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Los Alamos
NATIONAL LABORATORY

MCNP6 Developments: A 2022-23 Year in Review

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2023 MCNP® User Symposium

September 18–21, 2023

LA-UR-23-30362

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Thanks and Acknowledgements

Thanks to everyone for joining us for the 3rd Annual MCNP User Symposium!

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Outline

MCNP® Version 6.3.0

Released!

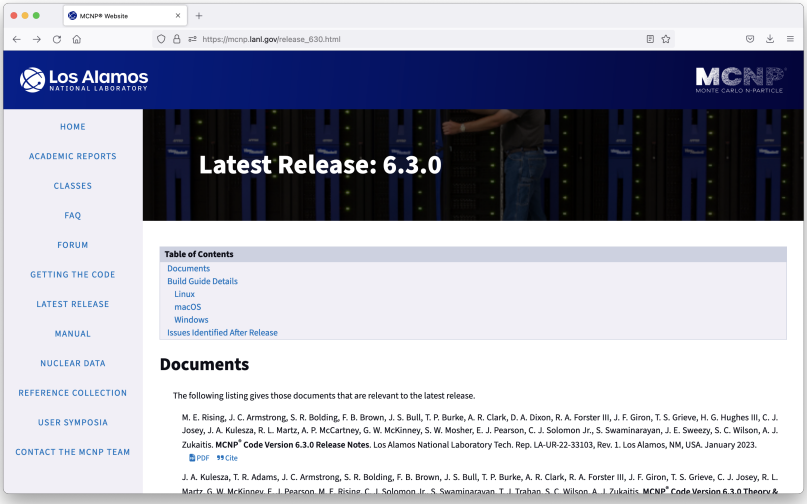
- **The MCNP6.3.0 code is now available to the public**
- Go request a license for the code from the Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory
  - MCNP6.3.0 package: https://rsicc.ornl.gov/codes/ccc/ccc8/ccc-870.html
  - Note that in the MCNP6.3 announcement on the RSICC webpage:

"Thanks to the support of the MCNP® team at Los Alamos National Laboratory RSICC will be waiving the cost recovery fee for all requests for the MCNP6.3 package that are submitted before September 30, 2023."

- For LANL employees, the process to request access to the code remains the same. See the How To Get The MCNP Code page on the MCNP website for details.

MCNP6.3 Release Webpage

- For the most up-to-date details on the latest release, see the Latest Release (https://mcnp.lanl.gov/release_630.html) tab on the MCNP website.

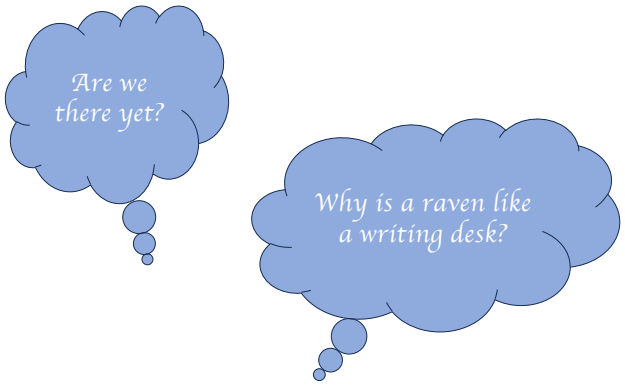


MCNP6.3 Release Installation Help

- A new MCNP6.3 installation video for Windows users was uploaded to the LANL YouTube channel (https://youtu.be/rUSV_apcXh8). Link also found on the Latest Release webpage.

How We Got Here

For many, it's probably not clear what caused such a delay in the public release ...



A Key?

← March 2022

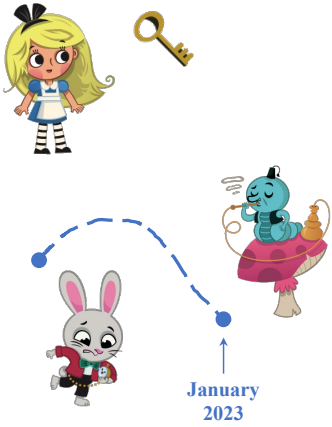
The Adventure Begins

← March 2022

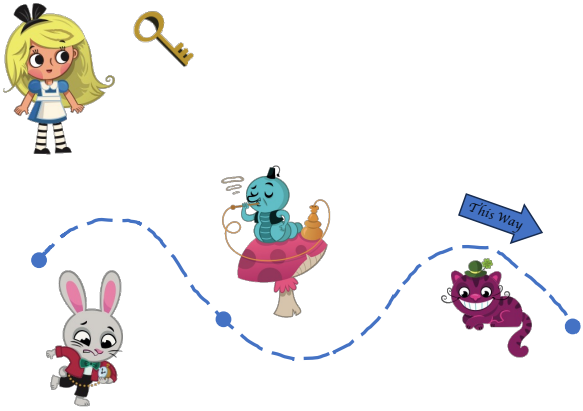
Down The Rabbit Hole

October
2022

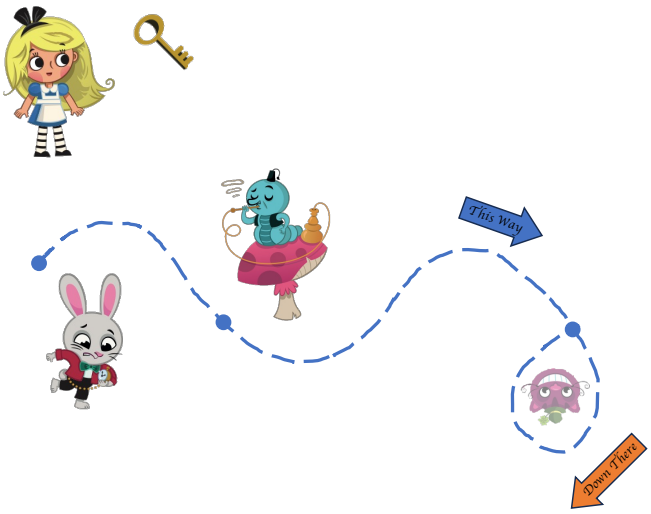
We're Late, We're Late



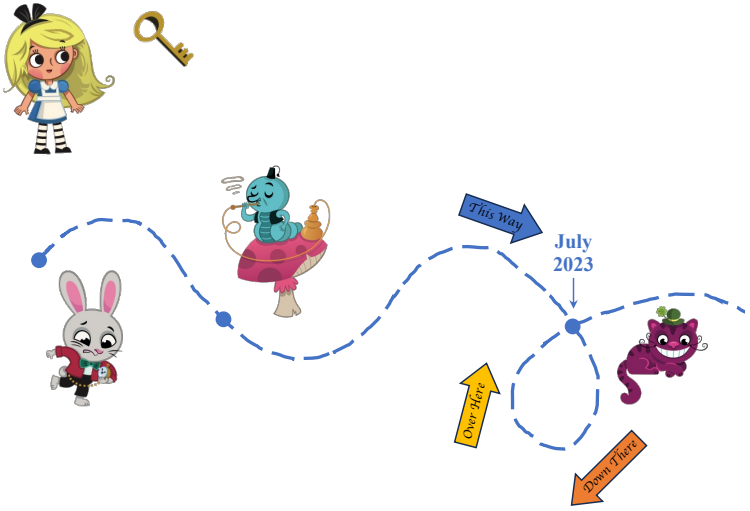
Which Way I Ought To Go From Here?



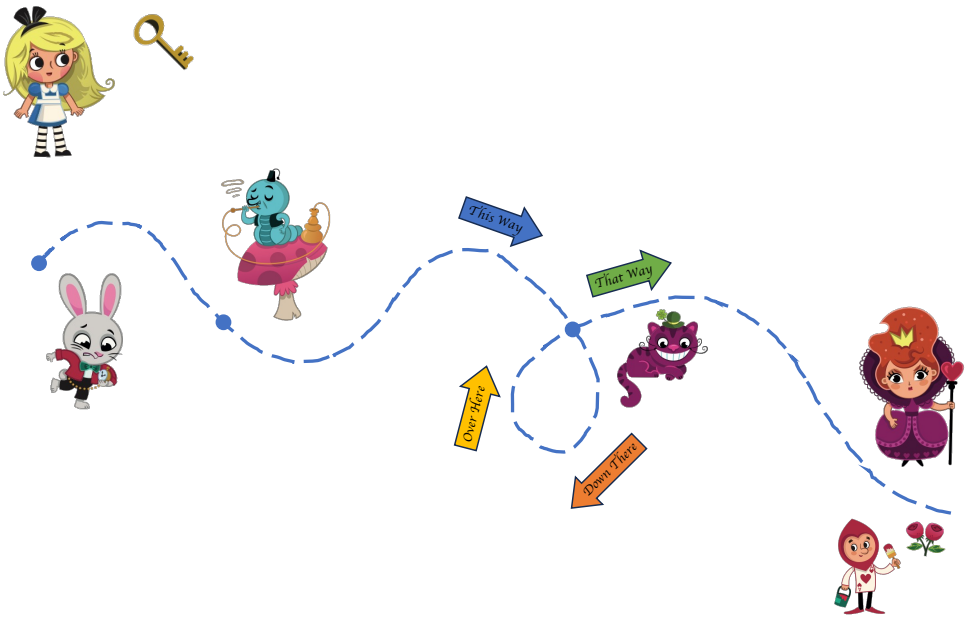
It Doesn't Matter Which Way You Go



You're Sure To Get Somewhere, If You Only Walk Long Enough



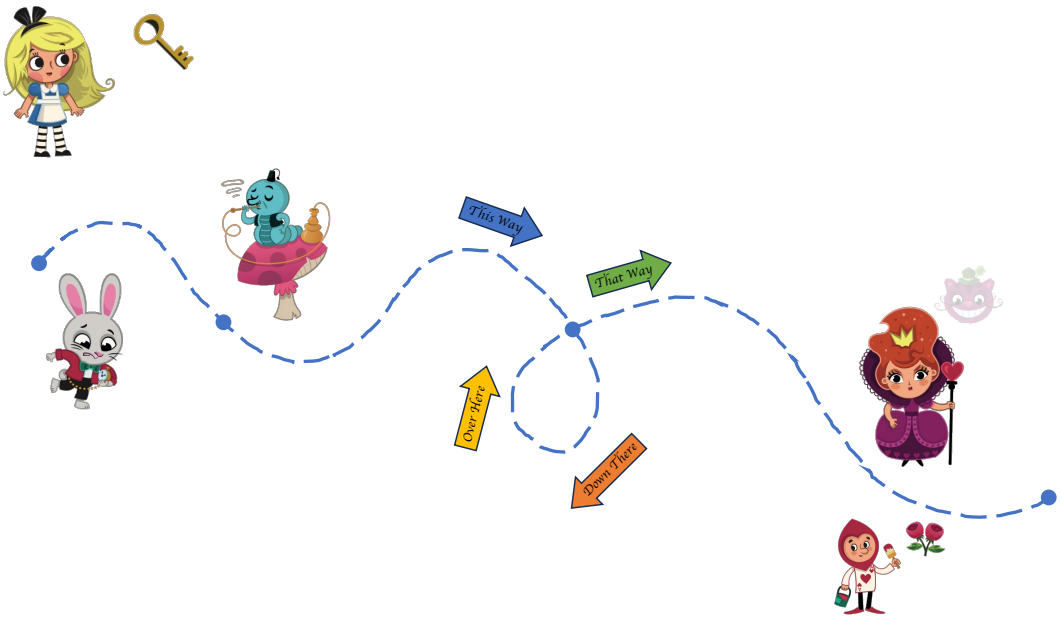
Off With Her Head? No.



The Adventure Concludes ...

August
2023

... Or Perhaps There Is More



The Abridged Version

March 2022 The Adventure Begins:

- It is determined that the MCNP code must have a license key

October 2022 Down the Rabbit Hole:

- The 2022 MCNP User Symposium takes place
- Modified versions of the MCNP6.2 code (**with** a license key enabled) are distributed by RSICC
- A LANL (Feynman Center for Innovation) – ORNL (RSICC) legal process is initiated

January 2023 We're Late, We're Late:

- The MCNP6.3 code, documents, etc., are completed, packaged, and sent to RSICC

July 2023 The Long and Winding Road:

- The LANL–ORNL legal paperwork is complete

August 2023 Conclusion:

- The MCNP6.3 code (**without** a license key enabled) package is distributed by RSICC

Through The Looking Glass

- At some point, a license-key-enabled version is supposed to replace the currently available MCNP6.3 version
  - The source-code package should still contain the executables we originally packaged
- Our Latest Release (https://mcnp.lanl.gov/release_630.html) webpage will continue to be updated including code patches
  - The source-code package will be required to apply code patches
- Most importantly:
  - The LANL–ORNL agreement is in place for all **MCNP6.*x*** versions
  - This will make future releases of the MCNP code a bit more deterministic

Our Team, Products, and Programs

MCNP Team

- To support a multitude of MCNP code and related products there are many folks directly involved at varying levels
  - Roughly 20 individuals involved
    - Covering all aspects of product development
    - Administrative (e.g., registrations, planning) support
    - Time and effort level ranges from 10-100%

- The core development team is likely smaller than expected
  - Roughly 6–8 core developers
    - Code and documentation changes
    - User support and training
    - Time and effort level ranges from 75-100%

MCNP Team Losses

- We have had a few changes to the core team composition over the past year
- A couple folks have left the team (and LANL):
  - Avery Grieve
    - Left LANL spring 2023
    - User support specialist for roughly 2 years
    - Active on the MCNP Forum, help email list, and in updating and teaching the classes
  - Stephen Wilson
    - Left LANL summer 2023
    - Worked on general code development and modernization for roughly 2 years
    - In the future, see the MCNP6.4 dynamic source and tally capabilities

MCNP Team Gains

- A couple folks have joined the team:
  - Cole Frederick
    - Joined the XCP-3 group in the summer of 2022
    - M.S. in Computer Science at Colorado State University, Fort Collins
    - Currently working on developer tools and infrastructure as well as the new Qt plotter
  - Pablo Vaquer
    - Postdoc appointment started in summer 2023
    - Ph.D. in Nuclear Engineering from Texas A&M University
    - Currently working on enhancing the MCNP unstructured mesh capabilities.
  - Colin Weaver
    - Staff scientist started in summer 2023
    - Ph.D. with distinction in Nuclear Engineering from the University of New Mexico
    - Currently working to expand the MCNP code verification test suite to include the "Ganapol benchmarks" and a new set of analytic benchmarks for sensitivity coefficients.

Monte Carlo Code and Nuclear Data Team Products (1)

- The MCNP code
  - ~500,000 lines of source code, build system, and utilities
  - Model data
  - Documentation
    - User and theory manual
    - Build guide
    - Verification and validation (V&V) report
    - Release notes
  - Supplementary scripts and tools
    - Data downloader
    - V&V framework

- Nuclear data libraries
  - Distributed on the nuclear data team website
  - https://nucleardata.lanl.gov/

Monte Carlo Code and Nuclear Data Team Products (2)

- MCNPTools
  - Open-source release in 2022
  - Available on GitHub (https://github.com/lanl/mcnptools)
- Whisper
  - Open-source release pending
- Intrinsic Source Constructor (ISC)
  - New version distributed with MCNP6.3 code including ENDF/B-VIII-based data
- CGMF fission event generator
  - Open-source release in 2020
  - Available on GitHub (https://github.com/lanl/CGMF)
- The GitHub LANL/MCNP team page will grow as we open-source more capabilities (https://github.com/orgs/lanl/teams/mcnp)

Monte Carlo Code and Nuclear Data Team Products (3)

- MCNP and NJOY user training
  - Introduction- and Intermediate-level courses
  - Advanced criticality, variance reduction, and data processing courses
  - Application-specific courses (e.g., nuclear criticality safety, safeguards)
- MCNP and nuclear data team websites
  - Collection of historic and modern resources
  - Distribution of processed nuclear data libraries
- Outreach
  - User forum
  - User symposium
  - American Nuclear Society workshops

Current Sponsors

- LANL Site Support Project
- DOE Nuclear Criticality Safety Program
- DOE Advanced Scientific Computing Program
- Engineering Campaigns
- LANL Laboratory Directed Research and Development Program(s)

LANL Site Support Project

- Institutional support for the MCNP code and nuclear data
- Support for existing capabilities
  - Modernization
  - Maintenance
  - Bug fixes
  - User support
- Examples
  - Qt-plotter technology preview
  - Supporting nuclear data availability online
  - MCNP User Symposium

DOE Nuclear Criticality Safety Program

- General support for criticality safety applications
- Methods development
  - Monte Carlo algorithms research
  - MCNP code improvements
  - Sensitivity / uncertainty upper subcritical limit (USL) calculations
- Verification and validation testing
- Advanced criticality calculations training
- User support
- Examples
  - Fission matrix convergence testing and acceleration
  - Whisper USL code and benchmark catalogue

DOE Advanced Scientific Computing Program

- Support development for advanced high performance computing platforms
- Methods development
- Algorithm improvements and optimization
- Advanced geometry and multiphysics coupling
- User support
- Examples
  - Remote memory access tallies at extreme scales
  - Unstructured mesh enhancements

Engineering Campaigns

- Support development for mesh geometry representations
- Algorithm improvements and optimization
- Advanced geometry and multiphysics coupling
- Tools for improved user workflow
- User support
- Examples
  - Unstructured mesh development
  - V&V of applications using UM geometry

LANL Laboratory Directed Research and Development Program(s)

- Short-term support, from months to 1–3 years
- Support development of new, targeted capabilities
  - New features
  - Extended/enhanced capabilities
  - Both within the MCNP code and external tools
- Examples
  - Recently completed
    - Multigroup cross section calculations
    - Multiphysics coupling tools
  - Ongoing
    - Generalized tally/nuclear data sensitivity capability
    - Delta-tracking implementation for nuclear reactor design

The Last Year in Review

Code Changes: New Features

- Added dynamic tally capability (`TALLYX` replacement) *
- Added extended ZAID support to code
  - No longer limited to 2-digit library indentifier to support upcoming ENDF/B-VIII.1 nuclear data library release
  - Example:
    - In MCNP6.3 and older versions of the code, only 2-digit ZAIDs could be used, i.e., `92238.00c`
    - In MCNP6.3.1+ a more general identifier could be used, i.e., `U-238.Lib80x-293.6K.c`
- Added `DENTYPE` keyword to `EMBED` card (for the `LNK3DNT` meshes)

Timeframe: October 2022–September 2023

*** Targeted for the MCNP6.4 code**

Code Changes: Enhancements

- Support for the newer Intel oneAPI compilers
- Improved portability of runtape files between standard, MPI, and Qt MCNP6.3 executables
- Updates to the “-v” version information printout *
- Eliminate reaction/nuclide limits for nuclear data file use
- Removed `MULTITRACK` option from `EMBED` card (for the UM)

Timeframe: October 2022–September 2023

*** Targeted for the MCNP6.4 code**

Code Changes: Bugfixes

- FMESH spontaneous fission normalization issue
- Improved input checks for tally specifications
  - T and C options on FM cards
  - FMESH boundaries and interval consistency
- Fix underallocated MPI buffer in KSEN implementation
- Fix rare floating-point errors in spontaneous fission sources
- Fix knock-on electron tally tagging bug
- Removed several bounds error and undefined behavior issues

Timeframe: October 2022–September 2023

*** Targeted for the MCNP6.4 code**

Code Changes: Clean-up

- Transitioned from Bitbucket to Gitlab for code repository management and issue tracking
- Brought documentation and code repository together for in-sync development
- Error and expire message formatting fixes
- Code comment typo fixes
- Unstructured mesh refactoring *
- Removed storage bookkeeping routines
- Added static Fortran code format analysis

Timeframe: October 2022–September 2023

*** Targeted for the MCNP6.4 code**

Documentation

- All MCNP6.3 documents available on website
  - Release notes (LA-UR-22-33103, Rev.1)
  - User and theory manual (LA-UR-22-30006, Rev.1)
  - Build guide (LA-UR-22-32851, Rev.1)
  - V&V report (LA-UR-22-32951, Rev.1)
- Additional enhancements and fixes for upcoming revisions of the manual
  - Add WWG card defaults
  - Fix tally relative error component discussion
  - Update incoherent scattering theory section
  - Various spelling, typo, grammar, and nomenclature fixes
  - Updates to acknowledgements section

Timeframe: October 2022–September 2023

Testing

- More extensive V&V and performance testing for the MCNP6.3 code (see talks during the symposium)
- Updates to V&V tests
  - Extending Lockwood electron transport validation tests
  - Adding subcritical multiplication validation test suite
  - Adding semi-analytic benchmarks to verification test suite

Timeframe: October 2022–September 2023

MCNP Classes

- Both in-person and virtual classes
  - 3 weeklong full-day in-person classes at LANL
  - 3 weeklong full-day virtual classes *at* LANL
  - 2 weeklong classes at OECD/NEA
- Topics covered
  - Introduction, Intermediate
  - Criticality, Variance Reduction
  - Unstructured Mesh, Nuclear Safeguards

Timeframe: October 2022–September 2023

Updated MCNP Help Resource

- Introduced a new ticketing system for the mcnp_help@lanl.gov help desk

MCNP Help Desk <gitlab.re-git@lanl.gov>
Wed 7/12/2023 10:08 AM
To:Rising, Michael Evan <mrising@lanl.gov>

Thank you for your mcnp_help request!

We are tracking your request and will respond as soon as we can.

If this is a question about how to obtain the MCNP code, more information can be found on the MCNP website here.

If this is a question related to the specifics of how to run the code or how to use certain features, please consider using one of the following resources:

- **MCNP forum**: This highly recommended resource is made up of a large community of users and developers that can provide faster and more diverse responses to a broad set of MCNP questions. More information on signing up for the forum can be found here.
- **MCNP user and/or theory manual**: The current and past user manuals can be found here.
- **MCNP classes**: Ranging from beginner- to advanced-level classes, find more information here on upcoming classes taught by MCNP developers and expert users at LANL.

If your request has been resolved through the use of one of these other resources, please reply back to this email indicating this issue can be closed.

This inquiry generated mcnp_help ticket #9.

Timeframe: October 2022–September 2023

Summary

Summary

- Over the past ~1 year we have focused on:
  - Supporting both internal and external releases
  - Applying fixes and enhancements for the MCNP6.3.1 release
    - Official patches to MCNP6.3.0 will be distributed on our website
    - When issues are identified, please send in bug reports to mcnp_help@lanl.gov
    - For those without source code, the MCNP6.3.1 release through RSICC is planned for the first quarter of 2024
  - Transitioned software configuration managment tools (Bitbucket to Gitlab)

- Once again, we want your feedback (mcnp_help@lanl.gov)
  - New features (e.g., HDF5-formatted files, fission matrix convergence acceleration)
  - Deprecated features
  - The new Qt-based Technology Preview executable

Questions?