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Title: Advances in the Development and Verification of MCNP5 and MCNP6

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Advances in the Development & Verification of MCNP5 & MCNP6

Forrest Brown, Brian Kiedrowski, Jeffrey Bull,
Tim Goorley, Grady Hughes, Mike James

Nuclear Criticality Safety Program

Abstract

Advances in the Development & Verification of MCNP5 & MCNP6

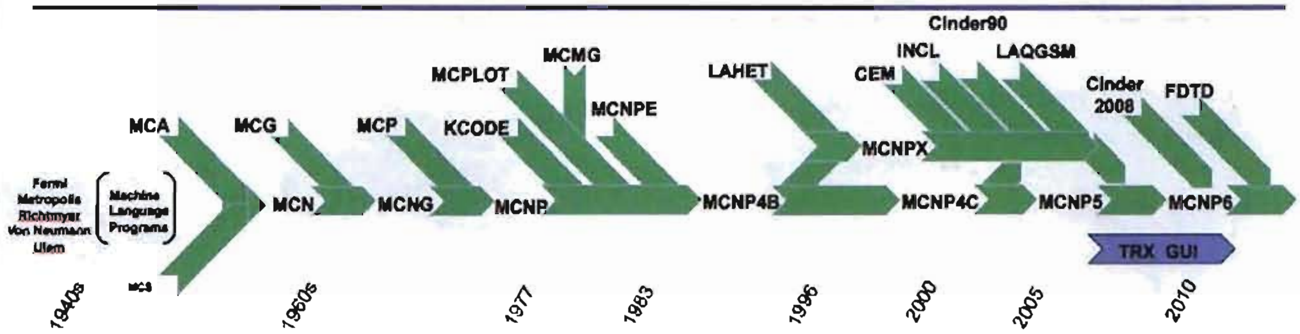
Forrest Brown, Brian Kiedrowski, Jeffrey Bull,
Tim Goorley, Grady Hughes, Mike James

The MCNP Monte Carlo code has been used for high-fidelity analyses of criticality safety problems since the 1970s. This talk reviews recent advances in the development and verification of MCNP, including the current production release of MCNP5 and the beta release of MCNP6. End-users in all application areas need to be aware of the forthcoming MCNP6 release and begin planning for the transition to the new code in 2012 and beyond.

- **MCNP**
  - History & Applications
- **MCNP5-1.60 Release**
  - Features & Bug-fixes
  - V&V Suites & Results
- **MCNP6-beta-1 Release**
  - Capabilities
  - Status
- **Future Plans**
  - MCNP5-1.60
  - MCNP6
  - References

MCNP
Monte Carlo Code

MCNP History



- **Monte Carlo transport of particles**
  - **MCNP5 - neutrons, photons, electrons**
  - **MCNPX - MCNP4 + high-energy physics**
  - **MCNP6 - merged code + more, 2011 - beta, 2012 - full release**

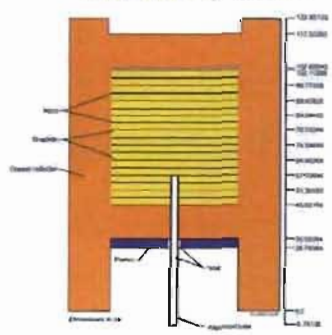
- 3D general geometry
- PC, Mac, Linux, Unix, Sun support
- Parallel (MPI + threads)
- 350K+ lines of code
- Extensive verification / validation

- 400+ person-years development
- 10,000+ users world wide
- 15,000+ reference citations
- Distributed by RSICC code center
- Export controlled

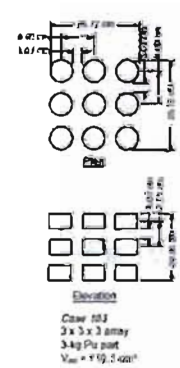
MCNP & Nuclear Criticality Safety (1)

HEU-MET-THERM-003

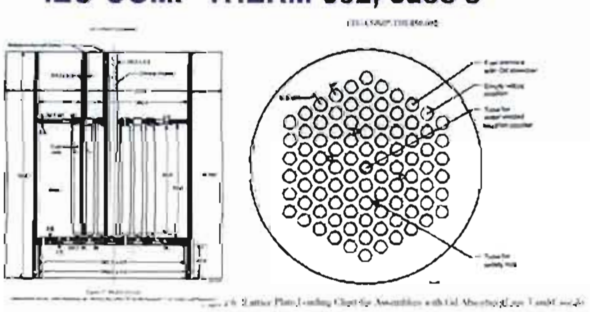
Zeus-2, HEU-MET-INTER-006, case 2



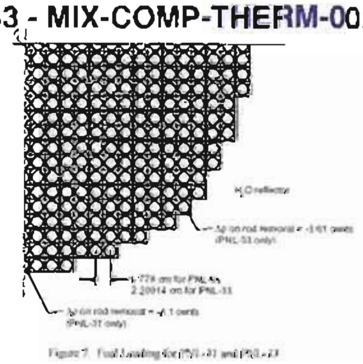
PU-MET-FAST-003, case 3



IEU-COMP-THERM-002, case 3



PNL-33 - MIX-COMP-THERM-002



MCNP & Nuclear Criticality Safety (2)

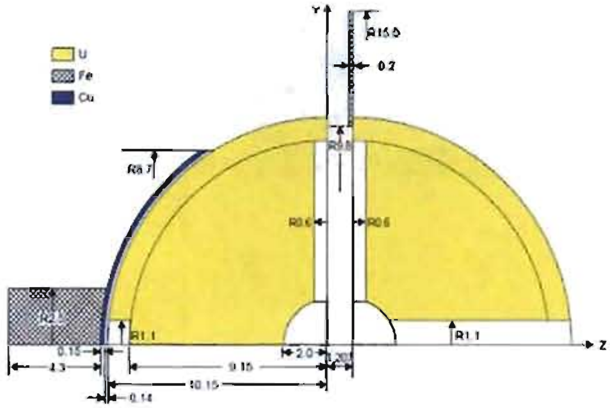


Figure 1. Unreflected HEU Sphere, heu-met-fast-008

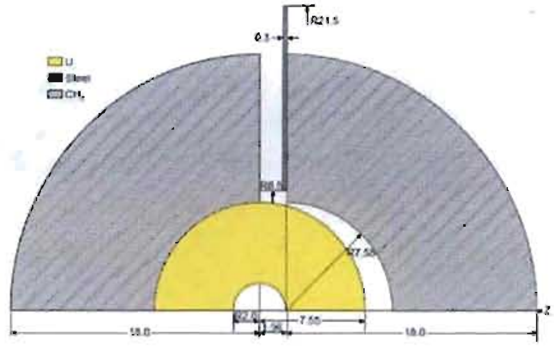


Figure 4. HEU Sphere Reflected by Polyethylene, heu-met-fast-011

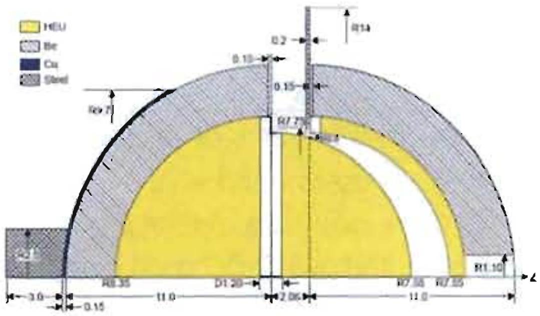
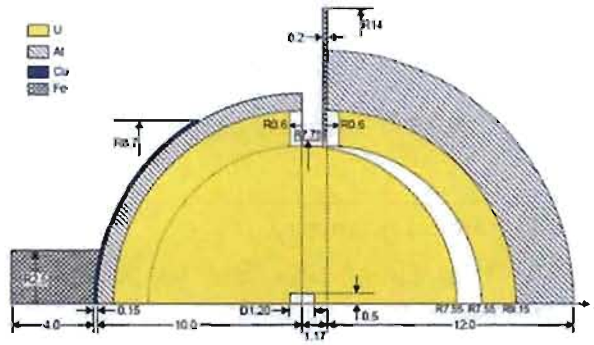
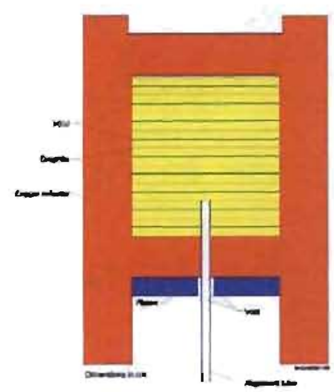


Figure 3. Incomplete HEU Sphere Reflected by Beryllium, heu-met-fast-009, case 1

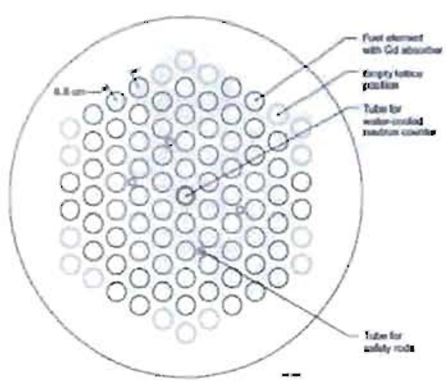


e 5. Incomplete HEU Sphere Reflected by Aluminum, heu-met-fast-012

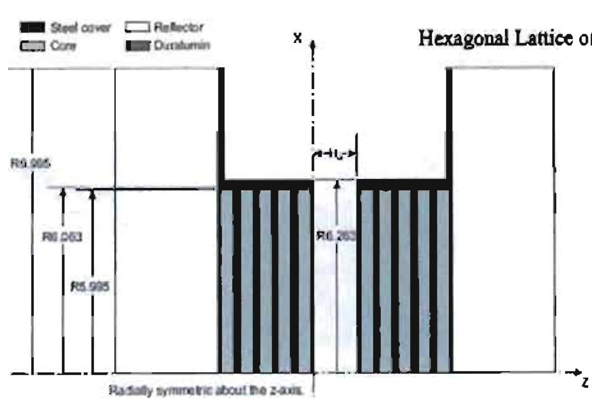
MCNP & Nuclear Criticality Safety (3)



Vertical Slice through the Center of the Zeus-2 Benchmark, heu-met-inter-006-case-2



Hexagonal Lattice of IEU Fuel rods, ieu-comp-therm-002-case-3



6. Stacked Plutonium Cylinder Reflected by Beryllium or Beryllium Oxide, pu-met-fast-021, case 1 or pu-met-fast-021, case 2

Nuclear Regulatory Commission Use of MCNP

Criticality Safety:
- To assess the criticality safety of licensed facilities that handle fissionable materials.

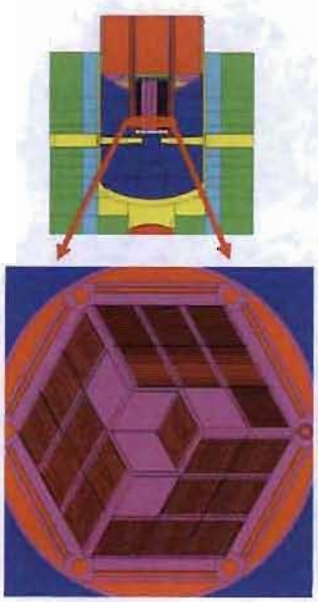
Radiation Shielding:
- To benchmark other shielding and dose calculation computer codes and methods used by NRC staff.
- To verify licensees' shielding and dosimetry calculations.

Radiation Dosimetry:
- Assess planned and unplanned worker radiation exposures.
- Assess public exposure from planned licensing actions.

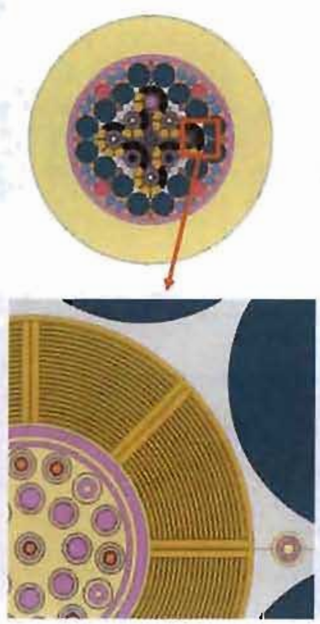
Medical:
- To understand the radiation safety implications of using radiation in medical diagnosis and treatments.

MCNP = Benchmark for Nuclear Reactor Design Codes

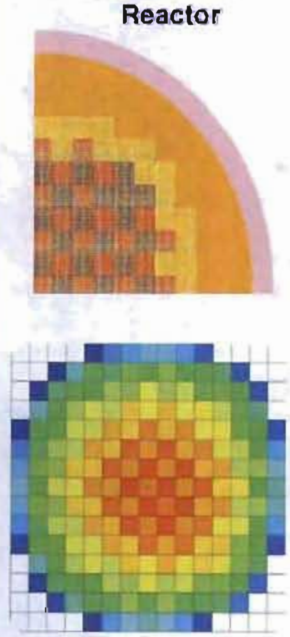
MIT
Research Reactor



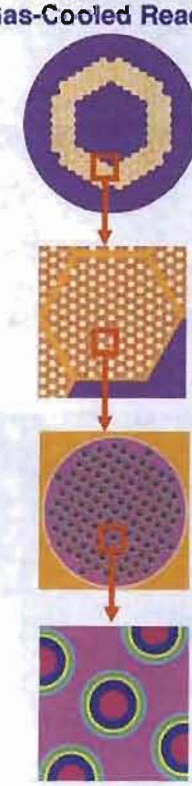
ATR
Advanced Test Reactor



PWR
Pressurized Water Reactor



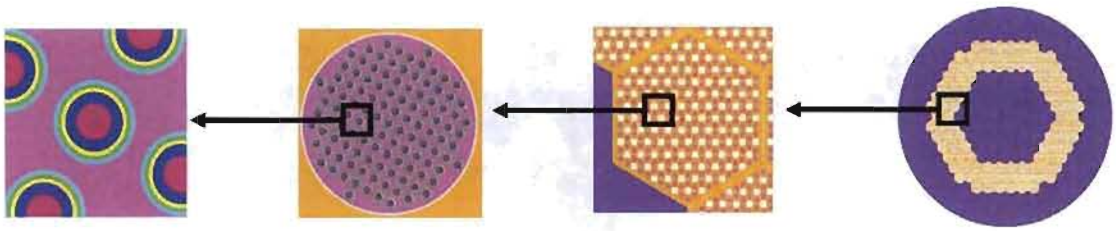
VHTR
Very High Temperatur Gas-Cooled Reactor



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

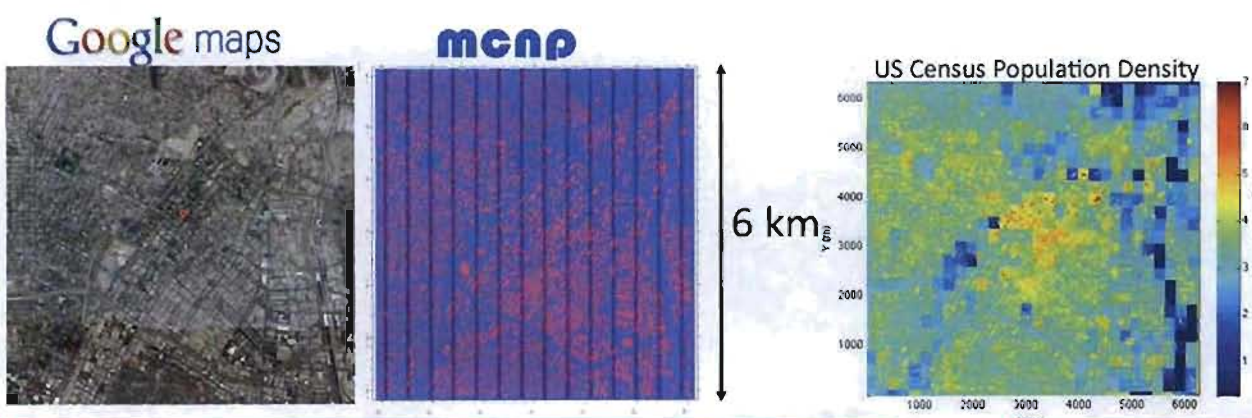
Advanced Reactor Design - VHTR, HTGR, ...

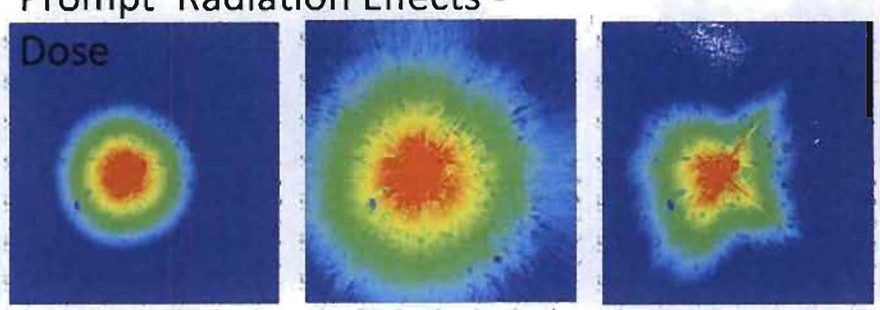
TRISO FUEL PARTICLES | FUEL COMPACTS | FUEL BLOCK | CORE



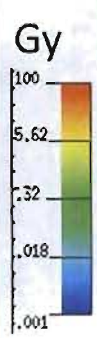
MCNP model - accurate & explicit at multiple levels

Analysis of IND Dose Effects





Neutron Dose (from neutron leakage) | Gamma Dose (from neutron capture) | Gamma Dose (from gamma leakage)

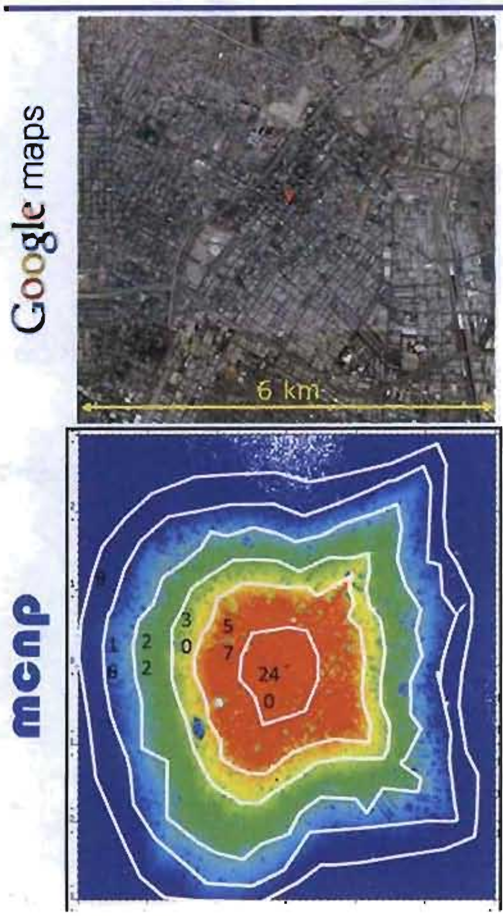


Gamma Dose

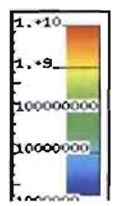
Dose contours from a 20 kT Little Boy device in downtown LA

Analysis of IND Circuit Effects

mcnp Monte Carlo Codes XCP-3, LANL



- Surface burst of Fat Man ~ 10 kT
- White contours: electric field strength in kV/m
- Circuit failure expected above 10 kV/m
- Color scale: photon flux
- Note 4 orders of magnitude decrease in underlying photon flux

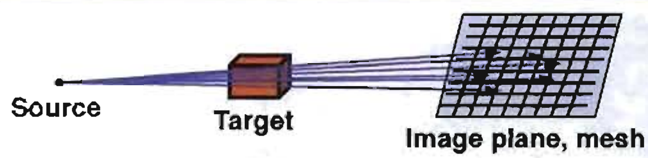


The results presented here are based on source region simulation levels from MCNP. This is part of the LANL EMP start-up project's goal of incorporating first physics principle source region calculations.

Radiography Calculations

mcnp Monte Carlo Codes XCP-3, LANL

- **Radiography tallies**



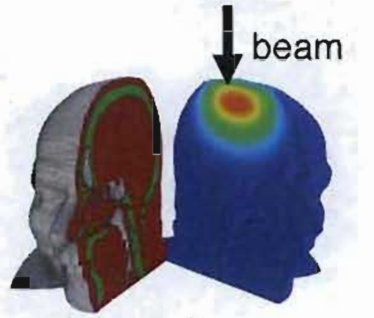
- **Neutron and photon radiography uses a grid of point detectors (pixels)**
- **Each source and collision event contributes to all pixels**

MCNP Model of Human Torso

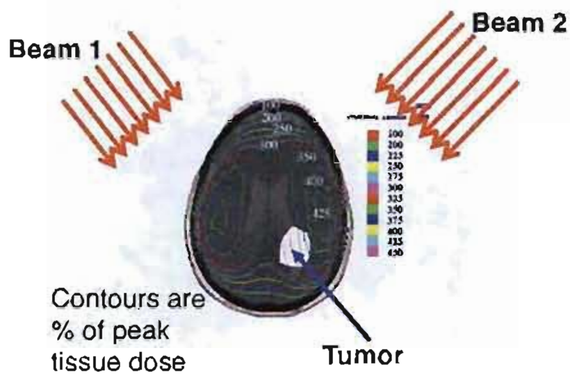
Simulated Radiograph - 1 M pixels

Medical Physics Treatment Planning

- MCNP is used to calculate dose distributions throughout a target region from different radiation beam orientations.
- Post processing programs are then used to (perhaps) combine different beams to maximize dose to tumor while minimizing dose to surrounding healthy tissue. These programs usually overlay the dose contours over patient specific CT images.
- While the peak tumor and tissue dose are usually based on in-phantom dose rate measurements, the simulation is necessary to determine more advanced parameters, such as the dose volume histogram.

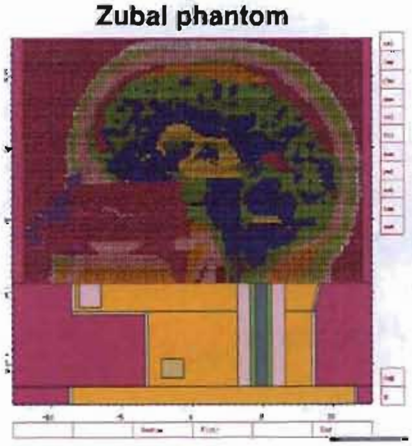


CT Based geometries are possible to represent in MCNP



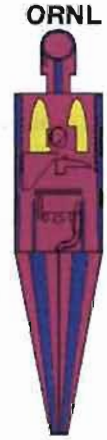
Medical Physics – Phantoms & Voxel Models

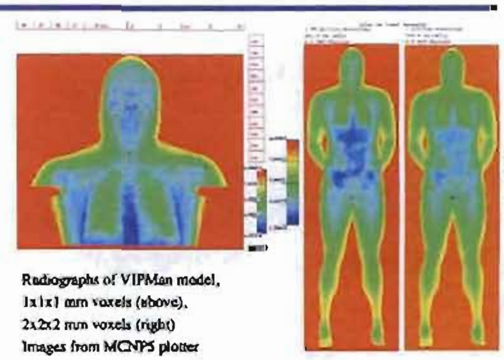
Zubal phantom



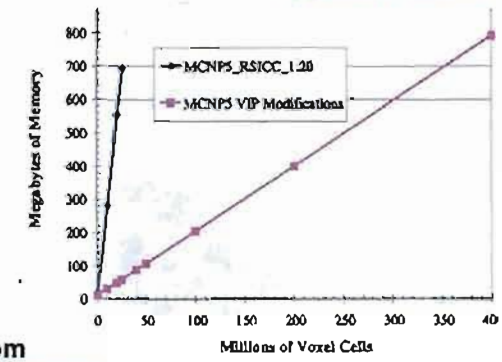
Yanch, MIT

ORNL

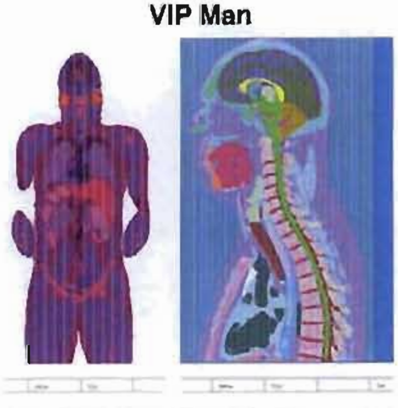




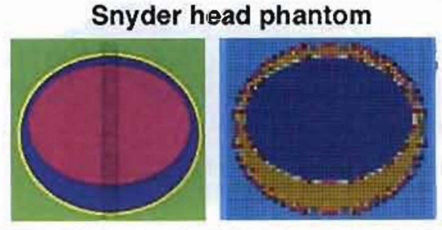
Radiographs of VIPMan model, 1x1x1 mm voxels (above), 2x2x2 mm voxels (right) Images from MCNP5 plotter



VIP Man



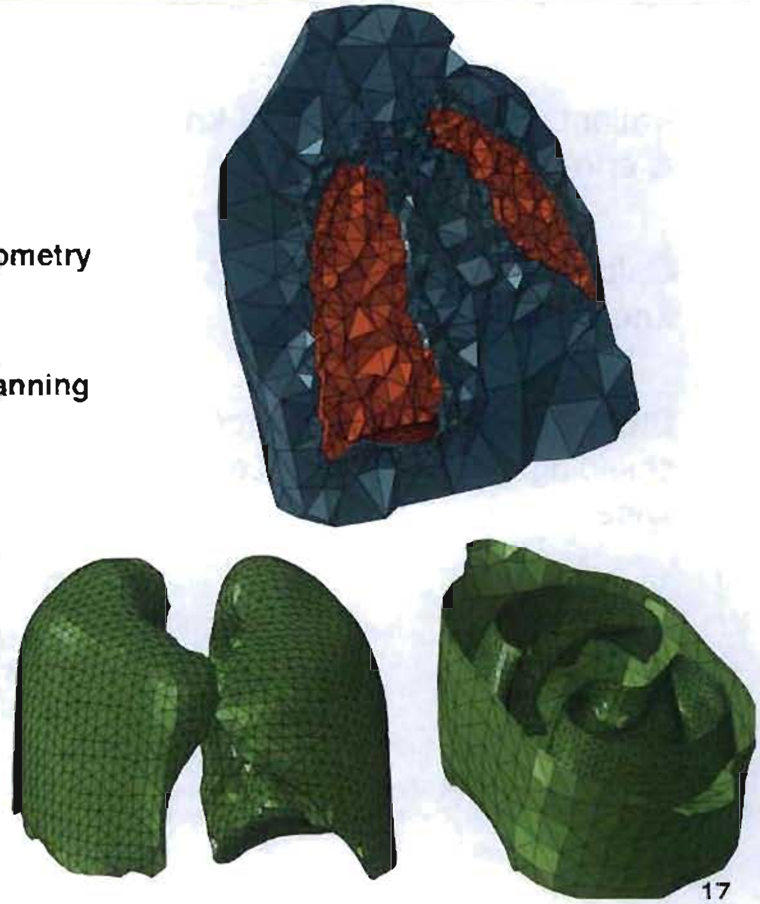
Snyder head phantom



Medical Physics - Treatment Planning

mcnp Monte Carlo Codes XCP-3, LANL

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



Radiation Cancer Therapy Research

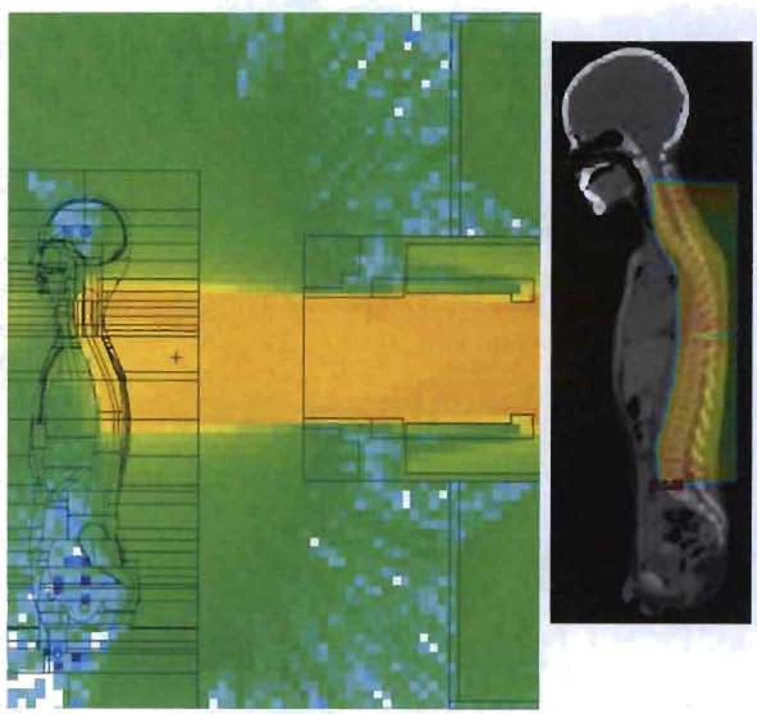
mcnp Monte Carlo Codes XCP-3, LANL

"The code is ideally suited for use in medical applications because of the accuracy of its physics models, the unique set of clinically relevant features, and the responsive support provided by the developers and the user community."

"We used MCNPX to verify the Mass General Hospital Proton Center, and this information has gone into the design of the MDACC proton center and others, which are used to treat > 5K people a year."

Wayne Newhauser, Ph. D.
Dept of Radiation Physics

THE UNIVERSITY OF TEXAS
MD ANDERSON
CANCER CENTER

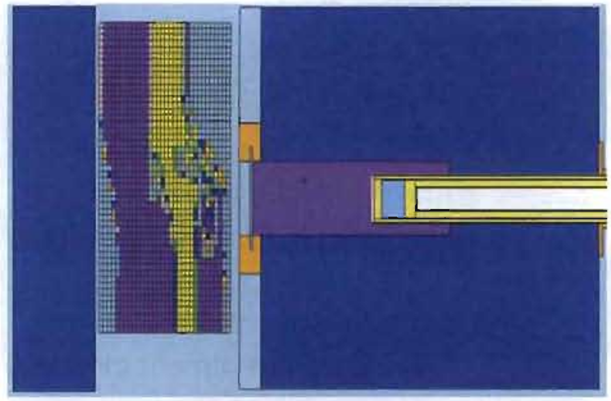


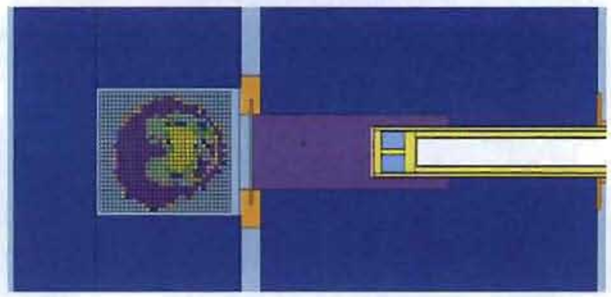
proton fluence and dose contours (arb units)

Medical Physics - Dose Calculations

mcnp Monte Carlo Codes XCP-3, LANL

- Patient-CT based model of **knee & end of accelerator**
- **Calculate dose throughout knee**
- Study impact of moderating/ shielding materials & B^{10} conc. in knee





Pictures from mcnp plotter

J. R. Albritton, "Analysis of the SERA treatment planning system and its use in boron neutron capture synovectomy," M. S. thesis, Massachusetts Institute of Technology, 2001.

Gierga DP, Yanch JC, Shefer RE, "An investigation of the feasibility of gadolinium for neutron capture synovectomy", Med Phys. 2000 Jul;27(7):1685-92.

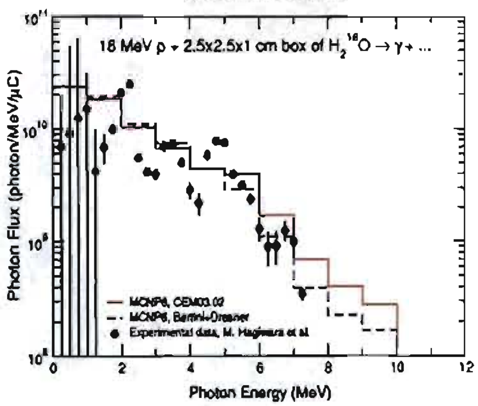
Proton & Carbon Therapy Applications

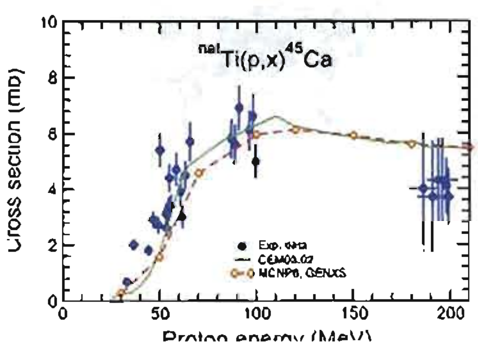
mcnp Monte Carlo Codes XCP-3, LANL

Proc. ND2010 April 26-30, 2010, Jeju Island, Korea, in press:

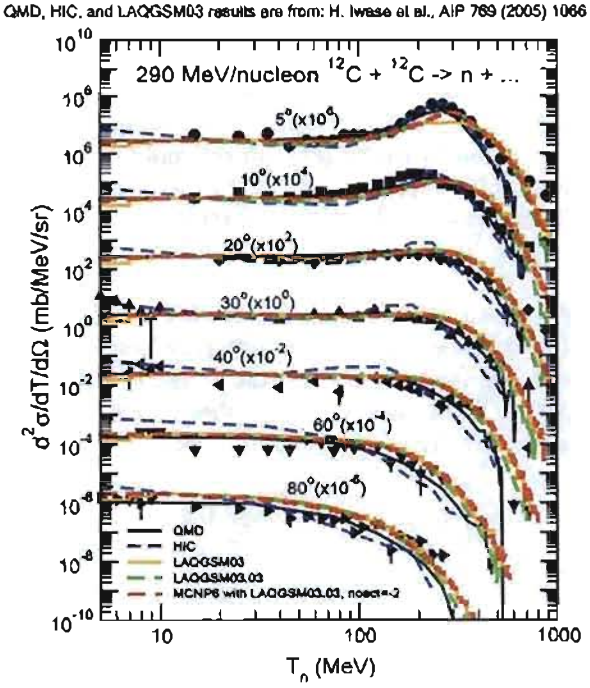
Spectrum Measurement of Neutrons and Gamma-rays from Thick $H_2{}^{18}O$ Target Bombarded with 18 MeV Protons

M. Hagiwara, T. Sanami, Y. Iwamoto, N. Matsuda, Y. Sakamoto, Y. Nakane, H. Nakashima, K. Masumoto, Y. Uwamino and H. Kaneko





Experimental data are from: Y. Iwata et al., Phys. Rev. C64 (2001) 054609; QMD, HIC, and LAQGSM03 results are from: H. Iwase et al., AIP 769 (2005) 1066



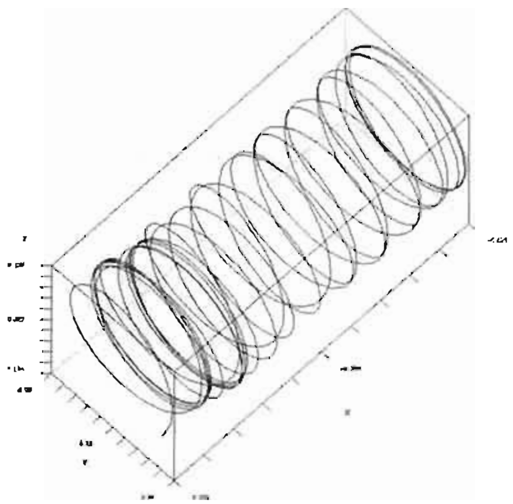
Radiochim. Acta 98, 447–457 (2010)

Excitation functions of nuclear reactions leading to the soft-radiation emitting radionuclides ^{45}Ca, ^{49}V and ^{204}Tl in beam collimator materials used in proton therapy

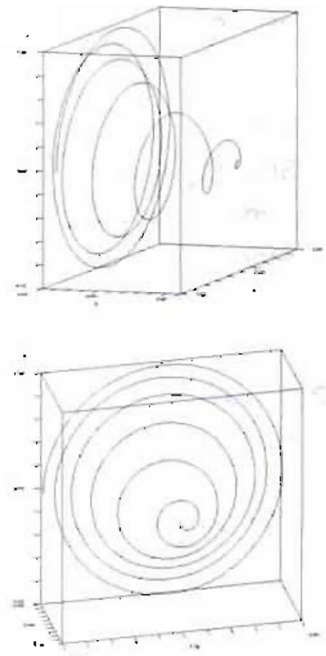
By S. M. Qaim, K. Kettern, Yu. N. Shubin, S. Sudar and H. H. Coenen

Proton in Air & Constant B Field

No Energy Straggling



With Energy Straggling



MCNP5-1.60
Release

MCNP5-1.60 Release

- **Chronology**
  - Development: Fall 2009 – Spring 2010
  - Extensive testing & V&V: Summer 2010
  - Sent to RSICC: September 2010
  - RSICC release: October 2010, July 2011

- **Focus**
  - **Stability + reliability for criticality calculations**
  - **Support for latest computers – multicore, Windows/Mac/Linux, 32/64 bit**
  - **Rigorous, extensive code V&V**
  - **A few new features, many minor bug-fixes**

- **Notable**
  - **Most rigorous & extensive MCNP testing ever**
  - **Over 5,000 hr computer time for V&V, mostly on criticality problems**
  - **First production release of adjoint-weighted tallies (kinetics parameters)**

New Features in MCNP5-1.60 (1)

- **Adjoint-weighted Tallies for Point Kinetics Parameters**
  - **First correct calculation of β_{eff}, Λ_{eff}, Rossi-alpha using continuous-energy Monte Carlo and adjoint weighting**
  - First production application of iterated fission probability to compute adjoint-weighted tallies
  - Thorough V&V against analytic, Sn, experiment

- **Mesh Tallies for Isotopic Reaction Rates**
  - Previously, could only do flux, dose, material reaction rates
  - **Important extension to specific isotopes**
  - Possible use in activation analysis or burnup

- **Increased Limits for Geometry, Tally, and Source Specifications**
  - **Allow up to 100M for cell, surface, material specs**. Previous 100K limit
  - Complex cell spec up to 9999 items, previous 999 limit
  - Needed to support complicated problems, CAD conversion, ...

New Features in MCNP5-1.60 (2)

- **Web-based documentation**
  - 280 MB of reference material – theory, coding, V&V, user manual
  - Installation instructions & scripts

- **Utility programs**
  - Improved **`merge_mctal`** for merging results from multiple runs
  - Improved **`merge_meshtal`** for merging results from multiple runs

- **Additional V&V suites – later in this presentation**

- **General**
  - Support for threading on multicore computers
  - Parallel processing efficiency for threaded criticality calculations
  - Arbitrary number of threads for restart (continue) runs
  - 12 other minor enhancements to code
  - 30 minor bug-fixes (none affect results for criticality calculations)

New Features in MCNP5-1.60 (3)

MCNP criticality problems with OpenMP threading:

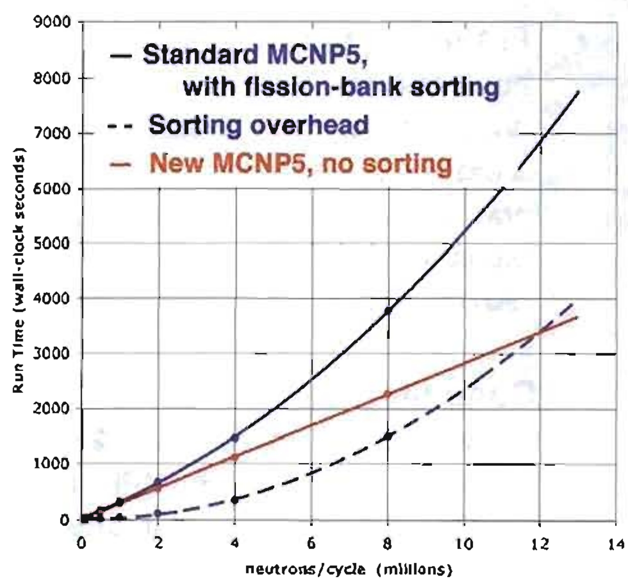
- Fission-bank needs to be reordered into a unique ordering that is independent of the number of threads or MPI processes.

- **Previous:**
  - Reorder by crude, inefficient sorting
  - Poor scaling for large neutrons/cycle

  T ~ *O*(N^2) N = neuts/cycle

- **MCNP5-1.60:**
  - New routine for unique reordering WITHOUT SORTING
  - Based on: FB Brown & TM Sutton, "Reproducibility and Monte Carlo Eigenvalue Calculations", Trans Am Nuc Soc 65, 235 (1992)

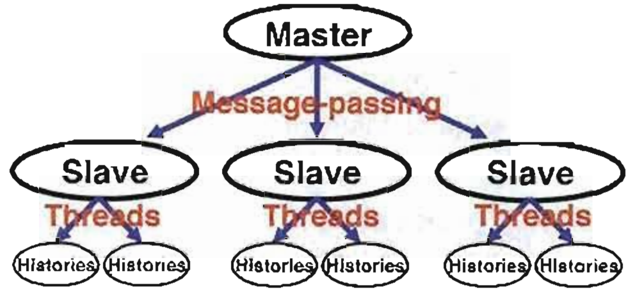
  T ~ *O*(N) N = neuts/cycle

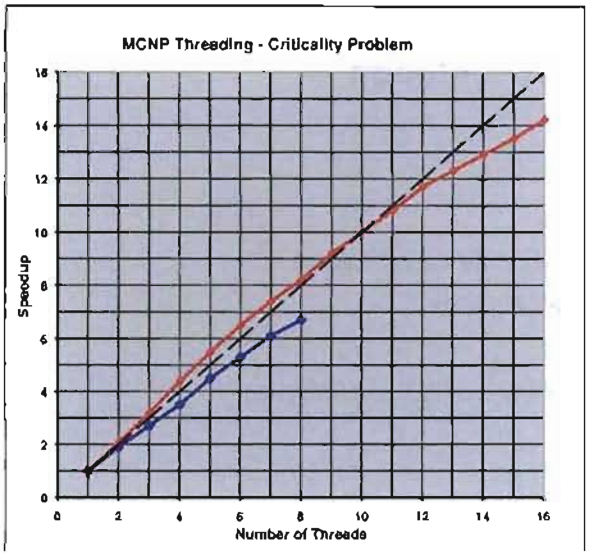


- 1/4-core, detailed PWR, 2D, ENDF/B-VII
- Run with 8 threads
- Times are wall-clock seconds for 5 cycles
- Identical results for old & new reordering

MCNP5 - Threading with OpenMP

- **Parallel performance**
  - MCNP5 has always used hierarchical parallelism with MPI + threading





Hardware

- Lobo – 16 threads/node
  - 4 x Quad-core AMD Opteron, 2.2 GHz, 32 GB memory
- Mac Pro – 8 threads
  - 2 x Quad-core Intel Xeon, 3GHz, 8 GB memory

Software

MCNP5-1.51, Intel-10 F90, "-O1 -openmp"

MCNP Criticality Calculation

BAWXI2 benchmark, kcode 25000 1 10 204

Verification / Validation for MCNP5-1.60 (1)

- **Testing + V&V Suites**

REGRESSION	- 66 installation & regression test problems
VALIDATION_CRITICALITY	- 31 ICSBEP Handbook cases
VERIFICATION_KEFF	- 75 analytic problems, exact results
VALIDATION_SHIELDING	- 19 shielding/dose problems vs experiment
KOBAYASHI [new]	- void & duct streaming, point detectors
POINT_KINETICS [new]	- adjoint weighted Rossi-α, β_{eff}, Λ_{eff}

- **Computers**
  - Mac / Linux / Windows, 32 / 64 bit
  - Sequential, threads, MPI, threads+MPI
  - Over 5,000 hr computer time
  - 2 students full-time + 2.5 staff part-time for 3 months

- **Criticality calculations**
  - Tested with ENDF/B-VI & ENDF/B-VII.0
  - All results should match previous versions of MCNP5

Verification / Validation for MCNP5-1.60 (2)

mcnp Monte Carlo Codes XCP-3, LANL

- **MCNP V&V Suites -- Focus**
  - **Physics-based V&V**
  - **Compare to experiment or exact analytic results**
  - Part of MCNP permanent code repository & RSICC distribution
  - Automated, easy execution
  - Automated, easy collection of results & comparison to experiment

- **Additional V&V Suites**
  - **VALIDATION_CRIT_EXPANDED** - 119 ICSBEP Handbook experiments
    - See paper for ICNC-2011 meeting
  - **Rossi Alpha Validation Suite** - 12 benchmark experiments
    - See paper for ICNC-2011 meeting
  - **VALIDATION_LANL_SB-CS** - 194 ICSBEP Handbook experiments
    - Provides V&V support for LANL criticality safety group

Verification / Validation for MCNP5-1.60 (3)

mcnp Monte Carlo Codes XCP-3, LANL

MCNP Criticality Validation Suite, Results on Mac OS X for ENDF/B-VII.0

	Experiment	MCNP5-1.51	MCNP5-1.60
J233 Benchmarks			
JEZ233	1.0000 (10)	0.9989 (6)	0.9989 (6)
'LAT23	1.0000 (14)	0.9990 (7)	0.9990 (7)
JMF5C2	1.0000 (30)	0.9931 (6)	0.9931 (6)
'LSTF1	1.0000 (83)	0.9830 (11)	0.9830 (11)
3B25	1.0000 (24)	1.0053 (10)	1.0053 (10)
)RNL11	1.0006 (29)	1.0018 (4)	1.0018 (4)
HEU Benchmarks			
;ODIVA	1.0000 (10)	0.9995 (6)	0.9995 (6)
rT2C11	1.0000 (38)	1.0018 (8)	1.0018 (8)
'LAT25	1.0000 (30)	1.0034 (7)	1.0034 (7)
;ODIVR	0.9985 (11)	0.9990 (7)	0.9990 (7)
JH3C6	1.0000 (47)	0.9950 (8)	0.9950 (8)
:EUS2	0.9997 (8)	0.9974 (7)	0.9974 (7)
;B5RN3	1.0015 (28)	0.9985 (13)	0.9985 (13)
)RNL10	1.0015 (26)	0.9993 (4)	0.9993 (4)

	Experiment	MCNP5-1.51	MCNP5-1.60
IEU Benchmarks			
IMF03	1.0000 (17)	1.0029 (6)	1.0029 (6)
BIGTEN	0.9948 (13)	0.9945 (5)	0.9945 (5)
IMF04	1.0000 (30)	1.0067 (6)	1.0067 (6)
ZEBR8H	1.0300 (25)	1.0195 (6)	1.0195 (6)
ICT2C3	1.0017 (44)	1.0037 (7)	1.0037 (7)
STACY36	0.9988 (13)	0.9994 (6)	0.9994 (6)
LEU Benchmarks			
BAWXI2	1.0007 (12)	1.0013 (7)	1.0013 (7)
LST2C2	1.0024 (37)	0.9940 (6)	0.9940 (6)
Pu Benchmarks			
JEZPU	1.0000 (20)	1.0002 (6)	1.0002 (6)
JEZ240	1.0000 (20)	1.0002 (6)	1.0002 (6)
PUBTNS	1.0000 (30)	0.9996 (6)	0.9996 (6)
FLATPU	1.0000 (30)	1.0005 (7)	1.0005 (7)
THOR	1.0000 (6)	0.9980 (7)	0.9980 (7)
PUSH2O	1.0000 (10)	1.0012 (7)	1.0012 (7)
HISHPG	1.0000 (110)	1 0122 (5)	1.0122 (5)
PNL2	1.0000 (65)	1.0046 (9)	1.0046 (9)
PNL33	1.0024 (21)	1.0065 (7)	1.0065 (7)

Verification / Validation for MCNP5-1.60 (4)

mcnp Monte Carlo Codes XCP-3, LANL

MCNP Criticality Verification Suite - VERIFICATION_KEFF

- **Compare MCNP5 vs Exact Analytic Results**
  - Mac OS X, Intel-10 f90
  - Same tests on Linux & Windows, with Intel, PGI, Absoft, gfortran, g95

Case	Name	Exact	intel-10
prob11	Ua-1-0-IN	2.25000	2.25000 (0)
prob14	Ua-1-0-SP	1.00000	1.00006 (10)
prob18	Uc-H2O(2)-1-0-SP	1.00000	1.00005 (11)
prob23	UD2O-1-0-CY	1.00000	1.00000 (6)
prob32	PUa-1-1-SL	1.00000	0.99995 (11)
prob41	UD2Ob-1-1-SP	1.00000	1.00003 (7)
prob44	PU-2-0-IN	2.68377	2.68382 (3)
prob54	URRa-2-0-SL	1.00000	1.00007 (13)
prob63	URRd-H2Ob(1)-2-0-ISLC	1.00000	0.99993 (6)
prob75	URR-6-0-IN	1.60000	1.59999 (1)

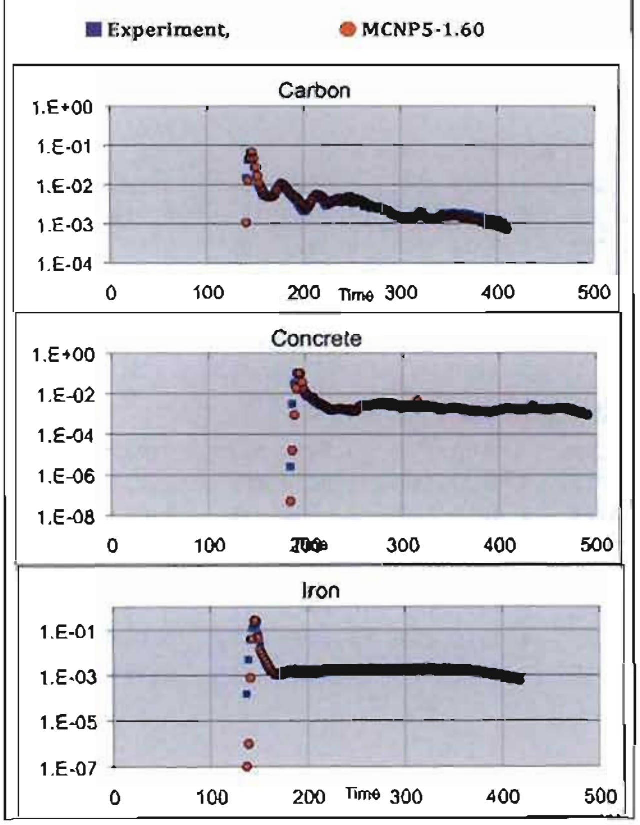
Verification / Validation for MCNP5-1.60 (5)

mcnp Monte Carlo Codes XCP-3, LANL

MCNP Kinetics Parameter Validation Suite Results on Linux

	Benchmark		MCNP5	
Rossi-Alpha vs Experiments				
GODIVA	-0.0011	2e-05	-0.001131	7e-6
JEZPU	-0.00064	1e-05	-0.000649	8e-6
BIGTEN	-0.000117	1e-06	-0.0001156	7e-7
FLAT23	-0.000267	5e-06	-0.0002931	3e-6
STACY29	-0.000122	4e-06	-0.0001222	9e-7
WINCO5	-0.001109	3e-06	-0.001124	1e-5
Generation Time vs Exact Analytic Solutions				
ONEINF	10		9.999	0.00085
TWOINF	14.17		14.16	0.00275
Generation Time vs PARTISN Solutions				
BARESLAB	9.793		9.792	0.00594
REFLSLAB	135.2		135.1	0.1068
THRESLAB	49.17		49.28	0.1018
INTRSLAB	112.1		112.7	0.4397
BARESPHR	1.721		1.722	0.00102
REFLSPHR	10.19		10.19	0.00737
SUBCSLAB	10.17		10.17	0.0073
SUPCSLAB	9.673		9.674	0.00526

Pulsed Sphere Problems (3 of 8)



Verification / Validation for MCNP5-1.60 (6)

mcnp Monte Carlo Codes XCP-3, LANL

Kobayashi Benchmark Results

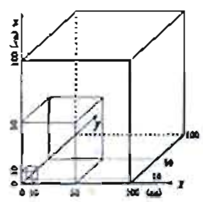
(1 of 6 problems)

Problem 1, Absorption + Scatter, 100M Histories

	x, y, z	Reference		MCNP-result		C/E
		Detector Set A				
f1405	5, 5, 5	8.29e+0	0.0002	8.22e+0	0.0002	0.99
f1415	5,15, 5	1.87e+0	0.0001	1.86e+0	0.0002	1.00
f1425	5,25, 5	7.13e-1	0.0000	7.13e-1	0.0001	1.00
f1435	5,35, 5	3.84e-1	0.0000	3.84e-1	0.0001	1.00
F1445	5,45, 5	2.53e-1	0.0001	2.54e-1	0.0001	1.00
F1455	5,55, 5	1.37e-1	0.0007	1.37e-1	0.0005	1.00
F1465	5,65, 5	4.65e-2	0.0012	4.68e-2	0.0007	1.01
F1475	5,75, 5	1.58e-2	0.0020	1.59e-2	0.0008	1.00
F1485	5,85, 5	5.47e-3	0.0034	5.48e-3	0.0012	1.00
F1495	5,95, 5	1.85e-3	0.0062	1.83e-3	0.0019	0.99
		Detector Set B				
F1505	5, 5, 5	8.29e+0	0.0002	8.22e+0	0.0002	0.99
F1515	15,15,15	6.63e-1	0.0000	6.63e-1	0.0001	1.00
F1525	25,25,25	2.68e-1	0.0000	2.69e-1	0.0001	1.00
F1535	35,35,35	1.56e-1	0.0001	1.57e-1	0.0001	1.00
F1545	45,45,45	1.04e-1	0.0001	1.04e-1	0.0002	1.00
F1555	55,55,55	3.02e-2	0.0006	3.01e-2	0.0009	1.00
F1565	65,65,65	4.06e-3	0.0007	4.08e-3	0.0015	1.01
F1575	75,75,75	5.86e-4	0.0012	5.89e-4	0.0034	1.01
F1585	85,85,85	8.66e-5	0.0020	8.73e-5	0.0087	1.01
F1595	95,95,95	1.12e-5	0.0038	1.16e-5	0.0236	1.03

	x, y, z	Reference		MCNP-result		C/E
Detector Set C						
F1605	5,55, 5	1.37e-1	0.0007	1.37e-1	0.0005	1.00
F1615	15,55, 5	1.27e-1	0.0008	1.28e-1	0.0005	1.00
F1625	25,55, 5	1.13e-1	0.0008	1.13e-1	0.0005	1.00
F1635	35,55, 5	9.59e-2	0.0009	9.65e-2	0.0006	1.01
F1645	45,55, 5	7.82e-2	0.0009	7.88e-2	0.0006	1.01
F1655	55,55, 5	5.67e-2	0.0011	5.65e-2	0.0007	1.00
F1665	65,55, 5	1.88e-2	0.0019	1.89e-2	0.0009	1.01
F1675	75,55, 5	6.46e-3	0.0031	6.50e-3	0.0012	1.01
F1685	85,55, 5	2.28e-3	0.0053	2.29e-3	0.0018	1.01
F1695	95,55, 5	7.93e-4	0.0089	8.00e-4	0.0029	1.01

1



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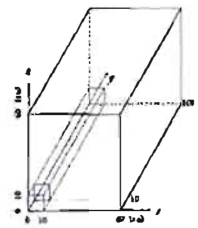

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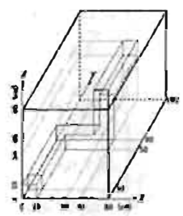


Verification / Validation for MCNP5-1.60 (7)

mcnp Monte Carlo Codes XCP-3, LANL

Parallel testing - OpenMP threads on Linux

Tests	Intel & gcc	PGI 7	PGI 9
Regression	Tu: seq, 1, 2, 4, 8, 16 Yr: seq, 1, 2, 4, 8	Tu: 1, 2, 4, 8, 16 Yr: 1, 2, 4, 8	Tu: 1, 2, 4, 8, 16 Yr: 1, 2, 4, 8
Validation Criticality	Tu: seq,1, 2, 4, 8, 16 Yr: seq, 1, 2, 4, 8	Tu: 1, 2, 4, 8, 16 Yr: 1, 2, 4, 8	Tu: 1, 2, 4, 8, 16 Yr: 1, 2, 4, 8
Verification Keff	Tu: seq, 1, 2, 4, 8, 16 Yr: seq, 1, 2, 4, 8	Tu: 1, 16 Yr: 1, 8	Tu: 1, 16 Yr: 1, 8
Kobayashi	Tu: seq, 1, 2, 4, 8, 16 Yr: 1, 8	Tu: 1, 16 Yr: 1, 16	Tu: 1, 16 Yr: 1, 8
Point Kinetics	Tu: seq, 1, 8, 9, 16	n/a	n/a
Validation Shielding	Tu: seq, 1, 2, 4, 8, 16 Yr: seq, 1, 8	Tu: 1, 16 Yr: 1, 8	Tu: 1, 16 Yr: 1, 8

Parallel testing - MPI nodes on Linux

Tests	*Intel-10*	*PGI-7*	*PGI-9*	*gfortran*
Regression	1, 3, 4, 8, 12, 17, 24, 33, 40, 48, 53, 64	1, 3, 12, 33, 40, 64	n/a	16
Validation Criticality	1, 3, 4, 8, 12, 17, 24, 33, 40, 48, 53, 64	1, 3, 12, 33, 40, 64	1, 12, 31	16, 31
Verification K-eff	1, 3, 4, 8, 12, 17, 24, 33, 40, 48, 53, 64	1, 3, 12, 33, 40, 64	n/a	16, 31
Kobayashi	1, 3, 4, 8, 12, 17, 24, 33, 40, 48, 53, 64	1, 3, 12, 33, 40, 64	n/a	n/a
Point Kinetics	n/a	64	n/a	n/a

Parallel testing - MPI+threads

Tests	*Number of MPI Processes*	*Number of OpenMP Threads Per MPI Process*	*Total Number of Threads*
Regression	2	7	14
	3	16	48
Validation Criticality	4	7	28
	3	16	48
Verification K-eff	4	7	28
	3	16	48
Kobayashi	4	7	28
	3	16	48
Point Kinetics	4	16	64

Rossi-alpha Validation Suite

mcnp Monte Carlo Codes XCP-3, LANL

- **MCNP5-1.60 can compute kinetics parameters**
  - Requires adjoint weighting techniques
  - Calculates Rossi-alpha ($-\beta_{eff}/\Lambda$)
- **Twelve benchmarks identified by Mosteller**
  - 4 HEU, 3 IEU, 3 Pu, 2 U-233
  - 8 fast, 2 intermediate, 2 thermal

	Rossi-alpha (10^4 gens/second)		
Name	Experiment	ENDF-VI	ENDF-VII.0
Jezebel-233	-100 ± 1	-109 ± 1	-108 ± 1
Flattop-23	-26.7 ± 0.5	-30.9 ± 0.4	-30.2 ± 0.4
Godiva	-111 ± 2	-117 ± 2	-111 ± 2
Flattop-25	-38.2 ± 0.2	-40.9 ± 0.2	-39.7 ± 0.2
Zeus-1	-0.338 ± 0.008	-0.372 ± 0.002	-0.360 ± 0.002
Zeus-4	-2.61 ± 0.02	-3.27 ± 0.01	-3.21 ± 0.01
BIG TEN	-11.7 ± 0.1	-12.5 ± 0.1	-11.8 ± 0.2
STACY-30	-0.0127 ± 0.0003	-0.0133 ± 0.0003	-0.0133 ± 0.0003
STACY-46	-0.0106 ± 0.0004	-0.0110 ± 0.0002	-0.0104 ± 0.0002
Jezebel	-64 ± 1	-64 ± 1	-65 ± 1
Flattop-Pu	-21.4 ± 0.5	-21.6 ± 0.3	-21.0 ± 0.3
THOR	-20 ± 1	-20 ± 2	-21 ± 1

Expanded Criticality Validation Suite

mcnp Monte Carlo Codes XCP-3, LANL

- **New, well-documented criticality suite**

  R.D. Mosteller, "An Expanded Criticality Validation Suite for MCNP",
  LA-UR-10-06230 (227 pages including MCNP inputs)

- **119 ICBEP Handbook experiments:**

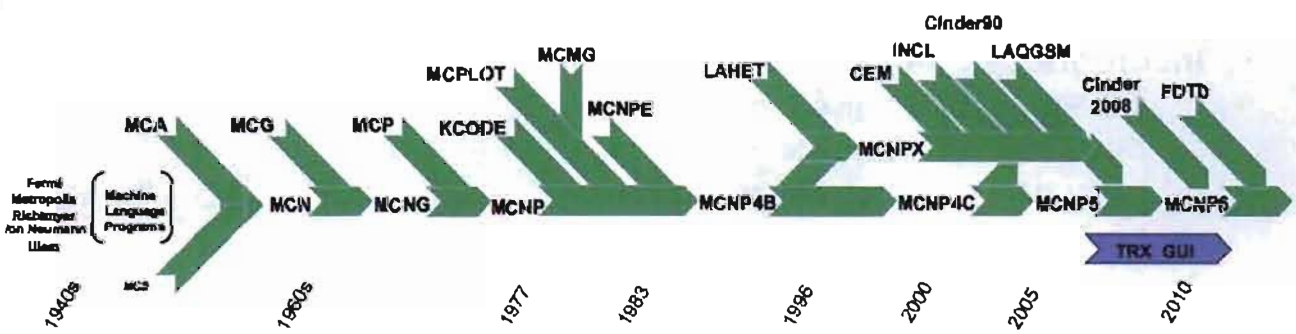
Fuel	Fast	Intermediate	Thermal	Total
U-233	10	1	7	18
HEU	29	5	6	40
IEU	10	1	6	17
LEU	-	-	8	8
Pu	21	1	14	36
Total	**70**	**8**	**41**	**119**

- **MCNP**
  - Automated execution & collection of results
  - Can run with ENDF/B-VI, T16+ENDF/B-VI, ENDF/B-VII.0 data
  - 7.75 hr on 8-core Mac Pro (714 M total neutron histories)

MCNP6 Status

MCNP6 Beta Release

mcnp Monte Carlo Codes XCP-3, LANL



- MCNP6 – beta release sent to RSICC for a limited set of beta testers
- MCNP6 – full release by RSICC expected in 2012
- Culminates 5 years of effort combining features of MCNPX into MCNP5
- MCNP5 & MCNPX are now frozen – future development will occur in MCNP6

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

Current & Future MCNP6 Efforts

mcnp Monte Carlo Codes XCP-3, LANL

The LANL MCNP6 team has more than 12 full time and 5 part time staff working on the following:

- Improved Physics
  - Incorporate new INCL, add delta rays, improve stopping power , add Rutherford scattering, allow particle to pick up charge as they slow down
- Improved Software parallelism
  - to be able to utilize >10K processors w/ mpi, R&D into Cray Fortran
- Improved Delayed Particle Emissions
  - better energy and angle correlations, beta and alpha emissions
- Efforts for EMP
  - Adding Electric Fields, Improved magnetic fields, specialized tallies
- Integration of Unstructured Mesh
  - work with weight windows mesh, charged particle tracking
- Optical Light
  - refraction, reflection, Cherenkov radiation
- Moving Objects
  - Realistic simulation of moving vehicles
- Sensitivity and Uncertainty
- Automatic Weight Windows Generation
  - from SN calculations – LANL's PARTISN.

MCNP contains a lot of physics

mcnp Monte Carlo Codes XCP-3, LANL

- Incorporates other codes as libraries:

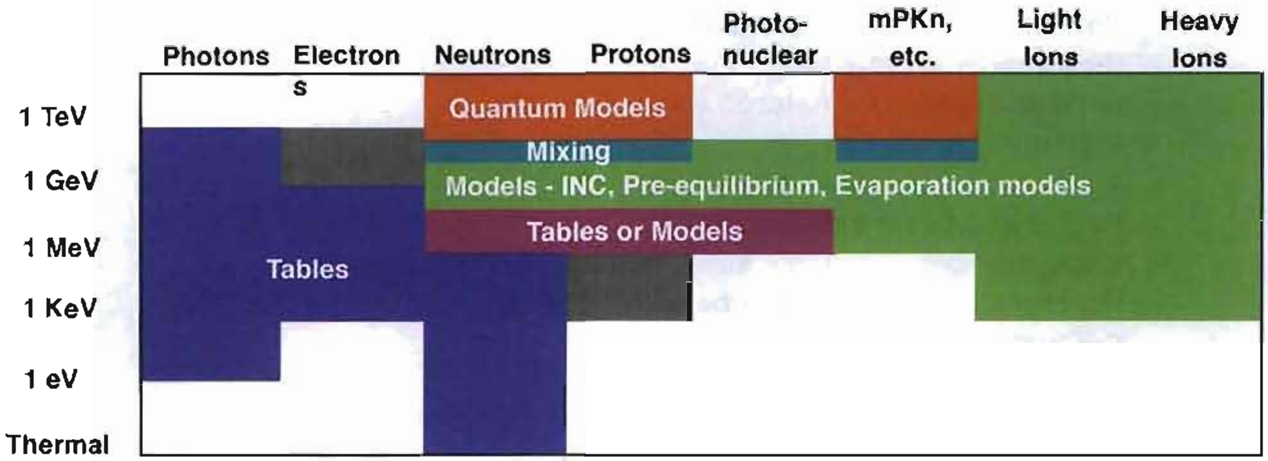
– LAHET	high energy transport	LANL
– CEM	high energy transport	LANL
– LAQGSM	high energy transport	LANL
– CINDER	unstable nuclei database	LANL
– ITS	electron transport	SNL
– MARS	high energy transport	FNAL
– HETC	high energy transport	ORNL

- Utilizes Nuclear and Atomic Data
  - LANL, LLNL, BNL, EU, Japan

- Large energy range (eV – 100s of GeV)

MCNP Physics

- **MCNP is physics rich – try to use best data, models, & theory**



- **Recent physics improvements include:**
  - Photon induced fission multiplicity
  - Characteristic muonic X-rays
  - Exact delayed gamma emissions
  - Visible light
  - Improved photoatomic form factors
  - Upgrades to CEM & LAQGSM 3.03
  - GEF photofission yield

MCNP6 Status

- **MCNP6 contains:**
  - MCNP6 = development version of MCNP at LANL, since 2004
  - Includes:
    - All MCNP5-1.60 capabilities (mpi + threads)
    - High energy protons & magnetic fields, for proton radiography
    - All MCNPX 2.7.D capabilities (mpi)
    - CINDER 2010 decay & depletion
  - Unstructured mesh, for linking with ABAQUS
  - Structured mesh, for linking with PARTISN
  - Adjoint-weighted perturbation estimators

- **MCNP6 in (very) limited beta release to outside LANL**
  - Recipients are active collaborators and sponsors
  - Full beta access within LANL and LLNL

MCNP6 Status

mcnp Monte Carlo Codes XCP-3, LANL

- **Active Validation Efforts**
  - Comparisons with experiments included in test suites
  - High energy proton, heavy ion interactions
  - Delayed photon and neutron spectra
  - Subcritical multiplication
  - Expanded criticality suite (119 problems)
  - Perturbation verification suite
  - Kobayashi benchmarks – streaming through ducts & voids
  - Reactor kinetics parameter benchmarks
  - Production / depletion (CINDER) soon

- **Nightly Regression Test suites**
  - 3 platforms (Linux 32, Linux 64, Windows 64)
  - 5 compilers (Intel 10+11, PGI 7, Pathscale 3, gfortran)
  - Serial, mpi, omp, mip+omp
  - Array bounds checking
  - 875 problem input files
  - Total: 10,000 runs each night

MCNP6 Status

mcnp Monte Carlo Codes XCP-3, LANL

- **MCNP & MCNPX teams have adopted MCNP6 as the base for all future development**

- **To go from Beta release to Production release:**
  - Assurance of reliability and accuracy for criticality
  - Assurance of reliability and accuracy for other apps
  - Comparable performance
  - Complete documentation

- **Future Work**
  - Cleanup coding style
  - Remove duplicate features
  - Extend parallel threading capability to new features
  - New Features

- **General release through RSICC**
  - 2012

Conclusions
&
Future Release Plans

MCNP5-1.60

- **Based on the excellent agreement found in all cases run:**
  - **All of the previous verification/validation efforts carried out in support of MCNP should carry over to the present version, MCNP5-1.60.**
- **We do not presume to declare MCNP5-1.60 as validated for any particular end-user application:**
  - That is the prerogative of the end-users, for their specific requirements and applications of the code
  - Such validation should be straightforward given the results reported herein for the MCNP5-1.60 verification testing
- **MCNP5-1.60 can be obtained from RSICC, rsicc.ornl.gov**

- **MCNP6 = MCNP5 + MCNPX merger**
  - Retains all capabilities in MCNP5 & MCNPX
    - High-energy physics (ie, GeV, TeV), 36 particle types, heavy ions, ...
    - Many new features for Homeland Security, detectors, ...
    - Depletion using CINDER-90, ...
- **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, not MCNP5/MCNPX/MCNP6**
- **MCNP6 is coming**
  - Beta-0 release: 1Q CY 2011 – very limited distribution
  - Beta-1 release: 4Q CY 2011 – general beta testing
  - Production release: CY 2012 – general public release

We need to plan for MCNP5 → MCNP6 transition

Questions ?