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Status of Cross-section Data Libraries for MCNP

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I. Monte Carlo Codes Group Recommendation and Summary

A. Recommended Action

Users of MCNP5, MCNPX, or MCNP6.1 should check the setting of the environment variable DATAPATH and make sure that it is set to the appropriate data directory for the system they are using:

- For the LANL HPC clusters, the proper settings for the typical user shells are

  bash: `DATAPATH=/usr/projects/mcnp/MCNP_DATA`

  csh,tcsh: `setenv DATAPATH /usr/projects/mcnp/MCNP_DATA`

- For the XCP-lan, the proper settings are:

  bash: `DATAPATH=/opt/local/codes/mcnp/MCNP_DATA`

  csh,tcsh: `setenv DATAPATH /opt/local/codes/mcnp/MCNP_DATA`

- For the upcoming MCNP6 release through RSICC, the install scripts for the codes set the DATAPATH variable to the location where the MCNP_DATA folder is installed.

B. Background

The Data Team, part of the XCP-5 group at LANL, uses the NJOY code and other codes to prepare the cross-section data files used by the Monte Carlo codes MCNP5, MCNPX, and MCNP6. They perform extensive quality assurance checking of those data files. The cross-section data files are included with the releases of MCNP that are distributed by RSICC.

MCNP5 is developed and supported by the Monte Carlo Codes group (XCP-3) at LANL. MCNPX is developed and supported by the NEN-5 group at LANL. MCNP6 is a merger of MCNP5 and MCNPX, with numerous additional features, and is jointly developed and supported by the XCP-3 and NEN-5 groups. MCNP5 and MCNPX are "frozen" codes, and all new development is being carried out only in the MCNP6 code.

In the past, when new types of data or improved representations were developed, the Data Team would incorporate the changes into the cross-section data files, and the Monte Carlo groups would make corresponding changes to the MCNP codes to use the new data. At present, however, only MCNP6 is updated to handle new data representations; MCNP5/X are not.

C. New Developments

The Data Team recently released a new, improved collection of cross-section data files that include the ENDF/B-VII.1 data. MCNP6 can make direct use of all of the new data from the Data Team, but requires

a few additional files that are not the Data Team's responsibility. MCNP5 and MCNPX can use nearly all of the new data, but cannot correctly handle the new continuous form of the S(alpha,beta) thermal neutron scattering data.

The Monte Carlo codes MCNP5, MCNPX, and MCNP6 determine the location of cross-section data libraries by examining the environment variable DATAPATH. This environment variable should contain the name of the directory (folder) where the files containing cross-section data are stored on a particular computer system. One of the files in the DATAPATH directory, *xsdir*, serves as a table of contents, providing MCNP with information on where and how the data are stored for each *zaid* found in a user input file.

To support the new cross-section data release while accommodating the differences between MCNP6 and the frozen MCNP5/X codes, The Monte Carlo group has provided a new data directory, MCNP_DATA, that includes symbolic links to the Data Team files, additional data files used by MCNP6, an MCNP5/X-specific *xsdir* file, and a new MCNP6-specific *xsdir* file called *xsdir_mcnp6.1*.

The following sections provide more details on the new cross-section data, the MCNP_DATA directory, and specific considerations for using MCNP5, MCNPX, and MCNP6 with the new data files.

II. Data Team Recommendations

In internal memo XCP-5:13-009 (U), the Data Team recommended the following for continuous Monte Carlo:

"c" -- continuous neutron data, ENDF/B-VII.1 data, *zaids*: .80c ...

"t" -- thermal neutron scattering S(a,b), continuous ENDF/B-VII.1 data, *zaids*: .20t ...

"p" -- photon data, mcplib84, *zaids*: .84p

"u" -- photonuclear data, la150u, *zaids*: .24u

"e" -- electron data, el03, *zaids*: .03e

"h" -- proton data, endf70prot, *zaids*: .70h

The Data Team files are stored in these directories:

XCP-lan: `/opt/local/codes/data/nuclear/mc/type1/`

HPC: `/usr/projects/data/nuclear/mc/type1/`

Release: `MCNP_DATA/xdata/`

In each of those directories, the *xsdir* file is set up to provide the recommended data as defaults. (If a *zaid*-suffix is not provided in user input, then the default data selected will match the Data Team recommendations.)

All older, previously released cross-section data files (e.g., ENDF/B-VII.0, ENDF/B-VI, ENDF/B-V, older photon and electron data, etc.) are also included in the Data Team directories, but are not the default. In general, older data files are retained forever, so that users can always rerun problems from past work.

III. Monte Carlo Codes Group Data for MCNP5 and MCNP6.1

MCNP6.1 requires some additional data that is not present in the Data Team directories. There is also some additional data available for use that has not been generated or QA'd by the Data Team.

The XCP-3 files are stored in these directories:

XCP-lan:	`/opt/local/codes/mcnp/MCNP_DATA/`
HPC:	`/usr/projects/mcnp/MCNP_DATA/`
Release:	`MCNP_DATA`

In each of these directories:

- The Data Team files are available via symbolic links, i.e., there are not duplicate copies of the Data Team files.

- There are additional files needed for MCNP6.1 features, such as cosmic ray background, depletion, delayed particles, high energy physics, etc.

- There are additional data files for photonuclear data (endf7u, *zaids*: .70u) and photoatomic data (eprdata12, *zaids*: .12p) that were not generated or QA'd by the Data Team.

- There is an MCNP6.1-specific *xsdir* file named *xsdir_mcnp6.1*. This *xsdir* file includes all of the same entries as in the Data Team *xsdir* file and provides exactly the same defaults as the Data Team *xsdir* file, except for:
  - There are additional (nondefault) entries for the .70u *zaids* from endf7u.
  - There are additional (nondefault) entries for the .12p *zaids* from eprdata12.

- There is an MCNP5/X-specific *xsdir* file named *xsdir*. This *xsdir* file includes all of the same entries as in the Data Team *xsdir* file and provides exactly the same defaults as the Data Team *xsdir* file, except for:
  - The continuous thermal neutron scattering S(a,b) data entries were deleted from the available *zaids*. Neither MCNP5 nor MCNPX can correctly use that data. Instead, the discrete S(a,b) data (endf70sab, *zaids*: .10t ...) are the defaults.
  - There are additional (nondefault) entries for the .70u *zaids* from endf7u.

Any new-style *zaids* with suffixes of the form .710nc, with 3-digit version numbers and 2-character type identifiers, cannot currently be used by MCNP5, MCNPX, or MCNP6. Any such entries found in the Data Team *xsdir* files are not included in any of the XCP-3 *xsdir* files.

The files in the XCP-3 directories will be copied to the physical DVD-2 and DVD-3 for the MCNP6.1 production release. The only changes that will be made are simply the compression of all data files using the zip utility. (*xsdir* files, scripts, and *readme* files will not be compressed.) The files from the Data Team directories will also be compressed and copied to the DVDs; symbolic links will not be used in creating the RSICC distribution package.

IV. Using MCNP5, MCNPX, MCNP6.1 and the XCP-3 Data

If the DATAPATH environment variable is set to the XCP-3 data directories, then

- MCNP6.1 will by default read the *xsdir_mcnp6.1* file. The default data will be the same as recommended by the Data Team. The additional MCNP6.1 data, the endf7u data, and the eprdata12 data will also be available.

- MCNP5 and MCNPX will read by default the *xsdir* file. The default data will be the same as recommended by the Data Team, except that discrete S(a,b) data will be used. The additional endf7u data will also be available, but the eprdata12 data will not be available.

V. Using MCNP5, MCNPX, MCNP6.1 and the Data Team Data

If the DATAPATH environment variable is set to the Data Team data directories, then

- MCNP6.1 will not find the *xsdir_mcnp6.1* file, and will proceed to read the *xsdir* file.
  - The default data will be the same as recommended by the Data Team.
  - The additional MCNP6.1 data, the endf7u data, and the eprdata12 data will not be available. Most problems will still run; some may fail due to missing data.

- MCNP5 and MCNPX will read the *xsdir* file.
  - The default data will be the same as recommended by the Data Team.
  - If explicit *zaid*-suffixes are supplied for discrete S(a,b) data (eg, lwtr.10t), then problems will run correctly.
  - If no *zaid*-suffix is supplied for S(a,b) data, or if the .20t suffix is used for the continuous S(a,b) data, then problems will not run correctly. There will be data failures in some problems, and silent wrong answers for some features.
  - The additional MCNP6.1 data, the endf7u data, and the eprdata12 data will not be available.

VI. Conclusions and Recommendations

Users of MCNP5, MCNPX, or MCNP6.1 should check the setting of the environment variable DATAPATH and make sure that it is set to the appropriate XCP-3 data directory for the system they are using.

For the LANL HPC clusters, the proper settings for the typical user shells are

bash: `DATAPATH=/usr/projects/mcnp/MCNP_DATA`

csh,tcsh: `setenv DATAPATH /usr/projects/mcnp/MCNP_DATA`

For the XCP-lan, the proper settings are:

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