LA-UR-22-30884
Approved for public release; distribution is unlimited.

Title: MCNP6.3 Code and Nuclear Data Installation Guide

Author(s): Josey, Colin James
Grieve, Tristan Sumner
Rising, Michael Evan

Intended for: 2022 MCNP User Symposium, 2022-10-17/2022-10-21 (Los Alamos, New Mexico, United States)

Issued: 2022-10-27 (Rev.1) (Draft)
MCNP6.3 Code and Nuclear Data Installation Guide

Colin Josey, Avery Grieve, and Michael E. Rising, XCP-3, LANL

2022 MCNP® User Symposium

October 17–21, 2022

LA-UR-22-30884 Rev. 1
MCNP® Trademark

MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the ® designation as appropriate.

▶ Please note that trademarks are adjectives and should not be pluralized or used as a noun or a verb in any context for any reason.

▶ Any questions regarding licensing, proper use, and/or proper attribution of Triad National Security, LLC marks should be directed to trademarks@lanl.gov.
Thanks and Acknowledgements

This work is supported by the Department of Energy through Los Alamos National Laboratory (LANL) operated by Triad National Security, LLC, for the National Nuclear Security Administration (NNSA) under Contract No. 89233218CNA000001.
Outline

Package Contents
   Source Distribution
   Executable(s) Distribution

Installation
   Nuclear Data Libraries and XSDIR(s)
   MCNP6.3 Code

Data Downloader and Updates
   General Usage and Getting Updates

Summary

Questions?
Package Contents
MCNP6.3 Source Distribution

Before diving into the executable(s) and nuclear data installation, some comments on the MCNP6.3 source code distribution may be of interest:

▶ The MCNP development team appreciates all forms of feedback
  ▶ For those generally using the code, requests for feature improvements, reported bugs or deficiencies, and any other issues that may simply be a matter of improved documentation, are always welcome
  ▶ For those modifying the source and/or building the code, patches are always welcome
  ▶ Send feedback to mcnp_help@lanl.gov

▶ In the past, any kind of feedback has been difficult to incorporate into the code in a *timely* fashion (i.e., multiple years between major releases)
  ▶ General requests need to be prioritized and well-aligned with respect to our funding sponsors and current efforts
  ▶ Code patches may be applied reasonably quickly with some caveats (see next slide)
MCNP6.3 Source Distribution: Existing Challenges

- Actual source code changes generally take very little time in comparison to all of the other necessary and complementary tasks
  - Verification, validation, and testing consistency across all code features is generally a significant amount of effort
  - Documenting the code changes in user manuals, release notes, V&V reports and/or build guides add to the overall cost of the code change effort

- A timely avenue for re-distribution of a patch-version of the MCNP6 code has not been previously possible

The MCNP6.3 source code distribution makes it possible to address the latter challenge
MCNP6.3 Source Distribution: What’s New?

- With the MCNP6.3 source code distribution, a functional git repository is distributed

- Therefore,
  - source code “git patches” will be distributed on the MCNP website
  - source code “git patches” can be sent to the MCNP team for consideration

- Note that we, the MCNP development team, do not keep track of the RSICC approved and licensed MCNP6.3 users

- We will communicate the availability of these patches on the MCNP website and through the MCNP forum
  - Instructions will be available on the website for each patch released
  - Announcements will be made on the forum and the website
MCNP6.3 Source Distribution: Summary

- Ultimately, this means that
  - we are planning on providing source code patches on the MCNP website on a regular basis
  - we are not planning on providing executables of these patch versions
  - all patches will be subject to our current code development practices, meaning extensive testing and proper documentation will be needed for any patch-level changes to be accepted and distributed

- When requesting the code from RSICC, “updating the source code with official MCNP development team patches” should be acceptable justification to obtain the source code, if desired
MCNP6.3 Executable(s) Distribution

- Available for each supported operating system
  - Windows
  - Linux
  - macOS

- Production executables
  - OpenMP thread-only build
  - OpenMP + MPI builds
  - For production MCNP calculations

- Qt Plotter Technology Preview executable
  - OpenMP thread-only build
  - For testing the new plotter, **not** for production MCNP calculations
MCNP6.3 Executable(s) Distribution: Production MPI Builds (1)

- For the first time, we are distributing MPI builds for all platforms
- The user’s system will need to have a compatible MPI library installed

<table>
<thead>
<tr>
<th>Platform</th>
<th>Supported MPI Library</th>
</tr>
</thead>
<tbody>
<tr>
<td>Windows</td>
<td>Microsoft MPI (MS-MPI)</td>
</tr>
<tr>
<td>Linux</td>
<td>OpenMP</td>
</tr>
<tr>
<td></td>
<td>MPICH</td>
</tr>
<tr>
<td>macOS</td>
<td>OpenMP</td>
</tr>
<tr>
<td></td>
<td>MPICH</td>
</tr>
</tbody>
</table>

Compatibility details not discussed here. Closely read and follow instructions with the installer and described in the release notes.
Due to the complexity of the general MPI landscape, these production builds are provided as “best-effort”

At this time, we can **not** guarantee that the distributed executables will be compatible on all possible platforms and configurations

If they are compatible, these MPI executables are considered production quality

When requesting the code from RSICC, “building an MPI-parallel version of the code” should be acceptable justification to obtain the source code, if desired

Closely read and follow instructions with the installer and described in the release notes to have the best chance for success.
MCNP6.3 Executable(s) Distribution: Qt Plotter Technology Preview Build

- Does not require an X11 server installed on user’s system – “It just works!”

- For testing the new plotter, **not** for production MCNP particle transport calculations

- Runtape-compatible with the production executables

- In the source code distribution, the source code for the technology preview is **not** distributed

- Send us feedback ([mcnp_help@lanl.gov](mailto:mcnp_help@lanl.gov))!
MCNP6.3 Executable(s) Distribution: Summary

- A *bit* more complex than previous releases
  - 3 production OpenMP builds
  - 5 production OpenMP + MPI builds
  - 3 technology preview OpenMP builds

- The distributed code installers will help
  - More extensive OS-specific compatibility checking
  - More interactive and intuitive
  - More information to read

Please read the installer instructions and messages provided during installation to have the best chance for success.
Installation
Read the README

▷ **FIRST**, open the README and actually read it!
  - For example, if you want to install any production MPI executables, you’ll likely want to install a compatible MPI library prior to launching the installer.

▷ Before proceeding, note that:
  - Python is required to use the data downloader (highly recommended).
  - HTTPS proxy may need to be set to access the online data.
  - On Windows, the installer can install MS-MPI if not found. **Requires administrator access.**
  - On Linux and macOS, a compatible MPI version needs to be installed separately.

▷ Now, open a terminal and launch the OS-appropriate installer:
  - `install_windows.bat` for Windows
  - `install_linux_mac.sh` for Linux or macOS
Launch the Installer

PS C:\Users\Work\rsicc_release mcnp630> .\install_windows.bat
Transcript started, output file is C:\Users\mcnp630_install_log.txt

Welcome to the MCNP 6.3.0 installer.

--------------------------
Checking Environment
--------------------------

Checking Python version...
Python 3.6+ found. Binary name: python

Checking if Microsoft MPI in path...
Microsoft MPI 10.1+ found. Path: C:\Program Files\Microsoft MPI\Bin\mpiexec.exe

Checking Complete.

--------
Main Menu
--------
Select an option:
[D] Install Data  [M] Install MCNP  [T] Test Installation  [A] All of the Above
[Q] Quit[?] Help (default is "A"):
Select Data Installation Location

Welcome to the MCNP 6.3.0 installer.

Checking Environment

Checking Python version
Python 3.6+ found. Bi

Checking if Microsoft MPI 10.1+ found
C:\Program Files\Microsoft MPI\Bin\mpiexec.exe

Checking Complete.

Main Menu

Select an option:
[D] Install Data  [M] Install MCNP  [T] Test Installation  [A] All of the Above
[Q] Quit[?] Help (default is "A"): d

The MCNP data can take over 100 GB to install. Do you wish to continue? [Y/n]: y

A prompt will open asking where you want to install the MCNP data.
Encountering a Proxy Error

A prompt will open asking where you want to install the MCNP data. Installing data at C:\Users\Nuclear Data
MCNP data already installed in this path. Do you want to continue? [Y/n]: y
Moving nuclear data manager to C:\Users\Nuclear Data ...
Configuring nuclear data manager with default configuration...
ERROR: <urlopen error [WinError 10061] No connection could be made because the target machine actively refused it>
ERROR: Unable to connect to the internet. Check your network and proxy settings.
ERROR: ------ Current proxy settings ------
ERROR: No HTTPS proxy detected.

**WARNING:** There appears to be something wrong with the data downloader.
Would you like to continue? [y/N]:

--------
Main Menu
--------
Select an option:
[D] Install Data  [M] Install MCNP  [T] Test Installation  [A] All of the Above
[Q] Quit[?] Help (default is "A"): 
Setting the HTTPS Proxy

May need to edit the install script to set the `https_proxy` environment variable to allow the data downloader to interact with the https://nucleardata.lanl.gov/ and https://mcnp.lanl.gov/ websites to obtain library installation information and actually download the necessary data.

---

```
:: Wrapper for running Powershell

@echo off

:: You can set environment variables here.
set https_proxy=your.proxy.here:portnumber

powershell.exe -ExecutionPolicy Bypass -File "%dp0\install_windows.ps1"
```
Data Downloading

The MCNP data can take over 100 GB to install. Do you wish to continue? [Y/n]: y

A prompt will open asking where you want to install the MCNP data.
Installing data at C:\Users\Nuclear Data
Moving nuclear data manager to C:\Users\Nuclear Data ...
Configuring nuclear data manager with default configuration...

[ ] [5.10 / 5.10 MiB], 100.00%
Downloading https://nucleardata.lanl.gov/lib/ENDF80SaB2.tgz
[ ] [0.70 / 2.39 GiB], 29.29%
Data Installing

Installing CGM [2.80 / 2.80 MiB], 100.00%
Installing CINDER [8.96 / 8.96 MiB], 100.00%
Installing DBRC_ENDF71 [6.72 / 6.72 MiB], 100.00%
Installing DBRC_ENDF80 [8.61 / 8.61 MiB], 100.00%
Installing FREYA [2.10 / 2.10 MiB], 100.00%
Installing Cosmic_Bkgnd
Updating **DATAPATH** Environment Variable

<table>
<thead>
<tr>
<th>Installation</th>
<th>Size (MiB)</th>
<th>Completion</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCPLIB</td>
<td>1.61 / 1.61 MiB</td>
<td>100.00%</td>
</tr>
<tr>
<td>DRE5</td>
<td>3.67 / 3.67 MiB</td>
<td>100.00%</td>
</tr>
<tr>
<td>ENDF5P</td>
<td>9.74 / 9.74 MiB</td>
<td>100.00%</td>
</tr>
</tbody>
</table>

Installation of the MCNP data completed.

Would you like to modify your user environment to set the DATAPATH? [Y/n]:
Select an option:
[D] Install Data  [M] Install MCNP  [T] Test Installation  [A] All of the Above
[Q] Quit[?] Help (default is "A"): m

----------
Installation
----------

In order to continue, please review the license agreement:

©2018. Triad National Security, LLC. All rights reserved.

This program was produced under U.S. Government contract 89233218CNA000001 for Los Alamos National Laboratory (LANL), which is operated by Triad National Security, LLC for the U.S. Department of Energy/National Nuclear Security Administration.

For a period of five years from February 14, 2018, the U.S. Government is granted for itself and others acting on its behalf a nonexclusive, paid-up, irrevocable, worldwide license in this data to reproduce, prepare derivative works, and perform publicly and display publicly, by or on behalf of the U.S. Government.
Select MCNP6.3 Code Installation Location

Do you agree to the terms? [Y/n]: y

A prompt will open asking where you want to install MCNP.
Installing MPI Version (1)

A prompt will open asking where you want to install MCNP.

**WARNING:** MCNP version 6.3.0 has been previously installed. This installer will remove it from the PATH if you update environment variables.

Installing the MCNP code at C:\Users\test

Both the default version and the Qt plotter preview version of MCNP will be installed. The MPI versions can also be installed.

Do you wish to install the Microsoft MPI version? [y/N]:
Installing MPI Version (2)

Expand-Archive
The archive file 'C:\Users\Work\rsicc_release mcnp630\bin\mpi\mcnp-6.3.0-Win
dows-MS-MPI.zip' expansion is in progress...
[00000000000000000000000000000000]

MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the ® designation as appropriate. Any questions regarding licensing, proper use, and/or proper attribution of Triad National Security, LLC marks should be directed to trademarks@lanl.gov.

LAHET, and LAHET Code System (LCS) are trademarks of Triad National Security, LLC.

Do you agree to the terms? [Y/n]: y
A prompt will open asking where you want to install MCNP.

WARNING: MCNP version 6.3.0 has been previously installed. This installer will remove it from the PATH if you update environment variables.

Installing the MCNP code at C:\Users\test
Both the default version and the Qt plotter preview version of MCNP will be installed. The MPI versions can also be installed.

Do you wish to install the Microsoft MPI version? [y/N]: y

Installing:
- Standard MCNP
- Qt Plotter Preview
- Microsoft MPI Build
Updating User Environment for MCNP6.3 Executable(s)

Installing:
- Standard MCNP
- Qt Plotter Preview
- Microsoft MPI Build

Would you like to modify your user environment to add the MCNP code to your PATH? [Y/n]: y

Environment variables will take effect when opening a new terminal window.

--------
Main Menu
--------
Select an option:
[D] Install Data  [M] Install MCNP  [T] Test Installation  [A] All of the Above
[Q] Quit[?] Help (default is "A"): 
Installation Complete

PS C:\Users> mcnp6
  Code Name & Version = mcnp6, 6.3.0, production
  Copyright Triad National Security, LLC/LANL/DOE - see LICENSE file

mcnp6 ver=6.3.0, ld=09/28/22 10/07/22 14:16:47
Source version = release/6.3-d70e4012cb
  Expire parameter is input file inp does not exist.

  bad trouble in subroutine exemes of mcnp

  input file inp does not exist.
PS C:\Users>
Data Downloader and Updates
Making Nuclear Data More Accessible

- Nuclear data libraries have historically been shipped with the MCNP code
- Getting updated nuclear data usually required
  - Waiting for new MCNP code release
  - Downloading the ENDF-format nuclear data and doing the NJOY processing manually
- Nuclear data team at LANL (XCP-5) have made available several nuclear data libraries on their website (https://nucleardata.lanl.gov/)
  - More easily provide nuclear data libraries
  - More timely delivery of nuclear data updates
- A Python tool for downloading and installing specific nuclear data libraries is provided with the MCNP6.3 package
  - Makes it simple to install and uninstall specific nuclear data library(ies)
  - Generates the nuclear data directory (XSDIR) file with user-specified ordering
nd_manager **Usage: Overview**

- The `nd_manager` tool and required atomic weight ratio data will ship with the MCNP code
- It requires Python3 – without a proper version, it won’t run:

  The nuclear data manager needs Python 3.6+ to run.

- There are multiple run modes that the tool has available to do various steps in the process:
  
  - `config` Adjust configuration options.
  - `list` List libraries available, downloaded, and installed.
  - `update` Query libraries for available libraries.
  - `download` Download list of data libraries.
  - `install` Install list of data libraries to datapath.
  - `uninstall` Uninstall list of data libraries from datapath.
  - `create-xsdir` Create xsdir based on the order of the listed libraries.
**nd_manager Usage: Initial Configuration**

- On the first run, or by using the `config` option, the script will generate a configuration file, defining where to retrieve nuclear data and the local installation location.

![nd_manager directory contents](image)

- Note this is where the `DATAPATH` environment variable should be set for the current profile.
**nd_manager Usage: Update and List Nuclear Data**

- Straightforward to update and view all available libraries and choose which ones to download and install

```
mrising@pn nd_manager % ./nd_manager update
mrising@pn nd_manager % ./nd_manager list
All libraries:
=================
CP2020 - This library contains data for incident charged particles for low Z isotopes and their interactions with other low Z isotopes [Production]
ENDF80SaB2 - ENDF/B-VIII.0-based thermal scattering library. [Production]
Lib80x - The general ACE library based on ENDF/B-VIII.0 containing continuous-energy incident neutron data [Production]
```
**nd_manager** Usage: Downloading Nuclear Data

- Can choose to download nuclear data libraries either by name/list (e.g. “Lib80x”) or using the “--all available” or “--all production” flags

```bash
ENDF5P - The ENDF5P library contains 76 evaluations from ENDF/B-V for which both full (extension .50c) and thinned (extension .51c) were developed.

XSDIR Order:

```

mrising@pn nd_manager % ./nd_manager_download Lib80x ENDF80SaB2
Downloading https://nucleardata.lanl.gov/lib/Lib80x.tgz
[==================================] [6.57 / 6.57 GiB], 100.00%
Downloading https://nucleardata.lanl.gov/lib/ENDF80SaB2.tgz
[==================================] [2.39 / 2.39 GiB], 100.00%
```
```
**nd_manager Usage: Installing Nuclear Data**

- Once downloaded, listings are updated:

```bash
mrising@pn nd_manager % ./nd_manager_list
All libraries:
==========
CP2020 - This library contains data for incident charged particles for low Z isotopes and their interactions with other low Z isotopes [Production]
ENDF80SaB2 - ENDF/B-VIII.0-based thermal scattering library. [Production] [Downloaded]
Lib80x - The general ACE library based on ENDF/B-VIII.0 containing continuous-energy incident neutron data [Production] [Downloaded]
```

- Now the downloaded libraries can be installed:

```bash
mrising@pn nd_manager % ./nd_manager_install ENDF80SaB2 Lib80x
Installing ENDF80SaB2
[ ] [2.39 / 2.39 GiB], 100.00%
Installing Lib80x
[ ] [6.57 / 6.57 GiB], 100.00%
mrising@pn nd_manager %
```

- Specifying the “--all available” or “--all production” flags will install the corresponding nuclear data libraries that were previously downloaded.
nd_manager **Usage: XSDIR File Creation**

- Order of libraries in the `xsdir` file is set in the config file

```
mrising@pn nd_manager % ./nd_manager_create-xsdir Lib80x ENDF80SaB2
The new XSDIR will have the following order:
  1: Lib80x
  2: ENDF80SaB2
Update XSDIRs? [y/N] y
```

- `xsdir` file:
nd_manager **Usage: Updating Nuclear Data**

- When new data is available on the website, it can be quickly and easily updated
- The tool can/will also update the `xsdir` file whenever new nuclear data libraries are installed/uninstalled

```
mrising@pn nd_manager % ./nd_manager update
The library "lib80x" has a new errata added on 2022-07-06:

B-10 Lib80x - After the release of ENDF/B-VIII.0 in February 2018, errors were discovered in the neutron on B-10 evaluation. A fix was provided for the errata; this update uses the fixed B-10 evaluation. For more information on the updated/fixed evaluation, please see: https://www.nndc.bnl.gov/endf-b8.0/errata.html. [Production]

Would you like to update? [Y/n] Y
Downloading https://nucleardata.lanl.gov/lib/B-10-Lib80x.tgz

[ ] 0.00% [ ] 15.93MiB [ ] 5.21 / 5.21 MiB], 100.00%

Installing B-10 Lib80x

[ ] 0.00% [ ] 15.93MiB [ ] 5.21 / 5.21 MiB], 100.00%

The new XSDIR will have the following order:

1: B-10 Lib80x
2: Lib80x
3: ENDF80SAB2

Update XSDIRs? [y/N] Y
```

```
mrising@pn nd_manager %
```
Summary
Summary

- MCNP6.3 release package
  - More MCNP6-specific executables and options available than ever before

- Installer
  - Streamlines the MCNP6.3 installation
  - Automatically downloads all production nuclear data and generates xsdir files for the user

- nd_manager
  - Allowing the LANL Nuclear Data and Monte Carlo teams to work and distribute their products independently
  - Updates, fixes (errata), and newly released data will be made available in a much faster timescale than ever before
Questions?