LA-UR-15-22754

Approved for public release; distribution is unlimited.

Title: **MCNP Workshop**

Author(s): Avneet Sood
Forrest Brown
Michael Rising
Steve Nolen
Travis Trahan

Intended for: M&C + SNA + MC 2015
Nashville, TN
2015-04-19

Abstract

MCNP Workshop

Avneet Sood, Forrest B. Brown, Michael E. Rising, Steve Nolen, Travis Trahan
Monte Carlo Codes Group, XCP-3, LANL

The Monte Carlo particle transport teams will review current activities occurring at LANL occurring in the (X) Computational Division, XCP. This includes what is new in MCNP6 released in July 2014 and recent work in MCATK, our Monte Carlo Applications Tool Kit. Additionally, the workshop will include an in-depth review of our recent work in MCNP6 on fission multiplicity modeling for the nuclear non-proliferation community, sensitivity and uncertainty calculations for eigenvalue and fixed source calculations for the criticality safety community, and recent nuclear data issues. Our MCATK team will review their current status, applications, and future direction.

• Introduction	Brown
• What's New in MCNP6 ?	Sood
• Fission Multiplicity	Rising
• Sensitivity / Uncertainty	Rising
• Whisper Methodology	Brown
• Data Issues	Brown
• Monte Carlo Application Toolkit	Nolen, Trahan
• Future Plans	Sood

Slides available at
mcnp.lanl.gov,
Reference Collection,
Technical Seminars
& Workshops

Los Alamos
NATIONAL LABORATORY
EST. 1943

MCNP Workshop

M&C + SNA + MC 2015

Nashville TN, 2015-04-19

Avneet Sood, Forrest Brown, Michael Rising, Steve Nolen, Travis Trahan

Monte Carlo Codes Group, XCP-3
X Computational Physics Division

LA-UR-15-22754

NNSA
National Nuclear Security Administration

Avneet Sood, Forrest B. Brown, Michael E. Rising, Steve Nolen, Travis Trahan
Monte Carlo Codes Group, XCP-3, LANL

• Introduction	Brown
• What's New in MCNP6 ?	Sood
• Fission Multiplicity	Rising
• Sensitivity / Uncertainty	Rising
• Whisper Methodology	Brown
• Data Issues	Brown
• Monte Carlo Application Toolkit	Nolen, Trahan
• Future Plans	Sood

Slides available at mcnp.lanl.gov → Reference Collection → Technical Seminars & Workshops

Introduction

Monte Carlo & MCNP History

ENIAC – 1945

30 tons

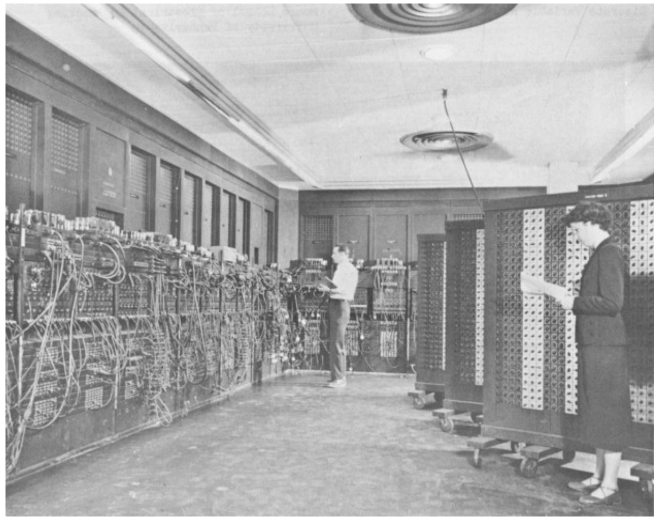
20 ft x 40 ft room

18,000 vacuum tubes

0.1 MHz

20 word memory

patchcords



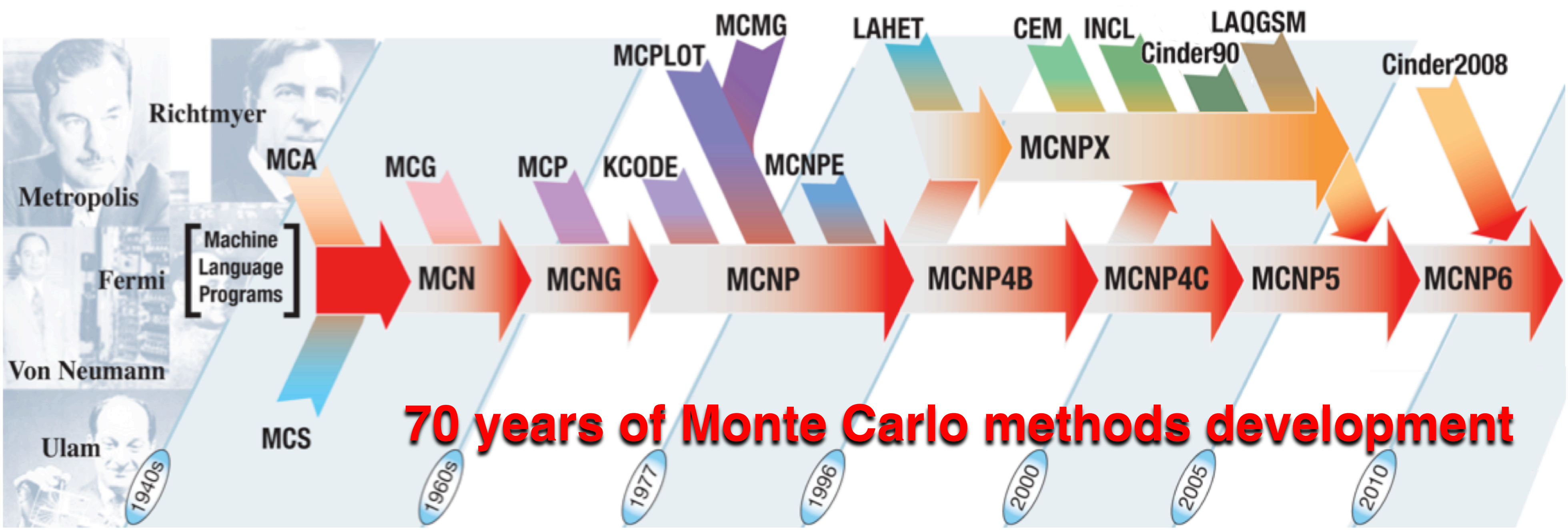
Manhattan Project – 1945...

Discussions on using ENIAC

Ulam suggested using the "method of statistical trials"

Metropolis suggested the name "Monte Carlo"

Von Neumann developed the first computer code



70 years of Monte Carlo methods development

MCNP6 Features

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

New Criticality Features
Sensitivity/Uncertainty Analysis
Fission Matrix
OTF Doppler Broadening

Fission
MCNP5/X multiplicity
LLNL fission package
CGM/LLNLGAM, CGMF (soon)

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

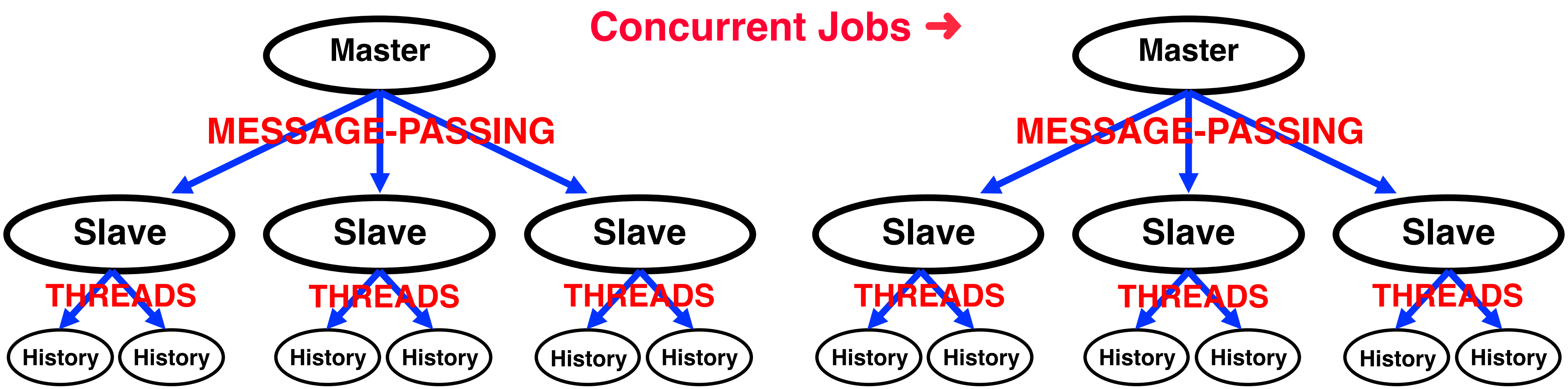
High energy physics models
CEM, LAQGSM, LAHET,
MARS, HETC

Continuous Testing System
~10,000 test problems / day

mcnp6.1 – 2013
mcnp6.1.1 – 2014

mcnp5 – 100 K lines of code, 12,000+ copies distributed by RSICC
mcnp6 – 500 K lines of code, 7,819+ copies distributed by RSICC

MCNP – Hierarchical Parallelism – Since 2000



Parallel Processes

– **Total processes = (# jobs) x (# MPI processes) x (# threads)**

– **Tradeoffs:**

- **More MPI processes** - lots more memory & messages
- **More threads** - contention from lock/unlock shared memory
- **More jobs** - system complexity, combining results

MCNP6 Status

- **MCNP6 releases by RSICC**

  MCNP6.1 – 2013, production version
  MCNP6.1.1 – 2014, same criticality, faster, beta features for DHS

  Nuclear Data – ENDF/B-VII.1 data, updates, & older data
  Reference Collection – 700^{+} technical reports
  V&V Test Collection – 1434 test problems

  $12{,}000^{+}$ copies of MCNP5 distributed by RSICC
  $7{,}819^{+}$ copies of MCNP6 distributed by RSICC

- **MCNP5 is frozen & unsupported. Last version 2010.**
- **Community needs to transition to MCNP6**

Support from DOE-NNSA-NCSP, DOE-NNSA-ASC, DOE, DOD, DTRA, DHS/DNDO, NASA, & others

What's New In MCNP6 ?

Motivation: We need accurate predictive capability

- Provide predictive capability to LANL, DOE/NNSA, DHS-DNDO, and DTRA sponsors
  - Some of the most powerful users are within our group!
  - We have access to engineering teams, high-performance computers, and unique experimental facilities
- Our biggest needs are:
  - Validated models of geometry and materials
  - Complex radiation source descriptions
  - Direct comparison to radiation detection instruments
- Our projects often have immediate, national-level impact
  - Criticality safety – assessing USL for facilities,
  - Design of new experiments – large scale DOE/NNSA-sponsored experimental facilities are being designed with MCNP
  - Radiation detector development – detecting nuclear threats
- External users directly benefit – often needs are similar
- Exciting research occurring with universities partners
- Attracting the best and brightest to LANL

MCNP6 Unstructured Mesh

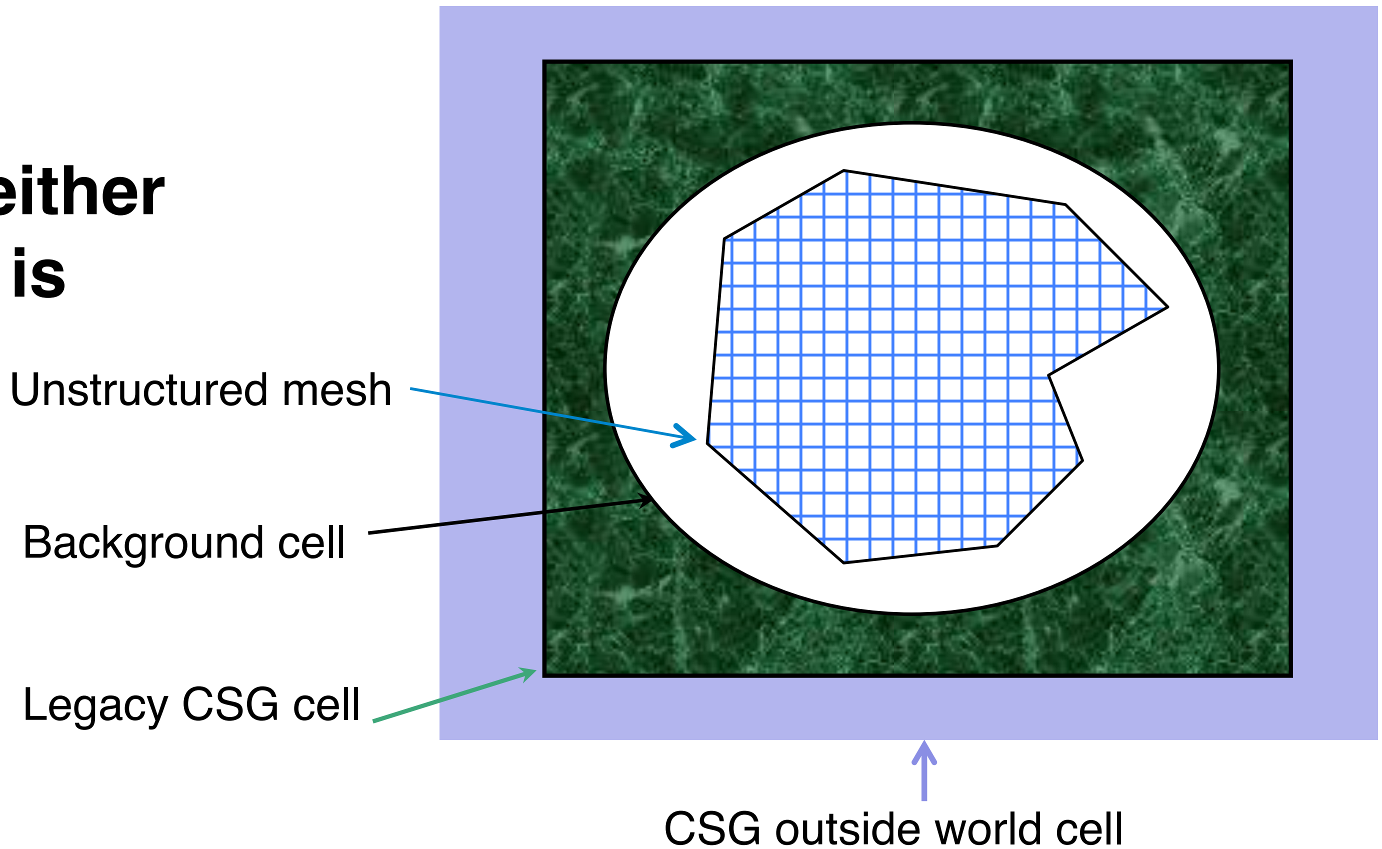
Current Capabilities

Roger L. Martz

April 2015

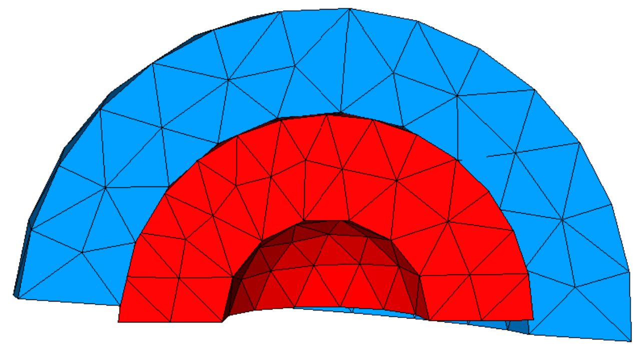
An unstructured mesh (UM) representation of the geometry is embedded in a traditional MCNP mesh universe giving rise to a hybrid geometry arrangement.

Any degree of complexity in either geometry type is permitted.

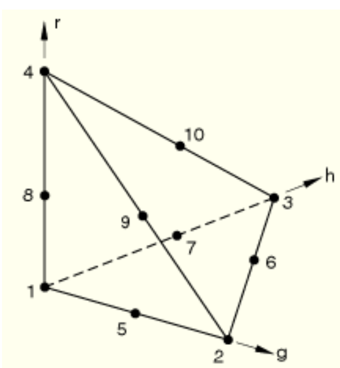


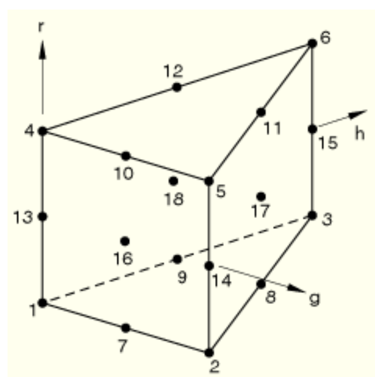
Some of the Initial Requirements

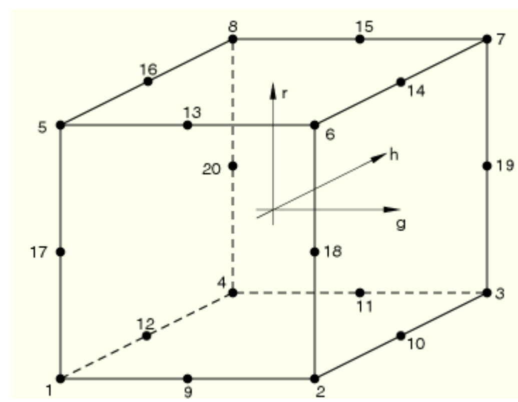
- Track through overlaps & gaps in a non-contiguous mesh
- Accumulate results on the mesh and output into a special file for post-processing



- Support unstructured polyhedrons with 4-, 5-, and 6-sides. Surfaces may be bilinear or quadratic depending on the number of nodes.







What is the UM capability?

A computer aided engineering (CAE) tool such as Abaqus/CAE or CUBIT can be used to create a 3-D solid model of the entity of interest.

Or

A computer aided design (CAD) tool such as SolidWorks or SpaceClaim can create the 3-D solid model for import into the Attila4MC GUI for problem setup.

Recent Features

- Supports multiple mesh files
- Improved tracking for electrons and heavy charged particles
  - All particle types now use the same top-level, UM tracking routine
- Allow non-uniform sampling of UM volume sources
- Select overlap treatment by part
- DXTRAN and point detector support
- Checking of twisted & deformed elements with the um_pre_op utility

Recent Important Bug Fixes, etc.

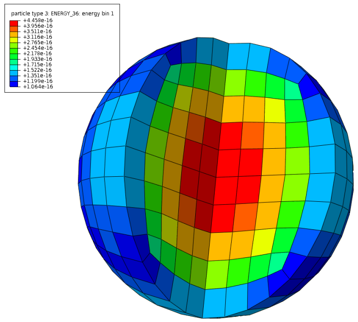
- Improved charged particle energy deposition
- Improved memory management
  - Reduction of by 20-50% of memory needed for calculations
- Improved background region tracking – now with an actual material assignment
- Resolved several tracking issues because of round off – includes handling large mesh elements
- Fix so that F8 tallies work with UM
- UM coding is Fortran 2003 compliant

Performance

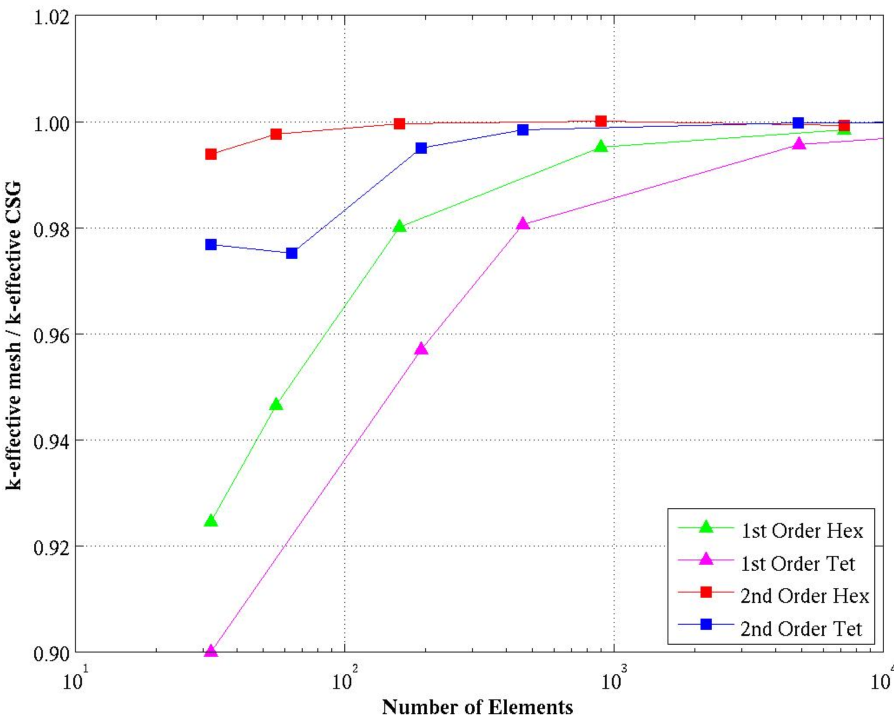
2nd Order Polyhedra Improve MCNP Mesh Calculations

- **Second order tetrahedral and hexahedral mesh elements more accurately reproduce the volume of curved objects.**
- **Fewer number of second order elements are required compared to first order.**
- **Fewer number of second order elements mean shorter calculation times by an order of magnitude to obtain the right answer with the same precision.**

See: LA-UR-09-7320



Godiva criticality benchmark sphere



Parallel Input

- **UM problem setup requires nested-loops in several parts of the code. These loops can be time-intensive.**
- **Can speed this up by running mpi.**
  - **Want 1 mpi slave node for each instance. The minimum number of mpi processes to specify should be 1 + number of instances in the model.**
  - **Each instance or part will then have a dedicated processor for its input.**
    At this time, multiple processors per instance or part are not implemented and there is no load balancing.
  - **Still limited by the instance / part with the largest number of elements.**
- **The most efficient parallel input processing takes place when all parts have approximately the same number of elements and there is more mpi processes than instances.**
  - **30,000 elements per part is a key # for efficient input processing.**
  - **When there are fewer processes than instances – round robin.**

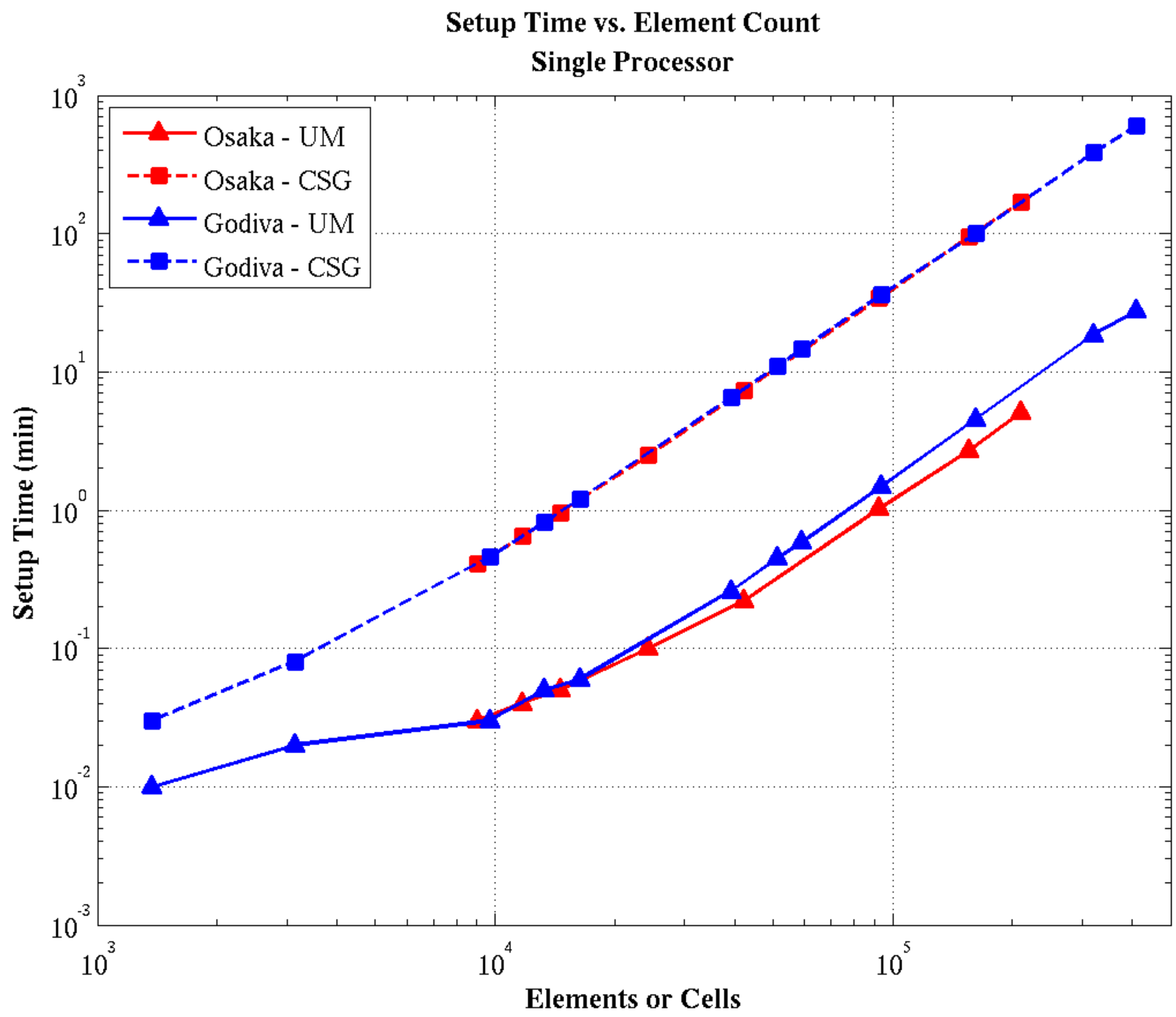
Direct Comparison

The following slides show a comparison between CSG and UM for the Godiva and Osaka benchmarks where

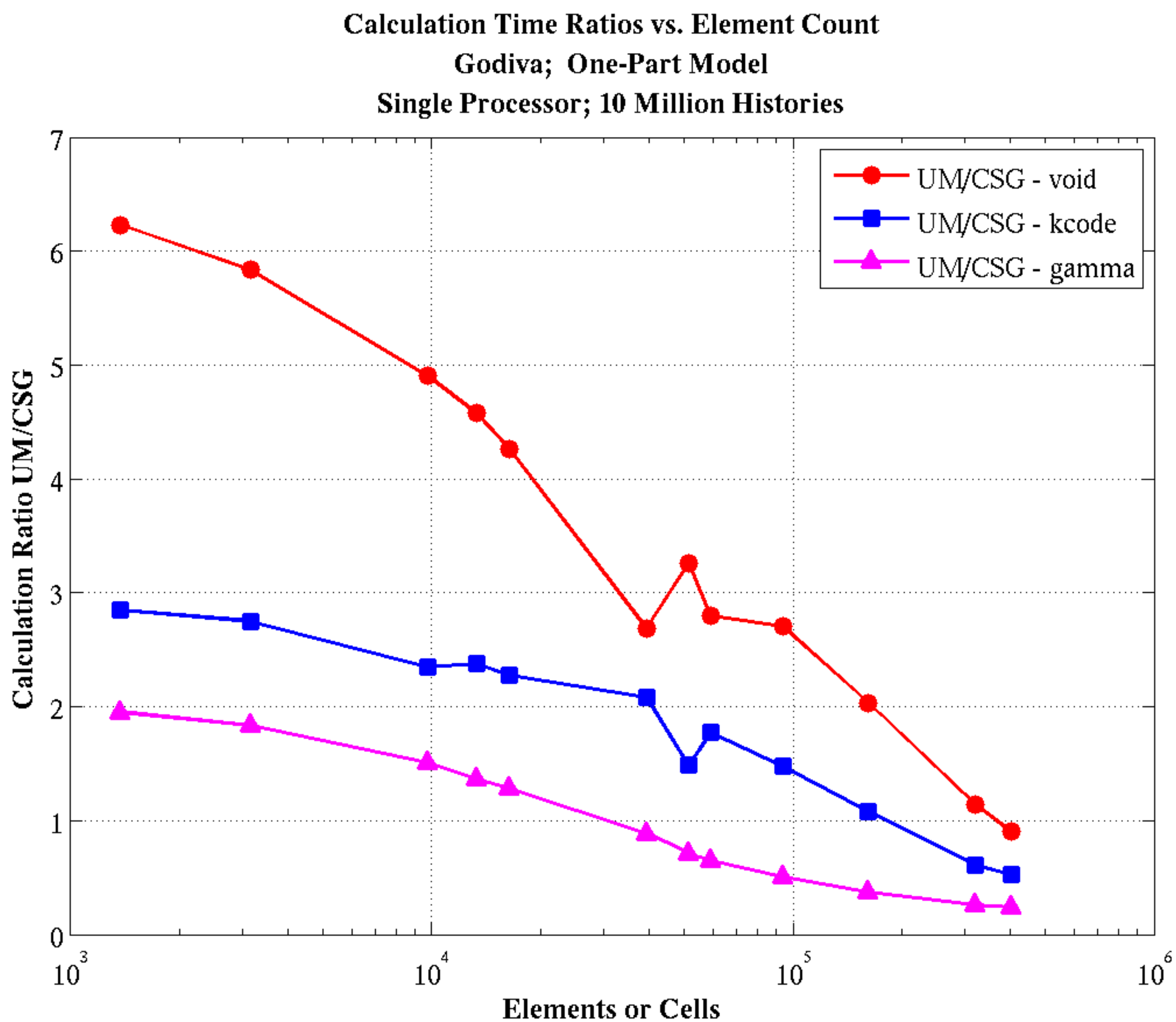
- The models use only 1st order tets.
- Each tet in the UM is modeled exactly in CSG using combinations of arb surfaces.
  - Thanks to Kevin Marshall, et al., of the Radiation Science's Group, AWE Plc. for providing the program to convert the Abaqus .inp file into an MCNP CSG input deck.
- The total number of histories were chosen so that the most detailed models could be run in a reasonable amount of time with 1 processor.

See: *Nuclear Technology*, Vol. 184, Nov. 2013.

Problem setup time for large element/cell counts is ~40 times faster with unstructured mesh.



As the problem detail increases, unstructured mesh calculation times are shorter.



Varian Medical's Attila4MC Setup Tool for MCNP6

Monte Carlo Codes
XCP-3, LANL

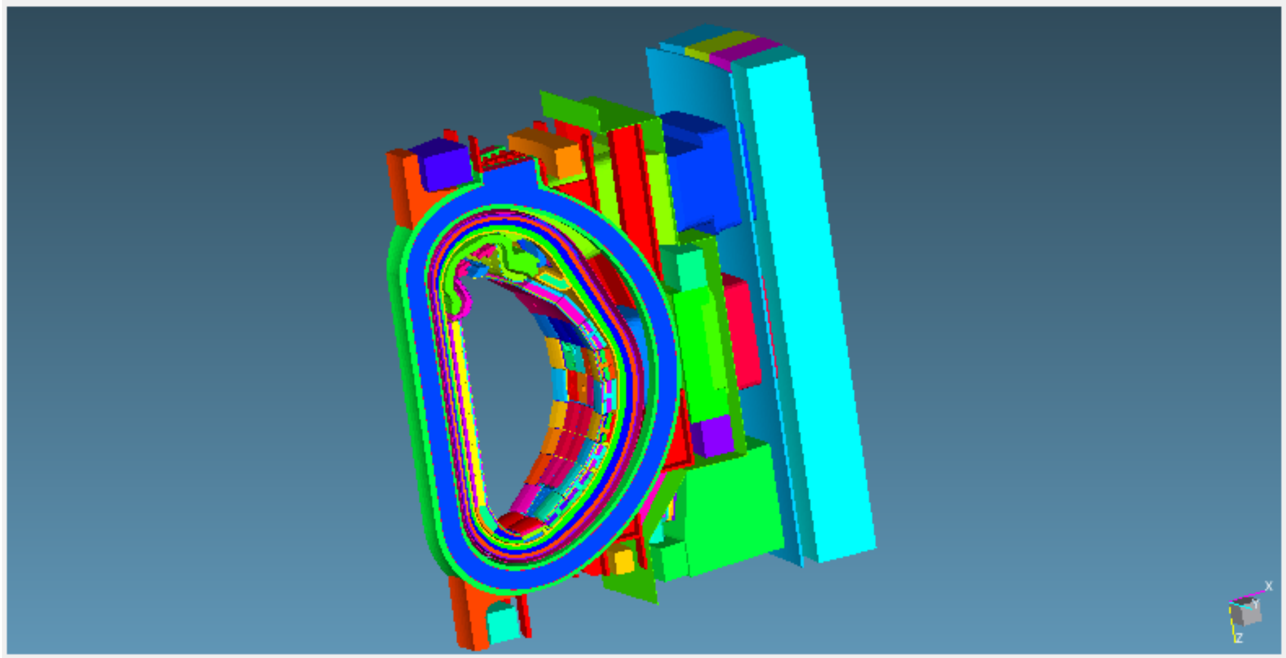
Generate geometry with SpaceClaim or Solidworks. (alternative to Abaqus/CAE)

Generate mesh with Simmetrix mesher in Attila4MC.

Setup MCNP6 input via Attila4MC GUI.

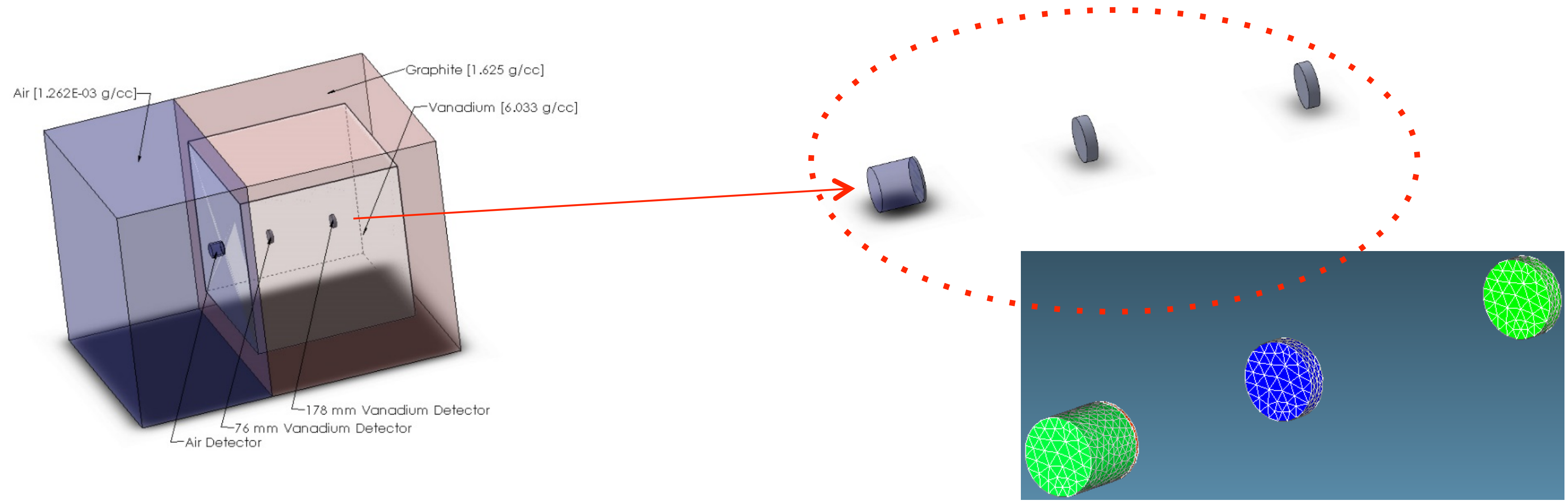
Generate deterministic weight windows via Attila

Cell Flag	User Region	Material	Density Scal
302 : M102_BSM_01-06_01_2	M102_BSM_01-06_01_2	m102_alite03	1
303 : m101_BSM_01-06_01_1	m101_BSM_01-06_01_1	m101_alite03	1
304 : m064_BSM_17-18_01-03_5	m064_BSM_17-18_01-03_5	m64_alite03	1
305 : m064_BSM_17-18_01-03_4	m064_BSM_17-18_01-03_4	m64_alite03	1
306 : m069_BSM_17-18_01-03_3	m069_BSM_17-18_01-03_3	m69_alite03	1
307 : m068_BSM_17-18_01-03_2	m068_BSM_17-18_01-03_2	m68_alite03	1
308 : m003_BSM_17-18_01-03_1	m003_BSM_17-18_01-03_1	m3_alite03	1
309 : VOID_FM_PLASMA	VOID_FM_PLASMA	void	0



Viewing: Attila + MCNP6

V&V with Vanadium Cube Benchmark

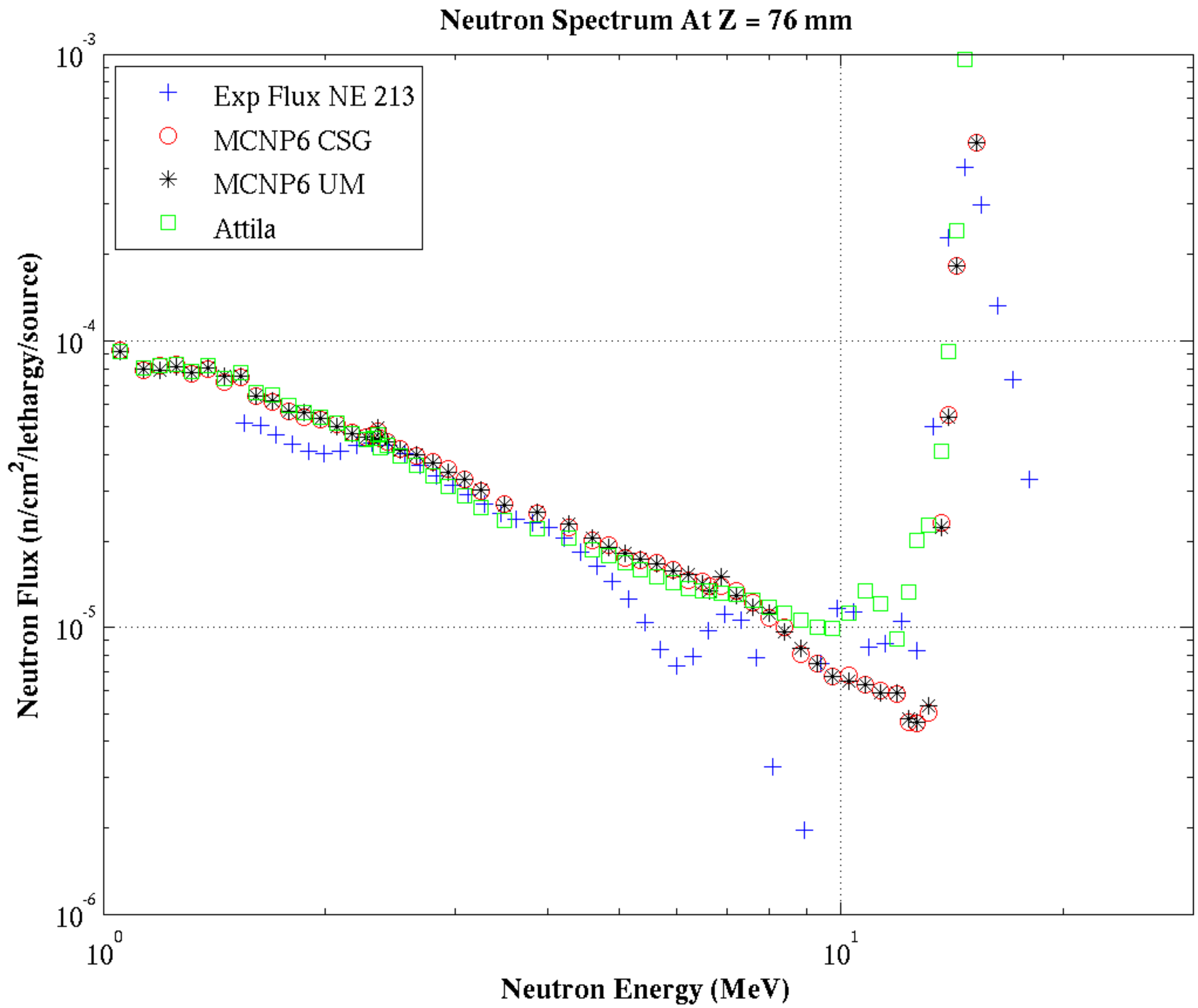


- Vanadium cube benchmark experiment from the Fusion Neutronics Source facility Japan Atomic Energy Research Institute.
- MCNP6 and Attila models developed from a single CAD model and used the same unstructured tet mesh.
- MCNP6 and Attila inputs prepared with the Attila4MC GUI.

See: Proceedings of the ANS, 2013 National Meeting

V&V with Vanadium Cube Benchmark

- 47,640 tet (1st order) mesh elements
- Attila: S24 triangular Chebychev-Legendre quadrature, P4, Galerkin scattering treatment, FENDL-2.1 multigroup cross sections (175 neutron/42 gamma)
- MCNP6: 3E8 histories, ENDF/B-VII cross sections (for available isotopes)



Neutron flux > 2 MeV at Z = 76 mm

Some Interesting Problems

ITER Demonstration Calculation

ITER model (20 degree section used for detailed analysis of diagnostic ports) calculation with MCNP6 Version 1.0

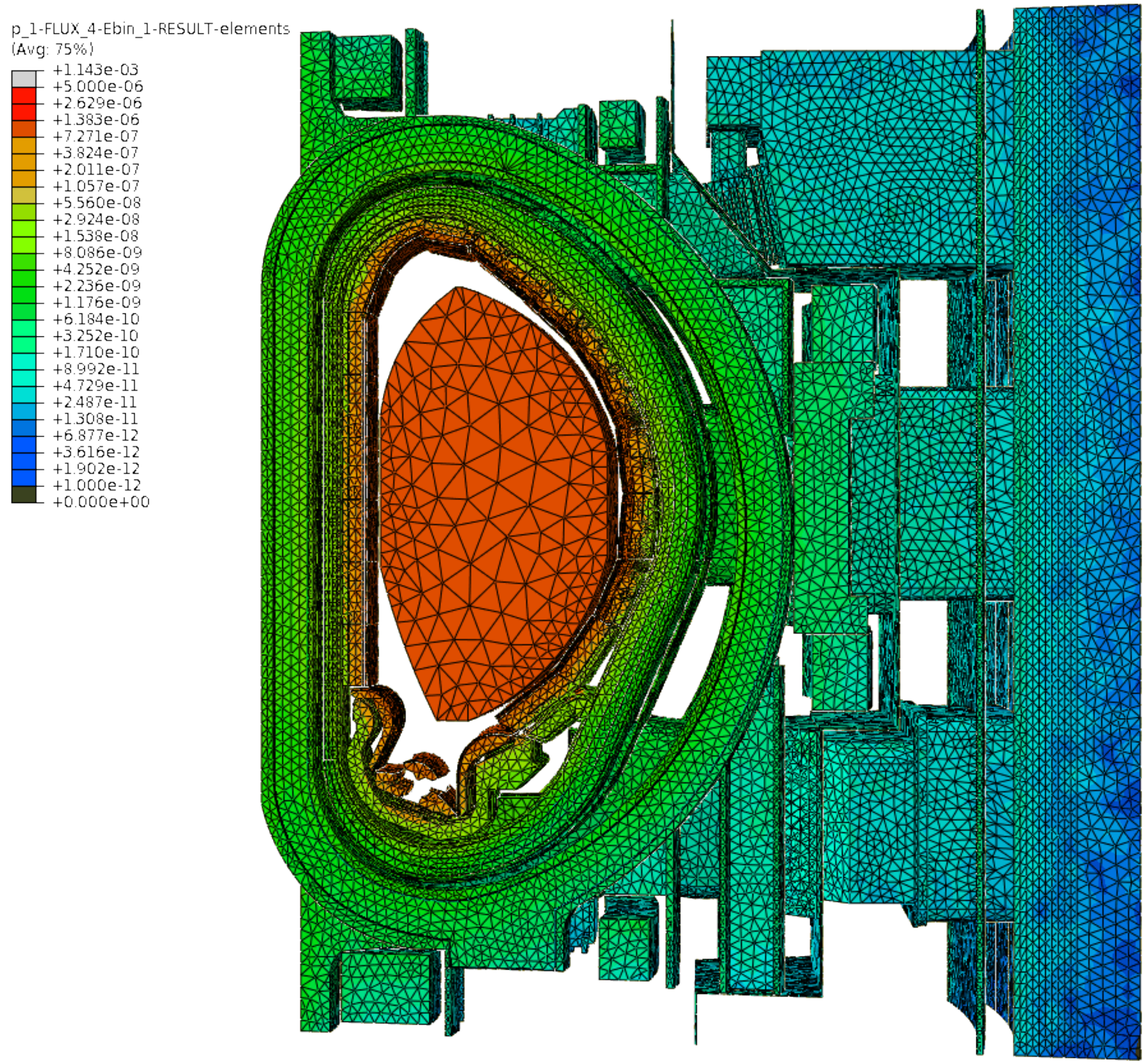
14.1 MeV mono-energetic neutron source using mesh volume source methodology.

Void region mesh removed to aid calculation performance and memory requirements (~4.5 GB/cpu).

2,073,968 1st order tets in 309 cells

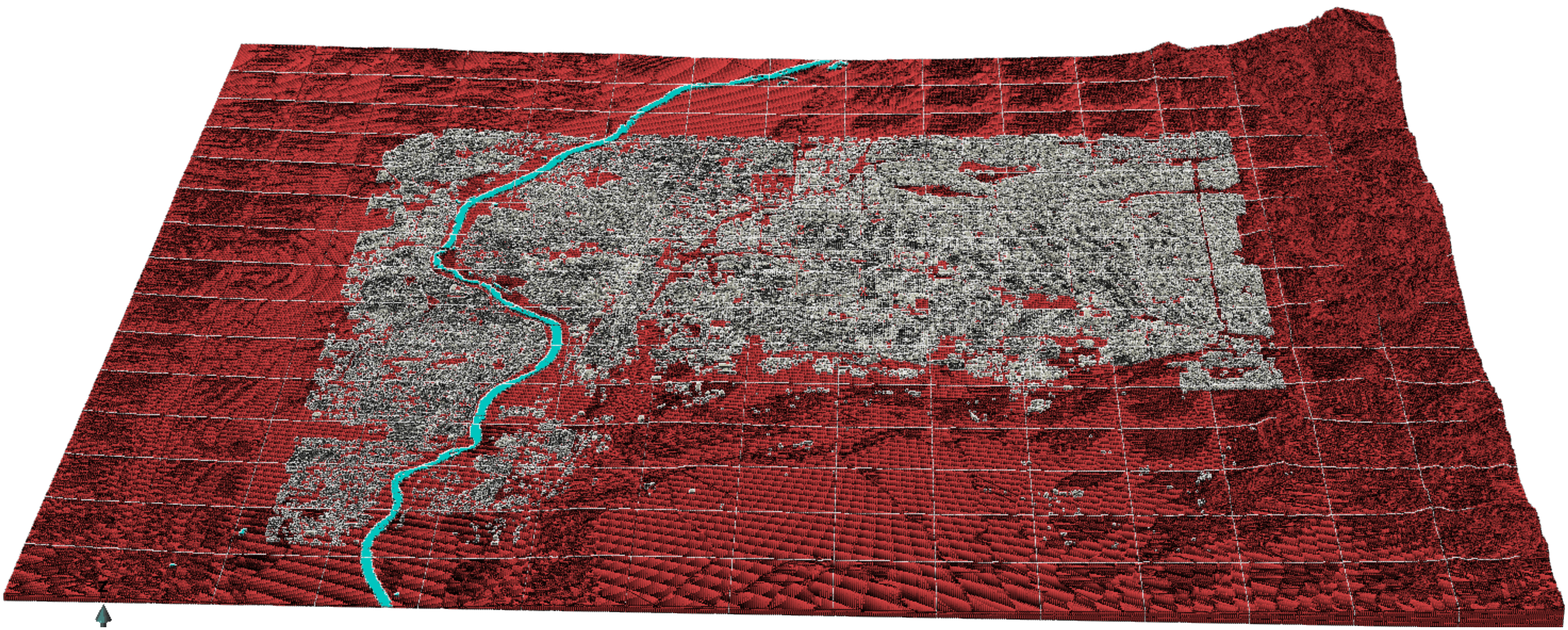
Reflecting boundary conditions

100 million histories run with 55 slave nodes. ~7.5 minutes setup time using parallel input processing.
~ 6.25 hours wall clock time with Intel Xeon E5-2670 chips @ 2.6 GHz running 64-bit Chaos Linux.

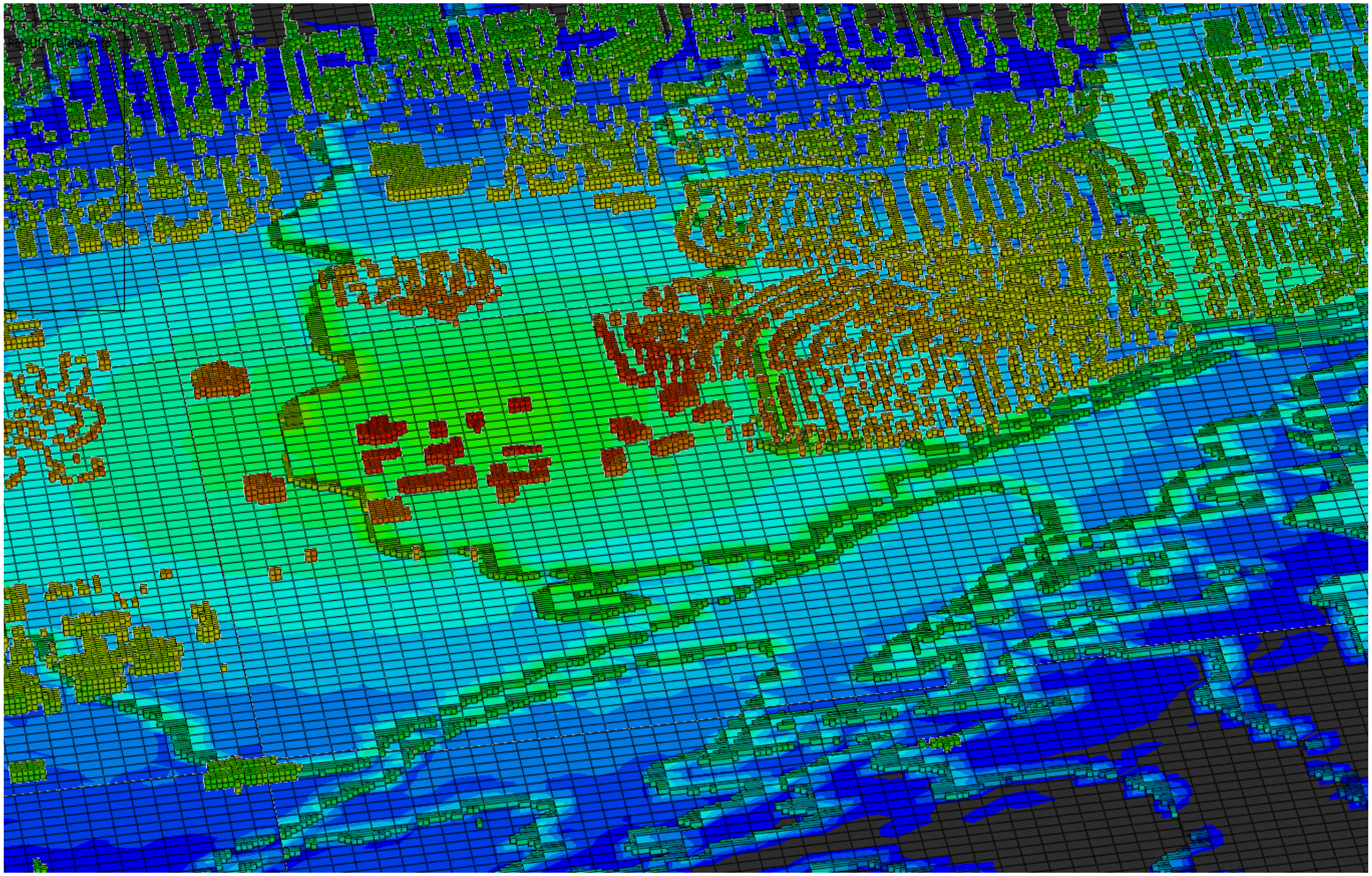


Total neutron flux

Hexahedral mesh converted from an MCNP lattice geometry using the um_pre_op utility.



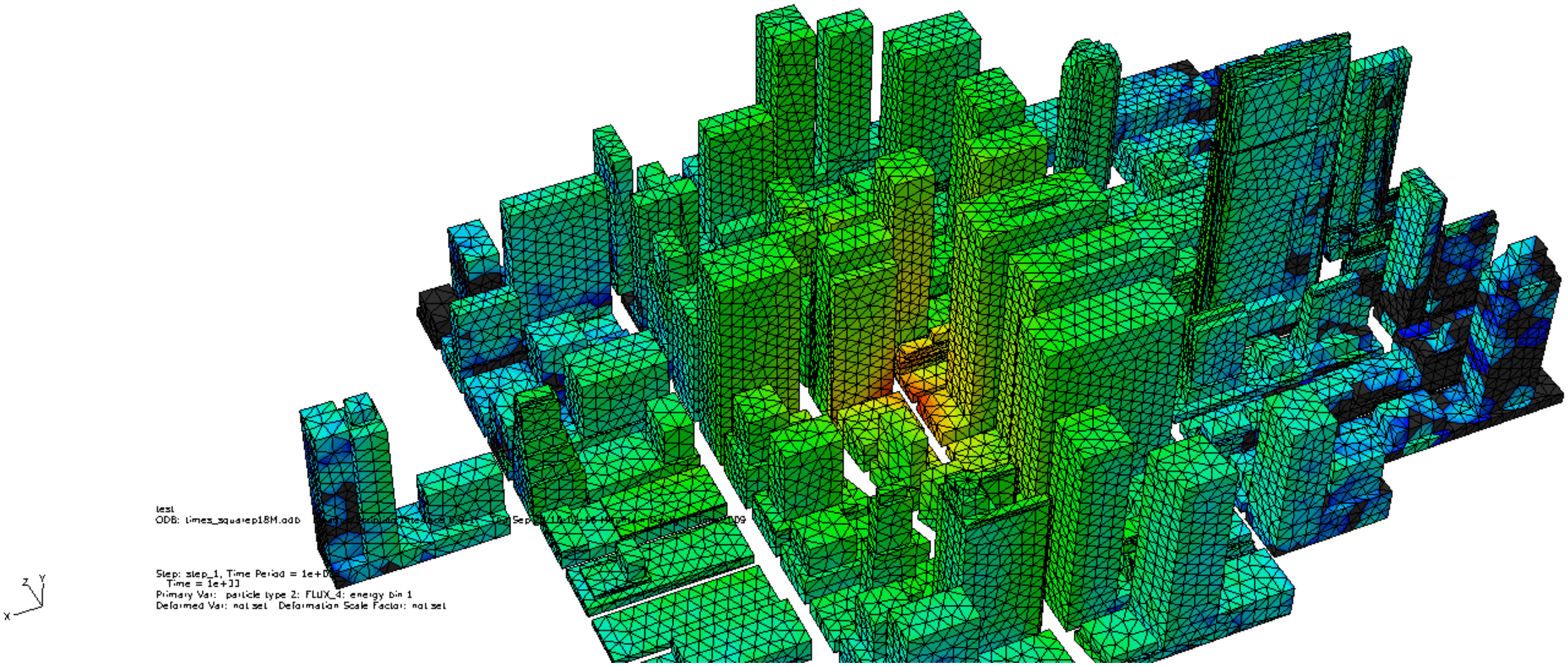
Gamma flux from an above ground "Fat Man-like" explosion



Times Square, New York City

Monte Carlo Codes
XCP-3, LANL

Gamma flux from a “Fat Man-like” explosion



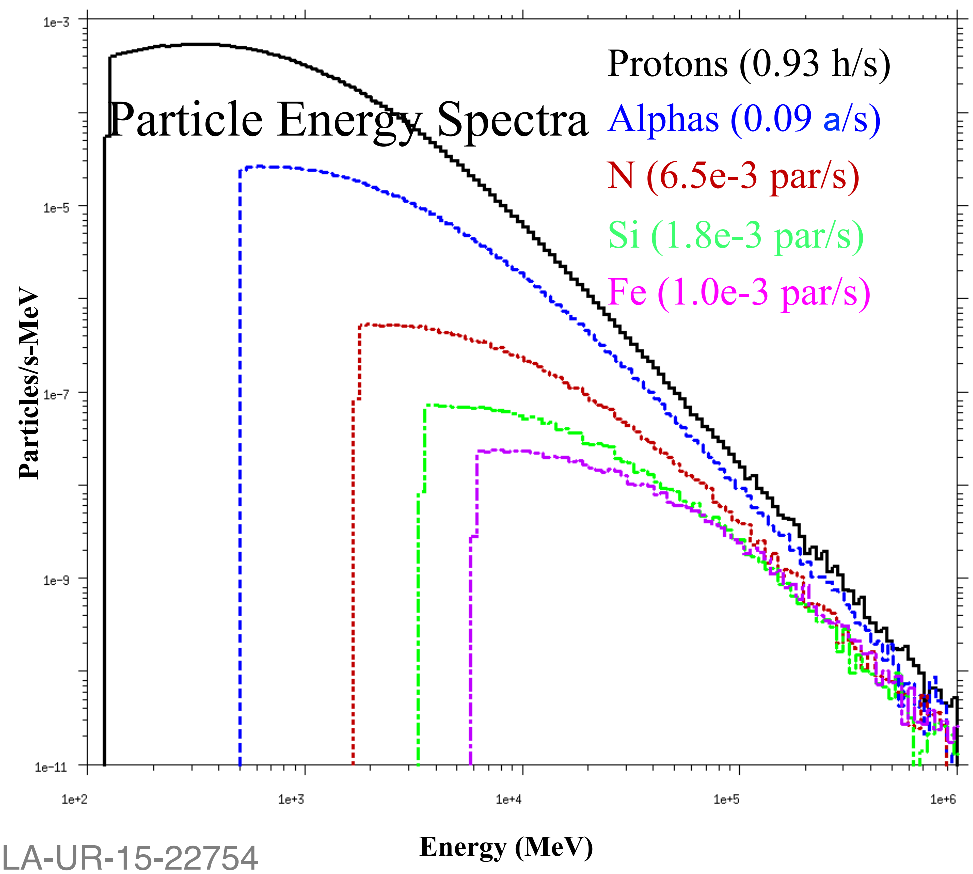
Radiation Sources

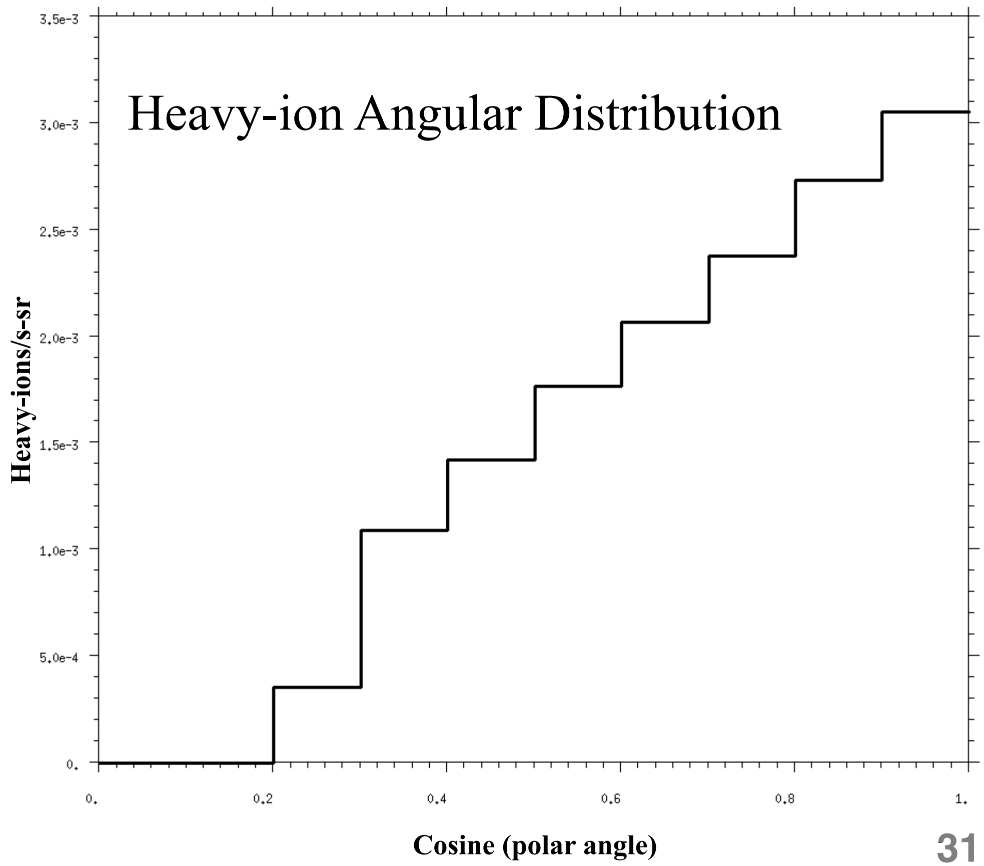
Gregg McKinney, Garrett McMath

What's New
In MCNP6 ?

Background Radiation Source: Cosmic Heavy ions

- Background radiation sources need to be accounted for development and evaluation of radiation detector performance.
- Cosmic radiation sources are often a large source of this background. MCNP previously had only proton and alpha sources
- University of Delaware model ^{14}N, ^{28}Si, and ^{56}Fe, each of which represents a range of actual cosmic-ray heavy ions.

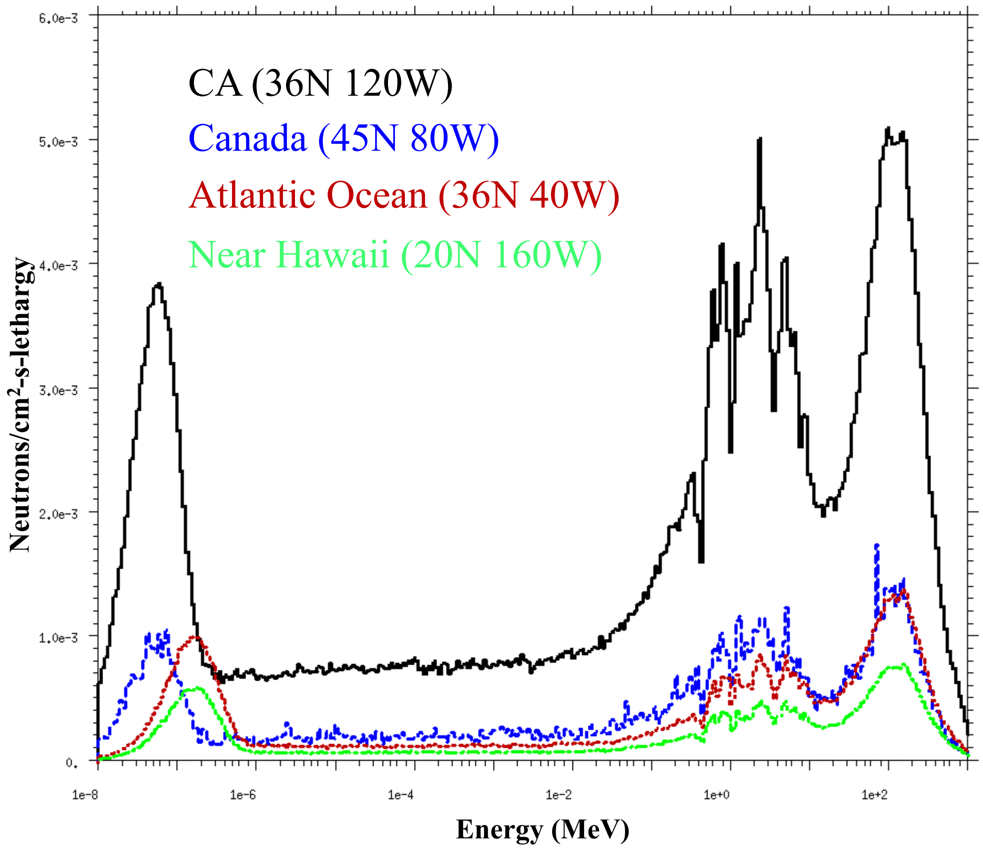




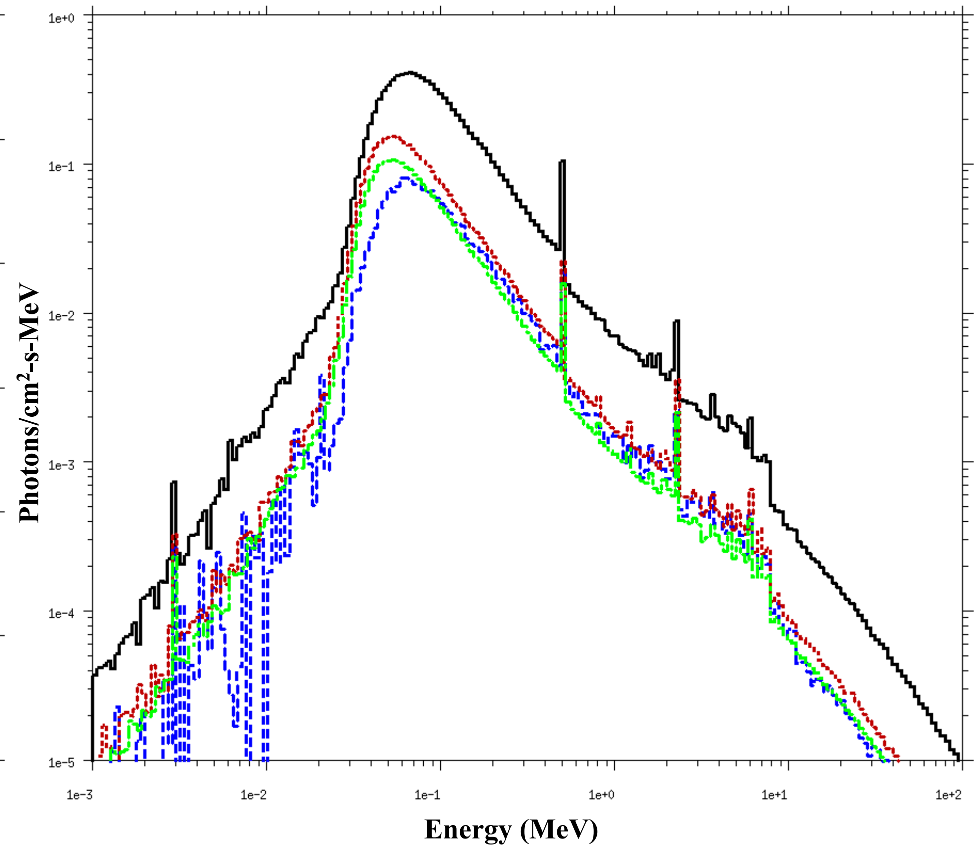
Background Radiation Sources

- **Spectra generated by MCNP6**
  - cosmic neutron sources
  - cosmic & terrestrial photon sources
- **1262 grid points**
  - every 5º in latitude
  - every 10º in longitude
- **Users can add their own data**
  - add location comment
  - create a unique lat/long
  - insert integral & differential data

Cosmic Neutron Spectra



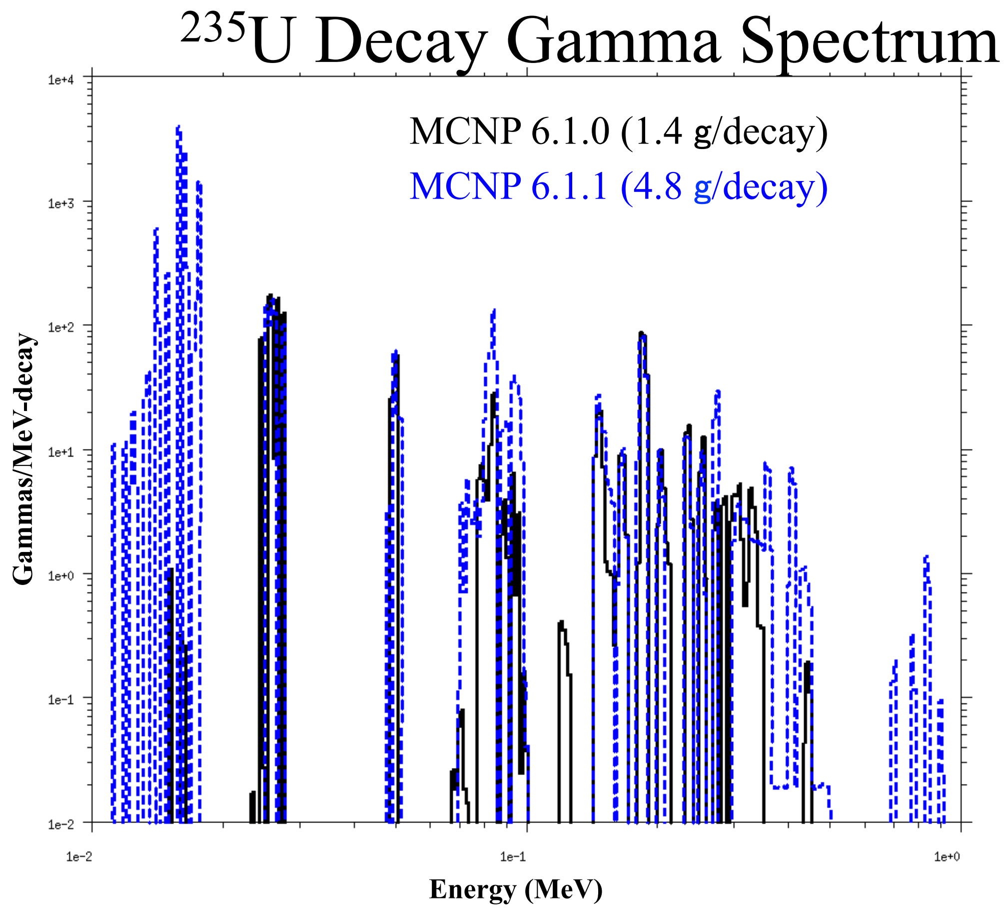
Cosmic+Terrestrial Photon Spectra



G. W. McKinney et al., "MCNP6 Cosmic & Terrestrial Background Particle Fluxes – Release 3," Proceedings of the ANS Winter Meeting, Washington, DC, Nov. 10-14 (2013).

Radiation source: Spontaneous Decay

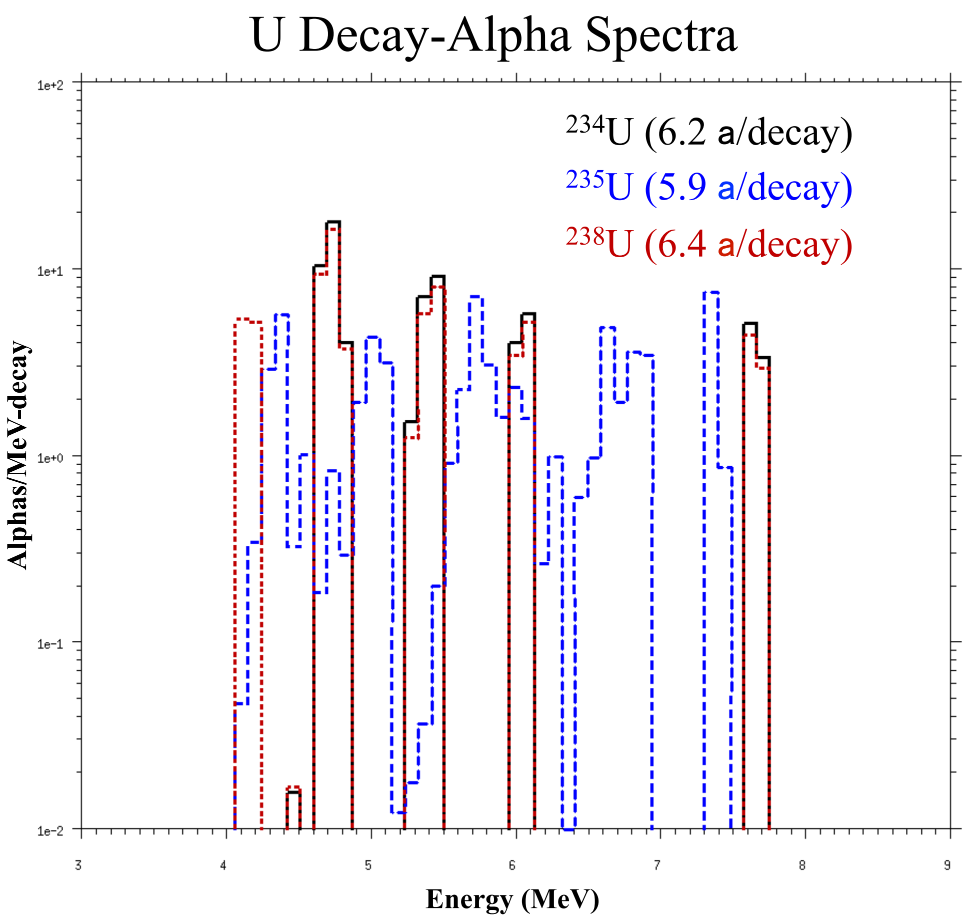
- Spontaneous gamma emissions have been in MCNP since 2008.
- User must specify a material-based source in material list or SDEF card.
- New feature allows spontaneous neutron and beta emissions
- New feature allows user to specify time where source is considered stable
- User can limit the number of decay daughters

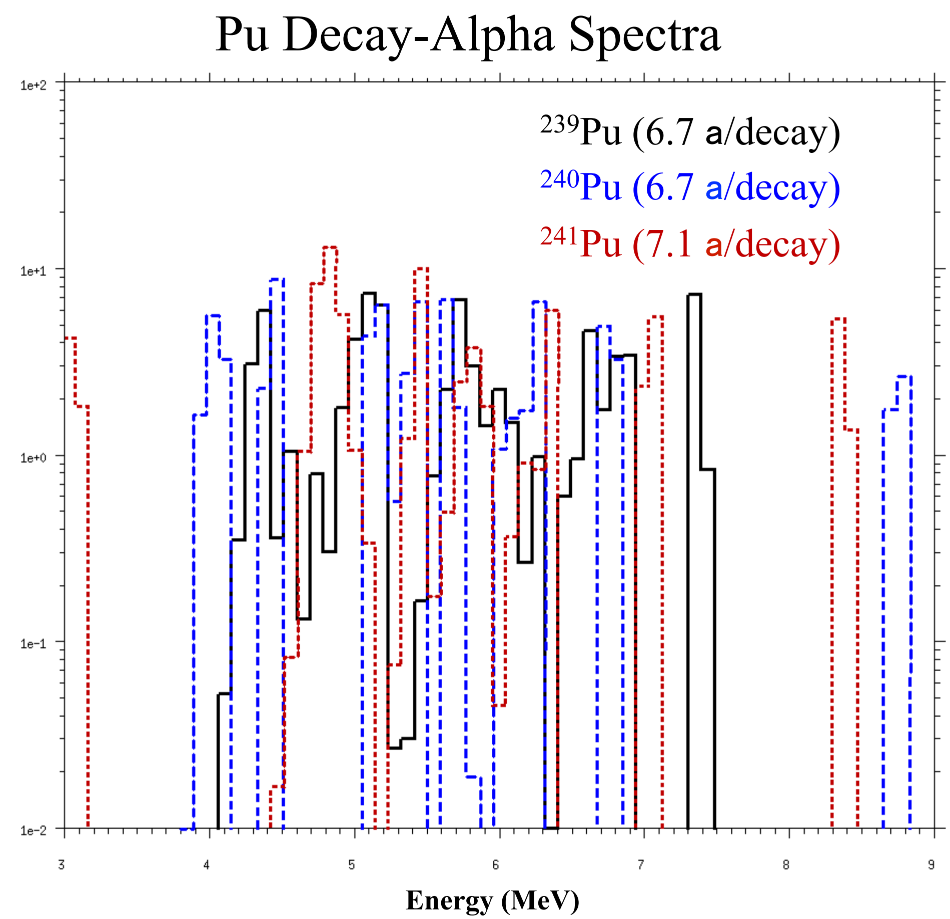


G. E. McMath et al., "MCNP6 Enhancements to Alpha Particle Production and Transport," Proceedings of the ANS Winter Meeting, Anaheim, CA, Nov. 9-13 (2014).

Spontaneous Alpha

- **New *delay_library_v3.dat* file with ENDF/B-VII.1 decay alpha data for 171 nuclides.**



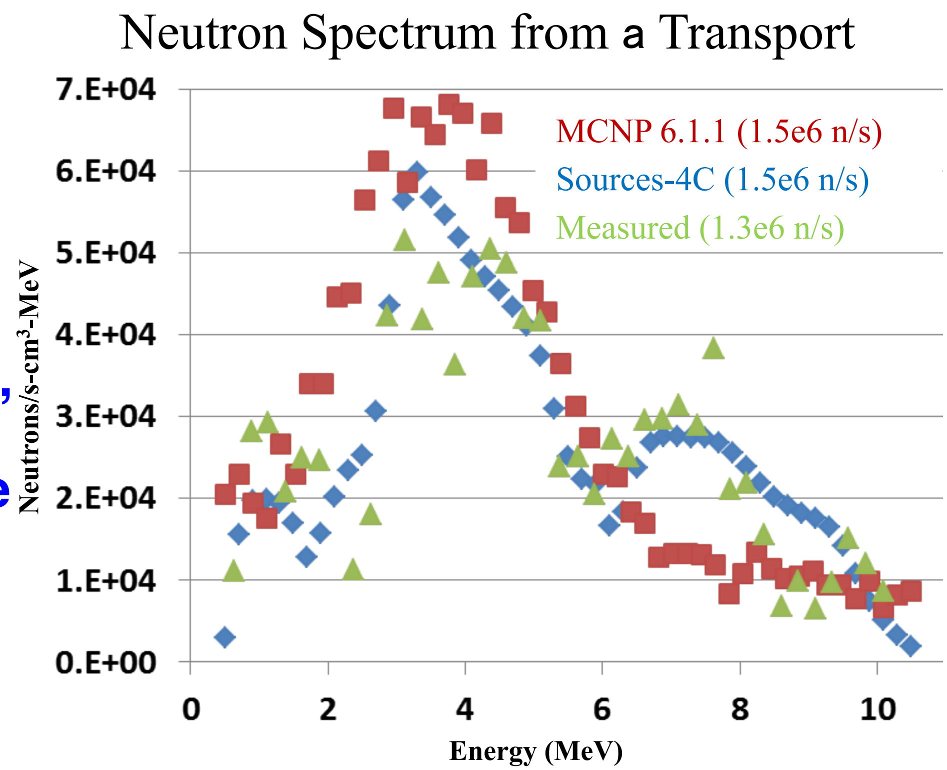


G. E. McMath et al., "MCNP6 Enhancements to Alpha Particle Production and Transport," Proceedings of the ANS Winter Meeting, Anaheim, CA, Nov. 9-13 (2014).

Transport Improvements

What's New
In MCNP6 ?

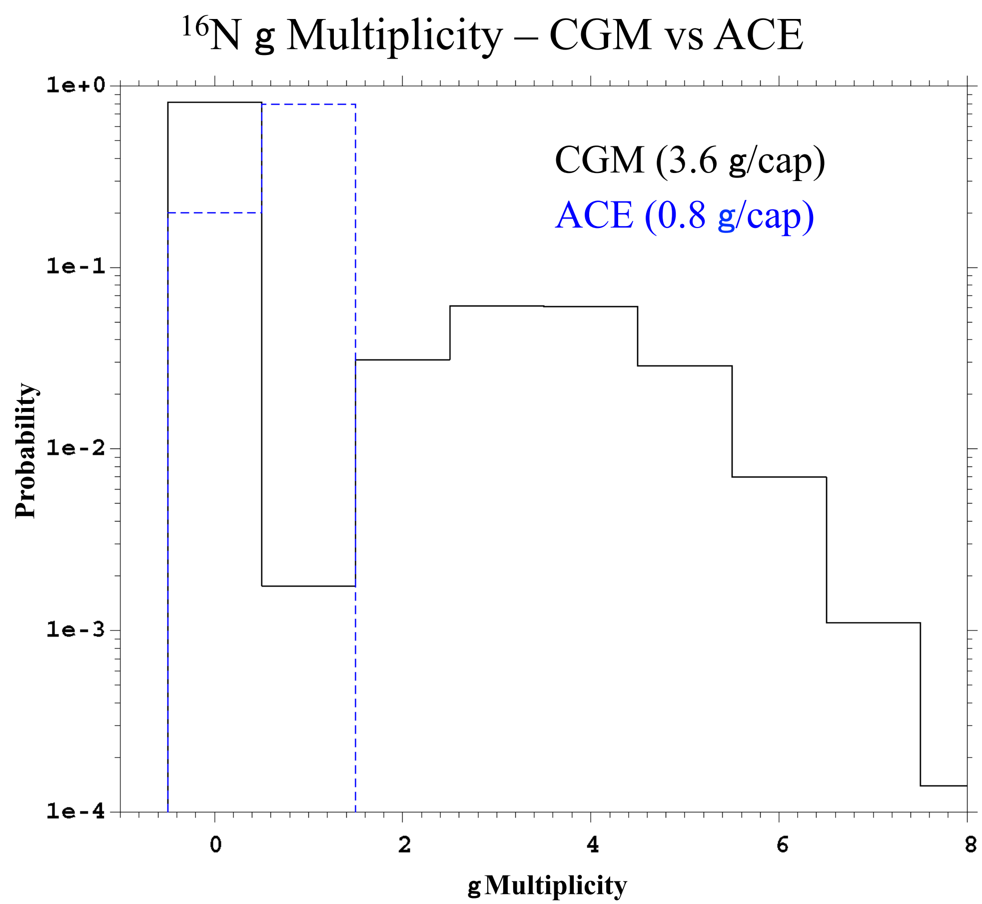
- Light-ion transport done via libraries/ data tables and models/event generators,
- Library-based transport very accurate collision physics and sampling speed for low-energy interactions (E<~100 MeV) compared to high-energy model-based transport.
- Library transport for neutrons, photons, electrons, and also protons. The light-ion library transport feature extends the proton library-based transport to other light ions, namely deuterons, tritons, helions, and alphas.
- When the incident light-ion energy is above the library maximum energy (E_{max}) it uses model transport, and when the ion energy is below E_{max} it uses library transport.



G. E. McMath et al., "MCNP6 Enhancements to Alpha Particle Production and Transport,"
Proceedings of the ANS Winter Meeting, Anaheim, CA, Nov. 9-13 (2014).

Correlated prompt gamma

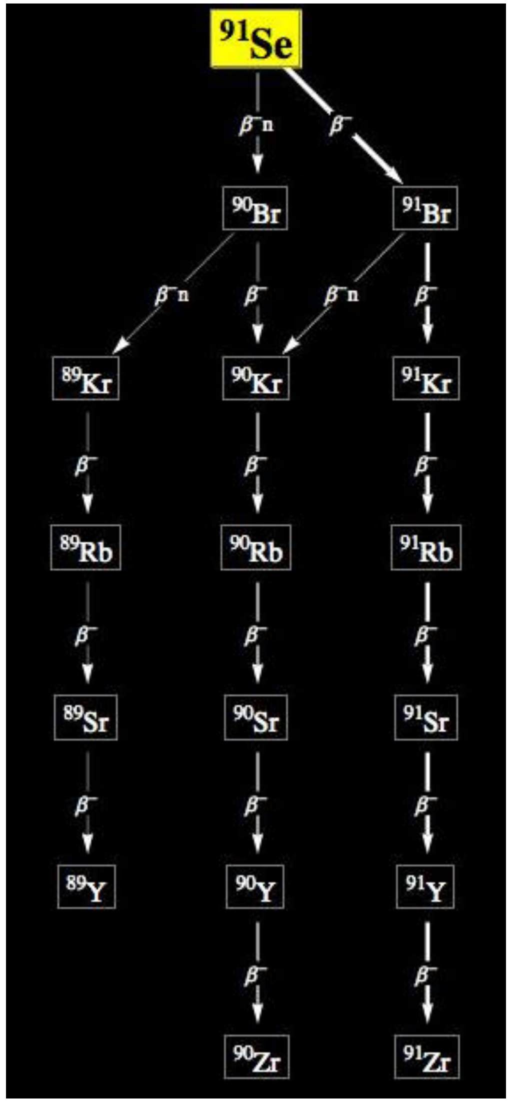
- Simulations of correlated emissions – both neutron and gamma – are required for supporting many experiments
- CGM and CGMF, Freya, are codes that perform the cascade of neutron and gamma emissions
- Emissions are correlated in number, energy, and angle
- MCNP is providing an API to interface with other codes for enhanced physics capabilities.



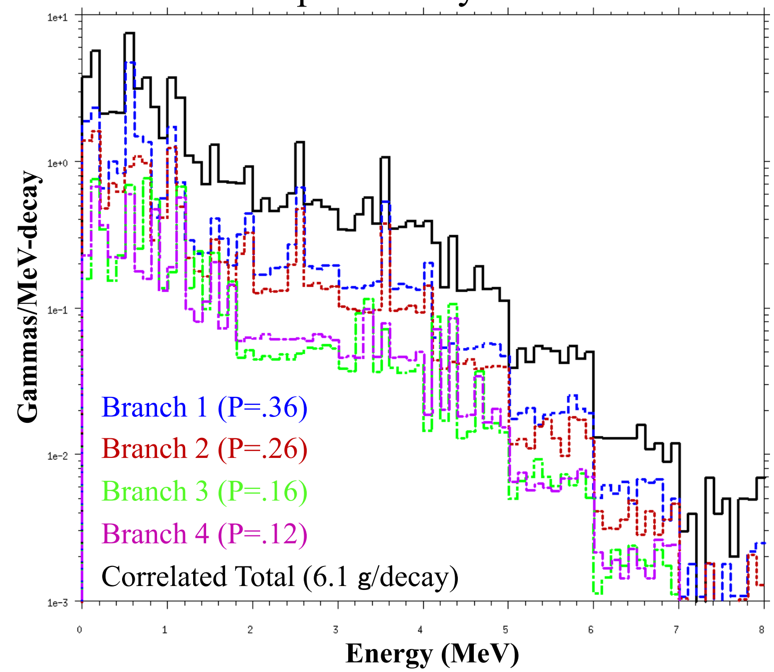
T. A. Wilcox et al., "MCNP6 Gets Correlated with CGM 3.4," Proceedings of the ANS RPSD Conference, Knoxville, TN, Sep. 14-18 (2014).

Correlated decay gamma

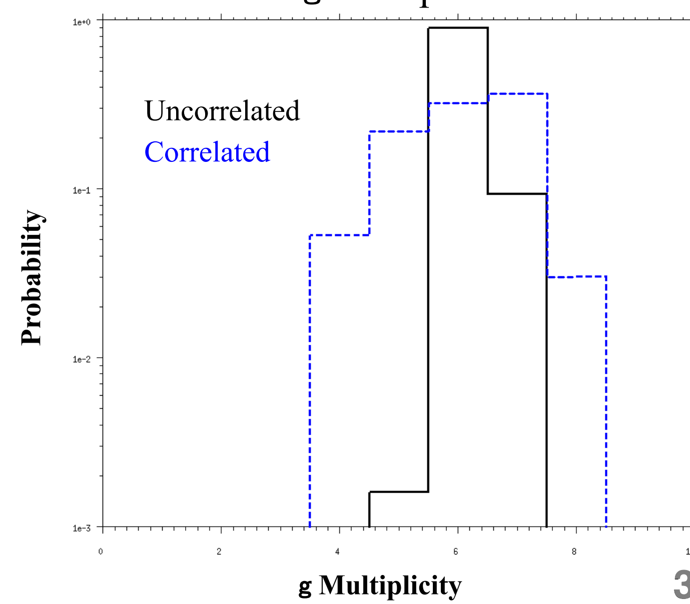
- **Delayed-particle production introduced into MCNP in 2006, via link to Cinder90**
- **Produces time-dependent nuclide production/depletion for an entire decay chain.**
- **New capability invokes Monte Carlo sampling of Cinder90 decay branches, leading to correlated delayed-particle production from a single decay branch**



Gamma Spectrum by Branch



^{91}Se g Multiplicities



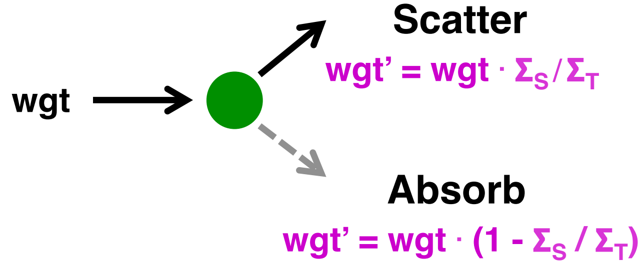
Fission Multiplicity
In MCNP6

Traditional “Weighted Simulation” Approach (1)

- **Default MCNP behavior relies on some non-analog simulation methods to evaluate integral quantities (why?)**
  – Monte Carlo method introduces variance into results
  – The more random sampling → more variance

- **Particle weights can modified based on the expected value of an event rather than randomly sampling the event**

Weighted Simulation



- **Survival biasing (implicit absorption shown above) is an effective variance reduction technique for many applications**
  – Always scatter, with a reduced particle weight
  – Using the expected value eliminates variance contribution from event

Traditional “Weighted Simulation” Approach (2)

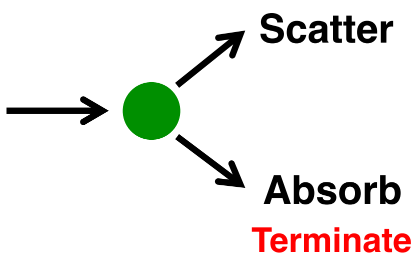
- **Criticality safety & reactor physics applications**
  - Survival biasing or implicit absorption is routinely used for neutron physics, where neutrons always survive collisions with reduced weight, Σ_S / Σ_T
  - For k-eigenvalue calculations, the fission reaction is included in the implicit absorption and the expected value of neutrons produced by fission, wgt $\cdot\ \nu\Sigma_F / \Sigma_T$, is often used at each collision
  - Sometimes the (n,xn) reaction, where x=2,3,…, is modeled by scattering and increasing neutron weight by x (not done in MCNP)
  - For neutron-induced photon production, the expected photons produced per collision, wgt $\cdot\ \Sigma_{n\rightarrow\gamma} / \Sigma_T$, is routinely used

- **Use of expected values implies uncorrelated outcomes**
  - On average, with sufficient sampling of all phase space, the integral quantities are correct
  - Detailed event-by-event physics modeling is incorrect and a more analog treatment of the random sampling is needed

Analog Simulation Approach (1)

- Using random sampling to select collision event type (scatter, capture, fission, etc.)
  - Without implicit absorption, the variance in the absorption event is non-zero
  - For many applications, the variance of the results will be increased

Analog Simulation



- In MCNP, the default implicit absorption option can be turned off and analog event sampling is turned on (cut or phys cards)

- However, getting away from using the expected value of secondary neutrons (fission) and photons (fission, capture, etc.) produced per collision is more complicated…

Motivation: Fixed Source Problems (1)

- **A predictive capability to detect special nuclear material (SNM) is of great importance to global security and nuclear nonproliferation applications.**
  - **To learn more about the unique signatures of SNM, detailed event-by-event physics (especially the fission process) needs to be studied**
    - List-mode detector responses
    - Multiplicity counters: p(n), p(γ)
    - Secondary particle correlations: n-n, n-γ, γ-γ
    - Average nuclear data quantities are insufficient, i.e. $\nu(E)$, $\chi(E,E')$
  - **The fission process has been theoretically and experimentally studied since the discovery of fission over 75 years ago**
  - **Recent revival of fission theory and experimental work has led to new capabilities that are in need of validation**

- **For MCNP to be used in this type of application, some more work needs to be done**
  - **Expand tabulated nuclear data → increased storage**
  - **Integrate event-by-event generators → increase computational cost**

Secondary Particle Event Generators (1)

MCNP6.1.1 contains two (low-energy) event generators:

- **LLNL Fission Library**
  - **Spontaneous, neutron-induced and photo-fission**
  - **Tabulated multiplicity and energy distributions from literature**
  - *** Fission Reaction Event Yield Algorithm (FREYA) isotopes:**
    - Spontaneous: ^{238}U, ^{240}Pu, ^{244}Cm and ^{252}Cf
    - Neutron-induced: ^{233}U, ^{235}U and ^{239}Pu
  - **If available, FREYA generates secondary neutrons and photons**

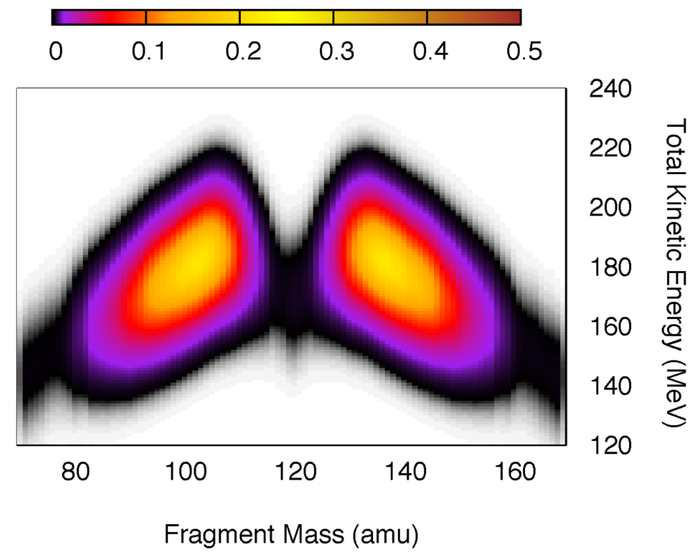
- **Cascading Gamma-ray Multiplicity (CGM) – LANL**
  - **Generates secondary particles from a variety of reactions**
  - **No fission! (** CGMF under active development)**

*** FREYA is not included in LLNL Fission Library in current MCNP6 distribution**

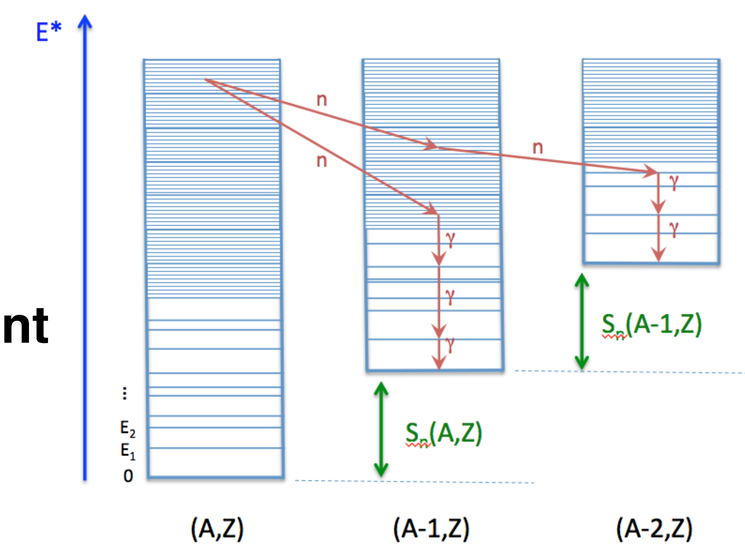
**** CGMF integration and testing currently in progress**

Secondary Particle Event Generators (2)

- **CGM:**
  - **Initial conditions of excited nucleus from specified collision reaction**
  - **Uses Hauser-Feshbach statistical theory of nuclear reactions**
  - **Monte Carlo is used to randomly sample each step in the de-excitation process**
  - **Currently used for non-fission secondary gamma ray emission in MCNP6**

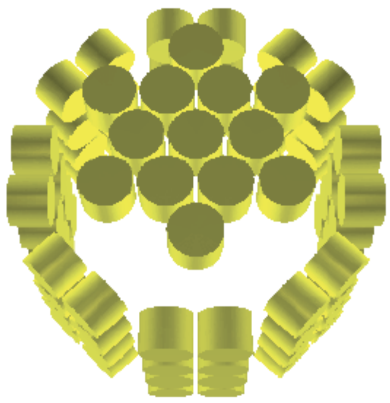


- **CGMF:**
  - **Superset of CGM with an added fission reaction capability**
  - **Fission fragments are sampled from a joint probability distribution function of mass, charge and total kinetic energy**
  - **Neutron/photon competition is treated during evaporation from fission fragments**

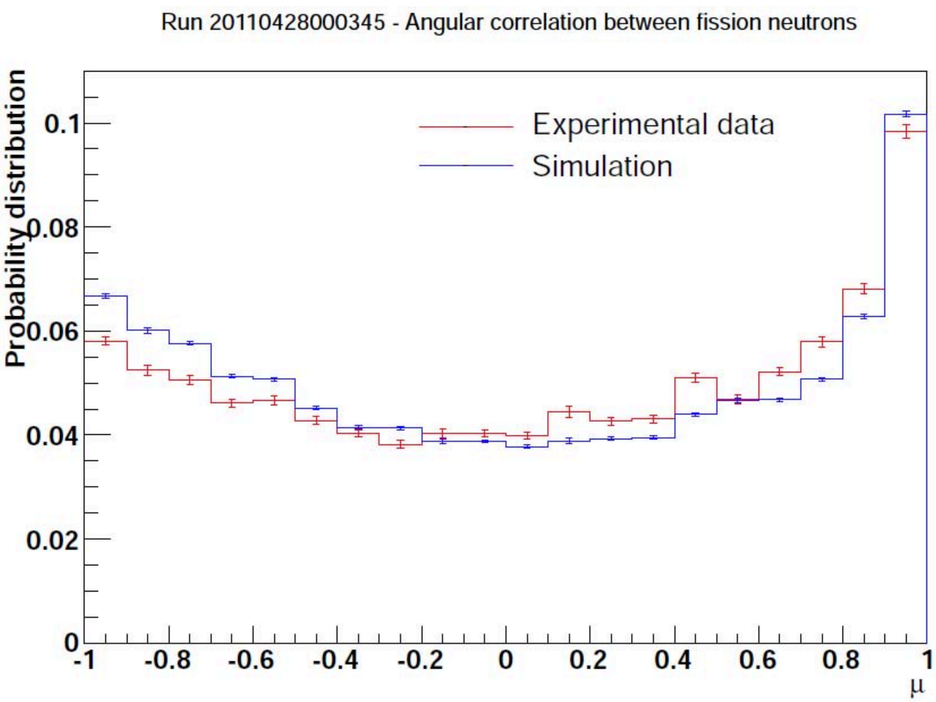


Secondary Particle Event Generators (3)

- **LLNL Fission Library:**
  - **Includes tabulated/fitted data for multiplicity and energy distributions of neutron and photon emissions (no angular correlations)**
  - **FREYA available via LLNL Fission Library**
  - **Default behavior is to use FREYA when isotope is available, tabulated/fitted data is used otherwise**



- **FREYA:**
  - **Similar to CGMF**
  - **Monte Carlo Weisskopf approach**
    - Neutrons emitted first from Weisskopf spectrum sampling
    - After neutrons are done emitting, photons are emitted from residual energy in fission fragment
  - **Computationally more efficient than MC Hauser-Feshbach approach in CGMF**

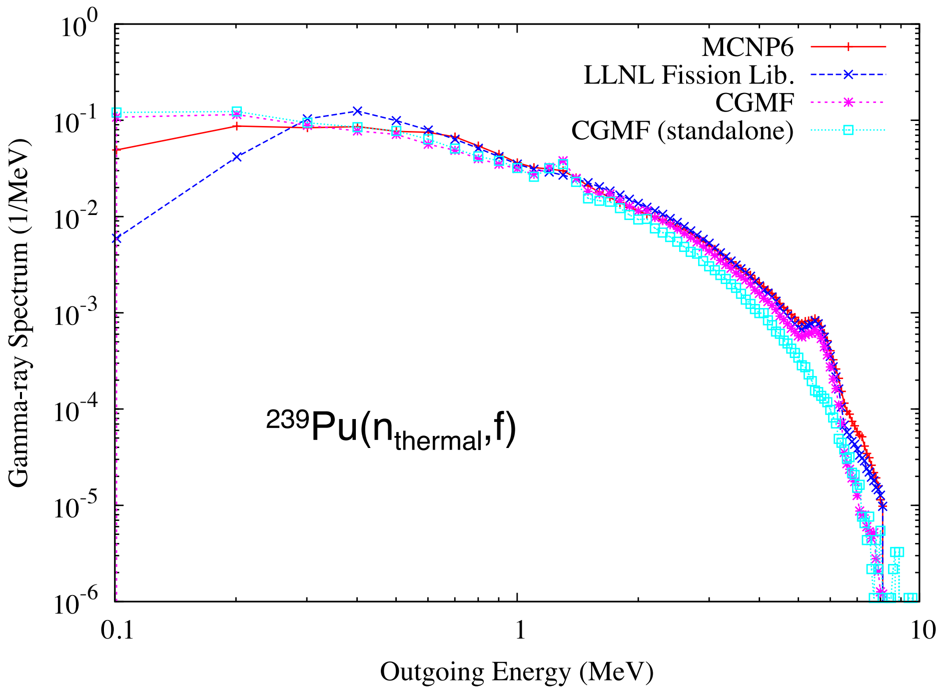


Correlated Data in Fission Events (1)

- **The primary goals of this NA-22 venture project:**
  - **Integrate CGMF & FREYA features into production version of MCNP6**
  - **Include thorough verification and validation testing**

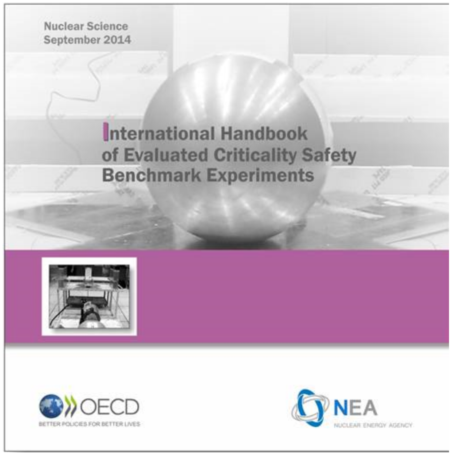
- **Code integration with MCNP6**
  - **Single common event generator interface**
  - **Integrate updated versions**
    - CGMF with speed improvements and new interface
    - LLNL Fission Library (version 1.9.1 released 2/25/15)
  - **Compare current test results with old test results**
  - **Develop more verification and validation tests**

Preliminary results are promising!

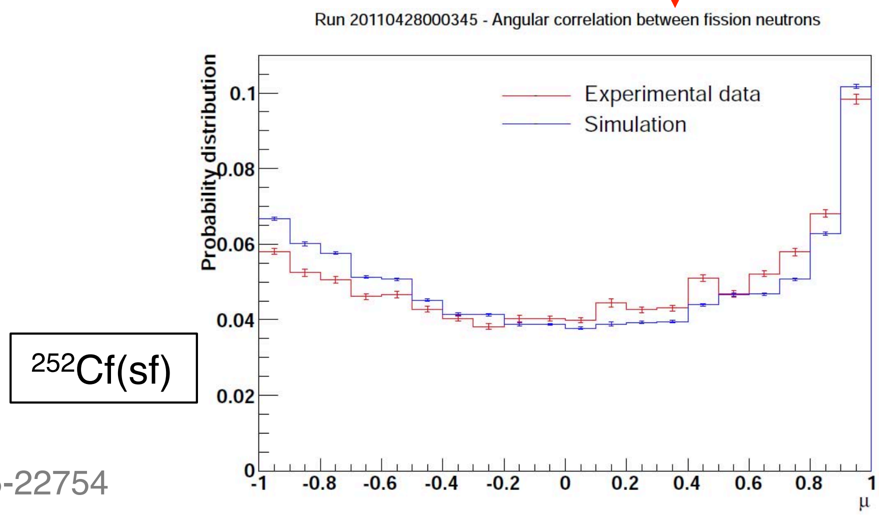


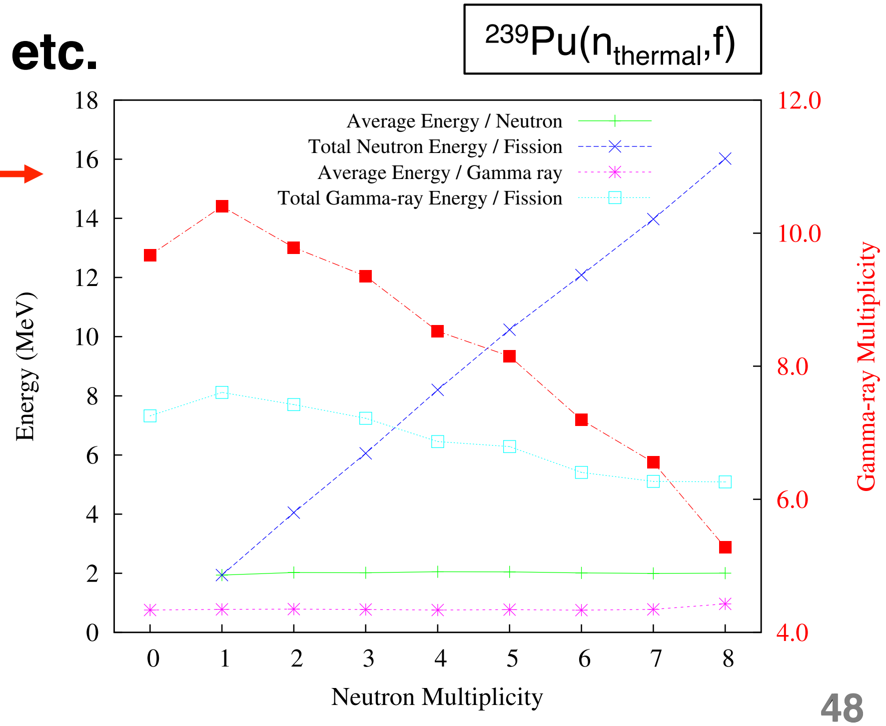
Correlated Data in Fission Events (2)

- **Validation of these models is desperately needed**
  - **Compare predictions of MCNP simulations of actual experimental measurements sensitive to the models**
  - **Subcritical work is being done and can be leveraged**



- **New measurements are currently underway (Univ. of Michigan) and are planned (LANL, LLNL, etc.) to look at quantities like:**
  - **Singlet and doublet counting rates, etc.**
  - **Multiplicity correlations**
  - **Angular correlations**





Motivation: k-eigenvalue Calculations (1)

- **For criticality calculations** [no external source, no spontaneous fission]
  - **Neutron multiplicity for fission is based on expected value of $wgt \cdot \nu\Sigma_F^{mat} / \Sigma_T^{mat}$ neutrons per collision in the material**
    - If more than 1 neutron, the energy & direction for each are sampled independently (no correlation)
  - **The spectrum used for the fission neutrons is randomly chosen using probabilities $\nu\Sigma_F^{iso} / \nu\Sigma_F^{mat}$ for the nuclides in the material**
    - Energy is sampled using ENDF spectrum data for the selected nuclide
    - Prompt vs delayed neutron selected first, then energy
    - If more than 1 neutron, energy is sampled independently for each one (no correlation), using the same spectrum data
  - **The direction for fission neutrons is sampled isotropically**
    - If more than 1 neutron, directions are sampled independently for each neutron (no correlation in direction)
  - **For KCODE problems with photons, photons are sampled independent of neutrons (no correlation between neutrons & photons)**

Motivation: k-eigenvalue Calculations (2)

- **Why is the expected value approach to fission neutron production used for criticality calculations? Why not use explicit fission neutron multiplicity data?**
  - **Traditional MC work in the criticality safety community has focused on k-effective, reflector & control material reactivity, etc.**
  - **The reactor physics community has traditionally used MC for k-effective, power distributions, control material reactivity, etc.**
  - **Very extensive collections of verification-validation data, MC vs benchmark experiments for those applications**

➜ **No verification-validation work has been done to date on using explicit fission neutron multiplicity options in MCNP for criticality safety or reactor physics applications**

MCNP6 – Work in Progress

- **For many years, patches to MCNP have existed for**
  - **Coincidence counting of fission neutrons**
    - Plan to incorporate the patches permanently into public version
  - **Intrinsic sources – spontaneous fission**
    - Plan to incorporate the patches permanently into public version
  - **List-mode data**
    - Can make use of exactly the same post-processing methods as for experimental data

- **CGMF & FREYA capabilities will be added to MCNP6**
  - **With improved verification and validation testing**
  - **Issues with parallel processing will be resolved**
  - **Double counting of fission photons needs to be resolved**

- **Investigate use of multiplicity for MCNP criticality calculations**
  - **Currently disabled for KCODE calculations**
  - **Needs validation against criticality benchmark suites**

Sensitivity/Uncertainty in MCNP6 & Nuclear Data Evaluations

MCNP6 Sensitivity/Uncertainty (1)

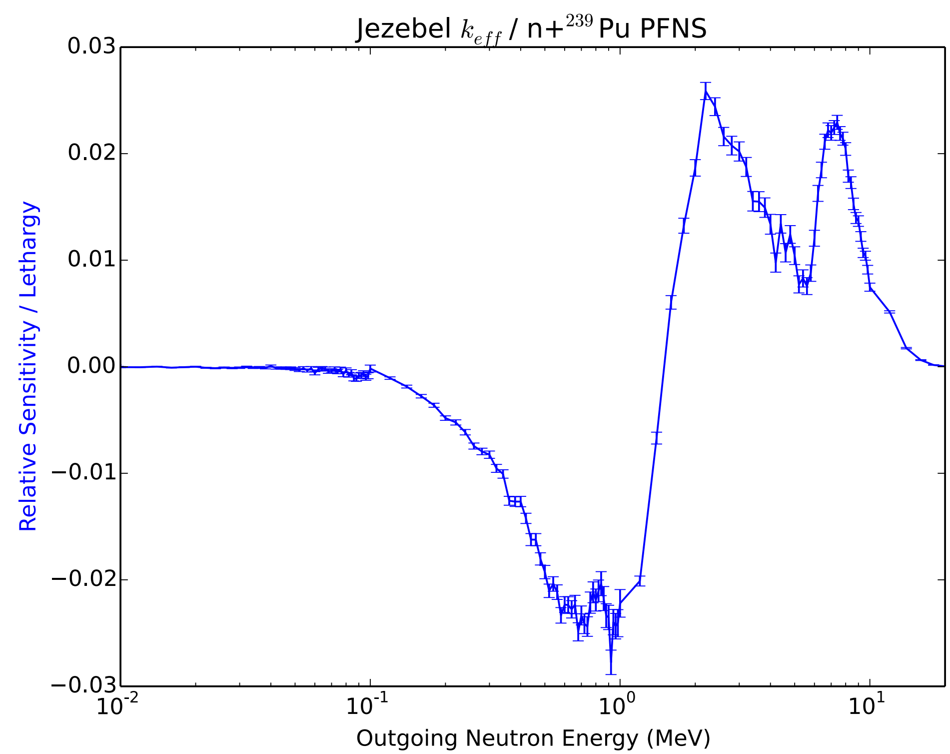
- Adjoint-weighted sensitivity coefficient tallies can be used to predict the impact on k_{eff} due to newly evaluated nuclear data

$$S_{k,\chi_i} = \frac{\chi_i}{k_{eff}} \frac{dk_{eff}}{d\chi_i}$$

- Simple ways to use:

$$k'_{eff} = k_{eff}\left[1 + \vec{S}_{k,\chi}\left(\frac{\vec{\chi}'}{\vec{\chi}} - 1\right)\right]$$

$$\frac{\sigma^2_{k_{eff}}}{k^2_{eff}} = \vec{S}^T_{k,\chi}\left(\frac{\boldsymbol{COV}_\chi}{\vec{\chi}\vec{\chi}^T}\right)\vec{S}_{k,\chi}$$



- With a recent evaluation of the ^{239}Pu(n,f) prompt fission neutron spectrum (PFNS), we can quickly validate this newly evaluated data against criticality safety benchmark simulations

MCNP6 Sensitivity/Uncertainty (2)

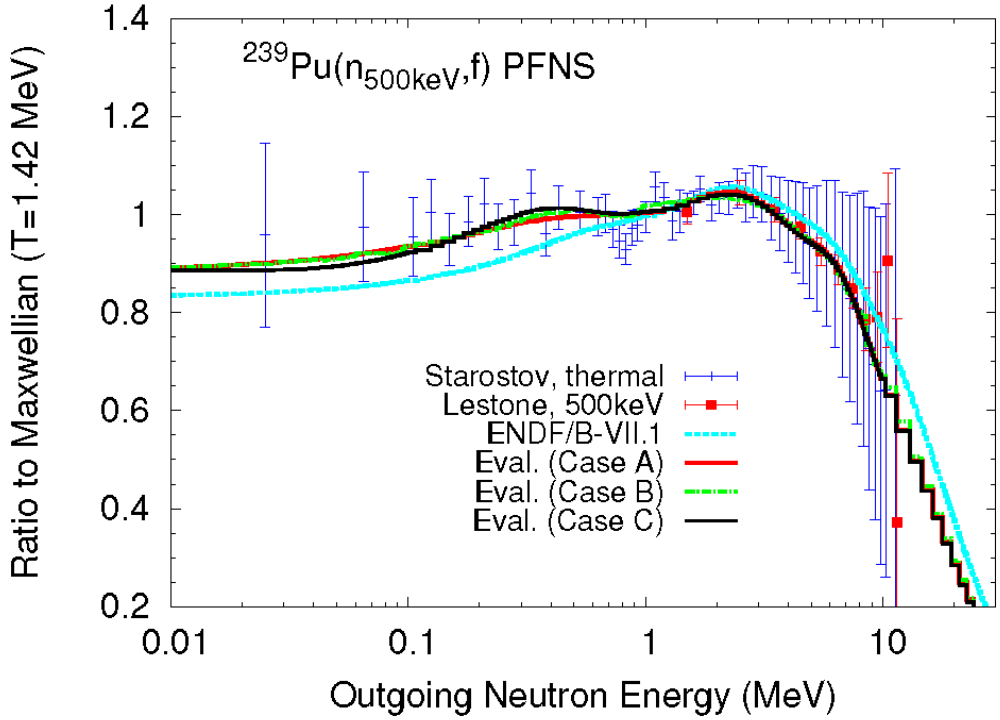
- When new theoretical methods or experimental measurements become available, the nuclear data community may find it necessary to update the nuclear data libraries to reflect these improvements

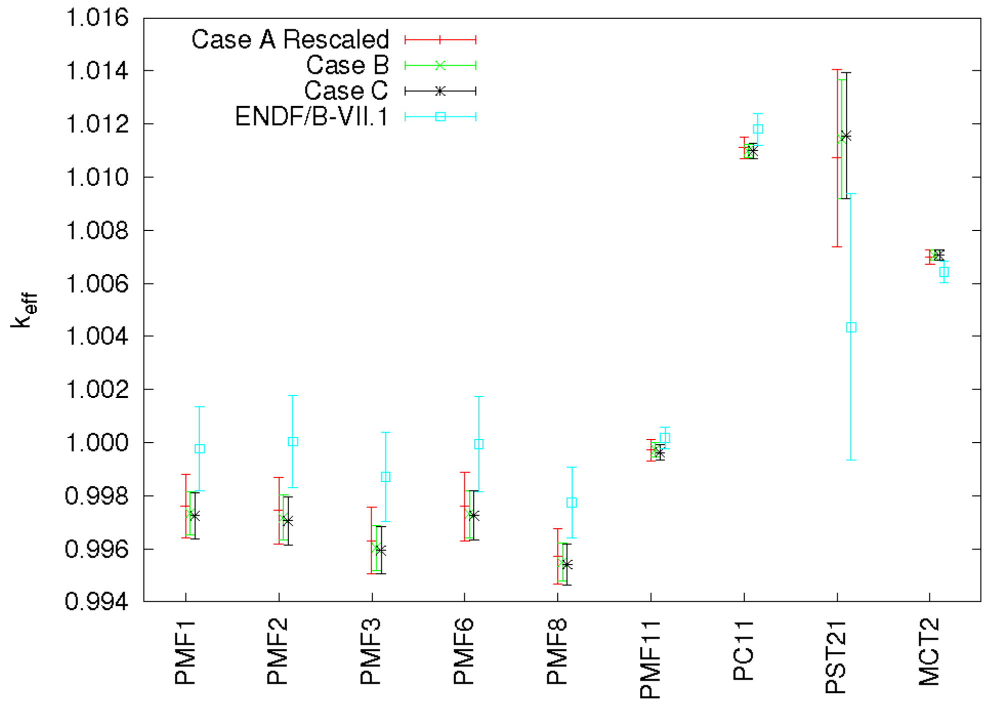
- At LANL, the impact on criticality calculations is one of the most important issues when new nuclear data (along with covariances) is being re-evaluated or released
  - Example: recent theoretical model improvements as well as experimental measurements were used in re-evaluating the $^{239}Pu(n,f)$ PFNS → this is an important quantity in fast metal systems (Jezebel)

- Using the adjoint-weighted sensitivity coefficients calculated by MCNP, collaborating with our theory and experimental colleagues was made easy
  - Obtain sensitivity of k_{eff} to the PFNS for a variety of benchmarks
  - Don't have to wait until new nuclear data library is released!

MCNP6 Sensitivity/Uncertainty (3)

- **During the evaluation process, immediate feedback is available**
  - **Don't need to process evaluated data into ENDF-6 format, run through NJOY to obtain new ACE formatted file and rerun MCNP6 calculations with different ACE files → especially cumbersome (and possibly error-prone) when making minor modifications to the evaluated data**
  - **Just use sensitivity profiles to estimate change in k_{eff} and uncertainty**





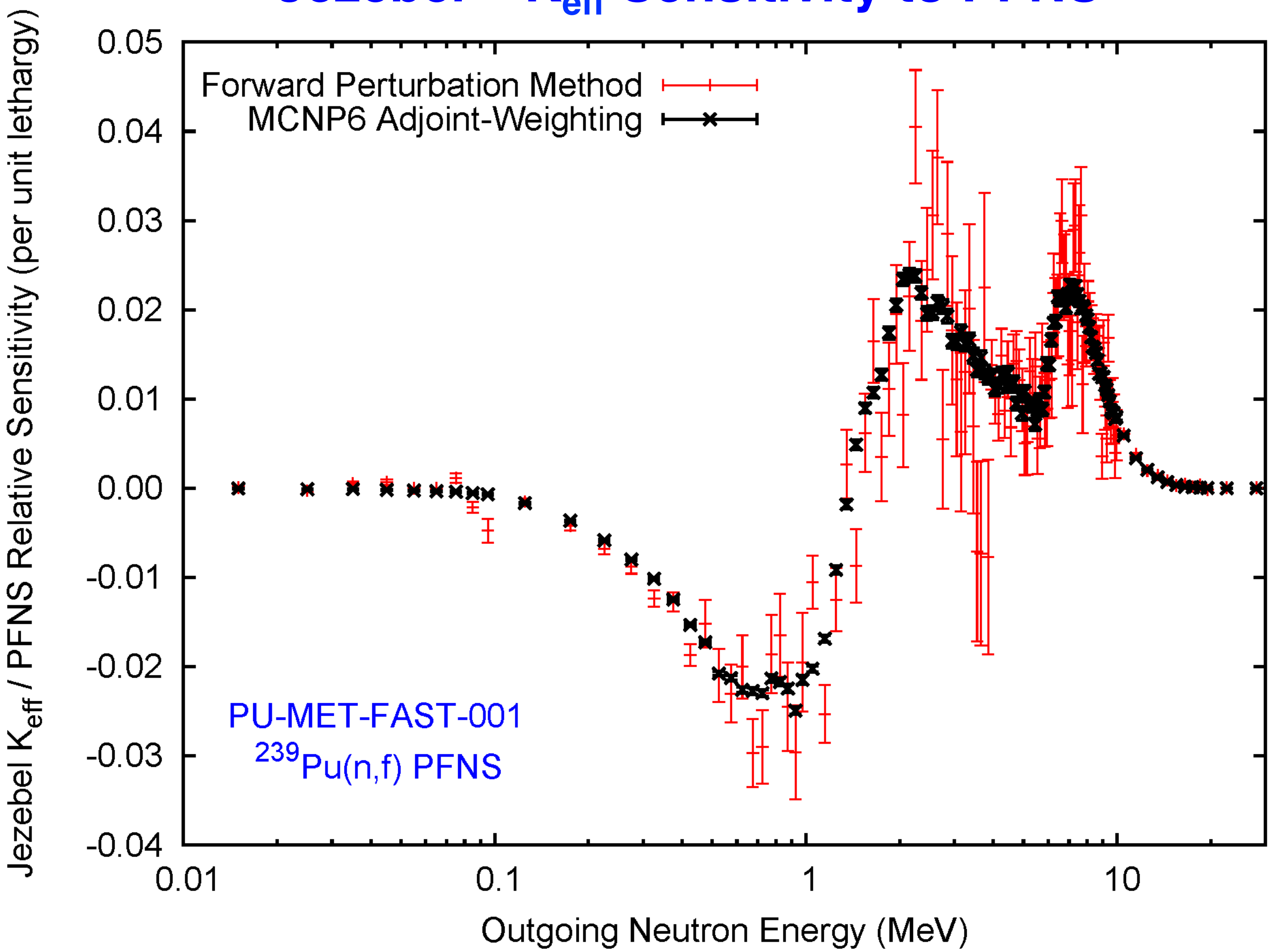
- **Impact of minor changes in PFNS (case A, B, C above) was easily compared to ENDF/B-VII.1 values of the benchmark calculations**

MCNP6 Sensitivity/Uncertainty (4)

- **MCNP6 sensitivity/uncertainty approach**
  - **Adjoint-weighted sensitivity calculation**
    - 1 MCNP6 calculation for adjoint-weighted results at all energy points in the sensitivity energy range
    - Simple linear algebra postprocessing to obtain change in k_{eff} and uncertainty

- **Some alternative approaches give poor results with more computational cost**
  - **Forward perturbation method**
    - Direct, simple, brute force – subtract base case & perturbed case for each energy point in the sensitivity energy range
    - Requires 100s or 1000s of separate MCNP calculations, with small statistics
    - Either edit ACE file directly for each calculation or edit ENDF-6 evaluation file, run NJOY to produce a new ACE file… not ideal!

Jezebel – K_{eff} Sensitivity to PFNS



Forward perturbation method = 2 MCNP6 calculations <u>per data point</u>

Adjoint-weighted sensitivity = 1 MCNP6 calculation for <u>ALL data points</u>

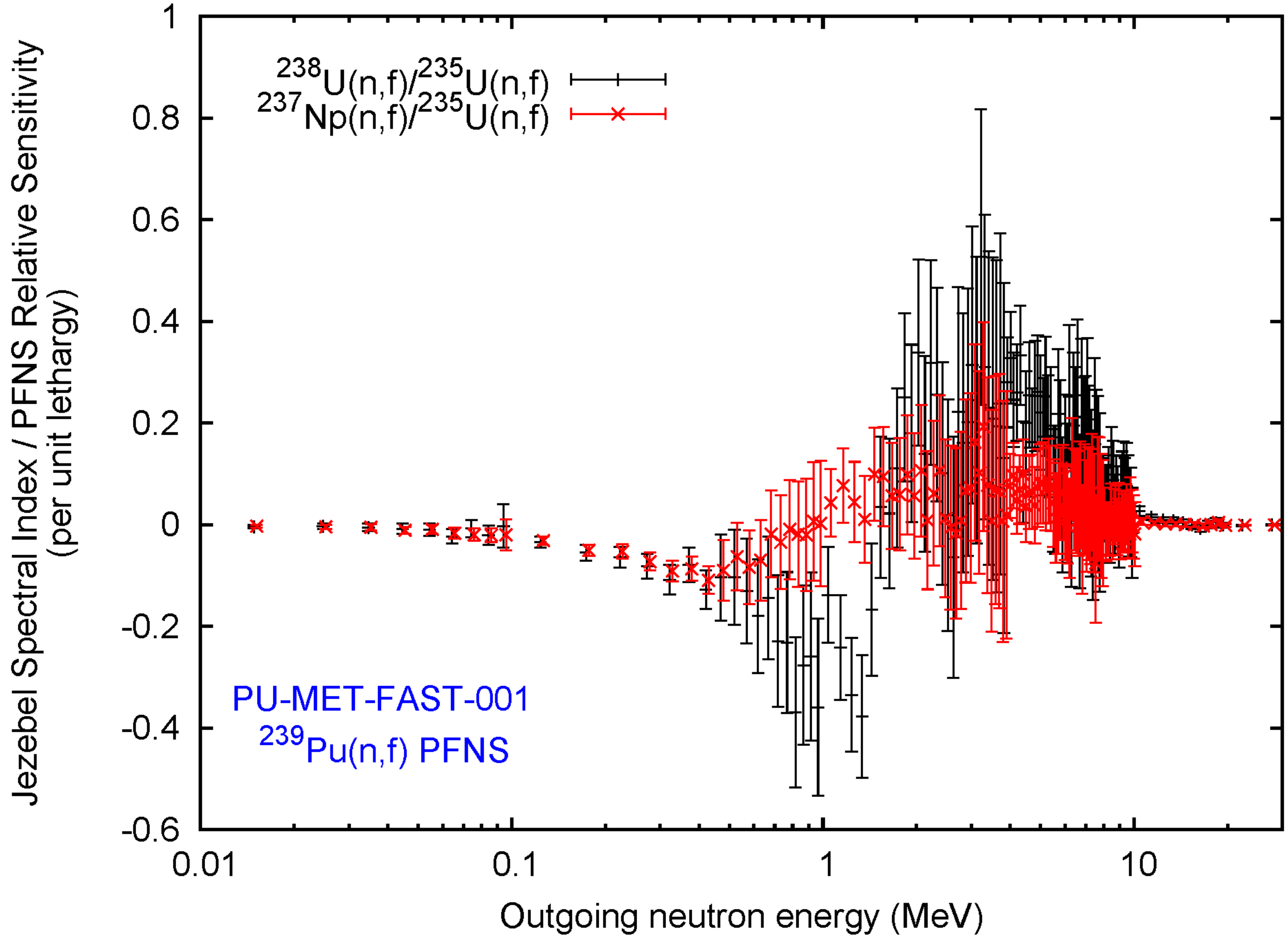
- Other integral & semi-integral data have been measured on critical experiments such as,
  - A variety of spectral indices (ratio of reaction rates)
  - Overall and energy-dependent leakage
  - Rossi-alpha
  - Reactivity worths

- When new nuclear data is available, we should compare our calculations of k_{eff} and these other integral & semi-integral quantities to provide feedback to the nuclear data community

- MCNP6 needs to be able to compute adjoint-weighted sensitivity tallies for quantities other than k_{eff}, such as spectral indices, to compare against other experimentally measured criticality data because the alternative approaches perform very poorly in comparison

MCNP6 Sensitivity/Uncertainty (7)

Jezebel – Spectral Index Sensitivity to PFNS



Forward perturbation method = 2 MCNP6 calculations <u>per data point</u>

Need adjoint-weighted sensitivity capability!

MCNP6 – Work in Progress

- **Continue to provide feedback to the nuclear data community on new evaluations regarding impact on criticality applications**
  - Ultimately, the tools in MCNP6 are available now for the nuclear data community to use to assess impact on k_{eff}
- **Currently, expanding the adjoint-weighted sensitivity calculations beyond k_{eff} is planned for in the not-so-distant future**
- **The nuclear criticality safety program is interested in having nuclear data covariance matrices in ACE format**
  - Modifications to NJOY are underway to process ENDF-6 covariances into ACE format covariances
  - MCNP6 will be able to compute k_{eff} uncertainties directly when available → eliminates postprocessing by users
  - The Whisper utility (discussed separately in this workshop) will make use of these ACE format covariances to establish the upper subcritical limits necessary for criticality safety analysts

References

Fission Multiplicity in MCNP6

J.M. Verbeke, C.A. Hagmann, J. Randrup and R. Vogt, Lawrence Livermore National Laboratory, LLNL-PROC-638986 (2013).

J.M. Verbeke, C. Hagmann, and D. Wright, Lawrence Livermore National Laboratory, UCRL-AR-228518 (2014).

R. Vogt and J. Randrup, *Phys. Rev. C*, vol. **84**, pp. 044612-1-14 (2011).

T. Kawano, P. Talou, M.B. Chadwick, and T. Watanabe, *J. Nucl. Sci. Tech.*, **47** (5), 462-69 (2010).

T. Wilcox, G.W. McKinney, T. Kawano, proceedings ANS RPSD 2014, LA-UR-14-21300 (2014).

B. Becker, P. Talou, T. Kawano, Y. Danon, and I. Stetcu, *Phys. Rev. C*, **87**, 014617 (2013).

M.E. Rising, A. Sood, P. Talou, T. Kawano and I. Stetcu, proceedings ANS Annual Winter Meeting 2014, Los Alamos National Laboratory, LA-UR-14-24979 (2014).

Sensitivity/Uncertainty & Nuclear Data Evaluations

B.C. Kiedrowski and F.B. Brown, *Nucl. Sci. Eng.*, **174**, 227-244 (2013).

B.C. Kiedrowski and F.B. Brown, proceedings ANS M&C 2013, Los Alamos National Laboratory, LA-UR-12-25966 (2013).

B.C. Kiedrowski, "MCNP6.1 k-Eigenvalue Sensitivity Capability: A Users Guide", LA-UR-13-22251 (2013).

M.E. Rising, *Nuclear Data Sheets*, **123**, 109-114 (2015).

D. Neudecker, P. Talou, T. Kawano, D.L. Smith, R. Capote, M.E. Rising and A.C. Kahler, *Nuclear Instruments and Methods in Physics Research A* (in press).

Whisper Methodology For Criticality Safety Validation & USLs

Whisper Methodology for Validation & USLs (1)

- **In early 2014, the XCP-3 & NCS groups at LANL undertook a major upgrade to the criticality safety computational capabilities**
  - **Previous:** **mcnp5-1.25, endf 4, 5, 6 (very old & unsupported)**
  - **Upgrade:** **mcnp6.1 + endf/b-vii.1, HPC cluster**
  - **Participants:**
    - Kiedrowski, Conlin, Favorite, Kahler, Kersting, Parsons, Walker, Brown, etc.
  - **References** **[all are on website mcnp.lanl.gov]**
    - LA-UR-14-26558, *Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits*
    - LA-UR-14-26436, *User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation*
    - LA-UR-14-23202, *Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation*
    - LA-UR-14-23352, *Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems*

Whisper Methodology for Validation & USLs (2)

- **Whisper ICSBEP Benchmark Suite**
  - **1086 ICSBEP benchmark problems from Mosteller, Kahler, others**
  - **Sensitivity profiles from adjoint-weighting for all isotopes/reactions/benchmarks**
- **Whisper methodology –** LA-UR-14-26558, LA-UR-14-26436, LA-UR-14-23352
  - **Verification of computer code system**
    - Installation tests, VERIFICATION_KEFF tests, config control, static linked, etc.
  - **Validation benchmarks**
    - Estimate missing uncertainties
    - Reject inconsistent benchmarks via iterated diagonal chi-squared method (~12%)
    - Correlation data from DICE; covariance data from ORNL (10% diag for missing)
    - Automated benchmark selection for AOA problem using sensitivity data to determine C_k values; C_k values used for weighting
  - **Calculational Margin**
    - Determine bias from non-parametric method based on Extreme Value Theory, using weighting determined from C_k values
    - Determine bias uncertainty numerically from distribution of worst-case k_{eff} bias
  - **Margin of Subcriticality**
    - Margin of 0.0050 for unknown code errors (expert judgment)
    - Margin for nuclear data uncertainty from GLLS method
    - Additional margin – analyst judgment for AOA & problem, conservatism, etc.
  - **USL = 1.0 – Calculational Margin – Margin of Subcriticality**

Whisper Methodology for Validation & USLs (3)

- **Current activities**
  - **NCS Division SQM for Whisper (XCP-3 assisting in review)**
    - *NCS-SQM Whisper Code Inspection (Sartor, in preparation)*
    - *NCS-SQM Whisper Verification & Validation (Sartor, in preparation)*
    - *NCS-SQM MCNP6 KCODE Verification & Validation (Sartor, in preparation)*
  - **Whisper software**
    - Potential use at other DOE sites
    - Well-documented and tested alternative to tsunami/tsurfer/etc
    - **To be included with standard MCNP6 distribution through RSICC**
  - **Whisper benchmark suite**
    - MCNP input for 1086 ICSBEP benchmarks
    - Valuable resource for all MCNP criticality-safety users & sites
    - **To be included with standard MCNP6 distribution through RSICC**
  - **Improved covariance data – produce with NJOY & new ACE formats**
    - **Minor mods to Whisper, when Nuclear Data Team produces improved data**
  - **Whisper training**
    - **Proposed to DOE-NCSP for LANL & other DOE crit-safety groups**
    - Local training at LANL (not DOE-NCSP funded)

Data Issues

Data Issues (1)

Over the last few years, a number of issues have come up regarding MCNP & its associated ACE datasets:

- Photon Doppler broadening
- NJOY purr temperature bug
- S(a,b) data for u-o2, zr-h, sio2
- S(a,b) data for h-zr at 1200 K
- Activation data interpolation
- makxsf temperature interpolation for S(a,b) data

- Some of these issues are mistakes in preparing ACE files, some are due to mismatches between NJOY & MCNP
- These & other data issues are usually discussed on the MCNP Forum & corrected in subsequent code releases from RSICC
- At present, there is no good mechanism for communicating these issues to all MCNP users (20k copies sent out in last 15 yr)

Data Issues (2)

Photon Doppler Broadening

- **Photon Doppler broadening data was included for all elements in the photoatomic libraries mcplib03 & mcplib04**
  - There was a mismatch between the data library description & mcnp5 coding – PDF data was stored, while CDF data was assumed in coding
  - New libraries mcplib63 & mcplib84 were provided on the mcnp.lanl.gov website in 2012, with the error corrected

- **Anyone using mcnp5:**
  - Use photon libraries mcplib63 or mcplib84, not mcplib03 or mcplib04

- **Anyone using mcnp6:**
  - The code checks the photon data, corrects if needed
  - Works correctly with mcplib03, mcplib04, mcplib63, mcplib84

NJOY purr temperature bug

- **A bug was found & corrected in NJOY in December 2012.**
  - A temperature parameter used in constructing the unresolved resonance probability tables for MCNP involved temperature, rather than the correct square-root of the temperature.
  - The bug in the PURR portion of NJOY was fixed in version njoy99.387 in December 2012. All prior versions have the bug; newer versions do not have the bug (including njoy2012).
  - Affects all ACE unresolved resonance data for temperatures greater than room temperature that were prepared using NJOY versions prior to njoy99.387
  - ACE files for ENDF/B-VII.1 were prepared with a correct version of NJOY, and do not have the problem.
  - All prior ACE files (including ENDF/B-VII.0) for temperatures greater than room temperature have the problem with incorrect probability table data.

Data Issues (4)

NJOY purr temperature bug – Impact for ENDF/B-VII.0

- If calculations are run using the ENDF/B-VII.0 data as released (with the njoy-purr bug) vs. corrected data, errors in Keff for some calculations are:

Typical PWR:	900 K:	Δk =	9 pcm	± 11 pcm
	2500 K:	Δk =	19 pcm	± 11 pcm
Intermediate, ZPR-III-48:	900 K:	Δk =	-37 pcm	± 14 pcm
	2500 K:	Δk =	-3 pcm	± 16 pcm
Godiva, HEU:	900 K:	Δk =	7 pcm	± 8 pcm
	2500 K:	Δk =	4 pcm	± 8 pcm
Inf medium, $H+U^{238}+Pu^{239}$:	900 K:	Δk =	-211 pcm	± 7 pcm
	2500 K:	Δk =	-188 pcm	± 7 pcm

ENDF/B-VII.1 data do not have this problem

S(a,b) data for u-o2, zr-h, sio2

- **For the continuous S(a,b) data released with ENDF/B-VII.1 (in the MCNP6.1 release in 2013)**
  - **ACE datasets with suffixes .20t - .29t, in directory xdata/ENDF71SaB**
  - **For u-o2, zr-h, sio2, the list of isotopes to match the S(a,b) data with was incorrect, so that the S(a,b) data was generally not used.**
  - **For u-o2, zr-h, sio2, the list of isotopes was corrected in the .30t - .37t datasets released with MCNP6.1.1 (2014)**

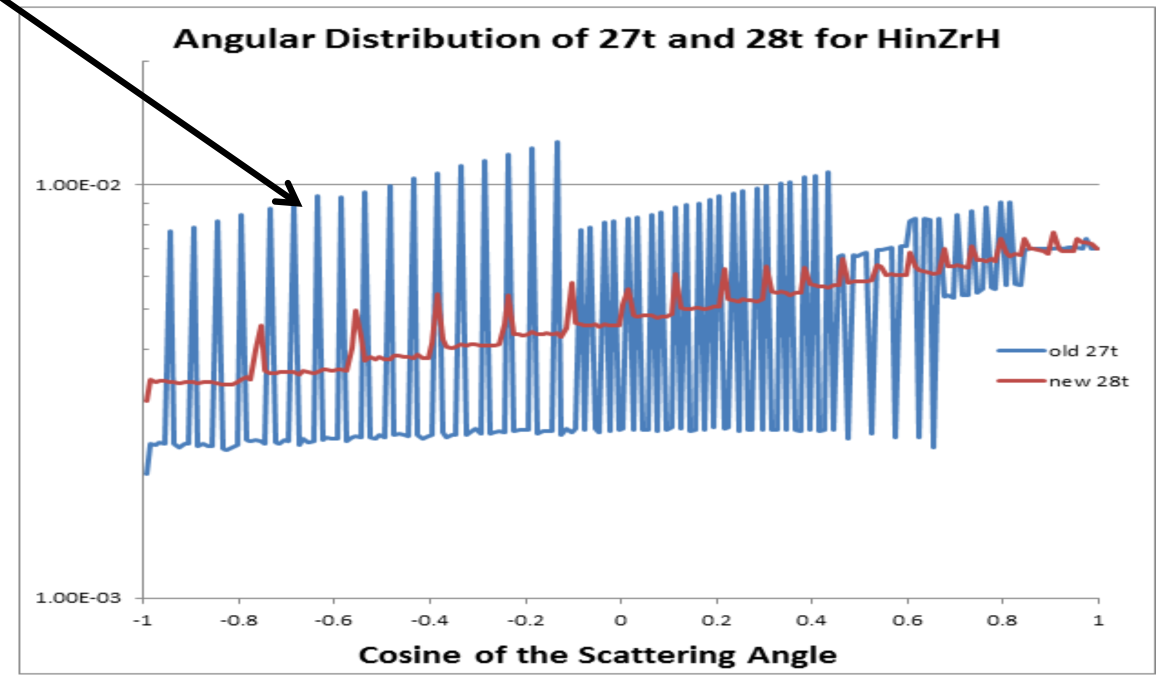
	.20t association	.30t association
u-o2	U-232, U-233, U-234	U-238
zr-h	Zr-90, Zr-91, Zr-element	Zr-90, Zr-91, Zr-92, Zr-93, Zr-94, Zr-95, Zr-96, Zr-element
sio2	O-16, Si-28, Si-29	O-16, Si-28, Si-29, Si-30

Data Issues (6)

S(a,b) data for h-zr at 1200 K for ENDF/B-VII.1 ACE files

- The S(a,b) data for h-zr.27t (1200 K) incorrectly flagged the elastic scattering data as “coherent” (Bragg data), when it is actually “incoherent”

- h-zr.27t (1200 K) S(a,b) dataset should not be used



- Corrected data has not yet been released

Activation data interpolation

- **Activation datasets, ".nnY", permit different interpolation schemes over different energy ranges**
  - **MCNP6 permits that**
  - **NJOY creates the ACE files correctly if there is only 1 interp scheme, incorrect format if there is >1 interp scheme**

- **This is not a problem for any existing ".nny" files distributed with MCNP; they all use only 1 interp scheme for activation data**

- **For researchers who create their own activation datasets, there will be errors if more than 1 interp scheme is used in NJOY**

makxsf temperature interpolation for S(a,b) data

- In 2006, the makxsf utility code was extended (based on MacFarlane's doppler utility code) to provide
  - Doppler broadening of ".nnC" ACE datasets
  - Temperature interpolation of URR probability tables
  - Temperature interpolation of thermal S(a,b) datasets
- Versions of NJOY used to prepare S(a,b) datasets for ENDF/B-VII.0 & ENDF/B-VII.1 are different
  - makxsf cannot handle newer continuous S(a,b) data, ".2nt"
  - makxsf cannot handle elastic S(a,b) data for ".1nt" where the data has been thinned (producing different energy grids at different temperatures)
  - makxsf OK for temperature interpolation on lwtr.1nt & hwtr.1nt, but not grph.1nt

Monte Carlo Application Tool Kit
MCATK

Outline

- MCATK Overview
- Development Strategy
- Available Algorithms
- Sources
- Geometry
- Cross Section Data
- Parallelism
- Miscellaneous Tools/Features
- Couple n-gamma Transport (In Progress)

What is MCATK?

- A C++ component-based Monte Carlo particle transport software library
  - Development began in 2008
- Designed to build specialized applications
- Designed to provide new functionality in existing general purpose Monte Carlo codes like MCNP
- Developed with Agile software engineering methodologies

Current MCATK Contributors

- Steve Nolen
- Jeremy Sweezy
- Travis Trahan
- Terry Adams
- Chris Werner
- Lori Pritchett-Sheats (CCS-2)
- Rob Aulwes (CCS-7)
- Grady Hughes

MCATK Motivation: Reduce Costs

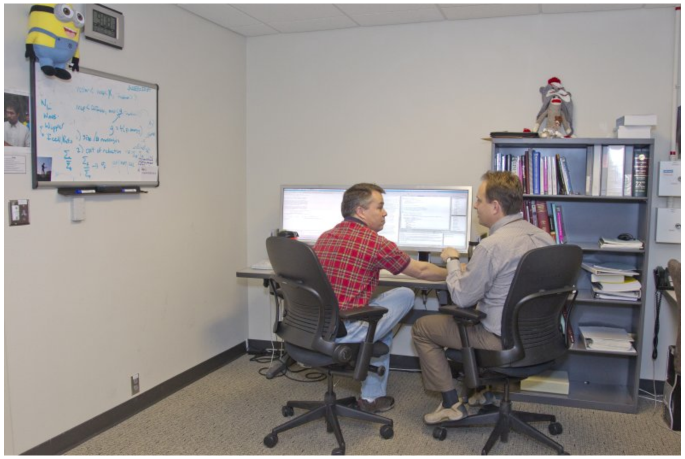
- **Reduce code duplication**
- **Reduce code complexity**
- **Reduce time to deliver custom solutions**
- **Leverage external packages**
- **Provide re-usable components**
- **Find defects earlier in the development cycle**

MCATK: Reusable Components

- Provide components for:
  - Existing codes (example: MCNP)
  - Stand alone applications (example: MCATK K_{eff} solver)
- Components are well tested
  - Unit testing – verification
  - Integrated physics tests – validation
- Flat API available for C and Fortran codes
- Object Oriented API for C++ codes

MCATK: Development

- **Agile software development methodology**
  - Incremental development
  - Short iteration cycles (2 weeks)
- **Test driven development (TDD)**
  - Test first philosophy
  - Unit testing with UnitTest++
  - Unit tests built and executed continuously (with each commit)
  - ~10 minute build
- **Pair-programming, Colocation**
  - Improves design and testing
  - Promotes knowledge sharing and collective ownership of code



MCATK: Continuous Testing and Reporting

Monte Carlo Codes
XCP-3, LANL

MCATK toolkitlib

Dashboard | Calendar | Previous | Current | Next | Project

No update data as of **Tuesday, March 24 2015 - 19:00 MDT**

Nightly tests
- run longer
- include more tests
- variety of platforms/ compilers

Nightly

Site	Build Name	Update Files	Configure Error	Configure Warn	Build Error	Build Warn	Test Not Run	Test Fail	Test Pass	Build Time
candycorn	linux-gnu4.6-Release	2	0	0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
cielito	linux-gnu4.8-Debug		0	0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
cielito	linux-gnu4.8-Release	0	0	0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
cielito	linux-intel14.0-Debug		0	0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
cielito	linux-intel14.0-Release	0	0	0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
moonlight	linux-gnu4.6-Debug	3	0	0	0	0	0	23^{+1}	888^{+1}_{-1}	Mar 24, 2015 - 20:05 MDT
moonlight	linux-gnu4.6-Release	0	0	0	0	0	0	0	994^{+1}	Mar 24, 2015 - 20:12 MDT
moonlight	linux-intel14.0-Debug	0	0	0	0	30	0	29	882^{+1}	Mar 24, 2015 - 20:22 MDT
moonlight	linux-intel14.0-Release		0	0	0	30	0	30	964^{+1}	Mar 24, 2015 - 20:32 MDT
pinto	linux-gnu4.6-Debug		0	0	0	0	0	22^{+1}	889^{+1}_{-1}	Mar 24, 2015 - 20:04 MDT
pinto	linux-gnu4.6-Release	0	0	0	0	0	0	0	994^{+1}	Mar 24, 2015 - 20:11 MDT
pinto	linux-intel14.0-Debug		0	0	0	30	0	29	882^{+1}	Mar 24, 2015 - 20:21 MDT
pinto	linux-intel14.0-Release	0	0	0	0	30	0	30	964^{+1}	[illegible]
retumbo	linux-gnu4.8-RelWithDebInfo	2	0	0	0	0	0	0	994	[illegible]
titegroup	linux-gnu4.6-RelWithDebInfo	2	0	0	0	0	0	3	991	[illegible]
varget	linux-intel14.0-RelWithDebInfo		0	0	0	30	0	30	964	[illegible]

Continuous

Site	Build Name	Update Files	Configure Error	Configure Warn	Build Error	Build Warn	Test Not Run	Test Fail	Test Pass
candycorn	linux-gnu4.6-Release		0	0	0	0	0	0	810^{+1}

New entry generated after **every** commit

Code coverage (nightly)

Site	Build Name	Update Files	Configure Error	Configure Warn	Build Error	Build Warn	Test Not Run	Test Fail	Test Pass	Build Time
[illegible]	linux-gnu4.6-Debug	3	0	0	0	0	0	1	808^{+1}	Mar 24, 2015 - 20:42 MDT
[illegible]	linux-gnu4.6-Debug	2	0	0	0	0	0	1	808	Mar 24, 2015 - 20:01 MDT

Site	Build Name	Percentage	LOC Tested	LOC Untested	Date
candycorn	linux-gnu4.6-Debug	86.57%	3067	476	Mar 24, 2015 - 20:01 MDT

Dynamic Analysis

Site	Build Name	Checker	Defect Count	Date
moonlight	[illegible]	Valgrind	452	Mar 24, 2015 - 20:42 MDT

Memory leaks etc. (even 3rd party libraries!) (nightly)

Power Iteration

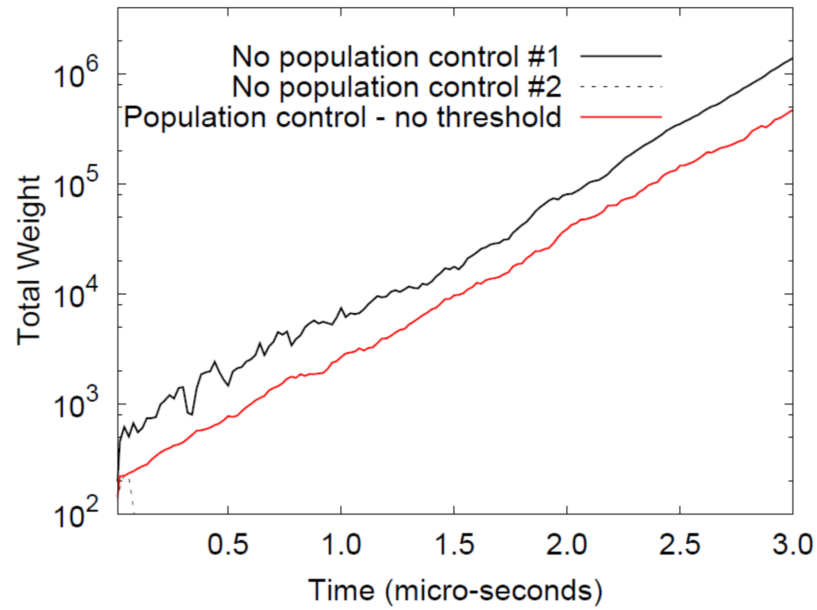
- **k-Eigenvalue solver**
- **α-Eigenvalue solver**
  - **The α-Eigenvalue is the inverse of the reactor period**
  - **Uses "time absorption" i.e.** $\alpha / velocity_{{}^{1}_{0}n}$
- **Validation suite covers many of the criticality test problems from the MCNP validation suite.**

Case	MCNP K_{eff}	MCNP Std. Dev.	MCATK Delta K_{eff}	MCATK Std. Dev.	# of Std. Dev.
JEZ233	0.9990	(8)	-0.0005	(12)	<1
FLAT23	0.9987	(11)	0.0018	(16)	<1
UMF5C2	0.9944	(9)	-0.0019	(13)	<2
FLSTF1	0.9895	(19)	-0.0039	(25)	<2
ORNL11	0.9930	(10)	-0.0022	(15)	<2
IMF04	1.0083	(10)	0.0018	(14)	<1
PUSH2O	1.0134	(11)	-0.0008	(16)	<1
HISHPG	1.0118	(9)	-0.0015	(15)	<1
PNL2	1.0146	(16)	-0.0022	(23)	<1

Note: Table shows a selection from suite which includes 24 systems

Time-Dependent Solver

- **Performs dynamic α-eigenvalue calculations**
- **Particles are added to "census" if they survive to the end of the time step**
- **Population control is applied to the census between time steps**
  - **This prevents exceeding memory limits for supercritical systems, and prevents the population from dying off in subcritical or stochastic systems (i.e., systems with small neutron populations)**



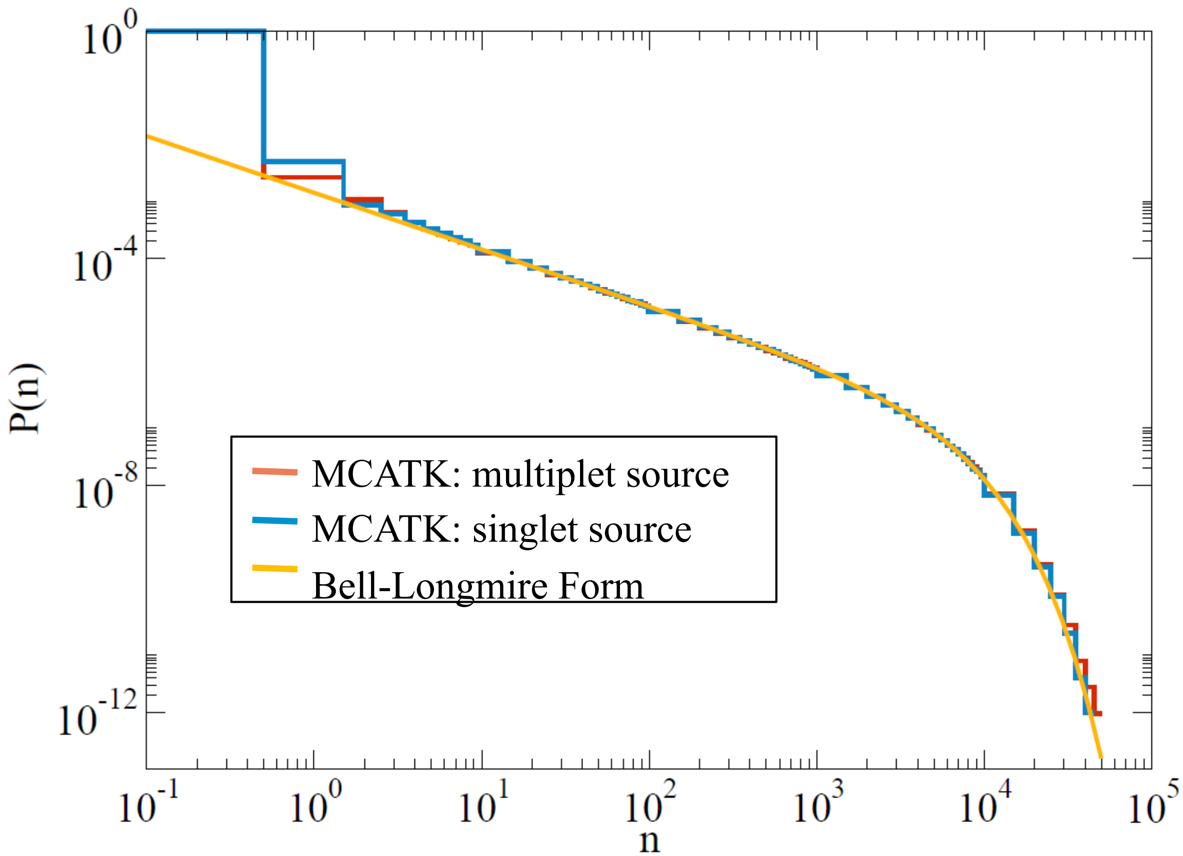
Total weight vs. time for a super-critical analytic problem using the MCATK time-dependent algorithm

Fission Chain Analysis

- Each source particle begins a fission chain
- Every descendent of the initiating particle is marked as being part of the same chain
- Tally quantities by fission chain
  - Total chain length
  - Number of fission events
  - Number of particles alive in a chain at a given time
- The fission chain analysis is particularly useful for analysis of stochastic systems (systems in which the neutron population is very small)
  - Probability of chains having a certain length at a given time
  - POI/POE
  - Multiplication

- **MCATK can be used to tally the expected number of chains comprised of n neutrons at a given time, $P(n)$.**

PDF of Neutron Number, n, for a Pu Sphere



Work performed by Erin Fichtl (LANL)

Fission Chain Analysis: POI/POE

- **Traditional method**
  - Set a cutoff for chain length
  - If a chain exceeds the cutoff, kill the entire chain and score it as a divergent chain
  - Tends to over-estimate POI by counting large, non-divergent chains as divergent
- **Booth's POE Guess method**
  - Rather than applying variance reduction to individual particles, apply rouletting and splitting to entire chains.
  - User supplies a guess for the POE
  - The chain is given an importance based on its current population, N, and the POE guess, POE_{Guess}:

$$I(N) = POE_{Guess}/POE_{Guess}^{N}$$

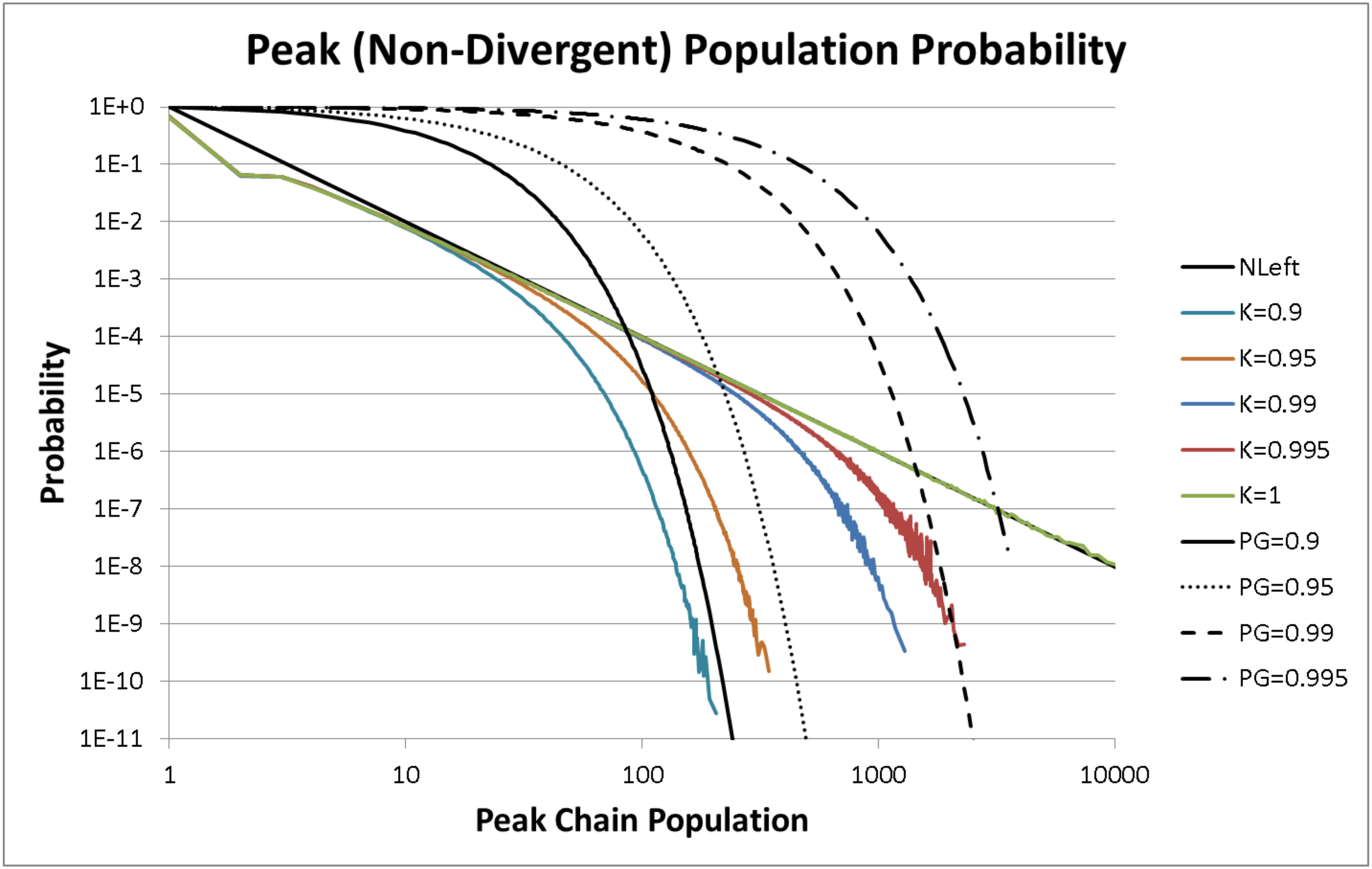
  - Can roulette chains too aggressively creating converge problems
- **MCATK "N Left" method**
  - The chain is given an importance based on its current population, N:

$$I(N) = C/N^2$$

  - The cutoff value, C, prevents rouletting below a certain chain population.

MCATK Fission Chain Analysis

Monte Carlo Codes
XCP-3, LANL



Sources

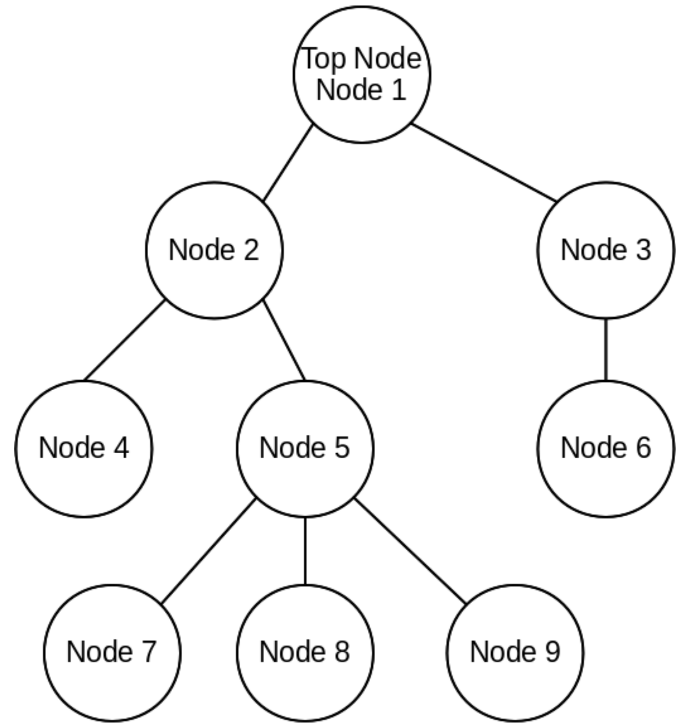
- **Burst**
- **Time-varying distributions**
- **Spatial-varying distributions**
- **Spontaneous fission**
  - **Can use average multiplicity or sample from actual multiplicity data**
- **Surface source files**
  - **Link to MCNP**

MCATK Geometry

- LNK3DNT mesh files
- Mesh specification through the API
- Mesh types supported:
  - Spherical: R
  - Cylindrical: R, RZ, RZΘ
  - Cartesian: X, XY, XYZ
- 3-D Solid Body Geometry
  - Available geometric primitives:
    - Spheres
    - Cylinders (right finite cylinder)
    - Boxes (right parallel piped)
    - Cones (truncated circular cones)
  - Each primitive can have rotations and translations

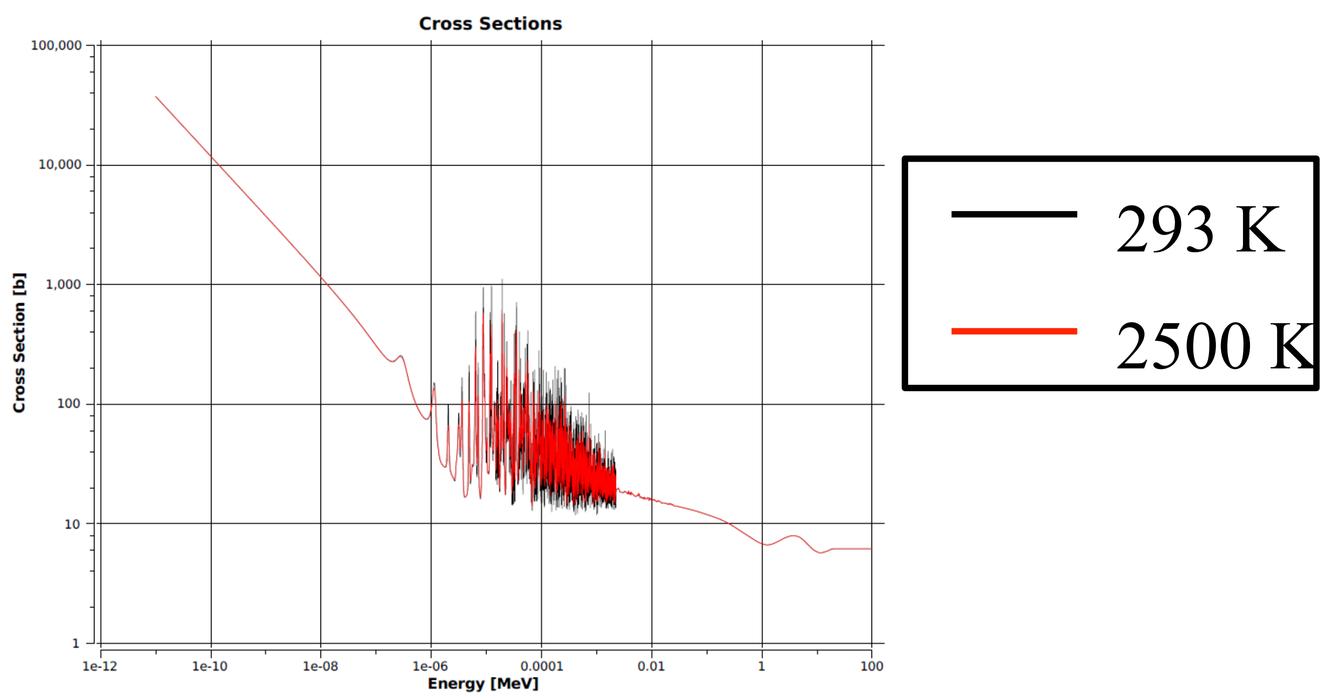
More on CSG

- **MCATK uses a scene graph hierarchy**
  - Each solid in the scene is assigned to a node in a tree
  - Each node is a childe of (contained by) the node above
  - Similar to CERN's ROOT and GEANT4 geometries
- **Nodes have the following properties:**
  - Each node is assigned a geometric primitive
  - Each node can have other nodes registered as children
  - A node can have an optional transformation that will be inherited by its children
  - Children are allowed to overlap, but MCATK applies an order of precedence
  - Parent containment and child precedence can be used to replicate combinatorial operators



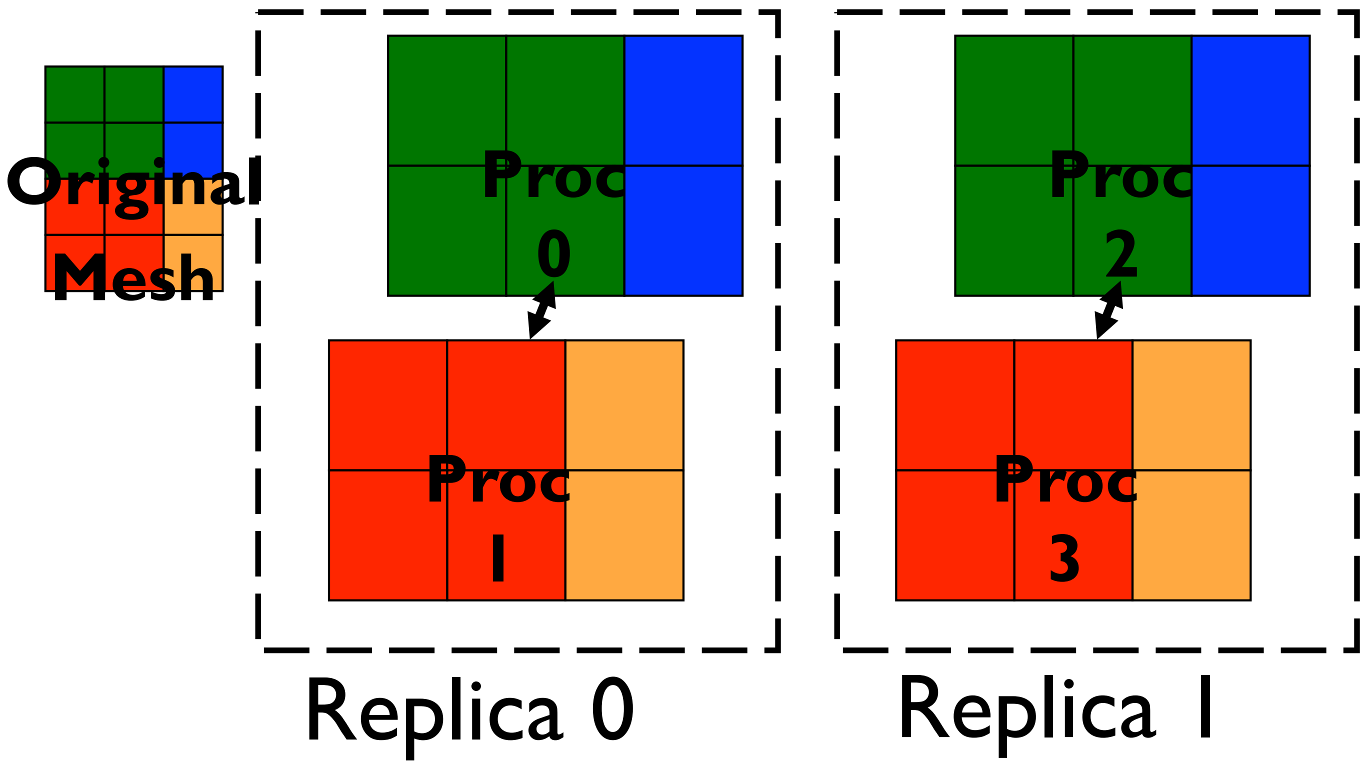
Cross Section Data and Multi-temperature Treatment

- **MCATK uses continuous energy data read from ACE data files**
- **Multi-temperature treatment:**
  - **MCATK is able to read in cross sections processed at more than one temperature**
  - **It picks the cross section table that was processed at the temperature that is closest to, but does not exceed the cell temperature**
  - **This capability is expected to be a step towards Doppler broadening on-the-fly and other multi-temperature treatments**



Parallel Models

- **MPI (distributed memory) only**
  - Domain decomposed
  - Domain replicated (particle decomposed)
  - Hybrid



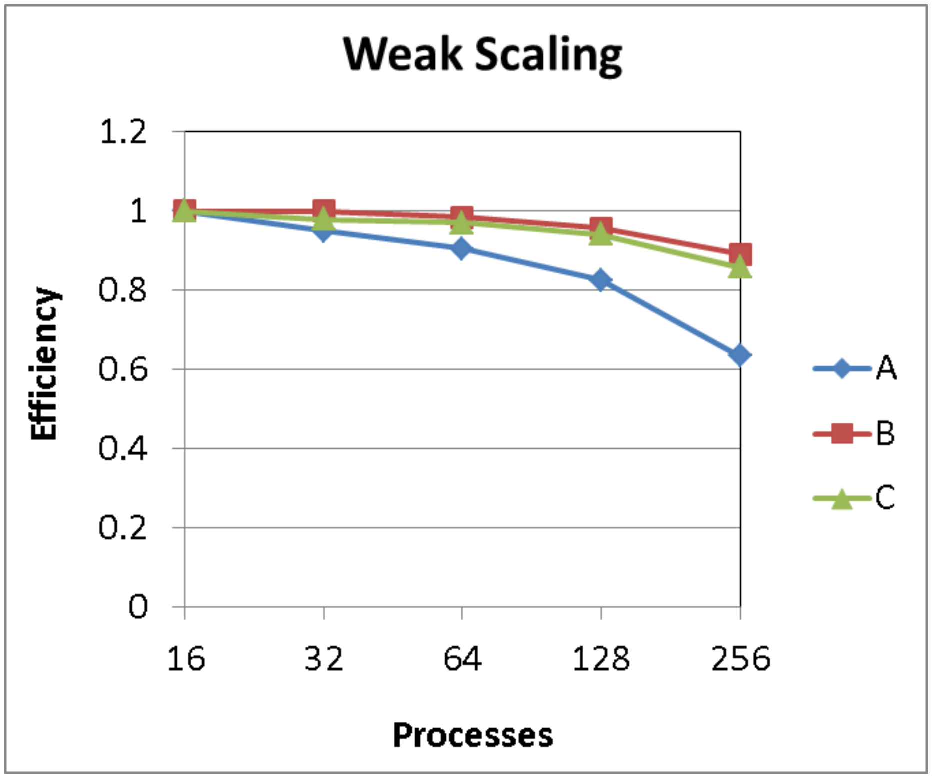
- **Threading models currently under investigation**
  - OpenMP, CUDA, TBB, Thrust, C++ Native

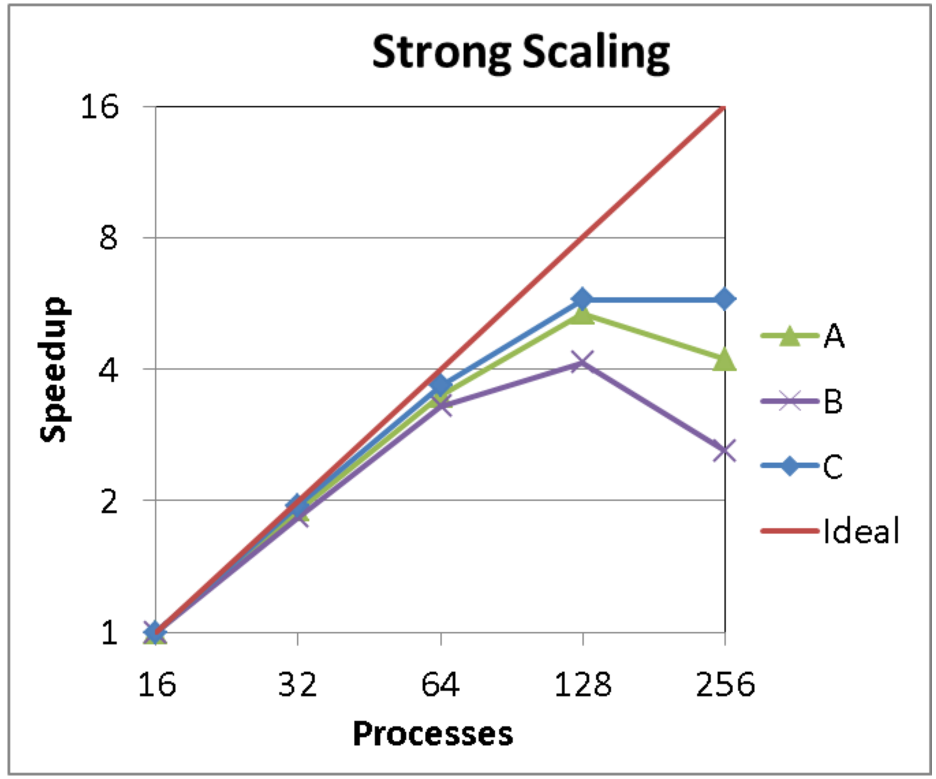
Parallel Performance

- A - Bare sphere of enriched uranium performing an static k prompt-eigenvalue
  - 1000 Active/50 Settles
  - 10000 particles/generation/process (weak)
  - 500,000 particles/generation (strong)
- B - Uranium sphere looking at time constant and scalar flux
  - 250,000 particles/proc (weak) : 500 steps @ 0.1sh
  - 1.5 M particles (strong) : 2500 steps @ 0.1 sh
- C - the ZEBR8H critical benchmark problem - static keff eigenvalue
  - 1000 Active Cycles/50 Settles
  - 5000/generation/proc (weak)
  - 100,000 particles/generation (strong)
- Performance tests are run as part of the weekly test suite
  - Tests may not involve enough work for all processors

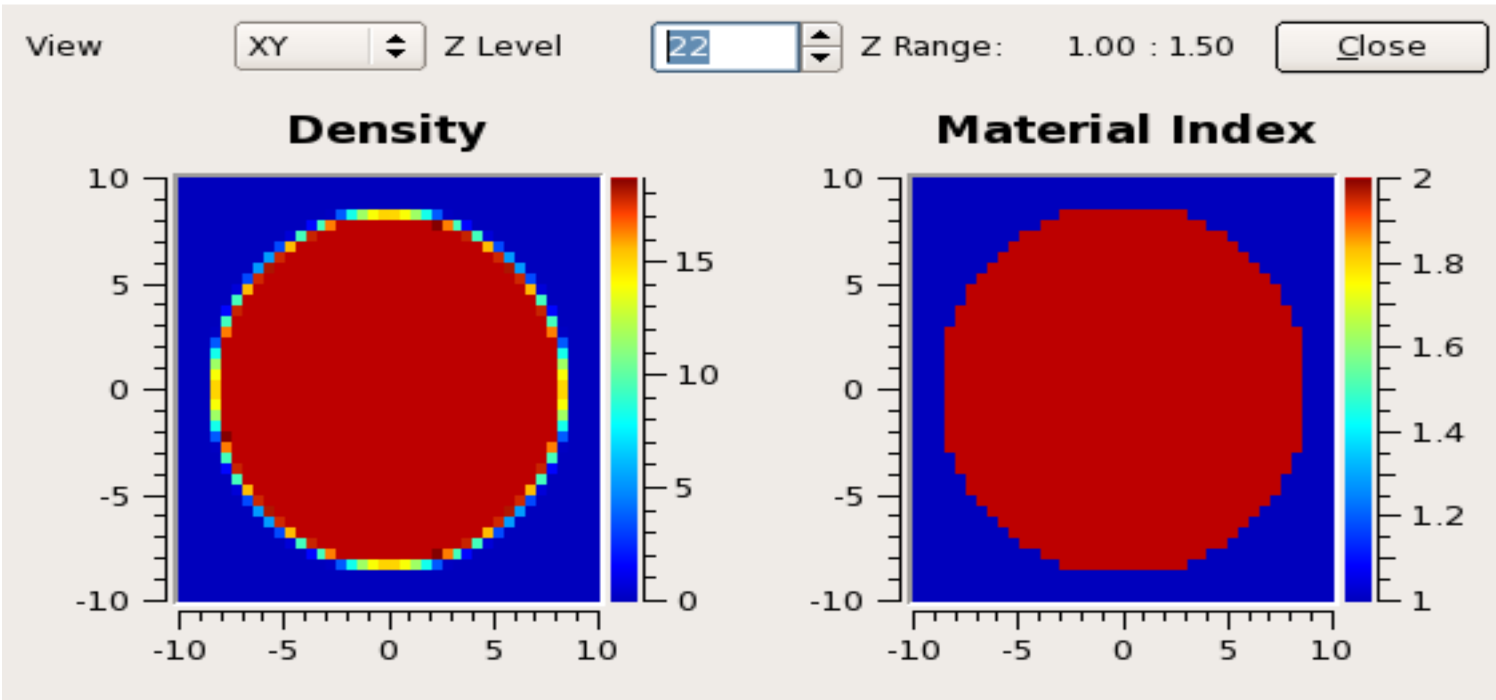
Parallel Performance

- **Need to run longer tests in the future to ensure that the processors are getting enough work, particularly for strong scaling**
- **There is considerable room for improvement in parallel performance.**
  - **To this point, the focus of MCATK has been on capability rather than performance.**





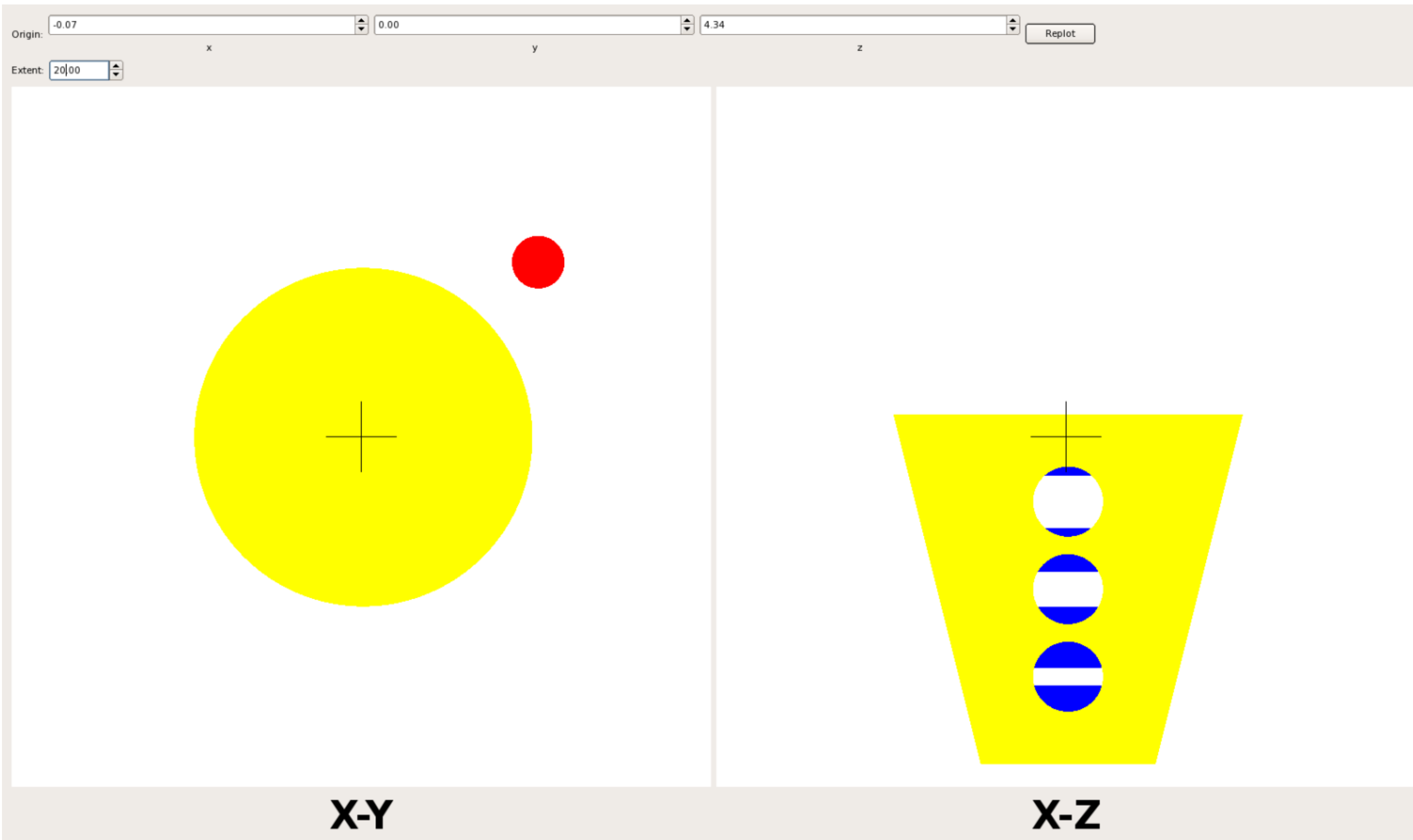
Godiva critical assembly via LNK3DNT file



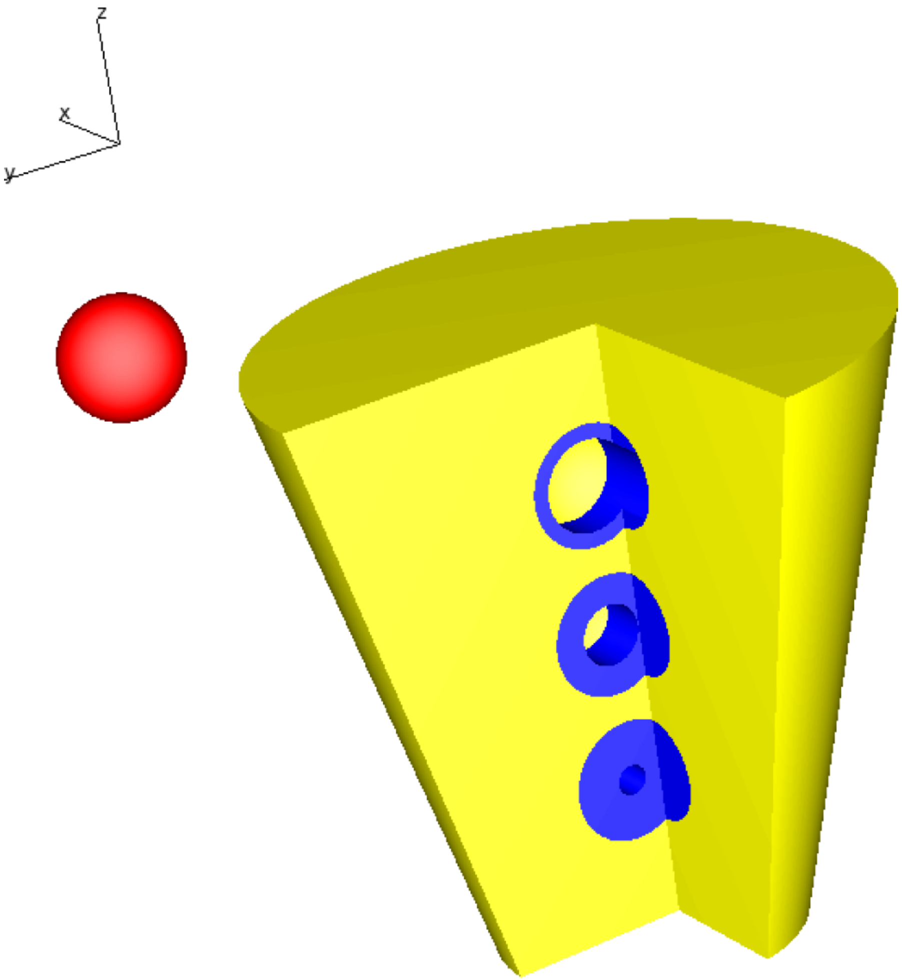
Geometry Plotting Tool

- Similar to MCNP's VisEd tool
  - 2 cross-sectional views with a common origin

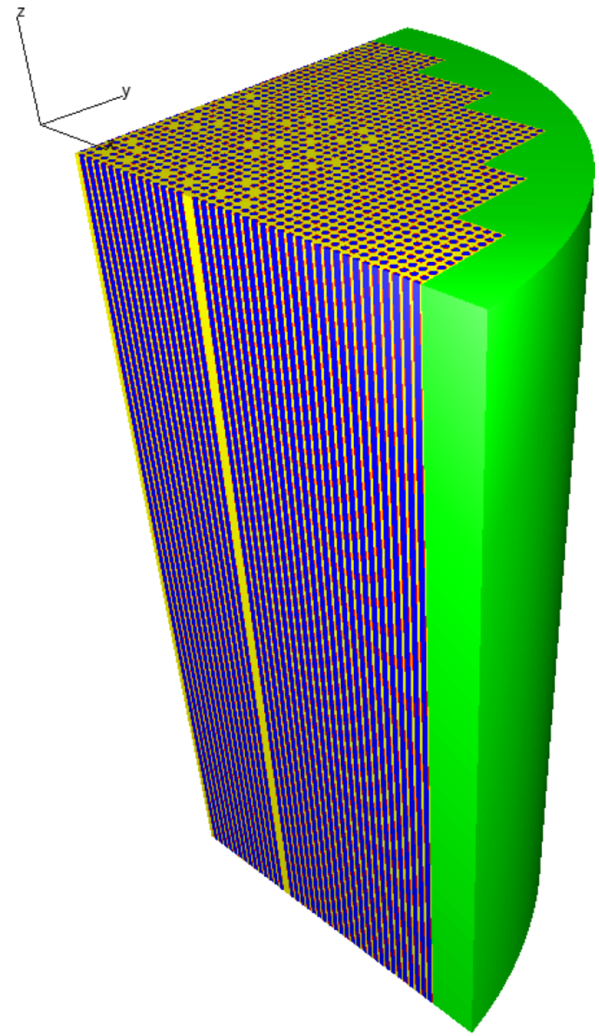
Radiographic Test Object



- 3-D Renderer
- Optional chop box for interior visualization

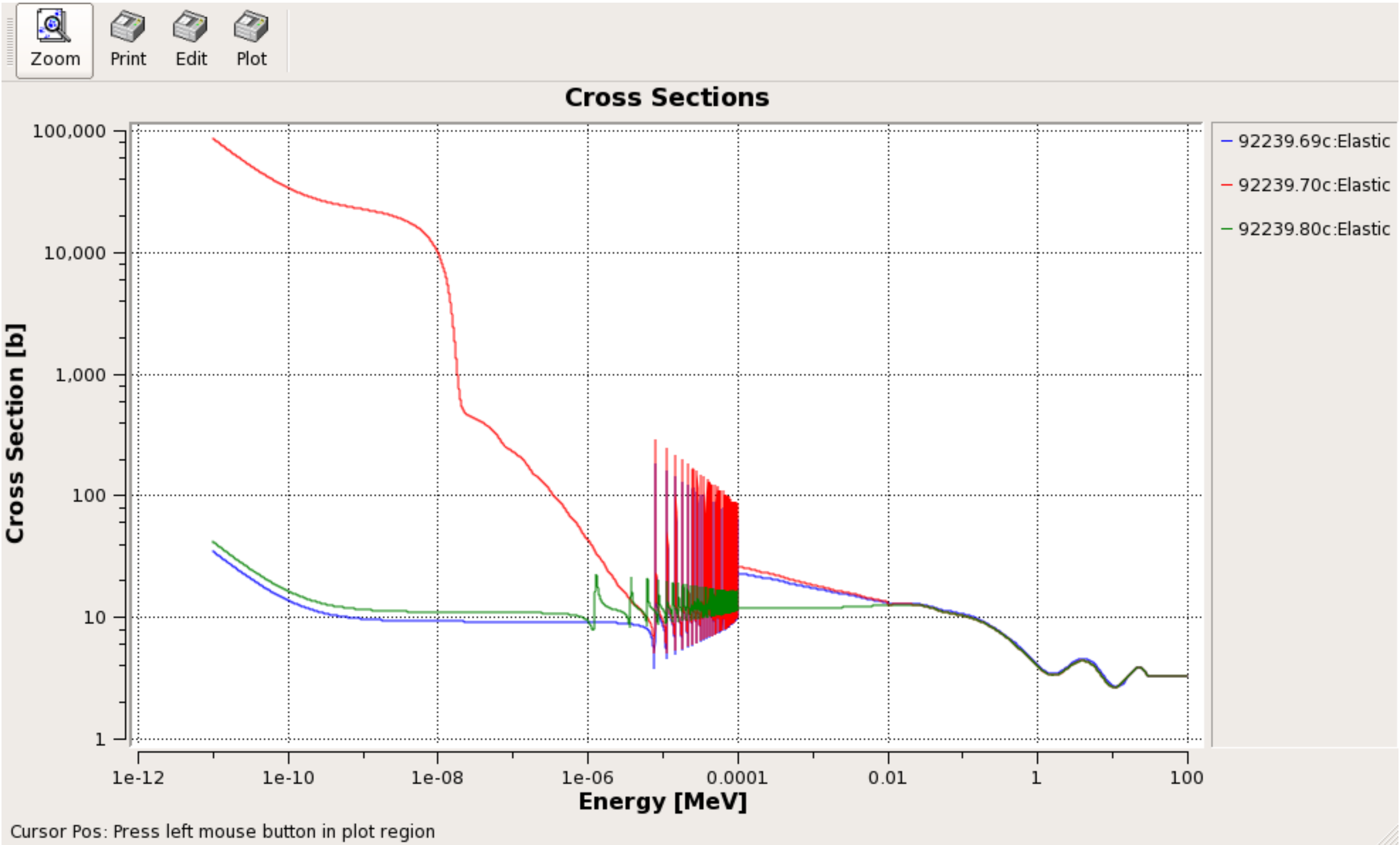


Radiographic Test Object



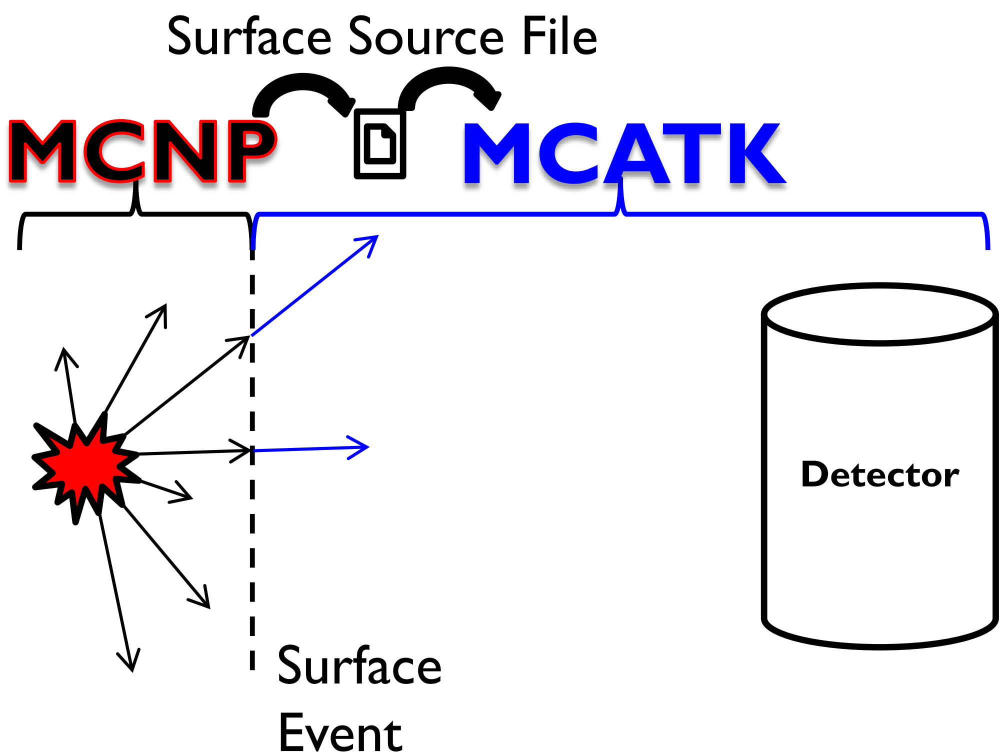
BAWXI2 Critical Benchmark

Cross Section Viewer



Surface Source Write/Read Capability

- **Compatible with MCNP SSW/SSR feature**
  - **Serves as a link between MCNP and MCATK**
- **Saves the state of each particle that exits the geometry**
  - **Could be extended to save particle states at other boundaries (e.g., interior surfaces or time/energy boundaries)**
- **Particles can be read in and treated as a source**



Surface Source File Manager

- **The SurfaceSrcFileManager application can be used to:**
  - Compare the contents of two surface source files
  - Convert a file from MCATK format to MCNP format and vice versa
  - Merge multiple surface source files into a single file
  - Sort the particles on a file according to their current time (useful for time-dependent calculations)
  - View the contents of a surface source file

```
./SurfaceSrcFileManager view mcatk file.ssr 1
```

```
NParticles:                  10000
NStartingParticles:          10000
Original Compilation Date:   07/29/14
Original Revision Number:    r3377
File created:                07/29/14
16:12:02
```

```
Particle 1:
    ID:              0
    Particle Type:   8
    Surface:         99999
    Weight:          1
    Energy:          14
    Time:            0.0005
    Position:        (0,0,0)
    Direction:       (1,0,0)
```

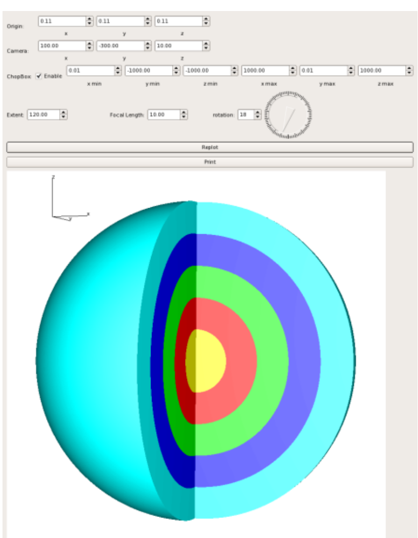
Status of Coupled n-gamma Transport

- **MCATK can produce photons from neutron collisions**
- **Photon production validation test:**
  - **Godiva inside a sphere of water (radius of 33.4717 cm)**
  - **k-eigenvalue calculation**
    - 5000 particles per cycle
    - 50 inactive cycles, 500 active cycles
  - **Tally number of Monte Carlo photons produced**
  - **Tally average energy and weight of photons produced per source neutron**

	MCNP	MCATK
MC Photons Created	6732584	6748119
Average Photon Weight per Source Neutron	4.54847	4.55595 ± 2.78392e-03
Average Photon Energy per Source Neutron	4.71901	4.72560 ± 3.09976e-03

Status of Coupled n-gamma Transport

- **No reading of real photon cross sections yet**
- **No photon scatter physics yet**
- **Can track photons through geometry with user-defined one-group total cross section.**
- **Photon tracking validation test:**
  - **Source neutrons Energy=1E-11 in the center of a hydrogen sphere, density=0.001 g/cc**
  - **Neutrons capture on H creates 2.2233-MeV Photons**
  - **Use user defined incoherent photon cross-section (0.137 barns).**
  - **Tally photon flux in 10-cm delta-R spherical geometry**



MCATK Rendering

Radius of Flux Volumes	MCNP Photon Flux	MCATK Photon Flux
<10 cm	2.32E-04	2.34E-04
10-20 cm	8.05E-05	7.99E-05
20-30 cm	3.97E-05	3.92E-05
30-40 cm	2.29E-05	2.28E-05
40-50 cm	1.41E-05	1.40E-05

MCATK: Summary

- **MCATK physics:**
  - Continuous energy neutron transport with multi-temperature treatment
  - Static eigenvalue (k and α) algorithms
  - Time-dependent algorithm
  - Fission chain algorithms
  - Coupled n-gamma transport in progress
- **MCATK geometry:**
  - Mesh geometries
  - Solid body geometries
- **MCATK provides:**
  - Verified, unit-tested Monte Carlo components
  - Flexibility in Monte Carlo applications development
  - Numerous tools such as geometry and cross section plotters
- **Public availability is a possibility**

Where to Learn More

MCATK Citation Paper (In press):

Adams, Nolen, Sweezy, Zukaitis, Campbell, Goorley, Greene, Aulwes. Monte Carlo Application ToolKit (MCATK). Ann. Nucl. Energy (2015). Online: URL http://dx.doi.org/10.1016/j.anucene.2014.08.047

MCATK at M&C/SNA/MC:

S. Nolen, T. Adams, J. Sweezy, T. J. Trahan, L. Pritchett-Sheats. Monte Carlo Applications Toolkit (MCATK): Advances for 2015. (Monte Carlo Methods, Wednesday PM B).

S. Nolen. Using Fission Chain Analysis to Inform Probability of Extinction/Initiation Calculations with MCATK. (Monte Carlo Methods, Tuesday AM B).

Future Plans

MCNP Future Plans

- **Continued focus on transport and physics improvements**
  - **Specific focus on sensitivity and uncertainty**
- **Next-generation high performance computers**
- **Applications: MCNP is often needed as radiation transport tool within other tools**
  - **Inputs are geometry, materials, sources, and “tallys”**
- **We are developing tools to assist users**
  - **Tools are external to MCNP**
    - Geometry: Collaborations with Varian (R. Martz)
      - Allows users to take CAD, modify through SpaceClaim, and develop mesh-based model using Attila4MC. Variance reduction with Sn calculation.
    - Radiation Source: MISC – generalized intrinsic radiation source (aged) from any decay-data libraries (CJ Solomon)
    - Tallies: MCNP tools – a package to facilitate user access to MCNP output files (CJ Solomon)
      - C++ library provides user access to MCNP’s mctal, meshtal, and ptrac files
      - User can produce tools to make plots, analyse data, etc without headache of having to parse data

[Discussion]

[Tuesday – MCNP 2020 initiative, in talk on MCNP6 Code Optimization]

Questions ?