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Title:

Verification of MCNP5-1.60

Author(s):

Forrest Brown, Brian Kiedrowski, Jeffrey Bull,
Matthew Gonzales, Nathan Gibson

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MCNP documentation and release

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Forrest Brown, Brian Kiedrowski, Jeffrey Bull, Matthew Gonzales, Nathan Gibson

Monte Carlo Codes, XCP-3
Los Alamos National Laboratory

Outline:

I. Introduction

A. Summary

The latest release of the MCNP5 [1] Monte Carlo code is designated MCNP5-1.60. This release includes many minor code modifications to fix reported bugs, output formats, error checking, and other difficulties present with previous versions of MCNP. In some cases, the problems that were fixed date back to the 1990s, but were only recently reported and fixed. In addition, there are enhancements to several MCNP capabilities: maximum number of cells, surfaces, materials, and tallies; isotopic reaction rates for mesh tallies; and adjoint-weighting for computing effective lifetimes and delayed neutron parameters. It should be noted that no errors were found that would affect the code results for basic criticality calculations. In nearly all cases, the bug fixes addressed problems with infrequently-used combinations of code options. All previously existing code capabilities have been preserved, including physics options, geometry, tallying, plotting, cross-section handling, etc. Tally results from MCNP5-1.60 are expected to match the tally results of problems that can be run with the previous MCNP5-1.51 [2,3,4], except where bugs were discovered and fixed. The bug fixes and enhancements are discussed in Reference [5], and supplemental pages for the MCNP manual are provided in Reference [6].

To verify that the MCNP5-1.60 is performing correctly, several suites of existing verification/validation problems have been run. For these benchmark suites, results have been compared with previously verified versions of MCNP5, with experimental or analytic results, and with results from running on different computer hardware/software platforms. In addition, 2 new verification/validation suites have been added, the Kobayashi benchmarks with problems containing voids and ducts, and a set of benchmarks for reactor kinetics parameters. The testing suites are:

- **Regression** - The standard MCNP5 Regression Test Suite [1,4],
- **VALIDATION_CRITICALITY** - The "Criticality Validation Suite" [7,8,9] consisting of 31 problems from the *International Handbook of Evaluated Criticality Benchmark Experiments* [10],
- **VERIFICATION_KEFF** - 10 problems from the suite of analytical criticality verification benchmarks [11],
- **VALIDATION_SHIELDING** - The "Radiation Shielding Validation Suite" [7,12,13] of problems,
- **KOBAYASHI** - The "Kobayashi Benchmarks" [14,15],
- **POINT_KINETICS** - The "Point Kinetics" validation suite [16,17]

Verification calculations for MCNP5-1.60 were run on Mac OS X, Linux, and Windows computing systems. Extensive testing of MCNP5 was performed using sequential execution (i.e., 1 CPU), threaded calculations using OpenMP with various numbers of threads, parallel message-passing using OpenMPI with various numbers of CPUs, and mixed threaded+MPI calculations using different combinations of threading and MPI. On each computer platform, several different Fortran-90 compilers were used in the testing. The total computing time used during the course of the testing was approximately 5,000 CPU-hours, over a span of several months calendar time. Results from these calculations have been compared to results from the previous, verified version of MCNP5 (Version 1.51), to known analytical results, and to results from experiments.

B. Objectives

The "correctness" of a computer code is traditionally discussed in terms of the verification and validation processes. Verification, generally performed by code developers, involves performing a series of calculations to determine whether a code faithfully solves the equations and physical models it was designed to solve. Verification 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. Validation may involve assessing the verification problems (to ensure that the end-user application is bounded), comparing calculations to relevant experiments, or by performing scoping studies (to ensure that parameter changes produce expected changes in results).

The MCNP5 developers have verified that MCNP5-1.60 produces the same results as the previous version, MCNP5-1.51 for a set of 143 verification test problems. A few test problems produce results that 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 some Monte Carlo calculations to roundoff. Computer roundoff issues are discussed in the next section.

The MCNP validation suites should not be used as an absolute indicator of the accuracy or reliability of MCNP5 or the nuclear data libraries. Many of the benchmarks are taken from sequences of similar benchmarks, and the sequence as a whole may display sensitivities that a single case cannot capture. Nonetheless, the suites can provide a general indication of the overall performance of a given library, and can alert the user to unexpected or unintended consequences resulting from changes to nuclear data. In addition, the test suites can help to identify areas where improvements are needed.

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, MCNP5-1.60. 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), but suggest that such validation should be straightforward given the results reported herein for the MCNP5-1.60 verification testing.

C. Discussion of Compiler Options and Computer Roundoff

When compiling MCNP5 using a particular Fortran-90 compiler on a particular computer system, the options used for compilation and the CPU characteristics can impact MCNP by introducing roundoff differences in computer arithmetic. For example, the *-r8* Fortran-90 compile option instructs the Fortran-90 compiler to convert (at compile time) all single-precision constants into their double-precision equivalents. That is, the Fortran-90 statements

```
real(8) x
x = .3
```

are converted at compile time to the statements

```
real(8)  x
x = .3d0
```

To a novice Fortran programmer, these 2 sets of statements may appear equivalent. For Monte Carlo calculations, however, the difference between the 2 sets can lead to roundoff differences in computer arithmetic (note: differences, not errors) due to the different precision of .3 as a single precision value and .3d0 as a double-precision value. If the first set of statements is compiled without the *-r8* option and the value of x is printed, and then compiled with the *-r8* option and the value of x is printed, these results are seen (on Mac OS X with the Intel Fortran-90 compiler):

```
Without -r8:        x = 0.3000000119209290
With -r8            x = 0.3000000000000000
```

While the relative difference between the 2 results is only 4x10^{-8}, such differences in numerical precision will lead to different particle tracking and collision analysis results in MCNP5 calculations. Because the number of accurate digits in the physical data (cross-sections) can be counted on one hand, computer roundoff differences as shown above have no physical significance, and any particle tracking differences caused by such roundoff are not errors in the code or data. Tracking differences due to computer roundoff do, however, complicate the verification and validation process.

In an attempt to reduce the computer roundoff differences between different compilers and systems (e.g., Intel F90 on Mac OS X vs. Linux, Intel F90 vs. Absoft F90 on Mac OS X, etc.), we deliberately chose to use the *-r8* compiler option for all systems and compilers in the release of MCNP5-1.60. In addition, we have chosen to use only moderate optimization levels with the various Fortran-90 compilers. For all systems, we have used the "*-O1*" optimization level. At higher levels of optimization, the Fortran-90 compilers generally achieve performance gains by rearranging the order of computations, combining common sub-expressions for intermediate results, holding much data in registers instead of storing to memory, utilizing vector hardware units rather than scalar CPU arithmetic, precomputing certain combinations of constants, and many other tried-and-true optimization tricks. Our testing typically shows only small gains in performance for Monte Carlo codes with these higher optimization levels, at the expense of tremendous complications in verification due to small roundoff differences. (The chief benefactors from the higher levels of compiler optimization are codes that are largely array-based, where vectorization of matrix-vector operations can lead to substantial code speedups.) We discourage users from invoking the higher optimization levels, unless they are willing to also perform the necessary additional verification of code correctness.

In general, we try to choose options for different Fortran-90 compilers and computer platforms that are as consistent as possible for building MCNP5. Nevertheless, computer roundoff differences will occur with different compilers/hardware. Roundoff differences are not considered errors. Careful examination of these differences is necessary in the verification/validation process to ensure that these differences are due solely to roundoff, and not to errors in coding.

II. Description of Verification/Validation Suites

A. Regression Test Suite

For many years, the MCNP distribution has included a set of installation tests to verify that installation and compilation of the code are carried out correctly on a given computer system. For these tests, reference "templates" are provided for both the printed code output and the resulting tally files (*mctal* files). These template files are compared with the actual output and *mctal* files. In the past, these tests took a few minutes each, so that the entire test set required ~1/2 hour or more. On today's computers, including PCs, the entire set of test problems executes in 1-2 minutes. Due to the short running time, the test set is typically run many times each day by an individual code developer and is now used for regression testing, rather than just installation testing. Today's code development process typically consists of modifying a few subroutines, incremental recompilation using GNU *make*, and then running the regression test set.

The regression test set was expanded from 52 problems to 66 problems, with new tests added to cover new code features or to explicitly test that particular bugs were fixed. Previous analysis of MCNP5 has indicated that the tests cover approximately 80-90% of the total lines of coding. The MCNP5 build system specifically includes capabilities for running any or all of the regression tests and for comparing results with the reference templates.

It is important to note that the regression tests do not verify code correctness; they are used only for the purpose of detecting unintended changes to the code. Also, many of the Regression Test problems have contrived input specifications, and even deliberate errors in some cases. These problems should most definitely not be used as good examples of MCNP5 problem input; they serve only to test the consistent operation of the code. Their extensive use on a daily basis serves to prevent the inadvertent introduction of bugs.

B. Criticality Validation Suite

The MCNP Criticality Validation Suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*. It contains cases for a variety of fuels, including ^{233}U, highly enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), and plutonium in configurations that produce fast, intermediate, and thermal spectra. For each fuel type, there are cases with a variety of moderators, reflectors, spectra, and geometries. The cases in the suite were chosen to include a variety of configurations. The fast-spectrum cases include bare spheres, cores reflected by a heavy material (normal U), and cores reflected by a light material (Be or water). The thermal-spectrum cases include lattices of fuel pins as well as homogeneous solutions. The number of

Table I. MCNP Criticality Validation Suite.

Spectrum	Fast			Intermediate	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins in Water	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05 (2)*	Falstaff (1)†	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (c-11)	Flattop-25	Godiver	UH$_3$ (6) Zeus (2)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H‡	IEU-CT-02 (3)	STACY-36
LEU					BaW XI (2)	LEU-ST-02 (2)
Pu	Jezebel Jezebel-240 Pu Buttons (3)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG‡	PNL-33	PNL-2

* Numbers in parentheses identify a specific case within a sequence of benchmarks

† Extrapolated to critical

‡ k_∞ measurement

experiments with intermediate spectra is much more limited, and those cases were chosen primarily for availability rather than specific attributes. All of the cases are at room temperature and pressure. The cases in the suite are summarized in Table I.

The 31 benchmark problems shown in Table II were run using both MCNP5-1.60 and the previously-released version MCNP5-1.51, using both the previous MCNP Data Libraries (ENDF/B-VI, T16, SAB2002) and the new ENDF/B-VII libraries. All calculations were performed with 250 generations of 5,000 neutrons each, and the results from the first 50

Table II. Description of Criticality Validation Problems

Name	Spectrum	Handbook ID	Description
Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of ^{233}U
Flattop-23	Fast	U233-MET-FAST-006	Sphere of ^{233}U reflected by normal U
U233-MF-005 (2)	Fast	U233-MET-FAST-005, case 2	Sphere of ^{233}U reflected by beryllium
Falstaff (1)	Intermediate	U233-SOL-INTER-001, case 1	Sphere of uranyl fluoride solution enriched in ^{233}U
SB-2 1/2	Thermal	U233-COMP-THERM-001, case 3	Lattice of ^{233}U fuel pins in water
ORNL-11	Thermal	U233-SOL-THERM-008	Large sphere of uranyl nitrate soln enriched in ^{233}U
Godiva	Fast	HEU-MET-FAST-001	Bare HEU sphere
Tinkertoy-2 (11)	Fast	HEU-MET-FAST-026, case 11	3x3x3 array of HEU cylinders reflected by paraffin
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	Intermediate	HEU-COMP-INTER-004	Infinite, homogeneous mix of HEU, H, graphite
ZEUS (2)	Intermediate	HEU-MET-INTER-006, case 2	HEU platters, graphite moderator, Cu reflector
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
Zebra-8H	Intermediate	MIX-MET-FAST-008, case 7	Plate of IEU (37.5 w/o) reflected by U & steel
IEU-CT-002 (3)	Thermal	IEU-COMP-THERM-002, case 3	Lattice of IEU (17 wt.%) fuel rods in water
Stacy (36)	Thermal	LEU-SOL-THERM-007, case 36	Cylinder of IEU (9.97 w/o) uranyl nitrate solution
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 soln 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.% ^{240}Pu)
Pu Buttons	Fast	PU-MET-FAST-003, case 3	3 x 3 x 3 array of small cylinders of Pu
Flattop-Pu	Fast	PU-MET-FAST-006	Pu sphere reflected by normal U
THOR	Fast	PU-MET-FAST-008	Plutonium sphere reflected by thorium
PU-MF-011	Fast	PU-MET-FAST-011	Pu sphere reflected by water
HISS/HPG	Intermediate	PU-COMP-INTER-001	Infinite, homog. mix of Pu, hydrogen, and 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

generations were discarded. Consequently, the results for each case are based on 1,000,000 active neutron histories.

C. Analytic Benchmarks for Criticality

Reference [11] provides a set of 75 criticality problems found in the literature for which exact analytical solutions are known. Number densities, geometry, and cross-section data are specified exactly for these problems. As part of the MCNP5-1.60 verification, 10 of these analytic benchmark problems were run to high precision. The 10 cases selected from [11] are listed in Table III along with the analytic results. For cases 11, 14, and 18, 2050 cycles of 20,000 neutrons were run, with the first 50 cycles discarded for settling. For the other cases, a total of 2100 cycles of 20,000 neutrons were run, with the first 100 cycles discarded for settling. For all cases, 40 million neutrons in active cycles contributed to the k_{eff} estimate from MCNP5.

Table III. Analytic Criticality Verification Problems

	Name	Description	Exact K-eff
11	Ua-1-0-IN	Infinite medium, 1 group	2.25
14	Ua-1-0-SP	Sphere, 1 group	1.0
18	Uc-H2O(2)-1-0-SP	Reflected sphere, 1 group	1.0
23	UD2O-1-0-CY	Cylinder, 1 group	1.0
32	PUa-1-1-SL	Slab, 1 grp, P1 scatter	1.0
41	UD2OB-1-1-SP	Sphere, 1 grp, P1 scatter	1.0
44	PU-2-0-IN	Infinite medium, 2 group	2.683767
54	URRa-2-0-SL	Slab, 2 group	1.0
63	URRd-H2O(1)2-0-ISLC	Slab, 2 group	1.0
75	URR-6-0-IN	Infinite medium, 6 group	1.60

D. Radiation Shielding Validation Suite

The radiation-shielding validation suite [7,12,13] contains three subcategories: time-of-flight spectra for neutrons from pulsed spheres, neutron and photon spectra at shield walls within a simulated fusion reactor, and photon dose rates. Two of the cases are coupled neutron-photon calculations, while the others are exclusively neutron or exclusively photon calculations.

Table IV. Summary of MCNP Radiation Shielding Validation Suite: Pulsed Spheres

MCNP Input	Target Material	Target Configuration	Thickness (mfp)	Detector Type	Detector Angle	Experiment Number
BE08	Beryllium	Bare Sphere	0.8	Pilot B	30E	9
C29	Carbon	Bare Sphere	2.9	NE 213	30E	14
CCR20	Concrete	Bare Sphere	2.0	NE 213	120E	52
FE09	Iron	Bare Sphere	0.9	NE 213	30E	31
PB14	Lead	Clad Sphere	1.4	NE 213	30E	37
LI616	^{6}Li	Dewar	1.6	NE 213	30E	4
N31	Nitrogen	Dewar	3.1	Pilot B	30E	18
H2O19	Water	Dewar	1.9	Pilot B	30E	40

The time-of-flight cases are a subset of the pulsed-sphere experiments that were performed at Lawrence Livermore National Laboratory from the late 1960s into the 1980s [18-20]. The objective of these experiments was to measure the neutron emission spectrum from a variety of materials bombarded by 14 MeV neutrons. These cases in the suite are summarized in Table IV.

The second subset of cases in the radiation-shielding validation suite is based on a series of experiments that was performed at Oak Ridge National Laboratory in 1980 [21]. The objective of the experiments was to simulate the deuterium-tritium 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. The fusion-shielding cases in the radiation-shielding validation suite are summarized in Table V. The last column indicates whether the detector was aligned with the axis of the particle beam.

Table V. Summary of MCNP Radiation Shielding Validation Suite: Fusion Shielding

MCNP Input	Configuration	Tally Type	On/Off Axis
FS1ONN	1	neutron	On
FS3OFN	3	neutron	Off
FS3ONP	3	photon	On
FS7ONN	7	neutron	On
FS7OFP	7	photon	Off

The cases in the last subset of the radiation-shielding validation suite are based on experimental measurements of photon dose rates. The first case is based on a 1980 measurement of air-scattered photon radiation far from the source ("skyshine") [22]. The second case is an idealization of a number of measurements of the radiation environment in an open field covered by fallout [23]. The remaining four cases model some of the Hupmobile thermoluminescent dosimeter (TLD) experiments performed at Lawrence Berkeley Laboratory between 1967 and 1969 [24,25]. The six cases are summarized in Table VI.

Table VI. Summary of MCNP Radiation Shielding Validation Suite: Photon Dose Rates

MCNP Input	Case	Source	Principal Media
SKYINP	Skyshine	^{60}Co	Air and Soil
KERMIN	Air over Ground	^{60}Co	Air and Soil
COAIR	^{60}Co through Air	^{60}Co	Air
COTEF	^{60}Co through Teflon	^{60}Co	Teflon
SMAIR	Sm K_α through Air	Sm K_α	Air
SMTEF	Sm K_α through Teflon	Sm K_α	Teflon

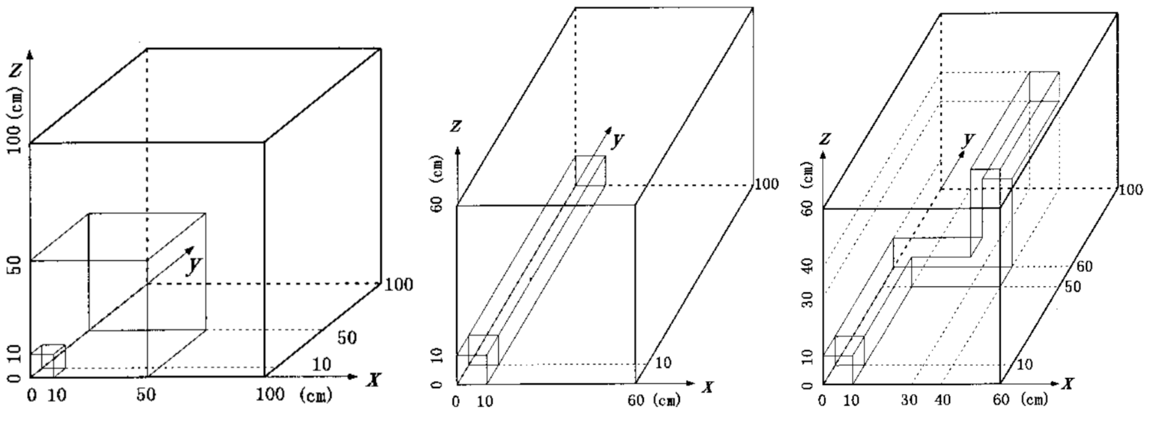
The MCNP calculations for the cases in this suite that include photons use the MCPLIB04 photon data library for all nuclides. The calculations for the radiation-shielding validation suite employed 1,000,000 particle histories for each case.

E. Kobayashi Benchmarks

This set of 3D benchmarks was defined by Kobayashi, Sugimura, and Nagaya in the OECD/NEA report “3-D Radiation Transport Benchmark Problems and Results for Simple Geometries with Void Regions” [14] and also described in [15]. The benchmark problems shown in Figure 1 consist of simple geometries that contain at least one void region and one mono-energetic, isotropic, cubic source region. Each configuration was simulated first with a purely absorbing and then with a fifty-percent scattering medium. One-group cross-sections are used for a purely absorbing material, and for a material with $\sigma_s/\sigma_t = .5$ and isotropic scattering. Fluxes were calculated at various points throughout the geometries using point detector tallies (F5). For the purely absorbing cases, Kobayashi supplied exact solutions obtained using numerical integration. For the cases with scattering, the reference solutions were computed by Y. Nagaya based on very long runs using the MVP Monte Carlo code.

For Problem 1, the results from 30 point-detector estimates of flux within the problem and on the boundary were compared to the exact analytic results (for the case with pure-absorber material) and to the reference MVP results (for the case with scattering). For Problem 2, the results from 16 point-detector estimates of flux were compared to the exact analytic results (for the case with pure-absorber material) and to the reference MVP results (for the case with scattering). For Problem 3, the results from 22 point-detector estimates of flux were compared to the exact analytic results (for the case with pure-absorber material) and to the reference MVP results (for the case with scattering). Overall, for 2 cases of each of the 3 problems, 136 different fluxes were compared between computed MCNP5 results and the reference.

Figure 1. Kobayashi Benchmark Problems



Problem 1 Problem 2 Problem 3

F. Point Kinetics Parameters Benchmark Suite

MCNP5-1.60 has, for the first time, the ability to compute adjoint-weighted tallies in criticality calculations using only the existing random walks. References [16,17] detail the ability to compute point reactor kinetics parameters: neutron generation times, Rossi-α, total and precursor-specific effective delayed neutron fractions, and average precursor decay constants. A series of verification and validation problems was added to the MCNP5 distribution. The verification problems are compared against both analytic solutions and with discrete ordinates results obtained from Partisn [16,17]. Unfortunately, Partisn does not handle delayed neutrons, so only the effective lifetime is validated this way. For validation, MC computes six values of Rossi-alpha and these values are compared against experimentally measured values.

Two infinite-medium test problems with analytic solutions are used to verify the methods for computing the kinetics parameters within MCNP. The problems specifically test the calculation of the effective lifetime using only prompt neutrons. The first problem is one group, and the second uses two energy groups.

Multigroup problems with finite geometries are tested using the discrete ordinates method with the code Partisn. Results for the effective lifetime are compared between MCNP and Partisn v6.26 (beta release). There are eight multigroup problems: (1) 4-group, bare, fast slab, (2) 4-group fissile slab with thermalizing reflector, (3) 2-group, three region slab problem involving fissile center, strong thermal absorber buffer zone, and moderating reflector, (4) 8-group, bare slab of homogeneous fissile/moderator mixture, (5) 4-group, bare, fast, sphere, (6) 4-group, sphere with reflector, (7) 4-group, bare, subcritical slab, and (8) 4-group, bare, supercritical slab.

Comparisons are made with experimental measurements of six criticality experiments from the OECD/NEA benchmark handbook [10]. These are: Godiva, Jezebel, BIG TEN, Flattop-233, Stacy (run 29), and WINCO (run 5). The corresponding designators are: HEU-MET-FAST-001, PU-MET-FAST-001, IEU-MET-FAST-007, U233-MET-FAST-006, LEU-SOL-THERM-007, HEU-SOL-THERM-038. The kinetics parameters are computed for each of the experiments. All calculations use 50k active cycles with 100k neutrons per cycle, a block size of ten, and ENDF/B-VII.0 data.

II. Verification/Validation Results on Different Computer Platforms

A. Linux Testing Results

Two Linux platforms are available at LANL for testing, the Yellowrail (Yr) and Turing (Tu) HPC clusters. Table VII provides a summary of each platform.

Table VII. Platform Summary for the Turing and Yellowrail clusters at Los Alamos National Laboratory

Name	Processor	OS	SUs or CUs	Nodes per SU/CU	CPU cores per Node / Total CPUs	Memory per compute Node / Total	Inter connect	Peak (TF)	Storage
Turing	AMD opteron	Linux (CHAOS)	1	64	16 / 1,204	32GB / 2TB	InfiniBand	9.4	144 TB Panasas
Yellowrail	AMD opteron	Linux	1	139	8/1,112	16GB / 2.22TB	InfiniBand	4.89	144 TB Panasas

In order to further validate and verify the code each test was compiled using different compilers:

- Intel v10.0.23 and gcc v4.3.3,
- Portland Group PGI v7.0-5,
- Portland Group PGI v9.0-3.
- gfortran

Shared Memory (Threading) Results

MCNP5 was compiled with only the shared memory (OpenMP or OMP) form of parallelism. For each compiler, the suites were run with varied numbers of threads to check for consistency. Table VIII offers an outline of the different environments used for each respective test and compiler.

Table VIII. List of platforms, compilers, compilation option (sequential or omp), and the number of OpenMP threads used in the run (if applicable).

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

With only a few peculiarities (see below), each of these tests ran with the expected outcomes (no differences). In all cases, bit-for-bit consistency is preserved between sequential and threaded runs. There are also no differences observed between the Turing and Yellowrail clusters. Between the Intel and PGI compilations, small differences in tally results are observed, likely because of numerical roundoff. Table IX summarizes the results from the Validation_Criticallity Suite and Table X summarizes the results from the Verification_Keff Suite.

The Regression tests, when run with more than one thread, always have output file differences (diff files with sizes ranging from 100 to 62,000 bytes), but no differences are observed in the tally results themselves. These differences are a result of the threads writing to the output file in a different order than for a sequential run, due to the asynchronous nature of the thread execution. Many of the differences found are in the DXTRAN transmission tables, weight window groups, print table 110, and print table 126. There were also many fatal errors (telling the user certain options are not thread-safe) and "tally not scored" warnings as a result of out-of-sync writing to the output file. Despite these differences, all *mctal* differences are zero with the exception of inp41, which is expected because the writes to the *mctal* file depend upon CPU speed, something not constant for threaded operations.

Tally results in Validation_Criticality and Verification_Keff are observed between the Intel and PGI-7 or PGI-9 compilations (different versions of PGI give the same results). The differences in MCNP results are within statistical bounds. The cause of these differences appears to be roundoff differences in the separate compilers.

The Verification_Keff test suites were run using ten of the 75 test cases provided in the suite; these numbers of these test problems are 11, 14, 18, 23, 32, 41, 44, 54, 63, and 75.

The results do not change for a different number of threads given the same compiler. Differences are observed between the Intel and PGI compilations, but not between different versions of PGI itself. The results differ within statistical bounds and appear to be numerical roundoff differences.

The Kobayashi test suite gives identical results for different compilers and number of threads. Results form the test suite are shown in Figures XIa – XId. The default number of histories run for all tests (Figures XIa, XIc, XId) was one million and almost all of the results converge to the reference solutions. Tests f1585, f1595, f3245, & f3255 do not converge to the reference solutions until one hundred million histories are run (Figure XIb). These tallies are deep within a thick shield, and variance reduction techniques have not (yet) been incorporated into the MCNP input for these cases, so that this behavior was expected.

Table IX. Validation_Criticality Results for Linux

LANL yellowrail & turing HPC clusters
MCNP Version = MCNP5-1.60
Data Version = ENDF/B-VI Data Libraries

	Experiment	MCNP-1.51	intel-10	pgi-7 & pgi-9
U233 Benchmarks				
JEZ233	1.0000 (10)	0.9911 (6)	0.9911 (6)	0.9911 (6)
FLAT23	1.0000 (14)	0.9996 (7)	0.9996 (7)	0.9996 (7)
UMF5C2	1.0000 (30)	0.9975 (7)	0.9975 (7)	0.9975 (7)
FLSTF1	1.0000 (83)	0.9898 (10)	0.9898 (10)	0.9898 (10)
SB25	1.0000 (24)	0.9953 (11)	0.9953 (11)	0.9953 (11)
ORNL11	1.0006 (29)	0.9978 (4)	0.9978 (4)	0.9978 (4)
HEU Benchmarks				
GODIVA	1.0000 (10)	0.9968 (6)	0.9968 (6)	0.9968 (6)
TT2C11	1.0000 (38)	0.9976 (8)	0.9979 (8)	0.9973 (8)
FLAT25	1.0000 (30)	1.0025 (6)	1.0025 (6)	1.0025 (6)
GODIVR	0.9985 (11)	0.9947 (8)	0.9947 (8)	0.9947 (8)
UH3C6	1.0000 (47)	0.9921 (8)	0.9921 (8)	0.9921 (8)
ZEUS2	0.9997 (8)	0.9934 (8)	0.9934 (8)	0.9949 (8)
SB5RN3	1.0015 (28)	0.9955 (14)	0.9955 (14)	0.9955 (14)
ORNL10	1.0015 (26)	0.9996 (4)	0.9996 (4)	0.9996 (4)
IEU Benchmarks				
IMF03	1.0000 (17)	0.9986 (6)	0.9986 (6)	0.9986 (6)
BIGTEN	0.9948 (13)	1.0072 (5)	1.0072 (5)	1.0072 (5)
IMF04	1.0000 (30)	1.0035 (6)	1.0035 (6)	1.0035 (6)
ZEBR8H	1.0300 (25)	1.0402 (6)	1.0406 (6)	1.0403 (5)
ICT2C3	1.0017 (44)	1.0007 (7)	1.0007 (7)	1.0003 (7)
STACY36	0.9988 (13)	0.9989 (7)	0.9989 (7)	0.9989 (7)
LEU Benchmarks				
BAWXI2	1.0007 (12)	0.9975 (7)	0.9975 (7)	0.9975 (7)
LST2C2	1.0024 (37)	0.9958 (6)	0.9958 (6)	0.9958 (6)
Pu Benchmarks				
JEZPU	1.0000 (20)	0.9977 (6)	0.9977 (6)	0.9977 (6)
JEZ240	1.0000 (20)	0.9988 (6)	0.9988 (6)	0.9988 (6)
PUBTNS	1.0000 (30)	0.9969 (6)	0.9969 (6)	0.9969 (6)
FLATPU	1.0000 (30)	1.0027 (7)	1.0027 (7)	1.0027 (7)
THOR	1.0000 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)
PUSH2O	1.0000 (10)	0.9956 (8)	0.9956 (8)	0.9956 (8)
HISHPG	1.0000 (110)	1.0105 (5)	1.0108 (6)	1.0105 (6)
PNL2	1.0000 (65)	1.0035 (9)	1.0035 (9)	1.0035 (9)
PNL33	1.0024 (21)	1.0044 (7)	1.0044 (7)	1.0044 (7)

Table X. MCNP Analytic Keff Criticality Verification Suite for Linux

MCNP Version = MCNP5-1.60

Case	Name	Exact	intel-10	pgi-7 & pgi-9
prob11	Ua-1-0-IN	2.25000	2.25000 (0)	2.25000 (0)
prob14	Ua-1-0-SP	1.00000	1.00006 (10)	1.00006 (10)
prob18	Uc-H2O(2)-1-0-SP	1.00000	1.00005 (11)	1.00005 (11)
prob23	UD2O-1-0-CY	1.00000	1.00000 (6)	1.00000 (6)
prob32	PUa-1-1-SL	1.00000	0.99995 (11)	0.99995 (11)
prob41	UD2Ob-1-1-SP	1.00000	1.00003 (7)	1.00003 (7)
prob44	PU-2-0-IN	2.68377	2.68380 (3)	2.68379 (3)
prob54	URRa-2-0-SL	1.00000	1.00007 (13)	1.00007 (13)
prob63	URRd-H2Ob(1)-2-0-ISLC	1.00000	0.99993 (6)	0.99993 (6)
prob75	URR-6-0-IN	1.60000	1.59999 (1)	1.59999 (1)

Table XIa. Kobayashi Benchmark Results for Linux – Problem 1

```
problem 1 - 3d, voids+absorbers

                x, y, z     Reference    Rel-Err      MCNP-result  Rel-err        C/E
      Detector Set A
            f1105  5, 5, 5    5.95659e+00  0.0000       5.98902e+00  0.0077         1.01
            f1115  5,15, 5    1.37185e+00  0.0000       1.37741e+00  0.0016         1.00
            f1125  5,25, 5    5.00871e-01  0.0000       5.02954e-01  0.0010         1.00
            f1135  5,35, 5    2.52429e-01  0.0000       2.53616e-01  0.0009         1.00
            f1145  5,45, 5    1.50260e-01  0.0000       1.51082e-01  0.0008         1.01
            f1155  5,55, 5    5.95286e-02  0.0000       5.98745e-02  0.0008         1.01
            f1165  5,65, 5    1.53283e-02  0.0000       1.54157e-02  0.0007         1.01
            f1175  5,75, 5    4.17689e-03  0.0000       4.20041e-03  0.0007         1.01
            f1185  5,85, 5    1.18533e-03  0.0000       1.19194e-03  0.0007         1.01
            f1195  5,95, 5    3.46846e-04  0.0000       3.48766e-04  0.0007         1.01
      Detector Set B
            f1205  5, 5, 5    5.95659e+00  0.0000       5.98902e+00  0.0077         1.01
            f1215 15,15,15    4.70754e-01  0.0000       4.72808e-01  0.0012         1.00
            f1225 25,25,25    1.69968e-01  0.0000       1.70924e-01  0.0008         1.01
            f1235 35,35,35    8.68334e-02  0.0000       8.74530e-02  0.0007         1.01
            f1245 45,45,45    5.25132e-02  0.0000       5.29738e-02  0.0006         1.01
            f1255 55,55,55    1.33378e-02  0.0000       1.34641e-02  0.0006         1.01
            f1265 65,65,65    1.45867e-03  0.0000       1.47220e-03  0.0006         1.01
            f1275 75,75,75    1.75364e-04  0.0000       1.76968e-04  0.0006         1.01
            f1285 85,85,85    2.24607e-05  0.0000       2.26640e-05  0.0006         1.01
            f1295 95,95,95    3.01032e-06  0.0000       3.03736e-06  0.0006         1.01
      Detector Set C
            f1305  5,55, 5    5.95286e-02  0.0000       5.98745e-02  0.0008         1.01
            f1315 15,55, 5    5.50247e-02  0.0000       5.53441e-02  0.0007         1.01
            f1325 25,55, 5    4.80754e-02  0.0000       4.83744e-02  0.0007         1.01
            f1335 35,55, 5    3.96765e-02  0.0000       3.99376e-02  0.0007         1.01
            f1345 45,55, 5    3.16366e-02  0.0000       3.18590e-02  0.0007         1.01
            f1355 55,55, 5    2.35303e-02  0.0000       2.37073e-02  0.0007         1.01
            f1365 65,55, 5    5.83721e-03  0.0000       5.87924e-03  0.0007         1.01
            f1375 75,55, 5    1.56731e-03  0.0000       1.57804e-03  0.0007         1.01
            f1385 85,55, 5    4.53113e-04  0.0000       4.56089e-04  0.0007         1.01
            f1395 95,55, 5    1.37079e-04  0.0000       1.37949e-04  0.0007         1.01

problem 1 - 3d, voids+abs+scat

                x, y, z     Reference    Rel-Err      MCNP-result  Rel-err        C/E
      Detector Set A
            f1405  5, 5, 5    8.29260e+00  0.0002       8.21008e+00  0.0023         0.99
            f1415  5,15, 5    1.87028e+00  0.0001       1.87171e+00  0.0015         1.00
            f1425  5,25, 5    7.13986e-01  0.0000       7.14294e-01  0.0010         1.00
            f1435  5,35, 5    3.84685e-01  0.0000       3.84947e-01  0.0008         1.00
            f1445  5,45, 5    2.53984e-01  0.0001       2.54409e-01  0.0009         1.00
            f1455  5,55, 5    1.37220e-01  0.0007       1.37618e-01  0.0050         1.00
            f1465  5,65, 5    4.65913e-02  0.0012       4.69768e-02  0.0065         1.01
            f1475  5,75, 5    1.58766e-02  0.0020       1.58611e-02  0.0083         1.00
            f1485  5,85, 5    5.47036e-03  0.0034       5.55882e-03  0.0125         1.02
            f1495  5,95, 5    1.85082e-03  0.0062       1.80738e-03  0.0194         0.98
      Detector Set B
            f1505  5, 5, 5    8.29260e+00  0.0002       8.21008e+00  0.0023         0.99
            f1515 15,15,15    6.63233e-01  0.0000       6.62661e-01  0.0011         1.00
            f1525 25,25,25    2.68828e-01  0.0000       2.69131e-01  0.0007         1.00
            f1535 35,35,35    1.56683e-01  0.0001       1.57175e-01  0.0008         1.00
            f1545 45,45,45    1.04405e-01  0.0001       1.04966e-01  0.0018         1.01
            f1555 55,55,55    3.02145e-02  0.0006       3.04680e-02  0.0087         1.01
            f1565 65,65,65    4.06555e-03  0.0007       4.05677e-03  0.0154         1.00
            f1575 75,75,75    5.86124e-04  0.0012       6.17315e-04  0.0374         1.05
            f1585 85,85,85    8.66059e-05  0.0020       7.53732e-05  0.0621         0.87
            f1595 95,95,95    1.12892e-05  0.0038       8.93999e-06  0.0904         0.79
      Detector Set C
            f1605  5,55, 5    1.37220e-01  0.0007       1.37618e-01  0.0050         1.00
            f1615 15,55, 5    1.27890e-01  0.0008       1.29261e-01  0.0053         1.01
            f1625 25,55, 5    1.13582e-01  0.0008       1.13956e-01  0.0055         1.00
            f1635 35,55, 5    9.59578e-02  0.0009       9.66584e-02  0.0059         1.01
            f1645 45,55, 5    7.82701e-02  0.0009       7.97329e-02  0.0065         1.02
            f1655 55,55, 5    5.67030e-02  0.0011       5.77584e-02  0.0073         1.02
            f1665 65,55, 5    1.88631e-02  0.0019       1.92730e-02  0.0090         1.02
            f1675 75,55, 5    6.46624e-03  0.0031       6.61780e-03  0.0121         1.02
            f1685 85,55, 5    2.28099e-03  0.0053       2.32574e-03  0.0176         1.02
            f1695 95,55, 5    7.93924e-04  0.0089       7.99651e-04  0.0271         1.01
```

Table XIb. Kobayashi Benchmark Results for Linux – Problem 1 with 100M Histories for the Case with Absorption + Scattering

```
problem 1 - 3d, voids+abs+scat

                     x, y, z     Reference    Rel-Err      MCNP-result  Rel-err        C/E
       Detector Set A
             f1405   5, 5, 5     8.29260e+00  0.0002       8.22128e+00  0.0002         0.99
             f1415   5,15, 5     1.87028e+00  0.0001       1.86969e+00  0.0002         1.00
             f1425   5,25, 5     7.13986e-01  0.0000       7.13968e-01  0.0001         1.00
             f1435   5,35, 5     3.84685e-01  0.0000       3.84885e-01  0.0001         1.00
             f1445   5,45, 5     2.53984e-01  0.0001       2.54296e-01  0.0001         1.00
             f1455   5,55, 5     1.37220e-01  0.0007       1.37760e-01  0.0005         1.00
             f1465   5,65, 5     4.65913e-02  0.0012       4.68619e-02  0.0007         1.01
             f1475   5,75, 5     1.58766e-02  0.0020       1.59539e-02  0.0008         1.00
             f1485   5,85, 5     5.47036e-03  0.0034       5.48436e-03  0.0012         1.00
             f1495   5,95, 5     1.85082e-03  0.0062       1.83720e-03  0.0019         0.99
       Detector Set B
             f1505   5, 5, 5     8.29260e+00  0.0002       8.22128e+00  0.0002         0.99
             f1515  15,15,15     6.63233e-01  0.0000       6.63223e-01  0.0001         1.00
             f1525  25,25,25     2.68828e-01  0.0000       2.69135e-01  0.0001         1.00
             f1535  35,35,35     1.56683e-01  0.0001       1.57088e-01  0.0001         1.00
             f1545  45,45,45     1.04405e-01  0.0001       1.04884e-01  0.0002         1.00
             f1555  55,55,55     3.02145e-02  0.0006       3.01899e-02  0.0009         1.00
             f1565  65,65,65     4.06555e-03  0.0007       4.08987e-03  0.0015         1.01
             f1575  75,75,75     5.86124e-04  0.0012       5.89316e-04  0.0034         1.01
             f1585  85,85,85     8.66059e-05  0.0020       8.73064e-05  0.0087         1.01
             f1595  95,95,95     1.12892e-05  0.0038       1.16588e-05  0.0236         1.03
       Detector Set C
             f1605   5,55, 5     1.37220e-01  0.0007       1.37760e-01  0.0005         1.00
             f1615  15,55, 5     1.27890e-01  0.0008       1.28498e-01  0.0005         1.00
             f1625  25,55, 5     1.13582e-01  0.0008       1.13990e-01  0.0005         1.00
             f1635  35,55, 5     9.59578e-02  0.0009       9.65330e-02  0.0006         1.01
             f1645  45,55, 5     7.82701e-02  0.0009       7.88423e-02  0.0006         1.01
             f1655  55,55, 5     5.67030e-02  0.0011       5.65785e-02  0.0007         1.00
             f1665  65,55, 5     1.88631e-02  0.0019       1.89793e-02  0.0009         1.01
             f1675  75,55, 5     6.46624e-03  0.0031       6.50277e-03  0.0012         1.01
             f1685  85,55, 5     2.28099e-03  0.0053       2.29937e-03  0.0018         1.01
             f1695  95,55, 5     7.93924e-04  0.0089       8.00893e-04  0.0029         1.01
```

Table XIc. Kobayashi Benchmark Results for Linux – Problem 2

```
problem 2 - 3d, voids+absorbers

                    x, y, z      Reference     Rel-Err       MCNP-result   Rel-err         C/E
      Detector Set A
            f2105   5, 5, 5      5.95659e+00   0.0000        5.92674e+00   0.0075          0.99
            f2115   5,15, 5      1.37185e+00   0.0000        1.37399e+00   0.0016          1.00
            f2125   5,25, 5      5.00871e-01   0.0000        5.02003e-01   0.0010          1.00
            f2135   5,35, 5      2.52429e-01   0.0000        2.53214e-01   0.0009          1.00
            f2145   5,45, 5      1.50260e-01   0.0000        1.50868e-01   0.0008          1.00
            f2155   5,55, 5      9.91726e-02   0.0000        9.96694e-02   0.0008          1.01
            f2165   5,65, 5      7.01791e-02   0.0000        7.05995e-02   0.0007          1.01
            f2175   5,75, 5      5.22062e-02   0.0000        5.25705e-02   0.0007          1.01
            f2185   5,86, 5      4.03188e-02   0.0000        4.06402e-02   0.0007          1.01
            f2195   5,95, 5      3.20574e-02   0.0000        3.23450e-02   0.0007          1.01
      Detector Set B
            f2205   5,95, 5      3.20574e-02   0.0000        3.23450e-02   0.0007          1.01
            f2215  15,95, 5      1.70541e-03   0.0000        1.71500e-03   0.0013          1.01
            f2225  25,95, 5      1.40557e-04   0.0000        1.41036e-04   0.0015          1.00
            f2235  35,95, 5      3.27058e-05   0.0000        3.27827e-05   0.0014          1.00
            f2245  45,95, 5      1.08505e-05   0.0000        1.08697e-05   0.0013          1.00
            f2255  55,95, 5      4.14132e-06   0.0000        4.14726e-06   0.0012          1.00

problem 2 - 3d, voids+abs+scat

                    x, y, z      Reference     Rel-Err       MCNP-result   Rel-err         C/E
      Detector Set A
            f2305   5, 5, 5      8.61696e+00   0.0006        8.56303e+00   0.0022          0.99
            f2315   5,15, 5      2.16123e+00   0.0001        2.16061e+00   0.0014          1.00
            f2325   5,25, 5      8.93437e-01   0.0001        8.94131e-01   0.0010          1.00
            f2335   5,35, 5      4.77452e-01   0.0001        4.78376e-01   0.0010          1.00
            f2345   5,45, 5      2.88719e-01   0.0001        2.89760e-01   0.0011          1.00
            f2355   5,55, 5      1.88959e-01   0.0001        1.89879e-01   0.0012          1.00
            f2365   5,65, 5      1.31026e-01   0.0002        1.31801e-01   0.0014          1.01
            f2375   5,75, 5      9.49890e-02   0.0002        9.55903e-02   0.0015          1.01
            f2385   5,85, 5      7.12403e-02   0.0002        7.18632e-02   0.0016          1.01
            f2395   5,95, 5      5.44807e-02   0.0002        5.50241e-02   0.0016          1.01
      Detector Set B
            f2405   5,95, 5      5.44807e-02   0.0002        5.50241e-02   0.0016          1.01
            f2415  15,95, 5      6.58233e-03   0.0024        6.91217e-03   0.0145          1.05
            f2425  25,95, 5      1.28002e-03   0.0034        1.30787e-03   0.0116          1.02
            f2435  35,95, 5      4.13414e-04   0.0036        4.17629e-04   0.0135          1.01
            f2445  45,95, 5      1.55548e-04   0.0045        1.60671e-04   0.0201          1.03
            f2455  55,95, 5      6.02771e-05   0.0060        5.83968e-05   0.0273          0.97
```

Table XId. Kobayashi Benchmark Results for Linux – Problem 3

```
problem 3 - 3d, voids+absorbers

                   x, y, z      Reference    Rel-Err      MCNP-result  Rel-err        C/E
      Detector Set A
            f3105   5, 5, 5     5.95659e+00  0.0000       5.93913e+00  0.0076         1.00
            f3115   5,15, 5     1.37185e+00  0.0000       1.37196e+00  0.0016         1.00
            f3125   5,25, 5     5.00871e-01  0.0000       5.01844e-01  0.0010         1.00
            f3135   5,35, 5     2.52429e-01  0.0000       2.53196e-01  0.0009         1.00
            f3145   5,45, 5     1.50260e-01  0.0000       1.50868e-01  0.0008         1.00
            f3155   5,55, 5     9.91726e-02  0.0000       9.96716e-02  0.0008         1.01
            f3165   5,65, 5     4.22623e-02  0.0000       4.24946e-02  0.0007         1.01
            f3175   5,75, 5     1.14703e-02  0.0000       1.15329e-02  0.0007         1.01
            f3185   5,85, 5     3.24662e-03  0.0000       3.26425e-03  0.0007         1.01
            f3195   5,95, 5     9.48324e-04  0.0000       9.53458e-04  0.0007         1.01
      Detector Set B
            f3205   5,55, 5     9.91726e-02  0.0000       9.96716e-02  0.0008         1.01
            f3215  15,55, 5     2.45041e-02  0.0000       2.46292e-02  0.0012         1.01
            f3225  25,55, 5     4.54477e-03  0.0000       4.56274e-03  0.0012         1.00
            f3235  35,55, 5     1.42960e-03  0.0000       1.43405e-03  0.0011         1.00
            f3245  45,55, 5     2.64846e-04  0.0000       2.65326e-04  0.0010         1.00
            f3255  55,55, 5     9.14210e-05  0.0000       9.15328e-05  0.0009         1.00
      Detector Set C
            f3305   5,95,35     3.27058e-05  0.0000       3.28347e-05  0.0014         1.00
            f3315  15,95,35     2.68415e-05  0.0000       2.69381e-05  0.0015         1.00
            f3325  25,95,35     1.70019e-05  0.0000       1.70565e-05  0.0016         1.00
            f3335  35,95,35     3.37981e-05  0.0000       3.39645e-05  0.0015         1.00
            f3345  45,95,35     6.04893e-06  0.0000       6.07755e-06  0.0014         1.00
            f3355  55,95,35     3.36460e-06  0.0000       3.37381e-06  0.0009         1.00

problem 3 - 3d, voids+abs+scat

                   x, y, z      Reference    Rel-Err      MCNP-result  Rel-err        C/E
      Detector Set A
            f3405   5, 5, 5     8.61578e+00  0.0004       8.52814e+00  0.0022         0.99
            f3415   5,15, 5     2.16130e+00  0.0001       2.16439e+00  0.0014         1.00
            f3425   5,25, 5     8.93784e-01  0.0001       8.96091e-01  0.0010         1.00
            f3435   5,35, 5     4.78052e-01  0.0001       4.79583e-01  0.0010         1.00
            f3445   5,45, 5     2.89424e-01  0.0001       2.90186e-01  0.0011         1.00
            f3455   5,55, 5     1.92698e-01  0.0001       1.93498e-01  0.0013         1.00
            f3465   5,65, 5     1.04982e-01  0.0008       1.06038e-01  0.0059         1.01
            f3475   5,75, 5     3.37544e-02  0.0011       3.44669e-02  0.0088         1.02
            f3485   5,85, 5     1.08158e-02  0.0016       1.09308e-02  0.0094         1.01
            f3495   5,95, 5     3.39632e-03  0.0027       3.45243e-03  0.0115         1.02
      Detector Set B
            f3505   5,55, 5     1.92698e-01  0.0001       1.93498e-01  0.0013         1.00
            f3515  15,55, 5     6.72147e-02  0.0002       6.72288e-02  0.0026         1.00
            f3525  25,55, 5     2.21799e-02  0.0003       2.21815e-02  0.0039         1.00
            f3535  35,55, 5     9.90646e-03  0.0003       9.88395e-03  0.0046         1.00
            f3545  45,55, 5     3.39066e-03  0.0019       3.35943e-03  0.0112         0.99
            f3555  55,55, 5     1.05629e-03  0.0033       1.06789e-03  0.0158         1.01
      Detector Set C
            f3605   5,95,35     3.44804e-04  0.0079       3.49978e-04  0.0249         1.02
            f3615  15,95,35     2.91825e-04  0.0066       2.88364e-04  0.0249         0.99
            f3625  25,95,35     2.05793e-04  0.0053       2.06502e-04  0.0308         1.00
            f3635  35,95,35     2.62086e-04  0.0008       2.67619e-04  0.0132         1.02
            f3645  45,95,35     1.05367e-04  0.0040       1.05811e-04  0.0448         1.00
            f3655  55,95,35     4.44962e-05  0.0044       4.17155e-05  0.0465         0.94
```

Shielding validation Suite

For the verification of MCNP5-1.60, special effort was made to obtain detailed experimental results from the reference documents and to plot the experimental results vs. MCNP5 results on a consistent basis. The results of this careful review of experiment and MCNP5-1.60 calculations are discussed in this section.

Pulsed Spheres

One set of problems chosen for inclusion in MCNP's shielding validation suite was the pulsed sphere experiments conducted at Lawrence Livermore National Laboratory though July 1971. In these experiments, a several materials were bombarded with 14 MeV neutrons, and their neutron emission spectra were measured with time of flight techniques. Eight of these cases, Table IV, were chosen as benchmarks. Experimental data can be found in [18,19,20] with the corresponding experiment numbers.

The eight cases shown in Table IV have been part of the MCNP Shielding Validation Suite since its initial development [7]. For the present work, the geometry, material compositions, source definitions, and other MCNP inputs were not changed from previous versions of the Suite. The tally bin structure, however, was modified for each of the 8 problems to match the time bin structure used in the references for reporting the experimental results. In the MCNP5 model, results were tallied in time bins corresponding to the intervals in the experimental measurements.

In addition, cases were run with MCNP5 without the spheres present, in order to determine the normalization factor for tallies in a manner consistent with the normalization procedure for the experimental results. The experimental measurements were normalized to dose without the spheres present. Thus, MCNP5 was run in the same configurations but without the spheres present. The total time-integrated dose of the no-sphere case was used as the normalization factor for the data in models.

MCNP5 results were plotted against the experimental data, as shown in Figures 2a and 2b. As is easily seen, the MCNP results correspond well with the experimental data, with the exceptions of the very early times (very high energy neutrons) and, to a lesser extent, the very late times (very low energy neutrons).

Figure 2a. Pulsed Sphere Problems, ■ Experiment, ● MCNP5

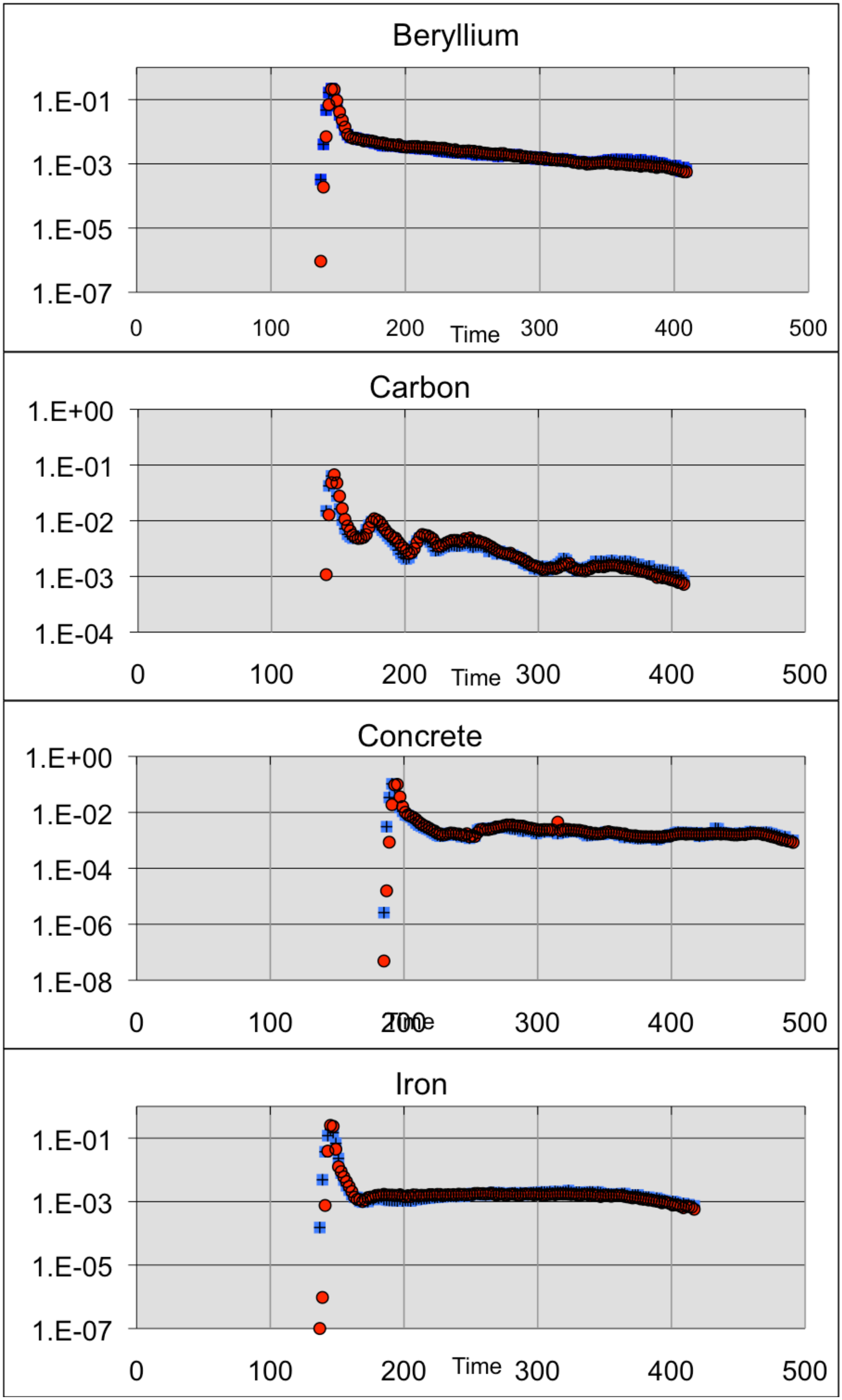
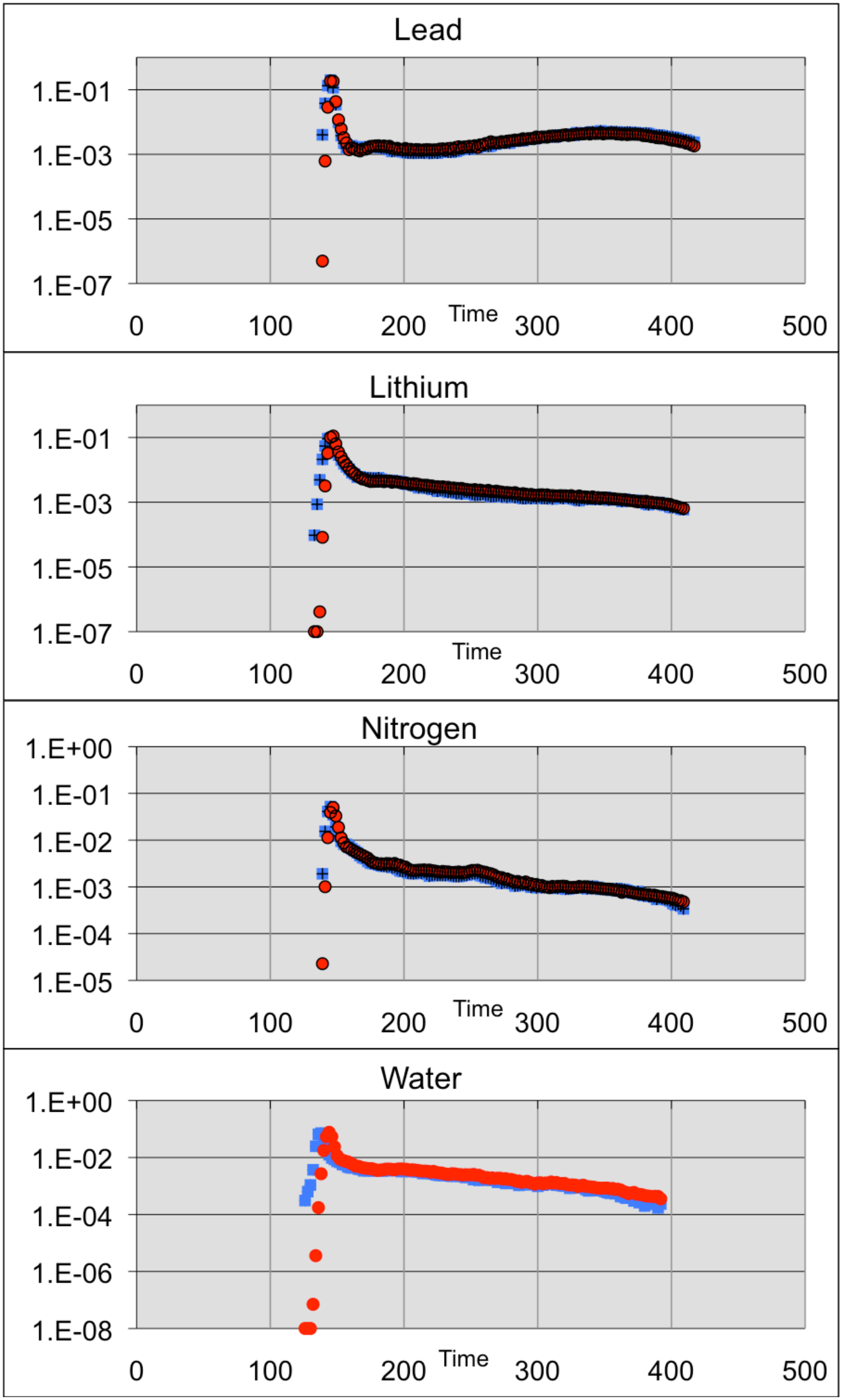


Figure 2b. Pulsed Sphere Problems, ■ Experiment, ● MCNP5



Fusion Shielding

The second series of problems in the Validation Shielding suite used for MCNP are those of fusion shielding, conducted at the Oak Ridge National Laboratory in 1980. These experiments contain measurements of both neutron and photon energy spectra. Experimental data can be found in [21]. Five cases were chosen for inclusion in the suite, summarized in Table V.

The five cases listed in Table V have been part of the MCNP Shielding Validation Suite since its initial development [7]. For the present work, the geometry, material compositions, source definitions, and other MCNP inputs were not changed from previous versions of the Suite. The tally bin structure, however, was modified for each of the 5 problems to match the energy bin structure used in the references for reporting the experimental results. In the MCNP5 model, results were tallied in energy bins corresponding to the intervals in the experimental measurements.

The experimental results give results as fluence with units of $\mathrm{MeV}^{-1}\mathrm{cm}^{-2}$ per source neutron. Thus, an F5 tally can be used in conjunction with an FM multiplier that includes the inverse of energy bin widths. No further normalization is needed, as both MCNP and the experimental results normalize results by the number of source particles. Comparisons for each of the 5 cases are shown in Figure 3. Experimental measurements are plotted as the center of the confidence interval. Very close agreement is seen for low and medium energy neutrons; some discrepancy is seen at very high neutron energies.

Skyshine

An MCNP photon shielding benchmark problem was selected to be the air-scattered photon radiation or “skyshine” experiment conducted by Nason, Shultis, and Faw at a shielding research facility on the Kansas plains in 1980. Experimental measurements can be found in [22].

The MCNP tally is modified such that the output is in units of $\mathrm{MeV/cm}^3$ per history. The experimental results, however, give exposure rates in microrads per hour per Curie. No changes to the input file geometry, materials, or sources were made from previous versions of the problem in the validation suite. The equation below shows the conversion from the tally output to this unit, using the density of air used in the MCNP calculation, 0.001124 $\mathrm{g/cm}^3$:

$$\frac{\dot{\mathrm{X}}}{\mathrm{Ci}} = \dot{\mathrm{X}}_{\mathrm{tally}} \cdot \left(1.602 \cdot 10^{-6} \frac{\mathrm{erg}}{\mathrm{MeV}}\right) \cdot \left(\frac{10^{6}\,\mu\mathrm{rad}}{100\ \mathrm{erg/g}}\right) \cdot \left(\frac{1}{0.001124\ \mathrm{g/cm^3}}\right) \cdot \left(3.7 \cdot 10^{10} \frac{\mathrm{histories/s}}{\mathrm{Ci}}\right) \cdot \left(3600 \frac{\mathrm{s}}{\mathrm{hr}}\right) = 1.898 \cdot 10^{15} \ \frac{\mu\mathrm{rad/hr} \cdot \mathrm{Ci}}{\mathrm{MeV/cm^3}} \cdot \dot{\mathrm{X}}_{\mathrm{tally}}$$

The experimental data were also multiplied by the surface area of the sphere subtended by the experimental geometry. When this is also applied to the MCNP results, the experimental data can be plotted against the MCNP results, as shown below in Figure 4.

Figure 3. Fusion Shielding Problems, ■ Experiment, ● MCNP5

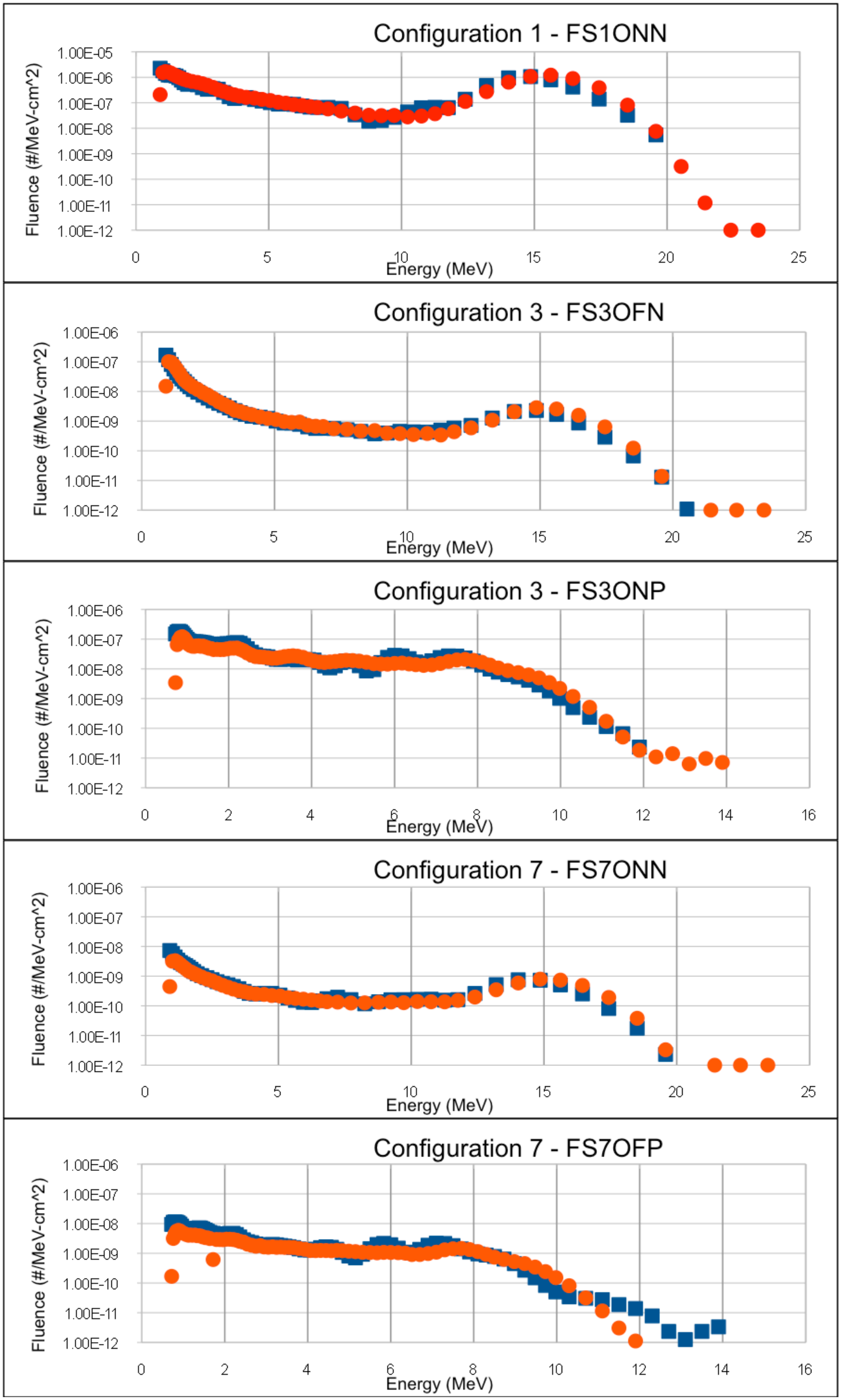
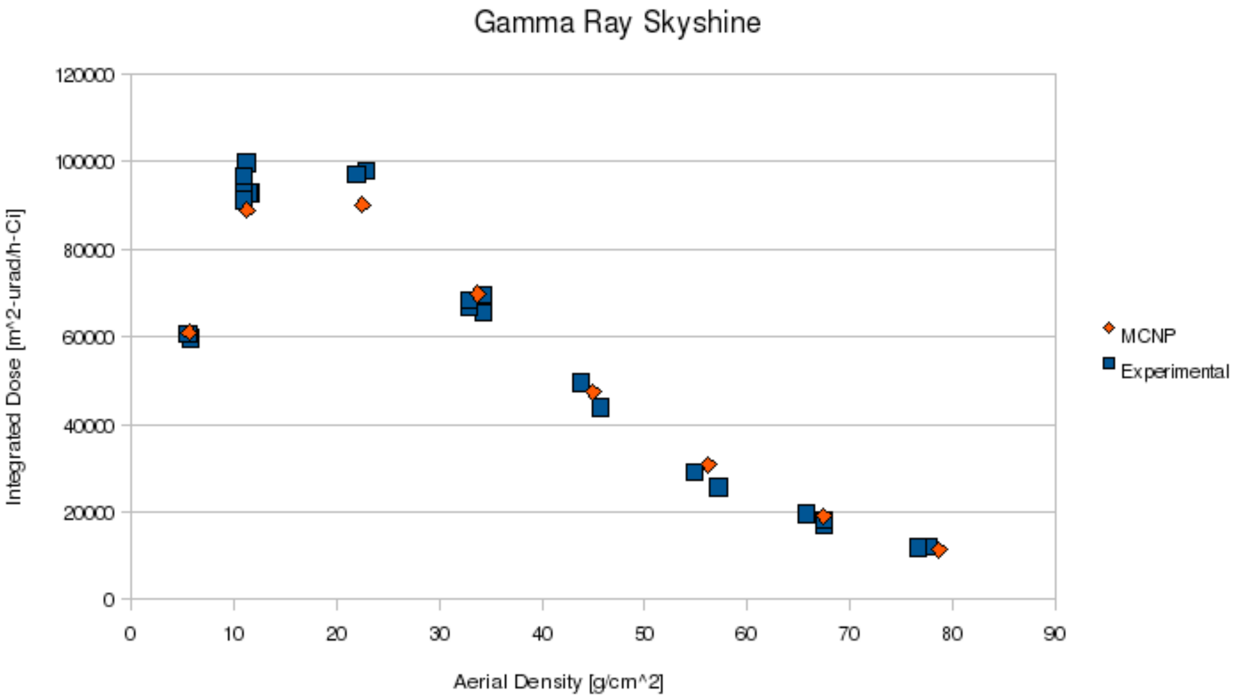


Figure 4. Results from Skyshine Benchmark



Other Shielding Benchmarks

For the remaining Shielding benchmarks (KERMIN, COAIR, COTEF, SMAIR, SMTEF), reconstruction of the experimental data and detailed plotting vs. MCNP5 results is in progress. For the air-over-ground problem (KERMIN), we are investigating inconsistencies in the specification of the problem compared to experiment. For the other cases, we were not able to obtain copies of the reports [24,25] containing the experimental results. Neither the LANL nor the LLNL technical report libraries had copies available, and none of the other LANL staff had old copies of the reports. Detailed comparison of the experimental measurements and MCNP5 results will be deferred until the reference reports can be located.

Point Kinetics Validation Suite

The Point Kinetics benchmark set was run on the Linux Turing HPC cluster using the Intel-10 executable for MCNP5-1.60 with 8, 9, and 16 OpenMP threads. Results from the 8, 9 and 16 thread runs were identical and are shown in Table XII. Since the capability to produce adjoint-weighted effective lifetimes and delayed neutron parameters is new with MCNP5-1.60, results from previous versions are not available. The results in Table XII are in complete agreement, however, with the verification results presented in Reference [17].

Table XII. MCNP Kinetics Parameter Validation Suite Results on Linux

MCNP Version = MCNP5-1.61

```
                Benchmark_Results        MCNP_Results

Rossi-Alpha (1/ns or 1/us) - Comparison with Experiments

    GODIVA        -0.0011   2e-05     -0.001131  7.414e-06
    JEZPU        -0.00064   1e-05     -0.000649  7.597e-06
    BIGTEN      -0.000117   1e-06    -0.0001156  6.907e-07
    FLAT23      -0.000267   5e-06    -0.0002931  2.567e-06
    STACY29     -0.000122   4e-06    -0.0001222  9.305e-07
    WINCO5      -0.001109   3e-06     -0.001124  9.942e-06

Generation Time (ns or us) - Comparison with Exact Analytic Solutions

    ONEINF             10       0         9.999  0.00085
    TWOINF          14.17       0         14.16  0.00275

Generation Time (ns or us) - Comparison with PARTISN Solutions

    BARESLAB        9.793       0         9.792  0.00594
    REFLSLAB        135.2       0         135.1  0.1068
    THRESLAB        49.17       0         49.28  0.1018
    INTRSLAB        112.1       0         112.7  0.4397
    BARESPHR        1.721       0         1.722  0.00102
    REFLSPHR        10.19       0         10.19  0.00737
    SUBCSLAB        10.17       0         10.17  0.0073
    SUPCSLAB        9.673       0         9.674  0.00526
```

Message Passing Results

Parallel MCNP5 was tested using the message passing interface (MPI) via the OpenMPI parallel libraries. All cases were run on the Turing cluster. Four compilers were considered, Intel Fortran v10.0.23, Portland v7.0-5, Portland v9.0-3, and gfortran. A summary of the cases run for verification and validation suites is given in Table XIII.

Table XIII. Summary of MPI test suite cases. The numbers shown are the number of MPI processes used. All tests were run on the Turing cluster.

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

Regression tests resulted in no differences in the tally results. However, some differences in standard output files were observed, with the size of generated difference files increasing with the number of processors. Many of these differences can be attributed to increasing numbers of warnings. However, in a few cases, differences were seen from other causes: Regression tests 18 and 38 have spacing differences in Table 110. Tests 23 and 47 result in Table 120 (cell importances) containing different cell neighbor listings in the test cases than in the reference output file. Test 28 has inconsistencies between the test case and reference output file for weight windows for cell 3. These sorts of differences in the diagnostics and information portions of the output files are typical for parallel MPI runs, and have always been seen in past verification tests. Most important, the *mctal* files are identical in the different runs, indicating that the Monte Carlo random walks were the same for all cases. (gfortran produced significant *mctal* differences, but after looking at the files, the differences were simply caused by "0.000" not matching "-0.000".)

All cases run for the Validation_Criticality suite compiled with Intel or PGI give bit-for-bit identical results when using different numbers of MPI processes. However, slight differences are observed between runs with Intel, PGI, and gfortran compilations. These differences, though, were found to be within statistical uncertainty and appear to be due to differences in numerical roundoff.

The 10 test cases selected from the Verification_Keff suite were run, and all results files are identical regardless of compiler or number of processors used.

For the Kobayashi test suite, all results files are found to be identical for all compilers and numbers of processors. The test cases were run with 100,000 histories and many tallies did not converge to the reference solutions. More histories should cause these results to converge to the reference solution; however, this was not investigated in this study, as this was addressed in the threading studies.

In addition to the above tests using just MPI for the parallel runs, the Intel-compiled executable was tested using both MPI message-passing and OpenMP threading for a number of cases shown in Table XIV. The combined MPI/OMP results were identical to those obtained with just MPI.

Table XIV. Summary of MPI/OMP test suite cases. All tests were run on the Turing cluster with the Intel-10 Fortran compiler.

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

B. Mac OS X Testing Results

Verification/validation testing was performed on Intel-based Macs, including a MacPro with 2 quad-core Xeon processors and on MacBooks with Intel Core2 Duo and Intel i7 processors. Both OS X 10.5.8 and 10.6.4 were used during the testing. The Fortran compilers used include: Intel-10.1, Intel-11.1, Absoft-11.0, g95, and gfortran. The only C compiler used in the testing was gcc. (It should be noted that C coding is used only for MCNP5 plotting, to interface with the X11 X-Windows graphics libraries, and is not used for computation during the Monte Carlo random walks.)

In testing MCNP5-1.60 with the various Fortran compilers, two particular compiler capabilities were investigated: including OpenMP threading, and generating 32-bit vs. 64-bit executables. The following conclusions were reached after extensive testing and experimentation:

- The Intel-10.1 Fortran compiler produces 32-bit executables with OpenMP threading that are correct and run efficiently. It was also tested with combined OpenMPI/OpenMP parallelism and worked correctly. (The ability to produce a 64-bit executable was not tested, due to difficulties with OS X 10.5.8 not having 64-bit X11 libraries.) This is the preferred compiler for current MCNP5-1.60 usage on the Mac. It was used to produce the executables for the RSICC code distribution package.

- The Intel-11.1 Fortran compiler produces either 32-bit or 64-bit executables with OpenMP threading, both of which worked correctly on OS X 10.6.4. There are some minor roundoff differences (for a few problems in the Criticality Validation Suite) that do not appear to be code or compiler errors. The 64-bit executable is roughly 10% faster than the 32-bit executable.

- The Absoft-11.0 Fortran compiler tested correctly in 32-bit mode without OpenMP threading. There were incorrect results from the 64-bit executable, so that option should not be used for MCNP5. Using OpenMP threading, there were errors and also some segmentation faults, so that option should not be used.

- The g95 Fortran compiler was tested with and without the OpenMP option. There were many errors with OpenMP, so that option should not be used. Without threading, the g95 version produced acceptable Regression test results.

- The gfortran Fortran compiler was tested with and without the OpenMP option. There were errors using OpenMP threading, so that option should not be used. Without threading, the gfortran version produced acceptable Regression test results.

To summarize, only the Intel-10.1 or Intel-11.1 Fortran compilers should be used for an OpenMP threaded version of MCNP5-1.60. At this time, other compilers can be used as long as OpenMP is not invoked for the compilation. Even though the 64-bit executable from Intel-11.1 was roughly 10% faster than the 32-bit version, the 32-bit version is our standard for testing and release since it is portable and executes correctly on all Intel-based Macs.

No testing was performed on the older PowerPC-based Macs. Those systems are now obsolete, since the last hardware was produced 5 years ago and the Fortran-90 compilers used for previous versions of MCNP5 are no longer available. In addition, MCNP5 performance on the older PowerPC Macs is about an order of magnitude slower than today's multicore Intel-based Macs. Users should not attempt to use the current MCNP5-1.60 on PowerPC-based Macs. Executables for those systems are not included in the MCNP5-1.60 release.

Regression Tests

The Regression test suite was tested primarily using a single thread (1 sequential process). For the Regression tests, all of the tally (*mctal* file) differences from the reference templates were zero, for all compilers tested. This indicates that the Monte Carlo random walks were performed correctly for all of the problems in the Regression suite, for all compilers. The reference templates for both output and tally files were generated on a Linux system, not a Mac OS X system. While the Mac testing gave *mctal* files that exactly matched the Linux templates, there were typically 2-5 output files that showed a few lines of differences from the Linux templates. These differences were in diagnostic information or incidental reports. As an example of roundoff effects, a common difference was the number of dxtran transmissions with weight less than 1.E-8 or some small number; this is clearly a roundoff effect since the tally results in the output and *mctal* files matched exactly. Typically, roundoff differences appear when testing in MCNP5 vs. some small threshold value.

Validation_Criticality Suite

The Criticality Validation Suite was tested using the Intel-10.1, Intel-11.1, and Absoft-11.0 Fortran compilers to build MCNP5-1.60. The basic reference results for this testing were the results produced by the previous version, MCNP5-1.51. OpenMP threading was used for the Intel compilers with 8 threads, but not for Absoft. Results for the experiments, reference results from MCNP5-1.51, and the MCNP5-1.60 results are shown in Table XV.

- The results for MCNP5-1.60 compiled with Intel-10.1 using OpenMP and 8 threads exactly matched the reference results.

- For the Intel-11.1 version of MCNP5-1.60, results matched the reference results (and Intel-10.1) for 28 of the 31 cases. Three cases showed small differences that are within statistics and appear to be acceptable roundoff differences. These differences are highlighted in Table XV. In running the tests, the 32-bit and 64-bit versions built with Intel-11.1 gave identical results to each other.

- For the Absoft-11.0 version of MCNP5-1.60, built without OpenMP threading, results matched the reference results (and Intel-10.1) for 28 of the 31 cases. Three cases showed small differences that are within statistics and appear to be acceptable roundoff differences.

The results in Table XV indicate that MCNP5-1.61 executes correctly for the Criticality Validation Suite problems. The preferred Fortran compiler is Intel-10.1, since it correctly supports efficient threading and exactly matches previous results from MCNP5-1.51. The Intel-11.1 Fortran compiler is entirely acceptable and also correctly supports OpenMP threading, but does show some small roundoff differences from the previous version. The Absoft-11.0 compiler is acceptable for non-threaded calculations. However, running the entire suite of problems takes 3 hours on a single thread, whereas the Intel versions with OpenMP threading take only 30 minutes using 8 threads. (The Intel-11.1 64-bit executable takes only 26 minutes with 8 threads.)

The Criticality Validation Suite was also run using the ENDF/B-VII data libraries, using MCNP5-1.51 and MCNP5-1.60 compiled with the Intel-10.1 Fortran compiler. Results from these tests are shown in Table XVI. The results from MCNP5-1.51 and MCNP5-1.60 match exactly for all problems, indicating that MCNP5-1.60 works correctly with either ENDF/B-VI or ENDF/B-VII data. (Since the release of ENDF/B-VII data, some of the benchmark problems in this test suite were modified to include isotopic rather than elemental data for ENDF/B-VII nuclides. As a result, the MCNP5-1.51 results in Table XV differ in a few cases from results reported in Reference [4]. The differences are due to the changes in benchmark compositions in the input files, and are not due to changes in either MCNP5-1.51 or the ENDF/B-VII data.)

Analytical Criticality Verification Suite

The analytical criticality verification suite [11] consists of 75 criticality problems for which exact results for k-effective are available from the literature. Reference [11] is included with the MCNP5-1.50 release documentation. A set of 10 problems was selected (Problems 11, 14, 18, 23, 32, 41, 44, 54, 63, 75) and run using both MCNP5-1.51 and MCNP5-1.60. These problems use a special set of cross-section data libraries, as specified in [11], and not the normal ENDF/B-VI or ENDF/B-VII data libraries distributed with MCNP5. Table XVII shows the results from these calculations, performed on a Mac Pro (2 quad-core Intel Xeon cpus, Mac OS X 10.4.11, Intel Fortran compiler 10).

For these problems, results calculated by MCNP5-1.51 and MCNP5-1.60 match each other exactly. Compared to the exact analytic benchmark results, 9 out of 10 cases for MCNP5-1.51 and MCNP5-1.60 agree with the exact results within one standard deviation, and 1 case (prob44) agrees with the exact result within 2 standard deviations.

Kobayashi Benchmark Suite

The Kobayashi benchmark suite was run on Mac OS X with MCNP5-1.60 executables built using the Intel-10 Fortran compilers. Results match exactly the results shown in Tables XIa, XIc, and XId for the Linux testing.

Others

The Point Kinetics Benchmark suite is very long-running and was not repeated on Mac OS X. Since the Shielding Validation Suite requires significant work to collect and plot the calculated vs. experimental results, it was also not tested in detail on Mac OS X. It was judged adequate to run the Regression tests, the Criticality validation Suite, the Analytic Criticality Verification Suite, and the Kobashi Suite on Mac OS X. While some minor roundoff differences were seen in output file results, no anomalies or errors were found during the testing.

Table XV. Validation_Criticality Results for Mac OS X

Mac OS X 10.5.8 & 10.6.4
MCNP Version = MCNP5-1.60
Data Version = ENDF/B-VI Data Libraries

	Experiment	MCNP-1.51	absoft-11	intel-10	intel-11
U233 Benchmarks					
JEZ233	1.0000 (10)	0.9911 (6)	0.9911 (6)	0.9911 (6)	0.9911 (6)
FLAT23	1.0000 (14)	0.9996 (7)	0.9996 (7)	0.9996 (7)	0.9996 (7)
UMF5C2	1.0000 (30)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)
FLSTF1	1.0000 (83)	0.9898 (10)	0.9898 (10)	0.9898 (10)	0.9898 (10)
SB25	1.0000 (24)	0.9953 (11)	0.9953 (11)	0.9953 (11)	0.9953 (11)
ORNL11	1.0006 (29)	0.9978 (4)	0.9978 (4)	0.9978 (4)	0.9978 (4)
HEU Benchmarks					
GODIVA	1.0000 (10)	0.9968 (6)	0.9968 (6)	0.9968 (6)	0.9968 (6)
TT2C11	1.0000 (38)	0.9976 (8)	0.9984 (9)	0.9976 (8)	0.9968 (8)
FLAT25	1.0000 (30)	1.0025 (6)	1.0025 (6)	1.0025 (6)	1.0025 (6)
GODIVR	0.9985 (11)	0.9947 (8)	0.9947 (8)	0.9947 (8)	0.9947 (8)
UH3C6	1.0000 (47)	0.9921 (8)	0.9921 (8)	0.9921 (8)	0.9921 (8)
ZEUS2	0.9997 (8)	0.9934 (8)	0.9952 (8)	0.9934 (8)	0.9934 (8)
SB5RN3	1.0015 (28)	0.9955 (14)	0.9955 (14)	0.9955 (14)	0.9955 (14)
ORNL10	1.0015 (26)	0.9996 (4)	0.9996 (4)	0.9996 (4)	0.9996 (4)
IEU Benchmarks					
IMF03	1.0000 (17)	0.9986 (6)	0.9986 (6)	0.9986 (6)	0.9986 (6)
BIGTEN	0.9948 (13)	1.0072 (5)	1.0072 (5)	1.0072 (5)	1.0072 (5)
IMF04	1.0000 (30)	1.0035 (6)	1.0035 (6)	1.0035 (6)	1.0035 (6)
ZEBR8H	1.0300 (25)	1.0402 (6)	1.0405 (6)	1.0402 (6)	1.0405 (6)
ICT2C3	1.0017 (44)	1.0007 (7)	1.0007 (7)	1.0007 (7)	1.0007 (7)
STACY36	0.9988 (13)	0.9989 (7)	0.9989 (7)	0.9989 (7)	0.9989 (7)
LEU Benchmarks					
BAWXI2	1.0007 (12)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)
LST2C2	1.0024 (37)	0.9958 (6)	0.9958 (6)	0.9958 (6)	0.9958 (6)
Pu Benchmarks					
JEZPU	1.0000 (20)	0.9977 (6)	0.9977 (6)	0.9977 (6)	0.9977 (6)
JEZ240	1.0000 (20)	0.9988 (6)	0.9988 (6)	0.9988 (6)	0.9988 (6)
PUBTNS	1.0000 (30)	0.9969 (6)	0.9969 (6)	0.9969 (6)	0.9969 (6)
FLATPU	1.0000 (30)	1.0027 (7)	1.0027 (7)	1.0027 (7)	1.0027 (7)
THOR	1.0000 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)
PUSH2O	1.0000 (10)	0.9956 (8)	0.9956 (8)	0.9956 (8)	0.9956 (8)
HISHPG	1.0000 (110)	1.0105 (5)	1.0105 (5)	1.0105 (5)	1.0115 (5)
PNL2	1.0000 (65)	1.0035 (9)	1.0035 (9)	1.0035 (9)	1.0035 (9)
PNL33	1.0024 (21)	1.0044 (7)	1.0044 (7)	1.0044 (7)	1.0044 (7)

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

	Experiment		MCNP5-1.51		MCNP5-1.60	
U233 Benchmarks						
JEZ233	1.0000	(10)	0.9989	(6)	0.9989	(6)
FLAT23	1.0000	(14)	0.9990	(7)	0.9990	(7)
UMF5C2	1.0000	(30)	0.9931	(6)	0.9931	(6)
FLSTF1	1.0000	(83)	0.9830	(11)	0.9830	(11)
SB25	1.0000	(24)	1.0053	(10)	1.0053	(10)
ORNL11	1.0006	(29)	1.0018	(4)	1.0018	(4)
HEU Benchmarks						
GODIVA	1.0000	(10)	0.9995	(6)	0.9995	(6)
TT2C11	1.0000	(38)	1.0018	(8)	1.0018	(8)
FLAT25	1.0000	(30)	1.0034	(7)	1.0034	(7)
GODIVR	0.9985	(11)	0.9990	(7)	0.9990	(7)
UH3C6	1.0000	(47)	0.9950	(8)	0.9950	(8)
ZEUS2	0.9997	(8)	0.9974	(7)	0.9974	(7)
SB5RN3	1.0015	(28)	0.9985	(13)	0.9985	(13)
ORNL10	1.0015	(26)	0.9993	(4)	0.9993	(4)
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)

Table XVII. MCNP Analytic Keff Criticality Verification Suite Results for Mac OS X

MCNP Version = MCNP5-1.60

```
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)
```

C. Windows Testing Results

Windows testing of MCNP5-1.60 was performed on a 32-bit Windows XP machine with 2 quad core Intel(R) Xeon(R) CPU X5550 @ 2.67GHz chips. The test suites were run with a variety of Fortran-90 compilers , including

- Absoft
    - Pro Fortran 11.0.0
    - Run with OpenMP
- CVF
    - Compaq Visual Fortran Optimizing Compiler Version 6.6 (Update B)
    - Compaq Visual Fortran 6.6-2518-47C86
    - Must be used with <u>no</u> optimization
- g95
    - configured with: /src/G95/gcc-4.0.3/configure --enable-languages=c --disable-nls
    - Thread model: single
    - gcc version 4.0.3 (g95 0.92!) Jun 17 2009
- Intel
    - Intel(R) Visual Fortran Compiler Professional for applications running on IA-32
    - Version 11.1 Build 20100203 Package ID: w_cprof_p_11.1.060

  - Run with OpenMP
- PGI
  - Portland Visual Fortran
  - pgf90 10.6-0 32-bit target on x86 Windows -tp penryn
  - Run with OpenMP

OpenMP threading was tested only for the Intel-11, Absoft-11, and PGI-10 compilers.

Regression Tests

The Regression test suite was tested primarily using a single thread (1 sequential process). For the Regression tests, all of the tally (*mctal* file) differences from the reference templates were zero, for all compilers tested. This indicates that the Monte Carlo random walks were performed correctly for all of the problems in the Regression suite, for all compilers.

While the Windows testing gave *mctal* files that exactly matched the Windows templates, there were typically 2-5 output files that showed a few lines of differences from the Windows templates generated using MCNP5-1.51 or the Linux templates. (Compiler optimization had to be turned off for the CVF version to match *mctal* results.) These differences were in diagnostic information or incidental reports. As an example of roundoff effects, a common difference was the number of dxtran transmissions with weight < 1.E-8 or some small number; this is clearly a roundoff effect since the tally results in the output and *mctal* files matched exactly. Typically, roundoff differences appear when testing in MCNP5 vs. some small threshold value.

It can be concluded that using different compilers can result in small differences due to arithmetic roundoff, but that the differences are small and within statistics.

Validation_Criticality Suite

The Criticality Validation Suite was tested using the Intel-11, PGI-10, Absoft-11, CVF, and g95 Fortran compilers to build MCNP5-1.60. The basic reference results for this testing were the results produced by the previous version, MCNP5-1.51. OpenMP threading was used for the Intel and PGI compilers with 8 threads, but not for other compilers. Results for the experiments, reference results from MCNP5-1.51, and the MCNP5-1.60 results are shown in Table XVIII.

- For the Intel-11 version of MCNP5-1.60, results matched the reference results for 28 of the 31 cases. Three cases showed small differences that are within statistics and appear to be acceptable roundoff differences. These differences are highlighted in Table XVIII.
- For the PGI, g95, and CVF versions of MCNP5-1.60 built without OpenMP threading, and for the Absoft version with OpenMP threading, results matched the reference results for 26 of the 31 cases. Five cases showed small differences that are within statistics and appear to be acceptable roundoff differences.

The results in Table XVII indicate that MCNP5-1.61 executes correctly for the Criticality Validation Suite problems on Windows. The preferred Fortran compiler is Intel-11, since it correctly supports efficient threading and most closely matches previous results from MCNP5-1.51. The other compilers are acceptable for non-threaded calculations.

Analytical Criticality Verification Suite

The analytical criticality verification suite consists of 75 criticality problems for which exact results for k-effective are available from the literature. A set of 10 problems was selected (Problems 11, 14, 18, 23, 32, 41, 44, 54, 63, 75) and run using MCNP5-1.60 on Windows. The results are shown in Table XIX. For these problems, results calculated by MCNP5-1.60 match the exact analytic benchmark results within statistics and show no errors.

Kobayashi Benchmark Suite

The Kobayashi benchmark suite was run on Windows with MCNP5-1.60 executables built using the Absoft-11, CVF, g95, and Intel-11 Fortran compilers.

- Results generated using the Intel-11, CVF, and g95 versions of MCNP5-1.60 match exactly the results shown in Tables XIa, XIc, and XId for the Linux testing.
- Results generated using the Absoft-11 version show roundoff differences in the individual tallies, but the same C/E values as the Linux results from Tables XIa, XIc, XId. The differences appear to be just simple arithmetic roundoff.

Others

The Point Kinetics Benchmark suite is very long-running and was not repeated on Windows. Since the Shielding Validation Suite requires significant work to collect and plot the calculated vs. experimental results, it was also not tested in detail on Windows. It was judged adequate to run the Regression tests, the Criticality validation Suite, the Analytic Criticality Verification Suite, and the Kobashi Suite on Windows. While some minor roundoff differences were seen in output file results, no anomalies or errors were found during the testing.

Table XVIII. Validation_Criticality Results for Windows

MCNP Version = MCNP5-1.60
Data Version = ENDF/B-VI Data Libraries

	Experiment	MCNP-1.51	absoft-11	cvf	g95	intel-11	pgi
U233 Benchmarks							
JEZ233	1.0000 (10)	0.9911 (6)	0.9911 (6)	0.9911 (6)	0.9911 (6)	0.9911 (6)	0.9911 (6)
FLAT23	1.0000 (14)	0.9996 (7)	0.9996 (7)	0.9996 (7)	0.9996 (7)	0.9996 (7)	0.9996 (7)
UMF5C2	1.0000 (30)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)
FLSTF1	1.0000 (83)	0.9898 (10)	0.9898 (10)	0.9898 (10)	0.9898 (10)	0.9898 (10)	0.9898 (10)
SB25	1.0000 (24)	0.9953 (11)	0.9953 (11)	0.9953 (11)	0.9953 (11)	0.9953 (11)	0.9953 (11)
ORNL11	1.0006 (29)	0.9978 (4)	0.9978 (4)	0.9978 (4)	0.9978 (4)	0.9978 (4)	0.9978 (4)
HEU Benchmarks							
GODIVA	1.0000 (10)	0.9968 (6)	0.9968 (6)	0.9968 (6)	0.9968 (6)	0.9968 (6)	0.9968 (6)
TT2C11	1.0000 (38)	0.9976 (8)	0.9981 (8)	0.9988 (8)	0.9983 (8)	0.9968 (8)	0.9972 (8)
FLAT25	1.0000 (30)	1.0025 (6)	1.0025 (6)	1.0025 (6)	1.0025 (6)	1.0025 (6)	1.0025 (6)
GODIVR	0.9985 (11)	0.9947 (8)	0.9947 (8)	0.9947 (8)	0.9947 (8)	0.9947 (8)	0.9947 (8)
UH3C6	1.0000 (47)	0.9921 (8)	0.9921 (8)	0.9921 (8)	0.9921 (8)	0.9921 (8)	0.9921 (8)
ZEUS2	0.9997 (8)	0.9934 (8)	0.9949 (8)	0.9937 (8)	0.9935 (7)	0.9934 (8)	0.9949 (8)
SB5RN3	1.0015 (28)	0.9955 (14)	0.9955 (14)	0.9955 (14)	0.9955 (14)	0.9955 (14)	0.9955 (14)
ORNL10	1.0015 (26)	0.9996 (4)	0.9996 (4)	0.9996 (4)	0.9996 (4)	0.9996 (4)	0.9996 (4)
IEU Benchmarks							
IMF03	1.0000 (17)	0.9986 (6)	0.9986 (6)	0.9986 (6)	0.9986 (6)	0.9986 (6)	0.9986 (6)
BIGTEN	0.9948 (13)	1.0072 (5)	1.0072 (5)	1.0072 (5)	1.0072 (5)	1.0072 (5)	1.0072 (5)
IMF04	1.0000 (30)	1.0035 (6)	1.0035 (6)	1.0035 (6)	1.0035 (6)	1.0035 (6)	1.0035 (6)
ZEBR8H	1.0300 (25)	1.0402 (6)	1.0406 (5)	1.0407 (6)	1.0403 (6)	1.0405 (6)	1.0397 (7)
ICT2C3	1.0017 (44)	1.0007 (7)	1.0003 (7)	1.0003 (7)	1.0003 (7)	1.0007 (7)	1.0003 (7)
STACY36	0.9988 (13)	0.9989 (7)	0.9989 (7)	0.9989 (7)	0.9989 (7)	0.9989 (7)	0.9989 (7)
LEU Benchmarks							
BAWXI2	1.0007 (12)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)	0.9975 (7)
LST2C2	1.0024 (37)	0.9958 (6)	0.9958 (6)	0.9958 (6)	0.9958 (6)	0.9958 (6)	0.9958 (6)
Pu Benchmarks							
JEZPU	1.0000 (20)	0.9977 (6)	0.9977 (6)	0.9977 (6)	0.9977 (6)	0.9977 (6)	0.9977 (6)
JEZ240	1.0000 (20)	0.9988 (6)	0.9988 (6)	0.9988 (6)	0.9988 (6)	0.9988 (6)	0.9988 (6)
PUBTNS	1.0000 (30)	0.9969 (6)	0.9969 (6)	0.9969 (6)	0.9969 (6)	0.9969 (6)	0.9969 (6)
FLATPU	1.0000 (30)	1.0027 (7)	1.0027 (7)	1.0027 (7)	1.0027 (7)	1.0027 (7)	1.0027 (7)
THOR	1.0000 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)	1.0054 (6)
PUSH2O	1.0000 (10)	0.9956 (8)	0.9956 (8)	0.9956 (8)	0.9956 (8)	0.9956 (8)	0.9956 (8)
HISHPG	1.0000 (110)	1.0105 (5)	1.0105 (6)	1.0113 (5)	1.0107 (5)	1.0115 (5)	1.0105 (6)
PNL2	1.0000 (65)	1.0035 (9)	1.0035 (9)	1.0035 (9)	1.0035 (9)	1.0035 (9)	1.0035 (9)
PNL33	1.0024 (21)	1.0044 (7)	1.0044 (7)	1.0044 (7)	1.0044 (7)	1.0044 (7)	1.0044 (7)

Table XIX. MCNP Analytic Keff Criticality Verification Suite for Windows

MCNP Version = MCNP5-1.60

Case	Name	Exact	absoft-11	cvf	g95	intel-11
prob11	Ua-1-0-IN	2.25000	2.25000 (0)	2.25000 (0)	2.25000 (0)	2.25000 (0)
prob14	Ua-1-0-SP	1.00000	1.00006 (10)	1.00006 (10)	1.00006 (10)	1.00006 (10)
prob18	Uc-H2O(2)-1-0-SP	1.00000	1.00005 (11)	1.00005 (11)	1.00005 (11)	1.00005 (11)
prob23	UD2O-1-0-CY	1.00000	1.00000 (6)	1.00000 (6)	1.00000 (6)	1.00000 (6)
prob32	PUa-1-1-SL	1.00000	0.99995 (11)	0.99995 (11)	0.99995 (11)	0.99995 (11)
prob41	UD2Ob-1-1-SP	1.00000	1.00003 (7)	1.00003 (7)	1.00003 (7)	1.00003 (7)
prob44	PU-2-0-IN	2.68377	2.68378 (3)	2.68378 (3)	2.68378 (3)	2.68382 (3)
prob54	URRa-2-0-SL	1.00000	1.00007 (13)	1.00007 (13)	1.00007 (13)	1.00007 (13)
prob63	URRd-H2Ob(1)-2-0-ISLC	1.00000	0.99993 (6)	0.99993 (6)	0.99993 (6)	0.99993 (6)
prob75	URR-6-0-IN	1.60000	1.60000 (1)	1.59999 (1)	1.59999 (1)	1.59999 (1)

IV Conclusions

The release notes for MCNP5-1.60 [5] describe the new features that are part of MCNP5-1.60 and a number of bugs in previous versions that have been fixed. Each of the coding changes for the new features and bug-fixes was independently checked to ensure that the changes were correct and did not interfere with the overall correctness of MCNP5 calculations.

The verification/validation testing described in the current report constitutes a set of integrated tests for a variety of criticality and shielding problems. The principal goal of this integrated testing is to ensure that the entire collection of changes in MCNP5 in going from MCNP5-1.51 to MCNP5-1.60 does not disrupt the integrity, correctness, and reliability of MCNP5 results for a varied set of typical application problems.

The conclusions of the testing described in this report can be summarized by:

- When MCNP5-1.51 and MCNP5-1.60 are compiled and run on the same computer hardware, using the same compiler, compiler options, code physics options, and data libraries, the two versions of MCNP5 produce identical results.

- The above statement is true, regardless of whether the code is run sequentially with 1-CPU, using threaded parallelism with multiple CPUs, using MPI parallelism with multiple CPUs, or using both threaded and MPI parallelism with multiple CPUs.

- When different compilers, compiler options, or computer hardware are used, MCNP5 results may differ slightly due to computer arithmetic roundoff. The observed differences were expected, reasonable, and explainable, with all results agreeing within statistics. The observed differences do not provide any indication of coding errors, execution errors, or data errors.

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