LA-UR-12-25950
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Title:	Verification of MCNP5-1.60 and MCNP6-Beta2 for Criticality Safety Applications
Author(s):	Kiedrowski, Brian C. Brown, Forrest B. Bull, Jeffrey S.
Intended for:	2012 ANS Winter Meeting and Nuclear Technology Expo, 2012-11-11/2012-11-15 (San Diego, California, United States)

Verification of MCNP5-1.60 and MCNP6-Beta2 for Criticality Safety Applications

Brian C. Kiedrowski, Forrest B. Brown, and Jeffrey S. Bull

Los Alamos National Laboratory

November 12, 2012

Abstract

The Monte Carlo code MCNP has been used for decades for high-fidelity criticality analysis. MCNP5-1.60 is the last production release, and MCNP6 is currently in beta testing. Verification and Validation has been done with the comparing code versions, compilers, platforms, and parallel options. The results show very strong consistency, confirming that MCNP is performing as expected.

Take-Away Message

- **All is well for MCNP criticality!**
- Comparisons between different code versions, compilers, platforms, and parallel options show strong agreement, often bit-for-bit.
- Observed differences are small and because of numerical round-off.

- Full report available online (**mcnp.lanl.gov**) under "Publications".
- Search for report number **LA-UR-12-21041**.
- Summary of numerical evidence to follow...

Overview

- MCNP5-1.60 and MCNP6 status
- Discussion of validation suites
- Compilers, platforms, etc.
- Results

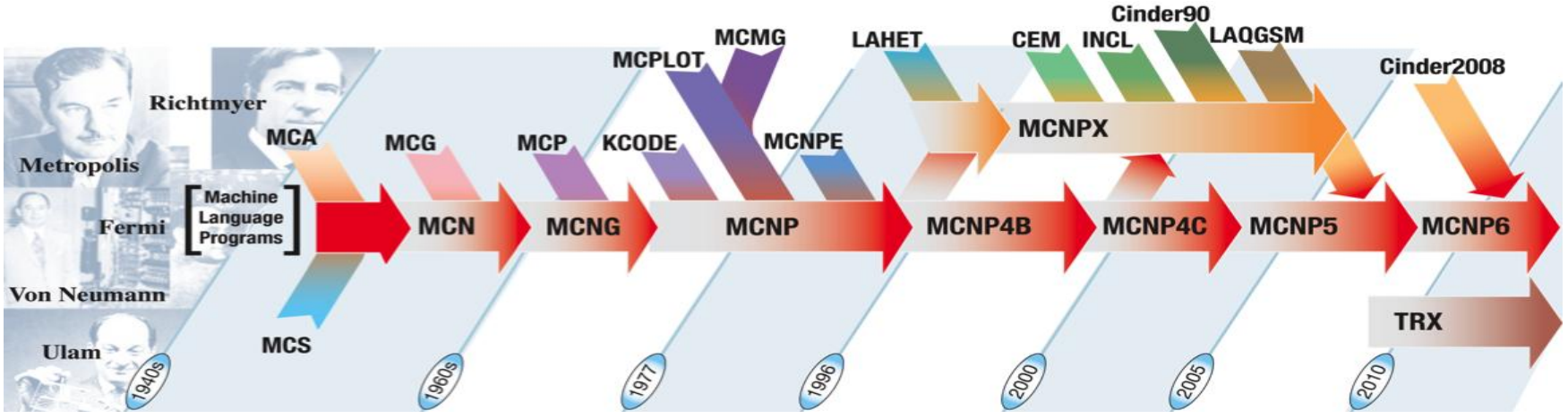
MCNP5-1.60 Status

- Released October 2010
- Stable, solid, maintenance mode, few bug reports
- Recommended working version for criticality safety users
- Most extensive V&V ever (thousands of CPU hours)
- Supports MPI + OMP forms of parallelism

MCNP5-1.60 New Features

- Adjoint-Weighted Tallies for Point Kinetics Parameters
- Mesh Tallies for Isotopic Reaction Rates
- Increased Limits for Geometry, Tally, and Source Specifications
- Web-based documentation
- Utility programs
- Additional V&V suites

MCNP6 Status



- Merger of MCNP5 and MCNPX complete!
- MCNP6 = merged codes + new features
- MCNP6-Beta2 currently available from RSICC.
- MCNP6-Beta3 being tested and available soon.
- Hopefully, production version of MCNP6 to follow.
- **Rigorous efforts made to preserve bit-for-bit tracking between MCNP5 and MCNP6!**

MCNPX

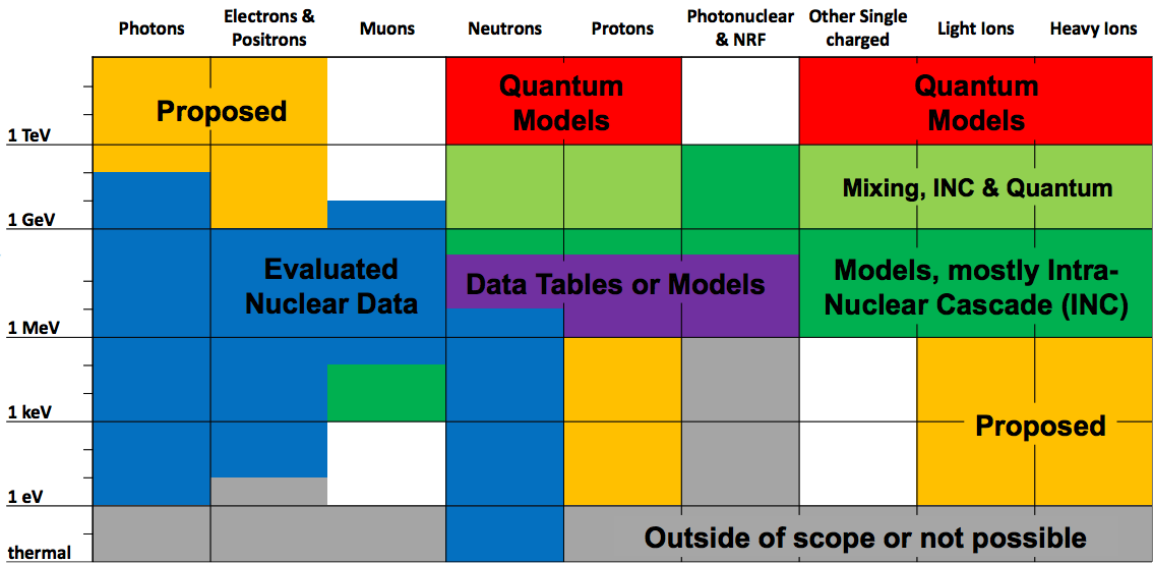
- Separate development path from MCNP4C.
- Contains core physics, with additional extensions for high-energy physics, exotic particles, detector calculations, etc.
- Not supported by criticality safety interests, minimal in-house V%V performed.
- Only new relevant feature for criticality safety is Monte Carlo depletion.

- **From a capability standpoint, MCNP6 contains all of MCNP5 and MCNPX.**

MCNP6 New Features for Criticality

- Fission Matrix
- Adjoint-Based Perturbations and Sensitivities

MCNP6 High-Energy Models



- High-energy physics models included in MCNP6.
- Off by default for classic problems and **NOT recommended for criticality!**
- OMP locks for thread safety recently installed.

Validation Suites

- Standard Suite: 31 problem set, ENDF/B-VII.0 or ENDF/B-VI
- Expanded Suite: 119 cases, ENDF/B-VII.0 or ENDF/B-VI
- LANL Safety Basis Suite: 194 cases, ENDF/B-VI and ENDF/B-V

Fortran 90 Compilers + Parallel Options

- The MCNP development team recommends the Intel compiler.
- MacOS X 10.6.8: Intel-10.1.008 (32-bit), 11.1.088 (32-bit), and 12.0.0 (32-bit)
- Windows 7: Intel-12.03.175 (32- and 64-bit)
- Redhat Linux: Intel-11.1.072 (64-bit)

- Parallel options:
  - MacOS X and Windows used OMP with 8 or 12 threads.
  - Linux used MPI with 128 processors.

Differences from Compiler Version (MacOS X)

	MCNP5-1.60		MCNP6-beta2	
	Intel 12 keff	Intel 10 deltak	Intel 11 deltak	Intel 12 deltak
TT2C11	1.0008 (7)	0.0010 (10)	0.0000 (9)	0.0000 (9)
ZEUS2	0.9972 (7)	0.0002 (9)	0.0000 (9)	0.0000 (9)
ZEBR8H	1.0196 (5)	-0.0001 (7)	0.0000 (7)	0.0000 (7)
HISHPG	1.0118 (5)	0.0004 (7)	0.0000 (8)	0.0000 (8)

Differences from Compiler Version (MacOS X)

1. Using the Intel-11 or Intel-12 compilers, results for MCNP5-1.60 and MCNP6-Beta-2 match exactly for all 31 cases.
2. MCNP6-Beta-2 compiled with the Intel-10 compiler shows round-off differences for 4 cases, and matches MCNP5-1.60 compiled with Intel-10.
3. MCNP6-Beta-2 compiled with the Intel-12 compiler in 64-bit addressing mode is roughly 20% slower than MCNP5-1.60.

Differences in Platform

- Standard Suite tested.
- No differences observed (31 out of 31 agree) for the same version and different platform.
- Intel 11 compiler (various versions) used.

Differences from Code Version (Linux, Intel 11.1.072)

- Expanded Suite tested.
- 116 of 119 problems match in Expanded Suite.
- Differences are around 1-σ of statistical uncertainty:

	MCNP5-1.60 keff	MCNP6-Beta2 deltak
heu-met-fast-019-case-2	1.0073 (2)	0.0001 (4)
heu-met-fast-011	0.9989 (2)	-0.0005 (4)
ieu-comp-therm-002-case-3	1.0044 (2)	-0.0002 (4)

Differences from Code Version, Safety Basis Suite

- Reference results run with MCNP5-1.25 (version in 2003) compiled with Intel-9.
- Cases run on MacOS X with MCNP5-1.60 and MCNP6-beta2 using ENDF/B-VI data.
- 140 out of 194 match within four decimal places of precision.
  - 43 agree within 1σ.
  - 11 agree between 1 and 2σ.

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Differences from Code Version, Safety Basis Suite

- 3 of the 11 problems showing differences between 1 and 2σ had input errors.
- 6 of these show round-off differences between MCNP5-1.60 and MCNP6-beta2.
- Testing with Intel-10.1 show that 192 out of 194 match, with disagreement within 1σ

- List of differences available in Transactions Summary and Full Report.

Summary

- Both MCNP5-1.60 and MCNP6-Beta-2 perform correctly for criticality safety applications.
- While small differences were noted for a few cases, these are strictly from computer round off and are not a concern for verification/validation.
- MCNP5-1.60 and MCNP6-Beta-2 yield the same results on different computer platforms – Mac OS X, Linux, and Windows – for criticality safety applications.
- MCNP5-1.60 and MCNP6-Beta-2 yield the same results using OMP threading and/or MPI message-passing parallelism.
- Using the Intel-12 compiler and 64-bit addressing produces roughly a 20% speedup in the MCNP executables compared to using older compilers.
- MCNP6-Beta-2 runs roughly 20% slower than MCNP5-1.60.

Recommendations

- Future development for MCNP be accomplished using the latest Fortran-90 compiler, Intel-12, rather than older versions of the compiler.
- Using the Intel-12 Fortran-90 compiler with 64-bit addressing permits the solution of very large problems that could not be run with older compilers and 32-bit addressing (where array sizes were limited to less than 2 GB), and also provides a speedup of roughly 20% in code execution.
- **No further development of MCNP5 is planned** and criticality safety analysts should consider testing MCNP6-Beta-2 on their particular problems and validation suites, to prepare for the eventual migration from MCNP5 to MCNP6.
- This migration should be accomplished within the next 1-2 years.

Acknowledgments

- Funding provided by the U.S. DOE/NNSA Nuclear Criticality Safety Program.

Questions?