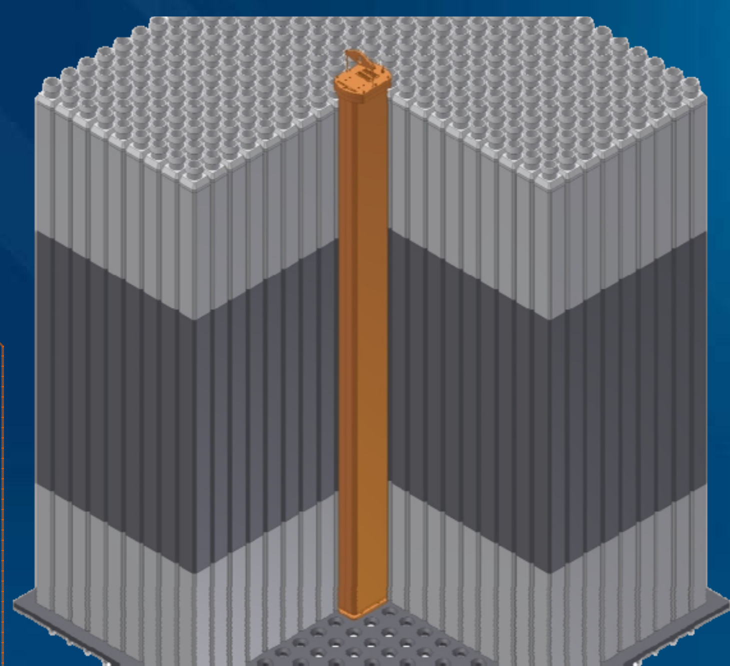
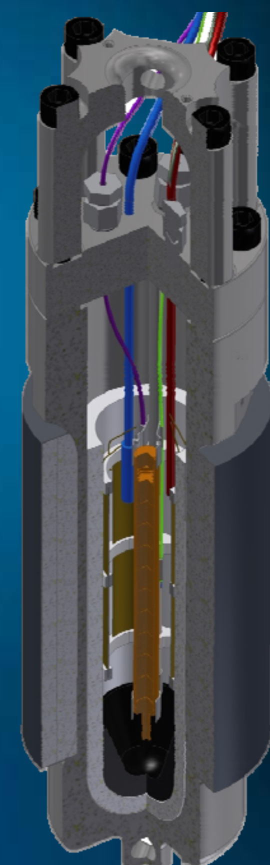
Rattlesnake, MAMMOTH and Research in Support of TREAT Kinetics Calculations

DOE NEUP-IRP Meeting
University of Michigan
May 24, 2016





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TREAT's mission is to deliver transient energy deposition to a target or targets inside experiment rigs.

1.21 Jigawatts

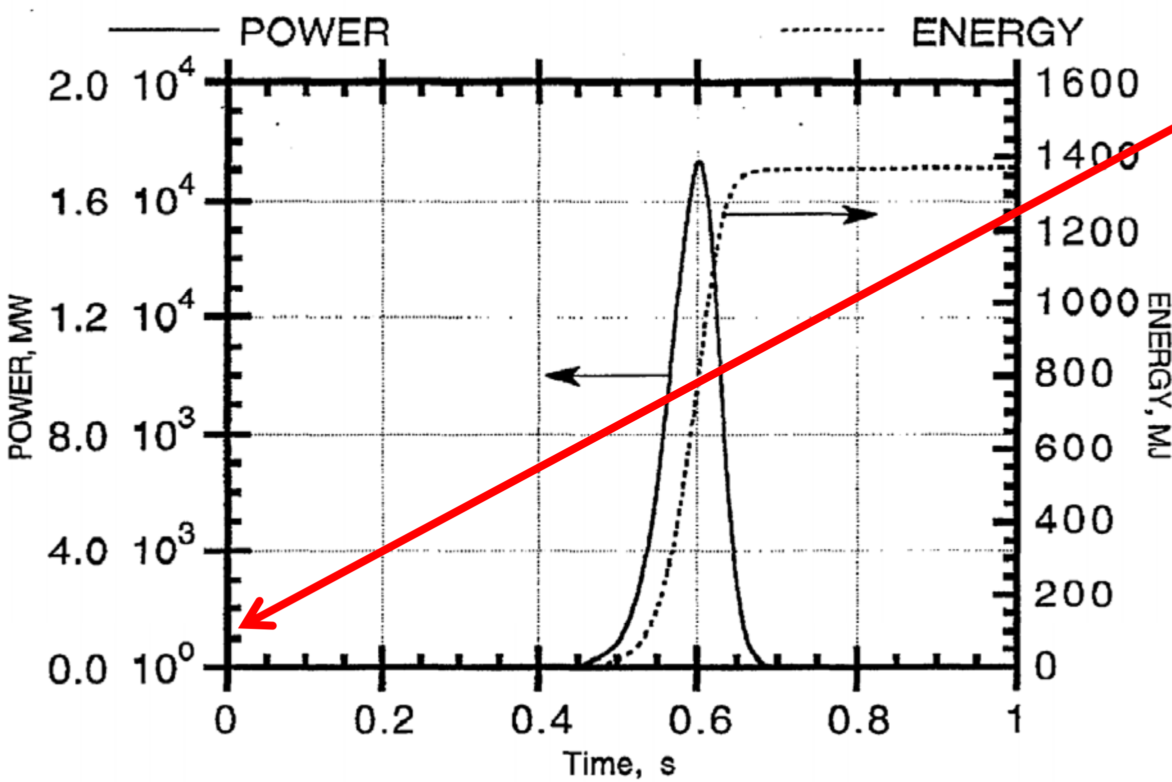

FIG. 5. Plot of TREAT reactor power and energy for hypothetical RIA-type transient resulting in 1400-MJ pulse with a 72-msec FWHM capable of depositing 1200 kJ of energy per kg of fuel (290 cal/g).

TREAT and Temperature Feedback

- Historically, failure conditions were determined by a number of transient experiments.
- In these experiments, very little predictive capability for core performance existed, and experiment models were somewhat limited.
- There is strong nonlinear coupling between the thermal feedback and the neutron radiation field distribution in TREAT.
- The best current practice is to apply a split operator approach the radiation transport equations and the heat transport equations. ANL is currently doing 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 temperature as a function of time and is also 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.
- 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.

- 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 is available to the solver(s) used.
- Nothing like this exists elsewhere – MAMMOTH is <u>earth-shaking</u>.

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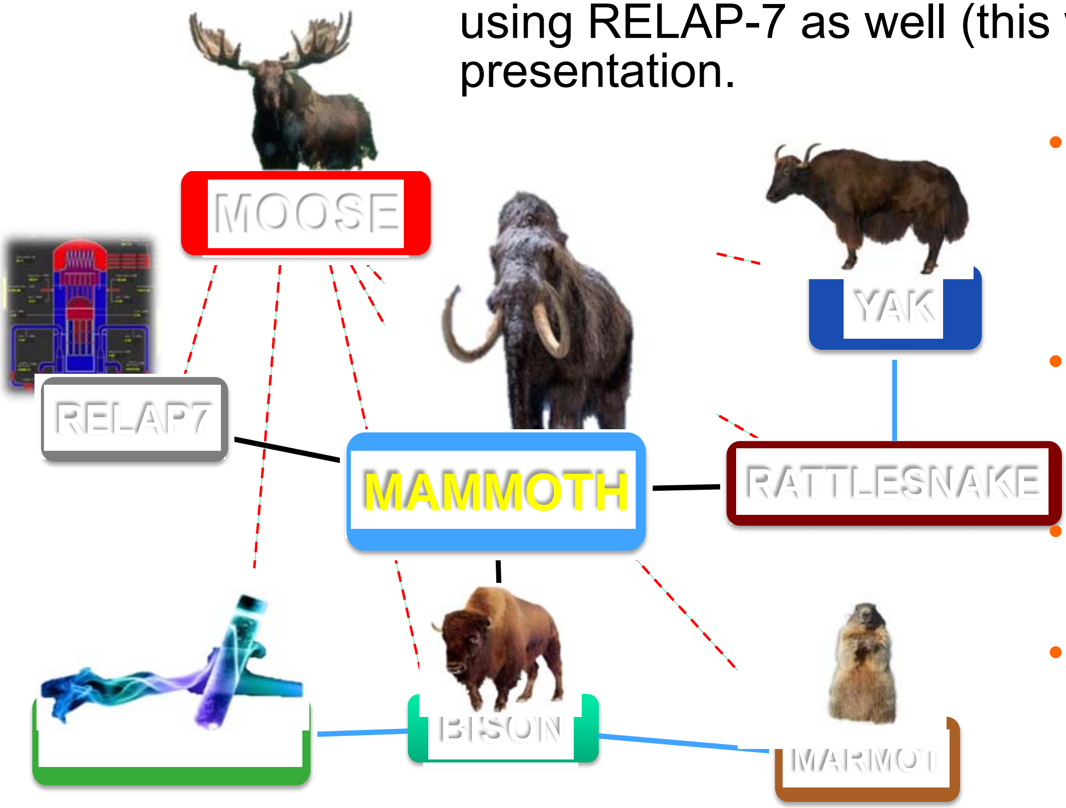
  - MAMMOTH is being evaluated LWR-type pin simulations using RELAP-7 as well (this would be another full presentation.



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- All codes are based on FEM – MOOSE routines perform all solutions.
- All data from all codes is available to the solver(s) used.
- One large matrix can be solved, although for practical applications individual physics are solved with iteration to converge (strong coupling)

The Magic of MOOSE

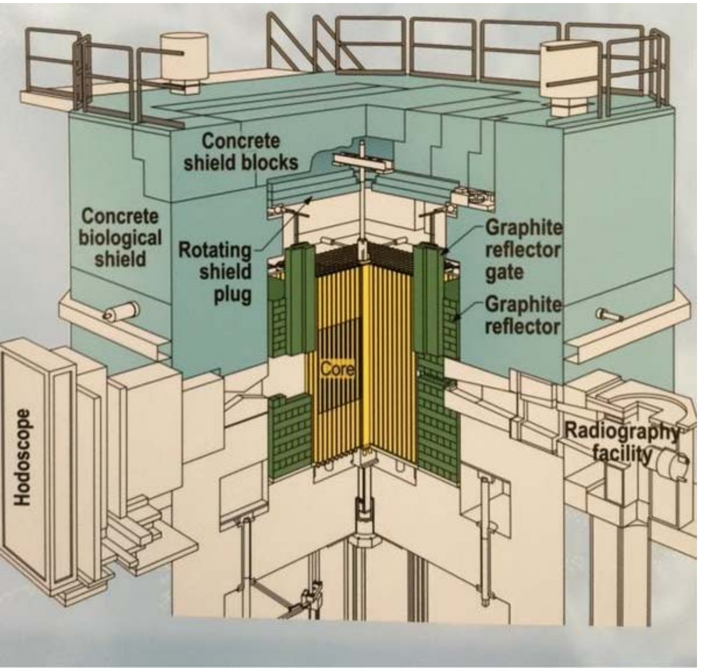
- MOOSE itself “simply” takes these equations and automatically expands them into the corresponding set(s) of finite element equations for user-specified mesh(es).
- These equations are all interdependent and can potentially result in a very large matrix, but but one that will yield a fully implicit 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

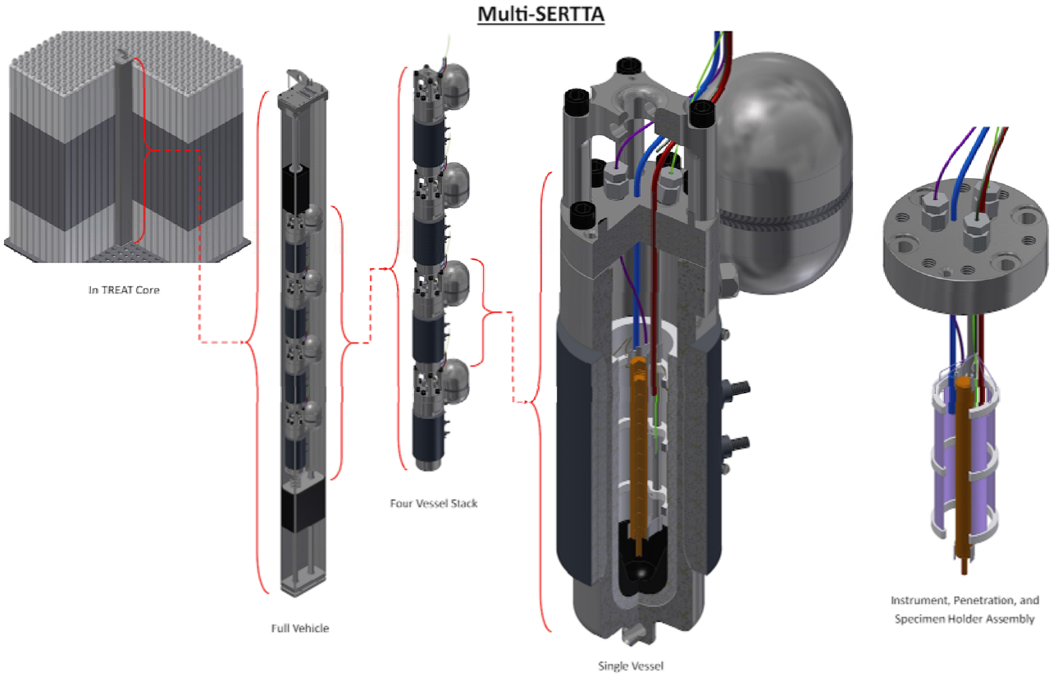
Rattlesnake – MOOSE-based Radiation Transport for Multiphysics Simulations

- **Rattlesnake solves the linear time-dependent Boltzmann equation**
- **It is a finite-element based solver:**
  - *CFEM* (continuous finite element method) and DG-FEM (Discontinuous Galerkin FEM) in space with
    - the *SAAF* (self-adjoint angular flux) formulation
    - the least squares formulation (LS)
    - First order S_N (FiS_N)
  - S_N, P_N or diffusion in space; multigroup in energy; method of lines in time.
- **Designed to support tightly coupled nonlinear multiphysics simulations including the fuel performance analysis.**
- **Built within the MOOSE framework, so it inherits provided by MOOSE:**
  - Various time integration schemes
  - Higher-order unstructured mesh
  - Massive parallelization
  - Mesh adaptability
  - 1D, 2D and 3D, user code agnostic of dimension
  - Flexible built-in postprocessing
  - Regression tests, test coverage report and etc.
  - And much more…

TREAT Modeling and Simulation

- NEAMS Funded ~$2.8M/yr
- No (unclassified) method exists for accurate 3D transient simulations for TREAT
- MAMMOTH focus was originally on modeling the core and matching to existing transient data
- Team is now turning focus on turning the power of MAMMOTH onto the multi-physics analysis of experiment vessels

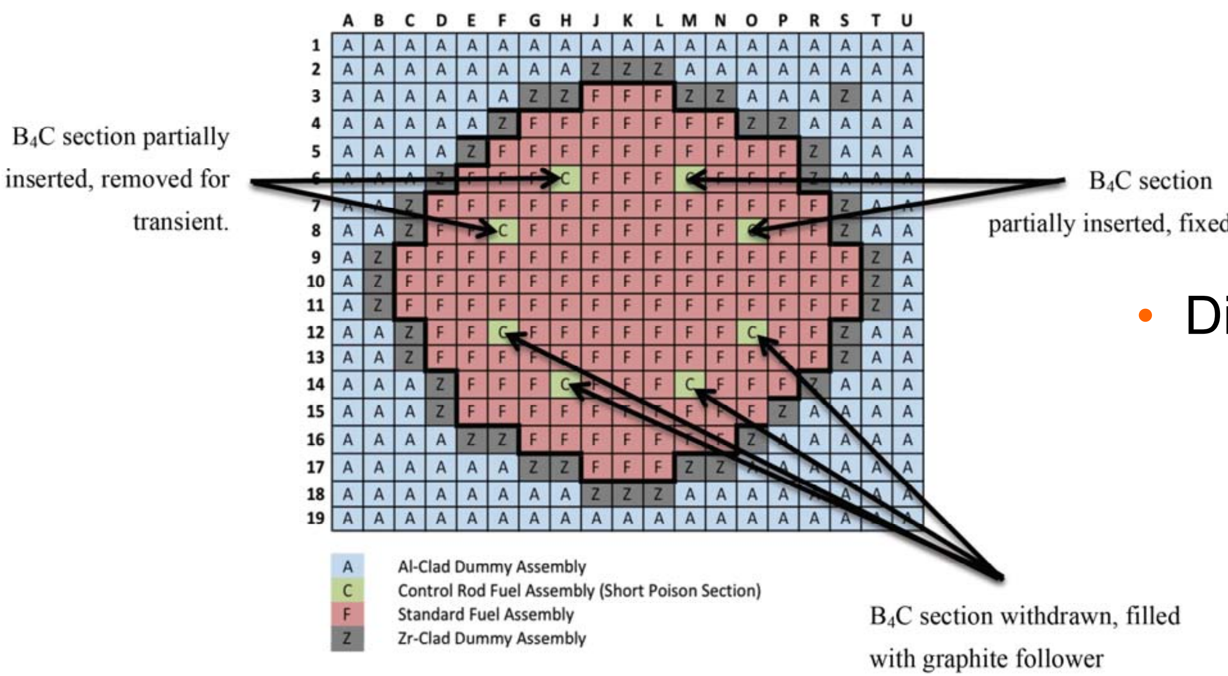




MD1

159 Element “Small Core” Configuration

- Developed solid understanding of modeling issues
  - Infinite media kinetics
  - Infinite lattice eigenvalue and transients
  - Simulation of TREAT Test 15 pre-operation transient testing.



- Advantages
  - Simple core
  - No in-core experiments or slots
  - Detector current data available
- Disadvantages
  - Exact rod movement not known
  - Asymmetric (control rod positioning)
  - Old instrumentation
- Starting point for transient validation

Slide 9

MD1 I don't understand what you are saying in the last bullet, beginning at "...with"

Mark DeHart, 11/18/2015

MD2

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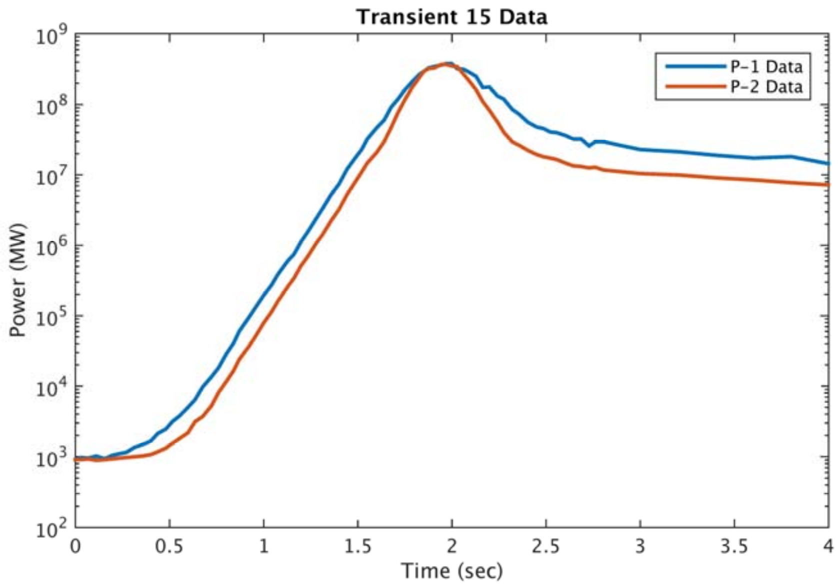
Neutron Kinetics – "Real" data

- Real Data
  - 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

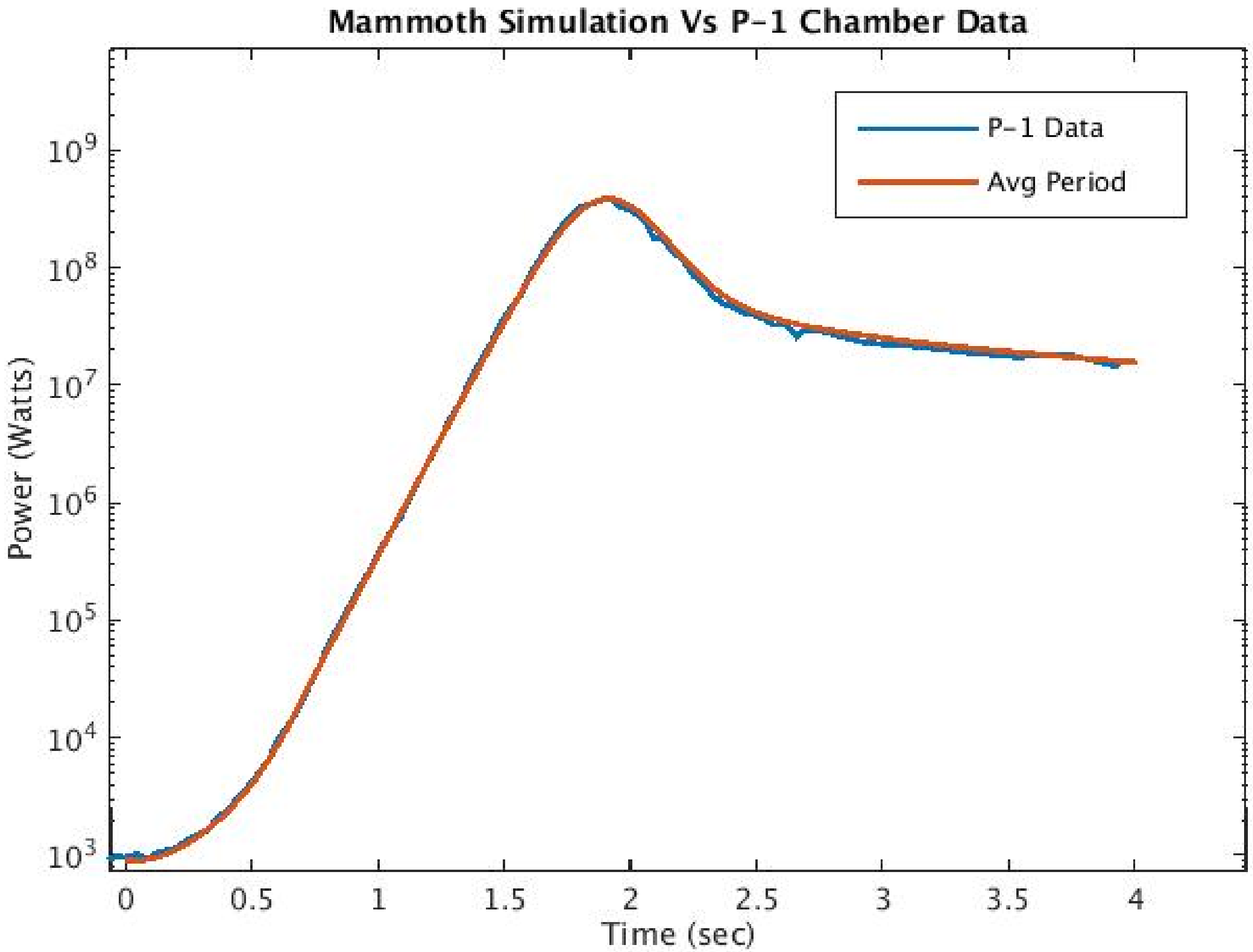
Slide 10

MD2 How are min, max calculated - from detector slopes? most probable is the mean?

Mark DeHart, 11/18/2015

Combined Kinetics and Feedback in Mammoth

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



Combine 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

Superhomogenization (SPH) Technique

- Cross section correction method
- Corrects spatial homogenization errors
- Reproduce the reaction rate and eigenvalue from a reference, heterogeneous problem
- Done with the use of a single new parameter
- First introduced by Kavenoky in 1978
- Generalized by Hébert in the 1980s

SPH procedure

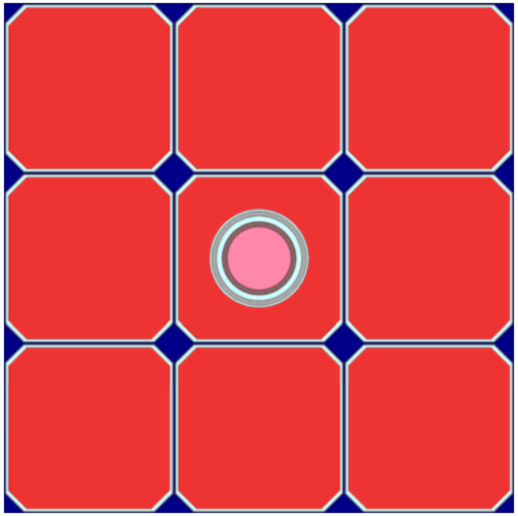
- The SPH problem is a nonlinear problem
- SPH is usually solved with an iterative method, called SPH procedure:

$$-\nabla \cdot \mu_{m,g} D_{m,g} \nabla \phi_{m,g} + \mu_{m,g} \Sigma^{r}_{m,g} \phi_{m,g} = \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \mu_{m,g'} \nu \Sigma_{f_{m,g'}} \phi_{m,g'} + \sum_{g' \neq g}^{G} \mu_{m,g'} \Sigma^{g \leftarrow g'}_{s0_m} \phi_{m,g'} \tag{4}$$

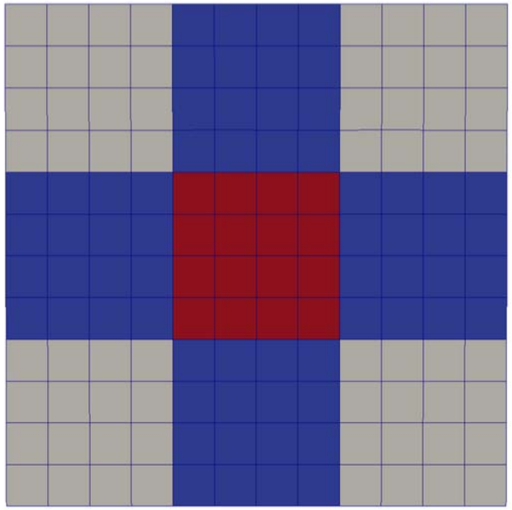
  - Calculate the source terms (right-hand side)
  - Solve for the fluxes
  - Renormalize and calculate the SPH factors
  - Repeat until convergence
- Using MOOSE's PJFNK solver, we are able to solve the nonlinear problem directly.
- Through all transport schemes (diffusion and low order to high order S_N/P_N), we reduce calculation time between factors of 5 to 45.
- Allows us to solve problems that were previously impossible to solve such as reflectors (without special surface corrections) and void boundary conditions.

SPH on a Simplified 3x3 TREAT model

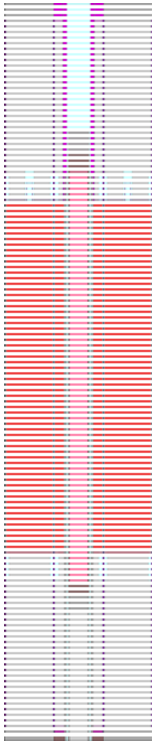
- Tested on a rodded 3x3 supercell with reflectors and vacuum boundary on the z axis. Tested on both 4 and 11 group structure.



X-Y Serpent geometry



X-Y Mammoth geometry



X-Z geometry

Results

Table II. SPH calculations with control rod inserted

Solver	Number of Energy Groups	Free SPH Iterations	CPU time [sec]
SPH iteration	4	-	660.0
PJFNK SPH	4	3	60.7
SPH iteration	11	-	9280.0
PJFNK SPH	11	5	202.9

[1]

- 11 groups do better, but 4 groups still very good

Table III. Diffusion results with 4 coarse energy groups for the 3x3 supercell

Control Rod	SPH	k_{eff} (pcm)	Fission Source Rate [% Difference]	Absorption Rate [% Difference]	Leakage Rate [% Difference]
Withdrawn	No	1.36036 (850.7)	-0.851	-0.418	-25.438
Withdrawn	Yes	1.35276 (287.7)	-0.295	-0.012	-16.307
Inserted	No	0.63081 (-6296.85)	6.029	6.663	-20.174
Inserted	Yes	0.67574 (378.39)	-0.415	-0.093	-13.653

[1]

Table IV. Diffusion results with 11 coarse energy groups for the 3x3 supercell

Control Rod	SPH	k_{eff} (pcm)	Fission Source Rate [% Difference]	Absorption Rate [% Difference]	Leakage Rate [% Difference]
Withdrawn	No	1.36275 (1028.4)	-1.025	-0.494	-31.273
Withdrawn	Yes	1.35278 (289.3)	-0.296	0.006	-17.383
Inserted	No	0.63081 (-6296.85)	7.406	6.708	-22.149
Inserted	Yes	0.67574 (378.39)	-0.062	-0.389	-13.851

[1]

Region Directional Diffusion Coefficients(RDDC)

- Challenge: Define diffusion coefficient in near-void regions for TREAT
- Idea: Use transport method (well-defined in voids) for computing
- Selected Trahan's region-wise DDC

Trahan Diffusion Coefficient

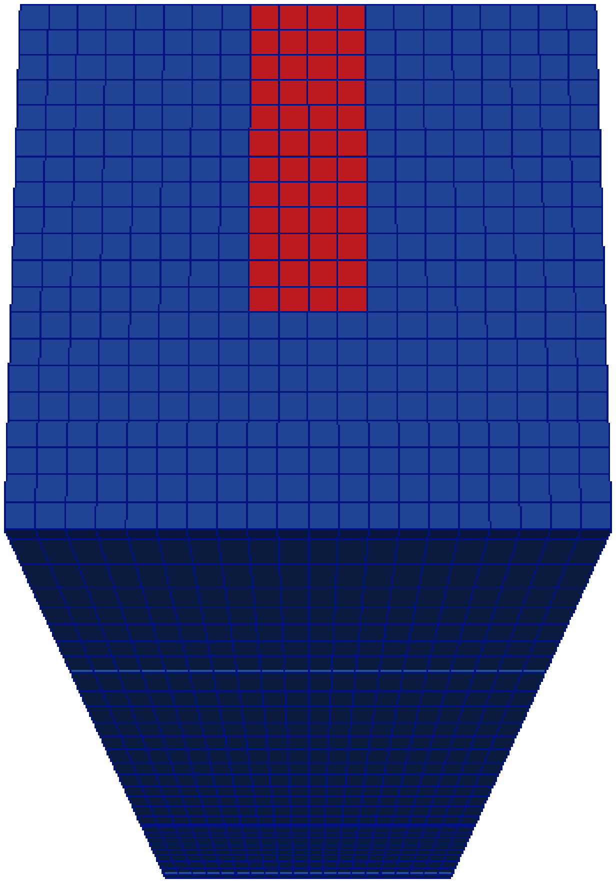
$$\left[\underline{\underline{D}}\right]_{i,j} = \frac{1}{4\pi}\int_{4\pi} d\Omega_i \Omega_j f$$

$$\vec{\Omega}\cdot\nabla f_g + \Sigma_{t,g} f_g\left(r,\vec{\Omega}\right) = 1 \text{ and Refl. BC}$$

- **Benefit:** Efficient & accurate TREAT solution using diffusion solver!
- Proven effective for VHTRs

SPH on a Simplified 5x5 TREAT model with slots

- This 5x5 problem contains 3 slotted assemblies
- It better represents some of the problem areas in the current core configuration
- These create a neutron streaming region in the axial and radial direction
- Directional diffusion coefficient will help improve the power distribution in the calculation



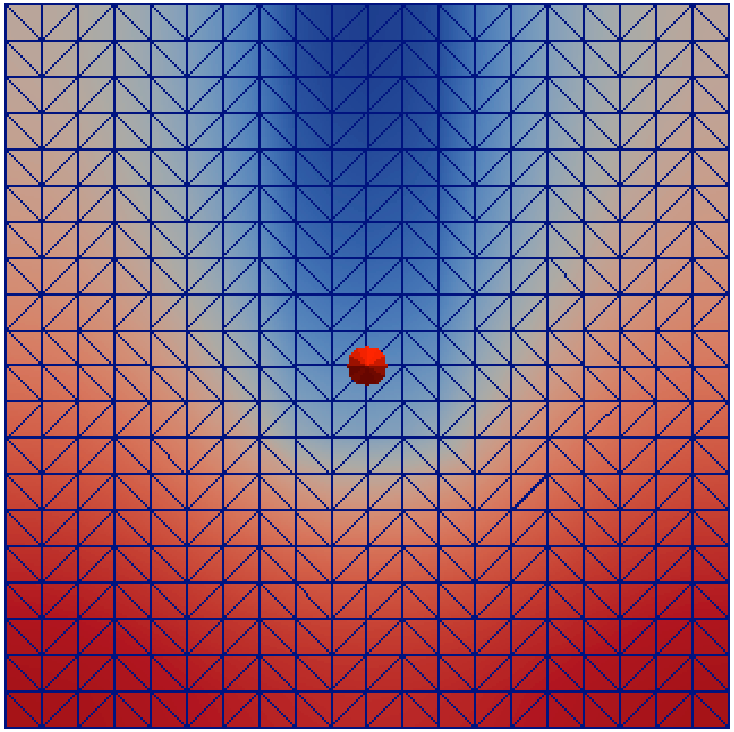
Reference Serpent	1.35115	
Rattlesnake no SPH	1.33685	(-1058.3)
Rattlesnake w SPH	1.35625	(377.5)

5x5 with Slots – Power Distribution

Diffusion no correction
TOTAL RMS 4.521
TOTAL MAX 8.669
TOTAL MIN -5.976

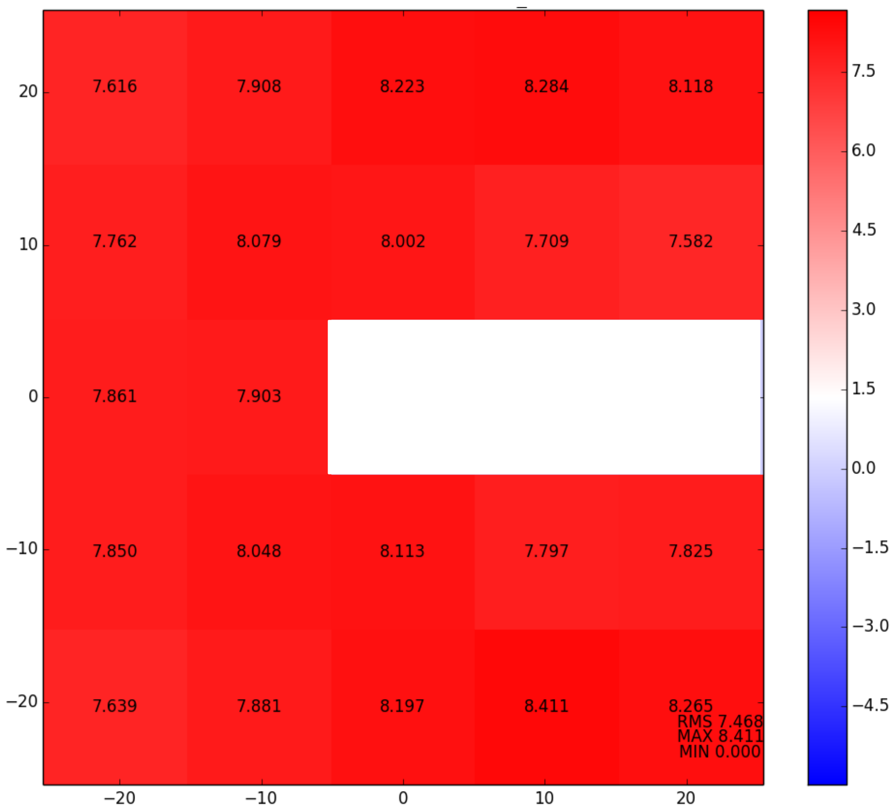
Diffusion SPH correction
TOTAL RMS 1.677
TOTAL MAX 3.338
TOTAL MIN -3.378

Diffusion with DDC and SPH correction
TOTAL RMS 0.730
TOTAL MAX 1.888
TOTAL MIN -2.063

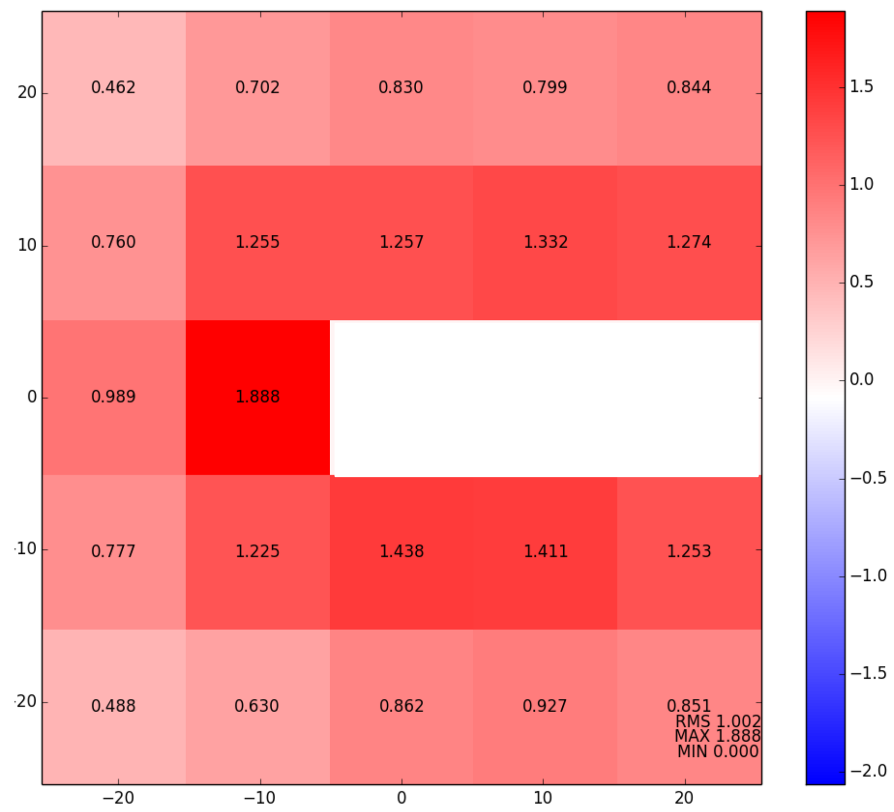


Thermal flux at midpoint

5x5 Midplane with peak % difference in power



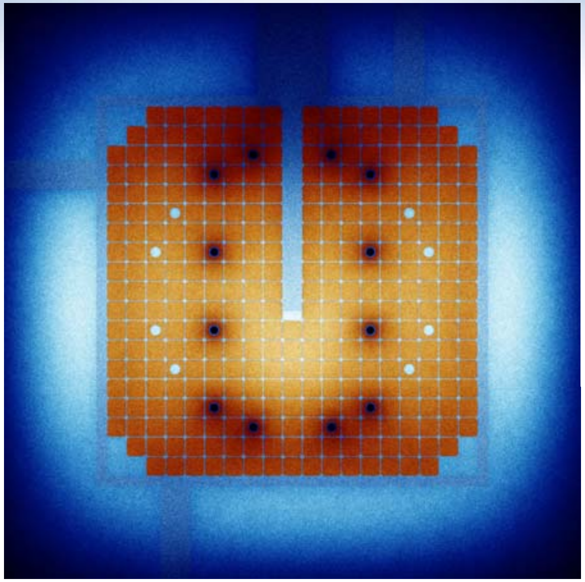
No SPH, no DDC

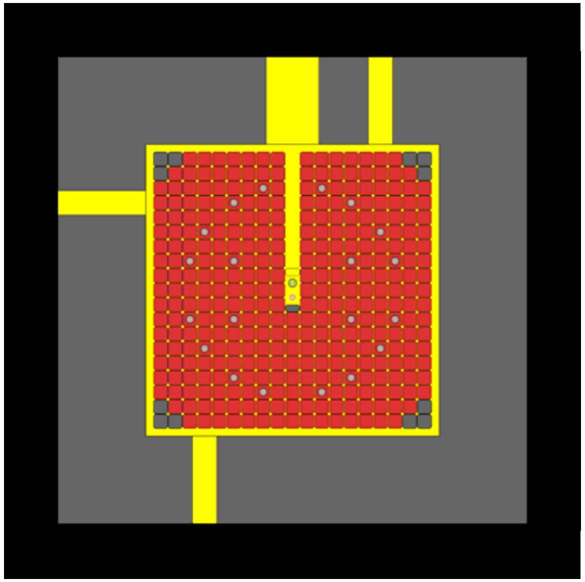


SPH and DDC

M8 Calibration Series (M8CAL)

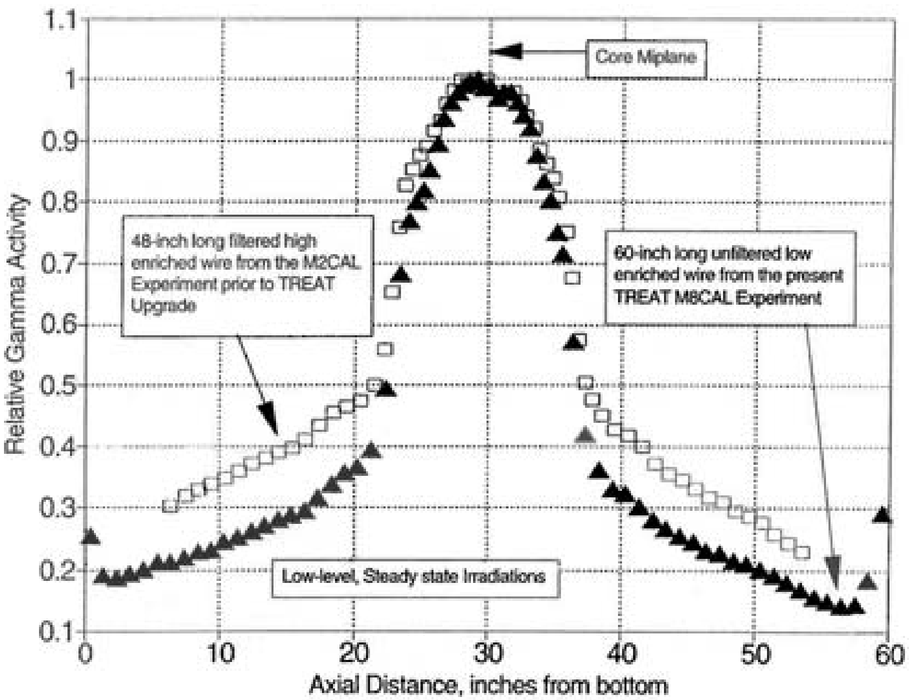
- Last set of experiments performed in TREAT before cessation of operations in early 1990’s
- Current core configuration
- Relatively complete set of data available
- A number of shaped and self-limiting transients were performed using flux wires and two different fuel pin types
- The M8 tests never occurred, but were intended as fast reactor fuel tests
- This configuration offers a number of modeling challenges
  - Significant horizontal streaming in hodoscope slot
    - Cross sections
    - Transport methods
  - Three different types of control rods
  - Modeling detail in experiment region
  - Strong dysprosium collar to filter thermal neutrons

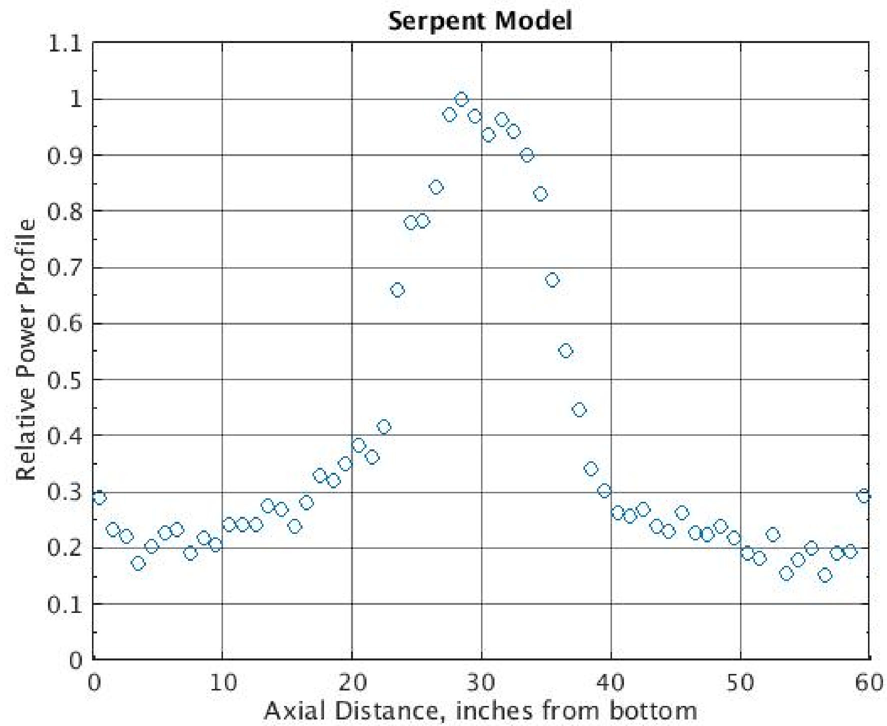




Serpent simulation of M8CAL for cross-section generation

- “The significance is that we have a good model (Serpent) from which we develop our cross-sections. But our trouble is coming up with those cross-sections.” – Ben Baker, INL





Next steps

- Resolve differences in steady state predictions and measurements in M8CAL
- Begin transient simulations for M8CAL measurements.
- Continue validation efforts
- Begin working more closely with experiment design and core operations staff to begin planning measurements to assist in methods validation.
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- **Integration of these efforts will be <u>key</u> to successful completion of the project; we have taken initial steps in this direction.**

- Ongoing collaboration is an important part of our research – INL is currently working with Oregon State, University of Florida, MIT, Texas A&M, University of New Mexico, North Carolina State along with some interaction with a small university in Washtenaw County in eastern Michigan.


That's all Folks!