

## Importance of All-in-one (MCNPX2.7.0+CINDER2008) Code for Rigorous Transmutation Study

Oyeon Kum<sup>a,c\*</sup> and Kwanghyun Kim<sup>b,c</sup>

<sup>a</sup>Institute for Modeling & Simulation Convergence, Daegu 42045, Korea

<sup>b</sup>RadTek Co., Ltd, Daejeon 34166, Korea

<sup>c</sup>University of Southwest America, CA 91701, USA

\*Corresponding author: okum@uswa.ac

### 1. Introduction

Nuclear transmutation (a conversion of one chemical element or isotope into another) is caused by a process that occurs either through nuclear reactions (in which an outside particle reacts with a nucleus), or through radioactive decay (where no outside particle is needed) although not all nuclear reactions or radioactive decay cause transmutation. Specifically, artificial nuclear transmutation may occur in machineries (i.e. accelerators or fission/fusion reactors) that have enough energy to cause changes in the nuclear structure of the elements. It can be utilized as a possible mechanism for reducing the volume and hazard of radioactive waste by transforming hazardous radioactive elements with long half-life into less hazardous elements with short half-life. Thus, the understanding of the transmutation mechanism and beneficial machinery design technologies are important and useful.

Although the terminology transmutation was rooted back to alchemy which transforms the base metals into gold in the middle ages, Rutherford and Soddy were the first observers by discovering the natural transmutation as a part of radioactive decay of the alpha decay type in early 20th century. Along with the development of computing technology, analysis software, for example, CINDER [1] was developed for rigorous atomic transmutation study. The code has a long history of development from the original work of T. England at Bettis Atomic Power Laboratory (BAPL) in the early 1960s. It has been used to calculate the inventory of nuclides in an irradiated material. CINDER'90 which is recently released involved an upgrade of the code to allow the spontaneous tracking of chains based upon the significant density or pass-by of a nuclide, where pass-by represents the density of a nuclide transforming to other nuclides.

CINDER2008 [2] code is a modern implementation of the CINDER'90 software package. The most notable improvements include (1) modern programming language and methods, (2) new algorithms to more accurately solve the underlying differential equations, (3) new extended data libraries developed using fission, fusion and constant weighting functions, (4) new data library development tool, (5) automatic post-processing capabilities, (6) accident analysis tools, (7) NAMELIST

input option, (8) constant power approximation and (9) high-fidelity beta-delayed gamma spectra.

In order to make use of the CINDER particle transmutation code, accurate knowledge of the average flux in the material that is to be transmuted is necessary. Thus, a transport code must be plugged onto the front end of the calculation to estimate the neutron distributions in the medium. As the transport wrapper, MCNPX2.7.0 code [3] is used with CINDER2008. At present, the connection uses ancillary scripts that provide an interface into the output files of the multi-particle transport code MCNPX. The inter-relation of the scripts and the CINDER and MCNPX codes is outlined in Fig. 1. One script, the ACTIVATION script, drives activation calculations of multi-region problems preparing for CINDER2008 input files and executing CINDER2008 with minimal user input. Another script, the GAMMASOURCE script, prepares decay gamma source decks that can be directly fed back into MCNPX calculation of gamma-ray radiation arising from activation products. Because of the separate modular structures and the use of additional script codes, CINDER2008 is hard to use and may provide inaccurate answers due to the lack of enough significant digits by the human interrogation of the process.

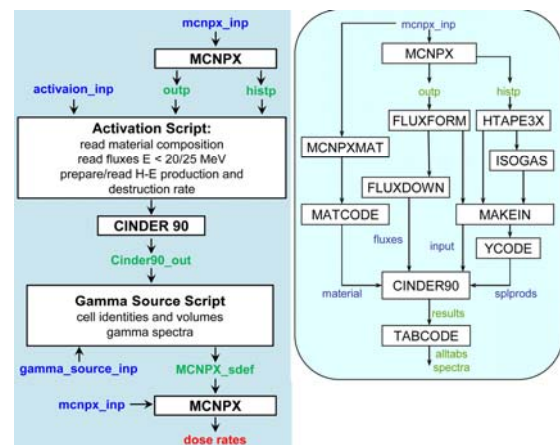


Fig. 1. Transmutation computation flow with two scripts. Right side shows the details of output and histp files. CINDER2008 also uses the results of the two scripts for CINDER90.

In this study, we propose an “all-in-one code” development by directly combining CINDER with MCNPX code. Specifically, the latest versions of MCNPX2.7.0 and CINDER2008 codes are used. The resulting “all-in-one” code structure is similar to FLUKA2011 [4]. An overview of the combined code performance is needed an input file which includes the transport calculation information and transmutation calculation requirement necessary for CINDER2008. All the intermediate information, for example, material data, volume, and fluxes are transmitted directly via computer memories with full significant digits to the next step calculation. Thus, the input file controls the range of simulation with optional flags, from simple particle transport simulation to atomic transmutation and radiation dose computations by the gamma ray distributions.

## 2. Methods and Results

In this section brief overviews of MCNPX2.7.0 and CINDER2008 codes are provided and the code merging processes are shown. Debugging tool of Fortran90/95 is used for analyzing the variables used in the independent codes and combination process.

### 2.1 MCNPX2.7.0

MCNP is a general purpose Monte Carlo radiation transport code that was developed to track many particle types over broad ranges of energies at Los Alamos National Laboratory nearly sixty years ago. MCNPX program began in 1994 as an extension of MCNP4B and LAHET 2.8 in support of the Accelerator Production of Tritium Project (APT) [5]. The work envisioned a formal extension of MCNP to all particles and all energies; improvement of physics simulation models; extension of neutron, proton, and photonuclear libraries to 150 MeV; and the formulation of additional variance-reduction and data-analysis techniques. The program also included cross-section measurements, benchmark experiments, deterministic code development, and improvements in transmutation code and library tools through the CINDER'90 project.

MCNPX2.7.0 is the latest public release version to the Radiation Safety Information Computational Center (RSICC), following the 2008 release of MCNPX2.6.0 and the 2005 release of MCNPX2.5.0 which was a superset of MCNP4C and MCNPX2.4.0.

MCNPX2.7.0 includes about 30 significant additional improvements from MCNPX2.6.0. Highlights are physics improvements, expanded tally options, additional source options, and improved plotting capability. Physics improvements include an upgrade of the Cascade-Excitation model (CEM), the addition of the LLNL fission multiplicity package, enhanced delayed-particle algorithms, an upgrade of the high-energy Los Alamos Quark-Gluon String model

(LAQGSM), and a variety of updated nuclear data files (nuclear resonance fluorescence, muonic x-rays, photo-fission, and fission-products, *etc.*). The code is compatible with MCNP5. Since MCNPX2.7.0 is now incorporated into MCNP6 which is merged code of the MCNP5 and MCNPX2.7.0, it is actually the last version in this series of Monte Carlo program.

### 2.2 CINDER2008

CINDER code system has been developed since 1960. Initially, the interests were focused on the reactor problems, but more recently include various accelerator problems. The development team began in 2005 with the intent to package CINDER'90 in a more user-friendly format, which was released from Radiation Safety Information Computing Center (RSICC) with the inclusion of relevant scripting tools. CINDER2008 is a significant upgrade in capability from CINDER'90.

Nuclear transmutation calculates the differential equation describing the rate of change in the atom density for a specific nuclide. The differential rate equation can be converted to Bateman equation via Markovian chains whose general explicit formula for the solutions can be found by taking the Laplace transform of the variables. While the Bateman formula can be implemented easily in computer code, if the rates of change are almost equal for some isotope pair, cancellation can lead to computational errors. Thus, other methods such as numerical integration or the matrix exponential method are also in use.

CINDER code system comes with an extensive library of neutron-induced reactions. There has been thought from time to time about developing photon-induced and proton-induced cross section libraries, but these are still underway. These neutron cross section libraries were completely reformulated for CINDER2008. Cross sections collapsed from pointwise ENDF using a hybrid fission-fusion weighting function. CINDER2008 has three reaction libraries covering energies  $10^{-11}$  to 25 MeV (20 MeV). Sixty six group fission-weighted library has the same group structure as the 63-group library (CINDER'90), except the lowest group ( $E_n < 10^{-9}$  MeV) has been broken into four groups. It has 321-group flat-weighted library, based on 315-group TRIPOLI [6] group structure. This library is expected to provide the best results overall due to higher fidelity. It has also 175-group fusion-weighted library, in the VITAMIN-J [7] group structure. This library doesn't have many groups at low energy and is probably best reserved for special problems for which the fusion spectrum serves as a good approximation to the actual neutron flux in the system. Maximum energy for each cross section is that from the respective reference data. Specifically, CINDER2008 package has a library maker code that the users can make their own group-averaged cross section library if desired. It is

recommended that the neutron flux must be specified using the same energy bin structure as the cross section library that you intend to use.

### 2.3 Debugging in source mode

The source languages of CINDER2008 and MCNPX2.7.0 are FORTRAN90/95 [8] which can be compiled with well-known Fortran compilers such as Intel [9], PGF [10], Absoft Pro [11], GNU fortran [12], Lahey fortran [13] *etc.* In this study, we used Portland Group fortran compiler to debug the codes. CINDER2008 is a “make-style” package, which is easier to change debug mode. Two options must be changed: FC=pgf90 and OTHERFLAGS= -g. The default compiler modes are gfortran and optimization level one. Then, we will have a debug command window as shown in Fig. 2.

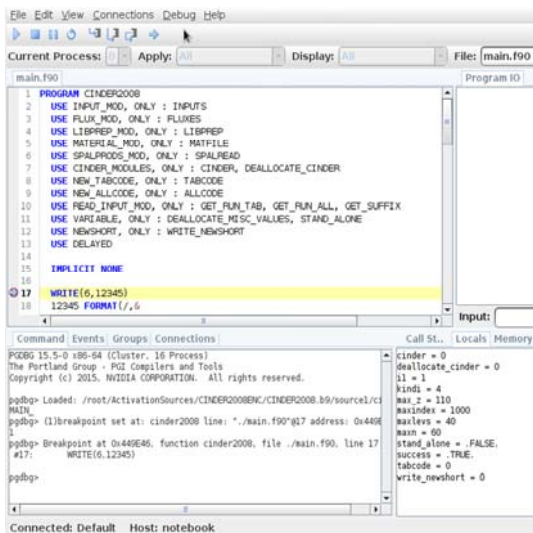


Fig. 2. Debug command window for CINDER2008 code.

MCNPX2.7.0 uses auto-configuration scheme to make use the maximum computer environments. Auto-configuration is noninvasive, at any point we can start to define our own configuration to replace specific parts of the auto-configuration. Most software packages that use “autoconf” have a basic unpack, build, and install procedure as follows:

```
gzip -dc DIRECTORY.tar.gz | tar xf -
cd DIRECTORY
./configure
make install
```

With the auto-configure function, MCNPX directory can be customized by using prefix option, for example, “./configure --prefix=/usr/mcnp.” Fortran compiler and optimization level can also be customized similarly although default compiler is gfortran. The following

example shows a case with debug mode of pgf90 compiler.

```
./configure --with-FC=pgf90 --with-DEBUG
make install
```

Then, the debug command window with MCNPX2.7.0 source is shown in Fig. 3.

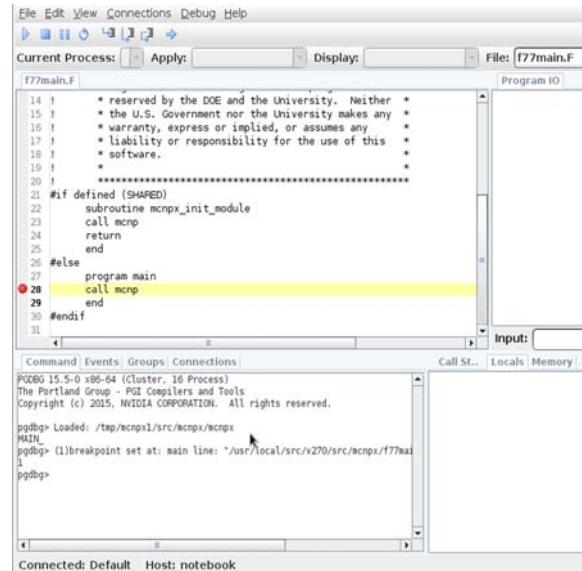


Fig. 3. Debug command window for MCNPX2.7.0.

### 2.4 Code merging strategy

In order to make use of the CINDER2008 particle transmutation code, accurate knowledge of the average flux in the material that is to be transmuted is necessary. Thus, MCNPX2.7.0 code must be plugged onto the front end of the calculation to estimate the neutron distributions in the medium. The inter-relationship between the CINDER2008 and MCNPX2.7.0 codes is shown in Fig. 1. Because the two scripts, the ACTIVATION and the GAMMASOURCE scripts, prepare all necessary input files for CINDER2008 and MCNPX2.7.0 codes, some arithmetic parts of the two scripts are rewritten with Fortran90/95 language. The necessary data variables are transported directly with memory bank. Because the number of data variables is not big, not so big memory size is required.

To make a “splprods” input file, HTAPE3X code is used to analyze the “histp” file provided by MCNPX2.7.0. Because many subroutines consisting of HTAPE3X code overlap with MCNPX2.7.0, this merging procedure is relatively simple. This merging reduces the real computing time with the avoidance of writing time of “histp” file. At present, parallel processing of the transmutation code was hard because parallel processing for “histp” file is not possible. However, this merging results in the transmutation code in parallel running, which is another benefit of “all-in-

one” code. Debug command window for HTAPE3X code is shown in Fig.4.

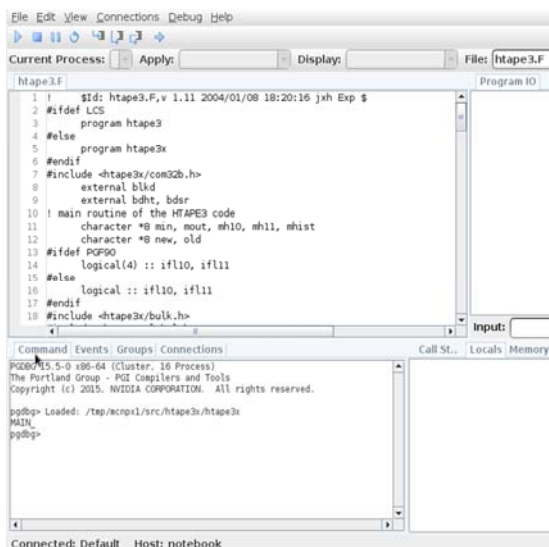


Fig. 4. Debug command window for HTAPE3X code.

### 2.5 All-in-one code

In all-in-one code, all previous intermediate information, for example, material data, volume, and fluxes are transmitted directly via computer memories with full significant digits for the next step calculation. The input file controls the range of simulation with optional flags, from simple particle transport simulation to atomic transmutation and radiation dose computations by the gamma ray distributions. Thus, the respective input files for CINDER2008 and MCNPX2.7.0 are also merged. Figure 5 is an example of the atom-density result (unit: atoms/barn-cm) of a specific problem which shows the dependence of the computed results on the number of significant digits of the input files. Problem definition, exact number of significant digits, quantitative differences of number densities will be shown in the presentation.

File	Edit	View	Search	Terminal	Help		
Mo 95	STABLE	1.744E-0025	2.466E-0025	2.494E-0025	4.641E-0015	4.641E-0015	4.641E-0015
Mo 96	STABLE	1.156E-0036	1.798E-0036	1.820E-0036	1.820E-0036	1.820E-0036	1.820E-0036
Mo 97	STABLE	3.972E-0049	6.844E-0049	6.961E-0049	6.961E-0049	6.961E-0049	6.961E-0049
A=66		1.336E-0012	1.336E-0012	1.457E-0012	1.457E-0012	1.457E-0012	1.457E-0012
65<A>173		4.284E-0002	4.284E-0002	4.284E-0002	4.284E-0002	4.284E-0002	4.284E-0002
172<A		0.000E+0000	0.000E+0000	0.000E+0000	0.000E+0000	0.000E+0000	0.000E+0000
TOTAL		4.284E-0002	4.284E-0002	4.284E-0002	4.284E-0002	4.284E-0002	4.284E-0002
Mo 95	STABLE	1.744E-0025	2.466E-0025	2.494E-0025	4.641E-0015	4.641E-0015	4.641E-0015
Mo 96	STABLE	1.156E-0036	1.798E-0036	1.819E-0036	1.819E-0036	1.819E-0036	1.819E-0036
Mo 97	STABLE	3.972E-0049	6.843E-0049	6.960E-0049	6.960E-0049	6.960E-0049	6.960E-0049
A=66		1.336E-0012	1.336E-0012	1.457E-0012	1.457E-0012	1.457E-0012	1.457E-0012
65<A>173		5.364E-0001	5.364E-0001	5.364E-0001	5.364E-0001	5.364E-0001	5.364E-0001
172<A		0.000E+0000	0.000E+0000	0.000E+0000	0.000E+0000	0.000E+0000	0.000E+0000
TOTAL		5.364E-0001	5.364E-0001	5.364E-0001	5.364E-0001	5.364E-0001	5.364E-0001

Fig. 5. Atomic density (unit: atoms/barn-cm) result for two input files with different significant digits.

As shown in the figure, the dependence is chaotic because of the non-linearity of the problem.

In some sense of flexibility of the CINDER2008 code, the “all-in-one” code reduces the value very much because the original CINDER2008 can be combined with arbitrary transport codes. This is a draw-back for the CINDER2008 code. However, the complexity problem for using CINDER2008 with independent scripts is resolved for the general users.

Debugging of the new code is necessary and uses the same compiler, pgf90. Inter-code comparisons are also important and underway now.

### 3. Conclusions

Nuclear transmutation process is governed by highly non-linear differential equation. Chaotic nature of the non-linear equation bespeaks the importance of the accurate input data (i.e. number of significant digits). Thus, reducing the human interrogation is very important for the rigorous transmutation study and “all-in-one” code structure is desired. Note that non-linear characteristic of the transmutation equation caused by the flux changes due to the number density change during a given time interval (intrinsic physical phenomena) is not considered in this study. In this study, we only emphasized the effects of human interrogation in the computing process solving nonlinear differential equations, as shown in the case of accidental discovery of chaos by Edward N. Lorenz [14]. Furthermore, excluding human interrogation, resulting in all-in-one code, will be more probable to include intrinsic physical problem such as flux changes in a given time interval.

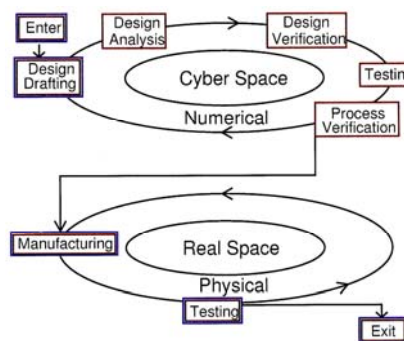


Fig. 6. Conceptual structure of the dual engineering design cycle. The key importance of the dual design cycle is to reduce the number of trials in the real physical space.

We showed the debugging steps of a new “all-in-one” code which combines the world best transportation code (MCNPX2.7.0) with transmutation code (CINDER2008). Moreover, efficient transmutation study is possible because “all-in-one” code structure makes the parallel processing easily

possible. Avoiding the necessity of scripts increases the user's conveniences. As a minor draw-back, flexibility of the CINDER2008 code is reduced by matching only with MCNPX2.7.0.

Future study is focused on developing a new customized transportation and transmutation simulation code to provide very efficient dual cycle engineering design environments in nuclear industry. The conceptual dual design cycle is shown in Fig. 6. Dual engineering design environment is expected to contribute much value to nuclear industry in cost-effectiveness and safety. Specifically, this or similar trials should be employed in the nuclear industry in order to, at least, reduce the concerns of those who oppose to the development of nuclear energy, which we believe the only way to achieve future national competitiveness.

## REFERENCES

- [1] W. B. Wilson, S. T. Cowell, T. R. England, A. C. Hayes & P. Moller, A Manual for CINDER'90 Version 07.4 Codes and Data, LA-UR-07-8412, Los Alamos National Laboratory, March 2008.
- [2] S. T. Holloway, W. B. Wilson, Charles T. Kelsey, IV, Hannah Little, Vladimir Mozin, A Manual for cinder2008 Codes and Data, LA-UR 11-00006, Los Alamos National Laboratory, March, 2011.
- [3] MCNPX User's Manual Version 2.7.0, LA-CP-11-00438, Denise B. Pelowitz, ed., April 2011.
- [4] <http://www.fluka.org>, as of August 2015.
- [5] M. B. Chadwick, P. G Young, S. Chiba, S. C. Fl'ankle, G. M. Hale, H. G. Hughes, A. J. Koning, R. C. Little, R. E. MacFarlane, R. E. Prael, and L. S. Waters, Cross-Section Evaluations to 150 MeV for Accelerator-Driven Systems and Implementation in MCNPX, NUCLEAR SCIENCE AND ENGINEERING: Vol.131, p.293, 1999.
- [6] <https://www.oecd-nea.org/tools>, as of August 2015.
- [7] A.B. Pashchenko and H. Wienke, FENDL2/A-MCNP, FENDL2/A-VITJ\_E and FENDL2/A-VITJ\_FLAT, IAEA-NDS-174, March 1997.
- [8] Tanja van Mourik, Fortran 90/95 Programming Manual, fifth revision, Chemistry Department, University College London, 2005.
- [9] <https://software.intel.com/en-us/fortran-compilers>, as of August 2015.
- [10] <http://www.pgroup.com>, as of August 2015.
- [11] <http://www.absoft.com>, as of August 2015.
- [12] <https://gcc.gnu.org/fortran>, as of August 2015.
- [13] <http://www.lahey.com>, as of August 2015.
- [14] James Gleick, Chaos: Making a New Science, New York, Penguin, 1987.