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Title: VERIFICATION OF MCNP5

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Los Alamos
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Verification of mcnp5

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Abstract

Verification of MCNP5

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MCNP Version 5 (MCNP5) comprises a complete modernization of the MCNP Monte Carlo code. A key requirement for MCNP5 was to preserve all previously-existing MCNP capabilities. Four sets of verification problems were used to ensure code correctness: a suite of 42 regression tests, a suite of 26 criticality benchmark problems, a suite of 10 analytic benchmarks for criticality, and a suite of 19 radiation shielding validation problems. In nearly all problems, MCNP5 results exactly match those of MCNP4C2. The few that differ agree well within statistics. It is concluded that MCNP5 is verified to be as reliable and accurate as previous versions and that all previously-existing capabilities have been preserved.

Outline

- MCNP 5
  - Modernization of MCNP
  - New Features in MCNP 5
- Testing / Verification Suites
  - Regression Test Suite
  - Criticality Validation Suite
  - Analytic Benchmarks for Criticality
  - Radiation Shielding Validation Suite
- Results
  - Criticality Validation Suite
  - Analytic Benchmarks for Criticality
  - Radiation Shielding Validation Suite
- Conclusions

mcnp 5

MCNP Tradition at Los Alamos

- The **MCNP** Monte Carlo radiation transport code has been developed and supported by the Monte Carlo team at LANL for **25 years**.
- Concurrently, the extensive nuclear and atomic **data libraries** have also been under constant development
- This tradition continues in the **Eolus ASCI Project** and related efforts in the Diagnostics Applications Group (X-5)
  - 12 MCNP code developers
  - Physical Data team also in X-5
  - Two application teams (user groups) in X-5

MCNP Development Team

Monte Carlo Development

Forrest Brown (Team Lead)

Tom Booth	Jeffrey Bull	Larry Cox
Art Forster	Tim Goorley	Russell Mosteller
Richard Prael	Elizabeth Selcow	Avneet Sood
Jeremy Sweezy	Grady Hughes	

Computer Support

Susan Post	Richard Barrett	Brian Jean
Teri Roberts	Skip Egdorf	Mark Zander

Research Associates

Taro Ueki (postdoc)

X-5 Data Team

Robert Little	Stephanie Frankle	Morgan White
Joanne Campbell	Stepan Mashnik	

University R&D	William Martin	Jerry Spanier
High-Energy Physics	Nikolai Mokhov	Sergei Strepanov
Visual Editor	Randy Schwarz	Lee Carter

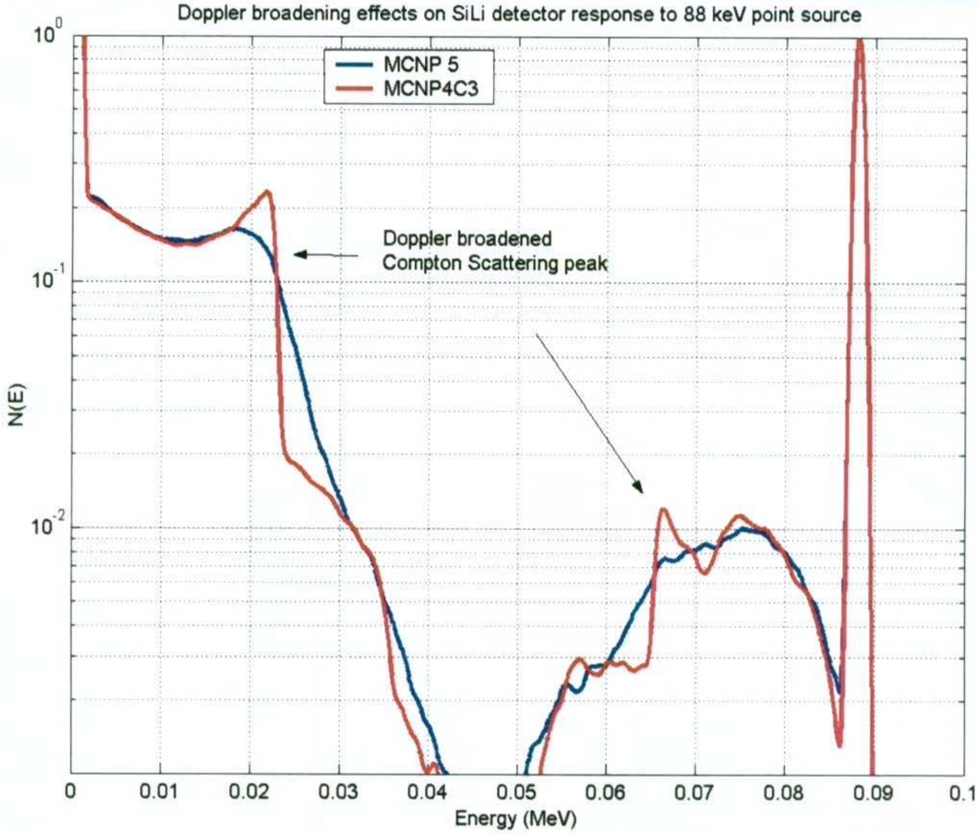
MCNP Version 5

- Modernization of MCNP
  - 2-year effort driven by ASCI Program needs for:
    - **Modern software engineering (SE) & software quality assurance (SQA),**
    - **Strict adherence to standards for Fortran-90 & parallel processing,**
    - **Preservation of all existing code capabilities,**
    - **Flexibility for rapid introduction of new features and advanced computers**
  - An evolutionary approach to MCNP modernization was followed, to minimize the chances of introducing new errors.
- MCNP5 is a rewrite of MCNP4C
  - Entire code is standard Fortran-90
  - Standard parallel coding: MPI (message-passing) + OpenMP (threads)
  - Fortran-90 dynamic memory allocation
  - Vastly improved modern coding style: spaces, blank lines, modules, replaced many thousands of GOTO's, ...
  - Some new features & new physics

New Features in MCNP Version 5

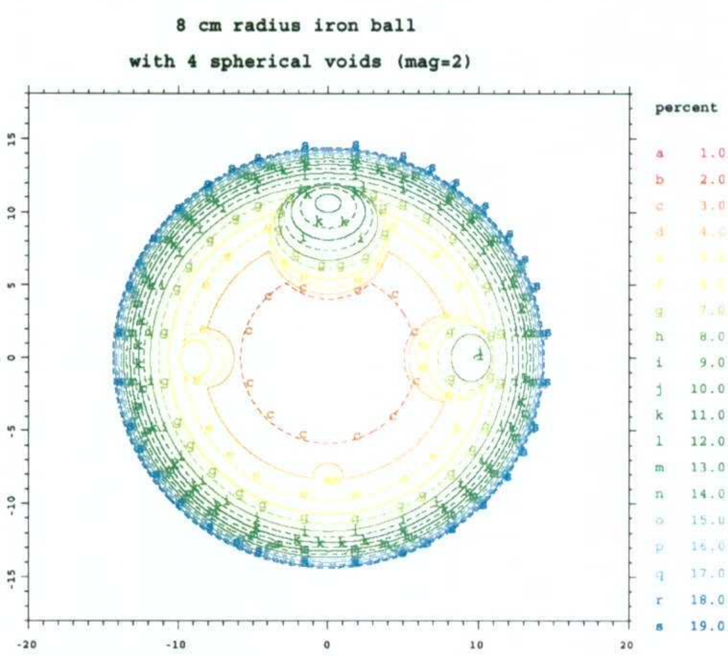
- Doppler Energy Broadening for Photon Transport
- Mesh Tallies
- Neutral Particle Image Tallies
- Sources: translate/rotate/repeat, Gaussian, particle type
- Easier specification of sources in repeated structures
- Time & energy splitting/rouletting
- Enhanced Parallel Processing Support
- Extended Random Number Package
- Unix-based build system, using GNU make
- Pulse height tally variance reduction (Spring, 2003)
- Radioisotope sources (Spring, 2003)
- Plotting options & more colors

Doppler Energy Broadening for Photons



Neutral Particle Image Tallies

- Release of long-term LANL feature
- Neutron and Photon radiography uses a raster of point detectors
- Each source and collision event contributes to all points
- Radiography Image Cards
  - FIR - flux image radiograph
  - FIP - flux image pinhole
  - FIC - flux image cylinder
- Two plotting options
  - Color contours
  - Color filled



An unscattered image from a 1 million pixel tally with a 6 MeV photon point source

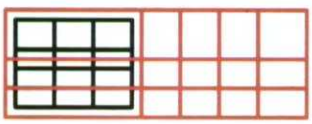
Neutral Particle Image Tallies

Simulated Radiograph – 1 M pixels

MCNP Model of Human Torso

Tally & Criticality Safety Enhancements

- Mesh Tallies
  - Arbitrary XYZ or RZ mesh superimposed on problem geometry
  - Multiple mesh tallies permitted, with separate mesh for each
  - Easy way to get assembly-tallies, dose fields, images, etc.



- Criticality Safety Parameters
  - Average energy of neutrons causing fission
  - Energy corresponding to average lethargy of neutrons causing fission
  - Fission to absorption ratios, etc.

New Random Number Generator

- Traditional MCNP RN generator
  - Based on 48-bit integers
  - Period ~10^{14}, stride = 152917
  - RNs reused after 500M histories
- New RN Generator
  - Based on 63-bit integers
  - Completely portable Fortran-90, modular
  - Efficient skip-ahead algorithm
  - Period ~10^{19} - 10,000x longer than previous
- Tested extensively
  - Knuth's statistical tests
  - Marsaglia's DIEHARD tests
  - Spectral test
- For now, traditional RN generator is default, new RN generators optional (will change next year)

Computer Systems Supported

- SGI IRIX64
- IBM AIX
- HP/Compaq OSF1
- Sun SunOS
- Linux with Absoft compiler
- Linux with Lahey compiler
- Linux with Portland Group compiler
- Windows PC with CVF compiler
- Windows PC with Absoft compiler
- Windows PC with Lahey compiler
- X11 graphics - all systems

- Mac OSX with Absoft compiler (soon)
- Itanium with Intel compiler (probably)

Must have Fortran-90 compiler - not F77 or g77

New Data Libraries - ENDF66

- To be released shortly by X-5 Data Team
- Based on ENDF/B-VI, Release 6
- 173 nuclides (ENDF60 has 122 nuclides)
  - 58 new nuclides
  - 40 new nuclide evaluations
  - Doppler broadening code included
- Smaller NJOY Processing Tolerance
  - 0.001 instead of ~0.005
- Probability tables, charged-particle production, and delayed neutron spectra and time constants
- Tabulated angular distributions
- Extensive verification and benchmarking

Verification / Validation

- The "correctness" of a computer code is traditionally discussed in terms of **verification & validation** processes.
- Verification
  - Generally performed by code developers
  - Involves a series of calculations to determine whether a code faithfully solves the equations and physical models it was designed to solve.
  - May involve comparison to other codes, to analytic benchmarks, or to experiments.
- Validation,
  - Generally performed by end-users,
  - Involves a determination of whether the code faithfully reproduces reality for a particular range of applications of interest.
  - May involve assessing the verification problems (to ensure that the end-user application is bounded), comparing calculations to relevant experiments, or scoping studies (to ensure that parameter changes produce expected changes in results).
- The MCNP5 developers have verified that MCNP5 produces the same results as the previous version, MCNP4C2, for a set of over 100 verification test problems.
  - A few test problems produce results which match within statistics, but do not agree bit-for-bit;
  - These differences are small and are attributed to computer roundoff due to the use of different compilers and the sensitivity of Monte Carlo eigenvalue calculations to roundoff.
- The verification problems used in this testing are grouped into 4 suites which are described below along with detailed discussion of the test results.

Verification Summary

- **Suite of 42 Regression Tests**
  - Run many times per day
  - Verifies code changes (not physics)
  - ~90% code coverage
- **Criticality Validation Suite**
  - 26 cases from International Handbook of Evaluated Criticality Benchmark Experiments
  - Run with ENDF60+URES data library, also with new ENDF66 data library
  - 52 cases run, 1,000,000 histories each
- **Analytic Benchmarks for Criticality**
  - 10 problems, from Sood/Forster report - exact solutions known
  - 8,000,000 histories each
- **Radiation Shielding Validation Suite**
  - 8 problems - time-of-flight spectra for neutrons from pulsed spheres
  - 5 problems - neutron & photon spectra at shield walls within simulated fusion reactor
  - 6 problems - photon dose rates
  - 1,000,000 histories for each problem

Regression Test Suite

- MCNP5 distribution includes a set of installation tests to verify that installation & compilation are carried out correctly on a given computer system
  - Reference "templates" are provided for both the printed code output & resulting tally files (mctal files)
  - Templates are compared with the actual output & mctal files.
  - During the development of MCNP5, the regression test set was expanded from 28 to 42 problems
  - Set of 42 problems executes in less than 5 minutes.
  - Previous analysis of MCNP has indicated that the tests cover approximately 80-90% of the total lines of coding. (Test coverage analysis for MCNP5 is in progrss.)
- Regression tests do not verify code correctness
  - Typically run many times each day by an individual code developer for regression testing
  - Used only to detect unintended changes to the code.
  - Extensive use on a daily basis serves to prevent the inadvertent introduction of bugs

Criticality Validation Suite - Problems

- 26 cases - wide variety of fissile materials & spectra
  - Three major fissile isotopes — U-233, U-235, Pu-239
  - Fast, intermediate, & thermal spectra
  - U-235 cases were chosen to include HEU, IEU, & LEU fuels
- Cases also chosen to include a variety of configurations
  - Fast-spectrum cases include bare spheres, cores reflected by a heavy material (normal U), cores reflected by a light material (Be or water).
  - Thermal-spectrum cases include lattices of fuel pins as well as homogeneous solutions.
  - Number of experiments with intermediate spectra is much more limited, cases chosen for availability rather than specific attributes.
- Specifications for all 26 cases taken from the International Handbook of Evaluated Criticality Benchmark Experiments
- Calculations
  - Single-processor mode on SGI Origin 2000 computer
  - Each case: 250 total generations, 50 initial generations discarded, 5000 neutron histories/generation, 1,000,000 active neutron histories
  - Calculations run with MCNP4C2 & MCNP5, using ENDF60+URES & ENDF66

Criticality Validation Suite

Name	Spectrum	Handbook ID	Description
Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of 233U
Flattop-23	Fast	U233-MET-FAST-006	Sphere of 233U reflected by normal U
U233-MF-005 (2)	Fast	U233-MET-FAST-005, case 2	Sphere of 233U reflected by beryllium
Falstaff (1)	Intermed	U233-SOL-INTER-001, case 1	Sphere of uranyl fluoride solution enriched in 233U
ORNL-11	Thermal	U233-SOL-THERM-008	Large sphere of uranyl nitrate solution enriched in 233U
Godiva	Fast	HEU-MET-FAST-001	Bare HEU sphere
Flattop-25	Fast	HEU-MET-FAST-028	HEU sphere reflected by normal U
Godiver	Fast	HEU-MET-FAST-004	HEU sphere reflected by water
HISS/HUG	Intermed	HEU-COMP-INTER-004	Infinite, homogeneous mixture of HEU, H, and graphite
ZEUS (2)	Intermed	HEU-MET-INTER-006, case2	HEU platters moderated by graphite and reflected by Cu
HEU-MT-003 (4)	Thermal	HEU-MET-THERM-003, case 4	Lattice of HEU cubes reflected by water
ORNL-10	Thermal	HEU-SOL-THERM-032	Large sphere of HEU nitrate solution
IEU-MF-003	Fast	IEU-MET-FAST-003	Bare sphere of IEU (36 wt.%)
BIG TEN	Fast	IEU-MET-FAST-007	Cylinder of IEU (10 wt.%) reflected by normal U
IEU-MF-004	Fast	IEU-MET-FAST-004	Sphere of IEU (36 wt.%) reflected by graphite
IEU-CT-002 (3)	Thermal	IEU-COMP-THERM-002, case 3	Lattice of IEU (17 wt.%) fuel rods in water
BAW XI (2)	Thermal	LEU-COMP-THERM-008, case 2	Large lattice of PWR fuel pins in borated water
SHEBA-2	Thermal	LEU-SOL-THERM-001	Cylinder of LEU fluoride solution enriched to 5 wt.%
Jezebel	Fast	PU-MET-FAST-001	Bare sphere of Pu
Jezebel-240	Fast	PU-MET-FAST-002	Bare sphere of Pu (20.1 at.% 240Pu)
Flattop-Pu	Fast	PU-MET-FAST-006	Pu sphere reflected by normal U
PU-MF-011	Fast	PU-MET-FAST-011	Pu Sphere reflected by water
Pu Buttons	Fast	PU-MET-FAST-003, case 3	3 x 3 x 3 array of small cylinders of Pu
HISS/HPG	Intermed	PU-COMP-INTER-001	Infinite, homogeneous mixture of Pu, hydrogen, & graphite
PNL-33	Thermal	MIX-COMP-THERM-002, case 4	Lattice of mixed-oxide fuel pins in borated water
PNL-2	Thermal	PU-SOL-THERM-021, case 3	Sphere of plutonium nitrate solution

Criticality Validation Suite - Results

- Keff results for 52 cases are shown in table
- MCNP5 & MCNP4C2 produce **identical** answers for 49/52 cases
- MCNP5 & MCNP4C2 agree within statistics for the other 3 cases
  - Zeus(2) cases:
    - Using ENDF60+URES data, tracked identically for 125 generations (0.625M histories), & final results agree within statistics.
    - Both code versions agree exactly using ENDF66 data
  - HEU-MT-003 (4) cases:
    - With ENDF60+URES data, both codes agreed exactly.
    - Using ENDF66 data, track for the first 225 generations (1.125M histories), & final results agree within statistics.
  - IEU-CT-002 (3) cases:
    - Matched using ENDF60+URES data
    - Differed slightly using ENDF66 data, with final results agreeing within statistics

- The statistically insignificant differences observed in 3/52 cases are attributed to roundoff associated with compiler differences.
  - MCNP4C2 compiled ~2 years ago using Fortran-77 compiler & associated math libraries
  - MCNP5 compiled using current version of SGI Fortran-90 compiler & associated libraries
  - Monte Carlo eigenvalue calculations are very sensitive to computer roundoff due to their iterative nature - small differences in even a single particle history will propagate through all future generations. (Fixed source calculations are less sensitive to roundoff, since generations are not used; roundoff differences affect only a single history and do not propagate.)

Criticality Validation Suite – K-effective Results

Name		ENDF60+URES Data		ENDF66 Data	
		MCNP5	MCNP4C2	MCNP5	MCNP4C2
1	Jezebel-233	0.99241 (57)	"	0.99106 (56)	"
2	Flattop-23	0.99931 (71)	"	0.99960 (72)	"
3	U233-MF-005 (2)	0.99785 (64)	"	0.99900 (59)	"
4	Falstaff (1)	0.99040 (104)	"	0.99017 (106)	"
5	ORNL-11	0.99596 (41)	"	0.99708 (37)	"
6	Godiva	0.99728 (63)	"	0.99647 (60)	"
7	Flattop-25	0.99790 (63)	"	0.99660 (59)	"
8	Godiver	0.99539 (80)	"	0.99675 (79)	"
9	HISS/HUG	1.01264 (47)	"	1.01016 (46)	"
10	ZEUS (2)	0.99722 (73)	0.99655 (71)	0.99538 (75)	"
11	HEU-MT-003 (4)	0.98257 (88)	"	0.98413 (79)	0.98374 (80)
12	ORNL-10	0.99874 (39)	"	0.99835 (40)	"
13	IEU-MF-003	1.00046 (57)	"	0.99973 (61)	"
14	BIG TEN	1.00987 (55)	"	1.00725 (54)	"
15	IEU-MF-004	1.00381 (62)	"	1.00315 (67)	"
16	IEU-CT-002 (3)	1.00024 (70)	"	1.00029 (74)	0.99987 (71)
17	BAW XI (2)	0.99837 (60)	"	0.99863 (70)	"
18	SHEBA-2	1.01064 (77)	"	1.01018 (82)	"
19	Jezebel	0.99694 (57)	"	0.99772 (60)	"
20	Jezebel-240	0.99883 (60)	"	0.99884 (57)	"
21	Flattop-Pu	1.00138 (66)	"	1.00266 (70)	"
22	PU-MF-011	0.99736 (76)	"	0.99700 (72)	"
23	Pu Buttons	0.99581 (67)	"	0.99735 (68)	"
24	HISS/HPG	1.01126 (59)	"	1.00936 (56)	"
25	PNL-33	1.00578 (79)	"	1.00545 (80)	"
26	PNL-2	1.00031 (104)	"	1.00219 (95)	"

Notes: " = result identical to that of column at left, (NN) = std deviation is NN x 10^{-5}

Analytic Benchmarks for Criticality

- LANL report describes 75 criticality problems found in the literature for which exact analytical solutions are known
  - A. Sood, R.A. Forster, D.K. Parsons, "Analytical Benchmark Test Set for Criticality Code Verification," LA-13511, Los Alamos National Laboratory (1999).
  - Number densities, geometry, & cross-section data specified exactly
- As part of the MCNP5 verification, 10 of these analytic benchmark problems were run to high precision using MCNP5
  - 2 different computer systems - SGI Origin 2000 & Pentium-III PC running Windows-2000.
  - For all cases, a total of 210 generations were run, with first 10 discarded
  - For cases 1-9, 40,000 histories were used per generation, for a total of 8M histories in the 200 active cycles.
  - For case 10, only 5,000 histories per generation were run, for a total of 1M histories in the active generations.
  - The 10 cases are listed in table along with both analytic & MCNP5 results
- In all cases, MCNP5 results were **identical** on the SGI & PC
- **All results in statistical agreement with exact k-eff's**

Analytic Benchmarks for Criticality - Results

	Name	Description	Exact K-eff	MCNP5 K-eff
1	Ua-1-0-IN	Infinite medium, 1 group	2.25	2.24996 (24)
2	Ua-1-0-SP	Sphere, 1 group	1.0	0.99990 (23)
3	Uc-H2O(2)-1-0-SP	Reflected sphere, 1 group	1.0	0.99985 (23)
4	UD2O-1-0-CY	Cylinder, 1 group	1.0	0.99996 (15)
5	PUa-1-1-SL	Slab, 1 grp, P1 scatter	1.0	0.99989 (26)
6	UD2OB-1-1-SP	Sphere, 1 grp, P1 scatter	1.0	0.99993 (17)
7	PU-2-0-IN	Infinite medium, 2 group	2.683767	2.68375 (7)
8	URRa-2-0-SL	Slab, 2 group	1.0	1.00001 (34)
9	URR-6-0-IN	Infinite medium, 6 group	1.60	1.59999 (2)
10	URRd-H2O(1)2-0-ISLC	Slab, 2 group	1.0	0.99986 (41)

Note: (NN) = std deviation is NN x 10^{-5}

Radiation Shielding Validation Suite

- Three subcategories:
  - Time-of-flight spectra for neutrons from pulsed spheres
  - Neutron and photon spectra at shield walls within a simulated fusion reactor
  - Photon dose rates
- Two of the cases are coupled neutron-photon calculations, while the others are exclusively neutron or exclusively photon calculations.
  - Photon data library
    - Cases that include photons use MCPLIB02 for all nuclides
    - MCPLIB02 was part of ENDF60 lib release, but not based on ENDF/B-VI
    - MCPLIB02 is an extension of the original MCPLIB photon library that has been used with MCNP for more than 20 years
    - MCPLIB02 extends the range of data for photon interactions up to 100 GeV, based on the LLNL Evaluated Photon Data Library
- Calculations performed in sequential mode on SGI Origin-2000
- Each case employed 1,000,000 particle histories

Pulsed Sphere Calculations

- Subset of the pulsed-sphere experiments that were performed at LLNL from 1960-1980s
- Objective was to measure neutron emission spectrum from a variety of materials bombarded by 14 MeV neutrons.

Target Material	Target Configuration	Thickness (mfp)	Detector Type	Detector Angle
Beryllium	Bare Sphere	0.8	Pilot B	30°
Carbon	Bare Sphere	2.9	NE 213	30°
Concrete	Bare Sphere	2.0	NE 213	120°
Iron	Bare Sphere	0.9	NE 213	30°
Lead	Clad Sphere	1.4	NE 213	30°
Li-6	Dewar	1.6	NE 213	30°
Nitrogen	Dewar	3.1	Pilot B	30°
Water	Dewar	1.9	Pilot B	30°

Fusion Shielding Calculations

- Based on experiments at ORNL in 1980
- Objective was to simulate the DT neutron spectrum that would exist at the first wall of a fusion reactor, as well as the spectrum of secondary photons that would be produced from neutron interactions within that wall

Configuration	Tally Type	On/Off Axis
1	neutron	On
3	neutron	Off
3	photon	On
7	neutron	On
7	photon	Off

last column indicates whether detector was aligned with axis of particle beam

Photon Dose Rates

- 1980 measurement of air-scattered photon radiation far from the source ("skyshine")
- Idealization of a number of measurements of the radiation environment in an open field covered by fallout
- Hupmobile thermoluminescent dosimeter (TLD) experiments performed at LBL 1967-69

Case	Source	Principal Media
Skyshine	Co-60	Air & Soil
Air over Ground	Co-60	Air & Soil
60Co through Air	Co-60	Air
60Co through Teflon	Co-60	Teflon
Sm Kα through Air	Sm Kα	Air
Sm Kα through Teflon	Sm Kα	Teflon

Radiation Shielding Validation Suite - Results

- If the tallies from two different versions of MCNP match, the final values necessarily will match as well.
- **MCNP5 produces exactly the same tally values as MCNP4C2** for all the cases in the validation suite, given the same data library
- This is true for both the older ENDF60 data and the new ENDF66 data.

Verification Summary

- **Suite of 42 Regression Tests**
  - Run many times per day
  - Verifies code changes (not physics)
- **Criticality Validation Suite**
  - **MCNP5 matches MCNP4C2 exactly in 51/52 cases, within statistics for other**
- **Analytic Benchmarks for Criticality**
  - 10 problems, from Sood/Forster report - exact solutions known
  - **All match exact solution within statistics**
- **Radiation Shielding Validation Suite**
  - 8 problems - time-of-flight spectra for neutrons from pulsed spheres
  - 5 problems - neutron & photon spectra at shield walls within simulated fusion reactor
  - **MCNP5 matches MCNP4C2 exactly in all cases**

Conclusions

- We have demonstrated by extensive verification testing that MCNP5 produces results which are as reliable and accurate as the previous version, MCNP4C2.
  - In nearly all cases, results from MCNP5 are in exact agreement with results from MCNP4C2.
  - For a few cases involving eigenvalue calculations (which are sensitive to computer roundoff), MCNP5 and MCNP4C2 results did not match exactly, but did agree within small statistics.
  - For fixed-source calculations (which are not sensitive to computer roundoff), all MCNP5 and MCNP4C2 results matched exactly.
- As a result of the excellent agreement found in all cases run, we conclude that all of the previous verification/validation efforts carried out in support of MCNP should carry over to the present version, MCNP5.
  - We do not presume to declare MCNP5 as validated for any particular end-user application (that is the perogative of the end-users, for their specific requirements and applications of the code), but suggest that such validation should be straightforward given the results reported herein for the MCNP5 verification testing.