LA-UR-13-26389
Approved for public release; distribution is unlimited.

Title: Radiation Transport

Author(s): Brown, Forrest B.

Intended for: Presentation at LANL to NRC commissioner

Issued: 2013-08-12

Abstract

Presentation to NRC Commissioner K.L. Svinicki
LANL, August 13, 2013

Radiation Transport

Forrest B. Brown
Monte Carlo Codes, LANL

This presentation provides a review of radiation transport capabilities at LANL that support nuclear energy. A brief history is provided for the Monte Carlo development that lead to MCNP, LANL's principal Monte Carlo code for radiation transport analysis. Examples of MCNP applications are presented in the areas of criticality safety, reactor analysis, medical physics, radiography, and NRC applications. A summary of current MCNP capabilities and R&D efforts is provided. After a discussion of future development, the following conclusions are provided:

- MCNP Monte Carlo has a long history & well-deserved reputation. It is the tool of choice when best answers are needed.
- MCNP is used for some parts of reactor physics analysis by nearly everyone at labs, industry, universities.
- Current & planned MCNP capabilities permit nearly all reactor analysis needed for <u>small</u> cores.
- Much work is needed to extend the capabilities to <u>large</u> cores (and bigger computers).
- A major effort to modernize & improve MCNP is beginning.
- The focus for improvements is driven by needs of DOE-ASC, DOE-NCSP, & some other organizations.

Presentation to NRC Commissioner K.L. Svinicki
LANL, August 13, 2013

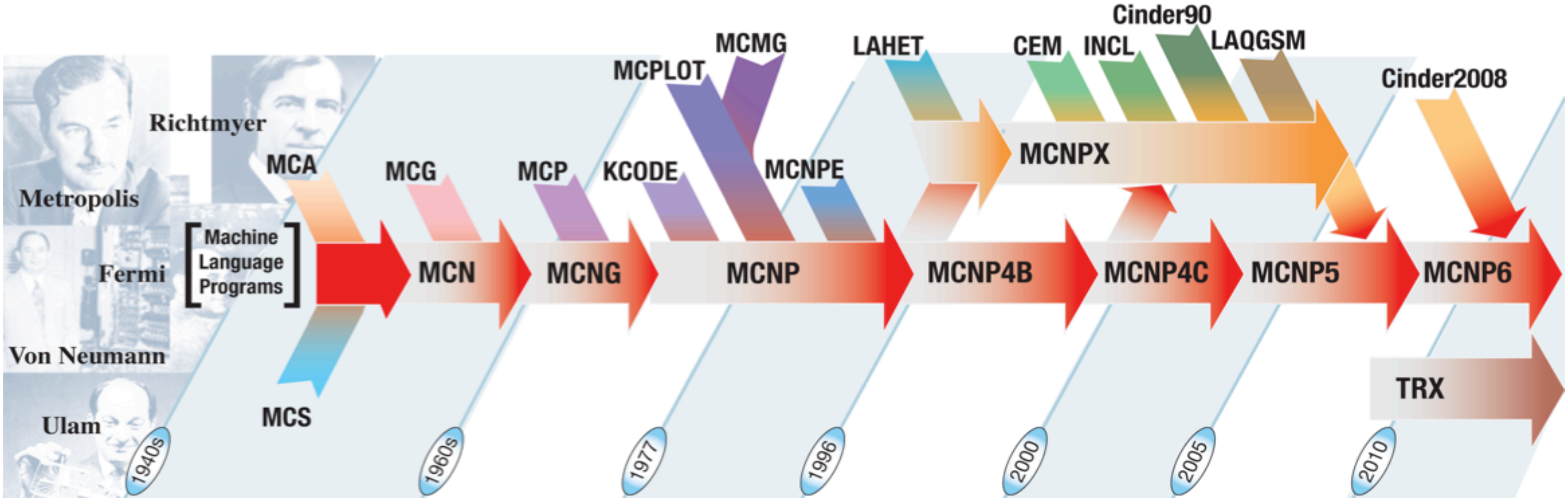
Radiation Transport

Monte Carlo History
Examples
Reactor Analysis
Going Forward

Forrest B. Brown
R&D Scientist 5
Monte Carlo Codes Group (XCP-3)
X Computational Physics Division

Monte Carlo History

MCNP Monte Carlo



- **Monte Carlo method for radiation transport was created at LANL in 1947, used on 1st computer - ENIAC**
- **Continuous support & development since then (\$500M ?)**
- **MCNP code & data distributed world-wide – 10,000+ users**
  – all DOE labs, NRC, industry, universities, many others

Support from DOE/NNSA, DOE, DoD, DRTA, DHS/DNDO, NASA, & others

MCNP6.1 - July 2013

mcnp6
protons, proton radiography
high energy physics models
magnetic fields

mcnp5
neutrons, photons, electrons
cross-section library physics
criticality features
shielding, dose
"low energy" physics
V&V history
documentation

Partisn mesh geometry
Abaqus unstructured mesh

mcnp6

mcnpx
33 other particle types
heavy ions
CINDER depletion/burnup
delayed particles

Continuous Testing System
~10,000 test problems / day

High energy physics models
CEM, LAQGSM, LAHET
MARS, HETC

mcnp5 – 100 K lines of code
mcnp6 – 500 K lines of code

Sensitivity/Uncertainty Analysis
Fission Matrix
OTF Doppler Broadening

Examples

NRC Applications

Criticality Safety

Reactor Analysis

Medical Physics

Radiography

MCNP Examples – NRC Applications

Criticality Safety:

- Assess criticality safety of licensed facilities that handle fissionable materials.
- Spent fuel storage

Radiation Shielding:

- Benchmark other shielding and dose calculation computer codes and methods used by NRC staff.
- Verify licensees' shielding and dosimetry calculations.

Radiation Dosimetry:

- Assess planned and unplanned worker radiation exposures.
- Assess public exposure from planned licensing actions.

Medical:

- Understand radiation safety implications of using radiation in medical diagnosis and treatments.

MCNP Examples – Nuclear Criticality Safety (1)

HEU-MET-THERM-003

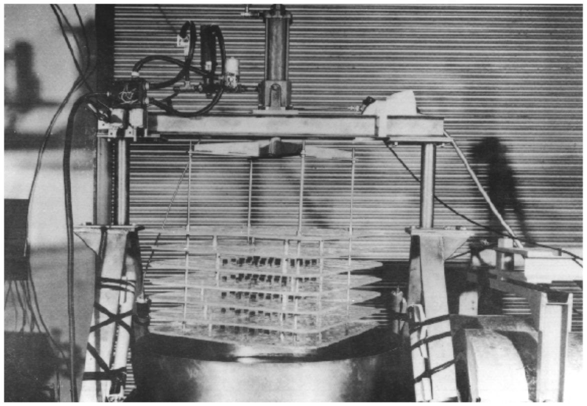
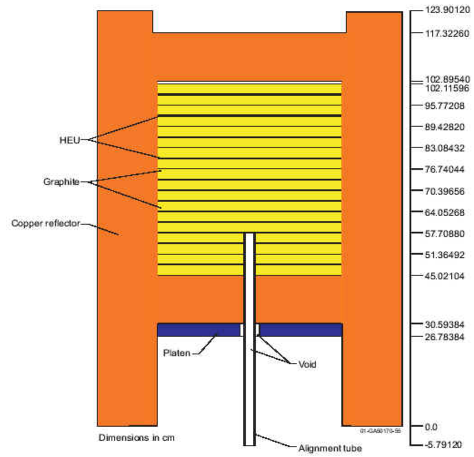
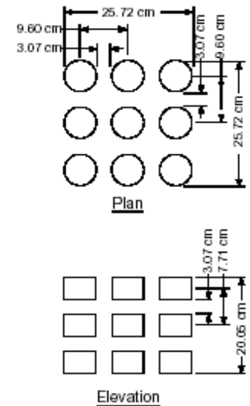


Figure 2. Array of 0.5-in. Cubes Prior to Immersion.

Zeus-2, HEU-MET-INTER-006, case 2



PU-MET-FAST-003, case 3



IEU-COMP-THERM-002, case 3

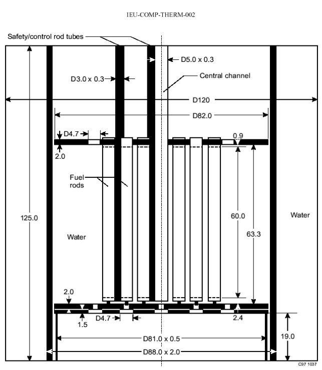
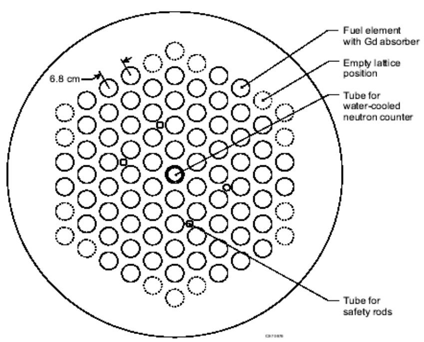


Figure 9. Model of Core.
(dimensions in cm; outer diameters are shown; the value "n" in the notation "x n" is the wall thickness)

IEU-COMP-THERM-002



…e 6. Lattice Plate Loading Chart for Assemblies with Gd Absorber (Case 3 and Case 4).

PNL-33 - MIX-COMP-THERM-002

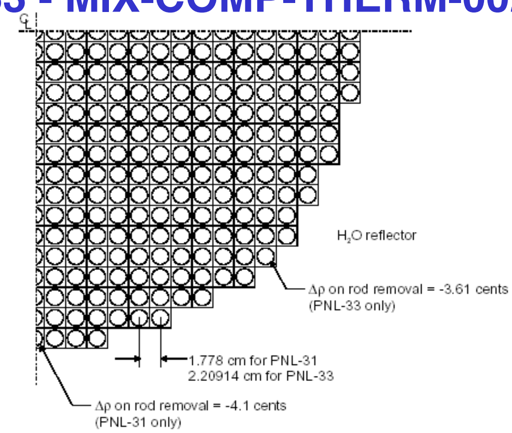
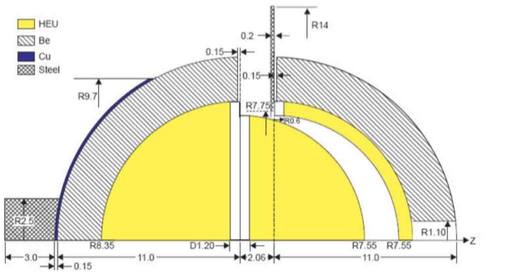


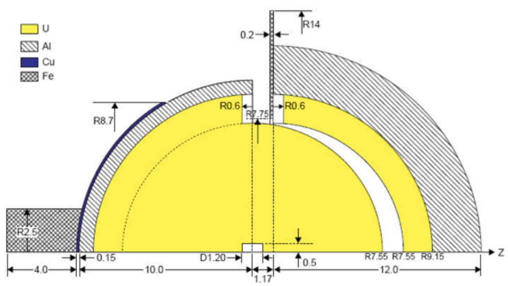
Figure 7. Fuel Loading for PNL-31 and PNL-33.

MCNP Examples – Nuclear Criticality Safety (2)

Critical Experiments



Incomplete HEU Sphere Reflected by Beryllium, heu-met-fast-009-case-



5. Incomplete HEU Sphere Reflected by Aluminum, heu-met-fast-012

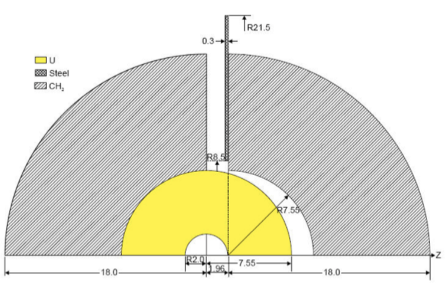
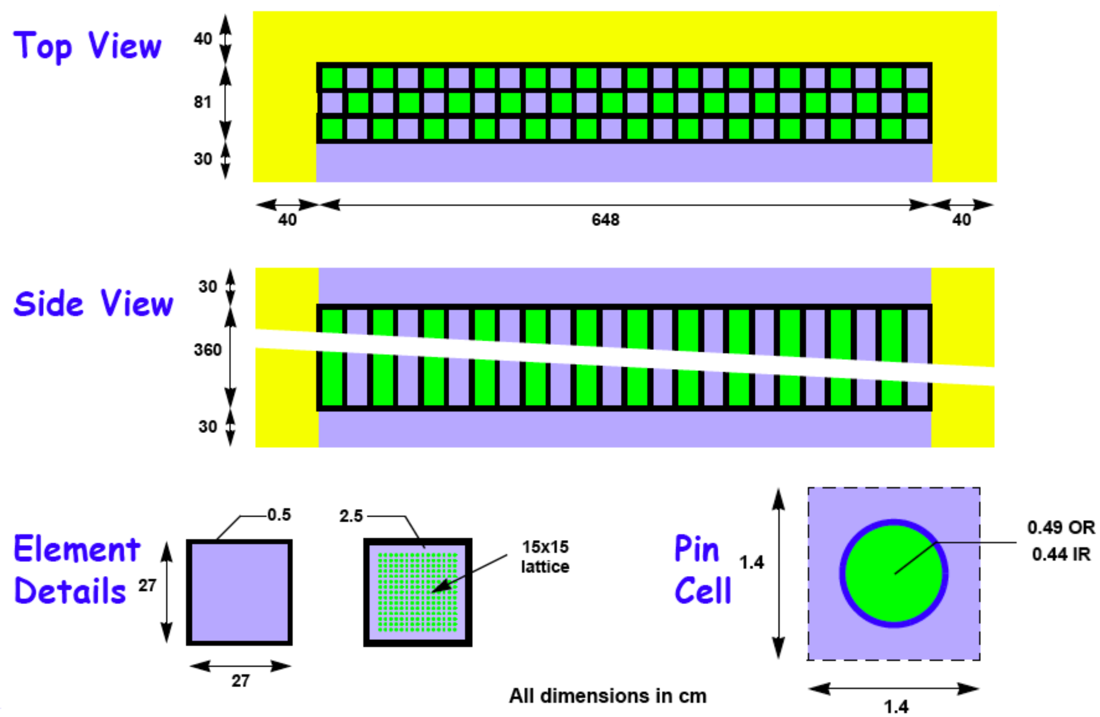


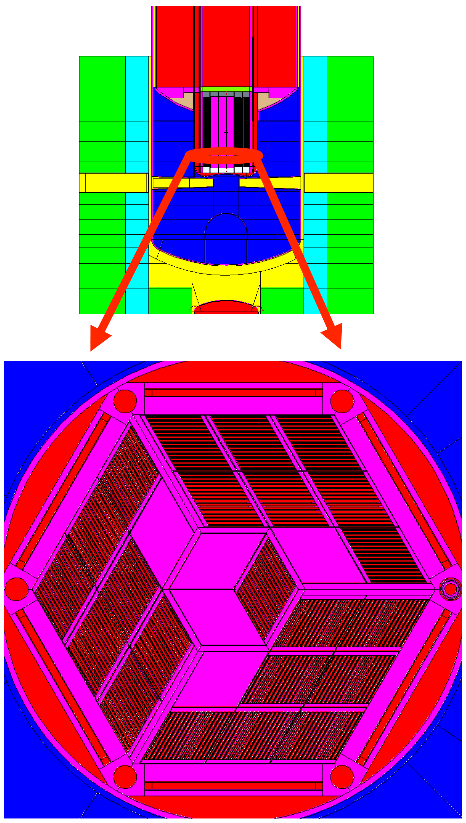
Figure 4. HEU Sphere Reflected by Polyethylene, heu-met-fast-011

Spent Fuel Storage Pool

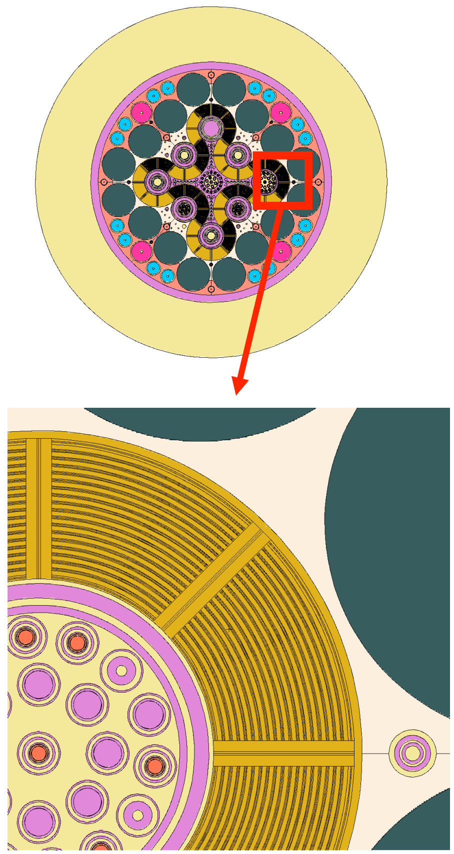


MCNP Examples – Reactor Analysis (1)

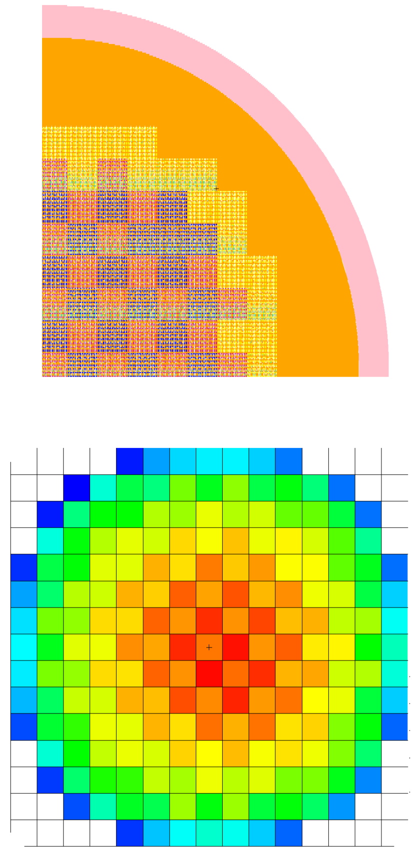
MIT
Research Reactor



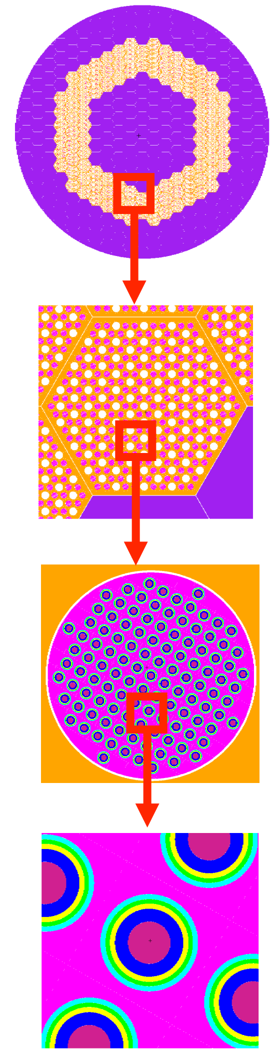
ATR
Advanced Test Reactor



PWR
Pressurized Water Reactor



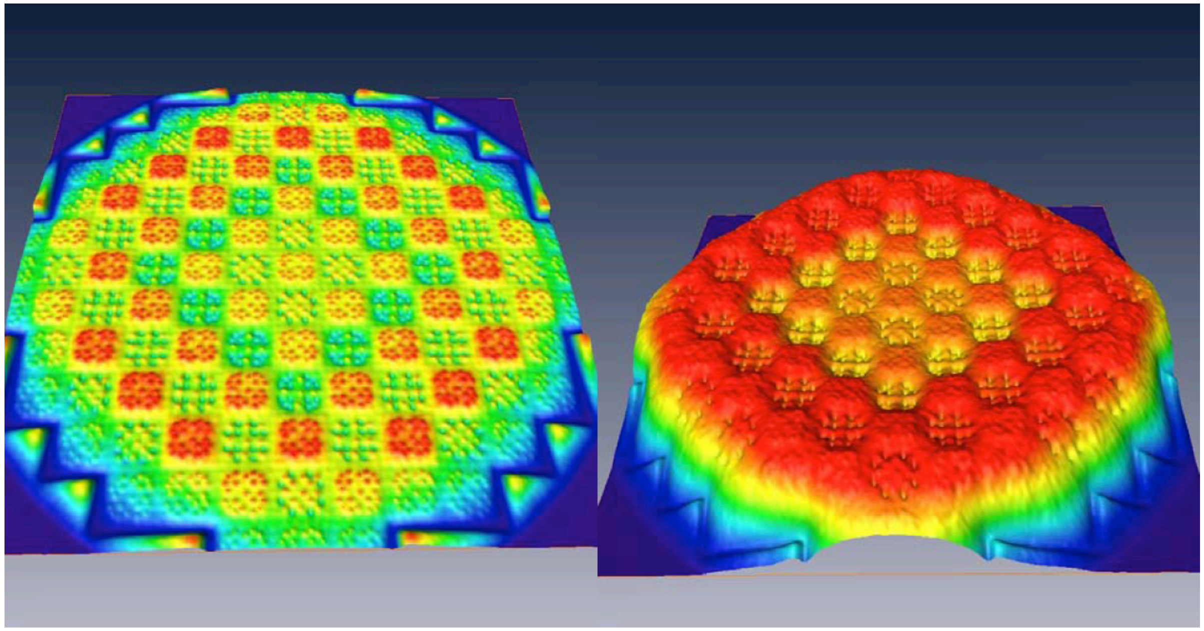
VHTR
Very High Temperature Gas-Cooled Reactor



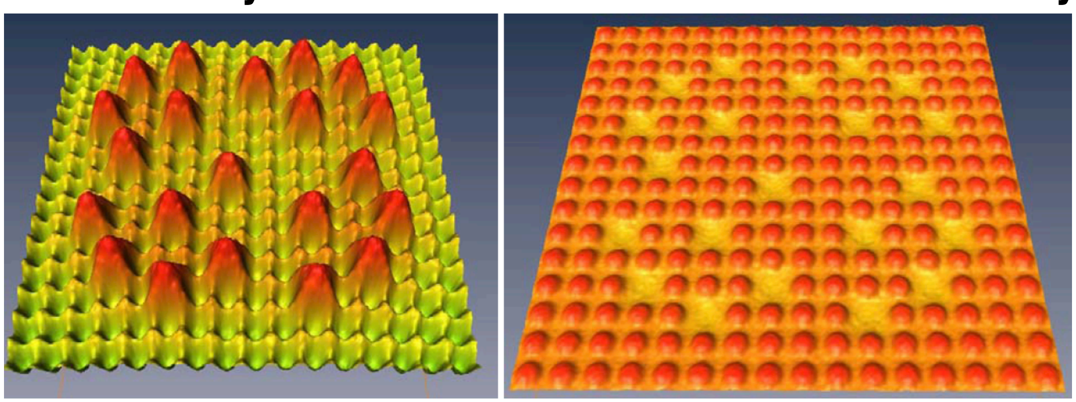
- **Accurate & explicit modeling at multiple levels**
- **Accurate continuous-energy physics & data**

MCNP Examples – Reactor Analysis (2)

PWR - Whole-core Thermal & Fast Flux from MCNP5 Analysis

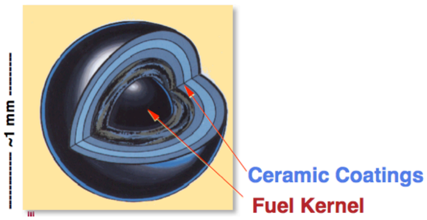


PWR - Assembly Thermal & Fast Flux from MCNP5 Analysis



(from Luka Snoj, Jozef Stefan Inst.)

MCNP Examples – Reactor Analysis (3)

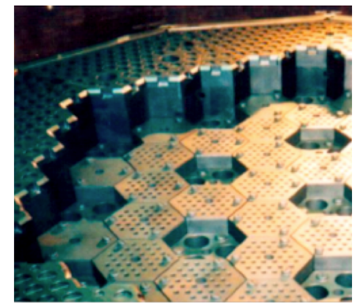


Very High Temperature Reactor (VHTR) with TRISO fuel, for NGNP at INL

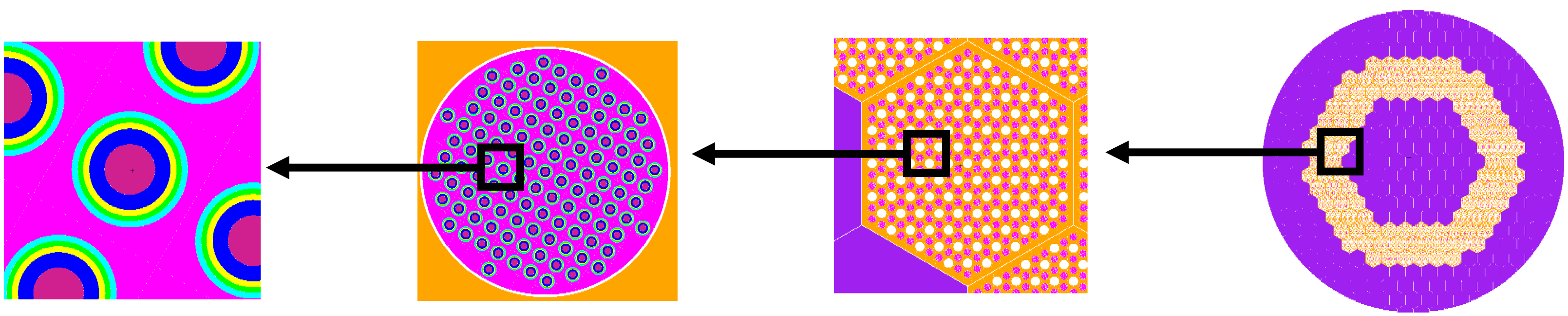
TRISO FUEL PARTICLES

FUEL COMPACTS

FUEL BLOCK



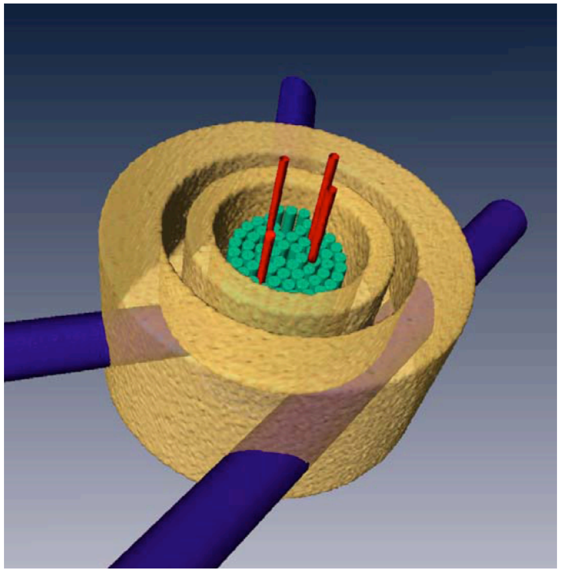
CORE

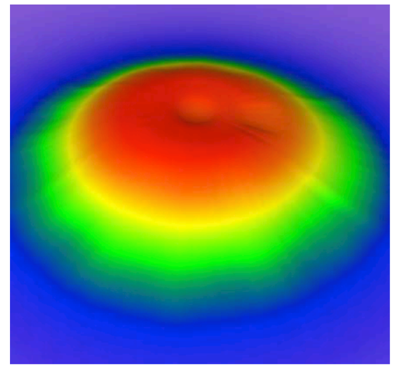
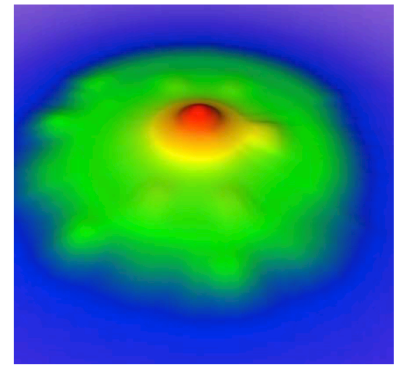
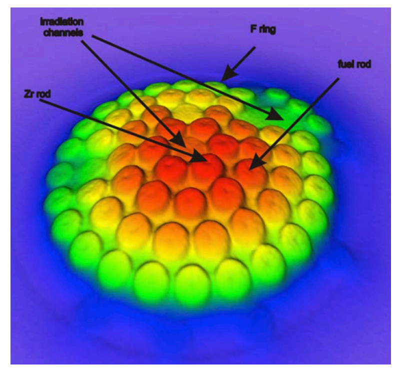
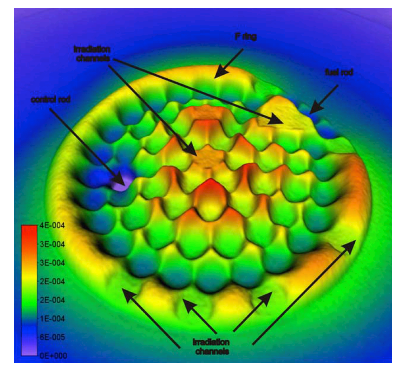


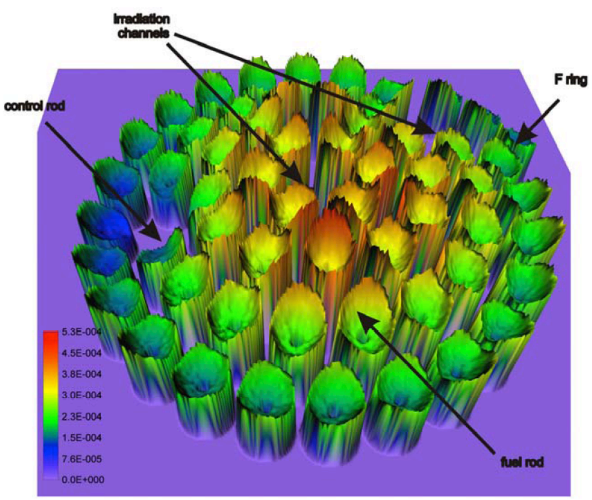
MCNP model - accurate & explicit at multiple levels

TRIGA Reactor LEU Conversion

3D geometry



	Fast Flux	Thermal Flux
Diffusion Theory Codes		
MCNP Analysis		

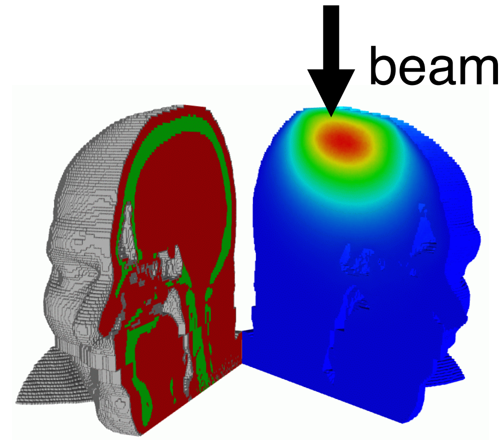


Radial Power Density From MCNP5 Analysis

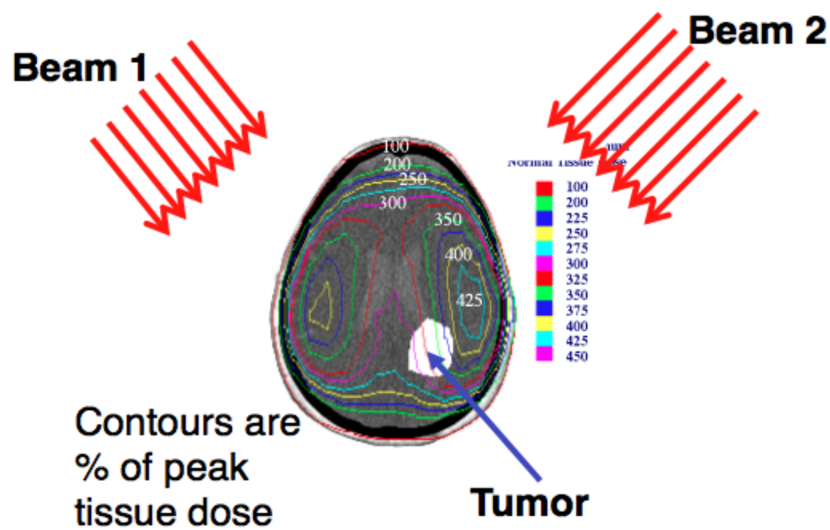
(from Luka Snoj, Jozef Stefan Inst.)

Treatment Planning

- **Calculate dose distributions** throughout target region for different beam orientations.
- Post-process, combine different beams to **maximize dose to tumor & minimize dose to healthy tissue**.
- While the peak tumor and tissue dose are usually based on in-phantom dose rate measurements, the simulation is necessary to determine more advanced parameters, such as the dose volume histogram.

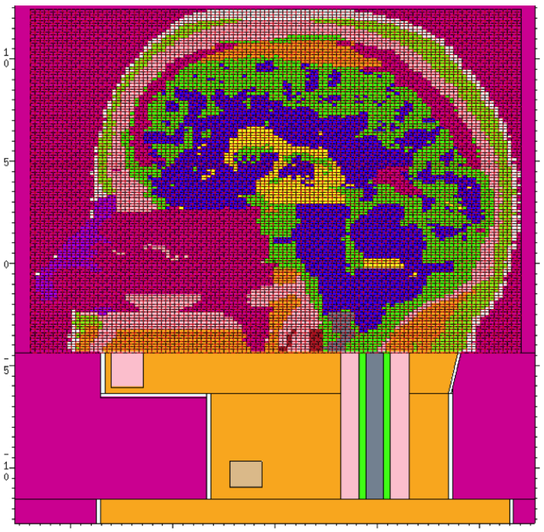


CT Based geometries are possible to represent in MCNP

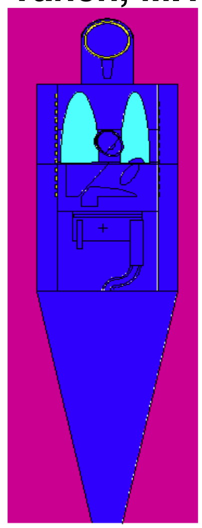


MCNP Examples – Medical Physics (2)

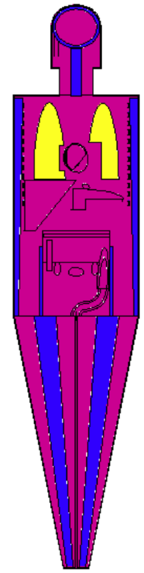
Zubal phantom



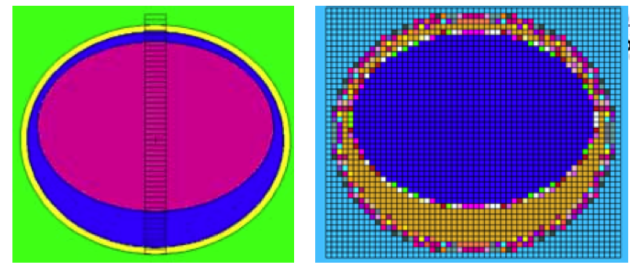
Yanch, MIT



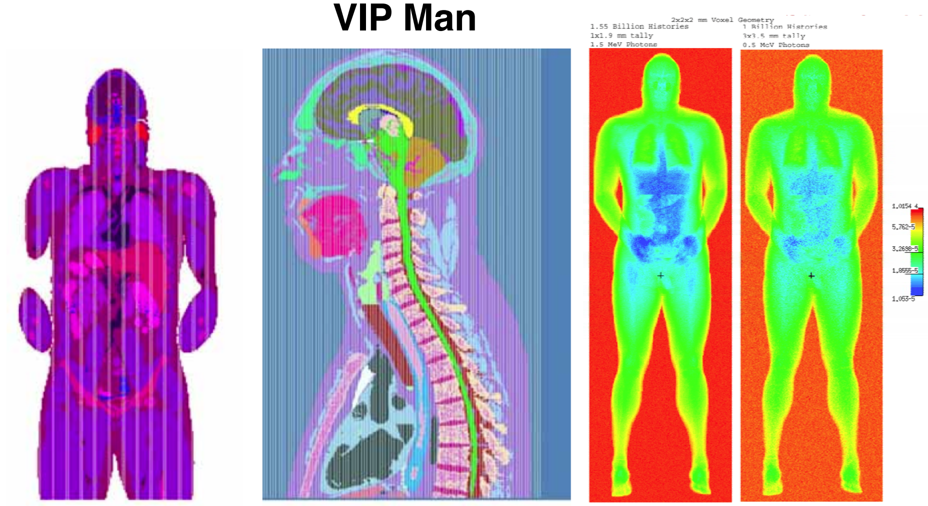
ORNL



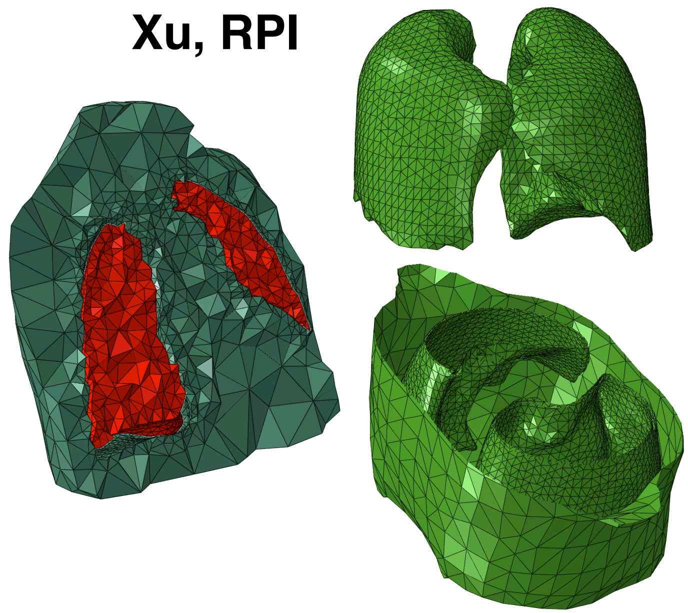
Snyder head phantom



VIP Man

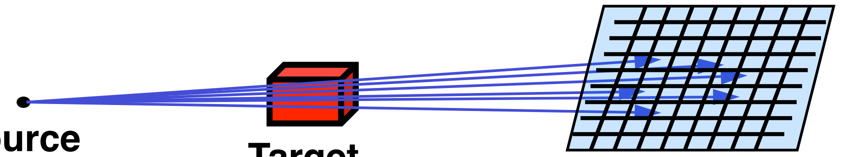


Xu, RPI



MCNP Examples – Radiography Calculations (1)

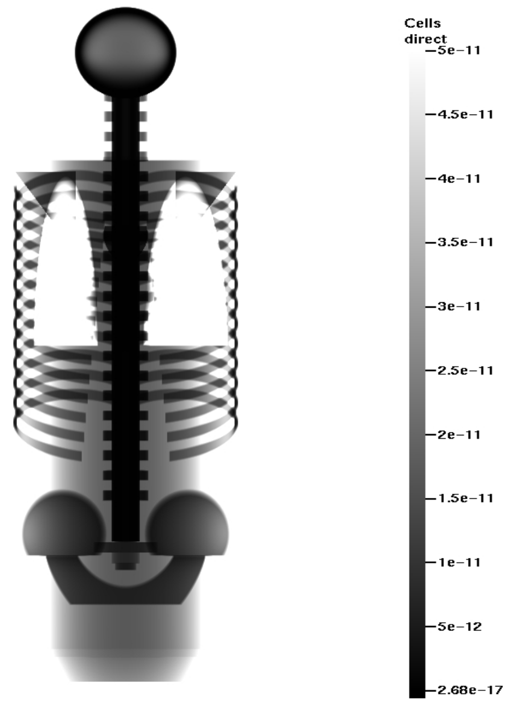
- Radiography tallies



- Neutron and photon radiography uses a grid of point detectors (pixels)
- Each source and collision event contributes to all pixels

MCNP Model of Human Torso

Simulated Radiograph - 1 M pixels

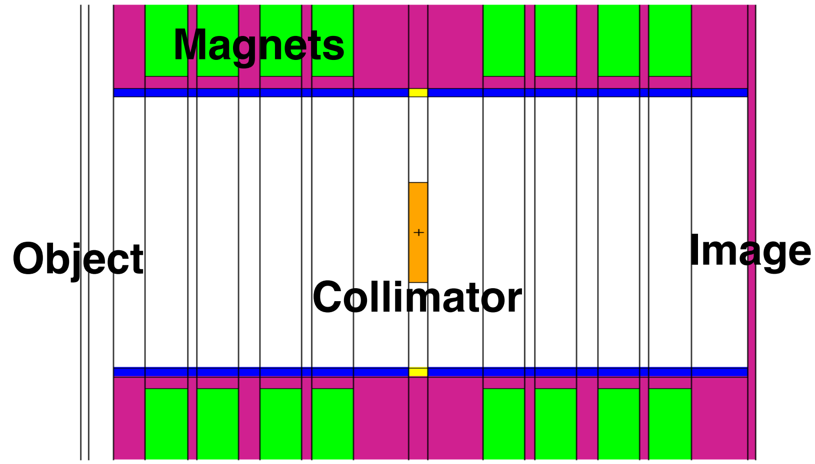


MCNP Examples – Radiography Calculations (2)

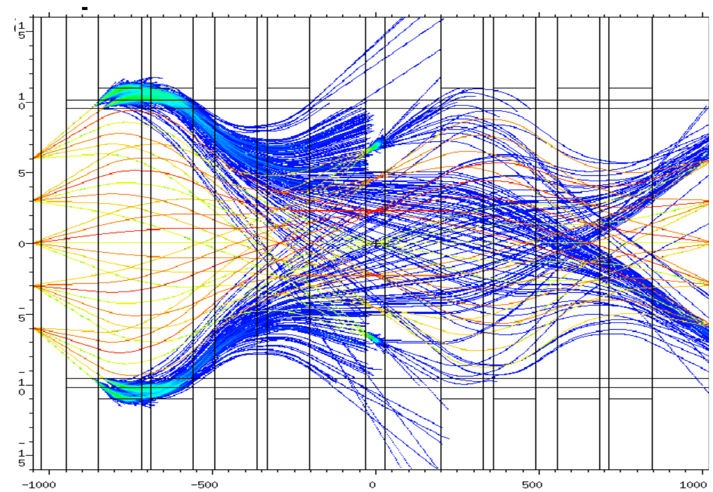
Proton Radiography at LANL & BNL

- Experiments at LANL & BNL use high-energy proton beams directed at test objects
  - LANL: 800 MeV proton beams
  - BNL: 24 GeV proton beams
  - Proposed: 50 GeV proton beams
- Proton beams are collimated & focused by magnetic lenses
- Radiography tallies simulate pixels from detectors
- Experiment design & analysis are modeled with MCNP6

LANSCE pRad, MCNP calculations



Horizontal axis - 0, 3, 6, and 9 mrads



Reactor Analysis with Monte Carlo

Trends
Reality
MCNP – Features
MCNP – R&D

Reactor Analysis with MC - Trends

Bigger, faster computers ➜ more Monte Carlo for reactor analysis

- Computers: 1 billion times faster than 30 years ago
- More: detail, tallies, neutrons, computer runs, …..

1960s:	K-effective [neutron multiplication factor for reactor]
1970s:	K-effective, detailed <u>assembly</u> power
1980s:	K-effective, detailed <u>2D whole-core</u>
1990s:	K-effective, detailed <u>3D whole-core</u>
2000s:	K-effective, detailed 3D whole-core, <u>depletion</u>, <u>reactor design parameters</u>
2010s:	All of above + <u>Total Uncertainty Quantification</u> (impact of uncertainties in cross-sections, manufacturing tolerances, methodology, …)

Reactor Analysis with MC - Reality

- **Realistic commercial PWR & BWR calculations have too much detail for anyone's Monte Carlo codes today**
  - **CASL is focused on PWRs, with conventional analysis tools**
    - MPACT (formerly PARKS) – deterministic, good but many approximations
    - Will extend to BWRs (if funding extended)

- **For <u>small</u> modular reactors (SMR) and <u>small</u> special-purpose reactors for DOD & NASA:**
  - **MUST use Monte Carlo for reactor core physics**
    - **High leakage**
    - **Close coupling in space & energy**
    - **Not separable into $\phi(x,y)$ and $\phi(z)$**
    - **Nearly everyone, everywhere, uses Monte Carlo for reactor core physics for SMRs & small special-purpose reactors**
    - **CASL approach will never get there**
      - **Serious difficulties with conventional multigroup, discrete angle approach used in conventional deterministic codes**

Reactor Analysis with MC – MCNP (1)

Current Features

- Criticality calculations - K-effective & alpha
- Coupled neutron-photon calculations
- 3D geometry, with hierarchical embedding
- Continuous-energy neutron physics & data
- $S(\alpha,\beta)$ thermal scattering treatment
- Perturbation theory
- Validation suites, based on ICSBEP benchmark experiments
- Mesh tallies for 3D power maps, etc.
- Burnup calculations with CINDER90
- Stochastic geometry, for random TRISO fuel
- Shannon entropy for convergence of power
- Adjoint-weighted reaction tallies
- Adjoint-weighted reactor kinetics parameters
- Sensitivity-uncertainty analysis of cross-section data
- etc., etc., etc.

R&D – in progress

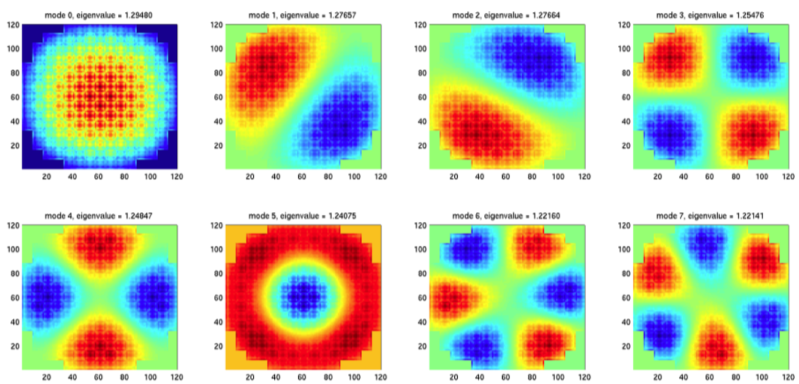
- On-the-fly Doppler broadening of neutron cross-sections
- Improved neutron free-gas scattering at epithermal energies
- Coupled MC & deterministic codes
- Automated variance reduction
- Coincidence, pulse height, light detectors
- Moving geometries
- Higher-mode eigenvalues & eigenfunctions
- Alpha eigenvalue methods, for time-dependent calculations
- Multiphysics
- Parallel calculation methods, for GPUs & MICs, for coming Exascale systems
- Code modernization & restructuring

Focus: faster, bigger, high fidelity, user needs, preserve V&V

Reactor Analysis with MC – MCNP R&D (2)

Monte Carlo Codes, XCP-3

- **Fission Matrix**
  - **Higher eigenvalues & eigenmodes**
  - Dominance ratio
  - Perturbation/transient analysis
  - Accelerate convergence
  - Novel sparse storage scheme provides high resolution, eliminates approximations

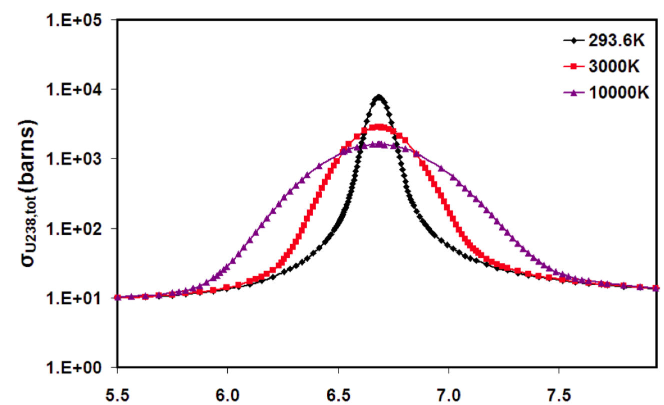


$$S_I = \frac{1}{K} \cdot \sum_{J=1}^{N} F_{I,J} \cdot S_J$$

- **On-The-Fly Doppler Broadening**
  - Continuous temperature capability, without precomputing 1000s of xsecs
  - Necessary for multiphysics:
    MC + TH + FEM + **...**

OTF Methodology (for each nuclide)

- Union energy grid for a range of T's
- High-precision fits for σ(E,T) vs T
- MCNP – evaluate σ(E,T) OTF during simulation



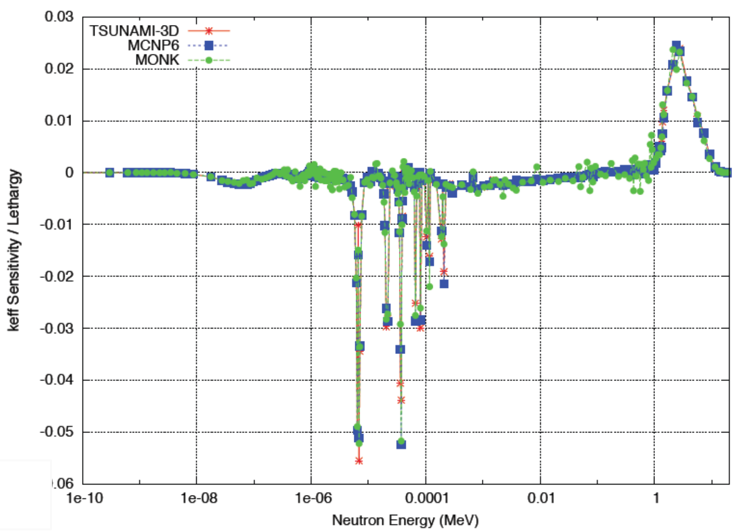
- Current R&D project on temperature coefficients with Univ. of New Mexico.

Both – collaboration with Univ. Michigan

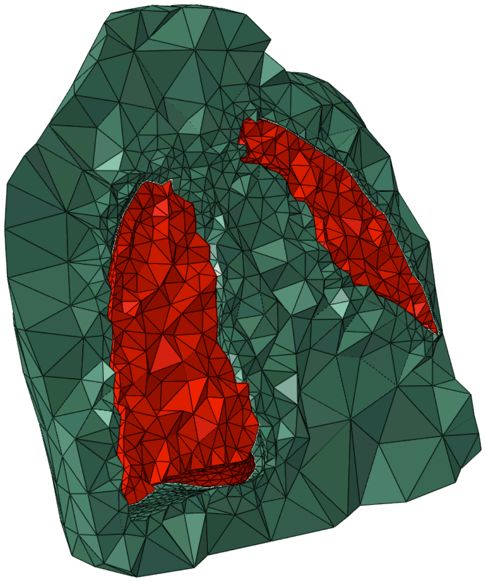
Reactor Analysis with MC – MCNP R&D (3)

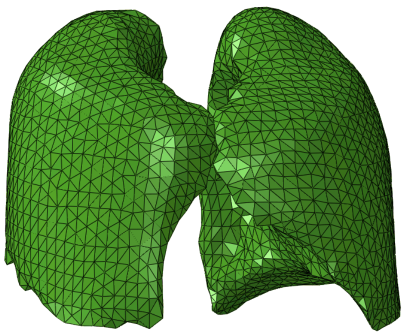
- **Sensitivity Coefficients to K_{eff} in Continuous-Energy**
  - Uses adjoint-weighted perturbations
  - Computes sensitivity coefficients for cross sections, fission, & scattering laws
  - User-defined energy resolution for results or tallies – no discretization

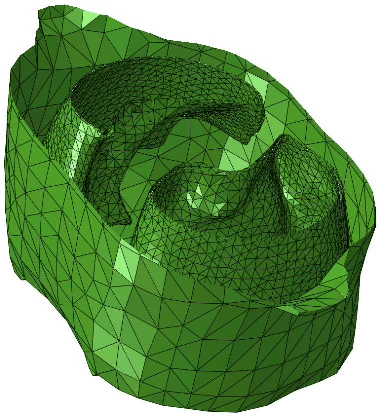
MOX Lattice: U-238 Total



- **MCNP6 Mesh Geometry**
  - 3D unstructured mesh
  - Embedded in 3D MCNP geometry
  - Many applications
    - Radiation treatment planning
    - Linkage to Abaqus







Going Forward

MCNP Work Needed for Reactors
Concerns
Conclusions

Going Forward – MCNP Work Needed for Reactors

- Limited to ~20K fuel materials with fission products, need millions
- Parallel threads+MPI for >10 years, needs work for petaflop systems
- Power defect: epithermal free-gas scatter ignores resonance scatter
- Reactor design depends on computing many design products (α_T, rod worth, etc.)
- Criticality searches – rods, boron, B^2
- Self-consistent equilibrium Xenon
- Temperature distributions
- Sensible units – °K, sec, W
- Combinations & ratios for tallies
- Multigroup cross-section generation
- More robust tracking gap/overlap fixup

- Library of standard materials
- Problem setup - more user-friendly
- Hexagonal meshes for geometry & tallies
- Improved output
- Standard file formats for linkage to other codes
- Reactor depletion improvements - branches, better predictor-corrector, inline equilibrium Xenon
- Automated weight-window generation
- Improved parallel processing efficiency for large reactor caclulations
- Simpler, automated setup for TRISO fuel
- Delayed-neutrons in alpha-eigenvalue calculations
- Etc., etc., etc.

Going Forward – Concerns

- **MCNP support**
  - **DOE/NNSA - Advanced Computing & Simulation (ASC)**
  - **DOE/NNSA - Nuclear Criticality Safety Program (NCSP)**
  - Some other odds & ends (DTRA, DHS, NASA, etc.)
  - No support from DOE/NE or NRC

  ➜ **Low priority for developing reactor core analysis features**

  ➜ **Serendipity with NCSP, but only goes so far …..**

- **Compare with another effort**
  - **US DOE Naval Reactors:**
    - **10 year effort, many people – total upgrade & overhaul of MC capabilities**
    - **Naval design labs will do nearly all reactor core physics analysis with MC, including burnup & coupling to thermal/hydraulics codes.**
  - **Same general approach proven for naval reactors analysis could be used for advanced analysis methods for current small reactors & future PWR/BWRs**

Going Forward – Conclusions

- **MCNP Monte Carlo has a long history & well-deserved reputation – tool of choice when best answers are needed**
- **MCNP is used for some parts of reactor physics analysis by nearly everyone at labs, industry, universities**
- **Current & planned capabilities permit nearly all reactor analysis needed for <u>small</u> cores**
- **Much work is needed to extend to <u>large</u> cores (and bigger computers)**
- **Major effort to modernize & improve MCNP is beginning**
- **Focus for improvements is driven by needs of ASC, NCSP, & some others**