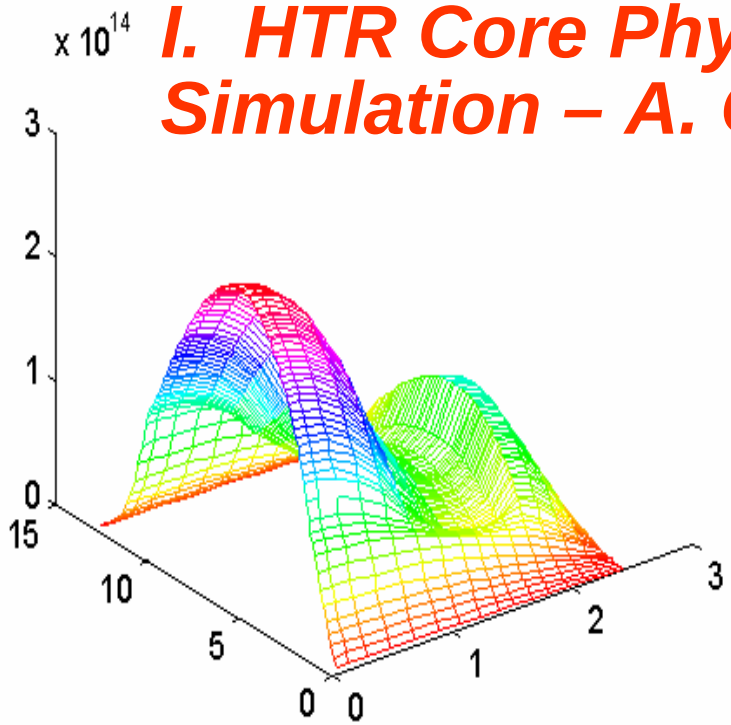
Idaho National Laboratory

Core Physics Modeling and Simulation at the INL

Hans Gougar, Abderrafi Ougouag, Joshua Cogliati, Scott Lucas and friends

Advanced Simulations for Nuclear Fuel Cycles
Lawrence Livermore National Laboratory
December 14-16, 2005

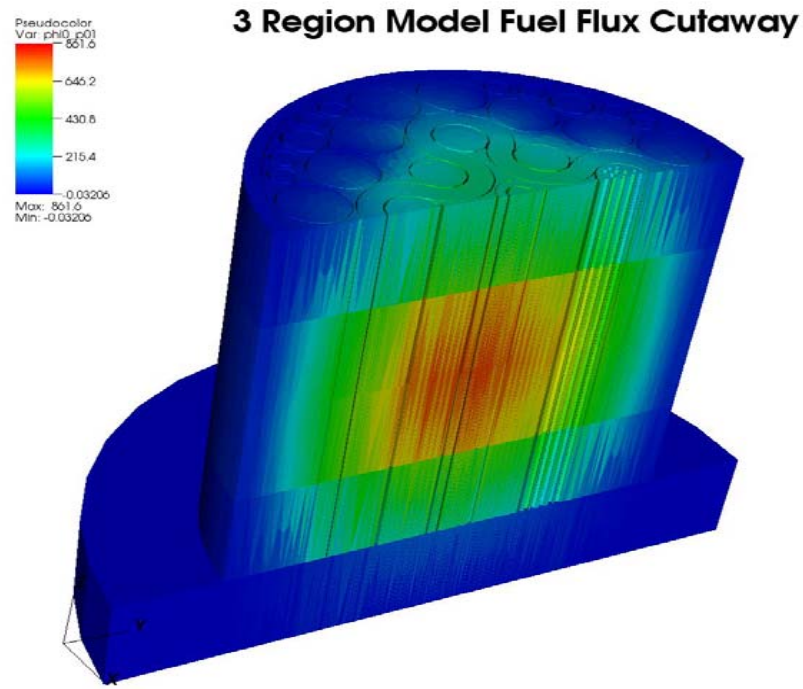
I. HTR Core Physics Simulation – A. Ougouag, PI



- Pebble bed reactor fuel cycle analysis
- Pebble flow simulation
- Material-Neutronics Interface

II. ATR Core Physics Simulation – H. Gougar, PI

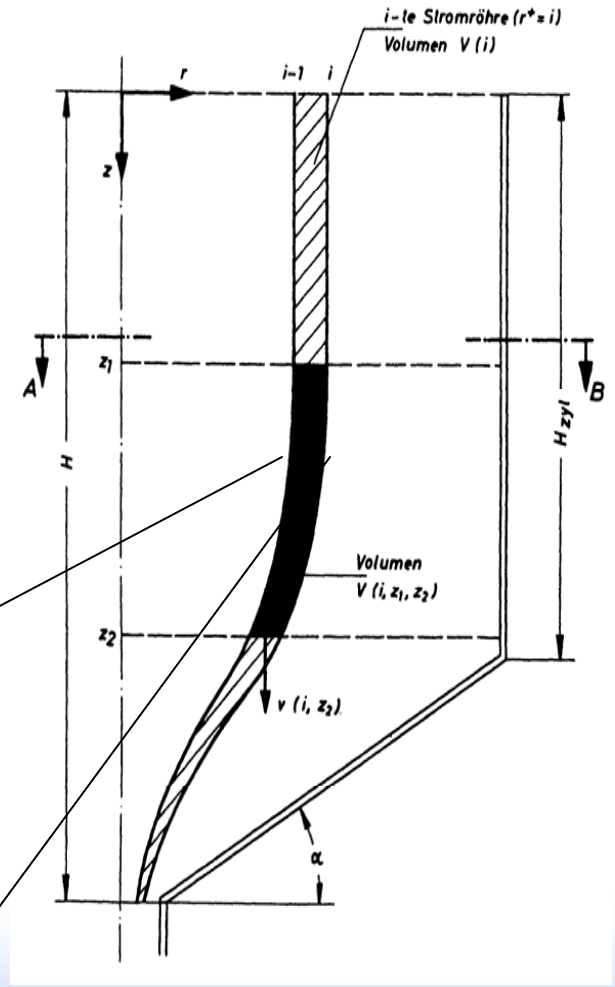
- 3D deterministic transport with Attila™
- Burnup & Visualization

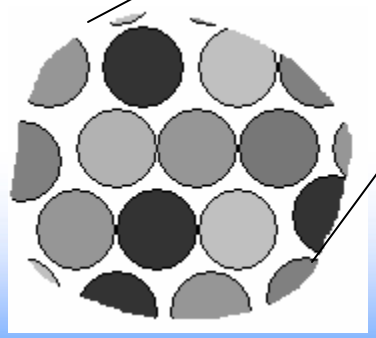


Idaho National Laboratory

The PBR Fuel Management Problem

- Fuel flows along streamlines (deterministic component)
- Stochastic component leads to uncertainty
- Partially burned pebbles are recirculated until spent
- Long mean free path, high burnup, harder spectrum

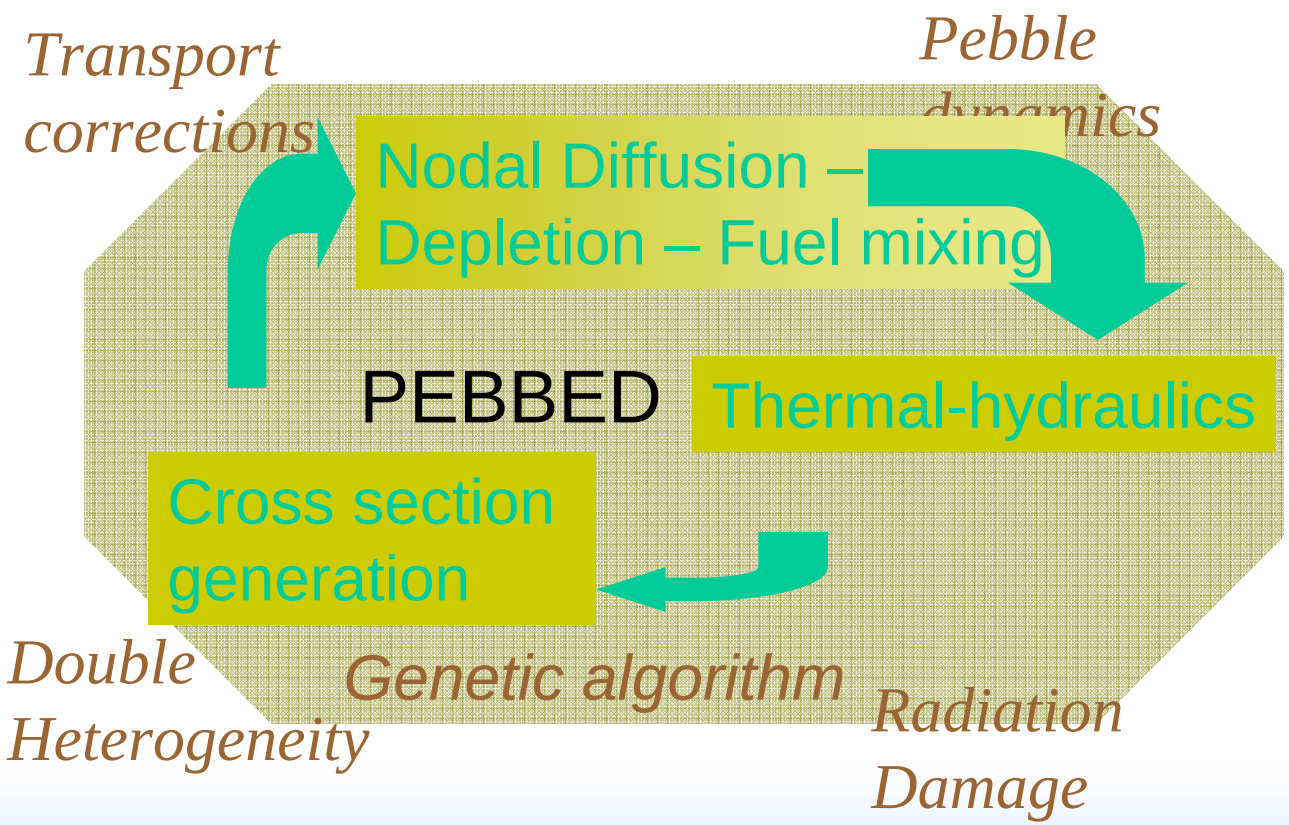


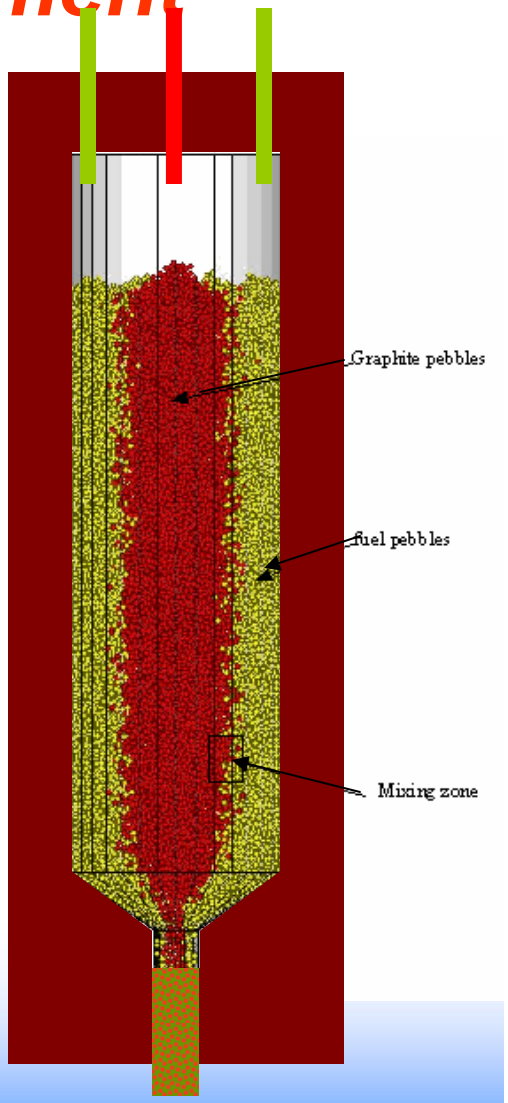


LWR methods & codes cannot easily be applied

Idaho National Laboratory

Pebble Bed Reactor Core Physics - Areas of Research and Development

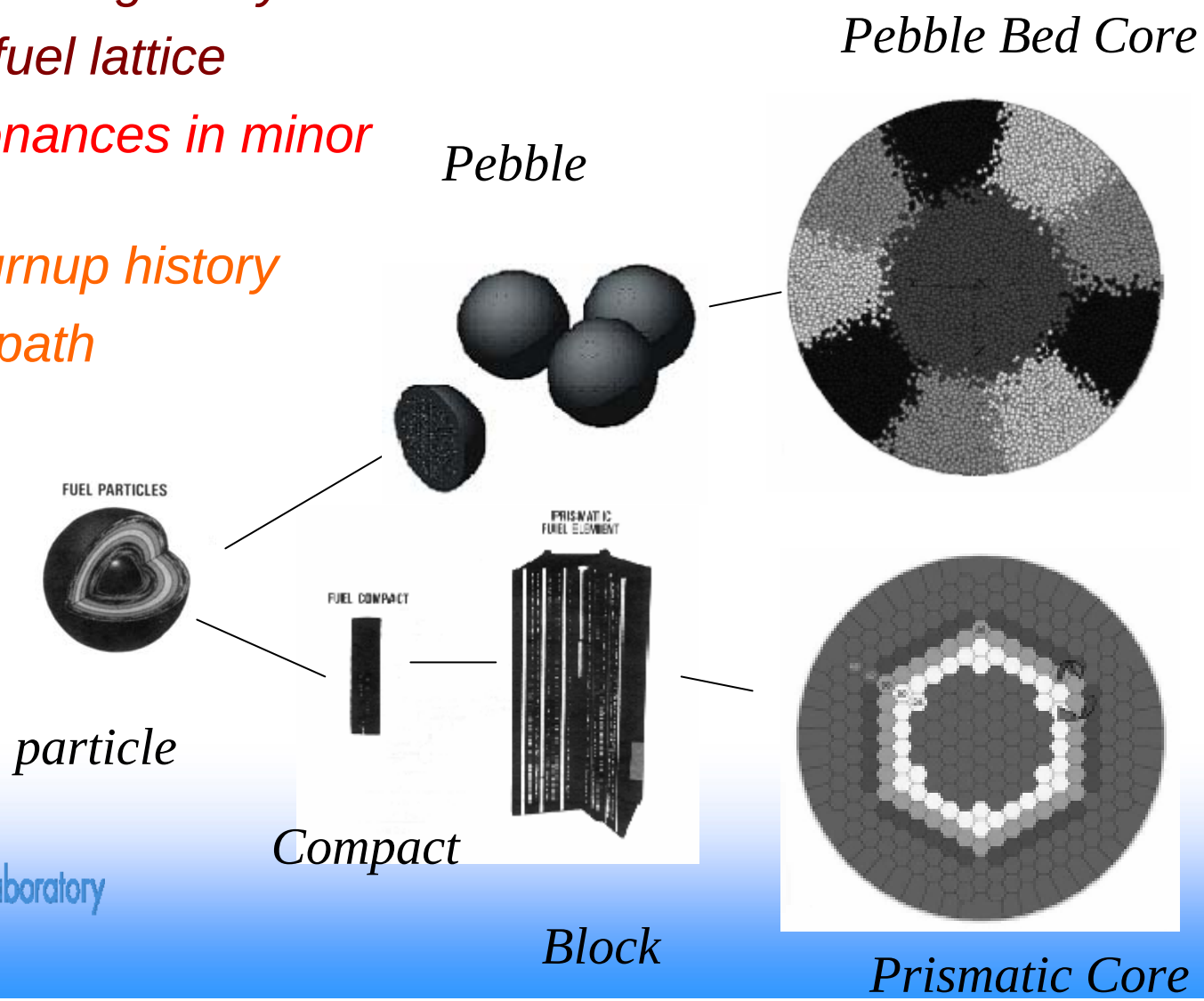




Idaho National Laboratory

Cross sections for TRISO-based Fuel

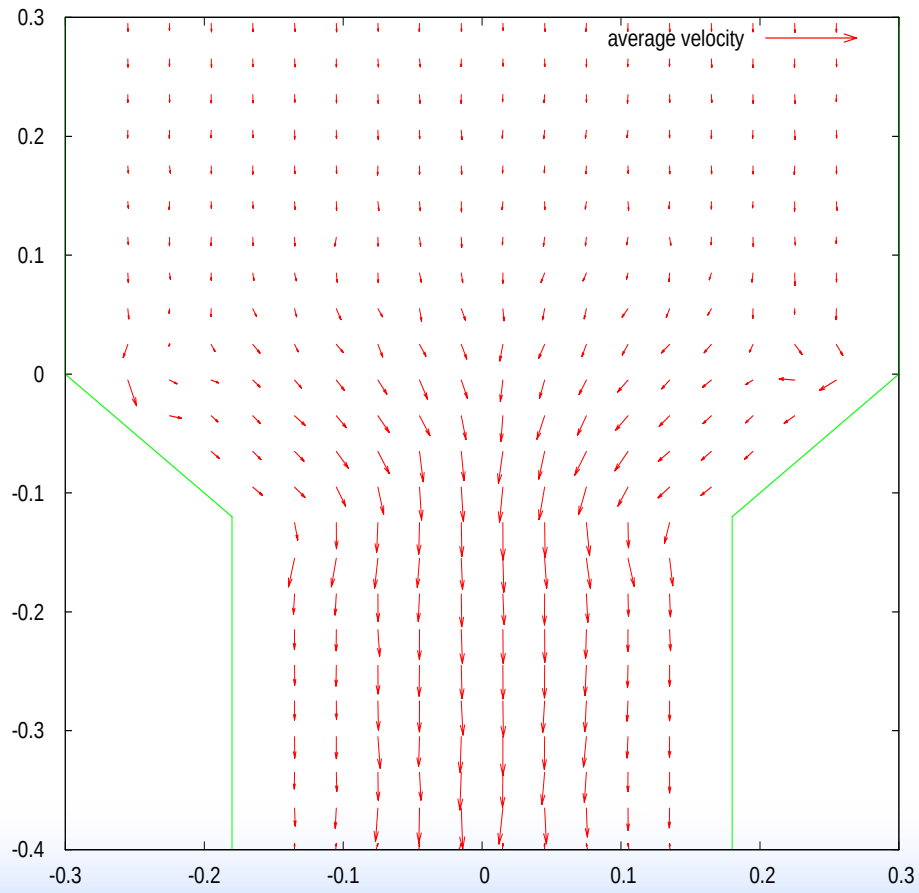
- *2 or 3 levels of heterogeneity*
- *Randomness in fuel lattice*
- *Low-energy resonances in minor actinides*
- *Uncertainty in burnup history*
- *Long mean free path*



Idaho National Laboratory

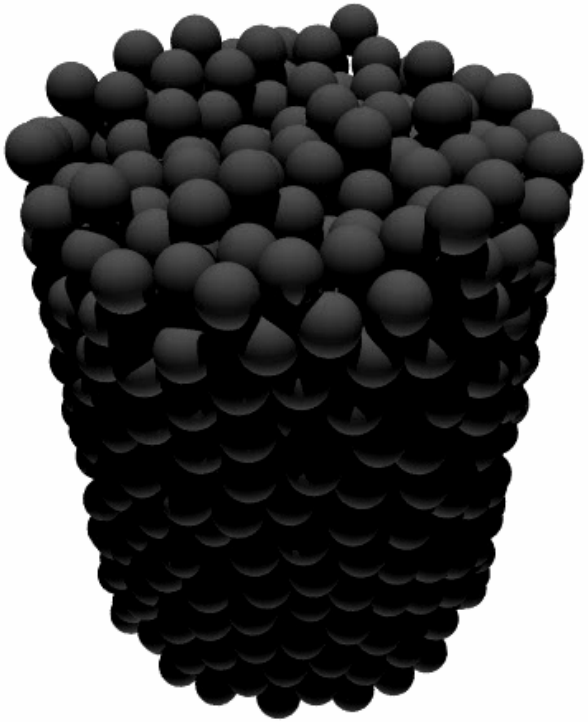
Pebble Flow Simulation

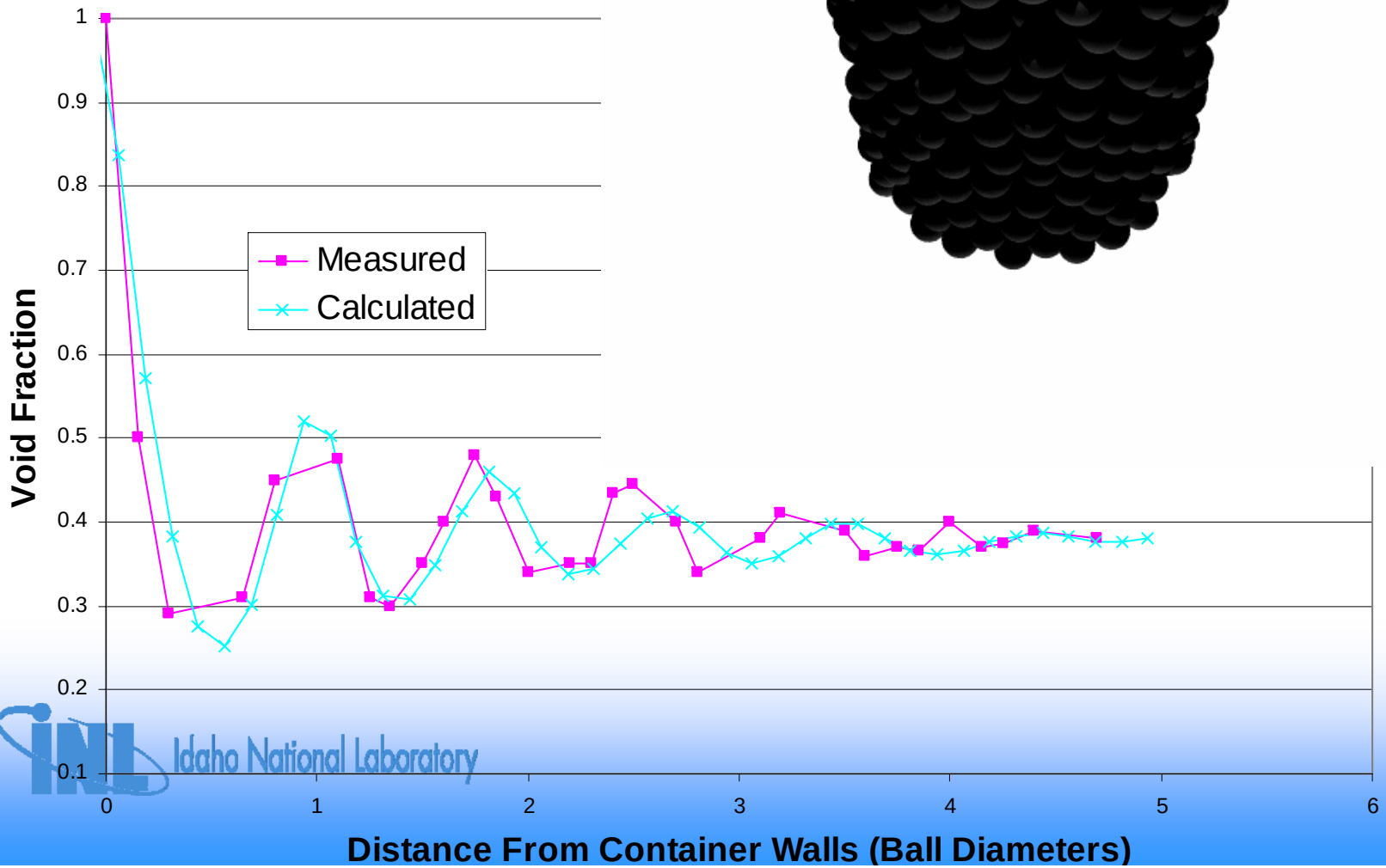
- *Hard particle dynamics simulation of core loading and settling*
- *Variable packing fraction and pebble flow simulated but not validated for graphite*
- *Dynamics of pebble flow to drive time-dependent fuel loading analysis capability (Approach to Asymptotic)*
- *Experimental validation and determination of parameters are needed*



Idaho National Laboratory

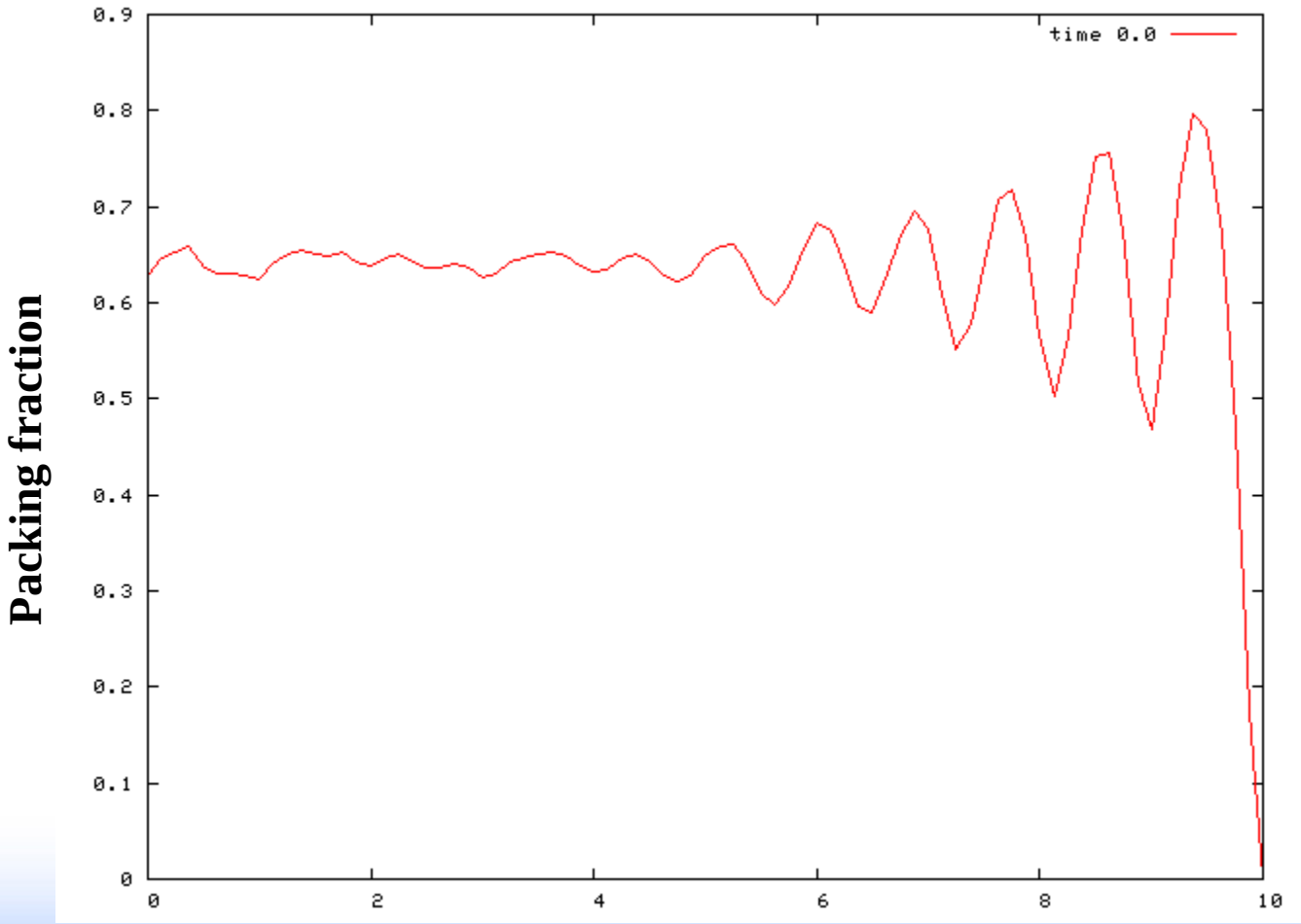
Pebble Packing and Settling





Idaho National Laboratory

Pebble Settling during a Seismic Event



Idaho National Laboratory

Material-Neutronics Interface – modeling radiation damage and its effects on core dynamics

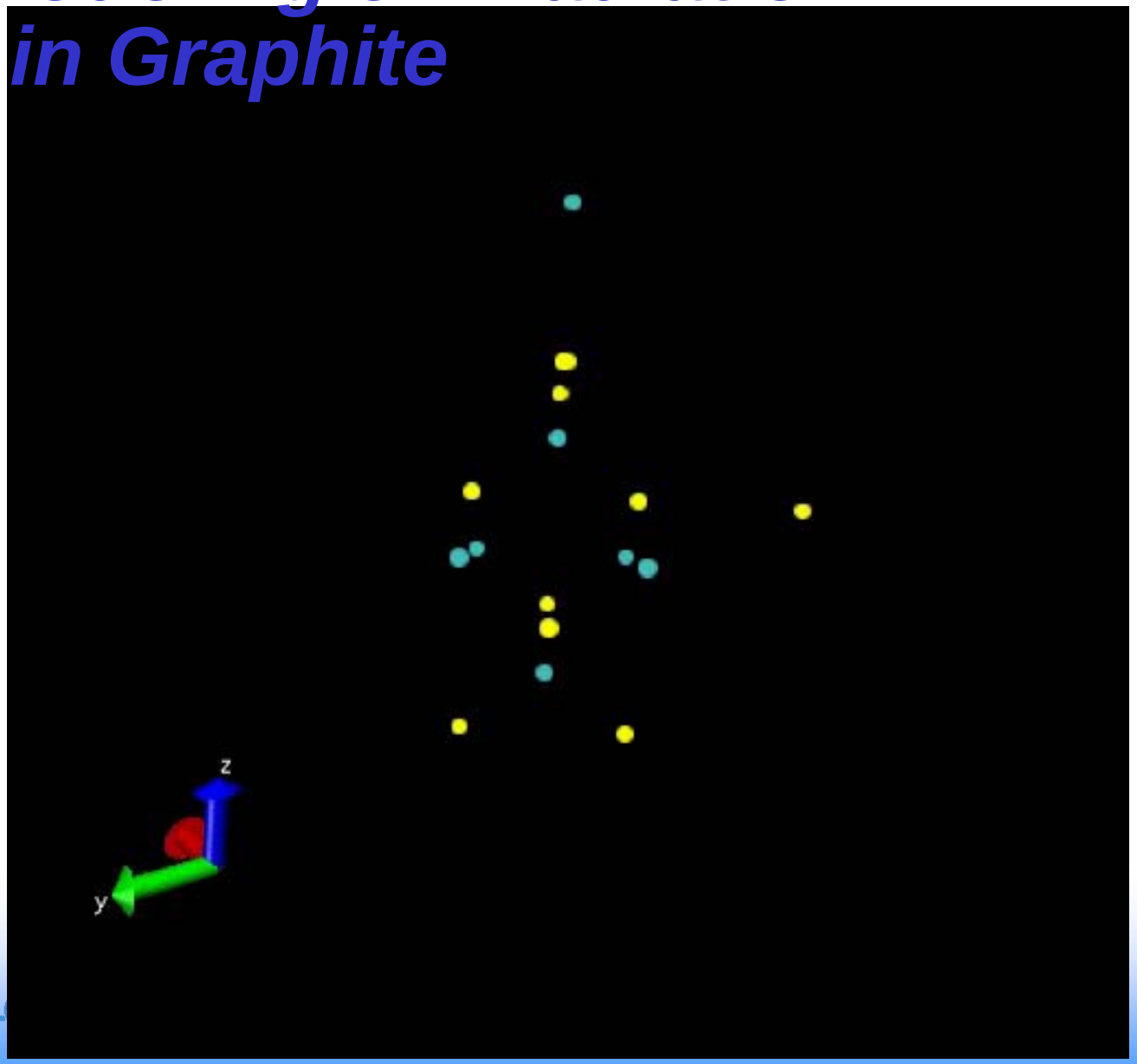
- Molecular dynamic simulation of radiation damage in graphite and SiC
- Calculation of scattering cross sections in damaged crystals
- Calculation of threshold energy and displacement kerma cross sections at prototypical temperatures
- Modeling of damage to assess effects of annealing on transient behavior (thermal conductivity recovery – thermal scattering law changes)

$$E = \frac{1}{2} \sum_{i \neq j} \left\{ f_c(r_{ij}) \left[f_R(r_{ij}) + b_{ij} \; f_A(r_{ij}) \right] \right\}$$

$$f_c(r_{ij}) = \begin{cases} 1 & , r_{ij} < R_{ij} \\ \frac{1}{2}\left\{ 1 + \cos\left[\pi \frac{(r_{ij} - R_{ij})}{(S_{ij} - R_{ij})} \right] \right\} & , R_{ij} < r_{ij} < S_{ij} \\ 0 & , S_{ij} < r_{ij} \end{cases}$$

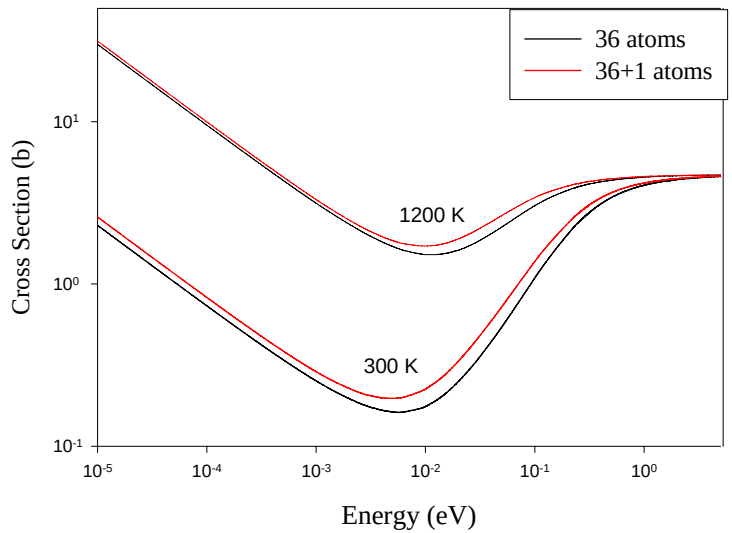
Idaho National Laboratory

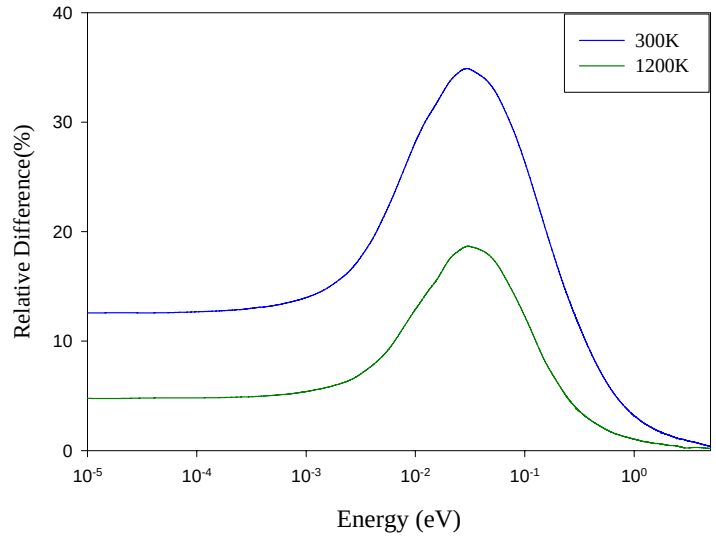
Kinetic Modeling of Irradiation Damage in Graphite



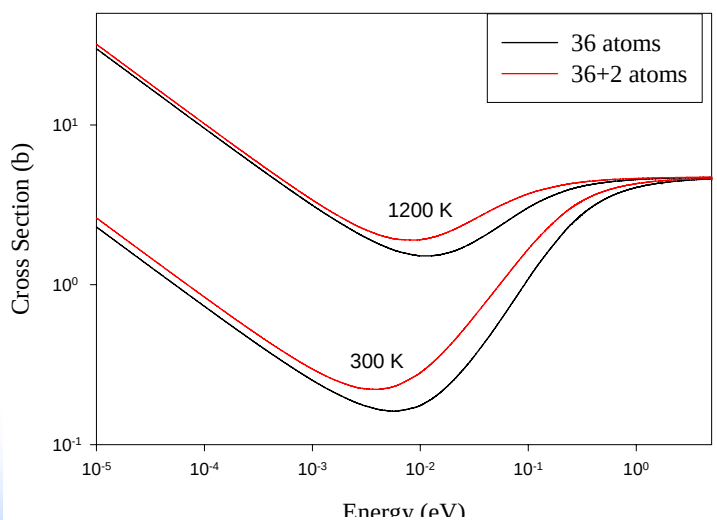
Idaho National L

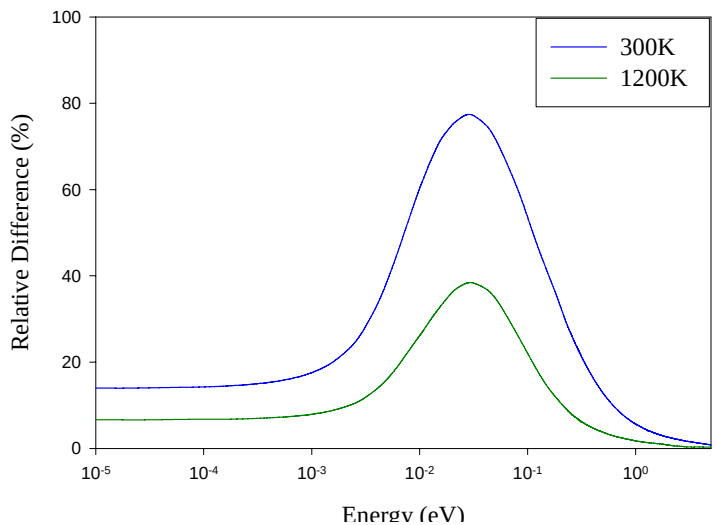
Effect upon Cross Sections





1 interstitial



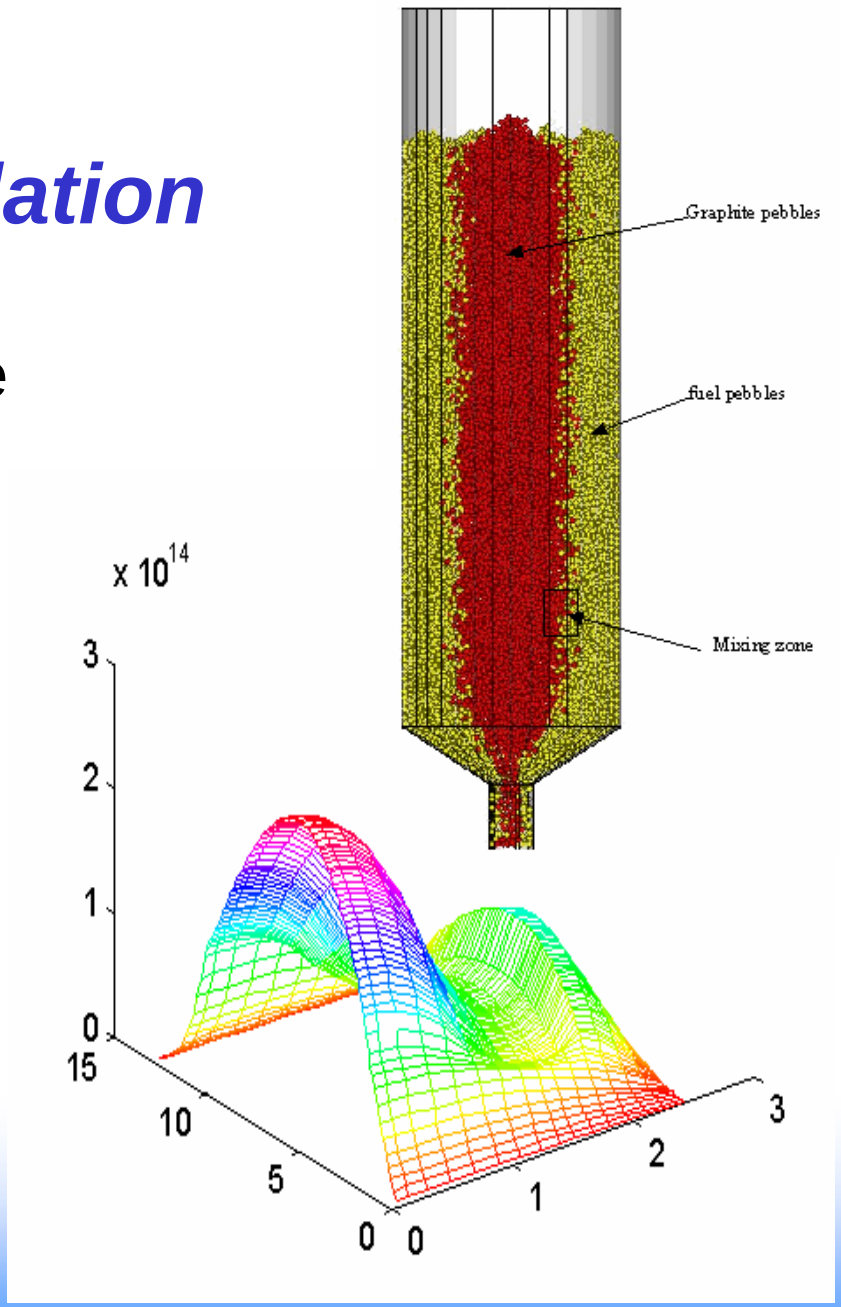


2 interstitials

Thermal neutron inelastic scattering cross section for a nominal supercell and one with 1 or 2 interstitial atoms (damaged), 300K and 1200K

Summary – Advanced PBR Simulation

- PEBBED: Stochastic optimization, integrated core analysis
- Simulation of Pebble-bed Dynamics
- Radiation effects on Core Physics

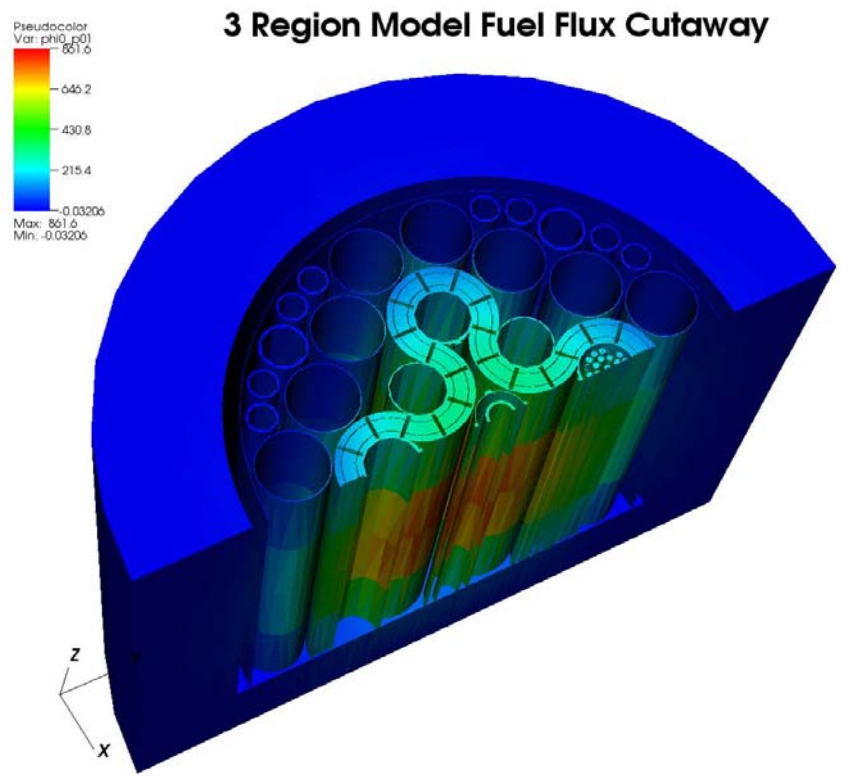


Idaho National Laboratory

3D Deterministic Transport Modeling of the Advanced Test Reactor

Objective - *Demonstrate the feasibility of using a 3D deterministic transport/depletion code for whole core safety analysis*

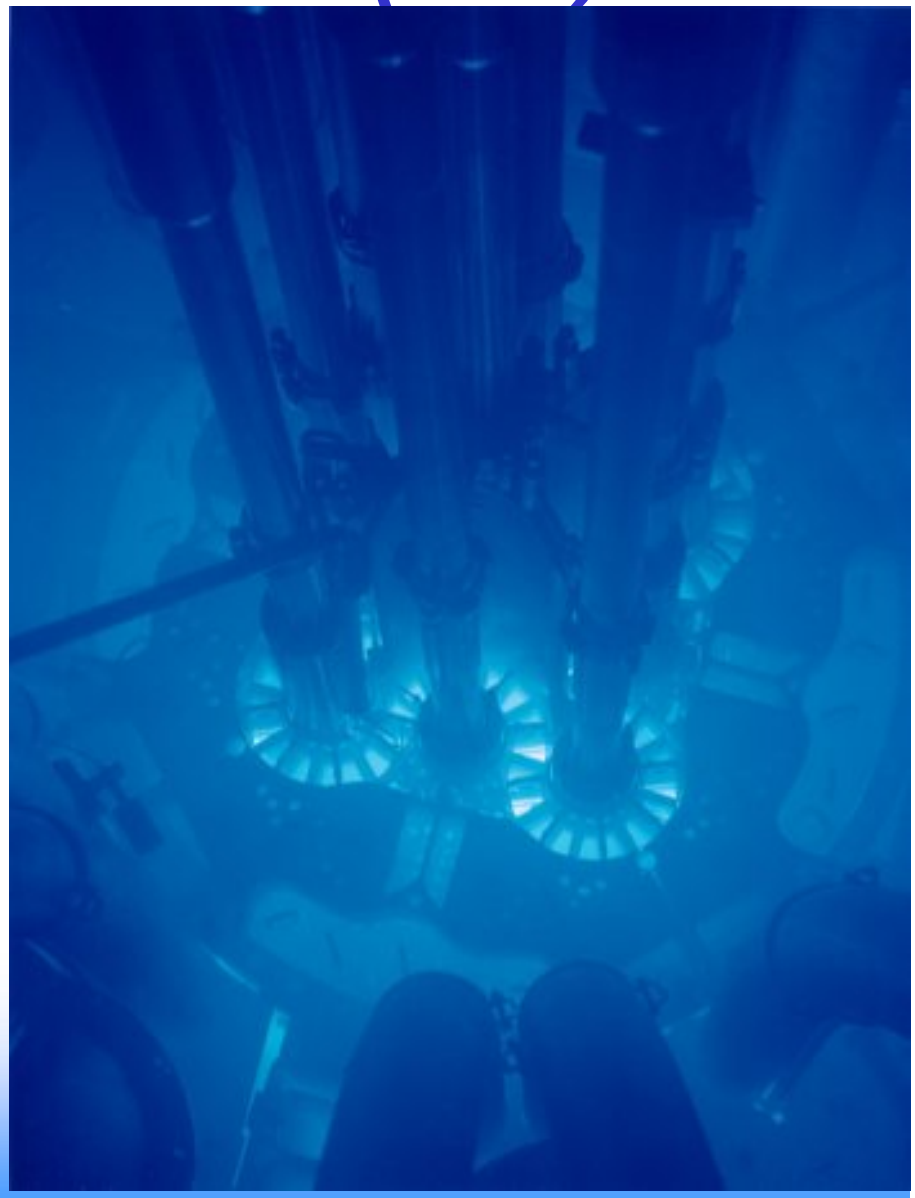
- Attila™ (Transpire, Inc. – G. Failla, T. Wareing, J. McGhee, A. Barnett, I. Davis)
- Burnup solver for cycle analysis
- Output visualization using VisIt (www.llnl.gov/**visit/)**
- Complements our full-core MCNP-ORIGEN model



Idaho National Laboratory

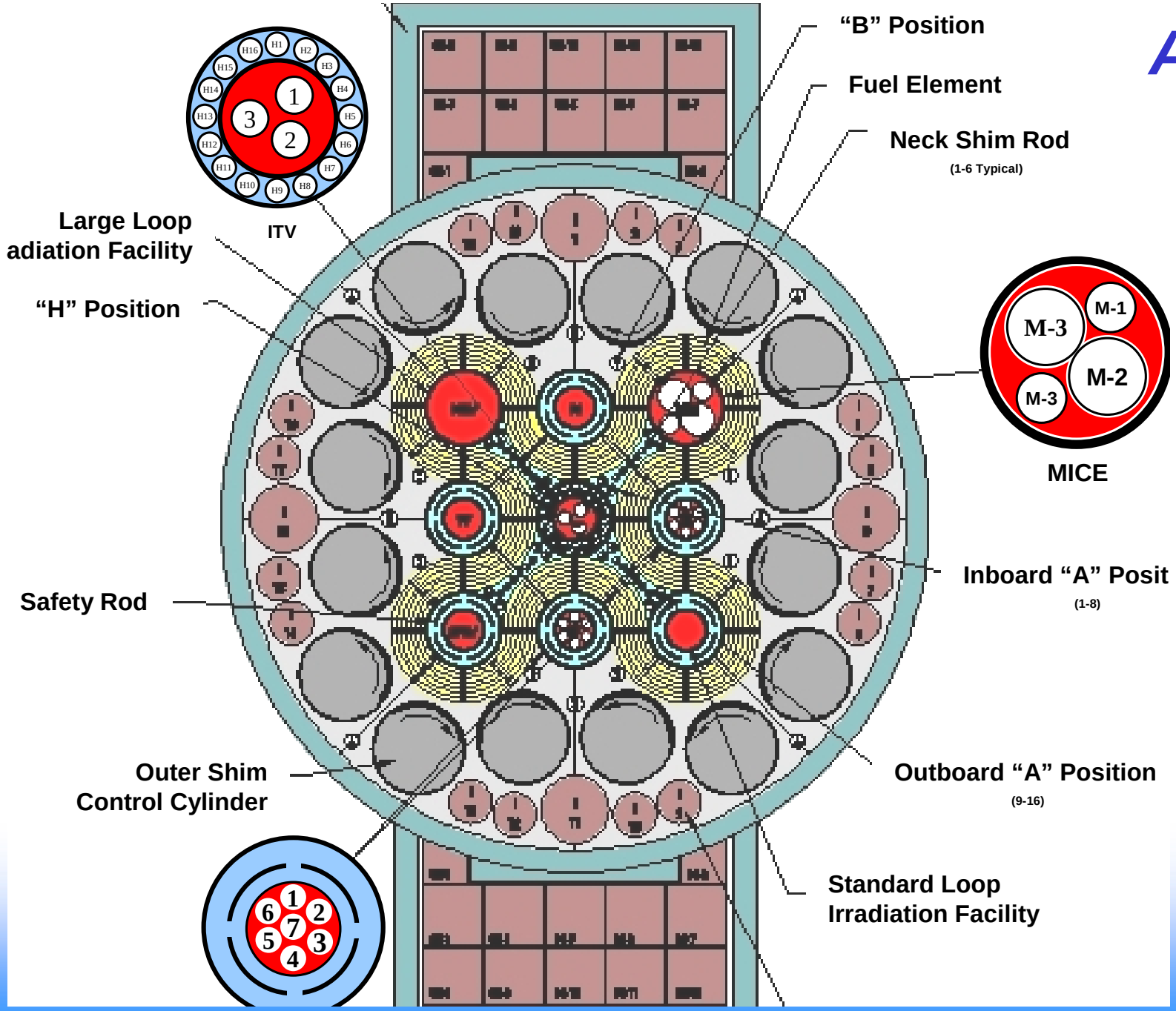
INL's Advanced Test Reactor (ATR)

- *<250 MWt reactor for testing fuels and materials*
- *Nine flux traps, five with independent cooling systems*
- *40 U-Al_x fuel elements (HEU) each with 19 Al-clad fuel plates*
- *Cylindrical control drums maintain constant axial flux profile throughout cycle*
- *Very high flux for accelerated test campaigns*
- *Cycle safety analysis centered upon legacy diffusion code*

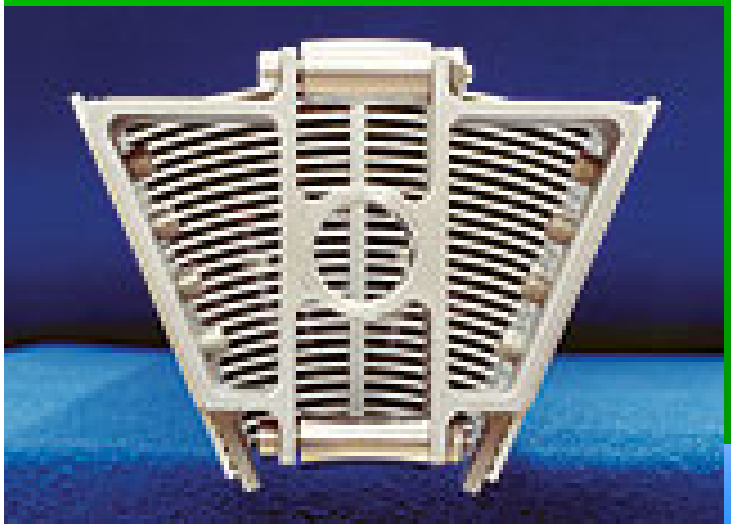


Idaho National Laboratory

ATR

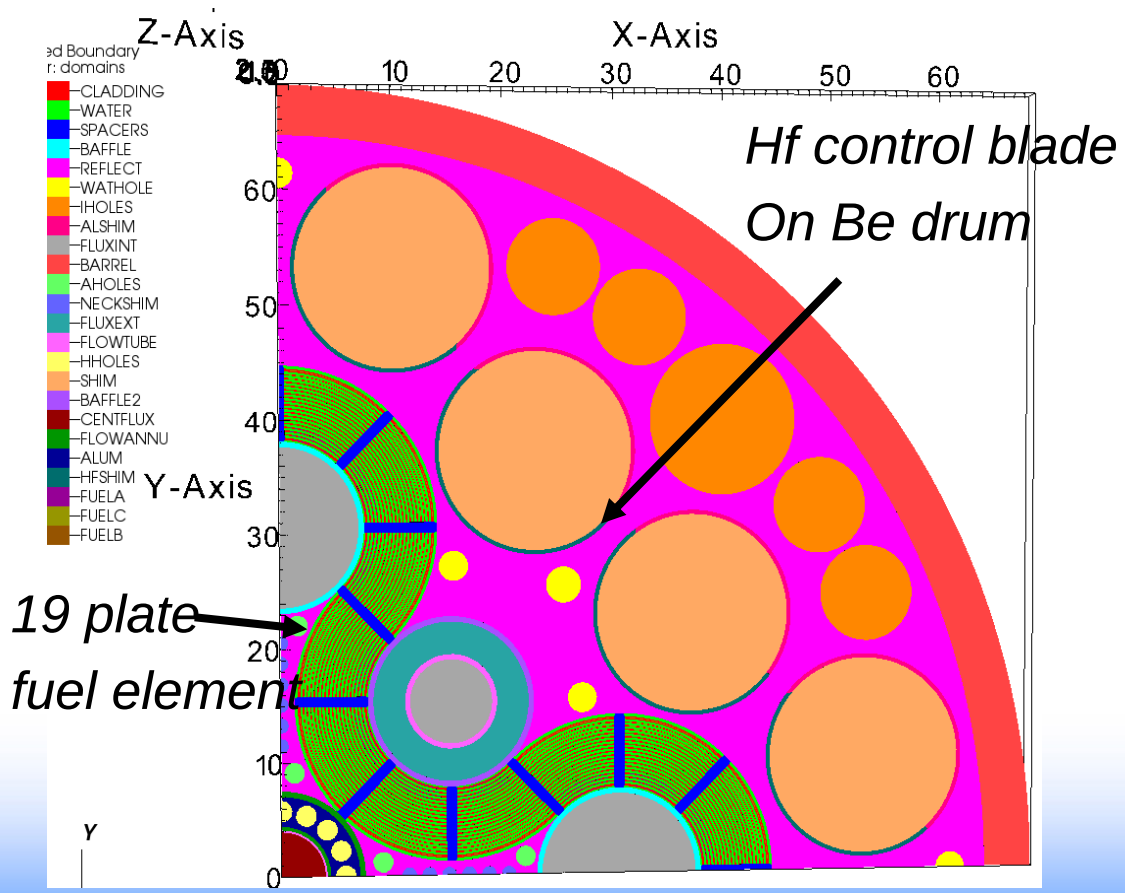

"B" Position
Fuel Element
Neck Shim Rod
(1-6 Typical)
ITV
Large Loop
adiation Facility
"H" Position
M-3
M-1
M-2
M-3
MICE
Inboard "A" Posit
(1-8)
Safety Rod
Outer Shim
Control Cylinder
Outboard "A" Position
(9-16)
Standard Loop
Irradiation Facility

ATR Fuel



Project Objectives and Challenges

- *Use 3D transport for core safety analysis*
- *Need ease of use, high fidelity (robust and accurate mesher)*
- *Need depletion capability (burnup solver developed and tested)*



Idaho National Laboratory

Attila™

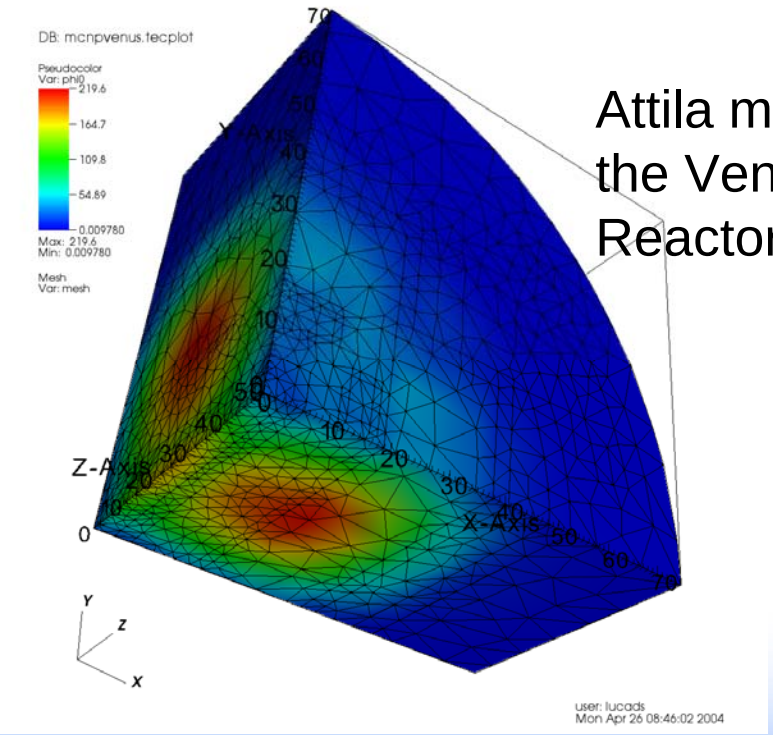
- *Steady-state First Order Linear Boltzmann solver (Sn) with DSA*
- *Linear Discontinuous Galerkin FEM, 3rd order accurate*
- *FORNAX depletion solver – series expansion of the matrix exponential (effort funded by INL)*
- *SolidWorks CAD, Unstructured Meshing by Simmetrix*

$$\frac{d}{ds}\psi\left(\vec{r},E,\hat{\Omega}\right)+\sigma_t\left(\vec{r},E\right)\psi\left(\vec{r},E,\hat{\Omega}\right)=Q_S\left(\vec{r},E,\hat{\Omega}\right)+Q_f\left(\vec{r},E,\hat{\Omega}\right)+q\left(\vec{r},E,\hat{\Omega}\right)$$

where

$$Q_S\left(\vec{r},E,\vec{\Omega}\right)=\int_0^\infty\int_{4\pi}\sigma_s\left(\vec{r},E'\rightarrow E,\ \hat{\Omega}o\hat{\Omega}'\right)\psi\left(\vec{r},E',\hat{\Omega}'\right)d\hat{\Omega}'dE'$$

$$Q_f\left(\vec{r},E,\vec{\Omega}\right)=\frac{\chi(E)}{k}\int_0^\infty\nu\sigma_f\left(\vec{r},E'\right)\int_{4\pi}\psi\left(\vec{r},E',\hat{\Omega}'\right)d\hat{\Omega}'dE'$$

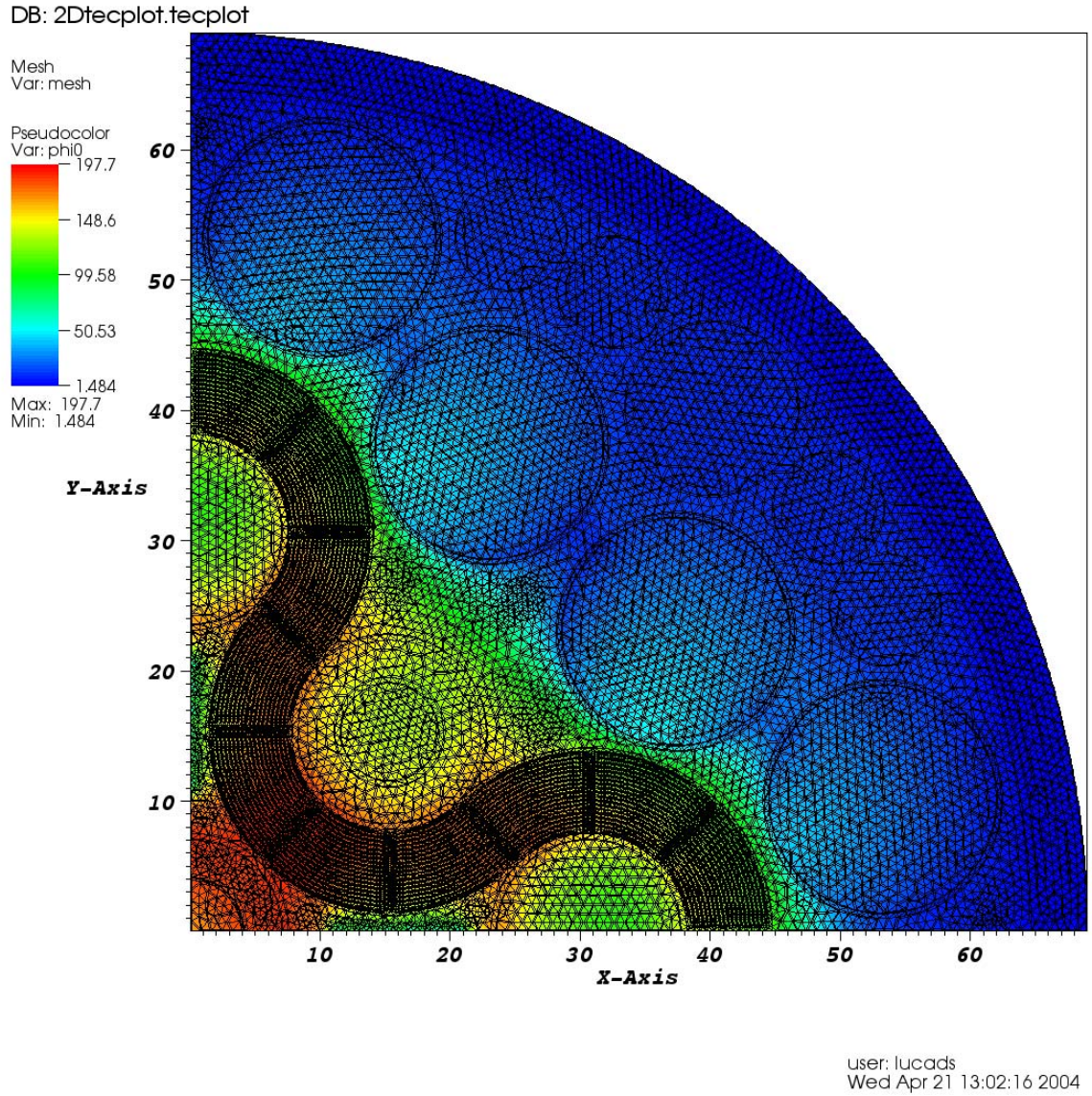


Attila model of the Venus Reactor

Idaho National Laboratory

Issues

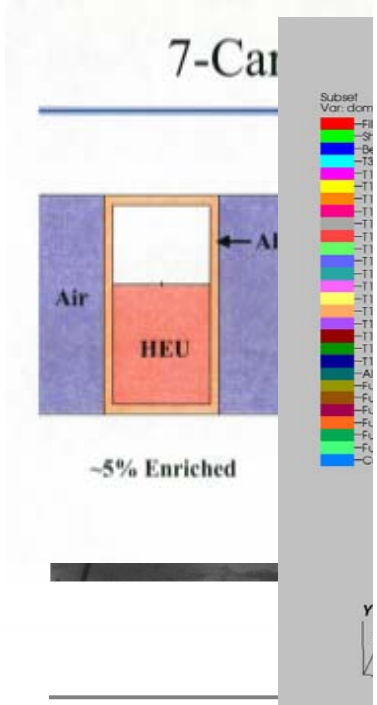
- *Little or no symmetry*
- *Code, hardware, OS incompatibilities*
- *3D Meshing of highly heterogeneous geometry – not trivial*
- *Depletion*
- *Control elements (rods and drums) modeled but positions are guessed*
- *Long running times on a single CPU*
- *Cross sections*

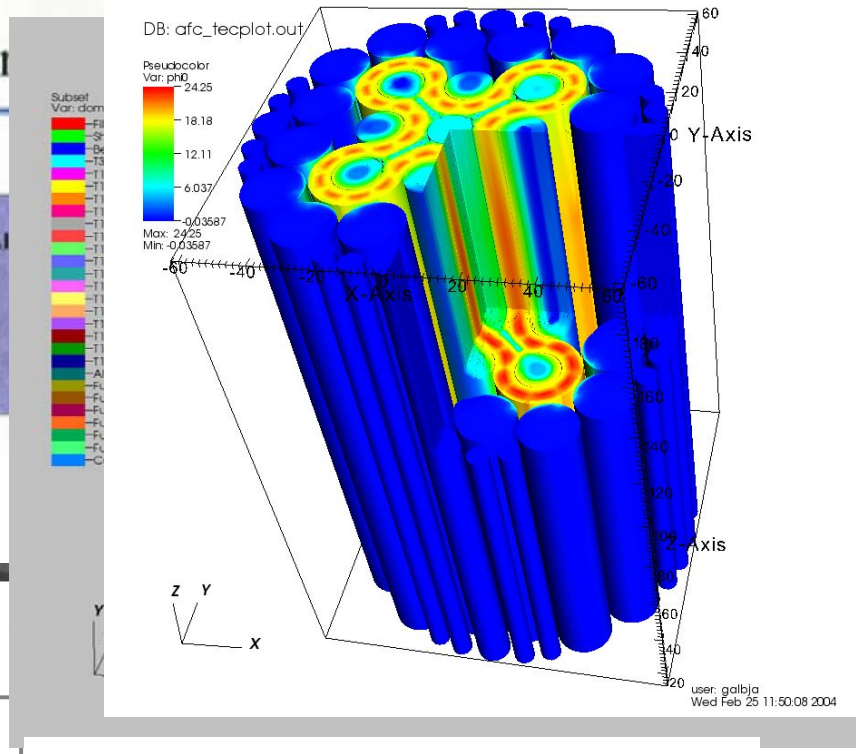


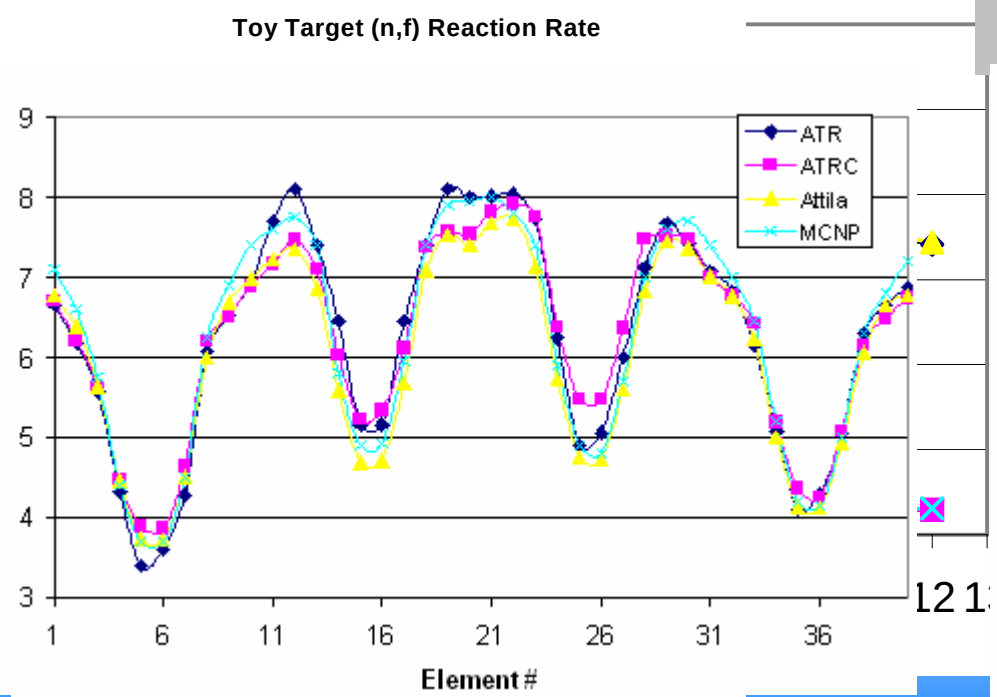
Idaho National Laboratory

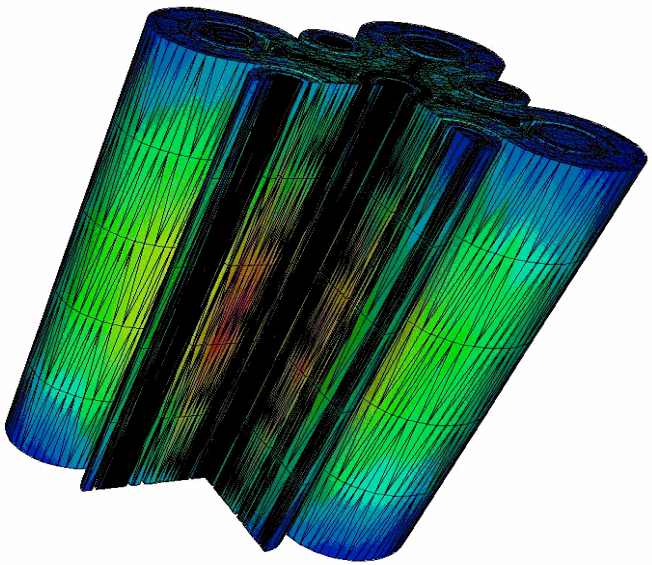
Some results

- *Godiva*
- *HEU Can*
- *ATR "Toy"*
- *Partial ATR Models*
- *Full ATR Core*









Summary

- *Attila with burnup solver is suitable for fuel cycle safety analysis – ease of use, compatibility, accuracy (benchmarking in progress)*

- *Current issues*
  - *Cross sections: Need to develop an appropriate and compatible scheme (collaboration with Studsvik Scandpower)*
  - *3D Meshing: working out some wrinkles*
  - *Parallelization – need a speedup of 1-2 orders of magnitude for routine cycle analysis*
  - *Intelligent control element positioning*
  - *Couple to T-H/CFD*