MCNP6® Recent Updates on Modernization, R&D, and Release Plans

Michael E. Rising, Jennifer Alwin, Forrest Brown, Christopher Perfetti, Bobbi Riedel, Kristy Spencer, and Daniel Timmons

NCSP Technical Program Review
February 23, 2021

LA-UR-21-21534
FY20 Updates
Overview

• MCNP Classes
  - Moved online in April 2020
  - Taught ~9 different online classes
  - In CY19, taught ~17 different in-person classes

• LANL MCNP Steering Committee formed
  - LANL NCS division represented
  - Early focus on user support

• Initiated efforts to improve several resources
  - MCNP website
  - MCNP user forum
  - MCNP support requests

### MCNP Classes Going Virtual

<table>
<thead>
<tr>
<th></th>
<th>CY 2019 (In-Person)</th>
<th>2020-21 (Online)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Days</td>
<td>75</td>
<td>41</td>
</tr>
<tr>
<td>Attendees</td>
<td>200</td>
<td>289</td>
</tr>
<tr>
<td>Attendee-Hours</td>
<td>6,300</td>
<td>6,400</td>
</tr>
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</table>
Modernization Highlights

• **New particle track output capabilities in parallel (NA-22, SS)**
  - Particle track output in HDF5 (PTRAC)
  - Needed for accurate analysis of subcritical experiment simulations

• **New mesh tally options and enhanced parallelism (ASC, SS)**
  - Mesh tally results in HDF5/XDMF (MESHTAL)
  - Batch tally options available
  - Remote memory access options for handling extreme scale mesh tallies

• **Unstructured mesh developments (ASC, SS)**
  - Unstructured mesh input/output model in HDF5/XDMF (EEOUT)
  - Improved input processing times
  - Extended V&V

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**NA-22**, DOE Nuclear Nonproliferation R&D Program
**ASC**, DOE Advanced Scientific Computing Program
**SS**, LANL Site Support Funding
FY20 R&D Activities
University R&D Activities

• Maintaining a pipeline of nuclear engineer graduates through new criticality safety research and development projects

• University of New Mexico
  – PI: Christopher Perfetti
  – Students: Bobbi Riedel & Daniel Timmons

• Oregon State University
  – PI: Todd Palmer
  – Student: Pavel Grechanuk

• University of Michigan and Rensselaer Polytechnic Institute subcontracts for dedicated Whisper and $S(\alpha, \beta)$ temperature R&D work, respectively.

Topics discussed on next few slides

Topic: Using Whisper and Machine Learning methods together to develop methodology for enhanced nuclear data validation

Fission Physics and Algorithm Developments for MCNP Criticality and Subcritical Simulations (Timmons, UNM)

- MCNP6.2 added fission models FREYA, CGMF, and the LLNL Fission Library for use in fixed-source simulations.

- Using a few nominal ICSBEP critical experiments, the new fission models typically result in increased bias as compared to the default ENDF/B libraries.

- While the new models are not validated for use in criticality safety applications, they are free from the historical calibration that has been done in the evaluation and validation of the ENDF/B libraries tuned to a subset of well-known critical experiments.

<table>
<thead>
<tr>
<th>Godiva Critical Assembly</th>
<th>$k_{\text{eff}}$</th>
<th>Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP6.2</td>
<td>1.00002(7)</td>
<td>-</td>
</tr>
<tr>
<td>CGMF</td>
<td>1.01306(112)</td>
<td>1304</td>
</tr>
<tr>
<td>LLNL</td>
<td>0.99861(6)</td>
<td>-141</td>
</tr>
<tr>
<td>FREYA</td>
<td>1.01520(61)</td>
<td>1518</td>
</tr>
</tbody>
</table>
Fission Physics and Algorithm Developments for MCNP
Criticality and Subcritical Simulations (Timmons, UNM)

• Accurate calculation of the system multiplication in the presence of a fixed-source in a multiplying medium (presented at 2020 ANS Winter meeting)

\[ M = 1 + \frac{k_q}{1-k_f}, \quad k_q = k_1, \quad k_f = \frac{\sum_{i=2}^{j} \prod_{i=2}^{j} k_i}{\sum_{i=2}^{j} \prod_{i=2}^{j-1} k_i} \]

• Continuing to investigate subcritical benchmarks and Monte Carlo algorithms for multiplying fixed-source simulations
  - Leakage Multiplication
  - Singles Count Rate
  - Doubles Count Rate

• Next steps: Calculating subcritical benchmark nuclear data sensitivities
Investigation of Region-wise Sensitivities for Nuclear Criticality Safety Validation (Riedel, UNM)

- Studying how Whisper selects benchmark populations and determines the baseline USL for loosely coupled systems.
  - Models of four distinct loosely-coupled systems were constructed (only two shown).
  - Parametric study of five separating distances between assemblies were used for each model.
- For each model and separation distance,
  - Region-wise and overall system sensitivity profiles calculated by MCNP6.
  - Whisper 1.1 selected benchmark populations and determined a baseline USL value.
  - Comparison between the models’ assemblies and the overall respective models.
Investigation of Region-wise Sensitivities for Nuclear Criticality Safety Validation (Riedel, UNM)

• Conclusions
  - Coupled system sensitivity profiles are usually dominated by a single assembly.
  - The overall (full model) Whisper baseline USL is not necessarily conservative.
  - It is recommended to calculate the regional baseline USL values and choose the more conservative value.

• Current Work
  - A comparison study between Whisper, Tsurfer and USLSTATS, and a 95/95 reference USL value.

• Future Work
  - This comparison study will be expanded to study multi-assembly models to develop more generalized guidance for loosely-couple systems.
Los Alamos Benchmark Suite & Whisper
Update on the Los Alamos Benchmark Suite (LABS)

- LABS is an effort to consolidate and peer-review benchmarks to share between groups at LANL (NCS, XCP-7, XCP-5, XCP-3)
- Status as of 02/04/2021:
  - Over 50% of the benchmarks from the Whisper 1.1.0 Suite added (112/218)
  - Nearly 500 individual cases added (475/1101)
  - All of the Pu benchmarks complete!
- MSIPP summer student selected to work on LABS for summer 2021
- Applied for NCSP funding to increase speed of benchmark review/revisions
LABS – Pu Revisions

A diagram showing a scatter plot of bias in pcm (Before Revision) vs. bias in pcm (After Revision). The plot includes data points for Pu Metal, PuO2, and Pu(NO3)4, with a dashed line indicating no change.

Top 12 Largest Changes

<table>
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<tr>
<th>Change in Bias (pcm)</th>
<th>Combined Error</th>
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<tbody>
<tr>
<td>pu-met-fast-042-001.i</td>
<td>-1430</td>
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<tr>
<td>pu-met-fast-042-002.i</td>
<td>-943</td>
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<tr>
<td>pu-met-fast-042-003.i</td>
<td>-724</td>
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<tr>
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<tr>
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<td>-500</td>
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<tr>
<td>pu-met-fast-042-011.i</td>
<td>-497</td>
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*Change in benchmark $k_{eff}$ value
FY21 Plans
FY21 Overview

• **MCNP 2021 User Symposium**
  - Save the date: *Week of July 12, 2021*
  - Held virtually this year. Details to come.
  - Presentations and panels with the development team and MCNP users.

• **Continue online MCNP classes**
  - Introduction class (recommended for all new users), May 24-28, 2021
  - Advanced Criticality class, June 7-9, 2021

• **Code developments continuing outside of MCNP6.3 Release**
  - Complete conversion to HDF5 file formats
  - Continue modernization of UM code and V&V
  - Begin replacement for geometry plotting GUI
FY21 Release Plans

• Release MCNP6.3
  - Complete upgrade of theory and user manual
  - Complete upgrade of automated V&V test suites
  - Complete Fortran 2018 compliance clean-up
  - Complete reorganization of code components

• All NCS-specific criticality and physics upgrades will be included (see. F. Brown’s talk)

• Scheduled to be release before Oct. 1, 2021
• Nuclear data is planned to be available via download from nucleardata.lanl.gov
Concluding Remarks

Summary

• FY20
  - Online classes
  - Modernization continues
  - Many ongoing R&D activities
  - Los Alamos Benchmark Suite reviews and revisions are important for future versions of Whisper

• FY21
  - MCNP6.3 Release
  - MCNP 2021 User Symposium

Acknowledgements

This work was supported in part by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.
Questions?

Contact: mrising@lanl.gov