LA-UR-12-26115

Approved for public release; distribution is unlimited.

Title:	MCNP Monte Carlo Progress – Nuclear Criticality Safety
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Intended for:	2012 ANS Winter Meeting, San Diego, CA, Nov 11-15, 2012

LA-UR-12-26115

MCNP Monte Carlo Progress
-
Nuclear Criticality Safety

Forrest Brown, Brian Kiedrowski, Jeffrey Bull
Monte Carlo Codes, XCP-3
Los Alamos National Laboratory

US DOE/NNSA Nuclear Criticality Safety Program –

What have we done for you lately ?

- MCNP5-1.60
- MCNP6-Beta
- Verification / Validation
- User Support & Training
- Work in Progress
- Future Release Plans

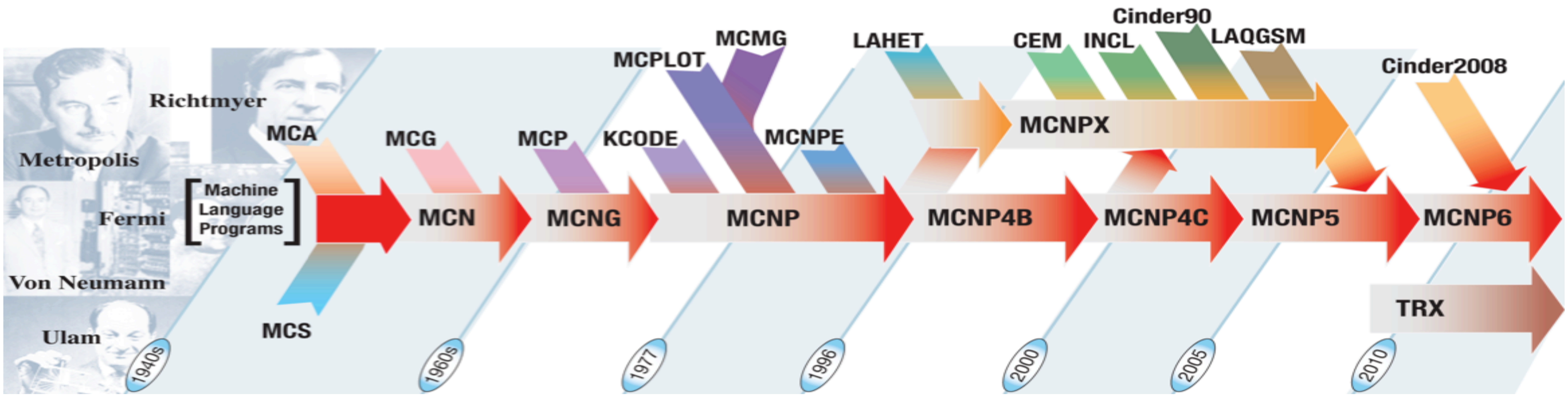
MCNP5-1.60
&
MCNP6-Beta

MCNP5-1.60 Status

- **MCNP5-1.60 Code Release**
  - **RSICC releases: October 2010, July 2011, February 2012**
    11,586 copies of MCNP distributed by RSICC, 2001 - 2011
  - **Stable, solid, maintenance mode, few bug reports**
  - **Workhorse for most MCNP users**
  - **Parallel MPI+threads on all computers**

- **Recent Features**
  - **Adjoint-weighted Tallies for Point Kinetics Parameters**
  - **Mesh Tallies for Isotopic Reaction Rates**
  - **Increased Limits for Geometry, Tally, and Source Specifications**
  - **Web-based documentation**
  - **Utility programs**
  - **Additional V&V suites**
  - **Most rigorous & extensive MCNP V&V testing ever**

MCNP6-Beta



- **MCNP release package now being distributed by RSICC**

  MCNP5-1.60 + MCNPX-2.70 + MCNP6-Beta-2 +
  Nuclear Data Libraries + MCNP Reference Collection

- **MCNP6-Beta-3 release late-2012, 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

MCNP5 vs 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

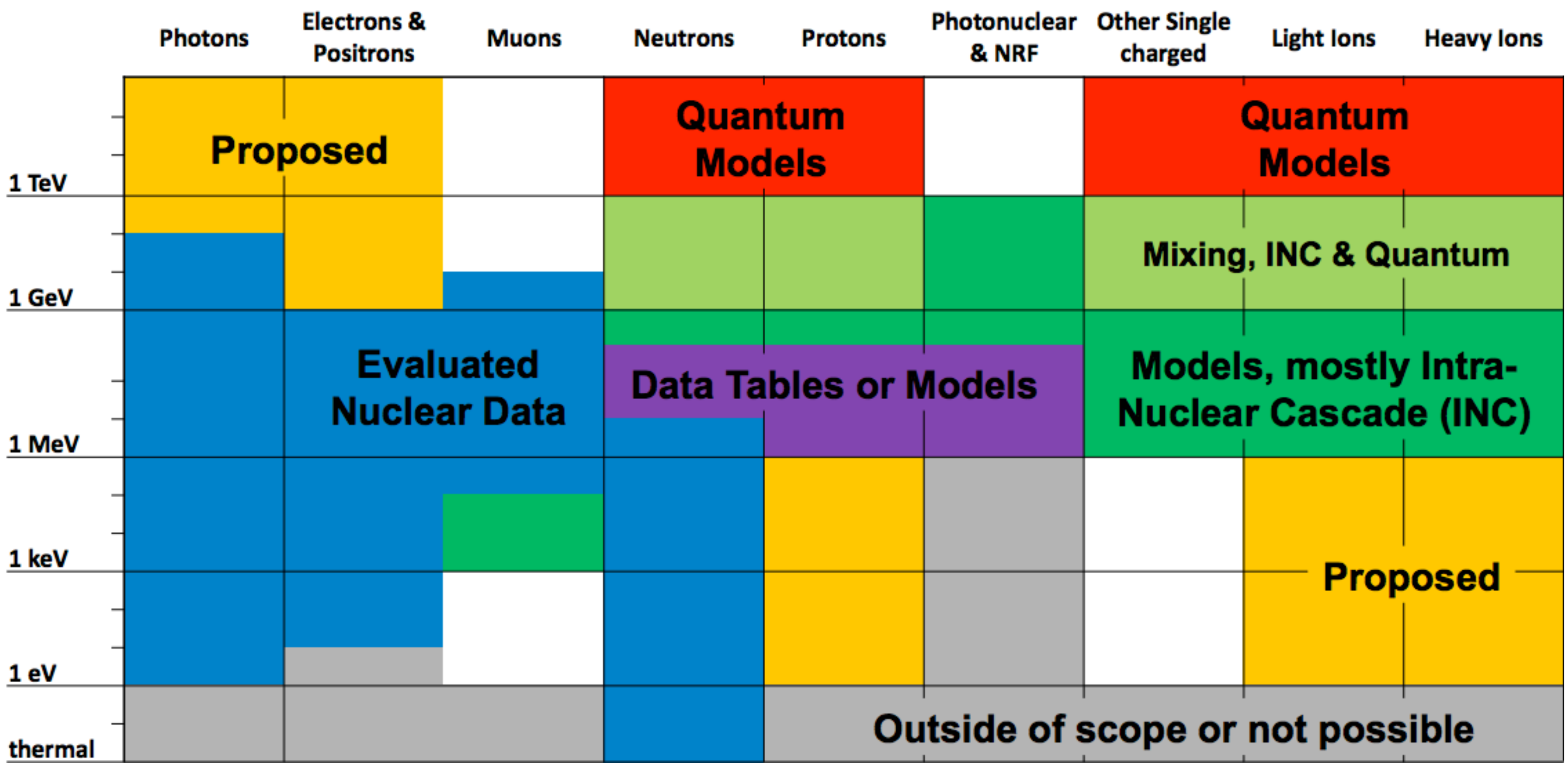
High energy physics models
CEM, LAQGSM, LAHET
MARS, HETC

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

MCNP6 – all particles & all energies, using best data + models + theory



Incorporates other codes:

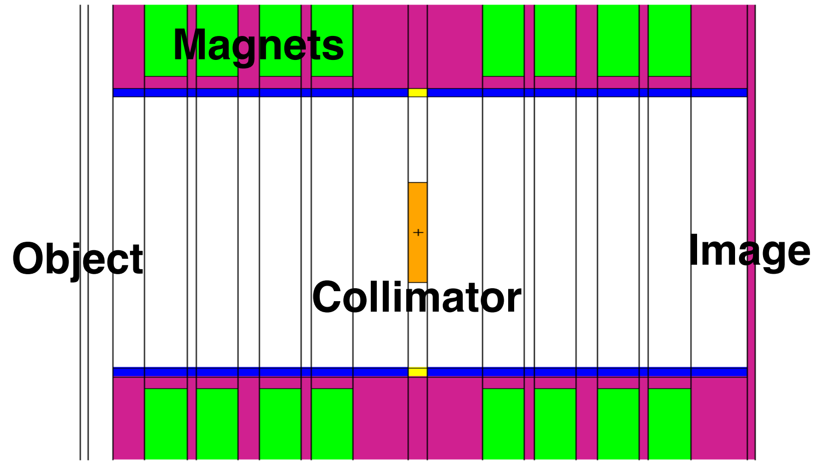
CINDER	burnup & decay	LANL	ITS	electron transport	SNL
LAHET	high energy transport	LANL	CEM	high energy transport	LANL
LAQGSM	high energy transport	LANL	MARS	high energy transport	FNAL
HETC	high energy transport	ORNL			

MCNP6 – Proton Radiography

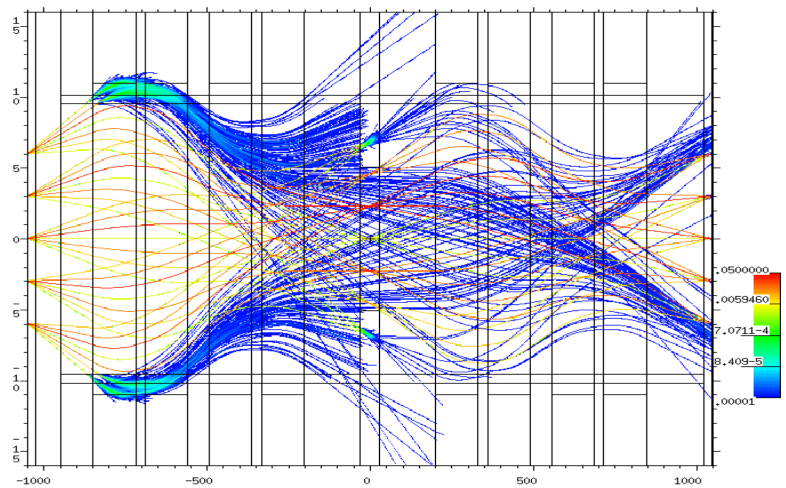
Monte Carlo Codes
XCP-3, LANL

LANSCE pRad, MCNP6 calculations

- Experiments at LANL & BNL use **high-energy proton beams** directed at test objects to produce **radiographic images**
  - LANL: 800 MeV proton beams
  - BNL: 24 GeV proton beams
  - Proposed: 50 GeV proton beams

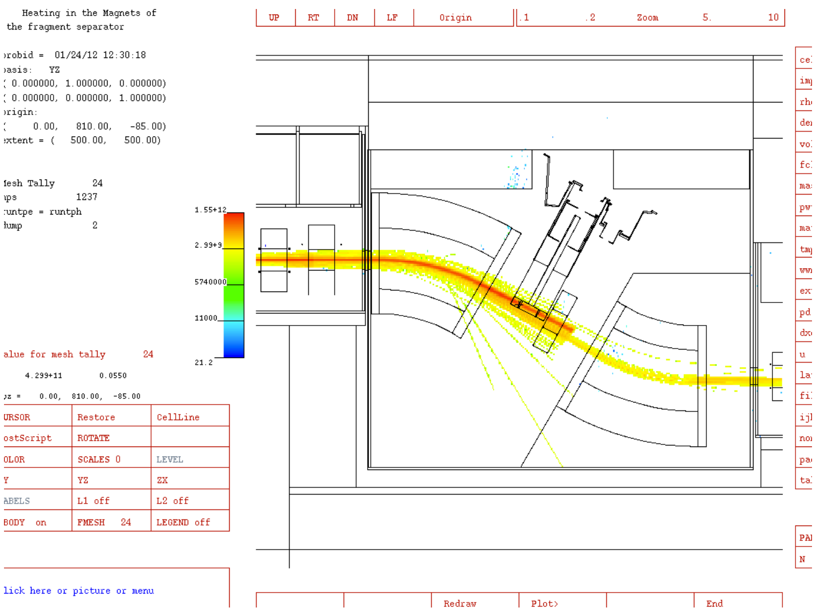


Horizontal axis - 0, 3, 6, and 9 mrads angles



- Proton beams are collimated & focused by **magnetic lenses**
- **Radiography tallies** simulate pixels from detectors
- Experiment design & analysis are modeled with MCNP6

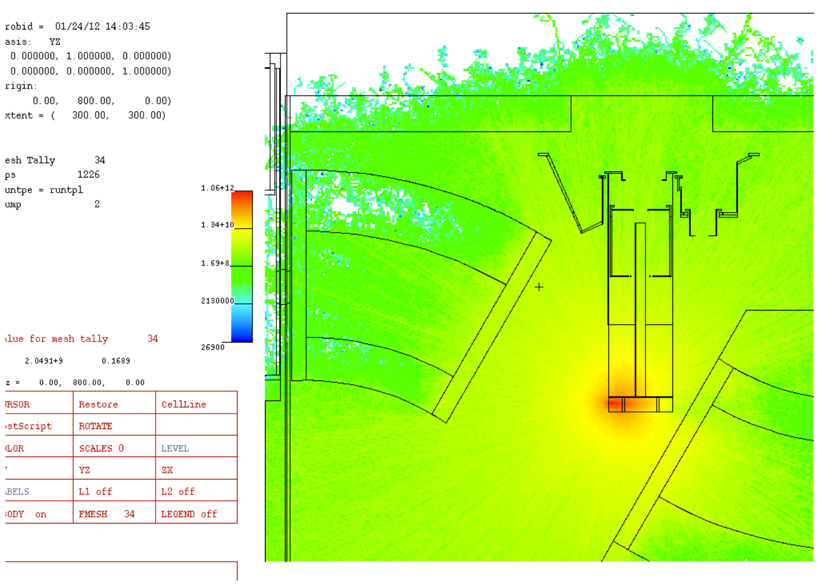
MCNP6 - User Example



Primary ion beam as it collides with the beam dump

^{48}**Ca ion beam**, **549 MeV/u (26.3 GeV/ion)**

With magnetic field focusing



Neutron field produced by ion beam collisions with target

MCNP6 - Medical Physics - Treatment Planning

Monte Carlo Codes
XCP-3, LANL

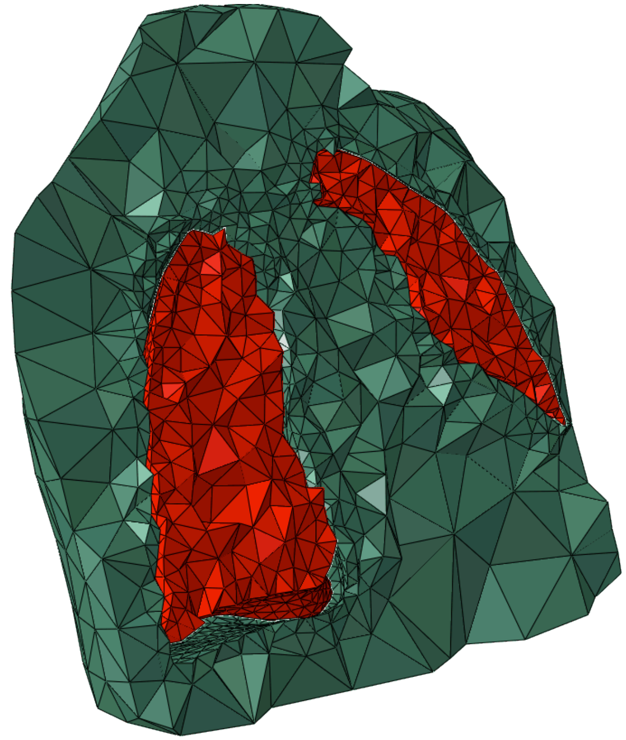
MCNP6

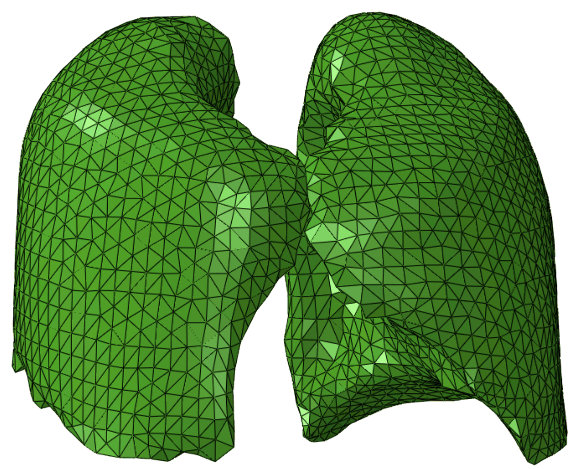
- 3D unstructured mesh
- Embedded in 3D MCNP geometry

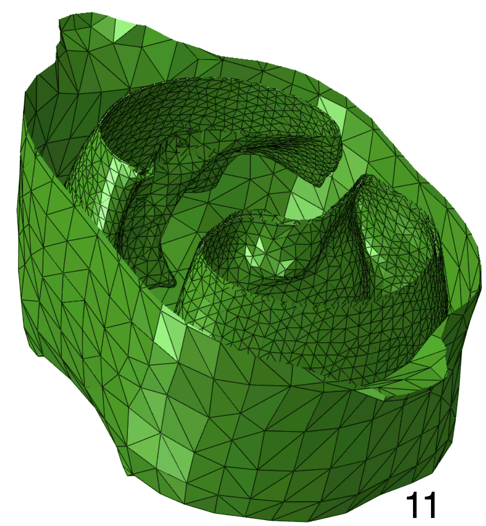
- Many applications
  - Radiation treatment planning
  - Linkage to Abaqus FE code

- MCNP6-Abaqus link for combined radiation energy deposition & structural analysis, using same mesh geometry

- Provides capability for CAD input (via Abaqus)







Verification
&
Validation

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
– **VALIDATION_ACODE**	static-alpha eigenvalue benchmarks
– **POINT_KINETICS**	reactor kinetics parameters
– **KOBAYASHI**	void & duct streaming, with point detectors, exact solutions
– **VALIDATION_SHIELDING**	19 shielding/dose experiments
– **REGRESSION**	66 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**

Current V&V Work

MCNP5-1.51 – 2008
MCNP5-1.60 – 2010
MCNP6-Beta-2 – 2012
MCNP6-Beta-3 – 2012
MCNP6 – 2013

- Detailed V&V for MCNP5 & MCNP6 presented separately at this meeting:
  Kiedrowski, Brown, Bull, "Verification of MCNP5-1.60 and MCNP6-Beta2 for Criticality Safety Applications", Tuesday AM - NCSD session

- Conclusions
  - Using the same F90 compiler,
    MCNP5-1.51, MCNP5-1.60, MCNP6-Beta all match results exactly for criticality safety applications
  - Switching from Intel-10 to Intel-11/12 introduces some small computer roundoff differences – compiler issue, not code or results

User Support

&

Training

User Support & Training

- **11,586 copies of MCNP distributed by RSICC, Jan 2001 – Oct 2011**
- **Classes**
  - **Theory & Practice of Criticality Calculations with MCNP5**
    FY11: PNNL/Hanford, LANL, Y-12, INL
    FY12: INL, PNNL/Hanford, LANL, SNL
  - **Introduction to MCNP5 – classes at LANL**
    FY11: 10/10, 5/11, 6/11
    FY12: 10/11, 5/12, 6/12, 10/12
  - **Advanced Variance Reduction – at LANL** 4/12
- **Conferences & Journals**
  - PHYSOR-2012 6 papers + Monte Carlo Workshop
  - ICNC-2011 6 papers
  - ANS Summer 2012 4 papers
  - RPI Colloquium invited
  - ANS Winter 2011 2 papers
  - NS&E journal 2 papers
  - PNST Journal 4 papers
- **Participated in ANS 10.7 Standards committee**

User Support & Training

- **MCNP Forum**
  - User-group – beginners & experts, ~1000 members
  - Feedback, bug reports, guidance
- **New MCNP Website**
  - Nice, modern, conforms to LANL requirements
  - Greatly expanded reference collection
- **Reference collection**
  - **1 GB+ of references on Monte Carlo & MCNP**, ~ 600 items
  - Web browser based
  - All MCNP5, MCNP6, & previous MCNP code documentation
  - Criticality, V&V, adjoints, electrons, detectors, parallel, benchmarks, …..
  - Includes 8 half-day Monte Carlo workshops
- **University collaborations**
  - Michigan, New Mexico, Wisconsin, RPI
  - Summer students at LANL

Work in Progress

R&D Work in Progress (1)

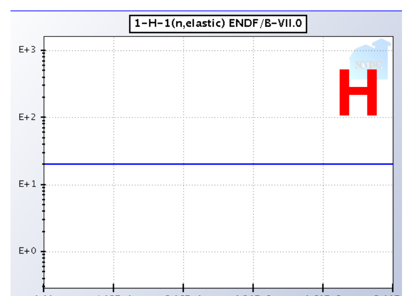
Continuous S(α,β) Scattering For Thermal Neutrons

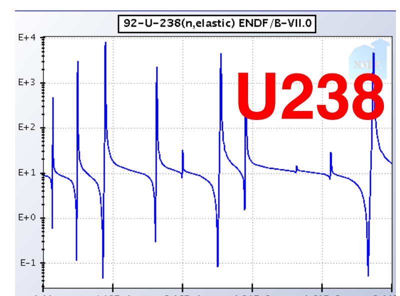
- **S(α,β) thermal neutron scattering**
  - Accounts for temperature, chemical-, & molecular-binding on collision physics
  - Traditional NJOY-MCNP uses discrete energy-angle data
- **Continuous S(α,β) treatment**
  - Developed by MacFarlane in early 2000s
  - Implemented in MCNP5 & MCNP6
- **Recent V&V effort**
  - A. Pavlou (U.Mich), 2011
  - Thorough V&V with ICSBEP benchmarks
  - **Conclusion: valid for crit-safety use**
  - Continuous S(α,β) data to be included with MCNP ENDF/B-VII.1 data libraries

Free-gas Resonance Scattering For Epithermal Neutrons

- **Free-gas scattering model**
  - Used to account for target nuclide thermal motion at epithermal energy
  - Traditional: assume constant $\sigma_{scatter}$
- **Resonance scatter can be important for free-gas model**

sig-scatter, 1 eV – 200 eV



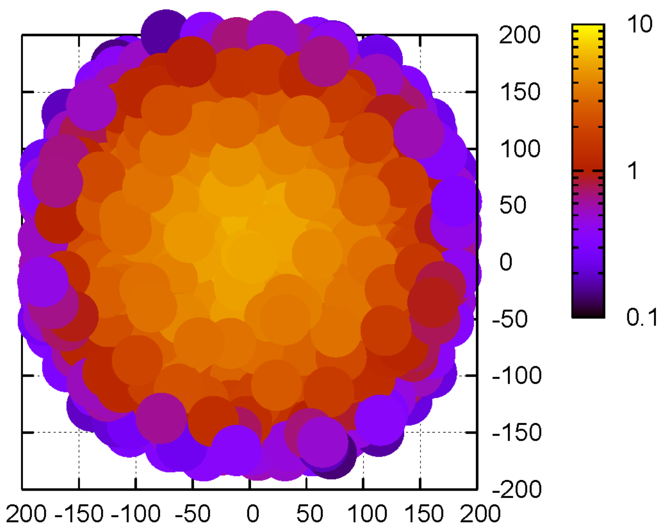


- **MCNP mods to include resonance scattering in free-gas model**

R&D Work in Progress (2)

Statistical Coverage of Fission Source

- **Kernel Density Estimators for fission source**
  - Automated placement based on distance between fission points
  - Provides robust estimate of sampling fissionable material
  - Can also be used to compute Shannon entropy



Alternate Eigenvalues for Criticality Searches

- **Collision or c-eigenvalue**
  - Like k, but for all collisions not just fission.

    c < 1 subcritical

    c = 1 critical

    c > 1 supercritical
  - Computing c versus k tends to be more efficient:

	k	c	Gain
Reflected Sphere	**0.9955**	**0.9954**	**31**
Pu Soln. Can Array	**0.9866**	**0.9989**	**60**
Full-Core PWR	**0.9992**	**0.9986**	**200**

R&D Work in Progress (3)

Improvements to Parallel MPI & Threading

- **For criticality calculations**
  - Reduce the amount of data exchanged at MPI rendezvous
- **MPI improvements**
  - Automatic chunking of large transfers
  - Asynchronous MPI messages
  - Improve Fortran/C interface
- **OpenMP threading improvements**
  - Replace private thread-safe storage for certain large arrays by OpenMP critical sections
  - Use OpenMP atomic operations with shared tally arrays

Parallel MC for Exascale Computers

- **Exascale computers are coming**
  - Millions of cpu cores
  - Reduced memory/cpu-core
  - Heterogeneous – GPUs & MICs
- **Need new parallel approach**

Parallel on particles

+

Distributed data

- Particles distributed among nodes
- Fetch data remotely as needed, do not move particles to data
- Eliminate synchronization
- Tally server nodes

R&D Work in Progress (4)

Monte Carlo Codes
XCP-3, LANL

The most significant advances in state-of-the-art for Monte Carlo criticality calculations in the past decade:

- **Multigroup sensitivity/uncertainty analysis (TSUNAMI)**
- **Hybrid Monte Carlo + deterministic**
- **Shannon entropy for source convergence diagnostics**
- **Adjoint-weighted tallies, via iterated fission probability**
- **Quantification of bias, uncertainty, & convergence theory**

- **On-the-fly neutron Doppler broadening with temperature**
- **Continuous-energy sensitivity/uncertainty analysis**
- **Fission matrix for higher modes & convergence acceleration**

The last 3 are in progress now, being introduced into MCNP6. Work reported at 2012 Chicago & San Diego ANS meetings.

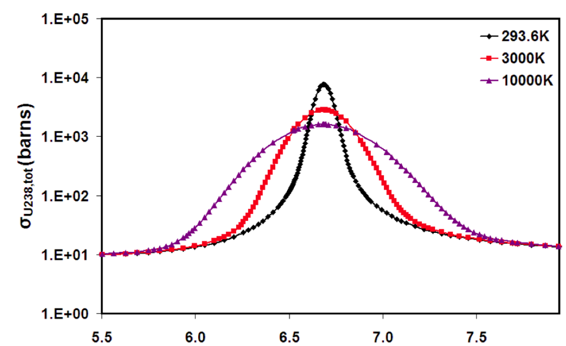
On-The-Fly Doppler Broadening (1)

Monte Carlo Codes
XCP-3, LANL

- **US DOE NEUP project with Univ. Michigan, ANL, LANL (2011-2012)**
  - **William Martin** & students (Mich), **Gokhan Yesilyurt** (ANL), **Forrest Brown** (LANL)
  - PhD thesis 2009, NSE article 2012, ANS Trans. 2012, workshops 2009 & 2012

- **Provide general temperature treatment for MCNP**
  - **Continuous temperature capability, without precomputing 1000s of xsec datasets**
  - **Necessary for multiphysics: MC + TH + FEM + ...**

- **OTF Methodology (for each nuclide)**
  - **Determine union energy grid for a range of T's**
  - **High-precision fits for σ(E,T) vs T**
  - **MCNP – evaluate σ(E,T) OTF during simulation**



  - 5-10x increase in xsec storage
  - No significant change in cpu time
  - Testing so far – matches explicit precomputed NJOY broadening

Brown, Martin, Yesilyurt, Wilderman, "Progress with On-The-Fly Neutron Doppler Broadening in MCNP", Trans. ANS 106, Chicago, 2012.

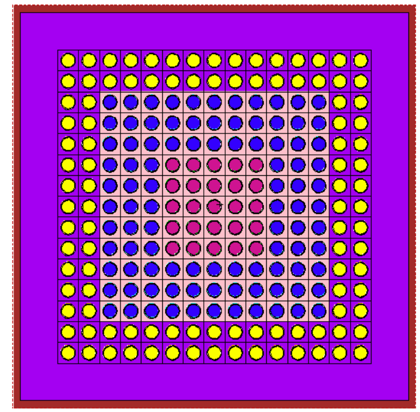
On-The-Fly Doppler Broadening (2)

mcnp Monte Carlo Codes XCP-3, LANL

STD = explicit njoy data for each T

OTF = 293 K data + OTF fits in T

Fuel 900K, clad 900K, mod 600K
Fuel 600K, clad 600K, mod 600K
Fuel 300K, clad 300K, mod 300K



k-effective:

STD	1.11599 (15)
OTF	1.11592 (15)

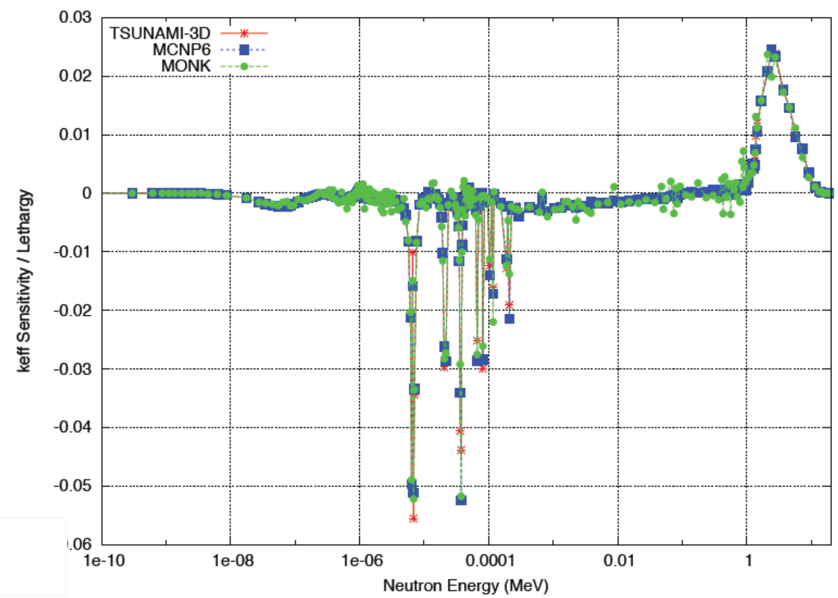
		900K	600K	300K
Total fission				
	STD	.045140 (.08%)	.161186 (.04%)	.248782 (.03%)
	OTF	.045081 (.08%)	.161329 (.04%)	.248731 (.03%)
Total capture in fuel				
	STD	.027672 (.09%)	.096276 (.05%)	.116745 (.04%)
	OTF	.027667 (.09%)	.096268 (.05%)	.116829 (.04%)
U235 capture in fuel				
	STD	.008993 (.08%)	.031910 (.04%)	.045998 (.03%)
	OTF	.008983 (.08%)	.031932 (.04%)	.045987 (.03%)
U238 capture in fuel				
	STD	.018547 (.11%)	.063887 (.06%)	.070236 (.05%)
	OTF	.018551 (.11%)	.063858 (.06%)	.070332 (.05%)
O16 capture in fuel				
	STD	1.15E-04 (.23%)	4.18E-04 (.14%)	4.37E-04 (.13%)
	OTF	1.15E-04 (.23%)	4.16E-04 (.14%)	4.37E-04 (.13%)

Continuous-Energy Sensitivity Coefficients (1)

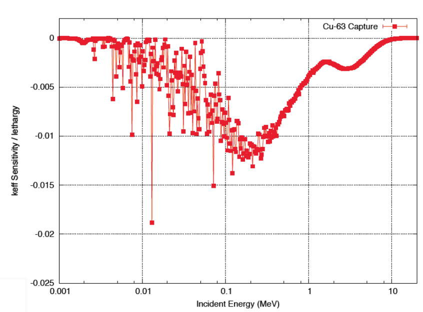
Monte Carlo Codes
XCP-3, LANL

- **MCNP6 can produce sensitivity coefficients in continuous-energy**
  - Uses adjoint-weighted perturbations
  - Computes sensitivity coefficients for cross sections, fission, & scattering laws.
  - User-defined energy resolution for results or tallies – no discretization
  - Nuclear Science & Engineering paper accepted and in publication (2013)
  - Can directly compare to TSUNAMI multigroup s/u results

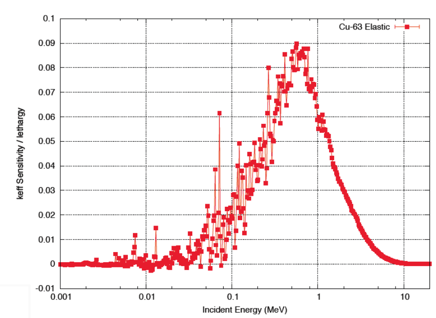
MOX Lattice: U-238 Total



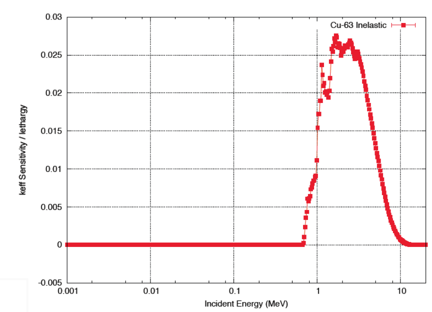
Zeus: Cu-63 Capture Cross-Section Sensitivity



Zeus: Cu-63 Elastic Cross-Section Sensitivity



Zeus: Cu-63 Inelastic Cross-Section Sensitivity



Kiedrowski, Brown, "Continuous-Energy Sensitivity Coefficient Capability in MCNP6", Trans ANS 107, San Diego, 2012.

Fission Matrix for MCNP (1)

Monte Carlo Codes XCP-3, LANL

- **Exact integral equation for fission source**

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

$$F_{I,J} = \int_{\vec{r}\in V_I} d\vec{r} \int_{\vec{r}_0\in V_J} d\vec{r}_0 \, \frac{S(\vec{r}_0)}{S_J} \cdot \int\iiint dE\, d\hat{\Omega}\, dE_0\, d\hat{\Omega}_0 \cdot \nu\Sigma_F(\vec{r},E) \cdot \frac{\chi(E_0)}{4\pi} \cdot G(\vec{r}_0,E_0,\hat{\Omega}_0 \to \vec{r},E,\hat{\Omega})$$

$$S_J = \int_{\vec{r}'\in V_J} S(\vec{r}')\, d\vec{r}' = \iiint_{\vec{r}'\in V_J} d\vec{r}'\, dE'\, d\hat{\Omega}' \nu\Sigma_F(\vec{r}',E')\Psi(\vec{r}',E',\hat{\Omega}'),$$

N = # spatial regions, F is NxN matrix

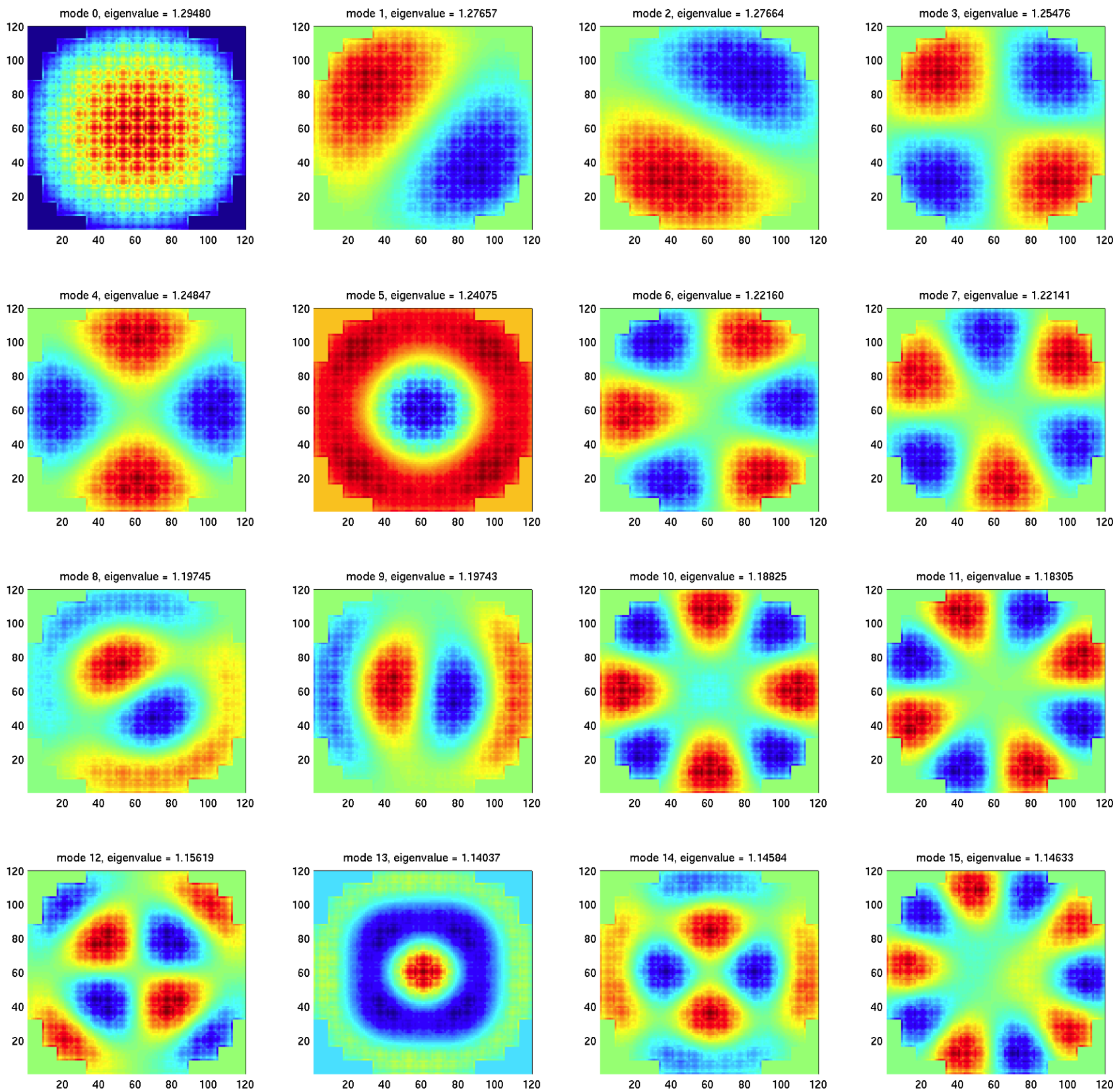
- **$F_{I,J}$ = next-generation fission neutrons produced in region I, for each fission neutron starting in region J (J→I)**
  - As region size decreases, unknown weight function $S(r_0)/S_J$ → 1, discretization errors → 0
  - Can accumulate tallies of $F_{I,J}$ even if not converged
  - Sparse storage scheme greatly reduces memory storage

- **Applications**
  - **Dominance ratio & higher eigenmodes**
  - **Accelerate convergence**
  - **Important advance in transport theory**

Carney, Brown, Kiedrowski, Martin, "Fission Matrix Capability for MCNP Monte Carlo", Trans ANS 107, San Diego, 2012

Fission Matrix for MCNP (2)

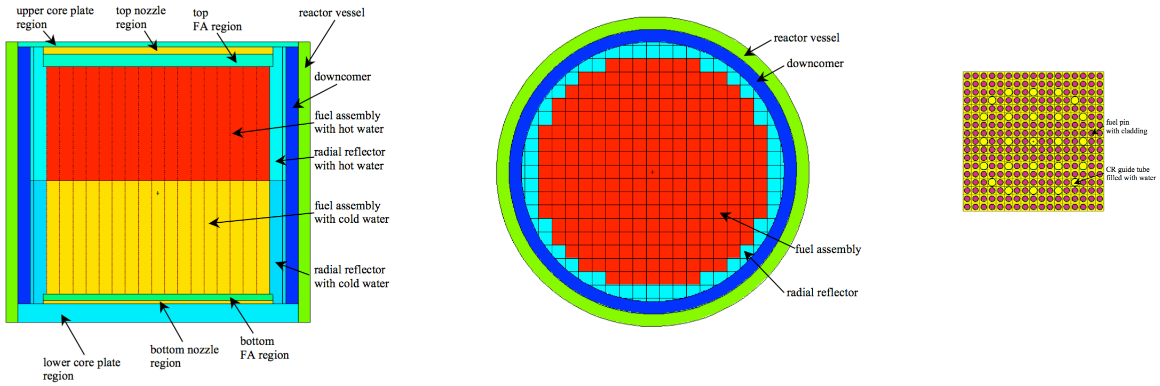
PWR – Eigenmodes for 120x120x1 Spatial Mesh



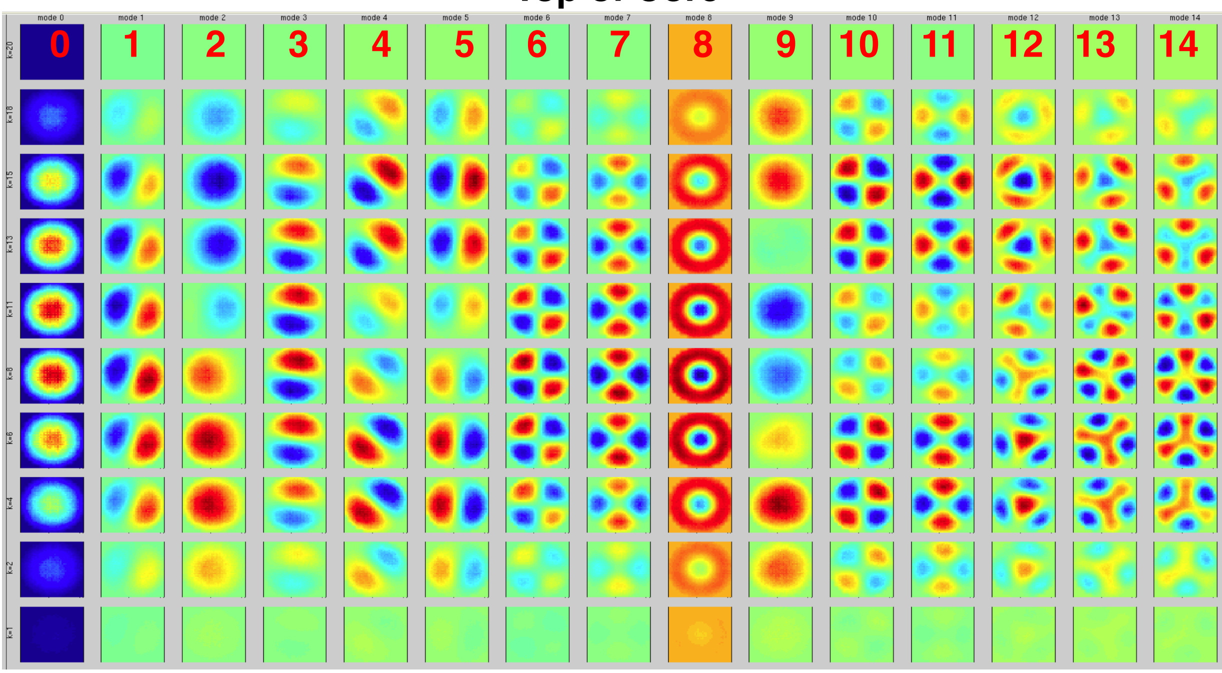
n	K_n
0	1.29480
1	1.27664
2	1.27657
3	1.25476
4	1.24847
5	1.24075
6	1.22160
7	1.22141
8	1.19745
9	1.19743
10	1.18825
11	1.18305
12	1.15619
13	1.14633
14	1.14617
15	1.14584

Fission Matrix for MCNP (3)

Full core, 3D reactor benchmark (Hoogenboom, Martin)



Top of Core



Bottom of Core

3D Eigenfunctions

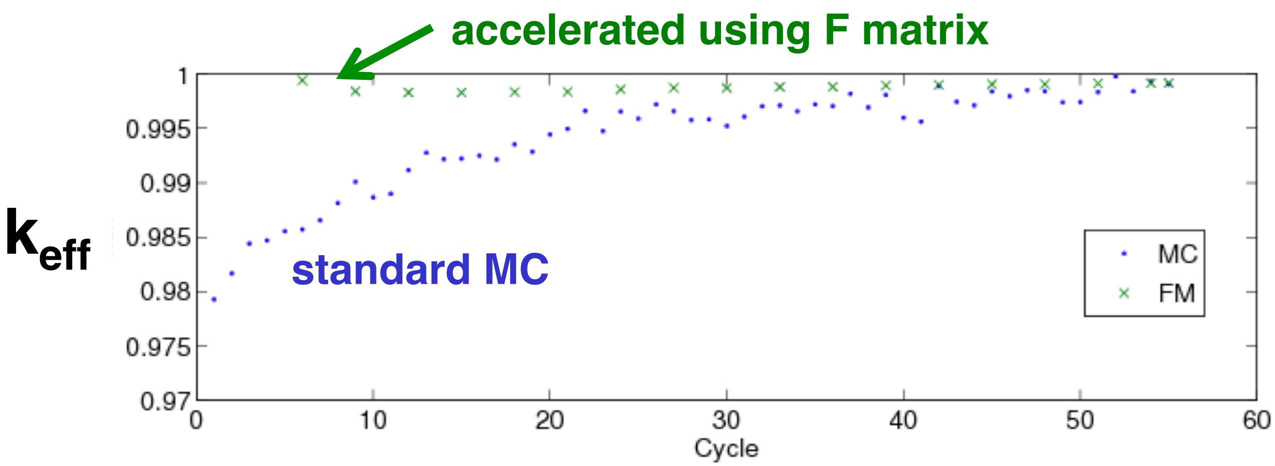
XY plots of eigenfunctions
at various Z elevations

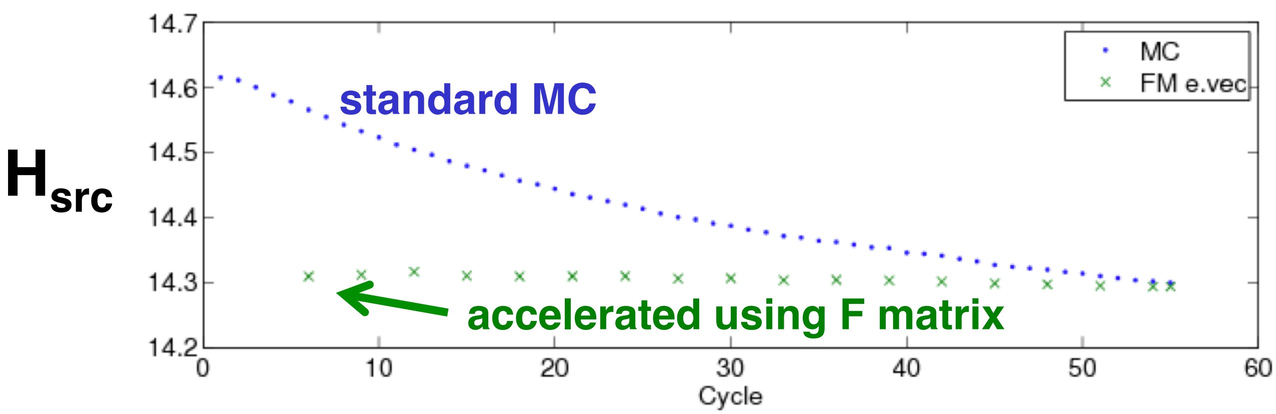
55 cycles, 1 M neuts/cycle

42 x 42 x 20 tally mesh,
35280 x 4913 fiss-matrix

Fission Matrix for MCNP (4)

- **Fission matrix can be used to accelerate convergence of the MCNP neutron source distribution during inactive cycles**
- **Very impressive convergence improvement**





Acceleration using fission matrix for 3D full-core reactor benchmark

Future Release Plans

MCNP6

- **MCNP6 = MCNP5 + MCNPX merger**
- **Impact on Criticality Calculations ➜ none**
  - **All KCODE criticality features same as for MCNP5**
  - **Matches results with MCNP5 for criticality suites**
- **Monte Carlo team will support MCNP6,
  no new features or releases of MCNP5 or MCNPX**
- **MCNP6 is here**
  - **Beta-2 release: 1Q CY 2012**
  - **Beta-3 release: 4Q CY 2012**
  - **Production release: 2Q CY 2013 (?)**
    - Need more V&V, documentation, code cleanup, installation scripts, etc.

Criticality-safety community needs to plan for MCNP5 ➜ MCNP6 transition over the next few years

Questions ?