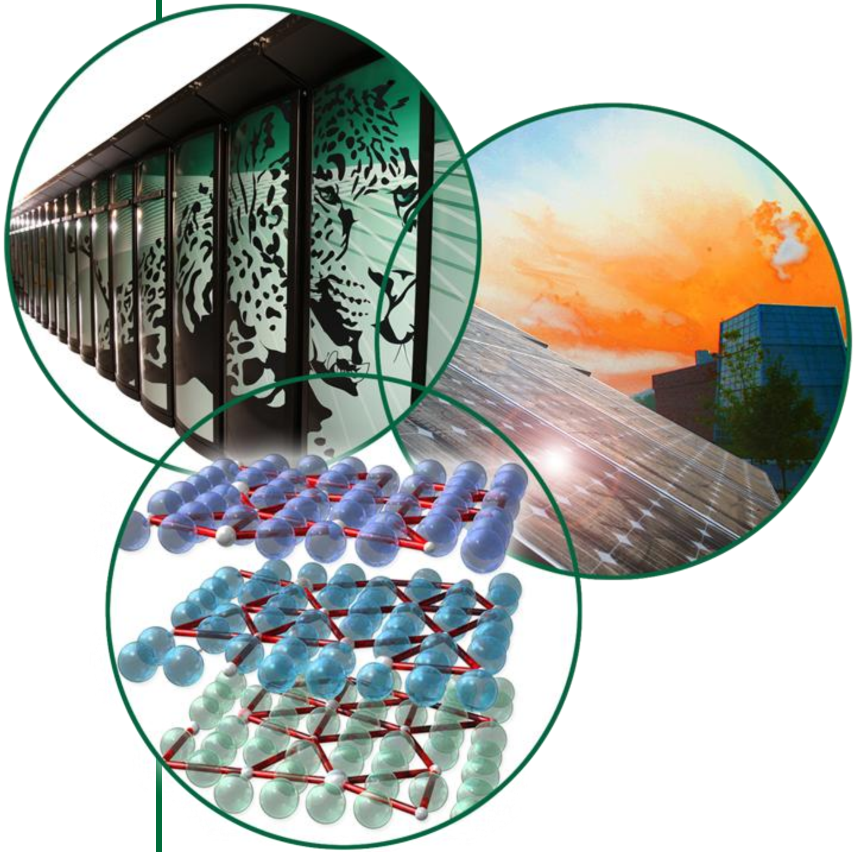
A Review of Nuclear Computational Information

SATIF-10
June 2-4, 2010
CERN



Bernie Kirk

ORNL/RSICC

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

Introduction

Updated Software since SATIF-9

Featured Software

- **MONACO/MAVRIC**
- **DENOVO**
- **MCNP/MCNPX**
- **TITAN**

CONCLUSION

MarketWatch
May 25, 2010

Cray Launches the Cray XE6 Supercomputer - The Next Generation of Its High-End Supercomputers

Attendees at the 2010 Cray User Group (CUG) meeting in Edinburgh, Scotland witnessed the formal introduction of Cray's highly anticipated new supercomputer, which combines the company's new Gemini interconnect with powerful AMD Opteron(TM) processors to bring production petascale computing to a new and expanded base of high performance computing (HPC) users.

And then, there is CUDA!

CUDA is NVIDIA's parallel computing architecture that enables dramatic increases in computing performance by harnessing the power of the GPU (graphics processing unit).

Updated Software since SATIF-9

C00657	Code System to Calculate Multigroup Beta-Ray Spectra.	BETA-S 6
C00684	Code System for Evaluating Routine Radioactive Effluents from Nuclear Power Plants with a Windows Interface.	NRCDOSE 2.3.15
C00726	One, Two- and Three-Dimensional Coupled Neutral and Charged Particle SN Code System.	CNCSN
C00728	GENII-LIN Multipurpose Health Physics Code System with a New Object-Oriented Interface, Release 2.0.	GENII-LIN 2.1
C00735	Inventory Code System for Neutron Activation Analysis.	EASY-2005.1
C00737	Environmental Radiation Dosimetry Software System.	GENII 2.09
C00740	Monte Carlo N-Particle Transport Code System Including MCNP5 1.51 and MCNPX 2.6.0 and Data Libraries (Source & Executables).	MCNP5/MCNPX
C00740	Monte Carlo N-Particle Transport Code System Including MCNP5 1.51 and MCNPX 2.6.0 and Data Libraries (Executables - No Source).	MCNP5/MCNPX-EXE
C00742	Gamma-electron Efficiency Simulator, Version 3.1	GES_MC
C00744	Visualization Code System for Gamma and Neutron Shielding Calculations.	EASY-QAD 1.0
C00745	Modular Code and Data System for Fast Reactor Neutronics Analyses	ERANOS 2.0
C00750	Modular Code System for Performing Criticality and Shielding Analyses for Licensing Evaluation with ORIGEN-ARP (Source & Executables).	SCALE 6
C00750	Modular Code System for Performing Criticality and Shielding Analyses for Licensing Evaluation with ORIGEN-ARP (Executables - No Source).	SCALE 6-EXE
C00753	Analytical Benchmarks; Case Studies in Neutron Transport Theory.	GANAPOL-ABNTT
C00755	Code System for Actinide Transmutation Calculations	CINDER 1.05
C00756	Code System to Perform Monte Carlo Simulation of Electron Photon Showers in Arbitrary Marerials.	PENELOPE2008.1
C00758	ACtivation ABacus Inventory Code System for Nuclear Applications.	ACAB-2008
C00761	Radiological Safety Analysis Code System.	RSAC7
C00764	MCNP Utility for Reactor Evolution.	MURE
C00766	Fine-flux Cross Section Condensation, 2D Few Group Diffusion and Transport Burnup Calculations	BOXER

P00158	Code System for Multilevel R-Matrix Fits to Neutron and Charged-Particle Cross-Section Data Using Bayes' Equations.	SAMMY-8
P00338	Code System for Inelastic and Elastic Scattering with Nucleon-Nucleon Potential	DWBA07/DWBB07
P00352	SCAMPI: Collection of Codes for Manipulating Multigroup Cross Section Libraries in AMPX Format.	SCAMPI
P00542	Code System to Determine Pu Isotope Abundances from Multichannel Analyzer Gamma Spectra.	MGA8
P00544	Covariance Matrix Interpolation and Mathematical Verification.	ANGELO-LAMBDA
P00545	Nuclear Properties and Decay Data Chart of Nuclides.	NUCHART
P00546	Nuclear Model Code System for Distorted Wave Born Approximation and Coupled Channel Calculations.	DWUCK-CHUCK
P00548	Nuclear Model Code System for Analysis and Prediction of Nuclear Reactions and Generation of Nuclear Data.	TALYS 1.0
P00550	Statistical Model Code System to Calculate Particle Spectra from HMS Precompound Nucleus Decay.	ALICE-2008
P00552	Plotting Program with Special Features for Windows Environment.	PLOT-S
P00553	Computer Code for the Analysis of Small-Break Loss-of-Coolant Accident of Boiling Water Reactors.	THYDE-B1/MOD2
P00554	Computer Code for PWR LOCA Thermohydraulic Transient Analysis.	THYDE-P2
P00555	Dynamic Analysis of Nuclear Energy System Strategies.	DANESS V1.0

Updated Data since SATIF-9

D00196	Power Reactor Embrittlement Data Base, Version 3.	PR-EDB
D00239	A Temperature-Dependent Linearly Interpolable, Tabulated Cross Section Library Based on ENDF/B-VII.0	POINT2009
D00242	Fine-Group Cross Section Library Based on JEFF3.1 for Nuclear Fission Applications.	MATJEFF31.BOLIB
D00243	TALYS-Based Cross Section Library for Use with MCNP(X).	TENDL-2008-ACE

M00005	Adjoint Function: Physical Basis of Variational & Perturbation Theory in Transport & Diffusion Problems.	JDL-IMPORTANCE
M00006	Nuclear Reactor Kinetics and Control.	JDL-REACTOR-KIN

BETA-S
A Code System to Calculate Multigroup Beta-Ray Spectra

BETA-S calculates beta-decay source terms and energy spectra in multigroup format for time-dependent radionuclide inventories of actinides, fission products, and activation products. Multigroup spectra may be calculated in any arbitrary energy-group structure. The code also calculates the total beta energy release rate from the sum of the average beta-ray energies as determined from the spectral distributions. BETA-S also provides users with an option to determine principal beta-decaying radionuclides contributing to each energy group. The SCALE code system must be installed on the computer before installing BETA-S, which requires the SCALE subroutine library and nuclide-inventory generation from the ORIGEN-S code.

- the BETA-S source code was converted to modern Fortran 90 standard
- dynamic memory allocation implemented
- the free-format input reading routines were replaced with reading modules in SCALE 5
- added the capability to obtain beta decay branching data from either a binary or card-image format ORIGEN data library (required for compatibility with ORIGEN-ARP)
- corrected an error associated with spectral calculation in highest energy group
- improved spectrum calculation by normalizing spectral energy to evaluated beta energy
- added capability to generate plot files compatible with PlotOPUS program.

Developer: Ian Gauld
ORNL

CNCSN: One, Two- and Three-Dimensional Coupled Neutral and Charged Particle SN Code System.

KATRIN-2.0: Three-dimensional neutral and charged particle transport.
KASKAD-S-2.5: Two-dimensional neutral and charged particle transport.
ROZ-6.6: One-dimensional neutral and charged particle transport.
ARVES-2.5: Preprocessor for the working macroscopic cross-section FMAC-M format for transport calculations.
MIXERM: utility for preparing mixtures on the base of multigroup cross-section libraries in ANISN format.
CEPXS-BFP: A version of Sandia National Laboratory's multigroup coupled electron-photon cross-section generating code CEPXS, adapted for solving the charged particle transport in the Boltzmann-Fokker-Planck formulation with the use of discrete ordinate method.
SADCO-2.4: Institute for High-Energy Physics modular system for generating coupled nuclear data libraries to provide high-energy particle transport calculations by multigroup method.

KATRIN, KASKAD-S and **ROZ-6** solve the multigroup transport equation for neutrons, photons and charged particles in 3D (and), 2D (, and) and 1D (plane, spherical and cylindrical) geometries, respectively.

Developer: A. M. Voloschenko et al
Russian Academy of Science

EASYQAD: A Visualization Code System for Gamma and Neutron Shielding Calculations, Version 1.0.

EASYQAD, Version 1.0, is a standalone Windows XP code system which facilitates gamma and neutron shielding calculations with user friendly graphical interfaces. It is used to analyze radiation shielding problems and includes:

- 8 kinds of geometry types,
- various flexible source options,
- common material library,
-various detector types.

EASYQAD, Version 1.0, is based on QAD-CGGP-A, which is a point-kernel code for calculating fast-neutron and gamma-ray penetration through various shield configurations defined by combinatorial geometry specifications. QAD uses a point-kernel ray-tracing technique for gamma-ray calculations and either a modified Albert-Welton kernel or kernels obtained from the moments method solution of the Boltzmann equation for neutron penetration calculations. The GP version optionally makes use of the Geometric Progression (GP) fitting function for the gamma-ray buildup factor.

Developer: Jong Kyung Kim
Hanyang University, South Korea

CINDER Version 1.05: Code System for Actinide Transmutation Calculations

This CINDER 1.05 package includes the CINDER’90 code Version 7.4.2, ACTIVATION 1.0, GAMMA_SOURCE 1.0.

CINDER’90 is the latest in the sequence of data and code evolution built upon the original work of T. England at Bettis Atomic Power Laboratory (BAPL) in the early 1960s. It is used to calculate the inventory of nuclides in an irradiated material.

In nuclear reactor applications, such a code is commonly called a burnup code. It may also be called an activation code since it well describes the conversion of stable nuclides to radioactive nuclides by particle bombardment.

The CINDER’90 library of 63-group cross sections describes 3400 nuclides in the range $1 \leq Z \leq 103$.

Developer: W. B. Wilson et al
Los Alamos National Laboratory

ALICE2008:
Statistical Model Code System to Calculate Particle Spectra from HMS Precompound Nucleus Decay

The HMS-Alice (Hybrid Monte-carlo Simulation) codes began evolution from the Alice code in 1995 with the development of the Monte Carlo precompound model. This new release designated HMS-ALICE2008 uses the HMS precompound decay model, the Weisskopf- Ewing evaporation model (optional with s-wave approximation) and Bohr- Wheeler fission models, all with multiple particle emission cascades, to estimate single and double differential emission spectra and product yields of nuclear reactions induced by probes from photons to heavy ions.

Developer: M. Blann

GES_MC: Gamma-electron Efficiency Simulator, Version 3.1

GES_MC (Gamma-electron Efficiency Simulator Monte Carlo) is written entirely in Java and is based on the EGSnrc (Electron Gamma Shower) source code. Although GES_MC is especially designed for the computation of the response function and peak efficiency for gamma detectors, it can also be used in various studies concerning photon or electron interactions with the matter in any cylindrical (RZ) geometry.

GES_MC is based on the radiation transport theory and algorithms (routines taken from EGSnrc software) developed by SLAC (Stanford Linear Accelerator Center , USA) and NRC (National Research Council, Canada).

http://tensp.academic.ro/download/fulea/.

Developer: Dan Fulea
Institute of Public Health, Romania

GENII 2.09: Environmental Radiation Dosimetry Software System.

The GENII system includes capabilities for calculating human and environmental radiation doses following chronic and acute releases. Radionuclide transport via air, water, or biological activity may be considered. Air transport options include both puff and plume models; each allows use of an effective stack height or calculation of plume rise from buoyant or momentum effects (or both). Building wake effects can be included in acute atmospheric release scenarios. The code provides risk estimates for health effects to individuals or populations; these can be obtained using the code by applying appropriate risk factors to the effective dose equivalent or organ dose. In addition, GENII Version 2 uses cancer risk factors from Federal Guidance Report 13 (FGR-13) to estimate risk to specific organs or tissues. Although the codes were initially developed at Hanford, they were designed with the flexibility to accommodate input parameters for a wide variety of generic sites.

Developer: Bruce Napier
Pacific Northwest National Laboratory

SAMMY-8.0.0: Code System for Multilevel R-Matrix Fits to Neutron and Charged-Particle Cross-Section Data Using Bayes' Equations

The purpose of the code is to analyze time-of-flight cross section data in the resolved and unresolved resonance regions.

The new features added to SAMMY include:

1. The value of ν (NU) for η (ETA) calculations can now be energy dependent.
2. Extensive revisions have been made to the self-shielding multiple-scattering (ssm) module.
3. Tabulated values (from Monte Carlo calculations) can be used instead of SAMMY-generated double-plus scattering corrections.
4. The "simple" resolution function may include a Gaussian whose width is a linear function of energy.
5. Input resonance parameters can now be presented as reduced width amplitudes γ instead of partial widths $\Gamma = 2P\gamma^2$.
6. For transmission measurements, the sample thickness may be non-uniform.
7. SAMMY now produces a third type of output file from which plots may be made – an ASCII file (with extension "LST") is created.

Developer: Nancy Larson
Oak Ridge National Laboratory

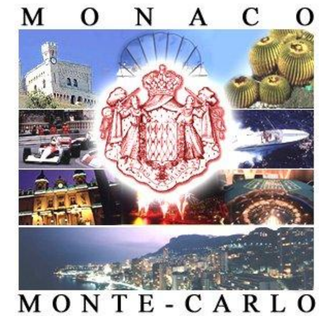
ERANOS 2.0: Modular Code and Data System for Fast Reactor Neutronics Analyses

The European Reactor ANalysis Optimized calculation System, ERANOS, has been developed and validated with the aim of providing a suitable basis for reliable neutronic calculations of current as well as advanced fast reactor cores. It consists of data libraries, deterministic codes and calculation procedures which have been developed within the European Collaboration on Fast Reactors over the past 20 years or so, in order to answer the needs of both industrial and R&D organisations. The whole system counts roughly 250 functions and 3000 subroutines totalling 450000 lines of FORTRAN-77 and ESOPE instructions.

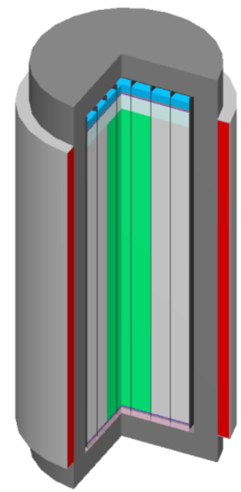
Nuclear data libraries:
The ECCO/ERANOS 2.0 code package contains four neutron cross section libraries derived from the JEF-2.2 nuclear data evaluated files. They are:
- 1968-group library (41 main nuclides)
- 33-group library (246 nuclides, including pseudo fission products)
- 175-group library (VITAMIN-J energy group scheme)
- 172-group library (XMAS energy group scheme, 246 nuclides, including pseudo-FP).

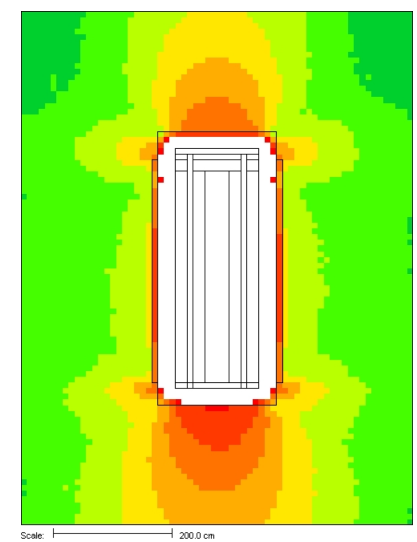
Developer: CEA Cadarache

ORNL's Monaco – Multigroup Monte Carlo



- Neutron/Photon
- Same geometry package as KENO-VI
- Flexible, friendly user input
  - Source description is separable:
    space, energy, direction
  - Region tallies, mesh tallies, point detector tallies
  - Integrates fluxes with response functions (dose)
- Variance Reduction capabilities
  - Weight windows based on region/energy
  - Mesh-based weight windows
- MeshView plotting software
  - Plot calculated responses on mesh grid

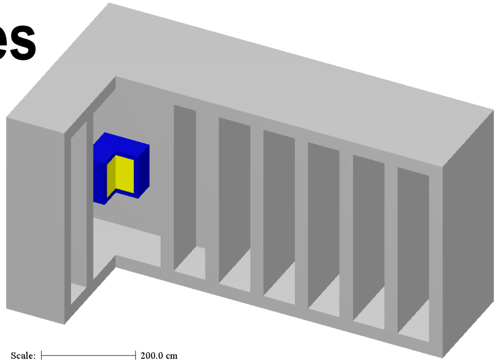


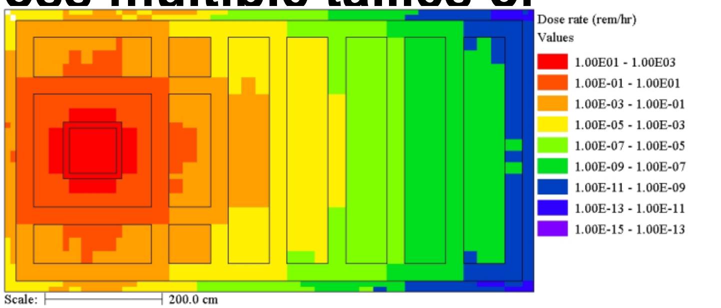


Developer: Douglas Peplow

MAVRIC – Auto Variance Reduction

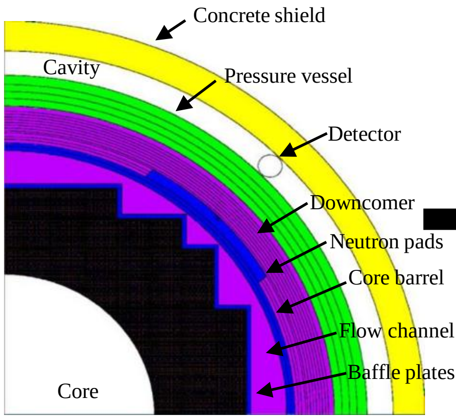
- Intended for challenging, deep-penetration problems
- CADIS (Consistent Adjoint Driven Importance Sampling)
  – Denovo is used to calculate the coarse-mesh adjoint flux for a specific tally
  – Creates importance map (space, energy) and biased source
  – Monaco is then optimized for that specific tally
- Forward Weighted CADIS
  – Denovo estimates forward fluxes, used in the adjoint source
  – Helps balance relative uncertainties across multiple tallies or large mesh tallies



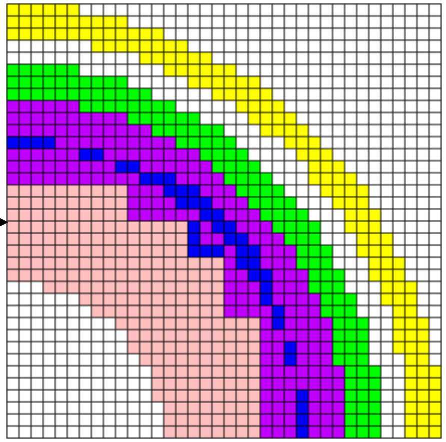


CADIS Methodology for Automated Variance Reduction

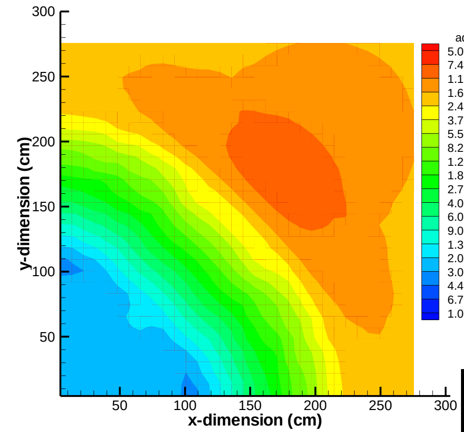
Example: PWR Ex-Vessel Thermal (^{10}B) Detector Response



Monte Carlo model

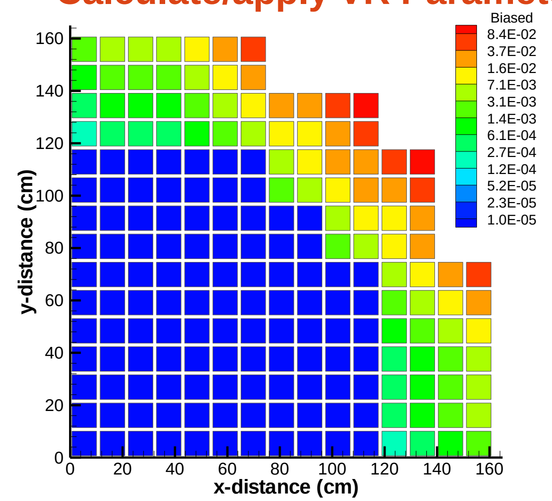


Deterministic model



Adjoint data

Calculate/apply VR Parameters

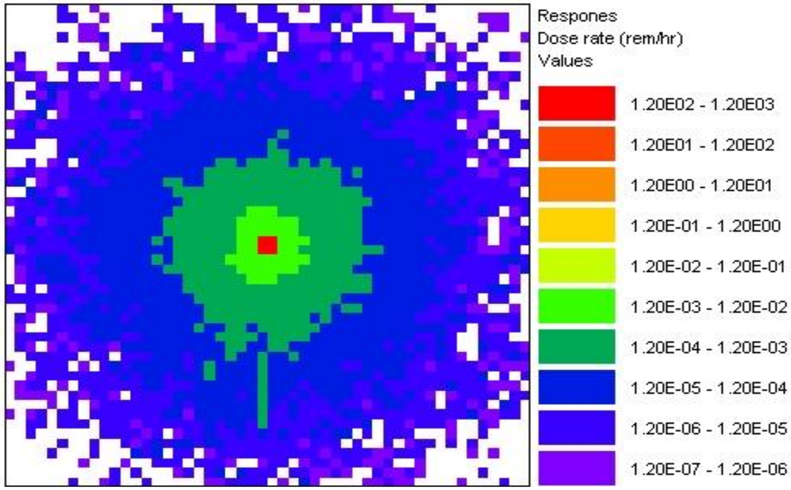


Faster Results

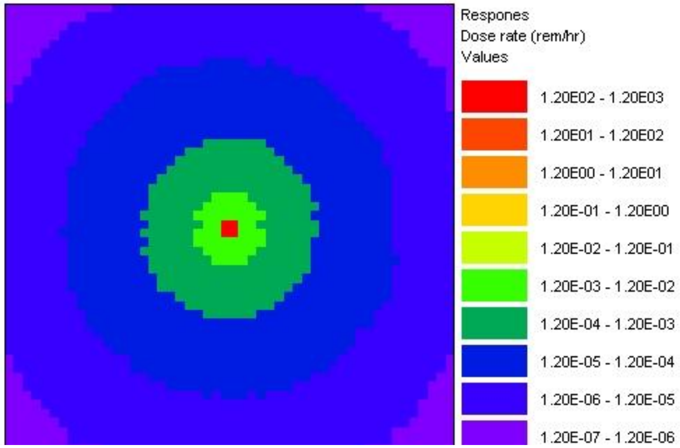
CASE	CPU TIME TO ACHIEVE RE=1% (h)	SPEEDUP
No VR	8.86E+4 (10.1 yrs)	1
Manual VR	13.6	6500*
CADIS VR	**1.02**	**87000**

* Required ~3 weeks by an experienced MC practitioner using all applicable MCNP4C VR capabilities

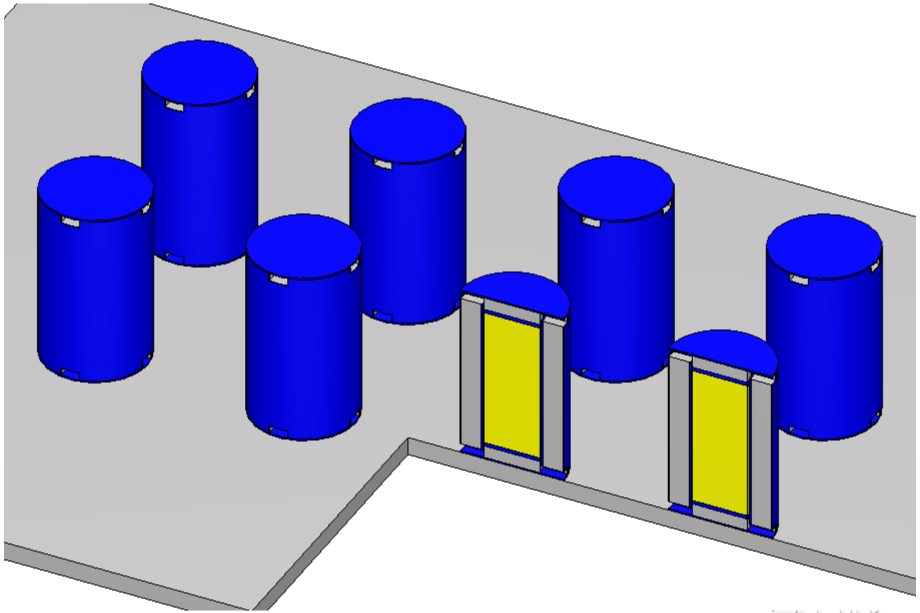
MAVRIC: Dose Rates from Cask Array



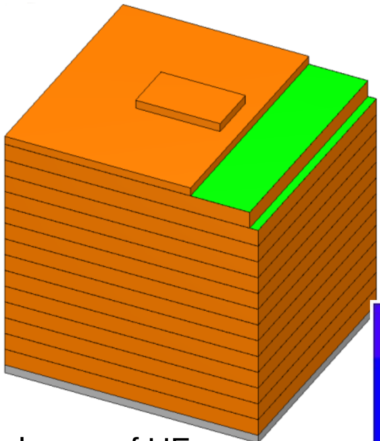
Analog calculation:
560 hours, poor resolution in mesh tally



Automated variance reduction: 109 hours,
80% voxels < 5% rel unc
97% voxels < 10% rel unc



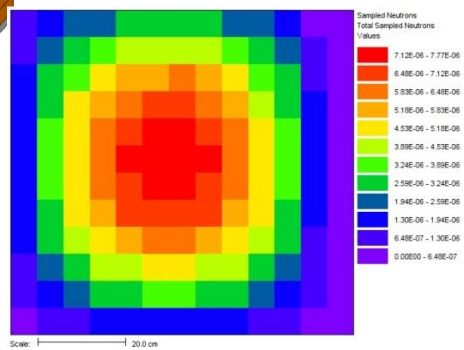
SCALE CAAS Capability

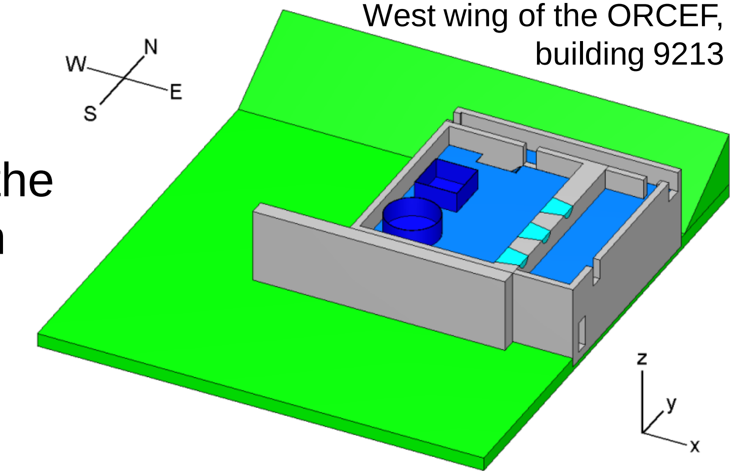


layers of UF_4

Step 1:

- Use KENO-VI to model the criticality accident and save the fission distribution as a mesh source

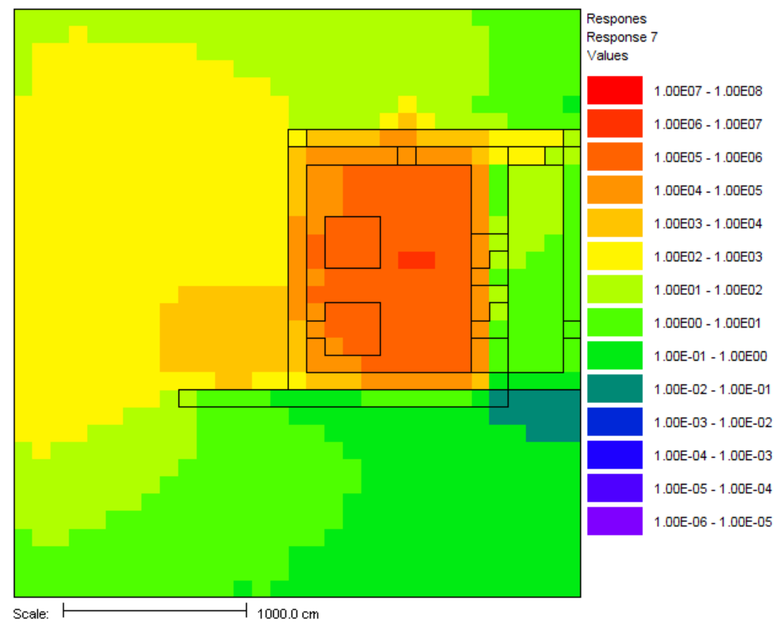




West wing of the ORCEF, building 9213

Step 2:

- Use MAVRIC to model particle transport
- Use KENO-VI fission distribution as the source for MAVRIC
- Calculate detector responses, dose rates at specific points or mesh tallies of dose rates



Dose in rem per 10^{19} fissions

Speedups of 3000 to 4500

ORNL's DENOVO

State of the Art Transport Methods

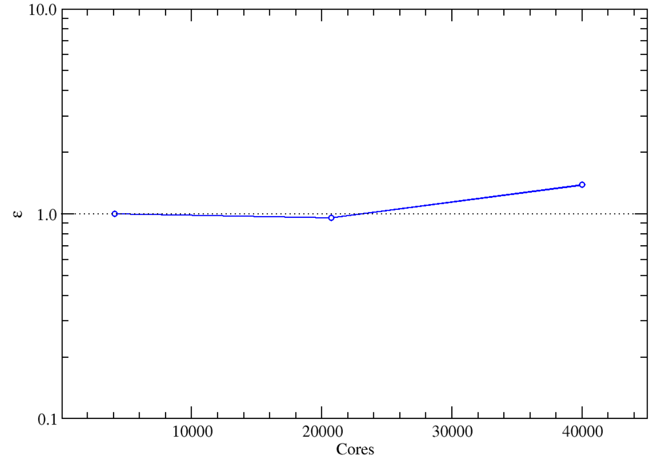
massively parallel deterministic radiation transport code

- **3-D regular grid, Discrete Ordinates (S_N)**
- **Multigroup energy, anisotropic P_N scattering**
- **6 spatial discretization algorithms (linear & tri-linear discontinuous FE, Step-characteristics, theta-weighted diamond, diamond difference + fixup)**

Developer: Tom Evans

Denovo

- **Advanced Methods**
  - GMRES (with DSA preconditioning) within-group solver
  - Transport, Two-Grid accelerated Gauss-Seidel for multi-group
  - Koch-Baker-Alcouffe (KBA) parallel domain-decomposition
  - Trilinos parallel solver package for highly efficient Krylov solvers and as an interface to the SuperLU direct solver library
  - Parallel first-collision source
  - 5 different spatial differencing schemes
  - Multiple input front-ends including Python
  - High-performance parallel I/O using HDF5

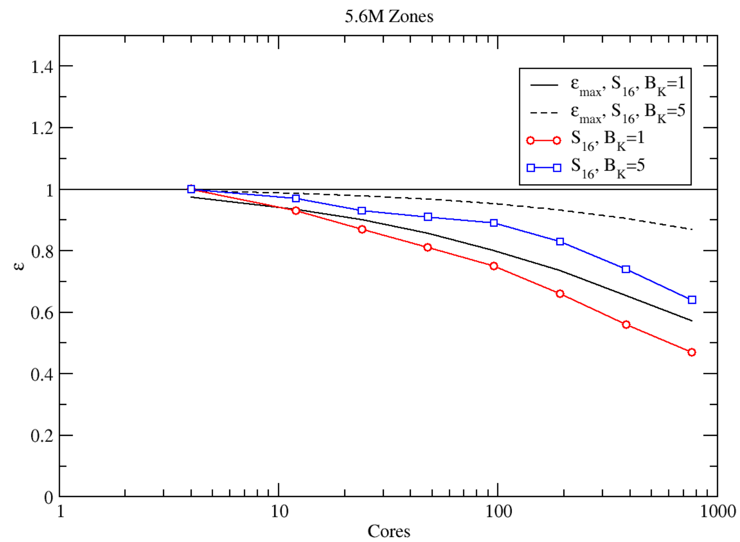


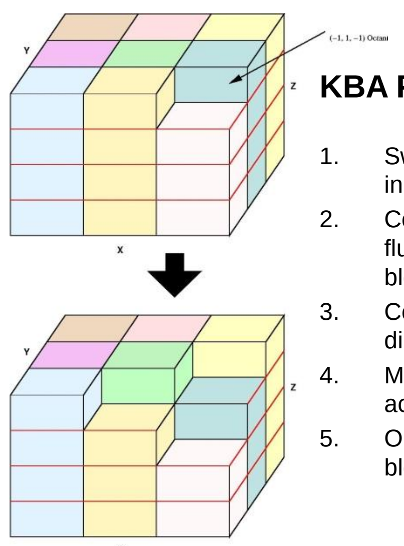
Weak Scaling

Denovo is designed to run high resolution problems scaled to thousands of cores.

Strong Scaling

Denovo's parallel algorithms are very efficient on cluster-level platforms as well.





KBA Parallel Sweep

1. Sweep each block starting in corner of octant.
2. Communicate outgoing fluxes to neighboring (x,y) blocks.
3. Continue sweep in z-direction.
4. MPI communication across blocks.
5. OpenMP on angles within block.

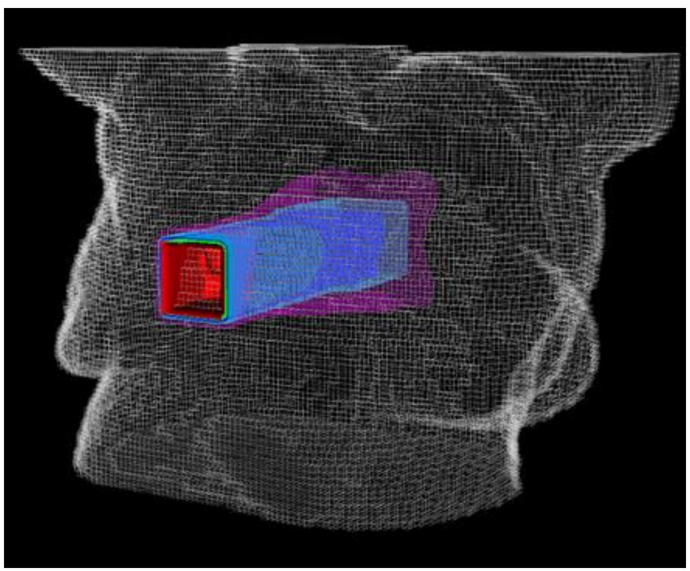
Denovo can run on PCs, workstation clusters, supercomputers

Jaguar – 1.64 PF Cray XT: 45,376 Quad-Core Processors, 362 TB memory

Cancer Therapy Planning with Denovo

Denovo generates a model directly from CT scans:

- 576,600 voxels
- lung/chest scan from UNC medical center

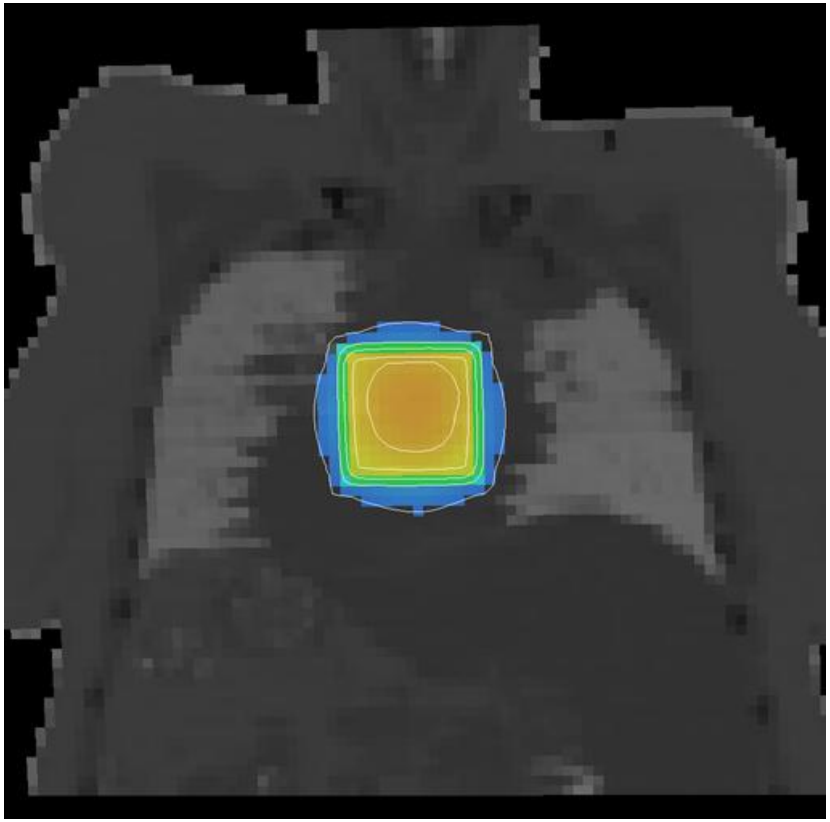


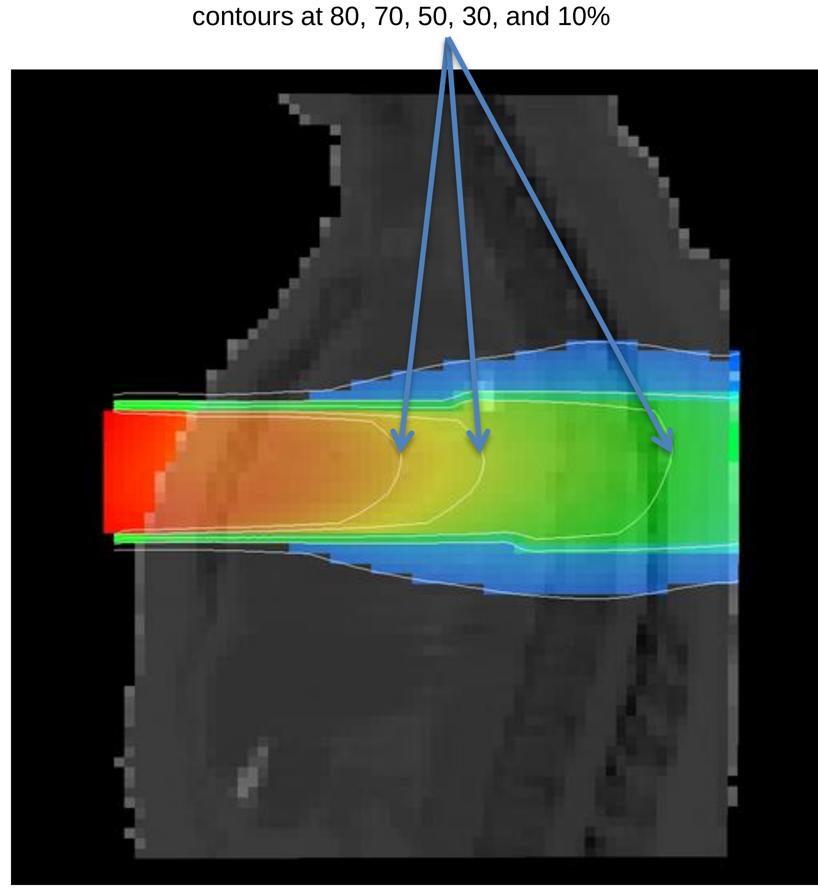
Using this model, Denovo can perform fast and accurate radiation transport calculations:

- S_8 angular quadrature
- P_3 scattering
- 40 energy groups

➔ **Calculation took 438 seconds on a 16 CPU AMD 64 Linux cluster**

Therapy Plan





Denovo outputs data that can be read directly by VisIt

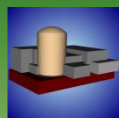
- inline, real-time visualization
- dynamic visualization for modulated therapy planning
- 2D/3D contours, color plots, etc.

Oak Ridge National Laboratory

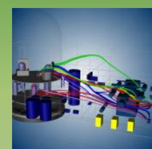
Denovo Capabilities for Treatment Planning

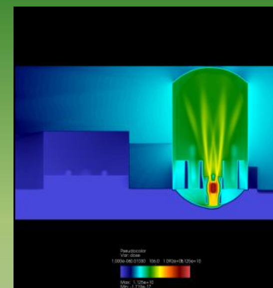
- Coupled photon-electron transport
  - Galerkin quadrature + CEPXS cross sections implemented
  - in testing and verification phase
- Boltzmann-Fokker-Planck planned for this year
- Photo-neutron library scheduled for testing ?
  - estimate neutron full-body doses to personnel and patients
- Coupled proton-neutron-photon physics planned after BFP implementation
  - used for proton therapy planning
  - occupational neutron dose calculations

Denovo – massively parallel deterministic radiation transport code enabling solutions to enormous nuclear energy applications

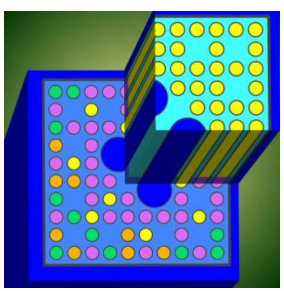


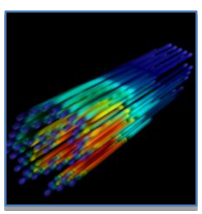
PWR Facility Modeling



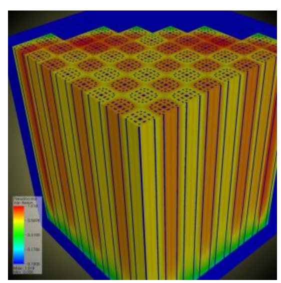


Zones	Angles	Groups	State Size (GB)	Output (GB)	Time (m)
103.7M	S_{24}/P_3	27	568.741	83.457	46.97
1,047.8M	S_{24}/P_3	27	5,746.180	843.189	79.43

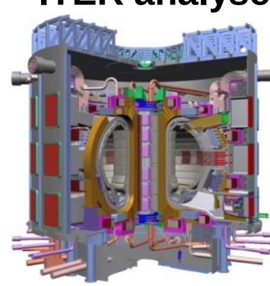


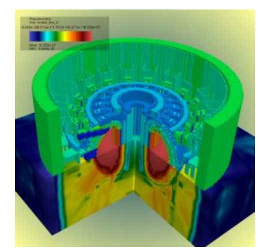


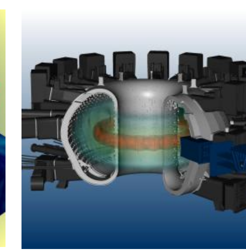
Nuclear Energy: LWR analyses



Fusion: ITER analyses

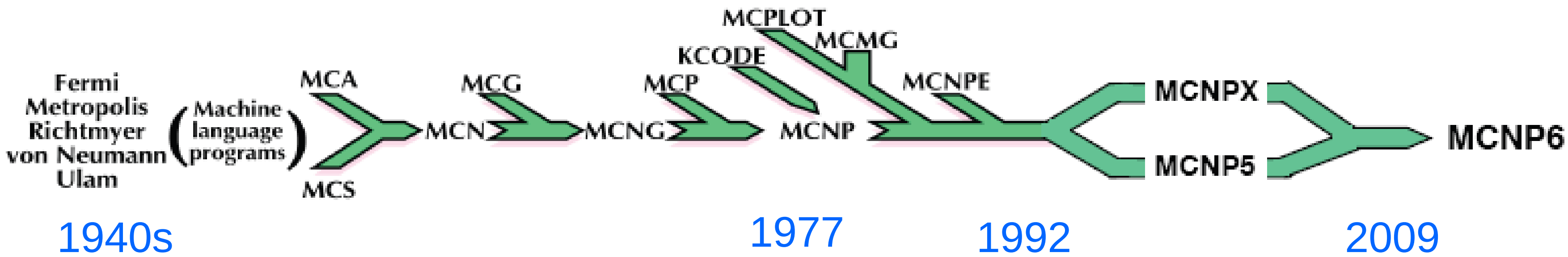






285M cell, S_{24}/P_3 model of the International Thermonuclear Experimental Reactor (ITER)

MCNP History



- **50+ years of code development!**
  - **World recognized experts in several fields**
- **Impressive physics, geometry, tally, variance reduction capabilities**
- **Modern Teraflop supercomputers can drive Monte Carlo calculations not dreamed possible more than a decade ago**
- **Now used for design of many systems (criticality example)**

1960s:	K-effective
1970s:	K-effective, detailed assembly power
1980s:	K-effective, detailed 2D whole-core
1990s:	K-effective, detailed 3D whole-core
2000s:	K-effective, detailed 3D whole-core, depletion, reactor design parameters

MCNP / MCNPX Teams Span X,D,N & T Divisions

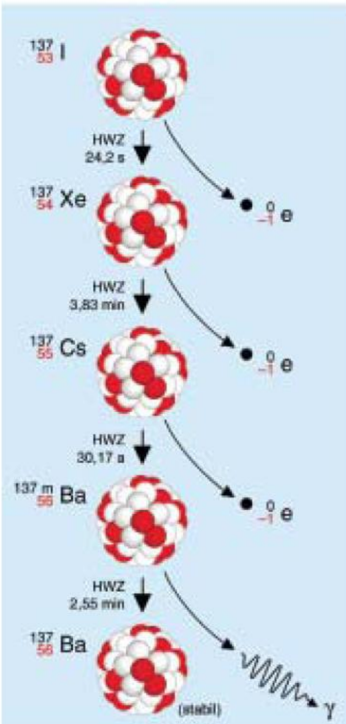
- MCNP
- Deputy Group Leader: Jeremy Sweezy
- Project Lead: Tim Goorley
- Tom Booth
- Forrest Brown
- Jeff Bull
- Art Forster
- John Hendricks
- Grady Hughes
- Roger Martz
- Stepan Mashnik
- Avneet Sood
- Tony Zukaitis

- MCNPX
- Team Lead: Gregg McKinney
- Project Lead: Laurie Waters
- Joe Durkee
- Jay Elson
- Michael Fensin (N-4)
- John Hendricks (X-3)
- Shannon Holloway (T-2 CINDER)
- Michael James
- Russell Johns
- William Johnson
- Toshihiko Kawano (T-2 CGM)
- Denise Pelowitz

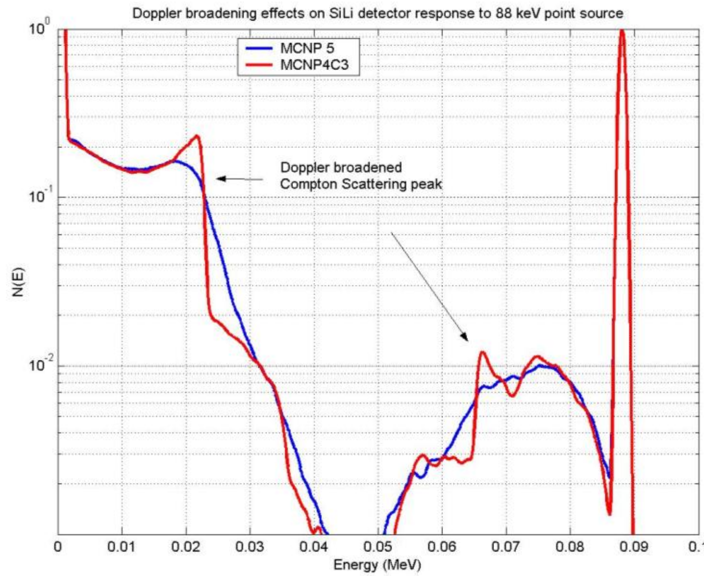
New Features of Summer 2009 Release

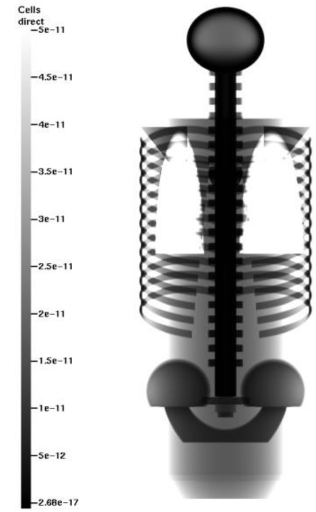
- **MCNP5 version 1.60**
  - Weilandt acceleration for criticality
  - Dominance ratio
- **MCNPX 2.7.0**
  - Delayed gamma spectral lines
  - LLNL photofission & neutron fission multiplicities
  - Muonic x-ray enhancements
  - Delayed neutron spectra
  - Pulsed Sources
  - Beam source options
  - Natural Background Sources
  - Activation Options

Recent Capabilities

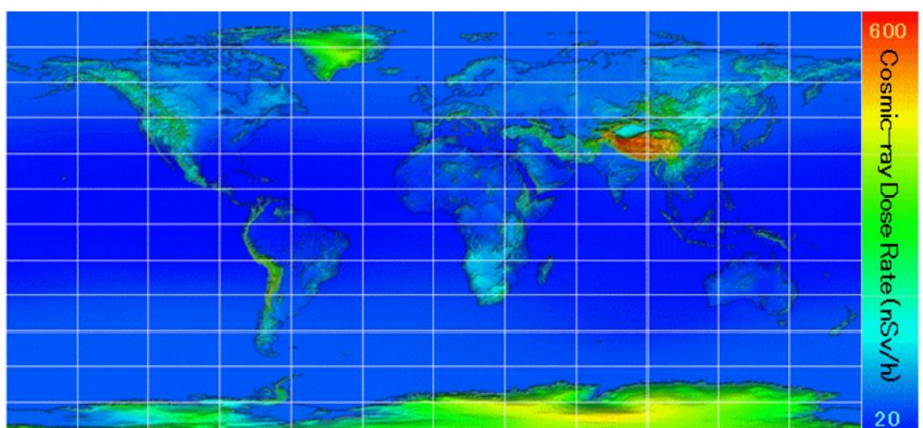


Decay Chains & their emissions





Simulated Radiographs



Background Neutron and Photon Radiation from lat, long, and elevation

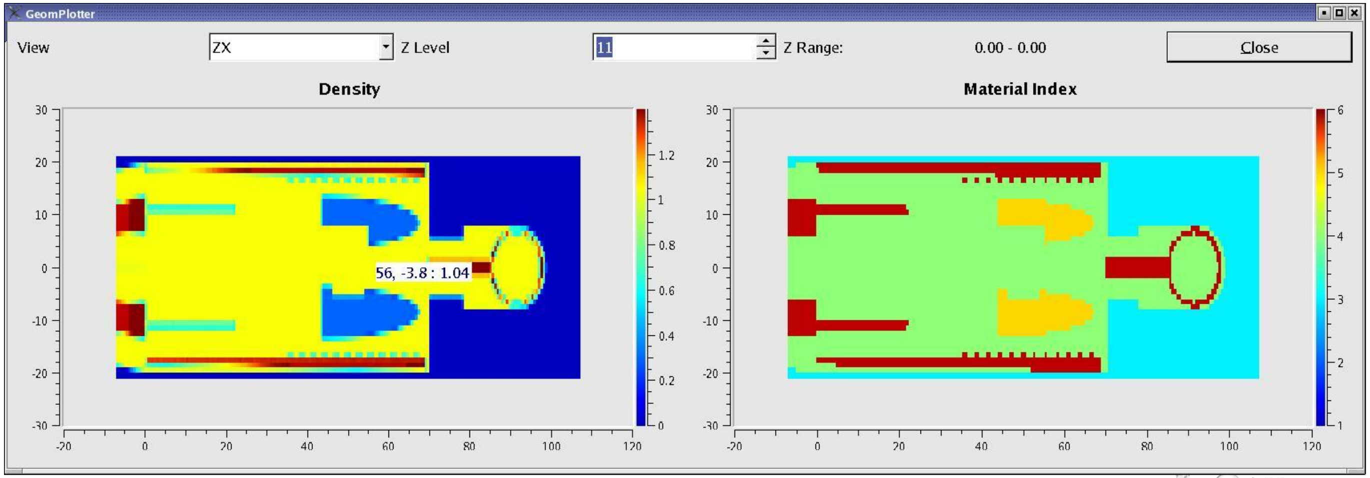
Top Ten List for Future Development

1. Monte Carlo Applications ToolKit
2. Unstructured Meshes
3. Lower Energy Thresholds
4. Reaction Specific Effects
5. Temperature Effects
6. Damage Effects
7. Better physics
8. Improved variance reduction
9. Criticality Efforts
10. Maintenance & Support

Monte Carlo Applications Tool Kit (aka MCATK)

- From scratch Monte Carlo radiation transport code in C++, using Agile-like processes, unit testing, pair programming, modular design
- Driven by desire to utilize GPUs & new hardware (which doesn't always have a FORTAN 90 compiler), as well as maintain MC expertise in new staff
- Intended to replace portions of MCNP
- Leverages Commercial + Open Source Software
  - Eclipse Development Environment
  - Unit Test++
  - QT
  - Doxygen
  - Boost

GUI tool to view geometry



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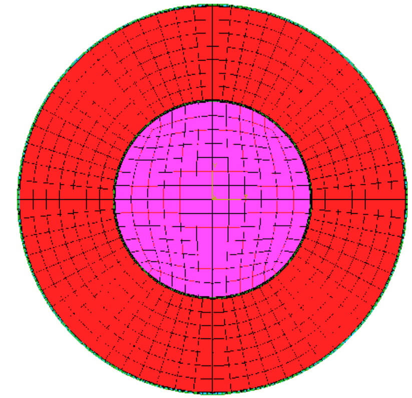
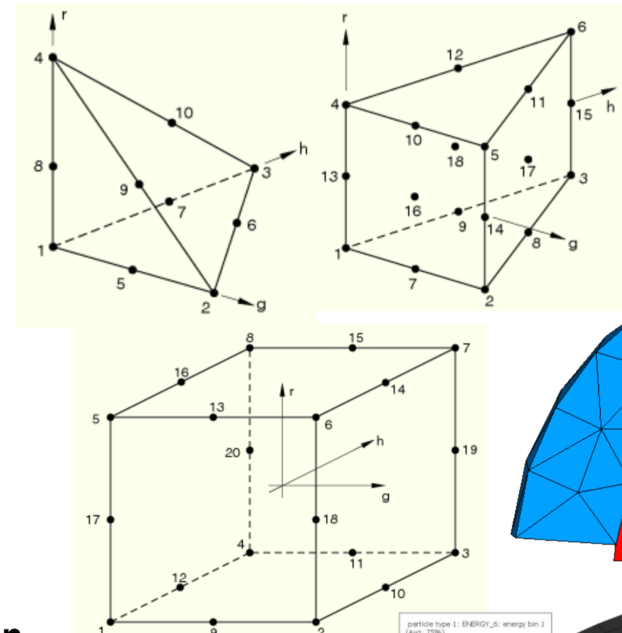
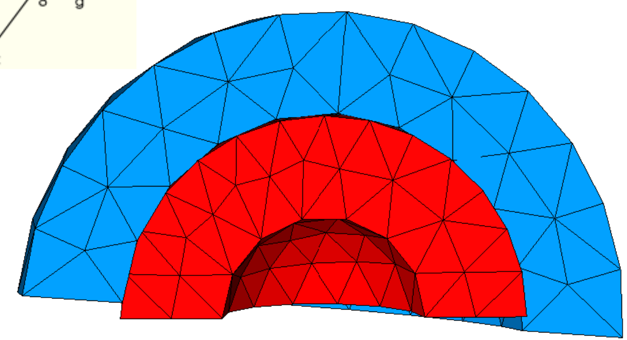
OAK RIDGE National Laboratory

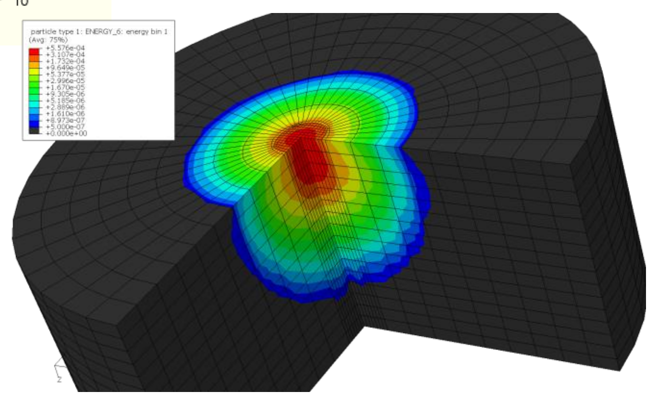
MCNP Unstructured Mesh



- track and tally on unstructured mesh
- mesh objects are mix of 4, 5 & 6 sided solids
- Boundaries of solids can be bi-linear.
- Mesh can be added into regular 3-D MCNP geometry
- Already in MCNP6, works in parallel
- Quadratic surfaces under development
- Want to expand to CAE codes other than ABAQUS
- Is currently used for thermo-mechanical analysis







Energy Deposition

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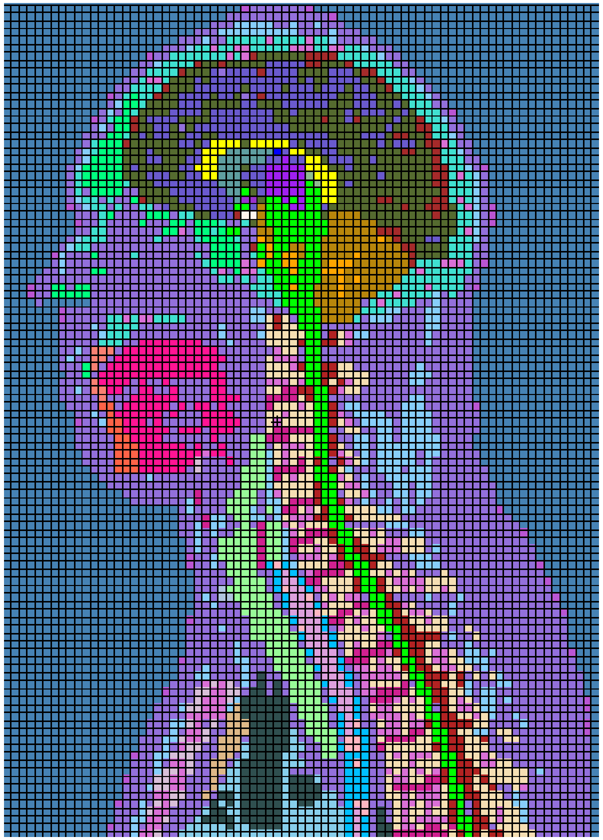
Low Energy Threshold

- **Current lower energy limit of photons and electrons is 1 keV**
- **Not sufficient for smaller geometries desired by medical community**
- **Also necessitates improved L-M-N shell fluorescence**



Millimeter or sub-millimeter patient –based geometry is frequent in user community

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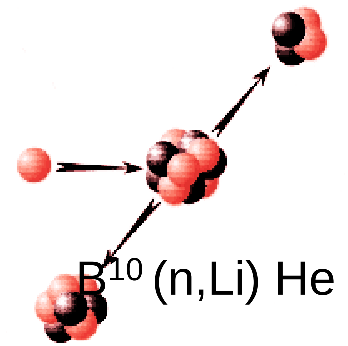
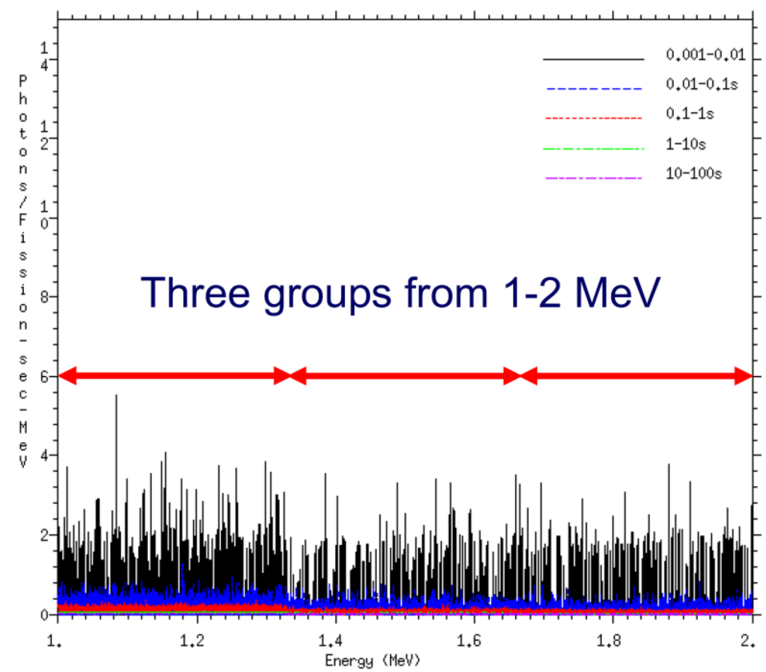
Reaction Specific Effects

- **Historically, average quantities (such as ν with fission and average E of daughter particles), have been used**



- **Today's detection applications (coincidence) require details of individual reactions to be correct. $E_{FissionN}(\nu)$, $E_{Fission\gamma}(\nu)$**

Multi-group delayed gamma spectrum from neutron-induced fission of ^{235}U



- **Include radioactive decay product emissions**

- **New data and even models are necessary**

MCNP Temperature Ef

- **Currently adjusts elastic scattering cross section and reaction kinematics as a function of material temperature**
- **Can pre-process data libraries to create new cross sections for all reactions (cumbersome)**
- **Want built-in neutron doppler broadening**
- **Want to include time dependant temperature effects**
- **Can we match the Godiva-IV experiment?**

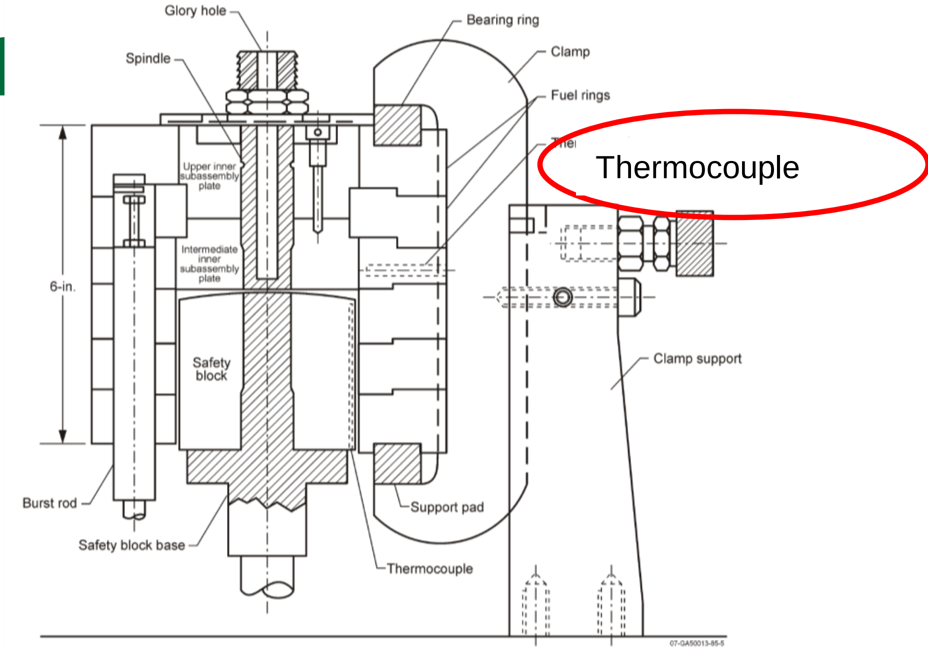
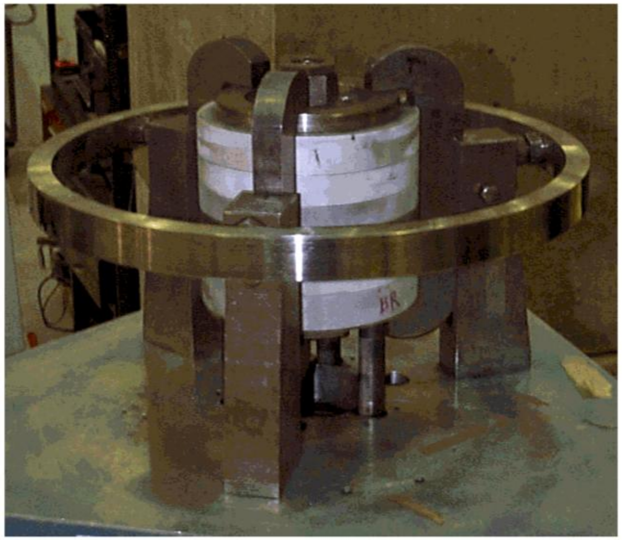


Figure 1. Cutaway View of the Godiva-IV Core and its Restraints.

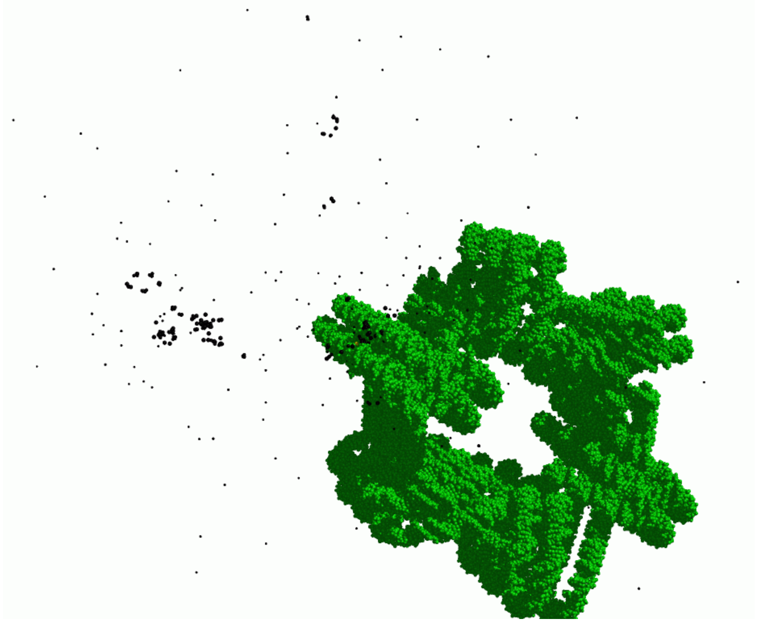


Side View of the Godiva-IV Assembly on Top of the Godiva Assembly Mounting Plate.

Damage / Material Interaction Effects

- **While MCNP can calculate energy deposition in a material very well, there is not a good way to assess what observable effects the energy produces**
- **Dose has widely accepted correlations**
- **Possible Interactions**
  - **Temperature rise**
  - **Ionization & Excitation**
  - **DNA strand breakage**
  - **Production of visible photons (scintillation)**
  - **Molecular changes**
  - **Atom dislocation**
  - **Phonons**
  - **Pressure vessel brittle fractures**

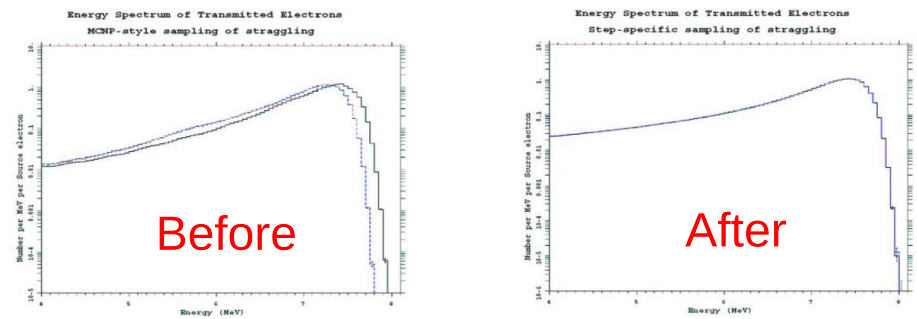
The amount of energy necessary to kill a person 1/2 the time (4 Gy), is equivalent to 280 joules = 67 calories. This would effectively raise a person's temperature by 0.002 deg C. (equal to a sip of warm coffee or lifting a man 16 inches off of the ground) – Eric Hall, Radiobiology for the Radiologist



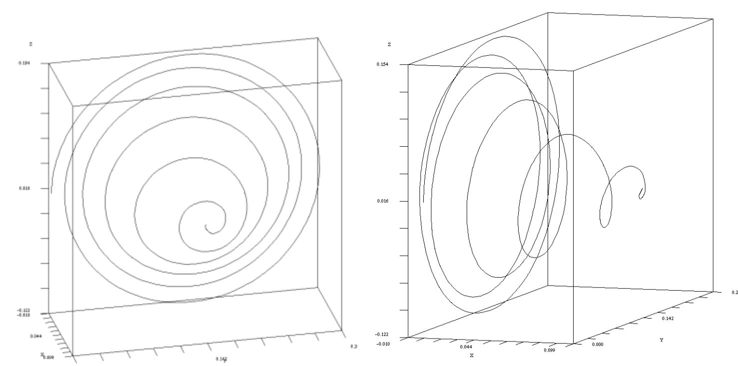
Production of free radicals in water surrounding a DNA chromosome (NOT MCNP)

Better Particle / Interaction Physics

- **MCNPX set of particles, always looking for more nuclear interaction physics**
- **Low-energy light-ion production of delta rays**
- **Improved electron transport**
- **Electrostatic Fields**
- **Fixed Source Transmutation**
- **Momentum & Ablation**

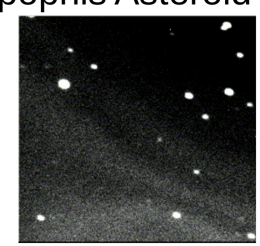


On-the-fly Landau Parameters for electron tracking



Proton track in magnetic field

Apophis Asteroid



Twenty years from today, on April 13th, 2029, http://neo.jpl.nasa.gov/apophis/ asteroid Apophis will buzz Earth only 18,300 miles above the planet's surface--well inside the belt of geosynchronous communications satellites. Represents a 1 in 800 year event for object of this size.

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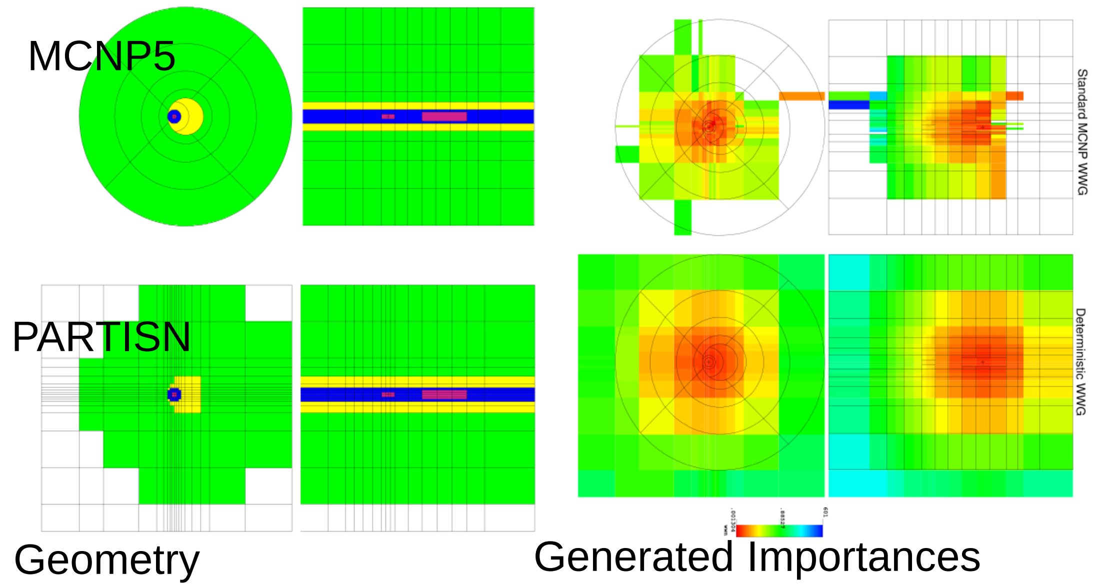
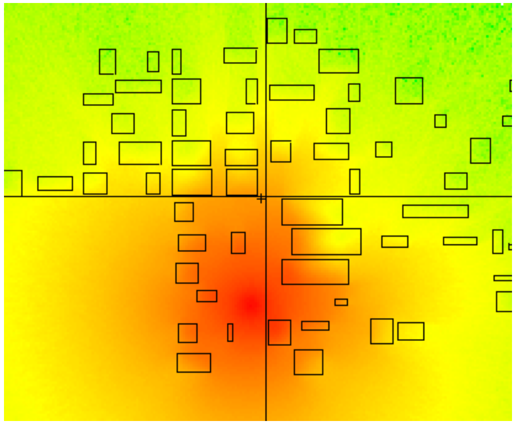
Improved Variance Reduction

- **Long time goal of linking together deterministic SN adjoint solutions to feed into foreward Monte Carlo calculations**
- **Variance Reduction needs reexamination. Many methods were developed to gain information in a few specific locations, not everywhere**
- **Continuous Energy Adjoint**
- **Not all pieces work together**





Dose from Hiroshima nuclear weapon detonation in Times Square, NY for FEMA.

The TITAN Code

*C. Yi and A. Haghighat, "SPECT Imaging Simulation Using the TITAN Transport Code," *Proc. M&C 2009*, Saratoga Springs, NY (2009).

- 3-D hybrid (S_N and Characteristic Method) deterministic transport code developed at the University of Florida (Yi and Haghighat, 2007)
- A new version of TITAN code* (2008) includes a simplified ray-tracing formulation in the collimator region
- Uses CEPXS multigroup photon cross sections
- Produces flux moment distribution
- Collimator blur simulated by integrating angular flux over the collimator solid angle

Developer: C. Yi, Ali Haghighat
University of Florida

Overview

- Monte Carlo codes are traditionally used to simulate SPECT
- TITAN, a hybrid deterministic code, was recently used for SPECT simulation
- For the same model:
  – Analyze results for SIMIND, a Monte Carlo code
  – Analyze results for TITAN and compare with SIMIND

SPECT Basics

- Single Photon Emission Computed Tomography (SPECT)
- Internalized radionuclide is the source
- Projection images acquired at various angles around the patient by a gamma camera
- Functional imaging

Image from Cornell University

Description of Model

- Simulate myocardial perfusion study with Tc-99m (140.5 keV gamma, $T_{1/2}$)
- 3 energy groups (lower bounds of 126.45, 98.35, and 10 keV)
- Torso phantoms generated by NCAT code

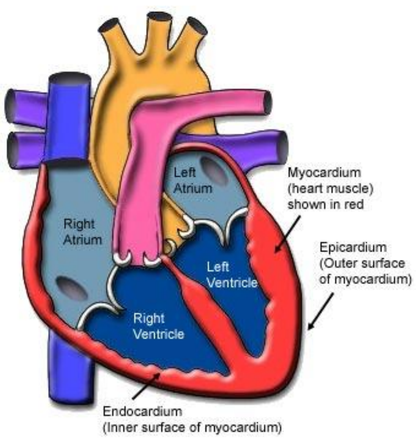
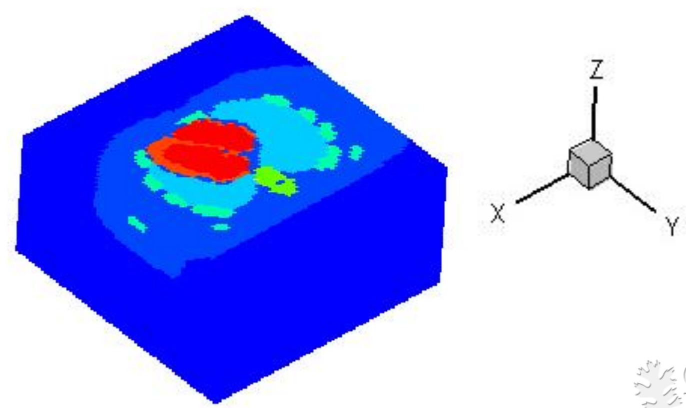


Image from www.perfusion.com

- NURBS-based cardiac-torso (non-uniform rational B-splines)
- 40x40x40 cm^3
- Thirteen materials
- Two voxel sizes:
  - 0.62x0.62x0.62 cm^3
  - 0.31x0.31x0.31 cm^3
- Two phantom volumes:
  - Attenuation distribution (densities)
  - Source distribution

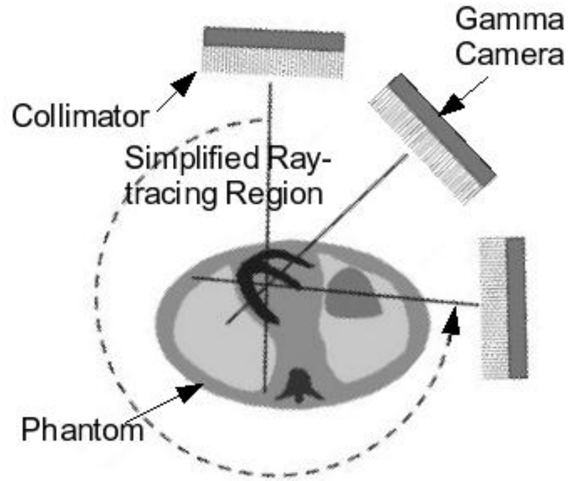


SIMIND Code

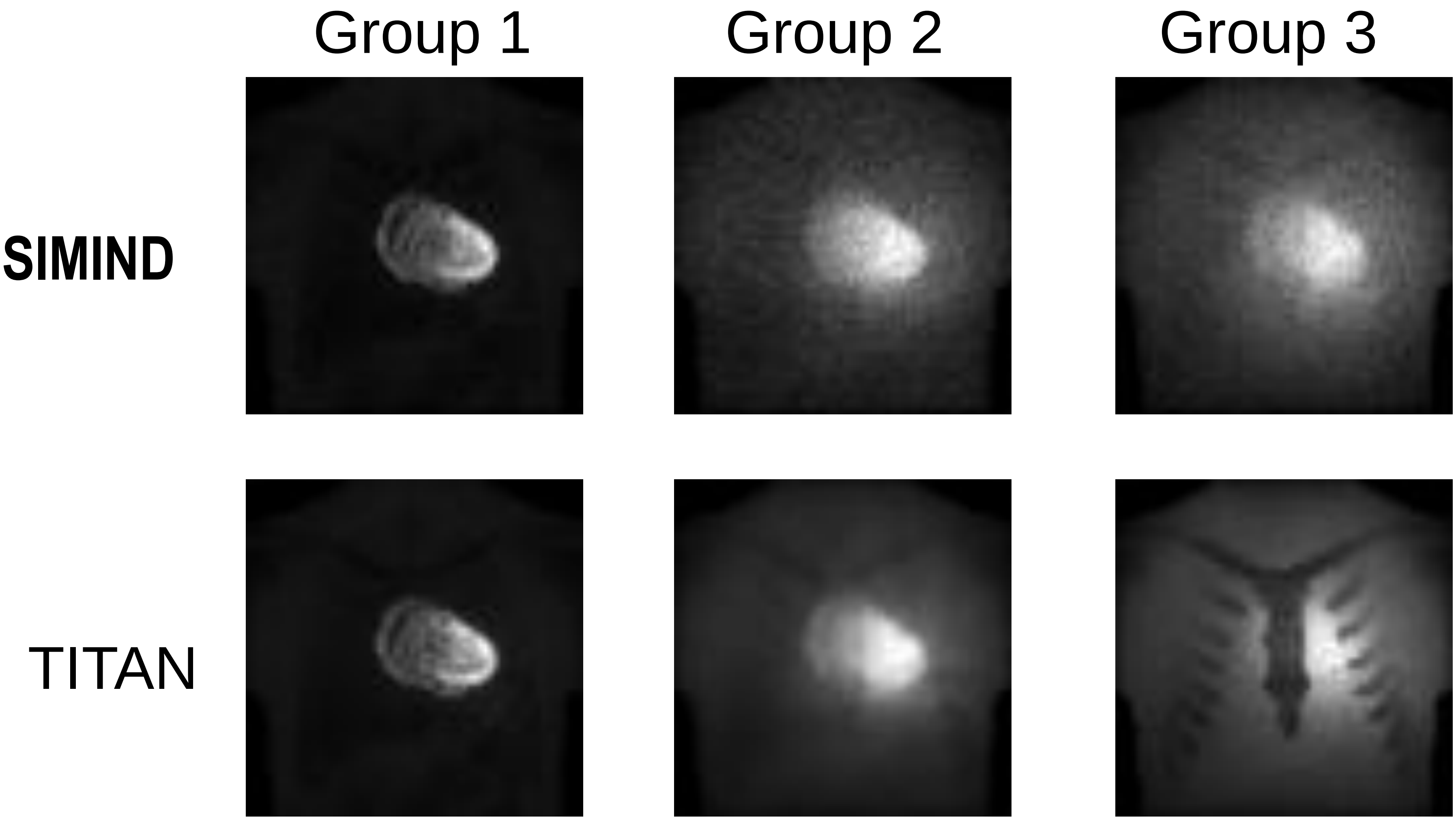
- Monte Carlo
- Specifically designed to simulate SPECT
- Requires a parameter file, material density phantom, and source phantom (no cross section file)
- Windowing to simulate energy groups
- Outputs projection images at each angle simulated
- No statistical information in output

TITAN Code

- Discrete ordinates method used in phantom
- Simplified ray-tracing method used between phantom and gamma camera
- Collimator and detector not modeled a



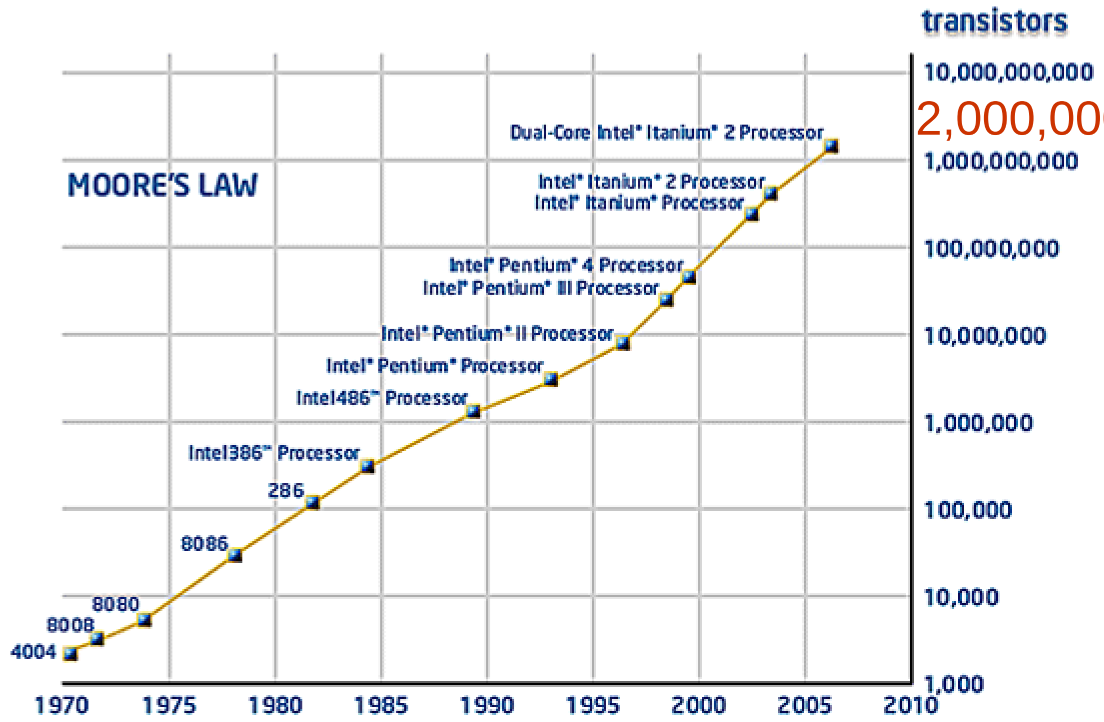
Results



Moore's Law

We are here!
Tukwila
processor

2,000,000,000



http://www.intel.com

ARE we headed for CLOUD COMPUTING?