Title: Verification and validation testing and tools: comparison between MCNP code versions and nuclear data libraries

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Verification and validation testing and tools: comparison between MCNP code versions and nuclear data libraries

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Overview

• Primary goal of software testing
• Results for individual suites
  – Validation
    ▪ Expanded criticality
    ▪ Pulsed spheres
    ▪ Rossi-α
  – Verification
    ▪ $k_{\text{eff}}$
    ▪ Kobayashi
Primary goal of software testing

• Test the code for *correctness*
• Correctness is defined with respect to some standard
  – Comparison to another code (version)
    – Comparison to (semi-)analytic results
    – Comparison to experiment measurements
Primary goal of software testing

• Test the code for correctness
• Correctness is defined with respect to some standard
  – Comparison to another code (version)
    Behavioral testing done for every code change during development
    Full end-to-end testing attempting to isolate behaviors / features
  – Comparison to (semi-)analytic results
    Ensuring the algorithms indeed solve the transport equation
    Simplified problems and mock data used to isolate code / algorithm implementation
  – Comparison to experiment measurements
    Ensuring the combination of algorithms and data compare well to nature / reality
    Applies only to application area being tested and compared
Primary goal of software testing

- Test the code for *correctness*
- Correctness is defined with respect to some standard
  - Comparison to another code (version)
  - Comparison to (semi-)analytic results
  - Comparison to experiment measurements

Current MCNP6 Testing Practices

REGRESSION
VERIFICATION
VALIDATION
Role of Verification and Validation

• Verification
  - Where analytical and semi-analytical solutions to the transport equation may exist, we want to ensure that MCNP is solving the correct equations

• Validation
  - Combination of code (MCNP) and nuclear data (ENDF/NJOY/ACE) work together to produce results comparable to reality

• Full end-to-end tests exercising many separate features
  (input parsing, problem setup, nuclear data usage & collision physics, transport & random walk algorithm, tallying, dose/response functions, output, etc.)

• Long-standing reputation can be linked to extensive and robust V&V
Results: Validation: Expanded criticality

• 119 criticality benchmarks selected from the ICSBEP handbook

• Includes systems with a variety of characteristics
  - Fast, intermediate, and thermal spectra
  - Light, heavy, or no reflectors
  - Lattices of fuel pins and liquid solutions
  - Low-, intermediate-, and highly-enriched uranium (LEU, IEU, HEU), mixed uranium and plutonium (MIX), U-233, and plutonium (PU) systems

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Results: Validation: Expanded criticality

Expanded criticality suite comparison between MCNP code versions 6.2.0 and 6.3 using ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data libraries. Plots are grouped by principal nuclide. Highlighted in the bottom plot are benchmarks that contributed significantly to the cumulative chi-squared.
Results: Validation: Pulsed spheres

- 6 LLNL pulsed sphere measurements\(^1\)
  - Spherical shell of material (beryllium, carbon, concrete, iron, lithium, and water)
  - Nominally 14-MeV (D,T) source
  - Leakage neutron time-of-flight (TOF) spectrum

- Two model types
  - Constructive solid geometry (CSG) modeling of only the pulsed sphere
  - Detailed CSG modeling the pulsed sphere, neutron source, and surroundings

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1. C. Wong et al., “Livermore Pulsed Sphere Program: Program Summary through July 1971,” Lawrence Livermore National Laboratory, Livermore, CA
Results: Validation: Pulsed spheres

Pulsed spheres suite comparison between MCNP code versions 6.2.0 and 6.3 using ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data libraries. From left to right; beryllium, carbon, and concrete. Top and bottom plots are “detailed” and “simple” geometries, respectively.
Results: Validation: Pulsed spheres

Pulsed spheres suite comparison between MCNP code versions 6.2.0 and 6.3 using ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data libraries. From left to right: iron, lithium, and water. Top and bottom plots are "detailed" and "simple" geometries, respectively.
Results: Validation: Rossi-α

• 14 criticality benchmarks selected from the ICSBEP handbook\(^1\)
• $\alpha$-eigenvalue is calculated via KOPTS card (“kinetics=yes”)
• Includes systems with a variety of characteristics\(^2\)
  – Fast, intermediate, and thermal spectra
  – Light, heavy, or no reflectors
  – Lattices of fuel pins and liquid solutions
  – Low-, intermediate-, and highly-enriched uranium, mixed uranium and plutonium, U-233, and plutonium systems

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Results: Validation: Rossi-α

Rossi-α suite comparison between MCNP code versions 6.2.0 and 6.3 using ENDF/B-VII.1 and ENDF/B-VIII.0 nuclear data libraries.
Results: Verification: $k_{\text{eff}}$

- 37 continuous energy (CE) and 68 multigroup (MG) $k$-eigenvalue analytic benchmarks\(^1\)

- These simple models include $k_\infty$, infinite slab, infinite cylinder, sphere, and two medium-reflected infinite slab problems

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Results: Verification: $k_{\text{eff}}$

$k_{\text{eff}}$ suite comparison between MCNP code versions 6.2.0 and 6.3 using a fictitious nuclear data library. Plots are grouped by energy representation.
Results: Verification: Kobayashi

- 6 analytic benchmarks with 3 distinct geometries\(^1\)
- Designed to test how 3D discrete ordinates codes deal with ray effects in problems with void and shield regions.
- Neutron source
  - Monoenergetic and isotropic
  - Uniformly distributed throughout a cube
  - Bounded by void and shield material regions
- Shielding
  - Pure absorber
  - 50% absorbing, 50% scattering

Kobayashi suite comparison between MCNP code versions 6.2.0 and 6.3 using a fictitious nuclear data library. From left to right: problems 1, 2, and 3. Top plots are pure absorbers and bottom plots are 50% absorbing, 50% scattering.
Summary

• V&V framework enables easy comparison between calculations performed with different code versions and/or nuclear data libraries
  - Expanded criticality: cumulative chi-squared is generally lower for ENDF/B-VIII.0
  - Pulsed spheres: some improvement in C/E vs TOF using ENDF/B-VIII.0
  - Rossi-α: cumulative chi-squared is generally lower for ENDF/B-VIII.0
  - $k_{eff}$: little difference between code versions (same “fictitious” nuclear data)
  - Kobayashi: little difference between code versions (same “fictitious” nuclear data)
• This entire framework will be distributed with the upcoming MCNP6.3 release
• V&V test suites shown and several that were not (Criticality, LAQGSM, Lockwood) will be distributed in new framework
Questions?

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