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MCNP6.3 Code and Nuclear Data Installation Guide

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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

Platform	Supported MPI Library
Windows	Microsoft MPI (MS-MPI)
Linux	OpenMP MPICH
macOS	OpenMP MPICH

Compatibility details not discussed here. Closely read and follow instructions with the installer and described in the release notes.

MCNP6.3 Executable(s) Distribution: Production MPI Builds (2)

- ▶ 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)!

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

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  
Microsoft MPI 10.1+ f
```

```
Checking Complete.
```

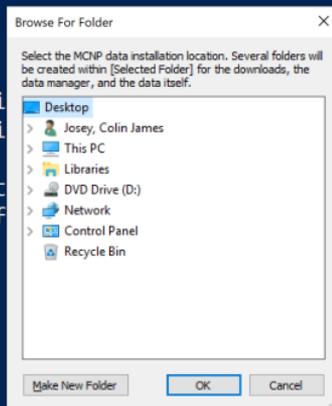
```
-----  
Main Menu  
-----
```

```
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.
```



```
...les\Microsoft MPI\Bin\mpiexec.exe
```

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 m
achine 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.

```
install_windows.bat x install_windows.ps1 x
1  :: =====
2  :: Wrapper for running Powershell
3  :: =====
4  @echo off
5
6  :: You can set environment variables here.
7  set https_proxy=your.proxy.here:portnumber
8
9  powershell.exe -ExecutionPolicy Bypass -File "%~dp0\install_windows.ps1"
```


MCNP6.3 Code Installation

```
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:

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splay publicly, by or on behalf of the U.S. Government.
```


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-Windows-MS-MPI.zip' expansion is in progress...  
[ooooooooooooooooooooooooooooo ]
```

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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"):
```


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 (XS DIR) file with user-specified ordering

nd_manager Usage: Overview

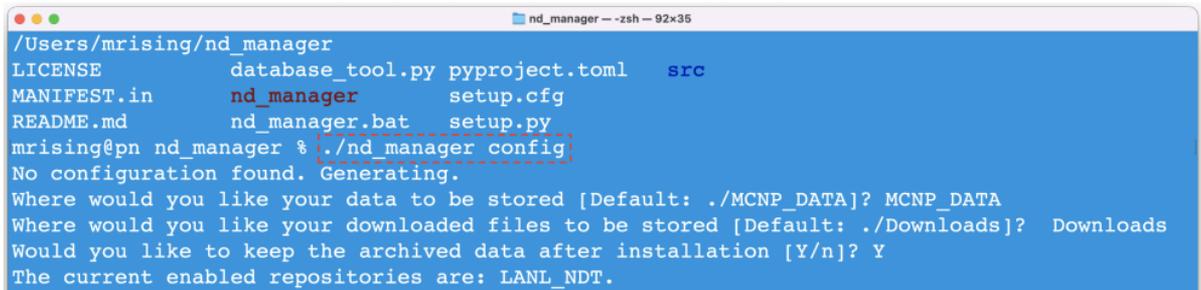
- ▶ The `nd_manager` tool and required atomic weight ratio data will ship with the MCNP code
- ▶ It requires Python3 – without a proper version, it won't run:

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-xmdir` Create xmdir 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 -- -zsh -- 92x35
/Users/mrising/nd_manager
LICENSE      database_tool.py pyproject.toml  src
MANIFEST.in  nd_manager      setup.cfg
README.md    nd_manager.bat  setup.py
mrising@pn nd_manager % ./nd_manager config
No configuration found. Generating.
Where would you like your data to be stored [Default: ./MCNP_DATA]? MCNP_DATA
Where would you like your downloaded files to be stored [Default: ./Downloads]? Downloads
Would you like to keep the archived data after installation [Y/n]? Y
The current enabled repositories are: LANL_NDT.
```

- ▶ 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: Installing Nuclear Data

- ▶ Once downloaded, listings are updated:

```
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:

```
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:

```
MCNP_DATA -- vi xsdir_mcnp6.3 -- 91x24
1 #-----
2 # xsdir
3 # This file was automatically generated by the nuclear data downloader tool.
4 #-----
5 atomic weight ratios
6   0001  1.000000   0001   1.000000
7   1000  0.99931697  1001   0.99916733   1002   1.99679968   1003   2.99013997
8   2000  3.96821760  2003   2.99012018   2004   3.96821897   2005   4.96916622
9   3000  6.99216250  3007   6.96764655   3008   7.96490665
10  4000  9.99703253  4009   9.99703253   4010  10.99159510
11  5000 12.99593624  5009  12.99593624   5010  13.99270115
-----
xsdir_mcnp6.3 1,1 Top
1129 10/18/2022
1130 directory
1131 # Library: Lib80x
1132 1001.00c 0.999167 Lib80x/H/1001.800nc 0 1 3 10257 0 0 2.530100E-08
1133 1001.01c 0.999167 Lib80x/H/1001.801nc 0 1 3 10257 0 0 5.170400E-08
1134 1001.02c 0.999167 Lib80x/H/1001.802nc 0 1 3 10257 0 0 7.755600E-08
1135 1001.03c 0.999167 Lib80x/H/1001.803nc 0 1 3 10257 0 0 1.034100E-07
1136 1001.04c 0.999167 Lib80x/H/1001.804nc 0 1 3 10257 0 0 2.154300E-07
1137 1001.05c 0.999167 Lib80x/H/1001.805nc 0 1 3 10257 0 0 8.617400E-12
1138 1001.06c 0.999167 Lib80x/H/1001.806nc 0 1 3 10257 0 0 2.154300E-08
xsdir_mcnp6.3 1138,1 144
```


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 `xmdir` 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?