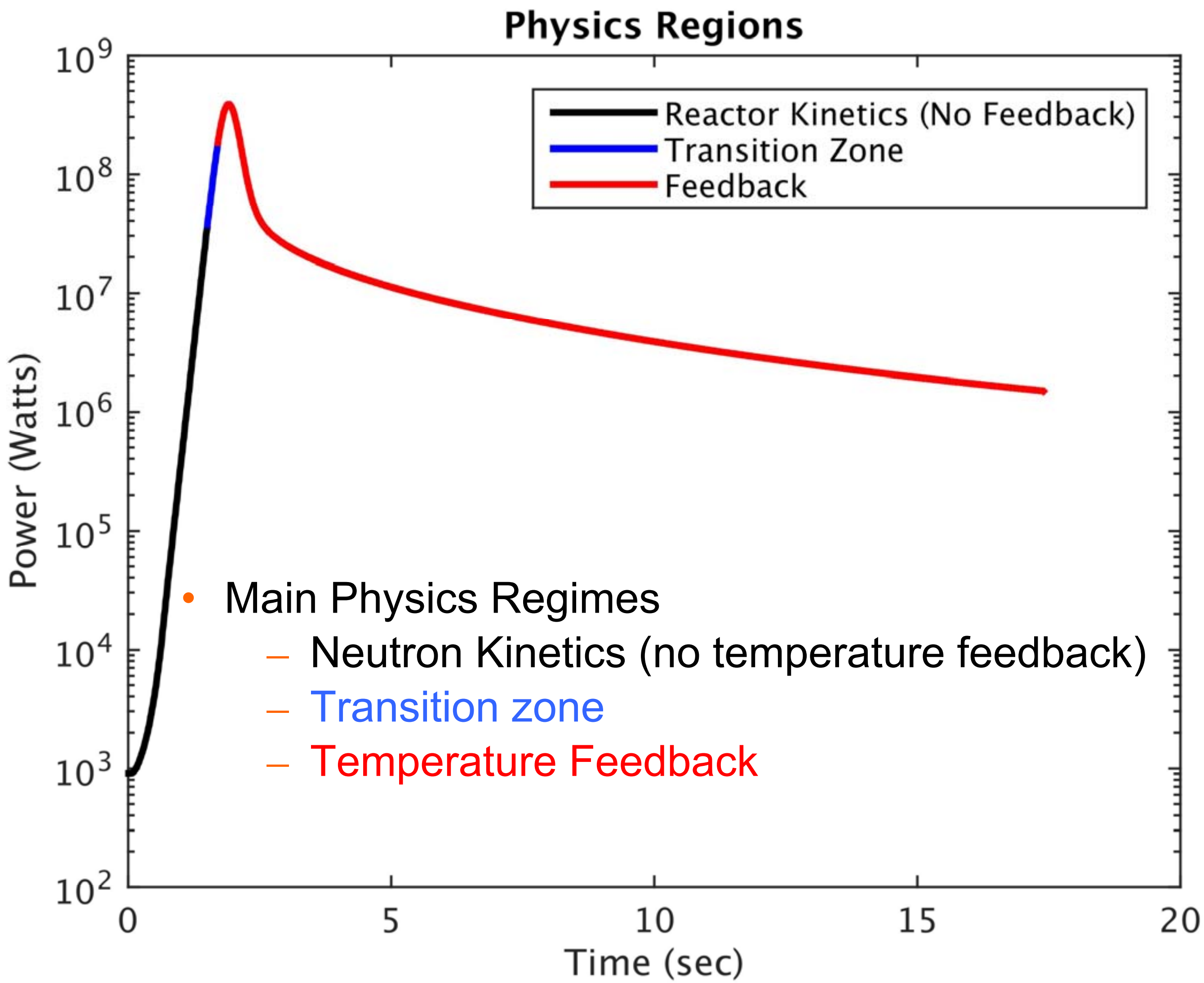
	A	B	C	D	E	F	G	H	J	K	L	M	N	O	P	R	S	T	U
1	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A
2	A	A	A	A	A	A	A	A	Z	Z	Z	A	A	A	A	A	A	A	A
3	A	A	A	A	A	A	Z	Z	F	F	F	Z	Z	A	A	A	Z	A	A
4	A	A	A	A	A	Z	F	F	F	F	F	F	F	Z	Z	A	A	A	A
5	A	A	A	A	Z	F	F	F	F	F	F	F	F	F	F	Z	A	A	A
6	A	A	A	Z	F	F	F	C	F	F	F	C	F	F	F	Z	A	A	A
7	A	A	Z	F	F	F	F	F	F	F	F	F	F	F	F	F	Z	A	A
8	A	A	Z	F	F	C	F	F	F	F	F	F	F	C	F	F	Z	A	A
9	A	Z	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F	Z	A
10	A	Z	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F	Z	A
11	A	Z	F	F	F	F	F	F	F	F	F	F	F	F	F	F	F	Z	A
12	A	A	Z	F	F	C	F	F	F	F	F	F	F	C	F	F	Z	A	A
13	A	A	Z	F	F	F	F	F	F	F	F	F	F	F	F	F	Z	A	A
14	A	A	A	Z	F	F	F	C	F	F	F	C	F	F	F	Z	A	A	A
15	A	A	A	Z	F	F	F	F	F	F	F	F	F	F	Z	A	A	A	A
16	A	A	A	A	Z	Z	F	F	F	F	F	F	F	Z	A	A	A	A	A
17	A	A	A	A	A	A	Z	Z	F	F	F	Z	Z	A	A	A	A	A	A
18	A	A	A	A	A	A	A	A	Z	Z	Z	A	A	A	A	A	A	A	A
19	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A

A	Al-Clad Dummy Assembly
C	Control Rod Fuel Assembly (Short Poison Section)
F	Standard Fuel Assembly
Z	Zr-Clad Dummy Assembly

- Transient Test 15 – 1.55% Δk
- Startup testing 1959-1960

- Advantages
  - Simple core
  - No in-core experiments or slots
  - Detector current data available
- Disadvantages
  - Exact rod movement not known
  - Asymmetric
  - Old instrumentation
- Starting point for transient validation
  - Many parameters & variables must be set within a model in order for the model to perform the same as the real experiment
  - It is nearly <u>impossible to model every detail</u>; the simulation is considered "good enough" if it captures the governing characteristics of the real event

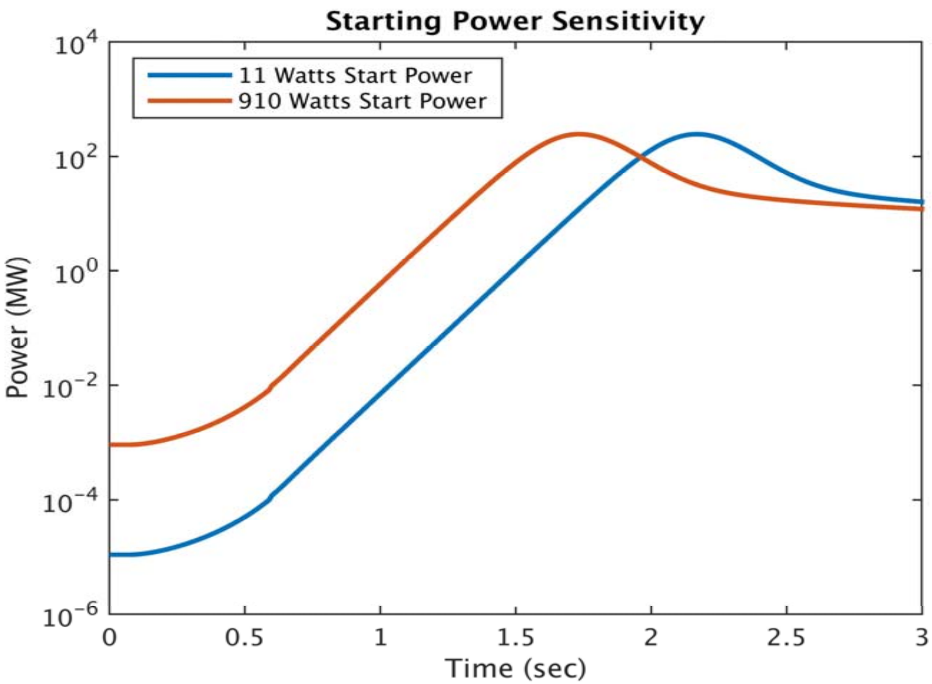
Validation Process



- Main Physics Regimes
  - Neutron Kinetics (no temperature feedback)
  - Transition zone
  - Temperature Feedback

Neutron Kinetics

- Sensitivity tests - Starting power
  - Peak power is fairly insensitive to starting power as long as the starting power is small in comparison with the peak power
    - May affect the ability to measure the asymptotic reactor period because of interference from the transition period
    - There will be shift in time when the peak is reached

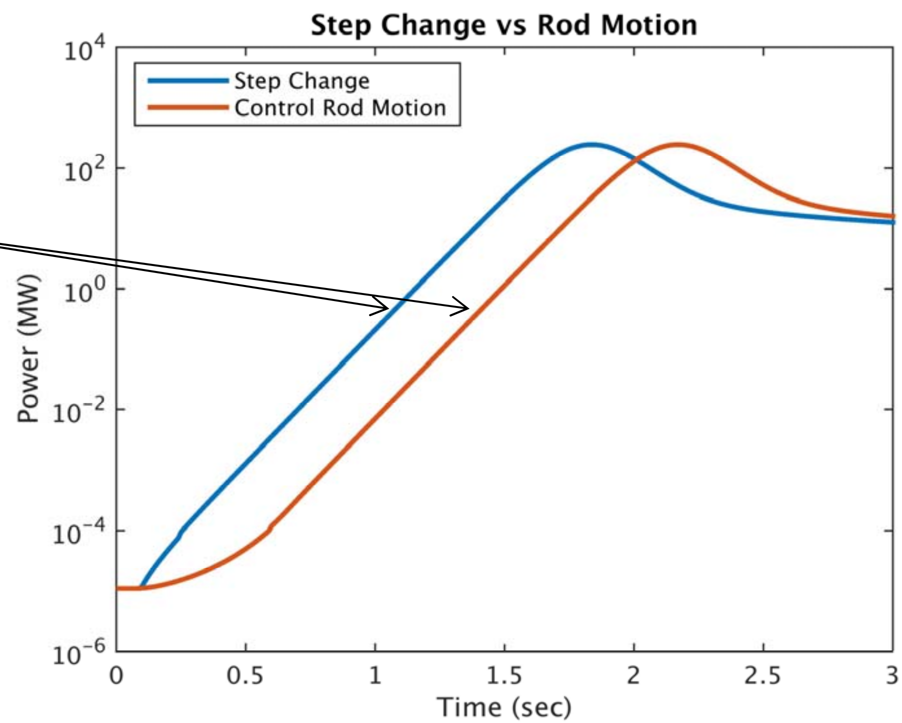


- Discovered Transient 15 could not have started at 11W as stated in ANL-6173. The transient must have started near 910W for the data to have reached the peak power

Neutron Kinetics

- Sensitivities
  - Rod Motion (reactivity as a function of time) vs Step Change in reactivity
    - Can ignore the rod motion as long as long as the rod motion is short before the transition period is reached
    - There will be shift in time when the peak is reached

Asymptotic Reactor Period might not be reached due to feedback

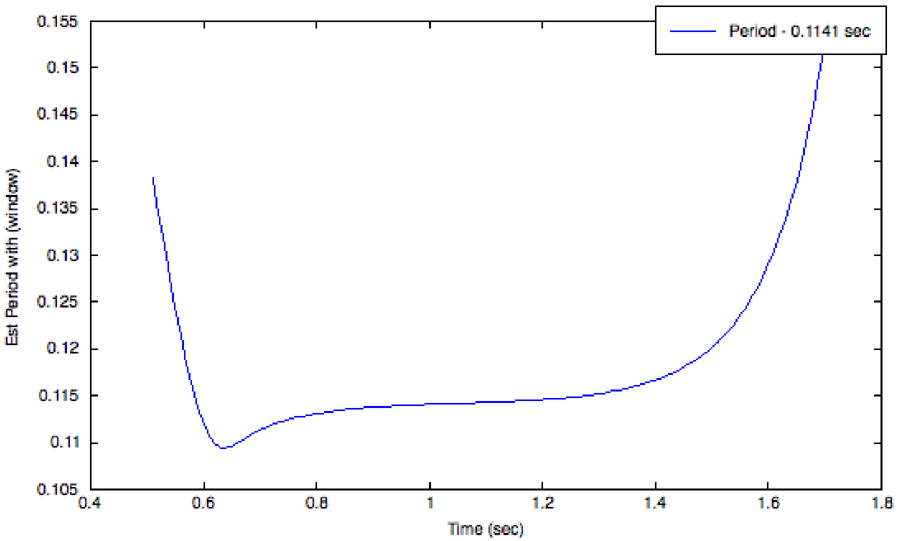


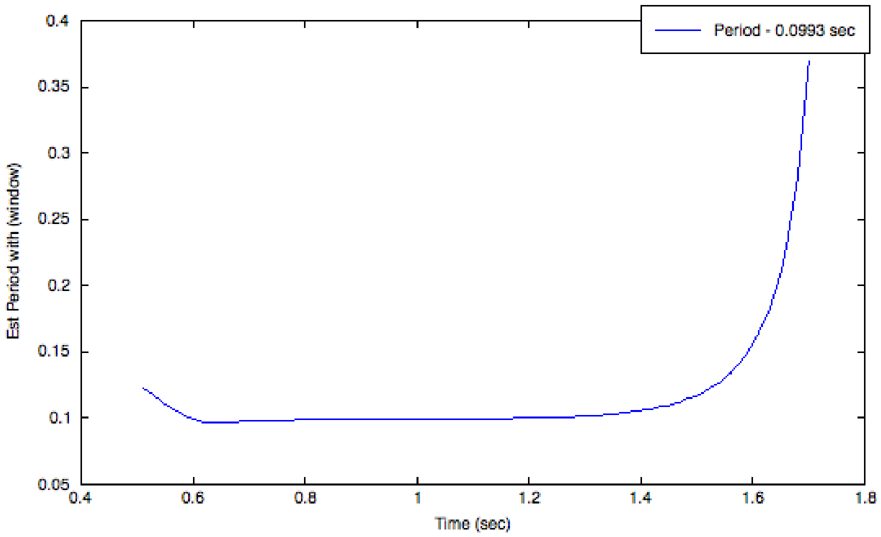
Neutron Kinetics

- Asymptotic Reactor Period Measurement
  - Grows as exp(time/T), T = Asymptotic Reactor Period
  - Most sensitive characteristic of a transient
  - Slight changes in period make large changes
    - For example: T1 = 0.105 sec vs T2 = 0.100 sec
      - Assume the effective transient time is 0.8 sec
      - P2/P1 = exp(0.8/0.1)/exp(0.8/0.105) = 1.46
      - P2 is 46% higher in power level (assuming no feedback)
  - Period is the directly measurable quantity in these experiments*
    - Reactivity is a derived quantity and depends on reactor parameters (e.g., positions of other rods, core configuration)
    - The asymptotic period is a result of the effective reactor parameters but does not depend on them for calculation
    - The chamber current is the direct measurement
      - Power is derived from current
      - Reactivity is derived from portion power history using either the asymptotic period or inverse-kinetics.
      - Asymptotic periods were used in the early transients

Neutron Kinetics

- Complications to Asymptotic Period Measurements
  - Time is required for the asymptotic period to be reached
  - Feedback starts to take effect as the power level increases
    - The power is increasing exponentially
  - A measurement may have contamination from the feedback thus the reactivity value is distorted as well!
  - These plots show the derivative of the power vs time (period) for T=0.1141 (left) and 0.0993 (right)





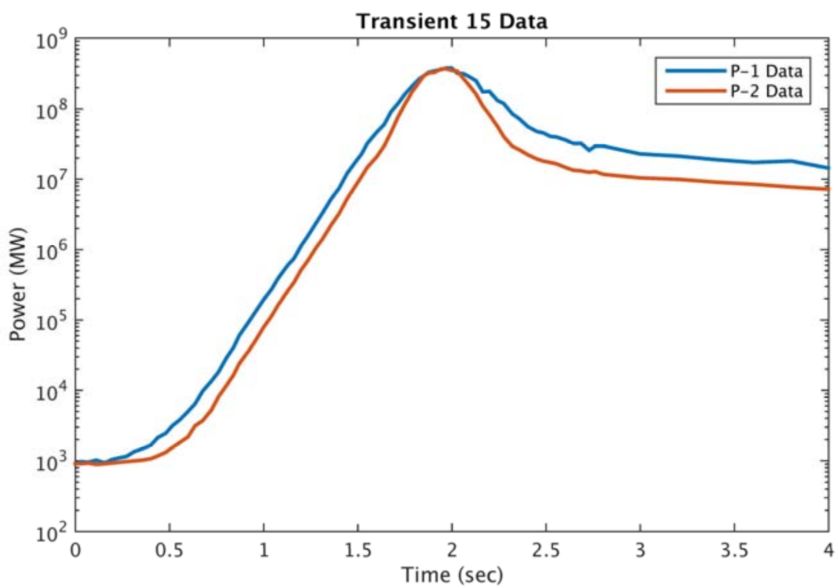
Neutron Kinetics

- For consistency, it is important to perform measurements on the simulation in the same manner as is performed in the real experiment
- Method:
  1. Determine reactor parameters at steady state
  2. Perform Asymptotic Period measurement (we can disable thermal feedback)
  3. Infer reactivity from the period measurement using the In-Hour equation and using the reactor parameters determined at steady state
- Note that there are two forms of the In-Hour equation.
  – They differ by the use of the lifetime and the generation time (up to ~13pcm different for Trans 15). The appropriate choice depends on the application.
  – It is hypothesized that the appropriate equation to use on the transient data should be the lifetime version since generation time changes as k changes and k changes greatly.

MD1

Neutron Kinetics (No Feedback)

- Real Data (And all that comes with it)
  - Transient 15: ANL-6173 Listed period = 0.105 sec and reactivity = 1.55%Δk/k
  - Original chamber current data was re-evaluated to determine appropriate bounds to place on these measurements
    - Period is the measured quantity, not reactivity
    - Chamber P-1 tented towards longer periods while P-2 tended toward shorter periods



Period	Reactivities
0.103 sec (min)	0.01552
0.1075 sec (most probable)	0.01515
0.112 sec (max)	0.01481

MD1 How are min, max calculated - from detector slopes? most probable is the mean?

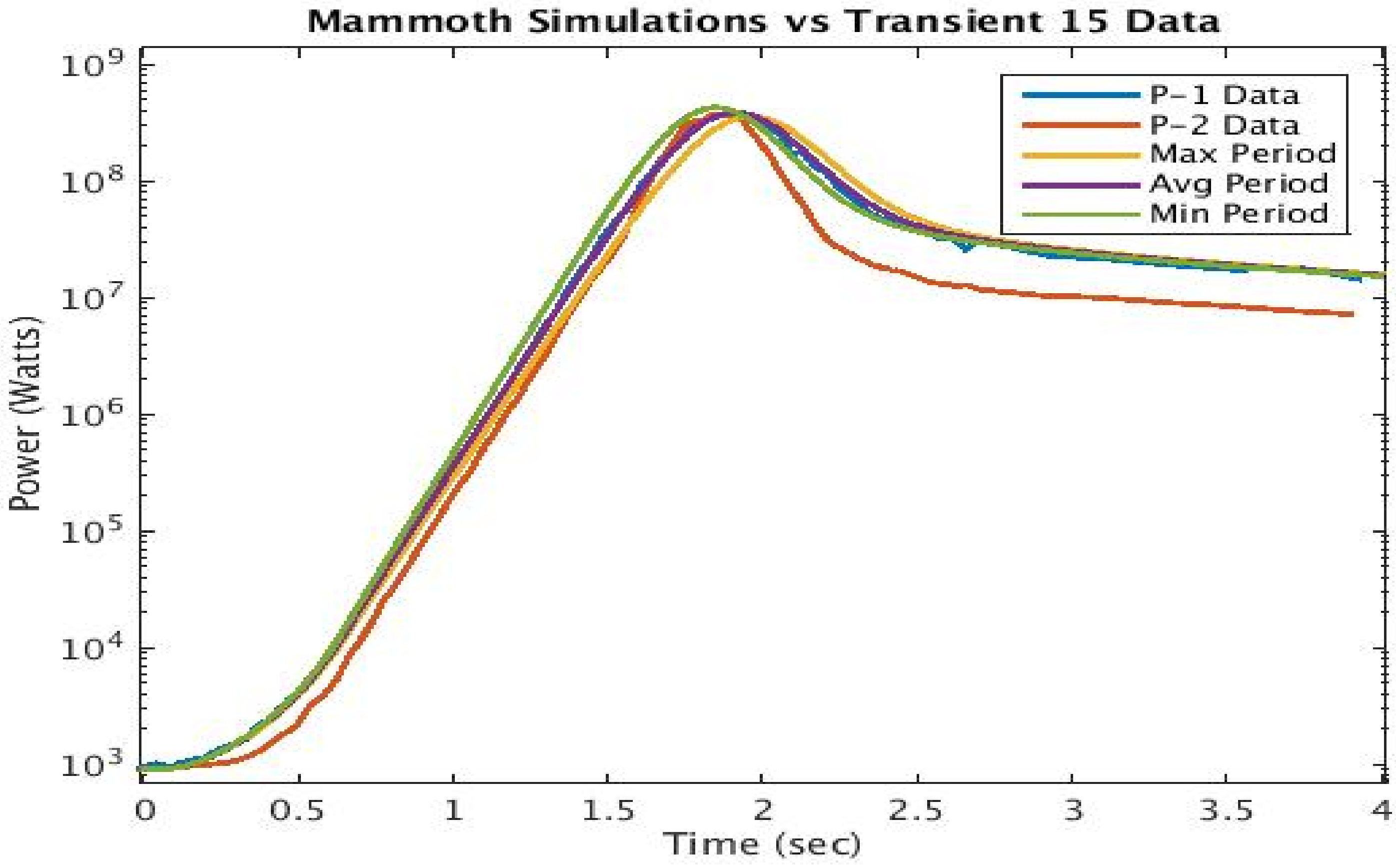
Mark DeHart, 11/18/2015

Feedback

- Feedback is governed by temperature which in turn is governed by the heat deposited in the core (i.e. integral power or energy)
- The relationship between the integral power and the temperature is related by the graphite's ability to hold heat, known as the specific heat (C_p)
- C_p is in of itself a function of temperature
  - Can be described as a polynomial
- To save on computation time the C_p was reduced to a constant
  - An effective C_p was calculated using the point kinetics solver capability in MAMMOTH, which had C_p temperature dependence
    - An effective temperature was determined by:
      - weighting the temperature by the power level at each time step,
      - summing and dividing the sum of the power levels at each step over the peak portion of the transient.
    - The effective temperature was used to select an effective C_p value to use as a first order approximation.

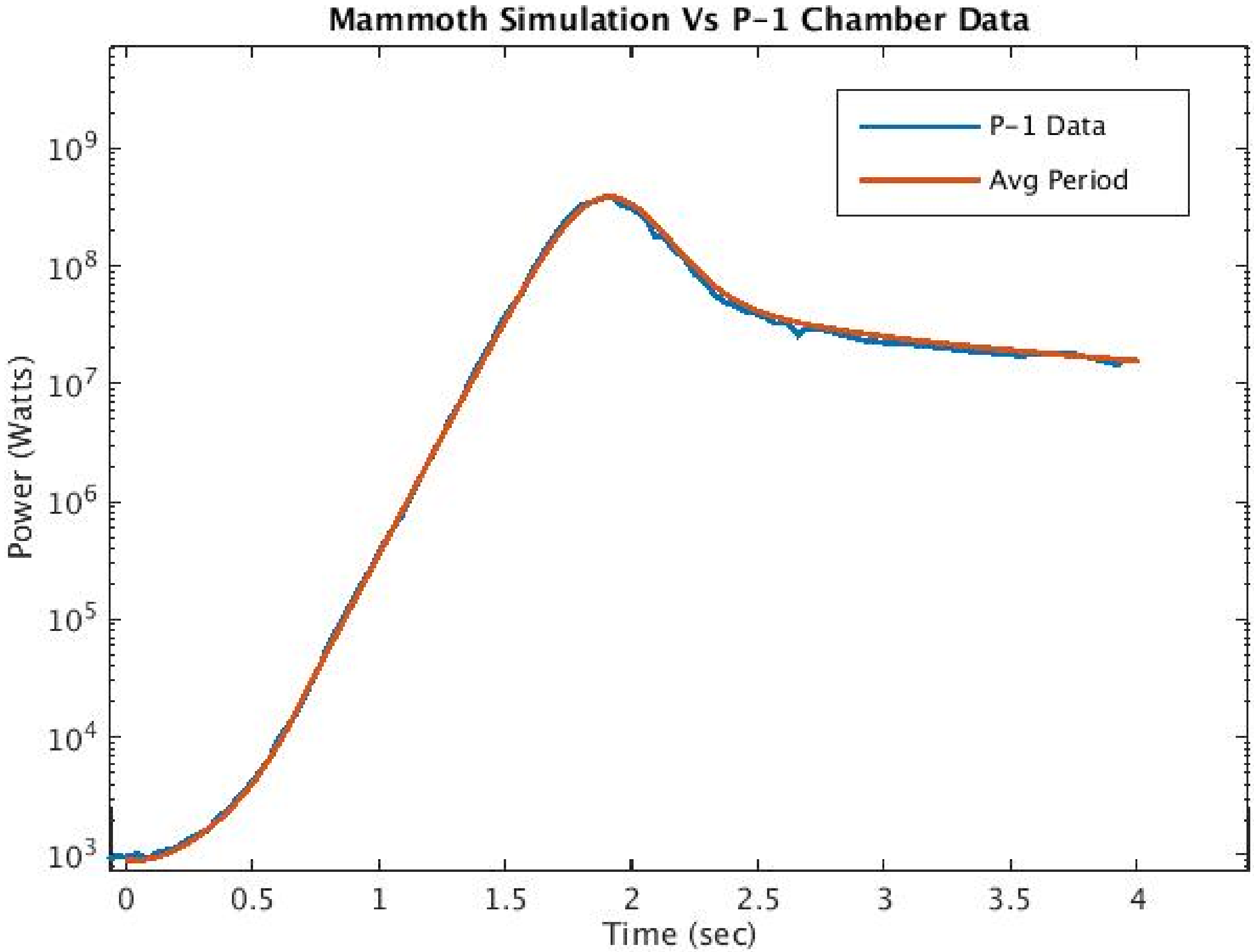
Combine Kinetics and Feedback in Mammoth

- Using the period bounds, effective C_p value and the simple model without any air channels (computationally less expensive)
  - All seem to follow P1 well, P2 has a larger dip (hypothesized that a control rod is in front of it)



Combine Kinetics and Feedback in Mammoth

- P1 Data (shifted in time by 0.07 sec) vs Average Period Result using Mammoth



Combined Kinetics and Feedback in Mammoth

- ANL – 6173 (Trans 15)
- Peak Power = 380MW
- Integral Power = 315 MW-sec or (MJ)
- ΔT at core center = 176 °C (K)
- Note: We have no uncertainties from the data on these values

Period	Peak Power (MW)	Peak Power (% Diff)	Integral Power (MJ)	Integral Power (% Diff)	ΔT max (Kelvin)	ΔT max (% Diff)
Min (0.1033 sec)	425	11.7	291	7.6	180	2.2
Avg (0.1082 sec)	384	1.1	281	10.7	174	1.3
Max (0.1126 sec)	355	6.5	268	14.9	166	5.8

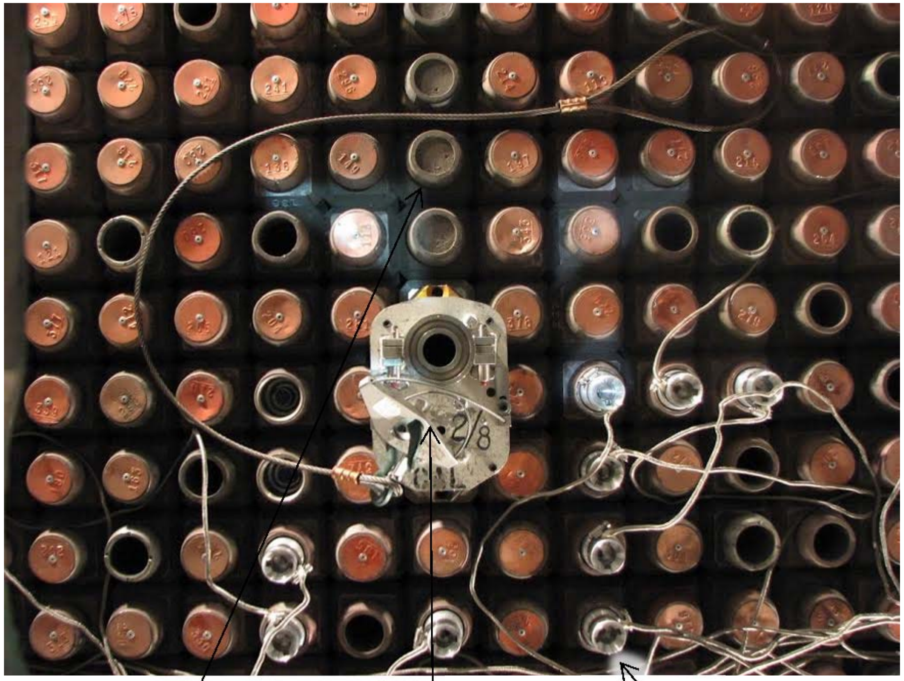
- We expect the results to improve with added complexity to the temperature portion of the model, C_p as a function of temperature

Challenges in Transient Modeling

- The key to obtaining a good transient lies mostly in matching the periods
  - Reported transients reactivity values are a best estimate and can contain contamination from feedback
  - Best practice is to use the measured period as the indicator for the simulation to follow
- Challenge will be in calculation of the true period – this is where uncertainties come in:
  - Boron
  - Graphitization
  - Channel streaming
  - Homogenization
- Thermal feedback will be important in capturing total energy deposition in target(s)
  - ~30% of the integral energy comes after the transient (>2.5sec)
- Although an IQS-based approach is being developed and will be valuable in design, it is not clear if large time steps will be appropriate for fully coupled multi-physics with experiments

Next steps

- Sensitivity analysis for transient calculations (period sensitivity)
- Begin to model more complex configurations with more complete data
- Initiate complete multi-physics modeling of experiments placed in center of the core using MAMMOTH
  - Neutronics
  - Fuels/materials performance
  - Fluids flow



- Continue validation efforts
- Improvements in cross section methods
- Improvements in calculational efficiency
- Begin working more closely with experiment design and core operations staff to begin planning measurements to assist in methods validation.

Questions?

"My presentation lacks power and it has no point.
I assumed the software would take care of that!"