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MCNP5-1.60 Development & Verification

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Abstract

MCNP5-1.60 Development & Verification

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The latest release of the MCNP5 Monte Carlo code is designated MCNP5-1.60. It includes 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. In addition, there are many minor code modifications to fix reported bugs, output formats, error checking, and other difficulties present with previous versions of MCNP. In nearly all cases, the bug fixes addressed problems with infrequently-used combinations of code options. In some cases, the problems that are fixed date back to the 1990s, but were only recently reported and fixed. All previously existing code capabilities are preserved, including physics options, geometry, tallying, plotting, cross-section handling, etc. No errors were found that would affect the code results for basic criticality calculations. Extensive verification and validation testing was performed, involving roughly 5,000 hrs of computing time. 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, except where bugs were discovered and fixed. In this presentation, we summarize the code enhancements and provide some results from the verification/validation effort.

MCNP5-1.60 Development & Verification

- **MCNP5-1.60 Release**
  - General Information
  - Features & Bug-fixes
- **Verification / Validation**
  - V&V Suites & Results
  - Parallel Testing with MPI & Threads
  - Additional V&V Suites
- **Conclusions & Future Plans**
  - MCNP5-1.60
  - MCNP6
  - References

MCNP5-1.60 Release

MCNP5-1.60 Release

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

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

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

New Features in MCNP5-1.60 (1)

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

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

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

New Features in MCNP5-1.60 (2)

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

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

- **Additional V&V suites – see part 3 of this presentation**

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

New Features in MCNP5-1.60 (3)

Monte Carlo Codes
XCP-3, LANL

MCNP criticality problems with OpenMP threading:

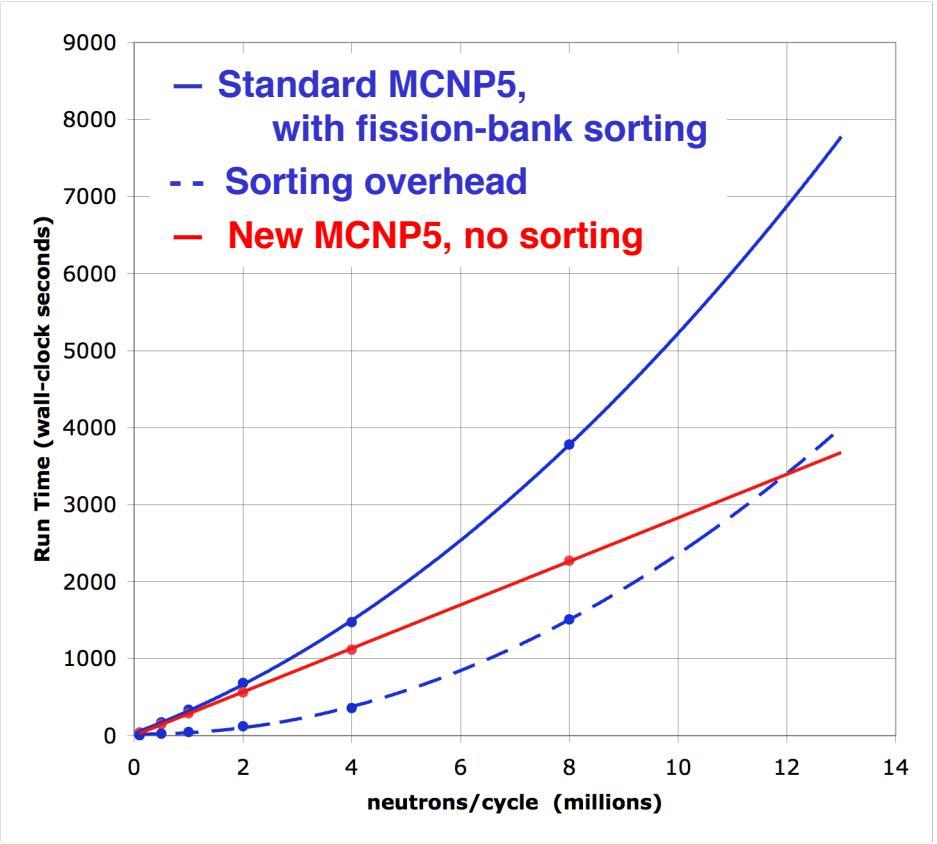
- Fission-bank needs to be reordered into a unique ordering that is independent of the number of threads or MPI processes.

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

$$T \sim O(N^2) \qquad N = \text{neuts/cycle}$$

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

$$T \sim O(N) \qquad N = \text{neuts/cycle}$$



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

Verification
&
Validation

Verification / Validation for MCNP5-1.60 (1)

- **Testing + V&V Suites**

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

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

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

Verification / Validation for MCNP5-1.60 (2)

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

- **Additional V&V Suites coming**
  - **VALIDATION_CRIT_EXPANDED** - 119 ICSBEP Handbook experiments
    - See talk at this meeting by Russ Mosteller
  - **Rossi Alpha Validation Suite** - 12 benchmark experiments
    - See paper for ICNC-2011 meeting

Verification / Validation for MCNP5-1.60 (3)

Monte Carlo Codes
XCP-3, LANL

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

	Experiment	MCNP5-1.51	MCNP5-1.60
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)

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

MCNP Criticality Verification Suite - VERIFICATION_KEFF

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

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

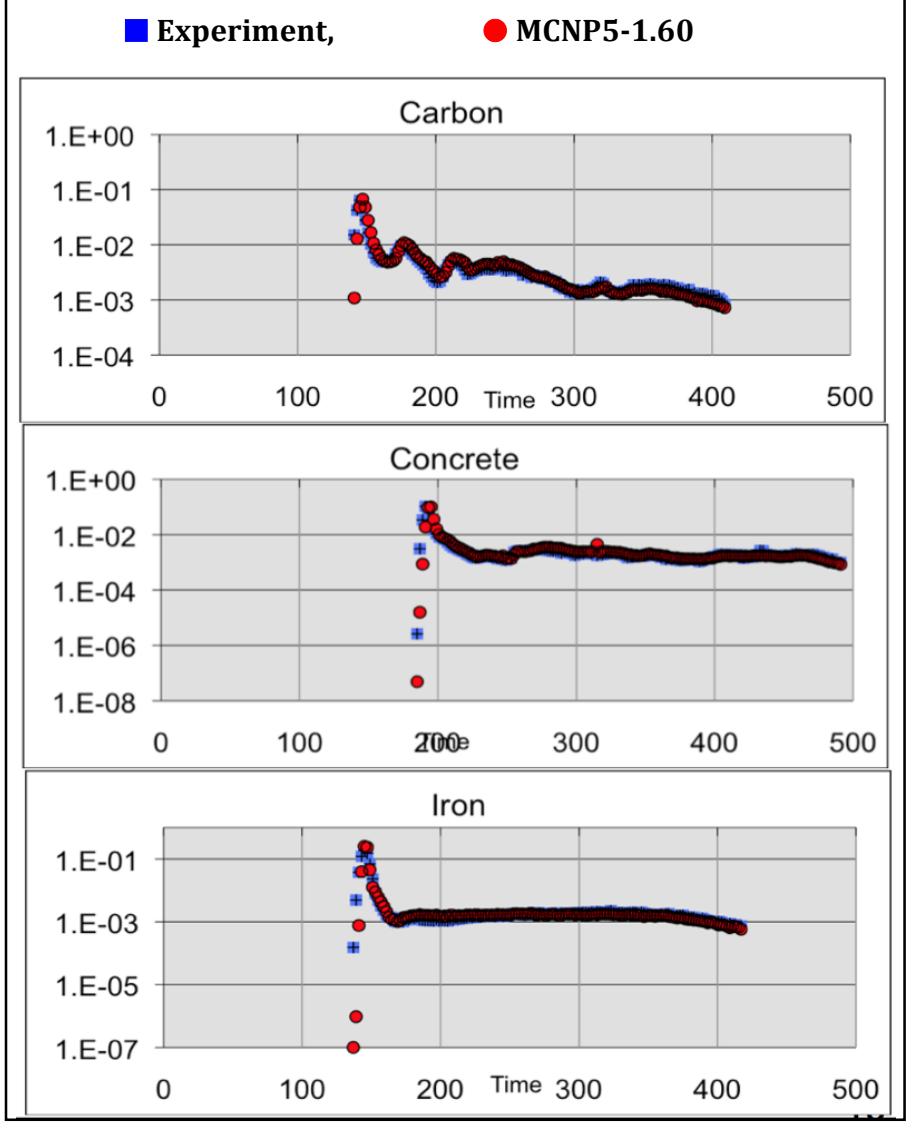
Verification / Validation for MCNP5-1.60 (5)

Monte Carlo Codes
XCP-3, LANL

MCNP Kinetics Parameter Validation Suite Results on Linux

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

Pulsed Sphere Problems (3 of 8)



Kobayashi Benchmark Results

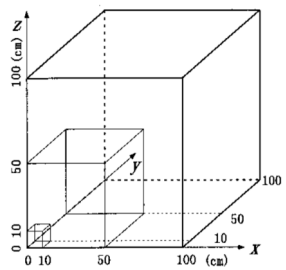
(1 of 6 problems)

Problem 1, Absorption + Scatter, 100M Histories

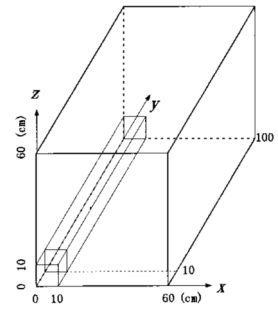
	x, y, z	Reference		MCNP-result		C/E
		Detector Set A				
f1405	5, 5, 5	8.29e+0	0.0002	8.22e+0	0.0002	**0.99**
f1415	5,15, 5	1.87e+0	0.0001	1.86e+0	0.0002	**1.00**
f1425	5,25, 5	7.13e-1	0.0000	7.13e-1	0.0001	**1.00**
f1435	5,35, 5	3.84e-1	0.0000	3.84e-1	0.0001	**1.00**
F1445	5,45, 5	2.53e-1	0.0001	2.54e-1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

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

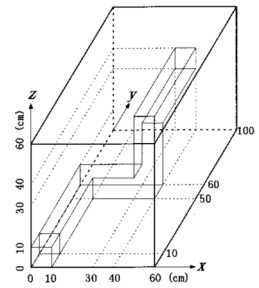
 # 1



 # 2



 # 3



Verification / Validation for MCNP5-1.60 (7)

Parallel testing - OpenMP threads on Linux

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

Parallel testing - MPI nodes on Linux

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

Parallel testing - MPI+threads

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

Rossi-alpha Validation Suite

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

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

Expanded Criticality Validation Suite

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

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

- **119 ICBEP Handbook experiments:**

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

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

Conclusions
&
Future Release Plans

MCNP5-1.60

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

MCNP6

- **MCNP6 = MCNP5 + MCNPX merger**
  - Retains all capabilities in MCNP5 & MCNPX
    - High-energy physics (ie, GeV, TeV), 36 particle types, heavy ions, …..
    - Many new features for Homeland Security, detectors, …..
    - Depletion using CINDER-90, …..
- **Impact on Criticality Calculations → none**
  - **All KCODE criticality features same as for MCNP5**
  - **Matches results with MCNP5 for criticality suites**
- **Monte Carlo team will support MCNP6, not MCNP5/MCNPX/MCNP6**
- **MCNP6 is coming**
  - Beta-0 release: 1Q CY 2011 – very limited distribution
  - Beta-1 release: 4Q CY 2011 – general beta testing
  - Production release: CY 2012 – general public release

Later this year, we need to plan for MCNP5 → MCNP6 transition

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Adjoint-weighted Tallies

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Questions ?