Verification of MCNP5-1.60 & MCNP6.1 for Criticality Safety Applications

Forrest Brown, Brian Kiedrowski, Jeffrey Bull
Monte Carlo Codes, XCP Division
Los Alamos National Laboratory
Abstract

Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications

Forrest Brown, Brian Kiedrowski, Jeffrey Bull

To verify that both MCNP5-1.60 and MCNP6.1 are performing correctly for criticality safety applications, several suites of verification/validation benchmark problems were run in early 2013. Results from these benchmark suites were compared with results from previously verified versions of MCNP5. Testing results for 354 problems on Mac OS X, Linux, and Windows systems indicate that: (1) Both MCNP5-1.60 and MCNP6.1 perform correctly for criticality safety applications. (2) Using the latest compilers, small differences were noted for a few cases compared to using older compilers, but these are strictly due to computer roundoff and are not a concern for verification. (3) MCNP5-1.60 and MCNP6.1 yield the same results on different computer platforms – Mac OS X, Linux, and Windows – for criticality safety applications. (4) MCNP5-1.60 and MCNP6.1 yield the same results using OpenMP threading and/or MPI message-passing parallelism. Criticality safety analysts should consider testing MCNP6.1 on their particular problems and validation suites, to prepare for the migration from MCNP5 to MCNP6. It is expected that this migration should be accomplished within the next 1-3 years.
US DOE/NNSA Nuclear Criticality Safety Program –

What have we done for you lately?

- MCNP6 Release, with ENDF/B-VII.1
- Verification / Validation
- User Support & Training
- New Criticality Methods

This talk: Verification & Validation
MCNP Progress

- MCNP release by RSICC in July 2013
  MCNP6.1 + MCNP5-1.60 + MCNPX-2.70
  Nuclear Data Libraries + MCNP Reference Collection

- Over 1 year of beta-testing + verification-validation for MCNP6

- MCNP5 & MCNPX were frozen – future development only in MCNP6

Support from DOE/NNSA, DOE, DoD, DTRA, DHS/DNDO, NASA, & others
MCNP5-1.60 vs MCNP6.1

**mcnp5**
- neutrons, photons, electrons
- cross-section library physics
- criticality features
- shielding, dose
- “low energy” physics
- V&V history
- documentation

**mcnp6**
- protons, proton radiography
- high energy physics models
- magnetic fields

**mcnp6**
- Partisn mesh geometry
- Abaqus unstructured mesh

**mcnp6**
- 33 other particle types
  - heavy ions
  - CINDER depletion/burnup
  - delayed particles

**mcnp6**
- High energy physics models
  - CEM, LAQGSM, LAHET
  - MARS, HETC

**mcnp6**
- Continuous Testing System
  - ~10,000 test problems / day

**mcnp5** – 100 K lines of code
**mcnp6** – 500 K lines of code

New Criticality Features
- Sensitivity/Uncertainty Analysis
- Fission Matrix
- OTF Doppler Broadening

High energy physics models
- CEM, LAQGSM, LAHET
- MARS, HETC
- Continuous Testing System
- ~10,000 test problems / day
Verification & Validation
MCNP V&V Work for Criticality Safety

We do a lot of verification/validation work, all the time:

MCNP Verification-Validation,  100+ reports on MCNP Website

• Brown, Kiedrowski, Bull, "Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications", LA-UR-12-21041 (2012).
• Brown, Kiedrowski, Bull, Gonzales, Gibson, "Verification of MCNP5-1.60", LA-UR-10-05611 (2010).

Nuclear Data

• Chadwick, et al., "ENDF/B-VII.0: ... Nuclear Data ...", Nuclear Data Sheets, Vol. 107, Number 12 (2006)
• Trellue, R. Little, "Release of New MCNP S(α,β) Library ... ENDF/B-VII.0", LA-UR-08-3628 (2008).
Recent V&V Work

• Very thorough testing of MCNP6.1 on many computer platforms:

Conclusions:

1. MCNP5-1.60 and MCNP6.1 perform correctly for criticality safety applications.

2. For a few cases, there are small differences using newer compilers. Strictly due to computer roundoff & not a concern.

3. MCNP5-1.60 and MCNP6.1 yield the same results on different computer platforms – Mac OS X, Linux, and Windows – for criticality safety applications.

4. MCNP5-1.60 and MCNP6.1 yield the same results using OpenMP threading and/or MPI message-passing parallelism.

• MCNP6.1 impact on criticality calculation results ➔ none
  – All MCNP5 KCODE criticality features preserved, + new features
  – Matches results with MCNP5 for criticality suites
Verification / Validation Suites

• **MCNP V&V Suites**
  - **VALIDATION_CRITICALITY** 31 ICSBEP experiment benchmarks
  - **VALIDATION_CRIT_EXPANDED** 119 ICSBEP experiments
  - **CRIT_LANL_SBCS** 194 ICSBEP experiments, from LANL crit-safety group
  - **VERIFICATION_KEFF** 75 analytic benchmarks, exact solutions
  - **VALIDATION_ROSSI_ALPHA** Rossi alpha vs experiment
  - **VALIDATION_ACODE** static-alpha eigenvalue benchmarks
  - **POINT_KINETICS** reactor kinetics parameters
  - **KOBAYASHI** void & duct streaming, with point detectors, exact solutions
  - **VALIDATION_SHIELDING** 19 shielding/dose experiments
  - **REGRESSION** 66 code test problems
  - many others for MCNP6

• **Focus**
  - Physics-based V&V, compare to experiment or exact analytic results
  - Part of MCNP permanent code repository & RSICC distribution
  - Automated, easy execution & comparison to experiments
### Table I. MCNP6.1 Results for Analytic Keff Benchmarks

<table>
<thead>
<tr>
<th>Case</th>
<th>Name</th>
<th>Analytic Exact $keff$</th>
<th>MCNP_Results $keff$</th>
<th>std</th>
</tr>
</thead>
<tbody>
<tr>
<td>prob11</td>
<td>Ua-1-0-IN</td>
<td>2.25000</td>
<td>2.25000</td>
<td>0.00000</td>
</tr>
<tr>
<td>prob14</td>
<td>Ua-1-0-SP</td>
<td>1.00000</td>
<td>1.00006</td>
<td>0.00010</td>
</tr>
<tr>
<td>prob18</td>
<td>Uc-H2O(2)-1-0-SP</td>
<td>1.00000</td>
<td>1.00005</td>
<td>0.00011</td>
</tr>
<tr>
<td>prob23</td>
<td>UD2O-1-0-CY</td>
<td>1.00000</td>
<td>1.00000</td>
<td>0.00006</td>
</tr>
<tr>
<td>prob32</td>
<td>PUa-1-1-SL</td>
<td>1.00000</td>
<td>0.99995</td>
<td>0.00011</td>
</tr>
<tr>
<td>prob41</td>
<td>UD2O_b-1-1-SP</td>
<td>1.00000</td>
<td>1.00003</td>
<td>0.00007</td>
</tr>
<tr>
<td>prob44</td>
<td>PU-2-0-IN</td>
<td>2.68377</td>
<td>2.68377</td>
<td>0.00003</td>
</tr>
<tr>
<td>prob54</td>
<td>URRa-2-0-SL</td>
<td>1.00000</td>
<td>1.00007</td>
<td>0.00013</td>
</tr>
<tr>
<td>prob63</td>
<td>URRd-H2O(1)-2-0-ISLC</td>
<td>1.00000</td>
<td>0.99993</td>
<td>0.00006</td>
</tr>
<tr>
<td>prob75</td>
<td>URR-6-0-IN</td>
<td>1.60000</td>
<td>1.59999</td>
<td>0.00001</td>
</tr>
</tbody>
</table>

**MCNP6.1, Intel-12 F90 - All results match**
### VALIDATION_CRITICALITY – F90 Compilers – Differences

<table>
<thead>
<tr>
<th></th>
<th>mcnp5-1.60 + ENDF/B-VII.0</th>
<th>mcnp5+Int-10</th>
<th>mcnp5_Int-11</th>
<th>mcnp5_Int-12</th>
<th>mcnp6_Int-12</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>deltak std</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>keff std</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>U233 Benchmarks</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>JEZ233</td>
<td>0.0000 ( 8)</td>
<td>0.9989 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>FLAT23</td>
<td>0.0000 ( 9)</td>
<td>0.9990 ( 7)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>UMFS2C2</td>
<td>0.0000 ( 8)</td>
<td>0.9931 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>FLSTF1</td>
<td>0.0000 (15)</td>
<td>0.9830 (11)</td>
<td>0.0000 (15)</td>
<td>0.0000 (15)</td>
<td></td>
</tr>
<tr>
<td>SB25</td>
<td>0.0000 (14)</td>
<td>1.0053 (10)</td>
<td>0.0000 (14)</td>
<td>0.0000 (14)</td>
<td></td>
</tr>
<tr>
<td>ORNL11</td>
<td>0.0000 ( 5)</td>
<td>1.0018 ( 4)</td>
<td>0.0000 ( 5)</td>
<td>0.0000 ( 5)</td>
<td></td>
</tr>
<tr>
<td><strong>HEU Benchmarks</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GODIVA</td>
<td>0.0000 ( 8)</td>
<td>0.9995 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>TT2C11</td>
<td>0.0010 (10)</td>
<td>1.0008 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>FLAT25</td>
<td>0.0000 ( 9)</td>
<td>1.0034 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>GODIVR</td>
<td>0.0000 ( 9)</td>
<td>0.9990 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>UH3C6</td>
<td>0.0000 (11)</td>
<td>0.9950 ( 8)</td>
<td>0.0000 (11)</td>
<td>0.0000 (11)</td>
<td></td>
</tr>
<tr>
<td>ZEUS2</td>
<td>0.0002 ( 9)</td>
<td>0.9972 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>SB5RN3</td>
<td>0.0000 (18)</td>
<td>0.9985 (13)</td>
<td>0.0000 (18)</td>
<td>0.0000 (18)</td>
<td></td>
</tr>
<tr>
<td>ORNL10</td>
<td>0.0000 ( 5)</td>
<td>0.9993 ( 4)</td>
<td>0.0000 ( 5)</td>
<td>0.0000 ( 5)</td>
<td></td>
</tr>
<tr>
<td><strong>IEU Benchmarks</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IMF03</td>
<td>0.0000 ( 8)</td>
<td>1.0029 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>BIGTEN</td>
<td>0.0000 ( 7)</td>
<td>0.9945 ( 5)</td>
<td>0.0000 ( 7)</td>
<td>0.0000 ( 7)</td>
<td></td>
</tr>
<tr>
<td>IMF04</td>
<td>0.0000 ( 8)</td>
<td>1.0067 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>ZEBR8H</td>
<td>-0.0001 ( 7)</td>
<td>1.0196 ( 5)</td>
<td>0.0000 ( 7)</td>
<td>0.0000 ( 7)</td>
<td></td>
</tr>
<tr>
<td>ICT2C3</td>
<td>0.0000 ( 9)</td>
<td>1.0037 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>STACY36</td>
<td>0.0000 ( 8)</td>
<td>0.9994 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td><strong>LEU Benchmarks</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BAWX12</td>
<td>0.0000 ( 9)</td>
<td>1.0013 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>LST2C2</td>
<td>0.0000 ( 8)</td>
<td>0.9940 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td><strong>Pu Benchmarks</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>JEZPU</td>
<td>0.0000 ( 8)</td>
<td>1.0002 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>JEZ240</td>
<td>0.0000 ( 8)</td>
<td>1.0002 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>PUBTNS</td>
<td>0.0000 ( 8)</td>
<td>0.9996 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>FLATPU</td>
<td>0.0000 ( 9)</td>
<td>1.0005 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>THOR</td>
<td>0.0000 ( 9)</td>
<td>0.9980 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>PUSH2O</td>
<td>0.0000 ( 9)</td>
<td>1.0012 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td>HISHPG</td>
<td>0.0004 ( 7)</td>
<td>1.0118 ( 5)</td>
<td>0.0000 ( 8)</td>
<td>0.0000 ( 8)</td>
<td></td>
</tr>
<tr>
<td>PNL2</td>
<td>0.0000 (12)</td>
<td>1.0046 ( 9)</td>
<td>0.0000 (12)</td>
<td>0.0000 (12)</td>
<td></td>
</tr>
<tr>
<td>PNL33</td>
<td>0.0000 ( 9)</td>
<td>1.0065 ( 7)</td>
<td>0.0000 ( 9)</td>
<td>0.0000 ( 9)</td>
<td></td>
</tr>
<tr>
<td><strong>Wall-clock:</strong></td>
<td><strong>34.7 min</strong></td>
<td><strong>34.0 min</strong></td>
<td><strong>30.5 min</strong></td>
<td><strong>38.5 min</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Rel. Speed:</strong></td>
<td><strong>0.98</strong></td>
<td><strong>1.00</strong></td>
<td><strong>1.11</strong></td>
<td><strong>0.88</strong></td>
<td></td>
</tr>
</tbody>
</table>
Summary of Verification Results

VERIFICATION_KEFF Suite – 10 analytical problems with exact $K_{\text{eff}}$ results
  – MCNP6.1, Intel-12 F90      All results match

VALIDATION_CRITICALITY Suite – 31 ICSBEP Cases, ENDF/B-VII.0
  – MCNP5  Intel-10 vs Intel-12: 4 diffs, within statistics
  – MCNP5 & MCNP6, Intel-12: All results match

VALIDATION_CRIT_EXPANDED Suite – 119 ICSBEP Cases, ENDF/B-VII.0
  Shortened Problems
  – MCNP5  Intel-10 vs Intel-12: 1 diff, within statistics
  – MCNP5 & MCNP6, Intel-12: All results match
  Standard Problems
  – MCNP5 & MCNP6, Intel-12: 4 diffs, within statistics

CRIT_LANL_SBCS Suite – 194 ICSBEP Cases, ENDF/B-VI
  MCNP5 vs MCNP6, Intel-10.1: 187 match, 4 diffs < 1σ, 3 diffs < 2σ
  MCNP5 (2013, Int-12) vs MCNP5 (2003, Int-9)
    142 match, 42 diffs < 1σ, 10 diffs < 2σ
Conclusions

• MCNP6 ↔ MCNP5, for standard criticality calculations

• MCNP6 impact on Criticality Calculations ➔ none
  – All KCODE criticality features same as for MCNP5
  – Matches results with MCNP5 for criticality suites

• MCNP6 currently runs ~ 20-30% slower than MCNP5 for criticality calcs
  – MCNP-2020 project underway, already providing improvements
  – Goal: 2X speedup over MCNP5 within 1-2 years

• Monte Carlo team will support MCNP6, no new features or releases of MCNP5 or MCNPX

• All new MCNP verification/validation/qualification efforts should be directed toward MCNP6, not MCNP5

• You need to plan for MCNP5 ➔ MCNP6 transition over the next few years
Questions ?