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Title: Features of MCNP6 Relevant to Medical Radiation Physics

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Features of MCNP6 Relevant to Medical Radiation Physics

H. Grady Hughes and Tim Goorley

Los Alamos National Laboratory

12th International Conference on Radiation Shielding (ICRS–12)

17th Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society (RPSD–2012)

Workshop on Computational Medical Physics

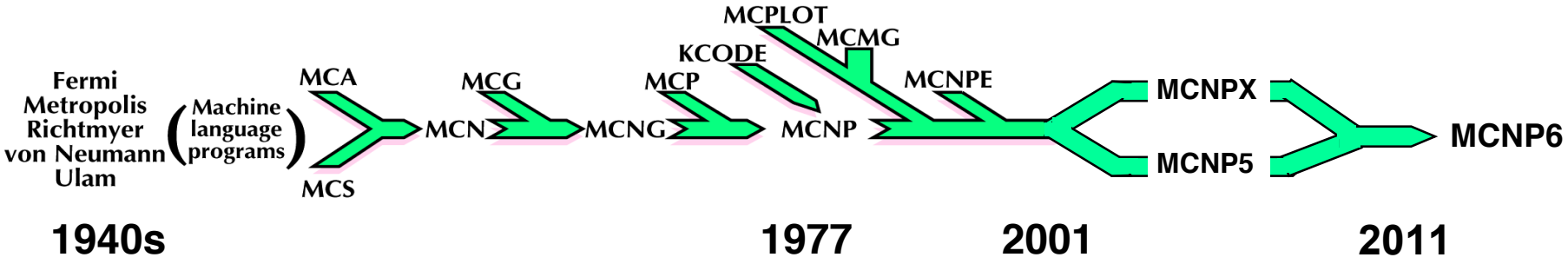
September 2–7, 2012

Nara, Japan

Abstract

MCNP (Monte Carlo N-Particle) is a general-purpose Monte Carlo code for simulating the transport of neutrons, photons, electrons, positrons, and more recently other fundamental particles and heavy ions. Over many years MCNP has found a wide range of applications in many different fields, including medical radiation physics. In this presentation we will describe and illustrate a number of significant recently-developed features in the current version of the code, MCNP6, having particular utility for medical physics. Among these are major extensions of the ability to simulate large, complex geometries, improvement in memory requirements and speed for large lattices, introduction of mesh-based isotopic reaction tallies, advances in radiography simulation, expanded variance-reduction capabilities, especially for pulse-height tallies, and a large number of enhancements in photon/electron transport.

MCNP History



- **Monte Carlo transport of particles**
  - **MCNP5 - neutrons, photons, electrons**
  - **MCNPX - neutrons, photons, electrons + many more particles & ions**
  - **MCNP6 - merged code + more, release in 2012**
- **For 30+ years, MCNP & its data libraries have been supported by the Monte Carlo team at LANL**
  - **Roots of MCNP go directly back to von Neumann, et al.**
  - **Continuous development, support, R&D, V&V**

MCNP Development Team

- Los Alamos groups XCP–3 and NEN–5

Forrest Brown	Jeffrey Bull	Larry Cox	Joe Durkee
Jay Elson	Michael Fensin	Tim Goorley	Grady Hughes
Michael James	Russell Johns	Brian Kiedrowski	Roger Martz
Stepan Mashnik	Gregg McKinney	Jeremy Sweezy	Trevor Wilcox
Tony Zukaitis			
active retirees:	Tom Booth	Art Forster	John Hendricks
	Denise Pelowitz	Dick Prael	Laurie Waters

- Other Los Alamos groups

XCP–5	Materials and Physical Data
XCP–7	Transport Applications

- External Collaborators

University of New Mexico	University of Southern Mississippi
University of Michigan	Lawrence Livermore National Laboratory
Sandia National Laboratory	CEA (France)
… and many others	

What Can MCNP Do?

Detailed models of geometry & physics

- General 3D combinatorial geometry
- Repeated structures
- Lattice geometries
- Unstructured mesh geometries (tet, hex)
- Geometry, cross section, tally plotting
- ENDF/B-VII physics interaction data
- Event-generator physics models

Calculate nearly any physical quantity

- Flux and current
- Energy and charge deposition
- Heating and reaction rates
- Response functions
- Mesh tallies and radiography images
- K-effective, α, η, ν, Λ
- Fission distributions
- Fission product distributions

Unique features for criticality calc's

- Shannon entropy of the fission source for assessing convergence
- Dominance ratio, k_1 / k_0
- Stochastic geometry
- Isotopic changes with burnup

> 10,000 users around the world

- Fission and fusion reactor design
- Nuclear criticality safety
- Radiation shielding
- Waste storage/disposal
- Detector design and analysis
- Nuclear well logging
- Particle accelerators
- Health physics and dosimetry
- Medical physics and radiotherapy
- Transmutation, activation, and burnup
- Aerospace applications
- Decontamination and decommissioning
- Nuclear safeguards

Portable to any computer

- Windows, Linux, Mac, Unix
- Multicore, clusters, netbooks, ASC, …
- Parallel, scalable - MPI + threads
- Built-in plotting

Support

- Extensive V&V against experiments
- Web site, user groups, email forum
- Classes: 1 week, ~ 6x / year
  general and special topics

Features of Interest to Medical Physics

- Extensions for problem size
  - More cells and surfaces
  - More detectors and tallies
  - Histories beyond the 32-bit limit (> 2 billion)
  - Lattice tally enhancements
  - Large lattice improvements
  - Optional initialization speedups
- Enhancements for tallying and visualization
  - Mesh tallies and mesh-based reaction tallies
  - Dosimetry and built-in response functions
  - Radiography tallies
- New kinds of geometry
  - CAD/CAE geometries (e.g. Abaqus)
  - PARTISN geometries (link to deterministic codes)
  - Third-party CT ⟶ MCNP geometry scripts (old methods)

Features of Interest to Medical Physics

- Improvements in Transport Capability
  - Pulse-height tally variance reduction
  - Condensed-history energy straggling logic
  - Stochastic geometry
- Physics Improvements
  - Photon Doppler broadening (for incoherent scattering)
  - Create temperature-specific neutron cross-section tables
  - Photon and atomic relaxation data extensions
  - Single-event electron transport
- On-Line Information
  - http://mcnp.lanl.gov especially → *Publications*
  - Medical physics MCNP Primer (LA–UR–07–4133)
  - Medical database(LA–UR–08–2468) with ICRP110 phantoms
    - Contact Tim Goorley (jgoorley@lanl.gov) to discuss or contribute.

Extended Limits on Problem Size

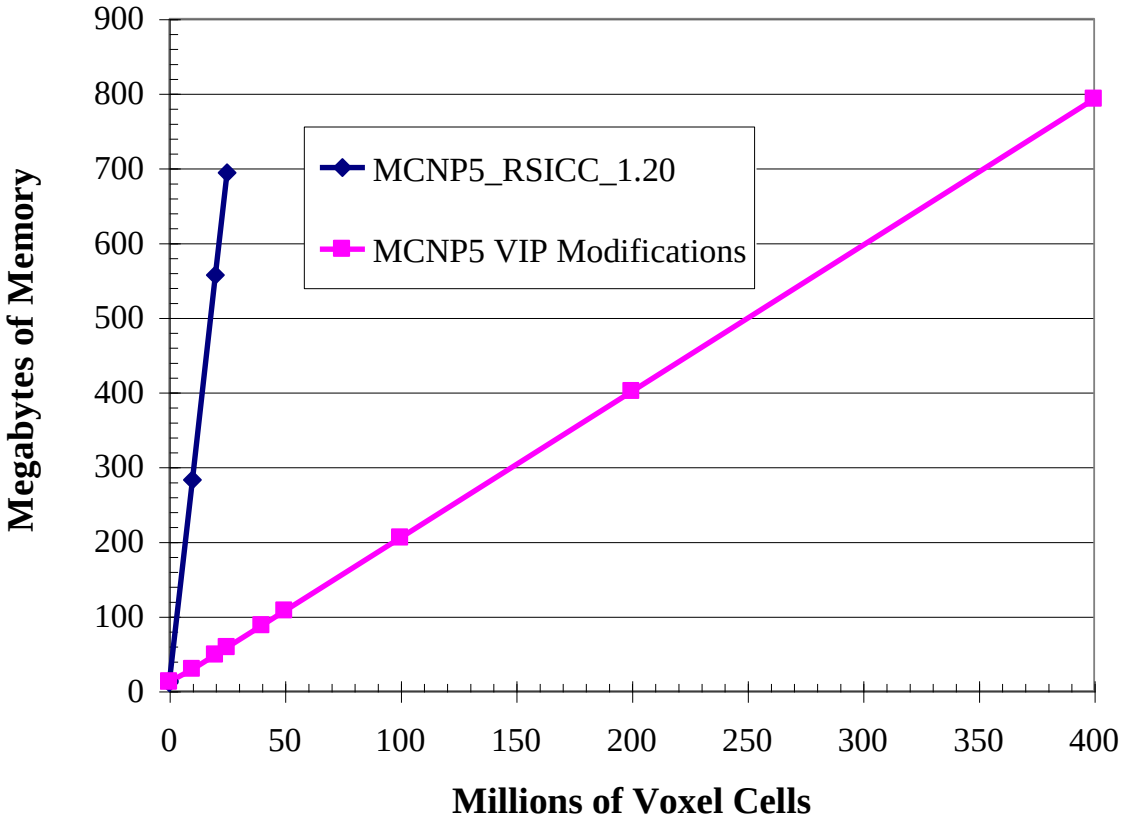
	MCNP5 1.51 and earlier	**MCNP5 1.60** and **MCNP6**
Cell numbers	99,999	99,999,999
Surface numbers	99,999	99,999,999
Material numbers	99,999	99,999,999
Universe numbers	99,999	99,999,999
Tally numbers	999	9,999
Geometry levels	10	20
Cell complexity (MLGC)	1,000	9,999
URAN universes	2	unlimited

Large Lattice Improvements: Tally Speed

- Under certain conditions, runtimes can be significantly reduced (5-500 times shorter, depending on problem).
- Stringent Conditions:
  - 1st level hexahedral lattice.
  - F4, optionally with DE–DF, each instance addressing the lattice.
  - No DXTRAN, GEB, E/C/T bins, flagging, WWG, perturbations, etc.
- MCNP will attempt to determine if these conditions are met and will attempt to use the enhancement if appropriate. Messages either way. Fast and slow runs will track.
- No tallied nested lattice, tallied partial lattice index range, or self-referencing fill entry. See LA-UR-04-3400.

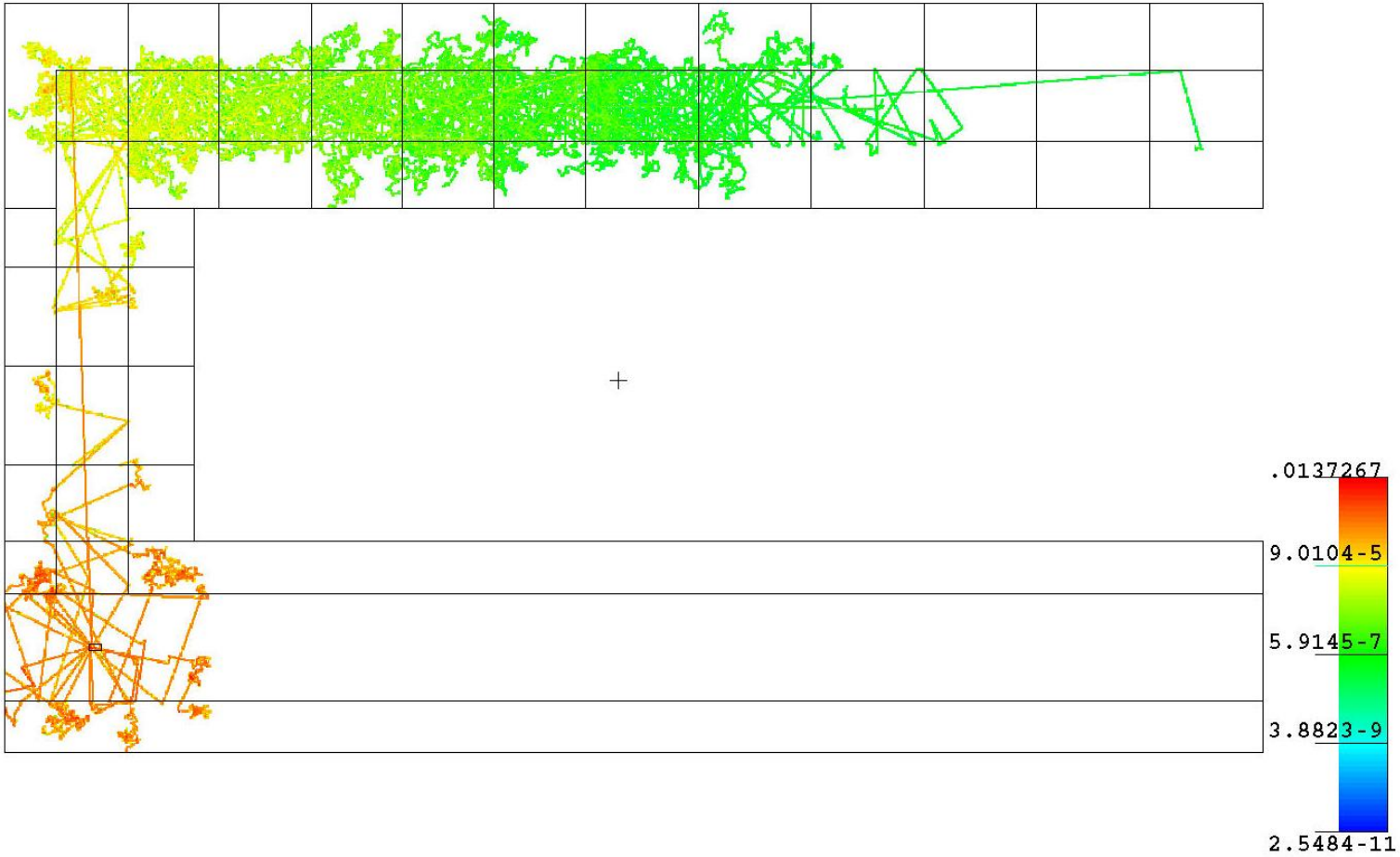
Large Lattice Improvements: Memory Use

- Increase voxel limit from ~20 million to ~800+ million (with recompilation).
- Reduce startup times from days to a few hours.
- Windows 32-bit OS limit: 2 Gbytes memory per program. (Use 64-bit chip & OS)



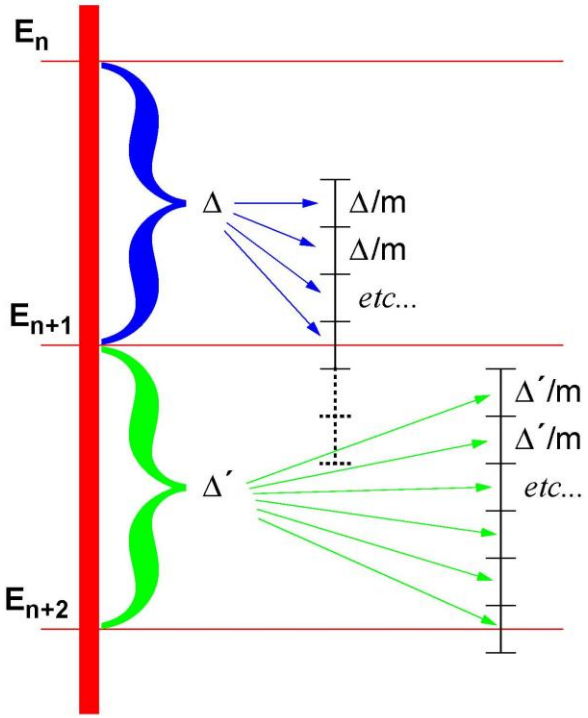
Goorley, "Issues Related to the use of MCNP code for an Extremely Large Voxel Model VIP-MAN," Monte Carlo 2005, Chattanooga TN.

Another View of Mesh Plots: Particle Tracks



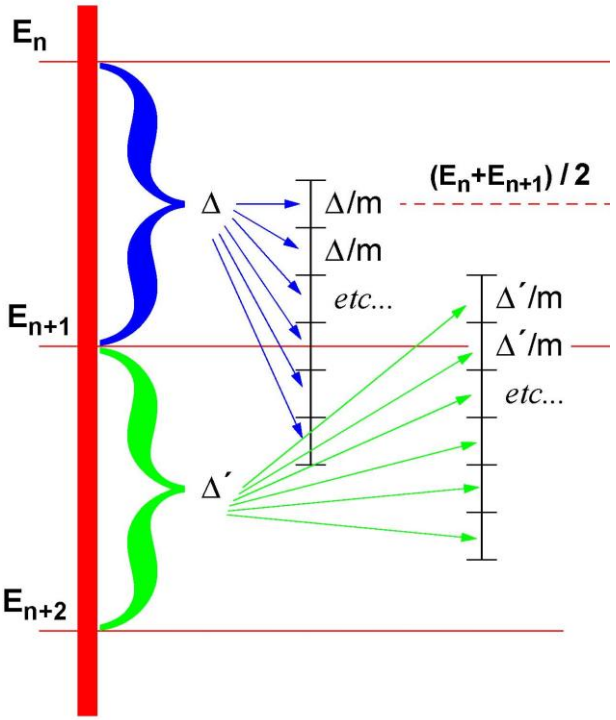
Electron Energy Straggling Improvements

Bin-Centered (MCNP) Logic



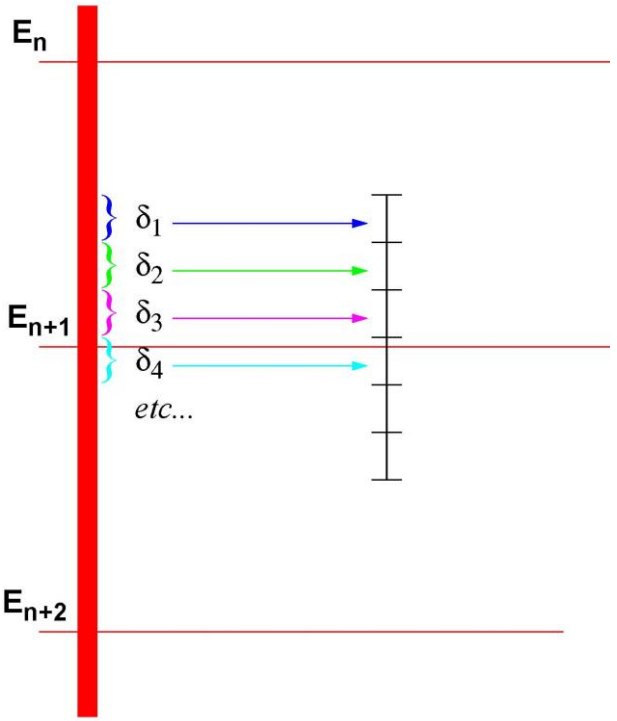
DBCN 17J 0.

Nearest-Group-Boundary (ITS) Logic



DBCN 17J 1.

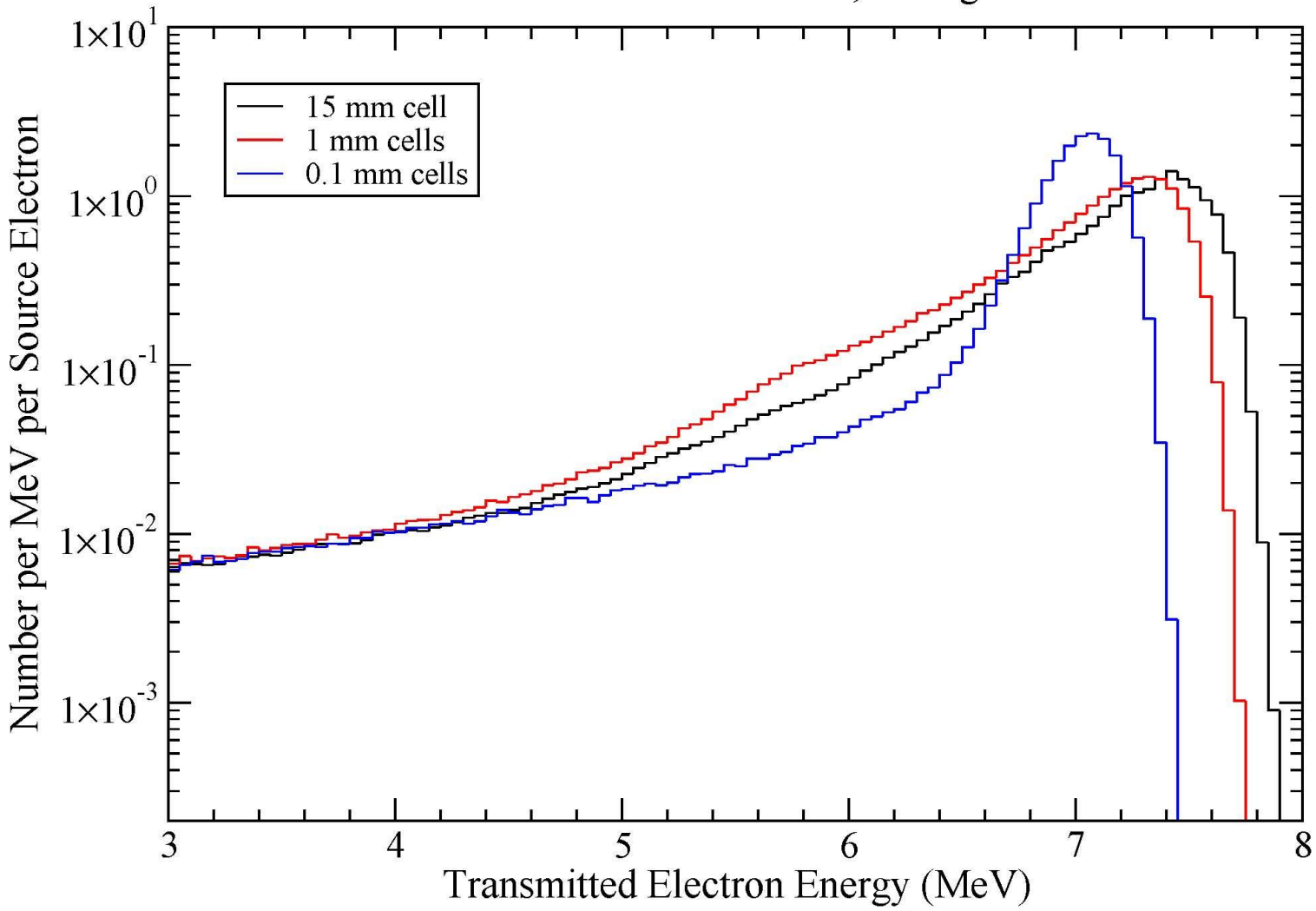
Energy- and Step-Specific Logic



DBCN 17J 2.

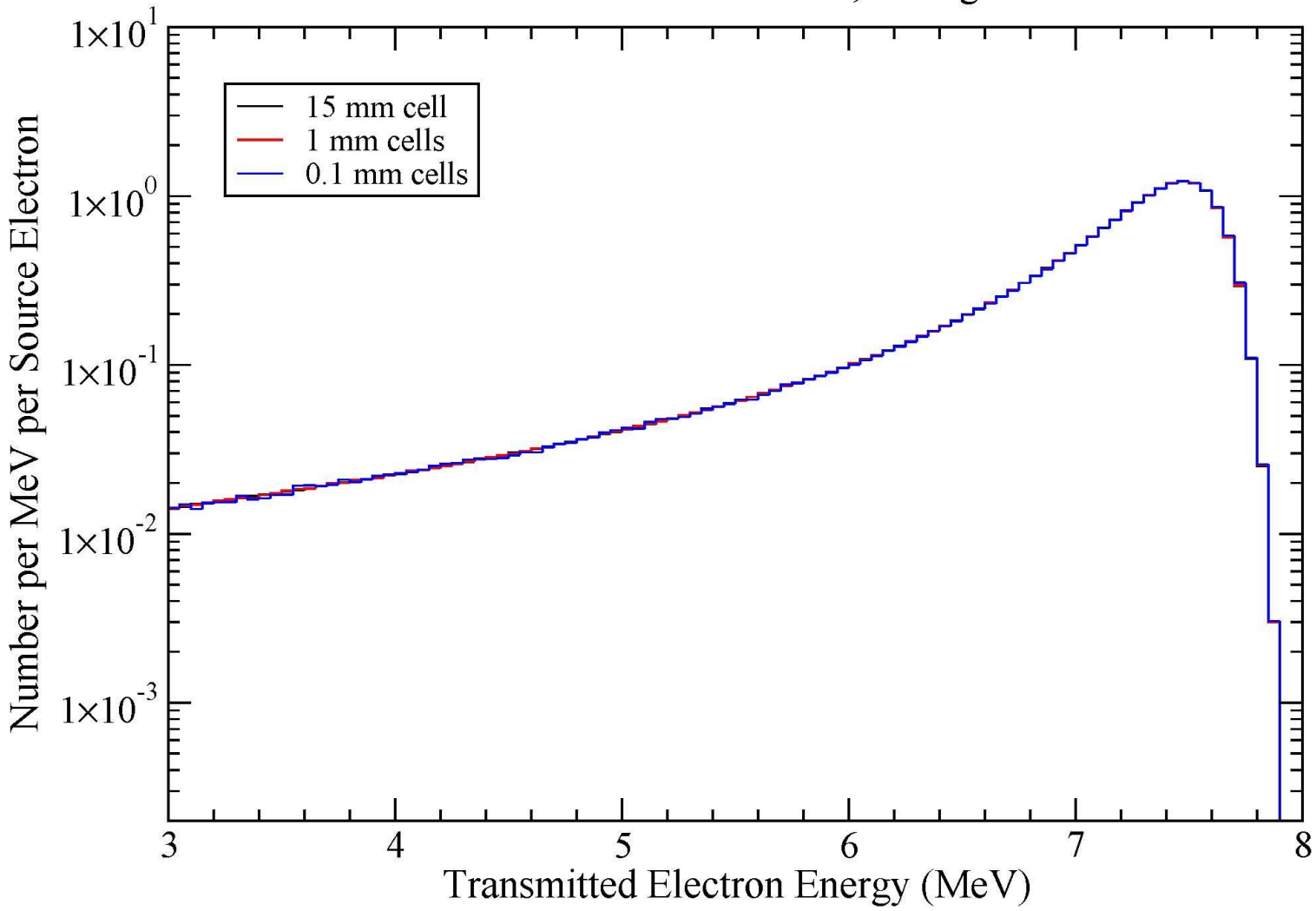
MCNP (bin-centered) Straggling Logic

10 MeV electrons after 15 mm water, no angular deflection



Step-Specific Straggling Logic

10 MeV electrons after 15 mm water, no angular deflection



Stochastic Geometry

- On-the-fly random translations of embedded universes in lattice
- Developed for pebble bed reactors.
- Medical physics applications?
  - Alveoli
  - Sinuses
  - Bone marrow
- Use URAN card
  - See MCNP5 Manual

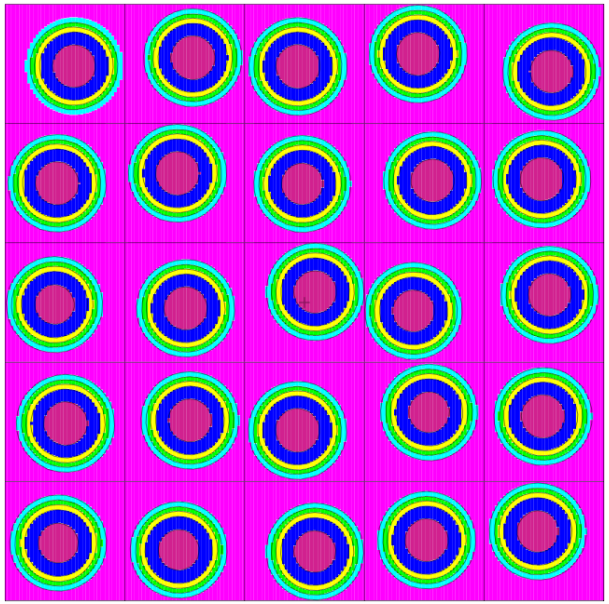


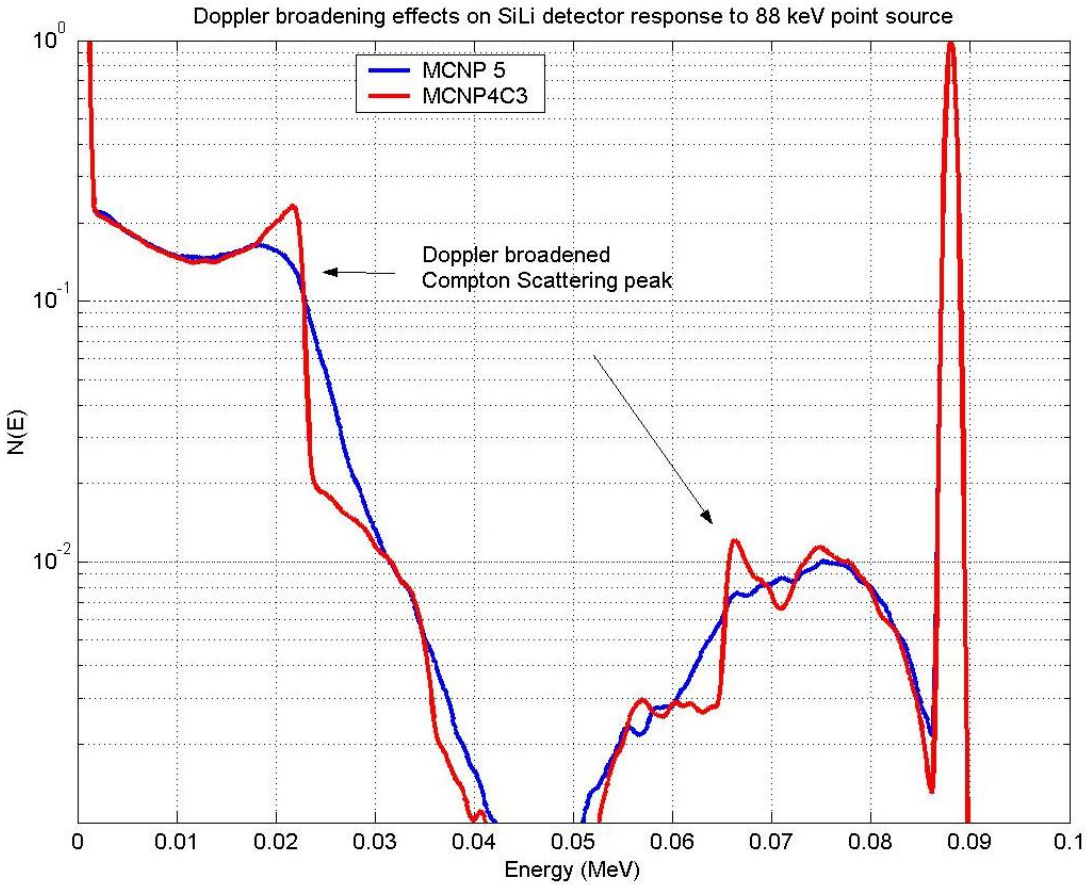
Image of the stochastic geometry of fuel kernels from MCNP5 plotter

Fuel kernel displaced randomly within lattice element each time that particle enters

Forrest Brown, "**Monte Carlo Methods and MCNP Code Development**" Monte Carlo 2005, Chattanooga TN.

Photon Doppler Broadening

- Released in MCNP5, RSICC_1.14
- Incoherent Compton event, includes electron binding energy.
- Causes reduction of the photon's total scattering cross section in the forward direction.
- Causes broadening of photons' energy spectrum.
- Important for $E_p < 1$ MeV.
- Bug fixes in MCNP5, RSICC_1.40, MCNP5, RSICC_1.60, and in MCNP6.



Temperature-Specific Neutron Cross Sections from MAKXSF

- **Now part of the cross-section library manager program MAKXSF**
- **Create cross-section tables at new temperatures**
  - **Doppler broaden resolved resonance data to higher temperature**
  - **Interpolate unresolved resonance probability tables to new temperature**
  - **Interpolate S(α, β) thermal data to new temperature**
- **Create new *xsdir* file which includes the changed cross-section tables.**

Photon Enhancements ENDF/B VI.8

- Extension of existing data: from ≥ 1 keV down to ≥ 1 eV
  - Coherent scattering
  - Incoherent scattering
  - Photoelectric absorption
- New kinds of photoatomic data
  - Subshell-wise photoelectric cross sections
    - Detailed sampling of initial vacancy now possible
  - Complete information for electron subshells
    - Binding energies, electron populations, transitions, etc.
- Extended scattering form factors
  - Coherent and incoherent scattering
  - Complete range of energy and angle
  - Accurate interpolation (especially for coherent scattering)
- Cold, neutral, atomic target materials Z = 1 … 100

Atomic Relaxation ENDF/B VI.8

- Consistent data for electron subshells
  - Binding energies
  - Electron populations
  - Number of transitions
  - Photoelectric subshell cross sections down to 1 eV
- Consistent data for transitions
  - Transitions with photon fluorescence (radiative)
  - Auger and Coster-Kronig transitions (non-radiative)
- Full analog sampling of the relaxation cascade
- New process: Compton-induced atomic relaxation
- Cold, neutral, atomic target materials Z = 1 … 100

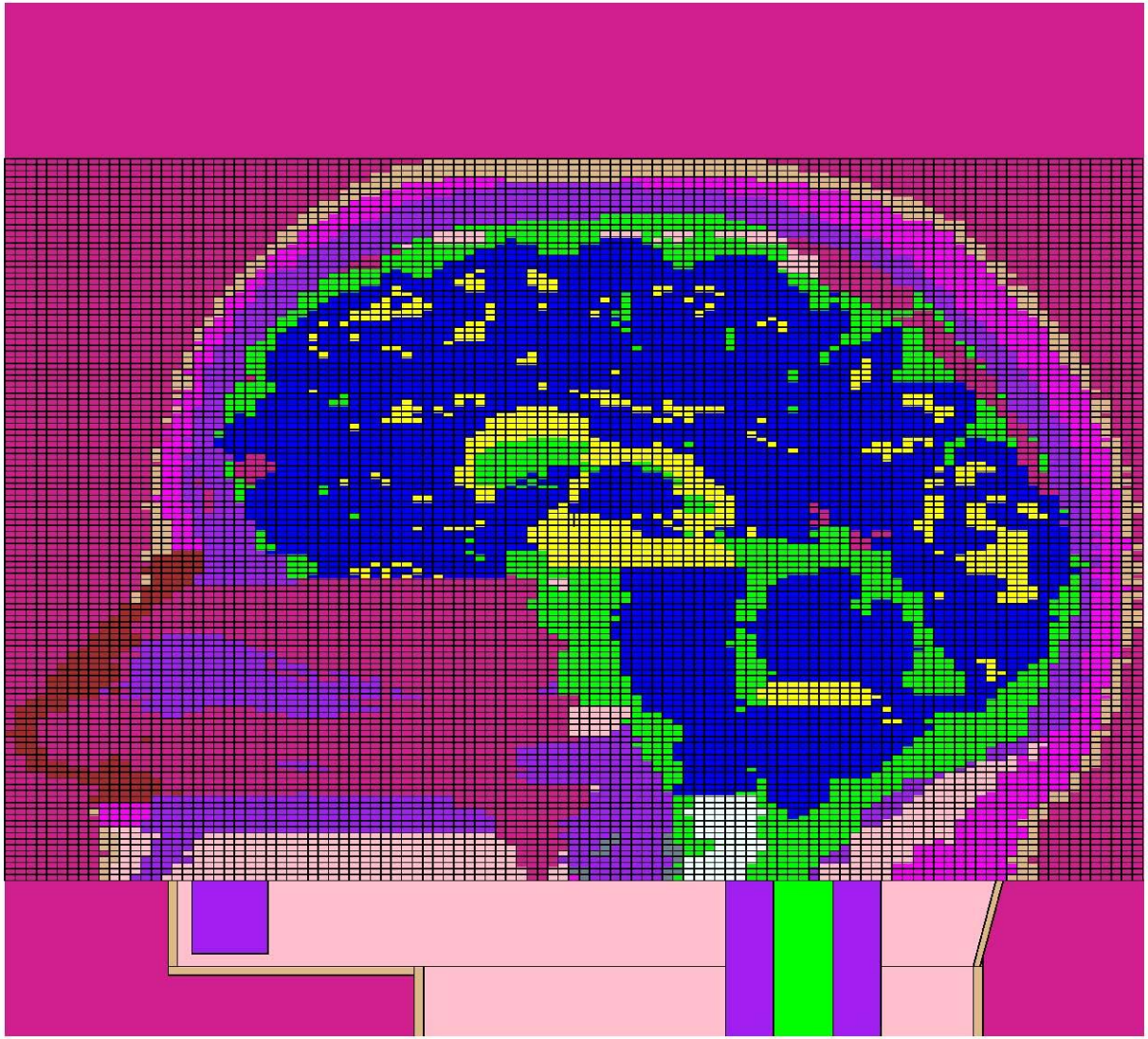
Electron Enhancements ENDF/B VI.8

- Cold, neutral, atomic target materials $Z = 1 \ldots 100$
- Microscopic electron cross sections down to 10 eV
- Electron elastic scattering
  - Electron angular distribution as function of electron energy
- Atomic excitation
  - Electron mean energy loss as function of electron energy
- Subshell-wise electroionization
  - Knock-on energy distribution as function of electron energy
  - Knock-on direction and primary energy loss from conservation
- Bremsstrahlung
  - Photon energy distribution as function of electron energy
  - Electron mean energy loss as function of electron energy
  - No photon angular data given (use existing MCNP methods)

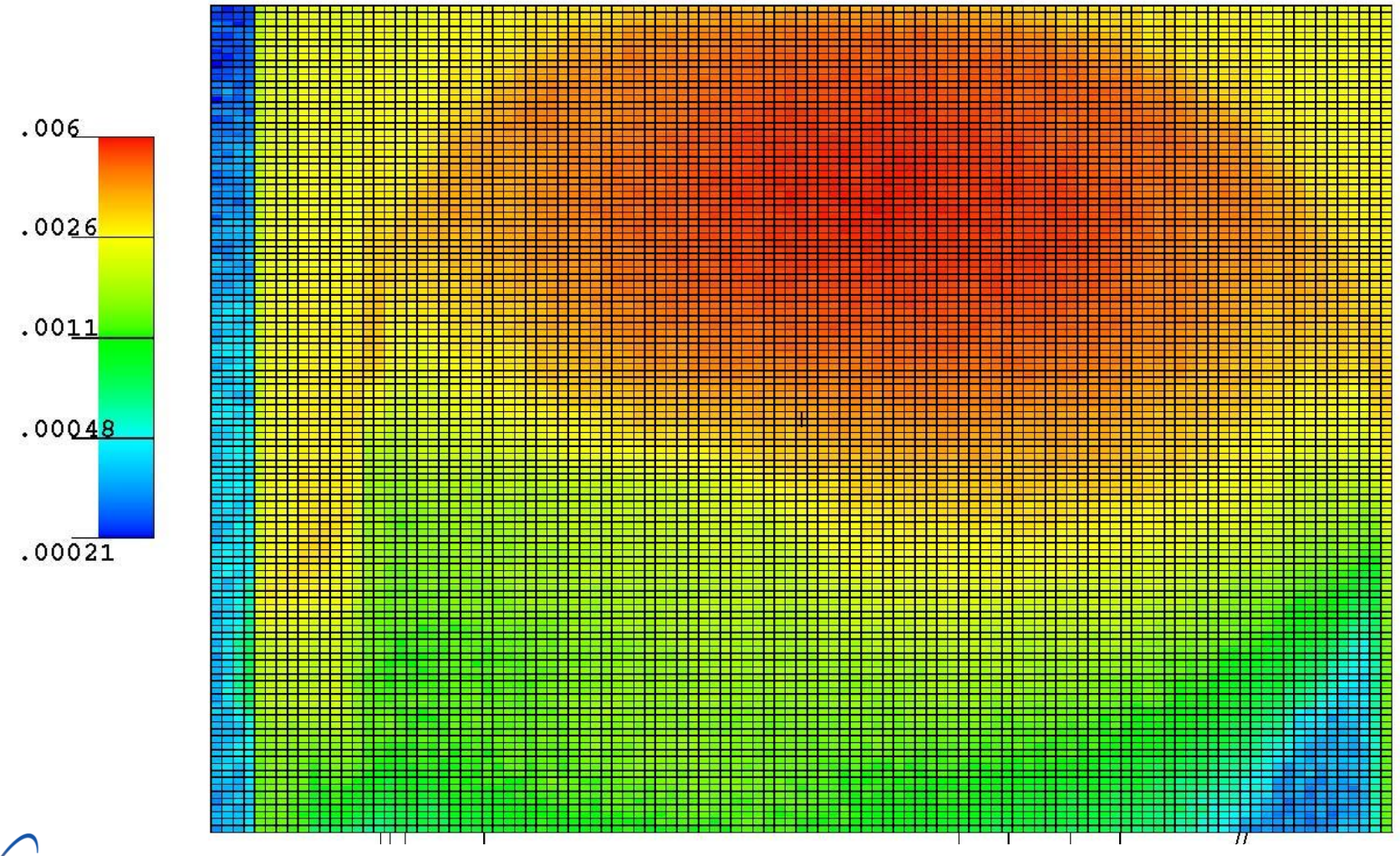
Example: the Zubal Head Phantom

- Voxel Phantom of Head – uses MCNP lattice geometry
- 85 × 109 × 120 = 1,111,800 voxels (small nowadays)
- X, Y, Z resolution: 2.2 mm × 2.2 mm × 1.4 mm
- 61 distinct brain and associated structures mapped
- References
  - Zubal, Harrell, Smith, and Smith, Proceedings of the International Workshop, National Radiological Protection Board, Chilton, UK, on 6 and 7 July 1995.
  - Modifications by Jeff Evans, Ohio State.
  - Lazarine, Alexis. "Medical Physics Calculations with MCNP: A Primer", April 2007. Texas A&M University Masters Thesis.

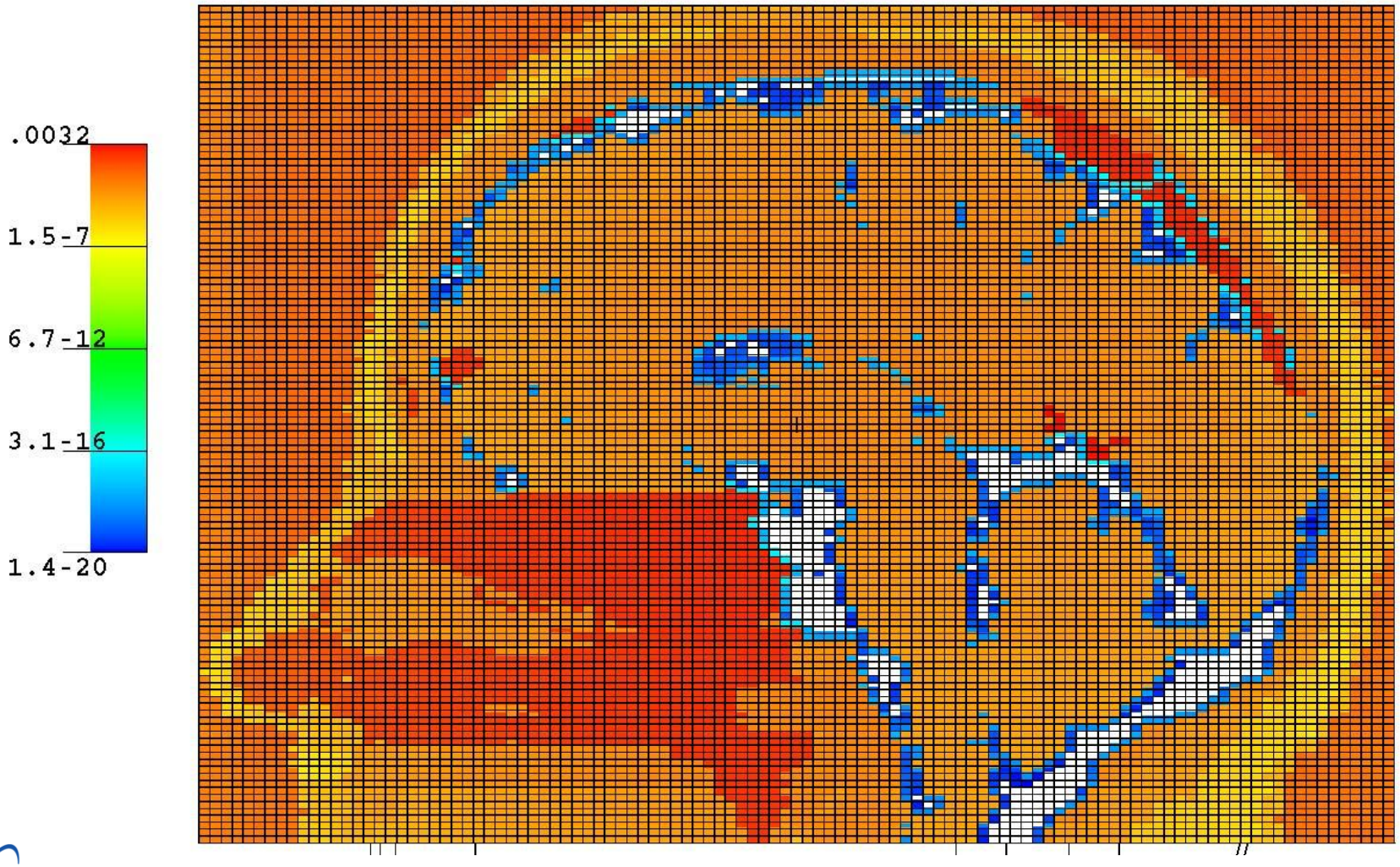
Zubal Head Geometry



Flux from Incident 1-MeV Neutrons

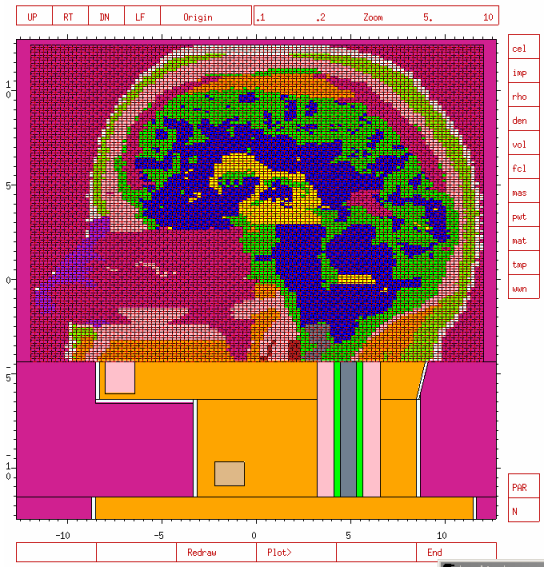


N14(n,p)C14 Reaction

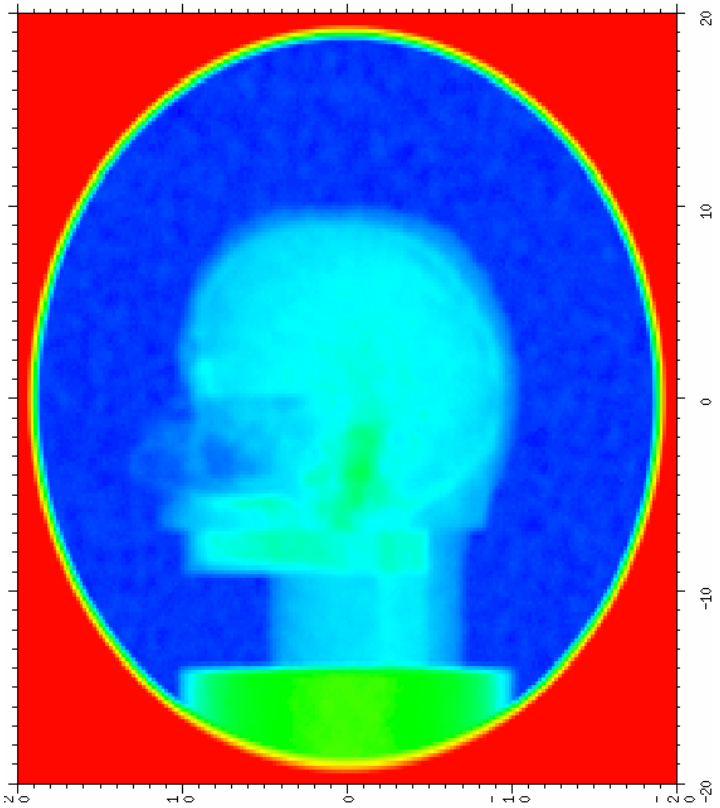


Zubal Head Phantom: Simulated Radiograph

CT Based Geometry



Simulated Radiograph

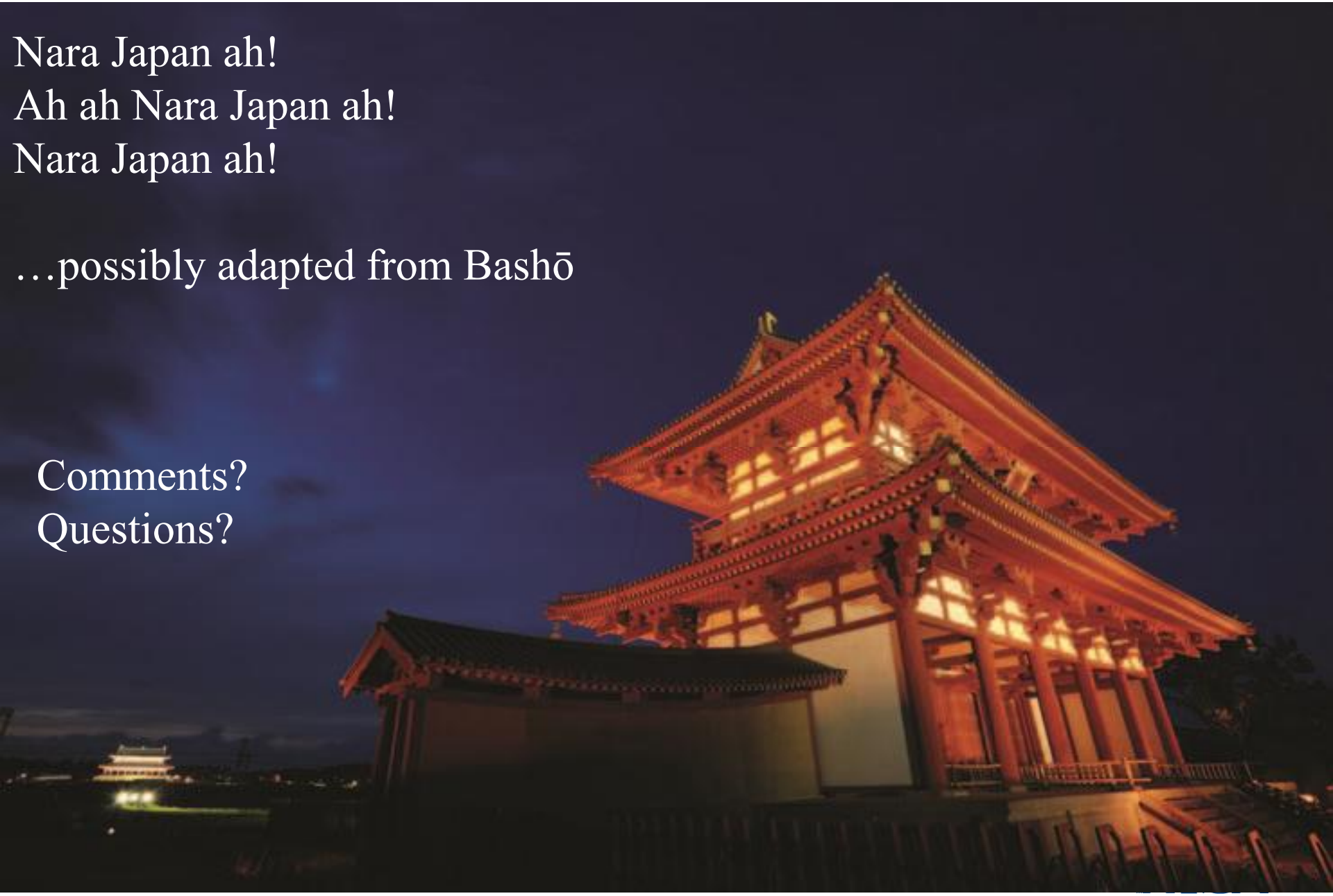


Alexis Lazarine, “Medical Physics Calculations with MCNP: A Primer”, April 2007. Texas A&M University Masters Thesis

Summary

- MCNP is a powerful general-purpose Monte Carlo particle transport code benefitting from an extensive program of development, validation, and verification.
- MCNP6 is the latest and most advanced version of the MCNP code family.
- MCNP6 contains a significant and growing set of features useful for medical radiation physics.
- The electron/photon transport capabilities of MCNP6 are being vigorously extended and improved.

Concluding Haiku



Nara Japan ah!
Ah ah Nara Japan ah!
Nara Japan ah!

…possibly adapted from Bashō

Comments?
Questions?