MCNP Progress
&
Performance Improvements

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Monte Carlo Codes, XCP-3
Los Alamos National Laboratory
US DOE/NNSA Nuclear Criticality Safety Program –

What have we done for you lately?

- MCNP6.1 Release, with ENDF/B-VII.1
- Verification / Validation
- User Support & Training
- Performance Improvements
- Work in Progress
MCNP6.1 Status (1)

- MCNP release by RSICC, July 2013
  - MCNP6.1 – production version
  - MCNP5-1.60, MCNPX-2.70 – old versions, no changes
  - Nuclear Data Libraries – including ENDF/B-VII.1 data
  - MCNP Reference Collection – 600+ technical reports

  12,000+ copies of MCNP distributed 2001-2012
  2,000+ copies of MCNP6 distributed 2013

- MCNP6.1.1 – beta release, planned for June 2014
  - Primarily for DHS users, no effect on crit-safety
  - Next production release targeted for 2015

- MCNP5 & MCNPX are frozen – all new development & fixes are in MCNP6

- Criticality safety community needs to transition to MCNP6

Support from DOE-NNSA-ASC, DOE-NNSA-NCSP, DOE, DoD, DTRA, DHS/DNDO, NASA, & others
Monte Carlo Codes
XCP-3, LANL

MCNP6.1 Status (2)

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

Partisn structured mesh
Abaqus unstructured mesh

mcnpx
33 other particles, heavy ions
CINDER depletion, delayed n γ

High energy physics models
CEM, LAQGSM, LAHET, MARS, HETC
cosmic ray background
LLNL fission multiplicity
Single-event electron physics

Continuous Testing System
~10,000 test problems / day

New Criticality Features
Sensitivity/Uncertainty Analysis
Fission Matrix
OTF Doppler Broadening
Performance Improvements
MPI & threading improvements

mcnp5 – 100 K lines of code
mcnp6 – 500 K lines of code
Verification & Validation (1)

We do a lot of verification/validation work - all the time, especially for MCNP6:

MCNP Verification-Validation, 100+ reports on MCNP Website

- Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications, LA-UR-12-210 (2012).
- Verification of MCNP5-1.60, LA-UR-10-05611 (2010).

Nuclear Data

- Continuous Energy Neutron Cross Section Data ...ENDF/B-VII.1, LA-UR-13-20137 (2013).
- LANL Data Testing Support for ENDF/B-VII.1, LA-UR-12-20002 (2012).
- ENDF/B-VII.0: ... Nuclear Data ..., Nuclear Data Sheets, Vol. 107, Number 12 (2006)
- Release of New MCNP S(α,β) Library ... ENDF/B-VII.0, LA-UR-08-3628 (2008).
### Table 1. MCNP6.1 and MCNP6.1.1-Beta Results for Analytic Keff Benchmarks

<table>
<thead>
<tr>
<th>Case</th>
<th>Name</th>
<th>Analytic k(\text{eff})</th>
<th>MCNP_Results k(\text{eff})</th>
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Results are identical for MCNP6.1 and MCNP6.1.1-Beta.

Wall-clock time, using 8 threads on Mac Pro:

- MCNP6.1: 151 min
- MCNP6.1.1-beta: 87 min
## Monte Carlo Codes
### XCP-3, LANL

**Verification & Validation (3)**

### mcnp5-1.60 + ENDF/B-VII.0

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<th>keff</th>
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### HEU Benchmarks

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**Wall-clock:** 34.7 min 34.0 min 30.5 min 38.5 min
**Rel. Speed:** 0.98 1.00 1.11 0.88
Verification & Validation (4)

**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, Intel-12) vs MCNP5 (2003, Intel-9): 142 match, 42 diffs < 1σ, 10 diffs < 2σ
• Very thorough testing of MCNP6.1 on many computer platforms:

  Conclusion:  MCNP6.1 is solid & reliable for crit-safety calculations

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

• Current MCNP6.1.1 beta exactly matches MCNP6.1 for crit-safety

• MCNP6.1 is 20-30% slower than MCNP5
  – Performance improvements address this, later in this talk
  – MCNP6.1.1 speed is comparable to or faster than MCNP5
User Support & Training (1)

- **12,000+ copies of MCNP distributed 2001-2012**
- **2,000+ copies of MCNP6 distributed 2013**

MCNP Forum - User-group, beginners & experts, >1000 members

- **Classes**
  - Theory & Practice of Criticality Calculations with MCNP
    - FY13: 3 classes (including special class for LANL NCS group certification)
    - FY14: 2 classes (both with some LANL NCS staff)
  - Introduction to MCNP – 5 classes FY13, 5 classes FY14
  - Advanced Variance Reduction – 1 class each FY
  - Intro + Variance Reduction – Kirtland AFB 2014

- **Conferences & Journals**
  - M&C 2013, NCSD 2013, SNA+MC 2013, PHYSOR 2014
  - ANS Washington, Reno, Anaheim

- **Other:** website, reference collection, summer students
Monte Carlo Codes

Performance Improvements (1)

• MCNP6.1
  – Preserves all criticality features
  – ENDF/B-VII.1 data libraries
  – RSICC release - July 2013

• MCNP6 Status
  – Many new capabilities
  – Last few years – focus on features, merger, testing, release
  – Needs upgrade of core software

• Path forward – MCNP 2020
  – Concerted effort to modernize the codebase, upgrade foundations
  – Goals: modular, flexible, faster
  – Necessary for MCNP to survive into the 2020’s

MCNP 2020

• Improve performance
  – 30-50% slowdown for MCNP6.1
  – Goal: 2X speedup within 2 years

• Upgrade core MCNP6 software
  – Restructure, clean up coding
  – Reorganize data structures
  – Evolution, not revolution
  – Reduce future costs for new development & maintenance
  – Goal: sustainable code

• Prepare for future
  – New computers – massive parallel but less memory per core
  – Improve MPI & thread parallelism
  – Goal: flexible, adaptable code
Performance Improvements (2)

- **Create a set of timing tests**
  - Stress different portions of MCNP coding
  - Helps determine effect of specific code optimizations

- **Initial performance improvements**
  - Eliminate strided f90 vector ops
  - Inline binary search, for neutron xsec routines
  - IF-guards, to avoid calling accessor functions
  - Inline code some other sections of coding
  - Eliminate unnecessary clearing of certain scratch arrays
  - Hash-based xsec energy lookups (algorithm change)
    - no work yet on tracking & geometry, or photon/electron routines
    - no work planned for any high energy physics

- **Intel compiler options**
  - Higher Fortran optimization levels do not provide improvements
  - Using –O2 instead of –O1 provides only ~ 0-5% speedup, but some test problems segfault
Performance Improvements (3)

Tests run on Mac Pro, 3.0 GHz Xeon, 2 quad-cores, with 8 threads. ENDF/B-VII.1, discrete S(a,b)

CRITICALITY PROBLEMS

ks1.txt  3D PWR, OECD perf. bench., Kord Smith, 60 isotopes, no tallies
ks2.txt  ks1.txt, 10 isotopes, no tallies
ks3.txt  ks1.txt, 10 isotopes, fmesh tallies
ks4.txt  ks1.txt, 60 isotopes, fmesh tallies
baw1.txt BAWXI2 ICSBEP problem, 31 isotopes, no tallies
baw2.txt BAWXI2 ICSBEP problem, 31 isotopes, fmesh tallies
fvf.txt  fuel storage vault, from OECD convergence benchmarks, 9 isotopes
g1.txt  Godiva problem, 3 isotopes
g2.txt  Godiva problem, 423 isotopes
pin.txt  AECL pin cell, with FPs, 147 isotopes

FIXED-SOURCE PROBLEMS

void1.txt ks1.txt, with VOID card & no tallies
void2.txt baw1.txt, with VOID card & no tallies
void3.txt fvf.txt, with VOID card & no tallies
det1.txt 3D porosity tool, Reg. problem 12, neutrons, weight windows, F4 tallies
med1.txta medical physics, modified 3D Zubal head, photons
pht1.txt PHTVR cylindrical test problem, photons
**Performance Improvements**

- **Speedups from recent performance improvements**

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<th>mcnp6.1,</th>
<th>mcnp5</th>
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<td>6/5</td>
<td>mcnp6.1</td>
<td>vs</td>
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5: mcnp5-1.60

6: mcnp6.1, released

NEW: mcnp6.1, + no strides
+ inlining
+ if guards
+ thrd-priv. common
+ etc.
+ hash-based xs lookup

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</table>
Performance Improvements (5)

- Timing results for the standard VALIDATION_CRITICALITY test suite with ENDF-B/VII data
  - Mac Pro (3 GHz, 8 cores), Intel 12.0 f90, run with 8 threads
  - Measured wall-clock times, including data I/O:

  - `mcnp5` release 34.7 min
  - `mcnp6.1` release 43.9 min
  - `mcnp6` NEW 27.9 min

  → 1.57 X speedup over `mcnp6.1`
  → 1.24 X speedup over `mcnp5`
### Speedups – NEW vs mcnp6.1
measured by Jeff Bull for mcnp performance test problems

<table>
<thead>
<tr>
<th>Test</th>
<th>MCNP6 1.0 Release (min)</th>
<th>MCNP6 NEW (min)</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>BAWXI2</td>
<td>63.58</td>
<td>14.55</td>
<td>4.37</td>
</tr>
<tr>
<td>mode p e in air</td>
<td>12.88</td>
<td>12.73</td>
<td>1.01</td>
</tr>
<tr>
<td>GODIVA</td>
<td>22.50</td>
<td>21.40</td>
<td>1.05</td>
</tr>
<tr>
<td>100M lattice cells in void</td>
<td>58.48</td>
<td>11.32</td>
<td>5.17</td>
</tr>
<tr>
<td>mode n p e in air</td>
<td>9.70</td>
<td>9.27</td>
<td>1.05</td>
</tr>
<tr>
<td>mode p in air</td>
<td>7.29</td>
<td>6.06</td>
<td>1.20</td>
</tr>
<tr>
<td>Pulse height tally</td>
<td>27.41</td>
<td>22.79</td>
<td>1.20</td>
</tr>
<tr>
<td>Radiography</td>
<td>33.30</td>
<td>31.06</td>
<td>1.07</td>
</tr>
<tr>
<td>Mode n in air with 750,000 tally bins</td>
<td>19.25</td>
<td>16.26</td>
<td>1.18</td>
</tr>
<tr>
<td>Well log (problem 12 from Regression suite)</td>
<td>57.89</td>
<td>30.27</td>
<td>1.91</td>
</tr>
</tbody>
</table>
## MCNP 2020

- **Improve performance**
  - Focus on geometry tracking

- **Upgrade core MCNP6 software**
  - Restructure, clean up coding
  - Reorganize data structures
  - Evolution, not revolution
  - Reduce future costs for new development & maintenance
  - **Goal:** sustainable code

- **Prepare for future**
  - New computers – massive parallel but less memory per core
  - Improve MPI & thread parallelism
  - **Goal:** flexible, adaptable code

## Parallel MPI & Threading

- **For criticality calculations**
  - Reduce the amount of data exchanged at MPI rendezvous
  - Tally server nodes

- **MPI improvements**
  - Eliminate synchronization
  - Asynchronous MPI messages
  - Improve Fortran/C interface

- **OpenMP threading improvements**
  - Replace private thread-safe storage for certain large arrays by OpenMP critical sections
  - Use OpenMP atomic operations with shared tally arrays
Physics & Temperature Dependence

- Implement modified free-gas scatter, to accurately model resonance upscattering for epithermal neutrons
- Full temperature dependence of $S(a,b)$ thermal scattering
- Investigate coupling MCNP into multiphysics calculations

Fission Matrix

- Automatically determine source convergence, without user input
- Apply to subcritical multiplication problems
- Accelerate source convergence

![Graphs showing $k_{eff}$ and $H_{src}$ convergence with and without F matrix]
Continuous-energy Sensitivity/Uncertainty Analysis

• Uses adjoint-weighted perturbations
• Computes sensitivity coefficients for cross sections, fission, & scattering laws
• Can directly compare to TSUNAMI multigroup s/u results
• See Kiedrowski presentation

Support for LANL PF-4 Nuclear Criticality Safety

• High priority
• See Kiedrowski presentation
Summary

- **MCNP6.1 & ENDF/B-VII.1 released**

- **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, no new features or releases of MCNP5 or MCNPX**

- **MCNP6 speed improved by 1.2 – 4 X for crit-safety**

- **More performance improvements in progress**

- **Criticality-safety community needs to plan for MCNP5 ➔ MCNP6 transition over the next few years**