Quality Assurance Procedures for ModCat Database Code Files

Revision 0

ER Siciliano
R Devanathan
ZC Guillen
RT Kouzes
JE Schweppe

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Pacific Northwest
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ER Siciliano
R Devanathan
ZC Guillen
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JE Schweppe

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Pacific Northwest National Laboratory
Richland, Washington 99352

Executive Summary

The Quality Assurance procedures used for the initial phase of the Model Catalog Project were developed to attain two objectives, referred to as "basic functionality" and "visualization." To ensure the Monte Carlo N-Particle model input files posted into the ModCat database meet those goals, all models considered as candidates for the database are tested, revised, and re-tested.

Acronyms and Abbreviations

ATTILA	A suite of deterministic radiation transport codes based upon solutions to the Boltzmann equation. [ATTILA]
Excel	The spreadsheet utility in the Microsoft Office suite of codes. The 2010 version is used for the files referenced.
cpu	Computer processing unit
DHS	U.S. Department of Homeland Security
DNDO	Domestic Nuclear Detection Office
DVD	Digital video disc
GEANT4	An object-orientated toolkit for Monte Carlo simulation of radiation detectors. [Allison 2006]
Linux	Open-source version of the UNIX operating systems.
Mac	The Macintosh line of personal computers and operating systems developed by Apple Inc.
MCNP	Generic reference to any of three Monte Carlo N-Particle radiation transport codes. [MCNP6; MCNP5;MCNPX]
ModCat	Model Catalog
OS	Computer operating system
PNNL	Pacific Northwest National Laboratory
Q/A	Quality Assurance
RAM	Random access memory
RSICC	Radiation Safety Information Computational Center, (https://rsicc.ornl.gov/Default.aspx)
TERT	Total-Elapsed Run Time
VisEd - VisPlot	Visual Editor – Visual Plotter [VisEd/VisPlot]
Windows	Generic reference to any one of several operating systems developed by Microsoft.

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Figures

1 Objectives for Code-File Test Procedures

The Model Catalog (ModCat) Project has the objective of creating a database of radiation transport models developed to simulate various detector and source configurations that were produced for national security applications. The Quality Assurance (Q/A) procedures used for the initial phase of the ModCat Project were developed to attain two objectives, referred to as "basic functionality" and "visualization." To ensure the Monte Carlo N-Particle (MCNP) [MCNP6; MCNP5;MCNPX] model input files posted into the ModCat database meet those goals, all models considered as candidates for the database are tested, revised, and re-tested.

Brief descriptions of these objectives and the Q/A procedures used to attain them are given here. The detailed tests used in those procedures are listed in the following sections. Although the type of code files addressed in this first phase of the project was limited to MCNP, additional testing procedures for other code types, such as GEANT4 [Allison 2006] and ATTILA [ATTILA], will be developed, and this document updated, to meet the same two objectives.

The primary goal of basic functionality was to provide the MCNP user with example output files (and in some cases example Excel analysis workbooks) as benchmarks for confirming the MCNP models downloaded from the ModCat database were not corrupted or otherwise altered during the download process. To provide results that would be useful to the widest group of MCNP users, these output files were produced using the single-thread or "sequential" versions of the binary (executable) files from the default Windows-installation of all three versions of the latest suite of MCNP (5, 6, X) codes. Because the input files were revised to attain this goal by using the simplest tally and other run-time options needed to attain this goal, the ModCat input files are expected to produce the same results when used on Linux or Mac systems. Limited testing for MCNP5 installations on those systems was conducted to confirm that expectation.

A secondary, task for basic functionality testing was to examine each input file to determine if there were a minimum amount of comments that help explain, or guide a user in understanding, the overall purpose, coding structure and parameters used in constructing the file. Although determining what amount and type of comments are sufficient to meet these criteria is a qualitative task, assuring that some "minimal" level of comments were included in all posted input files was deemed to be important.

The goal of visualization was to provide the user with an input file that could be visualized easily by using one of the Visual Editor Consultants (VEC) [VisEd/VisPlot] products, VisPlot or VisEd that are also included with the latest versions of the MCNP codes. For that purpose, a file with the extension "vis" is included with all ModCat models. It contains plot parameters that are automatically used by these visualization codes for an input file with the same name prefix. Providing this initial set of parameters helps the user quickly confirm via two different cross-sectional views that the downloaded model is indeed the one shown by the pictures posted in the ModCat database. Because the currently distributed versions of these VEC programs run only on systems using the Windows OS, the Visualization capability outlined above applies to Windows-system users only.

2 Computing Equipment and Software used for Testing

The following specifies the computing platform and software versions of MCNP that were used to produce all the code files posted in the ModCat database. They were established assuming most users would have access to similar or more capable computers upon which the same versions of MCNP (and associated cross-section libraries) have been installed. This information gives a scale of reference for what can be expected in computation speed and round-off differences that might result when the same ModCat input files are executed on different platforms (or older versions of MCNP or associated cross-section data libraries).

2.1 Computing Equipment

The computing equipment used for these tests was a typical, mid-level desktop workstation: a Dell Precision T3500 equipped with a 2.53 GHz, 4-core Intel Xeon cpu (model E5630) and 12 GB RAM. The installed operating system was the 64-bit Windows 7 Enterprise, with Service Pack 1.

This platform, as with almost all currently available computers, had a cpu that was capable of multi-core, multi-task co-processing. However, all the Q/A run-time testing for MCNP input files were performed using only the single-thread or "sequential" versions of the installed binary executable MCNP files. Because single-core evaluation takes the longest time to produce output, the tally summary values and the total elapsed run-times listed in the Code output files give the least-efficient baseline for comparison. The User should be able to confirm those results quickly, and then improve upon them easily by increasing the number of simulation histories and increasing the number of command-line "tasks" for multi-core execution of the installed "omp" binary versions. It is expected that the Total-Elapsed Run Times (TERT's) listed in the ModCat output files tests will decrease linearly with the inverse of cores used.

2.2 Software

All three versions of the MCNP codes (MCNP5_1.60, MCPNX_2.70, and MCNP6.1) [MCNP6; MCNP5;MCNPX], and the cross-section data libraries [ENDF] were installed from the most recent (2013) Radiation Safety Information Computational Center (RSICC) distribution DVD. The particular one used for these tests was labeled C00810MNYCP00 MCNP6.1/MCNP5/MCNPX, which includes both the executables and the source files. Testing was performed by using only the executable files. These files are the same as would have been installed from "executable-only" RSICC package number C00810MNYCP01. Information about moving from MCNP5 or MCNPX to the newer MCNP6 can be found in the Los Alamos reports "MCNP5 to MCNP6 Migration Notes" [Goorley 2013] and "MCNPX to MCNP6 Migration Notes" [James 2013]. These reports are also found in MCNP_DOCS\MCNP_REFS\pdf_files folder on Disk 1 "Codes and Documents" of the RSICC distribution package C810.

As mentioned above, only the single-thread or sequential versions of the installed binary executables files were used to produce the output files posted in the ModCat database. For reference, the command lines used for those tests are given below. Note that the names of the MCNP pre-compiled binary executables used and the environmental paths to them were those suggested or defined by following the installation instruction given in the file "INSTALL.html" in the MCNP_DOCS folder mentioned above.

For the MCNP5 results, the command line used was:

```
C:\MY_MCNP\MCNP_CODE\MCNP5\bin\windows\mcnp5_windows_i386_seq ixr
```

For the MCNPX results, the command line used was:

```
C:\MY_MCNP\MCNP_CODE\MCNPX\Executables\Win64_Seq\bin\mcnpx ixr
```

For the MCNP6 results, the command line used was:

```
C:\MY_MCNP\MCNP_CODE\MCNP6\bin\windows\mcnp6_windows_i386_omp tasks
1 ixr
```

All the input file names have the suffix "Input.txt," and run-time batch scripts were used to copy the resulting output file, and if present, mctal files using the same prefix as the input, but with the suffices "Output.txt," and if present, "Mctal.txt."

3   Details of Q/A Testing

For Reference Directories on MCNP-PC (Dell Precision T3500, PNNL P/N we19756), see Figure 1. c:\MCNP_ModCat_Testing, is the main directory typically accessed using a desktop shortcut.

1) Use subdirectory "FilesForTesting" to save and decompress ModCat downloads of zipped "code" folders.

2) Copy the input file of the model to each "ioAnalysis" folder, i.e. MCNP5-ioAnalysis, MCNP6-ioAnalysis, and MCNPX-ioAnalysis directories.

3) If present, copy the Excel .xlms file into (one) "ioAnalysis" folder (e.g. MCNP5-ioAnalysis).

4) Visualization Testing:

In the ioAnalysis folder with the input file, launch VisPlot (from the Start menu list) and use <alt-spacebar-x> to fill screen.

Figure 1: Directory Structure Used for Testing

Use the File menu in the VisPlot taskbar to select and load the input file. Document any problem at that point with loading the file. Use the (Microsoft utility) Snipping Tool to capture and save an image of the problem (in JPEG format).

If there is no problem loading the file into VisPlot, then use the Update Plots button on the VisPlot taskbar to get default views of model. Document it with the Snipping Tool and save the image in JPEG format.

At this point there will be one or two JPEG files. These files are used as part of the feedback report to the QA Lead.

5) I/O Testing:

> a) Execution:
> Go to each of the three MCNP "RunFiles" subdirectories, open a command window for each folder (via the command shortcut) in each folder), then use the RunAll..."bat" script files run each MCNP version for that same input file. Because the bat files are executing "sequential" runs, i.e., one core, and the MCPN-PC has a quad-core CPU, all three can be processed simultaneously, showing a ~75% cpu usage in the Task-Manager icon. The remaining cpu capacity also allows the user to access the PC for other tasks.

> b) Analysis:
> Copy the "out" and if present the "mctal" files from each of the MCNP "RunFiles" subdirectory into the corresponding MCNP "ioAnalysis" subdirectory.

> Use the "Beyond Compare" (or other installed file-comparison utility) to determine and document the differences between each out-file produced and the out-file downloaded
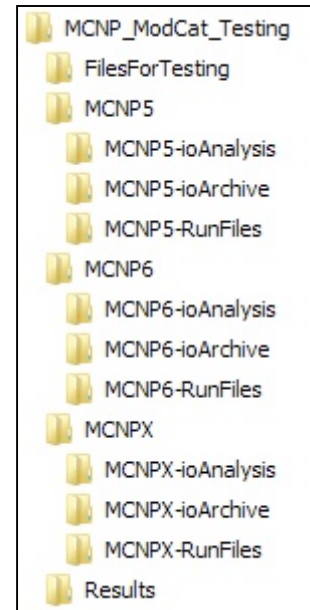
from the ModCat saved in the "FilesForTesting." A summary of any differences found will be saved and sent (along with the JPEGs from the Visualization Tests) to the QA Lead for changes in the model notes that the user will get along with the files to help the user view the model quickly and be aware of whatever differences he/she may find when using their particular version of MCNP or cross-section libraries.

6) Final Version Q/A: repeat all of the above after the QA Lead posts replies. Return all three versions of "out" files and if present, one version (e.g., MCNP5) of "mctal" file to the QA Lead for final postings.

4   References

Note for the MCNP references below, the LANL reports listed for MCNP6 and MCNP5 are available to anyone, but the MCNPX manual as well as the (unlisted) MCNP6 manuals are export controlled.

ATTILA is distributed by Transpire, Inc. Website: www.transpireinc.com/software/attilaAttila for further information and references.

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James MR, "MCNPX to MCNP6 Migration Notes", LA-UR-13-22964 (2013)

MCNP6: J.T. Goorley, et al., "Initial MCNP6 Release Overview - MCNP6 version 1.0", LA-UR-13-22934, (2013); also *Nuclear Technology* 180, pp 298-315 (Dec 2012).

MCNP5: X-5 MONTE CARLO TEAM, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory," LA-UR-03-1987, Los Alamos National Laboratory (April 2003).

MCNPX: "MCNPX User's Manual Version 2.7.0," LA-CP-11-00438, D. B. PELOWITZ, Ed., Los Alamos National Laboratory (Apr. 2011).

VisEd/VisPlot are two products developed by the Visual Editor Consultants, http://www.mcnpvised.com, and distributed by RSICC with the MCNP package.

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