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Title: Advances in Sensitivity Analysis with MCNP

Author(s): Kiedrowski, Brian C.

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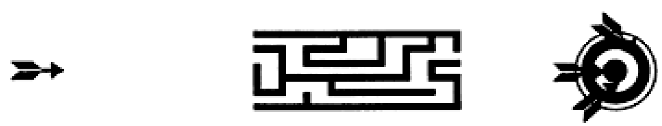
Advances in Sensitivity Analysis with MCNP



Brian Kiedrowski

Monte Carlo Codes (XCP-3)

Los Alamos National Laboratory

Presented at University of New Mexico (03/05/2013)

Abstract

Monte Carlo codes such as MCNP are used extensively in preventing inadvertent nuclear criticalities in processes involving fissionable material. Their ability to do this relies on the accuracy of the simulation tools, the underlying nuclear data libraries, and their validation of relevant experiments. Recent development of an inline method for importance or adjoint weighting with continuous-energy Monte Carlo in MCNP has allowed for the calculation of sensitivity coefficients without the need of meshes or multigroup collapse, unlike previously available tools. These capabilities allow for quantitative comparisons of processes to benchmark experiments and uncertainty quantification for the calculation of biases and safety margins. The current state-of-the-art is discussed, as well as future research avenues.

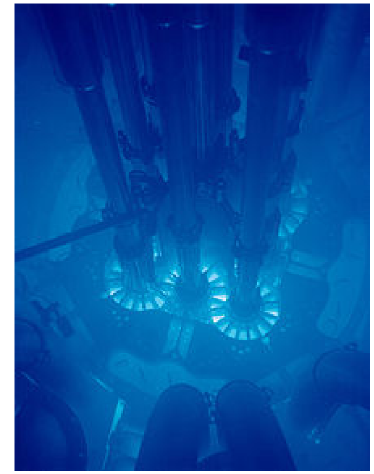
Overview

- How can we be confident that simulation tools can accurately predict criticality of a given process involving fissionable material?

- Roadmap of this talk
  - Overview of Monte Carlo method, MCNP
  - Code and Nuclear Data Validation
  - Inline Importance-Weighting Method in MCNP for Sensitivity Coefficients
  - Application of Sensitivity Analysis to Code Validation
  - Future Prospects

Fissionable Material Operations

- **Need to understand nuclear criticality of operations**



Accomplished by…

- **Experiments**
  - Ideal option, and only one in the early days
  - Difficult and expensive to perform in modern regulatory environment
  - Few facilities available today

- **Computer Simulations**
  - With modern computing, this has become the preferred option
  - Mature software, nuclear data, computational platforms
  - Often good quantitative agreement with experiment

- **Both supplement each other!**

Neutronics Simulation

Leakage Collisions Scattering

$$\left[\vec{\Omega}\cdot\nabla + \Sigma_T(\vec{r},E)\right]\cdot\psi(\vec{r},E,\vec{\Omega}) = \iint \psi(\vec{r},E',\vec{\Omega}')\Sigma_S(\vec{r},E'\rightarrow E,\vec{\Omega}\cdot\vec{\Omega}')\,d\vec{\Omega}'dE'$$

Fission

$$+ \frac{1}{k_{eff}}\frac{\chi(\vec{r},E)}{4\pi}\iint \nu\Sigma_F(\vec{r},E')\psi(\vec{r},E',\vec{\Omega}')\,d\vec{\Omega}'dE'$$

- **Solve the neutron transport equation.**

- **Methods of solution:**
  - **Deterministic methods: diffusion theory, discrete ordinates (SN), etc.**
  - **Monte Carlo**

Codes for Criticality Calculations

Code	Method	Space	Energy	Angle
MCNP5	Monte Carlo	exact	exact, groups	exact
MCNP6	Monte Carlo	exact, mesh (regular), mesh (unstructured)	exact, groups	exact
COG	Monte Carlo	exact	exact	exact
KENO-IV	Monte Carlo	exact	groups	exact
KENO-Va, -VI	Monte Carlo	exact	exact, groups	exact
SCALE / CSAS	Monte Carlo	exact	groups	exact
DENOVO	Sn, Discrete Ordinates	mesh (regular)	groups	rays
PARTISN	Sn, Discrete Ordinates	mesh (regular)	groups	rays
ATILLA	Sn, Discrete Ordinates	mesh (unstructured)	groups	rays

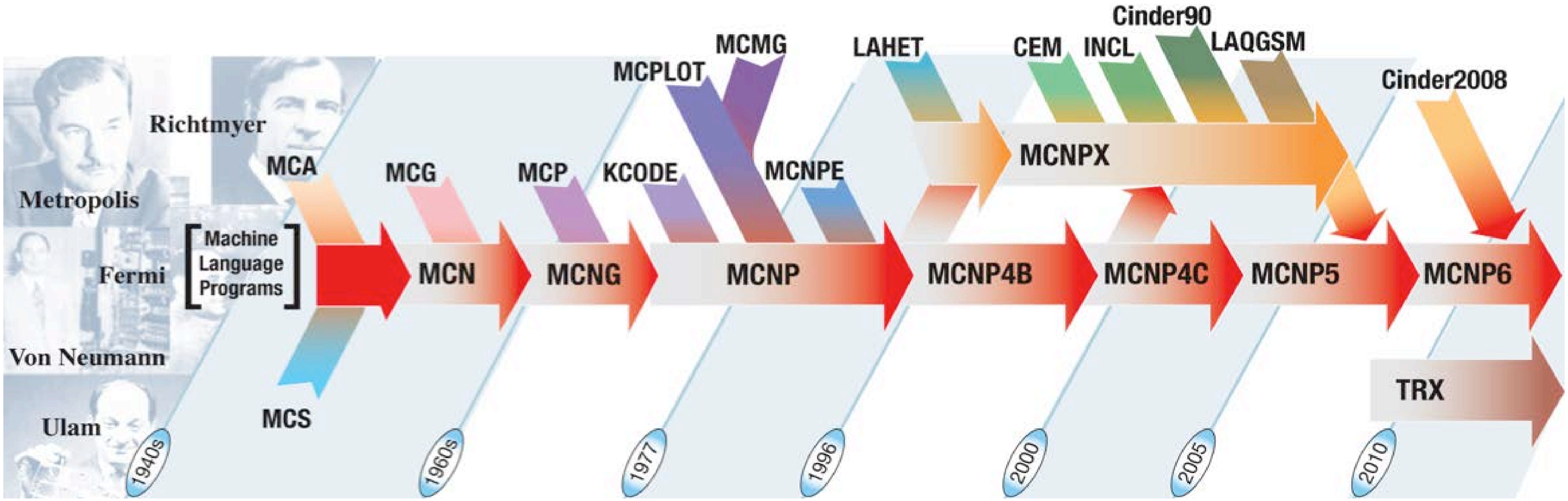
Monte Carlo Method

- **The Monte Carlo method does not "solve" the equations in a direct, mathematical sense**

- **Rather, it simulates the underlying radiation physics that the equation describes**
  - **The neutron transport equation describes mean-value radiation behavior.**
  - **Monte Carlo calculates "tallies" for quantities (e.g., reaction rates) that are mean values of the underlying radiation physics.**
  - **Because the tally quantities correspond to those from the neutron transport equation, its solution can be inferred.**

- **The eigenvalue problem is solved iteratively**
  - **Guess keff and flux, transport neutrons one iteration, which corresponds to a single fission generation.**
  - **After many iterations, the process converges and results may be obtained.**

MCNP History



- **MCNP release package distributed by RSICC**

  MCNP5-1.60 + MCNPX-2.70 + MCNP6-Beta +
  Nuclear Data Libraries + MCNP Reference Collection

- **MCNP6-Beta-3 release Jan-2013, MCNP6 production release mid-2013**

- **MCNP5 & MCNPX are frozen – future development will occur in MCNP6**

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

MCNP6

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

mcnp6

mcnp6
protons, proton radiography
high energy physics models
magnetic fields

Partisn mesh geometry
Abaqus unstructured mesh

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

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

Sensitivity/Uncertainty Analysis
Fission Matrix
OTF Doppler Broadening

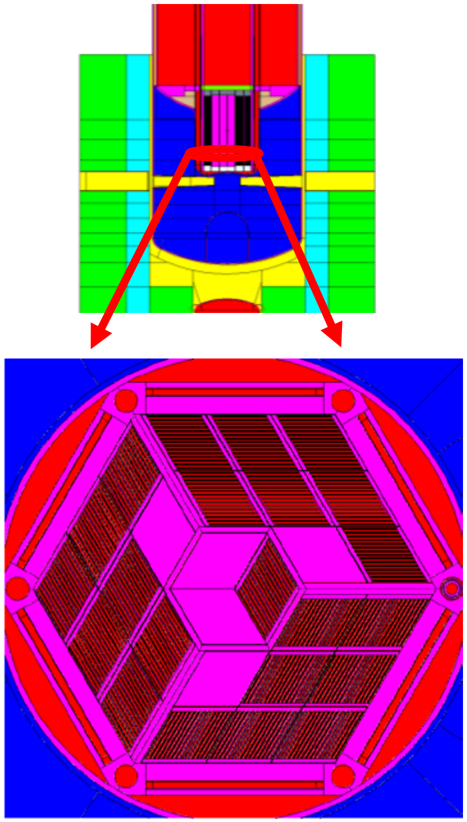
Continuous Testing System
~10,000 test problems / day

mcnp5 – 100 K lines of code
mcnp6 – 400 K lines of code

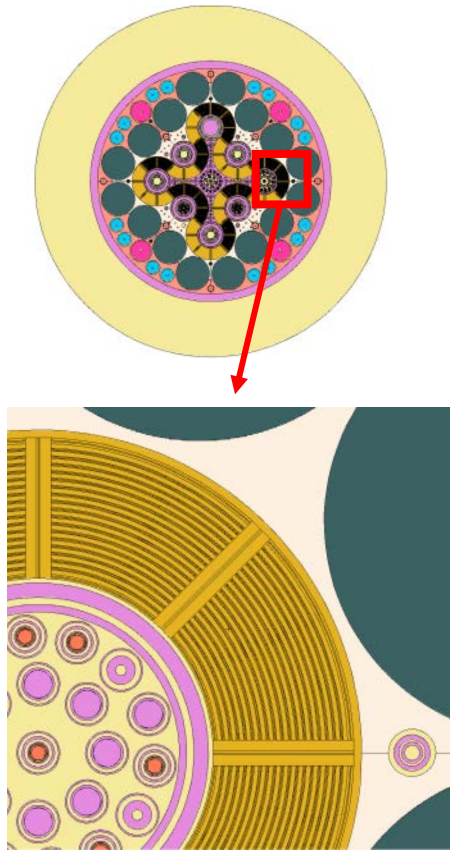
MCNP = Benchmark for Nuclear Reactor Design codes

Monte Carlo Codes
XCP-3, LANL

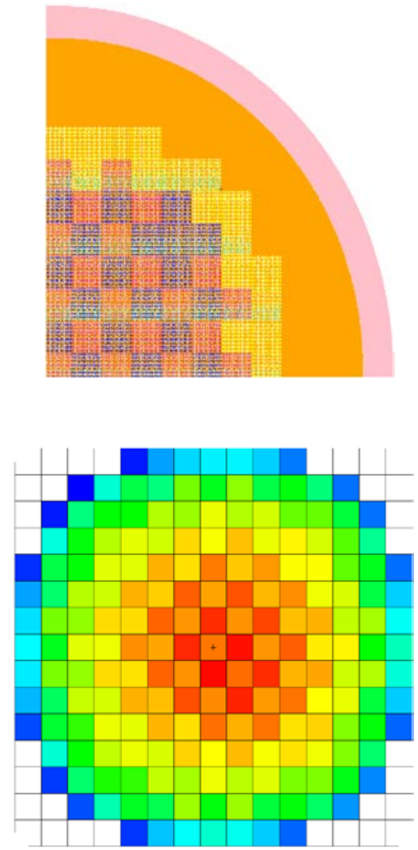
MIT
Research Reactor



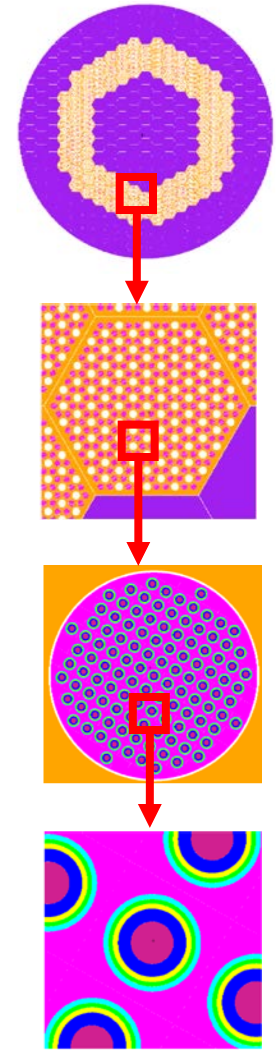
ATR
Advanced Test Reactor



PWR
Pressurized Water Reactor



VHTR
Very High Temperature Gas-Cooled Reactor

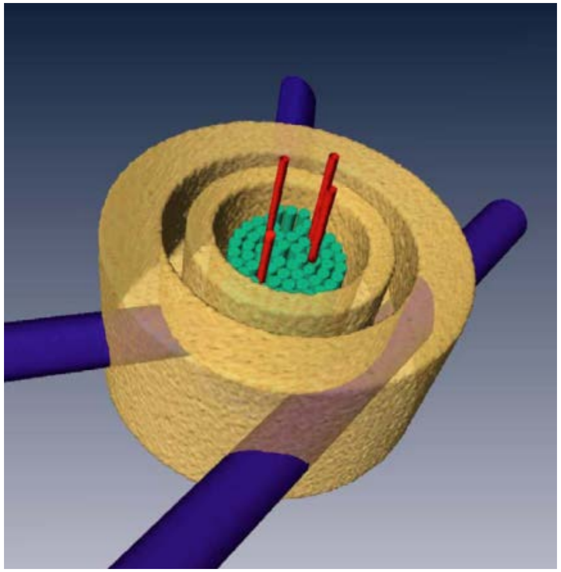


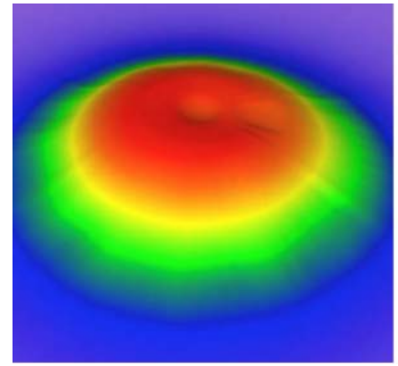
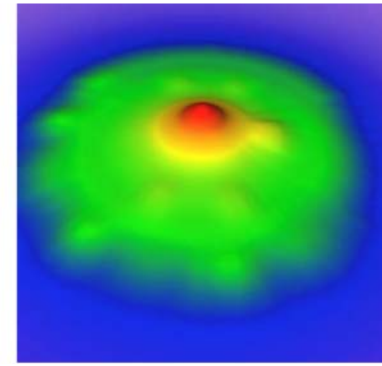
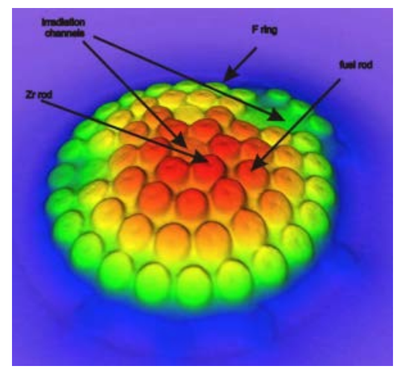
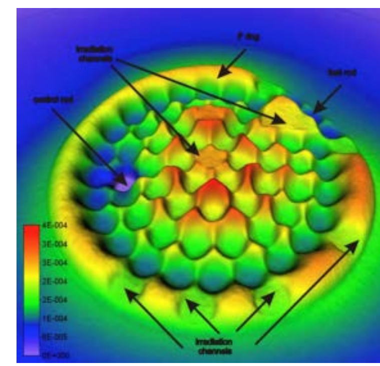
- **Accurate & explicit modeling at multiple levels**
- **Accurate continuous-energy physics & data**

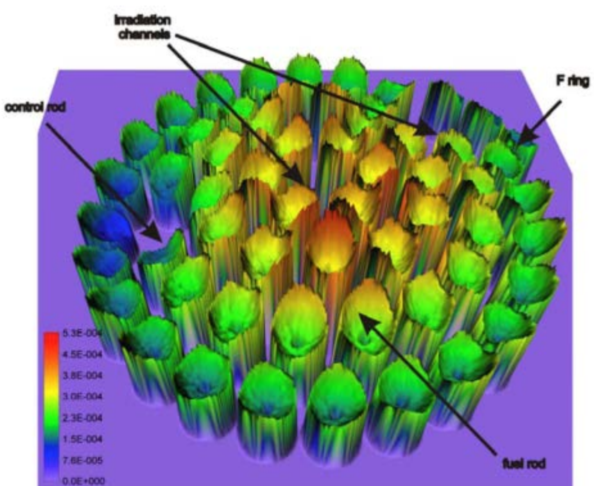
MCNP - TRIGA Reactor LEU Conversion

Monte Carlo Codes
XCP-3, LANL

3D geometry



	Fast Flux	Thermal Flux
Diffusion Theory Codes		
MCNP5 Analysis		

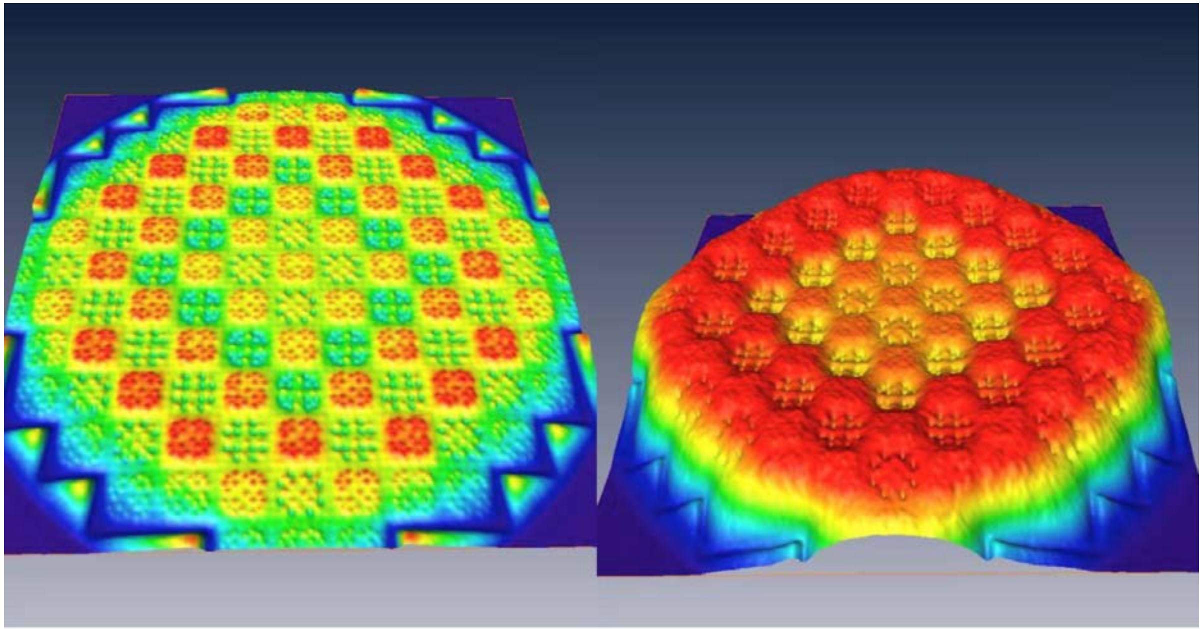


Radial Power Density From MCNP5 Analysis

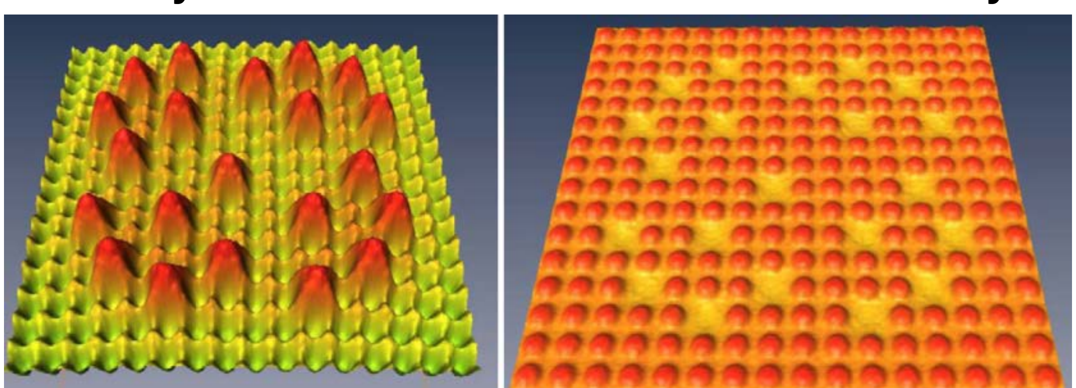
(from Luka Snoj, Jozef Stefan Inst.)

MCNP - PWR Analysis

Whole-core Thermal & Total Flux from MCNP5 Analysis



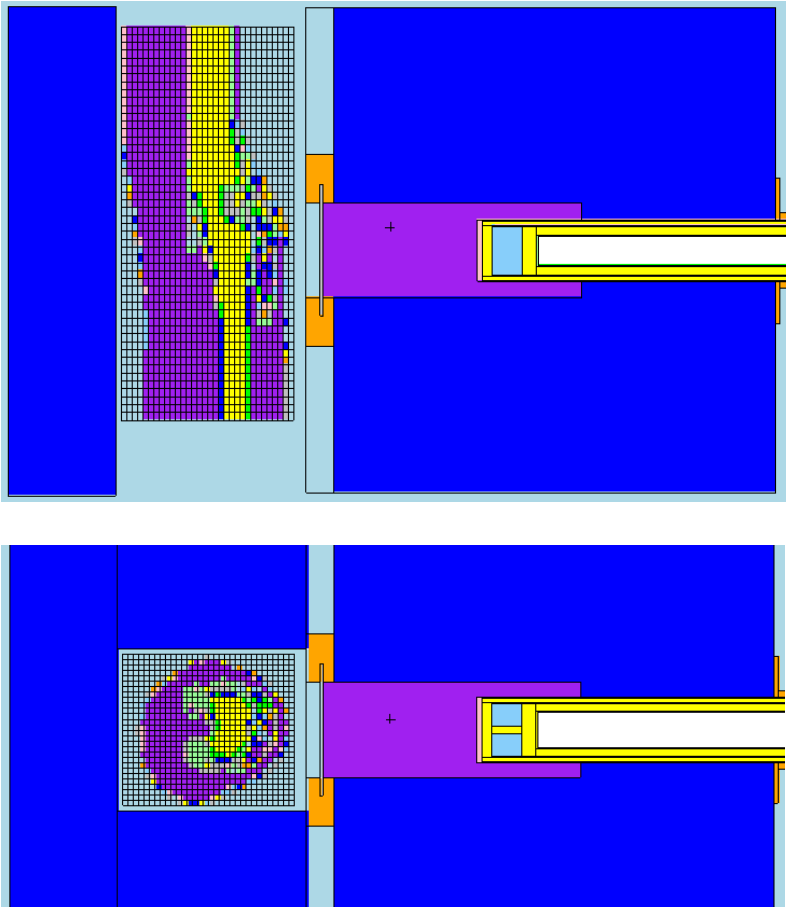
Assembly Thermal & Fast Flux from MCNP5 Analysis



(from Luka Snoj, Jozef Stefan Inst.)

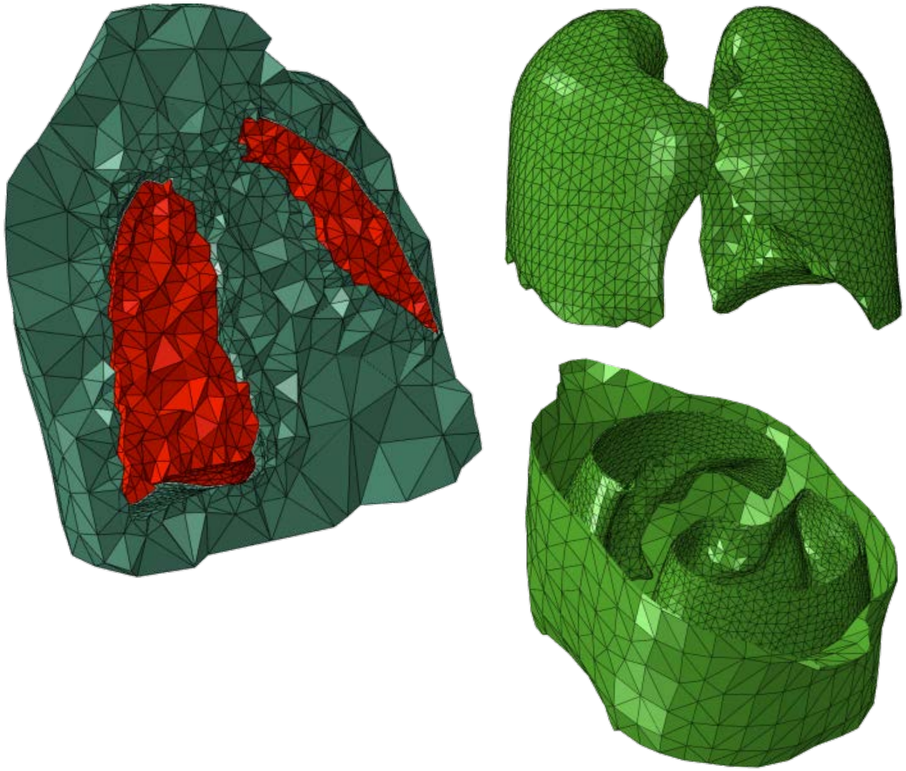
Medical Physics

- Patient-CT based model of **knee & end of accelerator**
- **Calculate dose throughout knee**



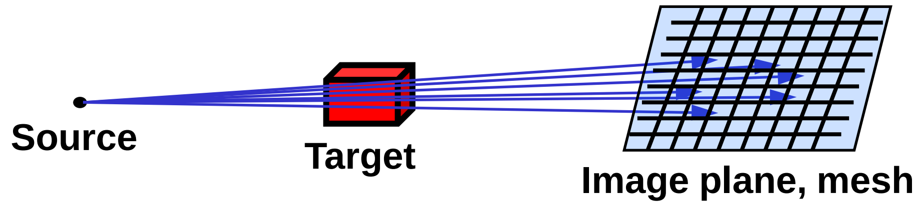
Pictures from mcnp plotter

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



Radiography Calculations

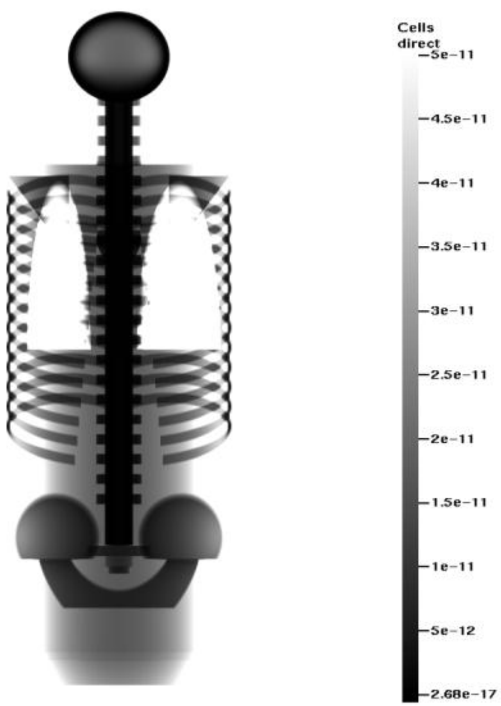
- Radiography tallies



- 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

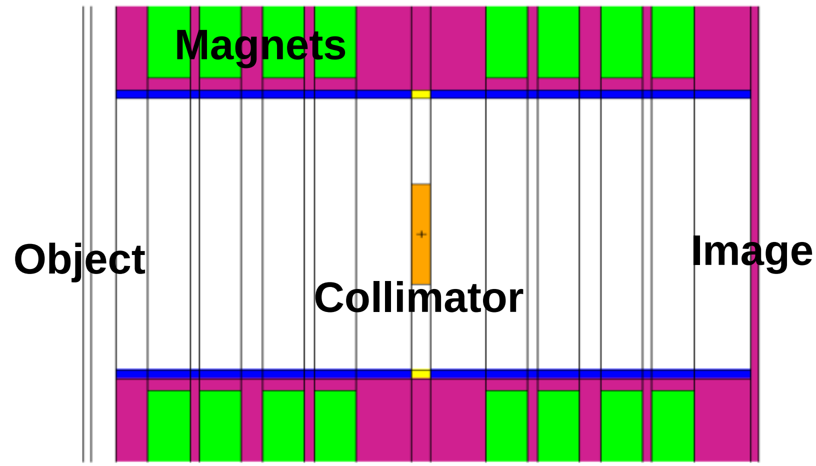
Simulated Radiograph - 1 M pixels



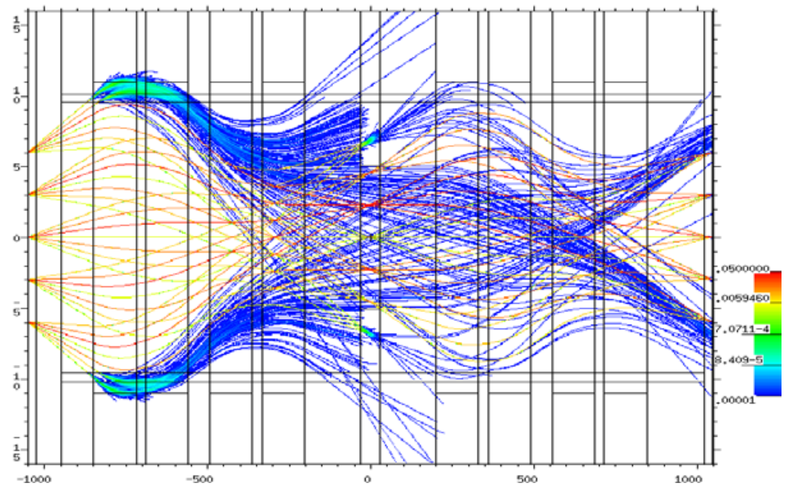
MCNP6 – Proton Radiography

- **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**

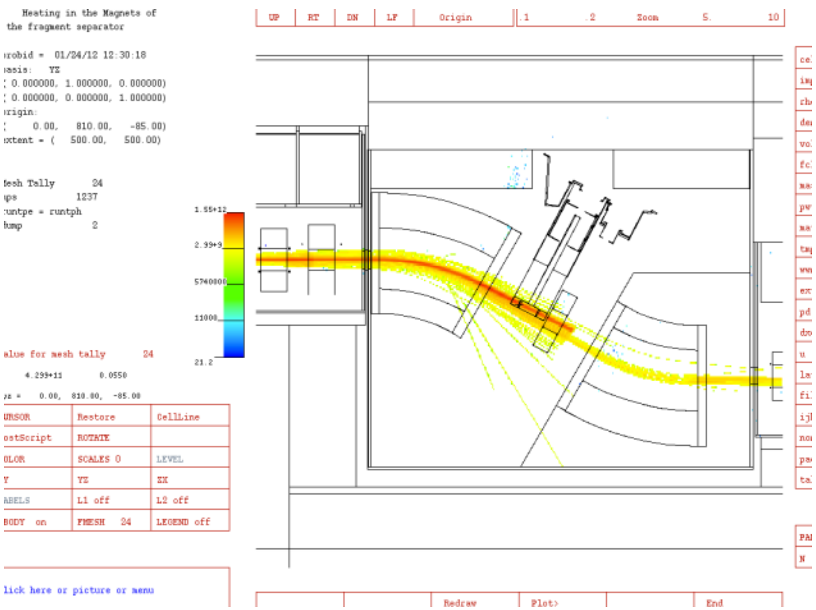
LANSCE pRad, MCNP6 calculations



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



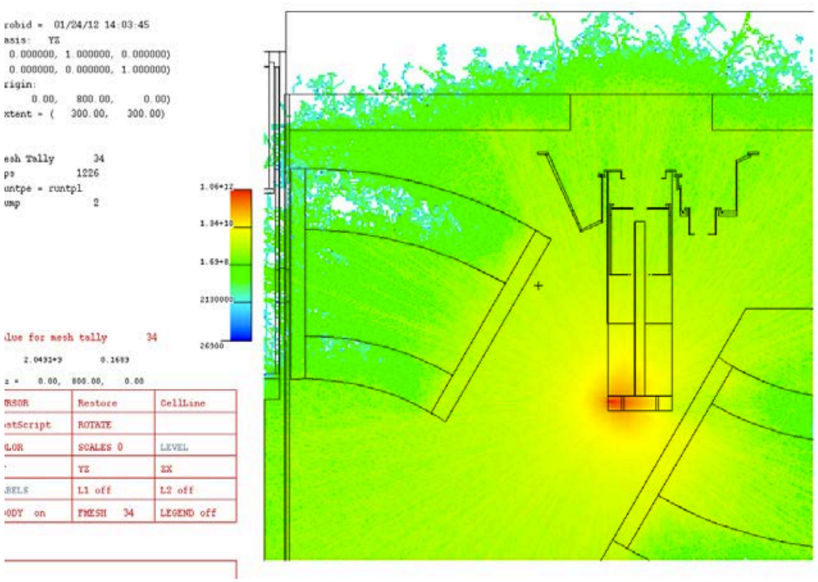
MCNP6 - User Example



Primary ion beam as it collides with the beam dump

^{48}Ca ion beam, 26.3 GeV/ion

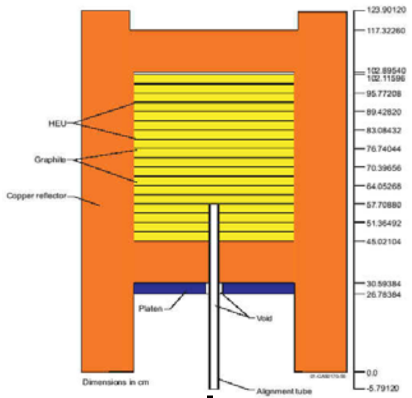
With magnetic field focusing



Neutron field produced by ion beam collisions with target

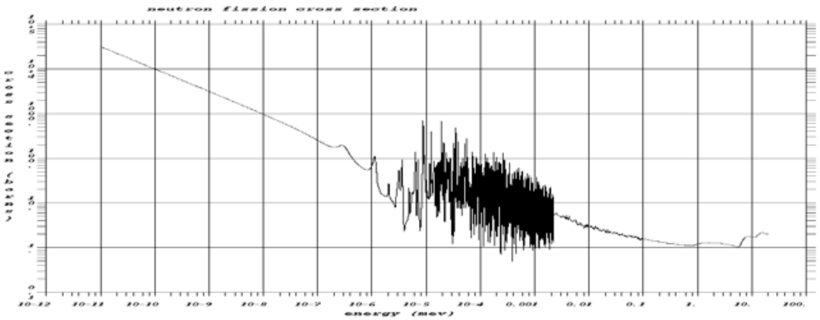
Neutronics Simulation

Code Model



Process/Experiment

Nuclear Data



MCNP

<u>Results:</u> keff, doses, reaction rates, etc.

How Can We Believe Codes?

- **Codes and nuclear data must be <u>verified</u> and <u>validated</u>.**

- **Verification**
  - **Testing that the code is performing the algorithms as expected.**
  - **Comparisons to analytic solutions, other methods, codes, etc.**
  - **Primarily done as part of the software quality assurance process.**

- **Validation**
  - **Testing that the code, methods, and data accurately predict reality.**
  - **Compare code results to measurements from experimental benchmarks.**
  - **Done by both the software development teams AND the end users, as validation is application specific.**

MCNP Verification & Validation Suites

- ## MCNP V&V Suites
  - **VALIDATION_CRITICALITY** — 31 ICSBEP experiment benchmarks
  - **VALIDATION_CRIT_EXPANDED** — 119 ICSBEP experiments
  - **CRIT_LANL_SBCS** — 194 ICSBEP experiments, from LANL crit-safety group
  - **VERIFICATION_KEFF** — 75 analytic benchmarks, exact solutions
  - **VALIDATION_ROSSI_ALPHA** — Rossi alpha vs experiment
  - **VERIFICATION_GEN_TIME** — Analytic + PartiSN solutions for neutron generation time
  - **KOBAYASHI** — void & duct streaming, with point detectors, exact solutions
  - **VALIDATION_SHIELDING** — 19 shielding/dose experiments
  - **REGRESSION** — 147 code test problems
  - many others for MCNP6 — electrons, protons, muons, high-energy physics, delayed particles, magnetic fields, point detectors, MCNP6/Partisn weight window generator, unstructured mesh & ABAQUS linkage, photons, pulse height tallies, string theory models

- ## Focus
  - Physics-based V&V, compare to experiment or exact analytic results
  - Part of MCNP permanent code repository & RSICC distribution
  - Automated, easy execution & comparison to experiments
  - Ongoing work task for **DOE/NNSA Nuclear Criticality Safety Program**

End-User Validation

- Users of computational tools like MCNP must ensure that the code and nuclear data is validated for their specific application.
  - Applies to all applications: shielding, detectors, reactors, etc.
  - Especially important when processes have inadvertent criticality as a concern.

- Identify experimental benchmarks that are similar to the process and have appropriate measured data.
  - Databases of experiments are available (e.g., International Criticality Safety Benchmark Evaluation Project Handbook).
  - However, must identify benchmarks that are like the process being analyzed.
  - Qualitative comparisons of geometry, materials, spectra, etc.
  - For nuclear data, quantitative comparisons may use sensitivity analysis.

Sensitivity Analysis

- The sensitivity coefficient gives the ratio of the relative change in a response *R* because of a relative change in some parameter *x*.

$$S_{R,x} = \left(\frac{\Delta R}{R}\right) \Big/ \left(\frac{\Delta x}{x}\right) = \frac{x}{R}\frac{\Delta R}{\Delta x}$$

- For this talk, the response *R* is the effective multiplication factor *k*, and x implies some nuclear data (e.g., cross section).
  - Nuclear data are usually the dominant source of uncertainty and error in Monte Carlo neutronics calculations.

- The magnitude of the sensitivity coefficient determines its ability to influence *k* of a system.

Sensitivity Capabilities

- **Sensitivity analysis is a well established technique**
  - **Decades at ANL with deterministic codes**
  - **About a decade at ORNL with multigroup Monte Carlo (TSUNAMI)**

- **MCNP6 includes a continuous-energy capability to compute sensitivity coefficients**
  - **More accurate: continuous in energy, space, and angle (no mesh).**
  - **No need to include effect of self shielding because of multigroup collapse.**
  - **Inline generation of “importance functions” means a single calculation.**
  - **First-of-a-kind capability, compares well with existing methods (see *Nucl. Sci. & Engr*. in July 2013).**

Sensitivities with Monte Carlo

- **Compute sensitivity coefficients with linear perturbation theory:**

$$S_{k,x} = \frac{x}{k}\frac{dk}{dx} = -\frac{\left\langle \psi^{\dagger}, \left(\Sigma_x - \mathbf{S}_x - k^{-1}\mathbf{F}_x \right) \psi \right\rangle}{\left\langle \psi^{\dagger}, \mathbf{F}\psi \right\rangle}$$

- **Description:**
  - **The brackets denote integration over relevant phase space (position, energy, direction).**
  - **The ψ with the dagger is an importance function (coming up!).**
  - **The boldface S and F represent the integrals for scattering and fission.**
  - **Sensitivities may be functions of position, energy, and (possibly) direction.**

Adjoint Transport Equation

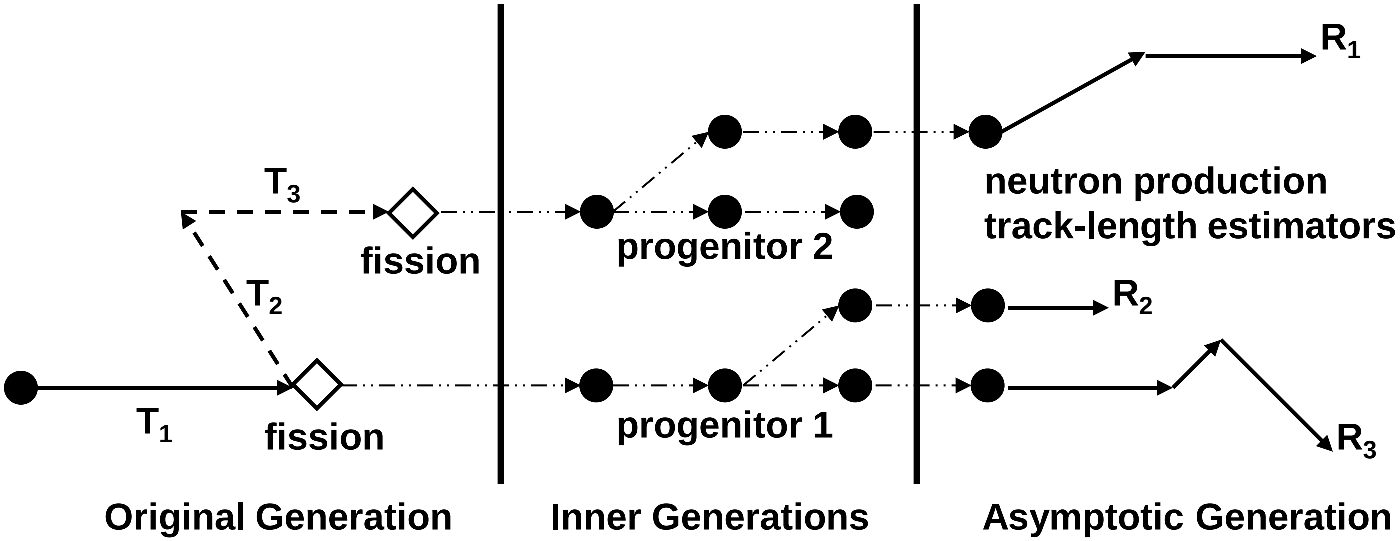
$$\left[-\vec{\Omega}\cdot\nabla + \Sigma_T(\vec{r},E)\right]\cdot\psi^{\dagger}(\vec{r},E,\vec{\Omega}) = \iint \psi^{\dagger}(\vec{r},E',\vec{\Omega}')\Sigma_S(\vec{r},E\rightarrow E',\vec{\Omega}\cdot\vec{\Omega}')\,d\vec{\Omega}'dE'$$

$$+ \frac{\nu\Sigma_F(\vec{r},E)}{k_{eff}}\iint \frac{\chi(\vec{r},E')}{4\pi}\psi^{\dagger}(\vec{r},E',\vec{\Omega}')\,d\vec{\Omega}'dE'$$

- **The adjoint transport equation gives the importance function**
  - **The importance function is proportional to the ability of a neutron at a specific position, energy, direction of driving the self-sustaining chain reaction.**
- **Physically, this can also be thought of this way:**
  - **Introduce a single neutron into an assembly at a specific position, energy, and direction.**
  - **Measure the neutron population in the reactor after an infinite amount of time.**
  - **Repeat this process, and the average is proportional to the importance or adjoint function at that location.**

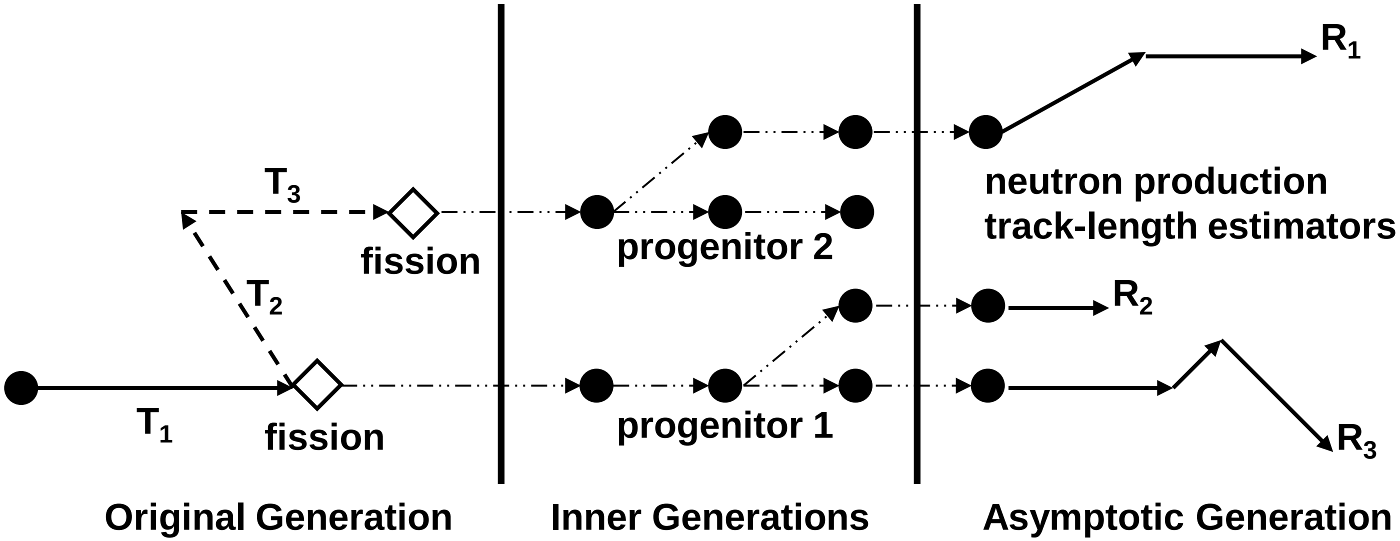
Inline Solution by Monte Carlo

- **Monte Carlo solves eigenvalue problem by an iterative process**
  - **Each iteration corresponds to a fission generation.**
  - **Introduce the concept of blocks or outer iterations of several generations (typically 5 to 10) to solve the adjoint function.**
  - **Purpose is to solve for an integral of an importance function times a kernel (e.g., scattering cross section) times the flux.**



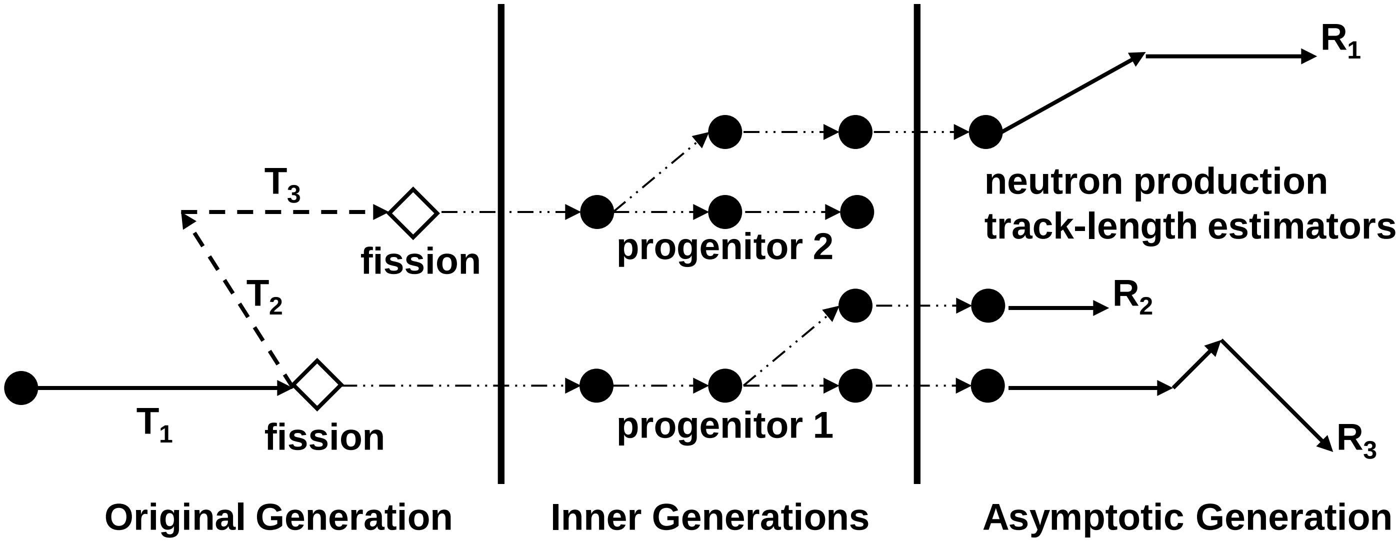
Inline Solution by Monte Carlo

- **In the first (original) iteration (generation):**
  - Record events representing the kernel times the neutron flux (normal Monte Carlo tallies).
  - For each recorded event, tag the neutrons, and associate tags with their events.
  - Events and tags should be combined as mathematically possible to limit storage requirements.
  - Progeny of neutrons from fission inherit their tags.



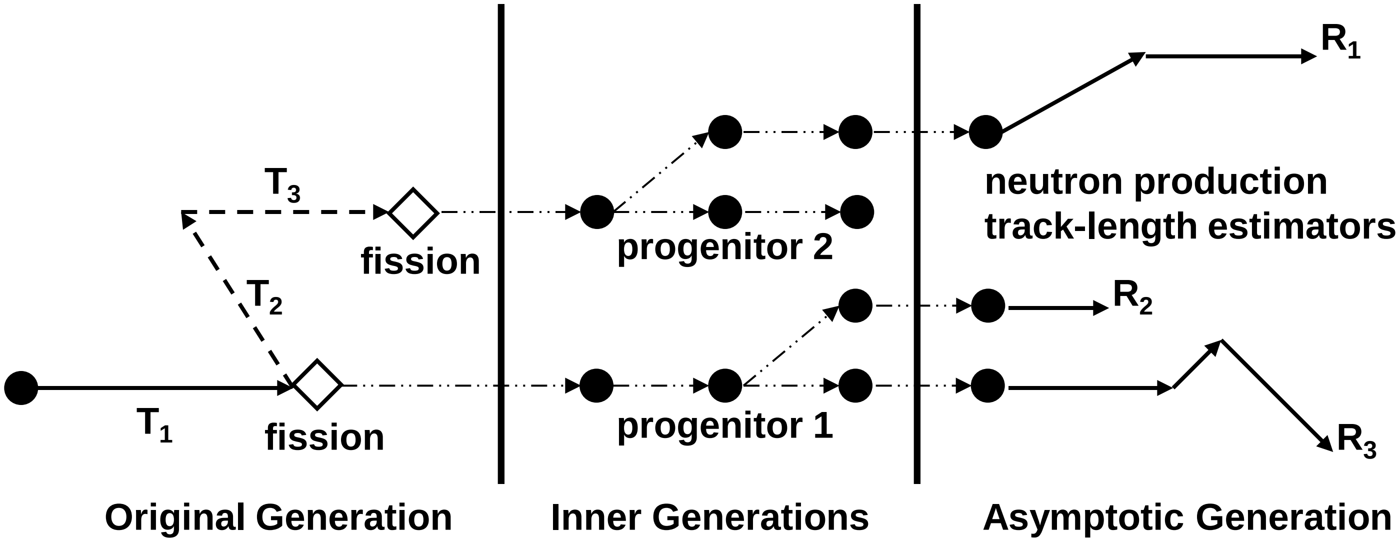
Inline Solution by Monte Carlo

- **In the subsequent (inner) iterations:**
  - Neutron progeny inherit their tags.
  - No additional scores made to the tallies until the final (asymptotic) generation.



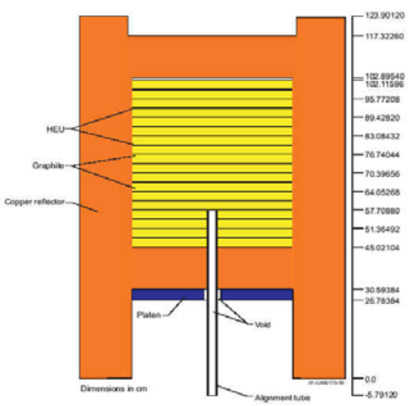
Inline Solution by Monte Carlo

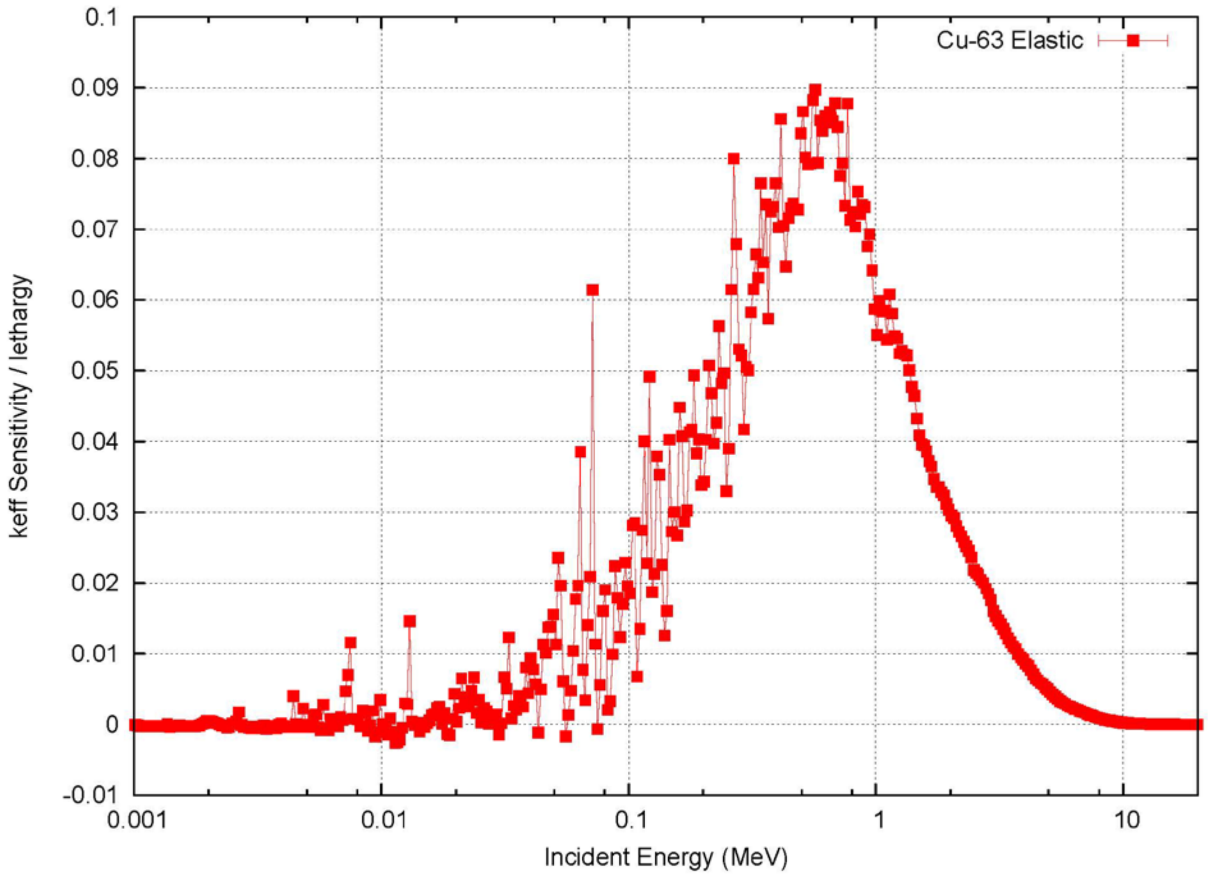
- **In the final (asymptotic) iteration in the block:**
  - **Neutron populations are assumed to be converged to their asymptotic value (i.e., infinite time).**
  - **Record the number of neutrons produced by a track-length estimator of fission neutron production.**
  - **Multiply these by their appropriate scores from recorded events to estimate the importance-weighted integrals by Monte Carlo.**
  - **Estimate sensitivity coefficients, repeat outer iterations.**



Example Sensitivity Profile

- **Cu-63 Elastic Scattering Sensitivity in Copper-Reflected Zeus experiment as a function of neutron energy:**





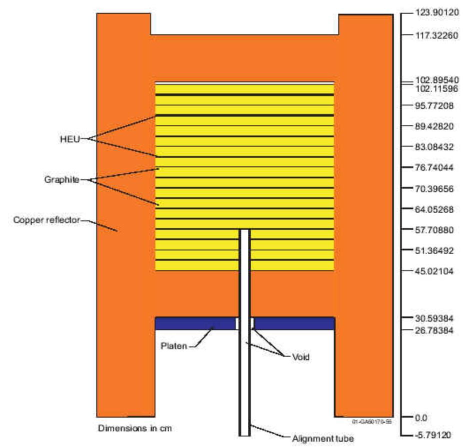
Verification of Sensitivity Method

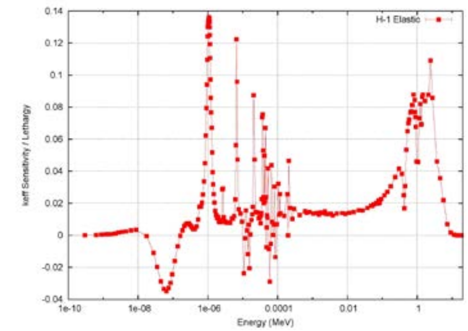
- **Method in MCNP was verified using:**
  - **Analytic solutions of multigroup infinite medium problems**
  - **Direct perturbations of material densities**
  - **Comparisons with TSUNAMI-3D and other codes using established benchmarks**

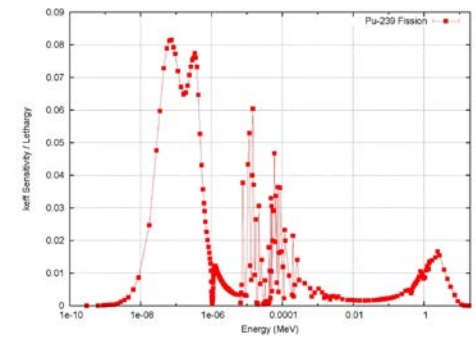
- **Results show agreement with existing results.**

Using Sensitivities

- **To determine if the code validation covers a particular process**





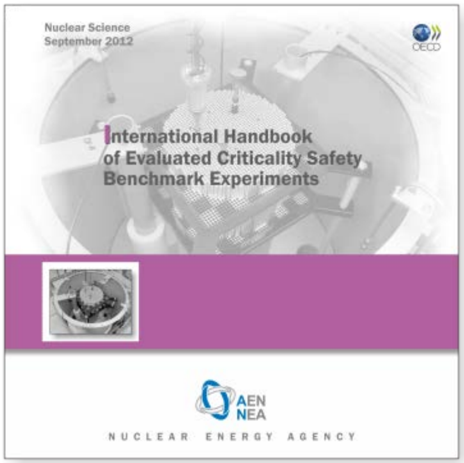


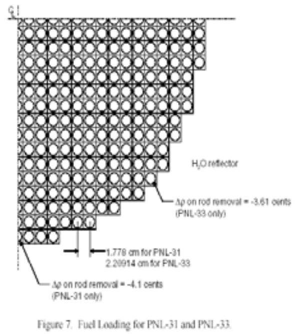
Identify process and upset conditions.

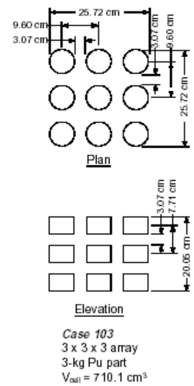
Prepare models for MCNP.

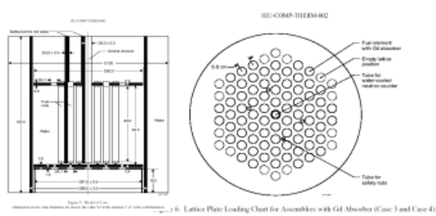
Generate sensitivity profiles with MCNP.

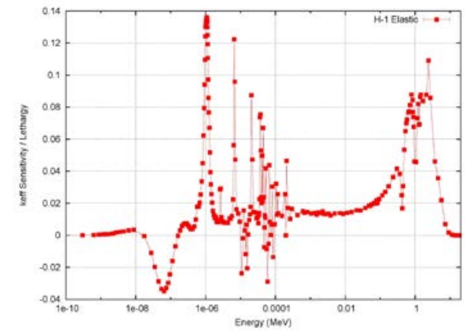
Using Sensitivities

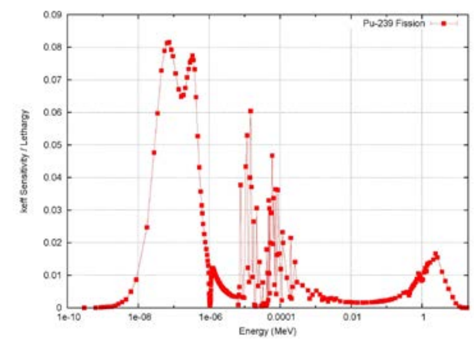












Find database of benchmarks.

Identify candidate benchmarks that have similar materials and spectra to process.

Generate sensitivity profiles and compare with process.

Using Sensitivities

- Once similar benchmarks are found, compare the codes ability to predict *k* to measured values.

- Establish a “bias” based on the inaccuracy of the calculation to form a conservative confidence interval.
  - Performance of the code and data on the benchmarks informs how well the code performs on the process (if the sensitivity profiles are similar).
  - Allows for the establishment of an appropriate criticality safety margin.

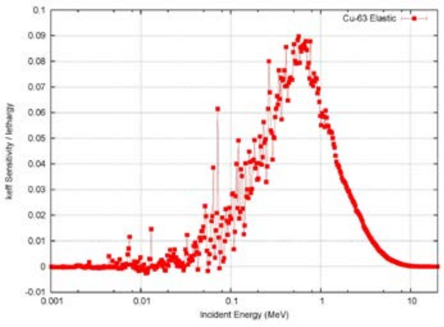
- What if there are no benchmarks like the process?

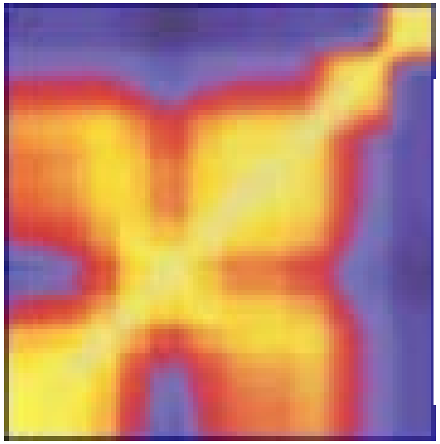
Lack of Benchmarks?

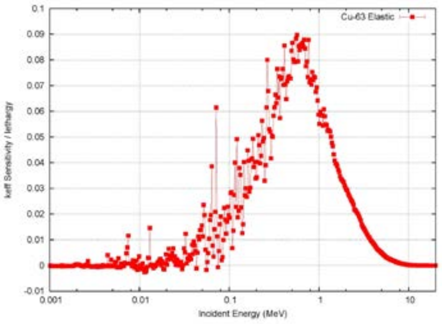
- **Perform an experiment that mocks the process.**
  - **Sensitivity coefficients may be obtained for both the proposed process and used to design the criticality experiment.**
  - **Critical experiment should be sensitive to the same nuclear data as the process in question.**

- **Establish the margin through the cross section uncertainties.**
  - **Convolve sensitivity coefficients with nuclear data covariances to estimate uncertainties.**

$$\sigma_k^2 = \mathbf{S}_k \mathbf{C}\, \mathbf{S}_k^{\mathbf{T}}$$







Neptunium Sphere

- Prior to 2002, there were no Np critical experiments, so how can the casting process to form the sphere used in the experiment be shown to be safe from criticality?
  - Conservatively set single parameter limits (ANSI/ANS 8.15) if applicable.
  - Otherwise, set the bias based on uncertainties in k from nuclear data using sensitivity analysis.

Future Development

- **Sensitivity analysis may also be used for uncertainty quantification of**
  - **Enrichment**
  - **Density/concentration**
  - **Geometry**
  - **Temperature**

- **Proof of concept work for geometric sensitivity work performed, R&D still needed**

- **Temperature work being done with UNM (Dr. Prinja)**
  - **Temperature sensitivities are effectively temperature coefficients in reactor analysis.**
  - **Goal is to develop the first continuous-energy Monte Carlo capability for reactor temperature coefficients.**

Future Development

- **Extend sensitivity capabilities beyond effective multiplication *k***
  - **Responses in fixed-source calculations (under development).**
  - **Other responses in eigenvalue calculations (e.g., foil activation) using generalized perturbation theory.**

- **<u>Long-term goal:</u> Develop an suite of easy-to-use, general-purpose, continuous-energy Monte Carlo capabilities for providing uncertainty estimates of calculated quantities.**

Questions?