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Eigenfunction Convergence and Transmutation Enhancements in MCNPX[(a)]

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This paper describes two new features developed for MCNPX. The first feature applies a variance reduction technique to achieve faster convergence of the eigenfunction in a criticality calculation. Results indicate that this new method converges nearly 100 times faster than the current approach. The second feature involves a transmutation option within MCNPX via a Fortran interface to the CINDER90 code. MCNPX burnup results for a simple criticality problem compare favorably to a Monteburns calculation.

KEYWORDS: Monte Carlo, MCNPX, CINDER, radiation transport, eigenfunction convergence, transmutation, burnup

1. Introduction

Recent versions of MCNPX [1] have focused on the needs of the reactor community by including such features as increased efficiency of parallel eigenvalue calculations (speedups of 10–100 for large clusters), speedup of lattice tallies (factors of ~10,000 for lattices with 10^6 elements), importing of external files (READ card), coincidence tallies (FT card, PHL and CAP options), and "mix-and-match" physics (enabling a seamless transition from library-based cross sections to models and providing model-based cross sections for missing library data). Future versions of MCNPX will include additional features of significance for this community, namely, the use of variance reduction to speed eigenfunction convergence and material transmutation via a CINDER90 [2] interface. These two features are complimentary in that a converged eigenfunction is necessary for an accurate transmutation calculation. This paper provides implementation details regarding these features and gives results for a simple criticality application.

2. Description of Features

2.1 Eigenfunction Convergence

A new Monte Carlo variance reduction technique [3] has been developed to enhance the convergence of an eigenfunction in critical or near-critical nuclear systems. The correct estimation of the underlying eigenfunction is essential for radiation protection and shielding near those systems, in addition to material transmutation, nuclear criticality, and other applications. This new method applies to Monte Carlo eigenvalue (k_{eff}) calculations, which work by treating fission events as capture and utilizing the fission sites as sources in subsequent generations. Although in most Monte Carlo transport codes the estimation of the eigenvalue is rigorous, the resulting eigenfunction for many applications may be off by orders of magnitude in symmetric parts of the problem.

(a) MCNPX is a trademark of the Regents of the University of California, Los Alamos National Laboratory.

This new method enhances the convergence of the eigenfunction by estimating F_i, the number of fission neutrons produced anywhere in the geometry per fission source in geometric region "i". Note that F_i is the local value of k_{eff} in region "i". Then the probability of producing a source neutron in geometric region "i" of the next generation is biased by a factor B_i, where

$$B_i = N*F_i*V_i / (k_{eff}*V*N_i) \quad (1)$$

with $N=\Sigma N_i$, $V=\Sigma V_i$, V_i=volume of region "i", and N_i=number of fission source neutrons produced in region "i" for some number of previous generations. The bias factor, B_i, must be properly normalized and damped so that it does not overcorrect from generation to generation. Furthermore, $B_i > 1$ for regions where the number of fission sources is low relative to their contribution to k_{eff}. This biasing function is updated and used during each generation to make the number of fission sources in each region proportional to their expected contribution to k_{eff}.

2.2 Transmutation

Another feature recently developed for MCNPX is the ability to perform transmutation calculations. Although this capability has been available to users via various scripting utilities, such as Monteburns [4], it is the first time that burnup calculations are entirely automated within MCNPX. This enhancement provides many benefits to the user by eliminating the need to learn other post-processing codes, reducing errors in normalizations and auxiliary input, and eliminating file manipulation and tracking issues.

This transmutation option is implemented with a batching scheme that updates material properties at various user-specified time steps. The number of particle histories sampled per batch is also specified by the user. At the beginning of each time step, MCNPX runs a batch of histories and accumulates a 63-group neutron flux averaged over each material. These fluxes, along with tabulated 1-group cross sections and related isotopic atom densities, are passed through an interface routine to CINDER90. In its usual fashion, CINDER90 uses the neutron fluxes and 1-group cross sections to perform activation, depletion, and decay for the specified burn time. It then updates the isotopic inventory, calculates burnup, and returns various quantities to MCNPX for use during the next time step (this procedure is similar to that done in Monteburns). As usual, users can perform various time-dependent tallies across this entire simulation process.

Due to complexities within MCNPX related to cross-section processing, it was necessary to develop an algorithm for predicting the list of transmuted isotopes. This list is generated during the "first pass" of input processing and is used to establish the appropriate storage for the various materials to be burned. During the "second pass" of the input processing, the nuclide list for each material is expanded to incorporate these transmuted isotopes. As described below, the user can add or remove isotopes from this list as they see fit.

A BURN card has been added to MCNPX to specify the various transmutation parameters. The format of this card is as follows:

BURN TIME=T_1,T_2,…
PFRAC=F_1,F_2,…
POWER=P
MAT=M_1,M_2,…
OMIT=J_1,N_1,I_{11},I_{12},…,J_2,N_2,I_{21},I_{22},…
AFMIN=A
BOPT=B_1,B_2,B_3

A BURN card without any keywords results in a single burn time of 1 day at a power level of 1 MW and includes all materials in the burn. A description of the various entries follows:

T_i = duration of the i^{th} burn step (days). Default is one time step of one day.
F_i = power fraction of each time step (0-1). Zero produces decay only. Default is 1.0.
P = power level (MW). Default is 1.0.
M_i = list of burn material numbers. Default is to burn all materials.
J_k = k^{th} material for which to omit nuclides. If J_1=-1, then the nuclide list is applied to all materials and J_2, J_3, etc. are not allowed.
N_k = number of nuclides listed for the k^{th} material.
I_{k1}, I_{k2}, ... = omitted nuclide list for the k^{th} material. Format is ZZAAA.
A = minimum atom fraction. Default is 1.0e-10.
B_1 = fission Q-value multiplier. Default is 1.0.

An example of the BURN card follows:

BURN TIME=15,30,30 MAT=3,4 POWER=2.0
OMIT=3,3,8017,92234,92239,4,1,92234

This card specifies a power level of 2 MW for a total duration of 75 days (time steps of 15 days, 30 days, and 30 days). Materials 3 and 4 are included in the burn with isotopes 8017, 92234, and 92239 excluded from material 3 and isotope 92234 excluded from material 4.

New tables are provided in the MCNPX output file, which give the updated atom fractions, cell densities, and burnup details for each time step.

3. Results

3.1 Eigenfunction Convergence

The sample problem chosen for use in this paper consists of seven cans of highly enriched uranium (HEU) solution arranged on a hexagonal grid (see Fig. 1). The MCNPX input file for this problem is given in Table 1.

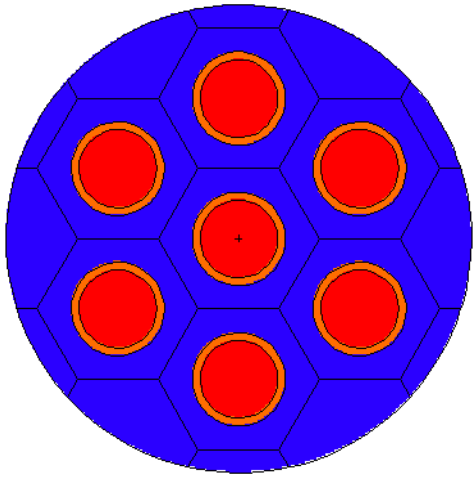

Fig. 1 A cross-sectional view of the seven cans of HEU solution surrounded by air.

Table 1 MCNPX input file for the seven-can sample problem.

```
cylinders containing critical fluid
1 1 -8.4       -1       u=1    imp:n=1
2 0            -2       u=1    imp:n=1
3 2 -2.7       -3 1 2   u=1    imp:n=1
4   3 -.001     3       u=1    imp:n=1
10 3 -.001     -6 lat=2 u=2    imp:n=1 fill=-2:2 -2:2 0:0
                                        2 2 2 2 2
                                        2 2 1 1 2
                                        2 1 1 1 2
                                        2 1 1 2 2
                                        2 2 2 2 2
11 0           -8               imp:n=1 fill=2
50 0            8               imp:n=0

1 rcc 0   0 0   0 12 0   5
2 rcc 0 12 0   0 8   0   5
3 rcc 0 -1 0   0 22 0   6
6 rhp 0 -1 0   0 22 0   9 0 0
8 rcc 0 -1 0   0 22 0   30

m1     1001 5.7058e-2    8016 3.2929e-2
       92238 2.0909e-3   92235 1.0889e-4
m2    13027 1
m3    7014 .8 8016 .2
kcode 1000 1 10 100
ksrc    0 6   0   18 6   0   -18 6   0   9 6 15   -9 6 15   9 6 -15   -9 6 -15
```

Clearly the eigenfunction in the outer cans of this configuration should all be equal; however, an eigenfunction tilt of 3–4 (ratio of maximum to minimum) for 1000 particles/cycle is typical (see Fig. 2a). The eigenfunction convergence technique,

described in section 2.1, reduces this eigenfunction tilt to only 6% (see Fig. 2b). It requires nearly 100,000 particles/cycle to achieve this eigenfunction convergence using the existing "analog" approach, thus this new technique enhances convergence by nearly two orders of magnitude. When a deliberately poor initial source distribution is used, this eigenfunction tilt can exceed a factor of 90 in a standard Monte Carlo calculation. With the new method, this extreme case resulted in an eigenfunction tilt of only 3. The correct calculation of the eigenfunction in Monte Carlo eigenvalue problems improves computational efficiency and enables reliable fluxes to be calculated for use in isotope production and depletion.

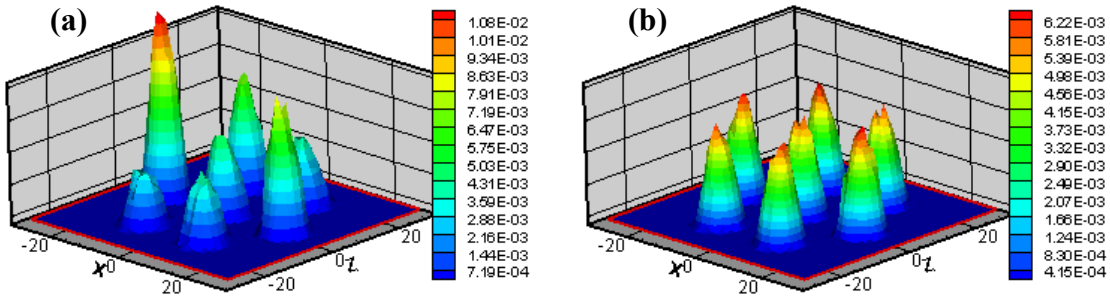

Fig. 2 Graph (a) shows the eigenfunction from a standard calculation, with a tilt of 3.5. Graph (b) shows the eigenfunction from the new method, with the tilt nearly eliminated.

3.2 Transmutation

During this first phase of the transmutation implementation, we focus on comparisons between MCNPX and Monteburns. As the MCNPX implementation approaches that of Monteburns, it is expected that the results will be quite similar. For this comparison, the Monteburns input file is given in Table 2, and the MCNPX KCODE and BURN cards are as follows:

```
KCODE 5000 1.0 20 120
BURN TIME=15.22,30.44,30.44,30.44,30.44,30.44,
          30.44,30.44,30.44,30.44,30.44,30.44
     MAT=1  OMIT=-1,9,8017,92234,92239,
     93235,93236,93238,93239,94236,94237
```

For both calculations, the seven-can configuration was burned at 1 MW for 1 year. Figure 3 presents the k_{eff} and burnup results for each timestep (the standard deviation on the k_{eff} values is about .001). While this preliminary comparison is quite good, discrepancies have been attributed to differences in cross-section data (Monteburns creates its 1-group data from the 63-group fluxes), average fission Q values, and average fission ν values. Figure 4 shows the difference in MCNPX burnup between the central and outer cans, indicating a ~20% increase in burnup in the central can (in this case each can was assigned a different material so burnup could be calculated individually).

Table 2 Monteburns input file for the seven-can sample problem.

```
cylinders containing critical fluid
UNSU
1
1
6597.34
1.0
-200.
365.24
12
40
1
0
CINDER
/path/to/origen/libraries
.0001
0
9
92235.60c
92236.60c
92237.50c
92238.60c
93237.60c
94238.60c
94239.60c
94240.60c
94241.60c
```

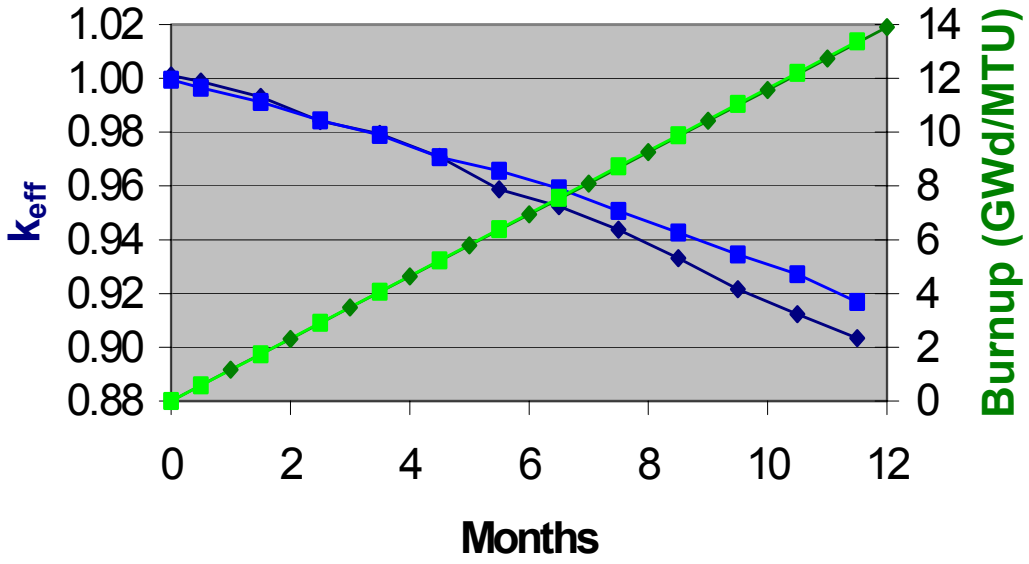

Fig. 3 MCNPX and Monteburns k_{eff} and burnup results for the seven-can HEU problem. MCNPX values are denoted by squares and Monteburns values by diamonds.

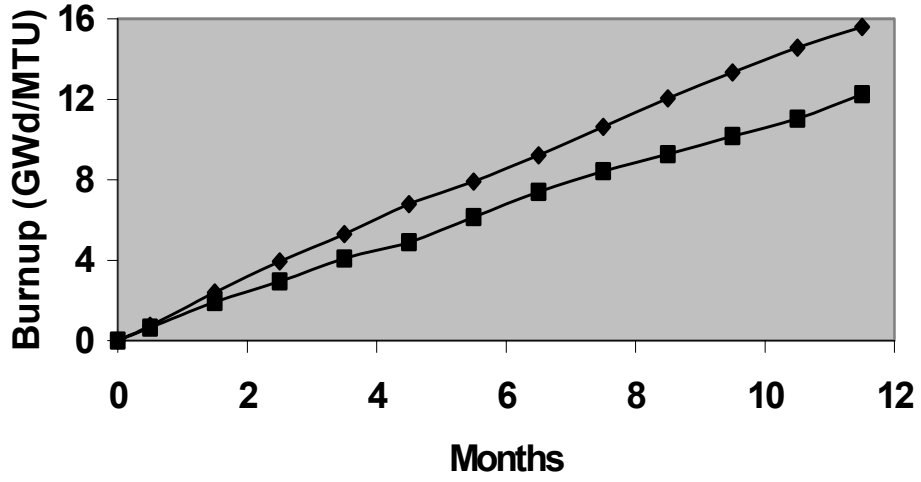

Fig. 4 MCNPX burnup results for the central and outer cans. Values for the central can are denoted by diamonds and those for the outer can by squares.

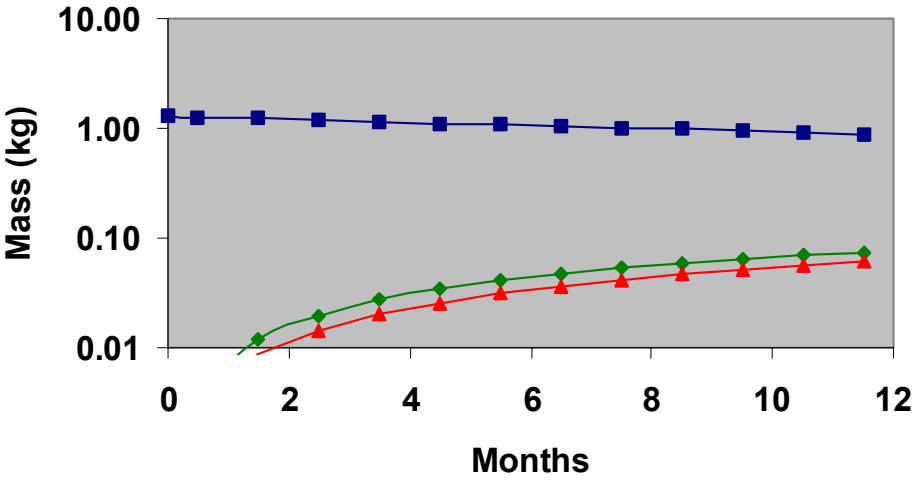

Fig. 5 MCNPX actinide inventories for the seven-can HEU problem. ^{235}U values are denoted by squares, ^{236}U by triangles, and ^{239}Pu by diamonds.

Figure 5 provides a plot of the mass inventory of various actinides as a function of time, and Figure 6 gives the fission product inventories at the end of the 1-year burn.

4. Conclusion

MCNPX continues to meet the needs of the reactor community by implementing features of interest to criticality users. A variance reduction technique was successfully implemented for criticality calculations and is shown to enhance eigenfunction

convergence by nearly two orders of magnitude in some applications. A transmutation option was also developed to automate burnup calculations. Results for a seven-can HEU sample problem are shown to be in good agreement with Monteburns.

MCNPX features currently under development include delayed neutron and gamma models (for all nuclides), 2-D contour plots of mesh tallies, variance reduction with pulse-height tallies, and possibly a cubic-spline tracking capability.

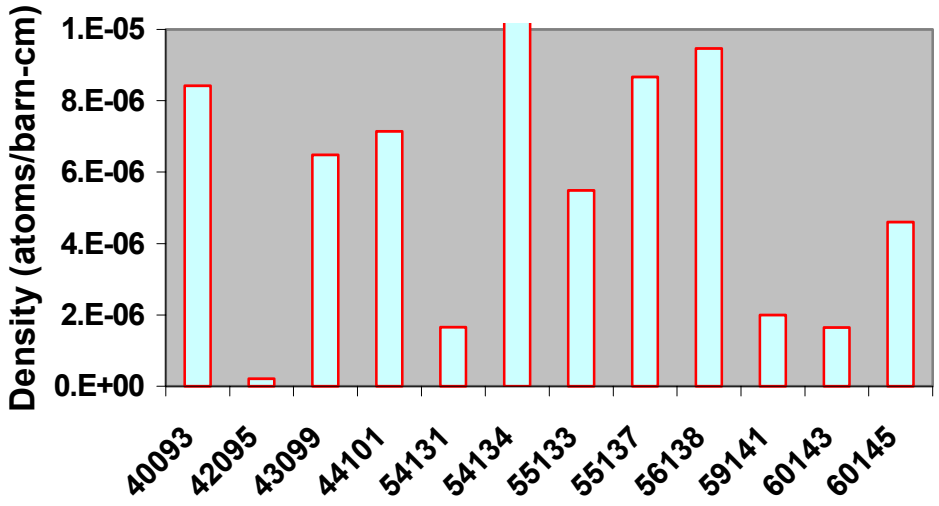

Fig. 6 MCNPX fission product inventories for the seven-can HEU problem. The values along the horizontal axis represent various isotopes (e.g., 40093=^{93}Zr).

References

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3. J. S. Hendricks, J. P. Finch, and C. Choi, "*Calculation of Eigenfunction Fluxes in Nuclear Systems*," Los Alamos National Laboratory document LA-UR-03-6889 (2003).
4. H. R. Trellue and D. I. Poston, "*User's Manual, Version 2.0, for Monteburns, Version 5B,*" Los Alamos National Laboratory document LA-UR-99-4999 (1999).