Hybrid Deterministic-Monte Carlo Methods for Neutral Particle Transport

Deokjung Lee

Ulsan National Institute of Science and Technology, UNIST-gil 50, Eonyang-eup, Ulju-gun, Ulsan, 689-798, Korea *deokjung@unist.ac.kr*

1. Introduction

In the history of transport analysis methodology for nuclear systems, there have been two fundamentally different methods, *i.e.*, deterministic and Monte Carlo (MC) methods [1-5]. Even though these two methods coexisted for the past 60 years and are complementary each other, they never been coded in the same computer codes. Recently, however, researchers have started to consider to combine these two methods in a computer code to make use of the strengths of two algorithms and avoid weaknesses [5-9]. Although the advanced modern deterministic techniques such as method of characteristics (MOC) can solve a multigroup transport equation very accurately, there are still uncertainties in the MOC solutions due to the inaccuracy of the multigroup cross section data caused by approximations in the process of multigroup cross section generation, *i.e.*, equivalence theory, interference effects, *etc.* Conversely, the MC method can handle the resonance shielding effect accurately when sufficiently many neutron histories are used but it takes a long calculation time. There was also a research to combine a multigroup transport and a continuous energy transport solver in a computer code system depending on the energy range [10,11]. This paper proposes a hybrid deterministic-MC method in which a multigroup MOC method is used for high and low energy range and continuous MC method is used for the intermediate resonance energy range for efficient and accurate transport analysis.

2. Methodology

2.1 Deterministic Method

This section briefly summarizes the deterministic MOC. After integration over energy and space, the Boltzmann neutron diffusion equation can be written as below for a direction of Ω_m [1,2]:

$$
\frac{d\varphi_{m,i}^s}{ds_m} + \Sigma_{t,i}^g \varphi_{m,i}^g = Q_{m,i}^g,
$$
\n(1)

where g is the energy group index, i is the mesh index, *m* represents the direction of neutron motion Ω_m , and

 $Q_{m,i}^g$ is the angular source in the direction *m*, group *g*, mesh *i* which can be written as:

$$
Q_{m,i}^s = \frac{1}{4\pi} \left[\sum_{s'} \sum_{s,i}^{g'\rightarrow s} \phi_i^{s'} + \frac{\chi^s}{k_{\infty}} \sum_{s'} \nu \sum_{f}^{g'} \phi_i^{s'} \right].
$$
 (2)

With the assumption of constant source and constant material property in each mesh, Eq. (1) can be integrated along the neutron motion path, S_m , from the entering point ($s_m = 0$) to the exiting point of the mesh *i*:

$$
\varphi_{m,i}^{s}(s_m) = \varphi_{m,i}^{s}(0)e^{-\sum_{i,j}^{s} s_m} + \frac{Q_{m,i}^{s}}{\sum_{i,i}^{s}}(1-e^{-\sum_{i,j}^{s} s_m}) ,\qquad (3)
$$

where $\varphi_{m,i}^{s}(s_m)$ is the outgoing angular flux from the

mesh *i*, in direction *m*, group *g*. Using Eq. (3), a multigroup transport problem can be solved by tracing the neutron trajectories along rays laid out over the problem geometrical domain with uniform spacings along the quadrature set directions. Usual fission source update and power method will be used to update system eigenvalues.

2.2 Monte Carlo Method

The MC method can be written formally as below to represent the probabilistic process [12]:

$$
\Psi(\mathbf{r}, E, \Omega) = \int \left[\int \int \Psi(\mathbf{r}', E', \Omega') C(\mathbf{r}', E' \to E, \Omega' \to \Omega) dE' d\Omega' \right] \tag{4}
$$

$$
\times T(\mathbf{r}' \to \mathbf{r}, E, \Omega) d\mathbf{r}'
$$

where $\Psi(\mathbf{r}, E, \Omega)$ is the particle collision density, $C(\mathbf{r}', E' \to E, \Omega' \to \Omega)$ is the collision kernel, $T(\mathbf{r}' \to \mathbf{r}, E, \Omega)$ is the transport kernel, and $Q(\mathbf{r}', E, \Omega)$ is the fission source term. In the MC simulation, the two kernels are realized using random numbers and probability distribution functions (PDF) based on the underlying physics.

2.3 Hybrid Method

Hybrid method uses the MOC and MC together in the solution process of Boltzmann transport equation. The approach in this paper is to use MOC for high and low neutron energy groups and MC for intermediate energy groups in an anticipation to use MC for resonance energy groups with continuous energy cross sections. As in the conventional methods, the group sweeping order in the hybrid method is from the highest energy group (*g*=1) to the lowest energy group (*g*=*ng*) where *ng* is the total number of groups. The groups for MC simulation are from *gb* to *ge*. In this hybrid method, the method for the neutron source calculation is same as the conventional MOC except for the fact that the MC tallied fluxes are used for those MC groups. And the flux updates for the groups of high energy MOC, from 1 to (*gb*-1), are same as the conventional MOC. The hybrid algorithm is shown in Fig. 1.

Fig. 1. Hybrid deterministic-MC algorithm

The MC simulation in the hybrid method is a fixed source problem using the source from upper energy groups. The sites of source neutrons are sampled uniformly in each cell and the total number of source neutrons, n_i^g , in cell *i*, group *g*, is proportional to the source from the high energy MOC groups, *i.e.*,

$$
n_i^g = N \times p_i^g \tag{5}
$$

where N is the total number of starting neutrons in each cycle and p_i^g is the fraction of the source neutrons in cell *i*, group *g*, and calculated as follows:

$$
p_i^g = \frac{Q_i^g}{Q_{sum}}; \ Q_{sum} = \sum_i \sum_{g'=gb}^{ge} Q_i^{g'}
$$
 (6)

With the number of source neutrons by Eq. (5), the MC simulation for the multigroup neutron slowingdown problem is performed for the groups from *gb* to *ge*, and neutron fluxes are tallied. This MC simulation will repeats K times and the tallied fluxes are used to update scattering sources for low energy groups and fission sources for the next outer iterations.

3. Numerical Results

A model pin cell problem is designed to test the proposed method. Fig. 2 shows the model problem geometry with fuel, clad, and coolant regions. The coolant region is subdivided into two calculation meshes in the radial direction for MOC. Three sets of 8 group macroscopic cross sections are provided for those three regions. The COO1 and COO2 regions use the same cross sections. The boundary conditions are all reflective.

Fig. 2. Model problem

Fig. 3 shows the k_{eff} values over the cycles for hybrid calculation. Due to the statistical nature of MC method applied to the intermediate energy groups, the solution of hybrid method in Fig. 3 fluctuates similarly to the MC solution. It does not monotonically converge like MOC-only method but it is noted that it reaches stationary condition after 100 iterations. Therefore, the hybrid solutions in Table I were averaged over the iterations from 100 to 200 and statistically processed to obtain variances. The numbers (0/10/10000) at the title represents the number of inactive/active/histories per cycle.

Fig. 3. Keff behavior in hybrid method

Method	inactive/ active/ histories	k_{eff}	Std. dev. (pcm)	Error (pcm)
МC	50/1600/20k	1.27804	15	
МC	50/100/10k	1.27834	97	30
MOC		1.27815		11
HYBRID	0/10/10k	1.27842	59	38
HYBRID	0/100/10k	1.27831	19	27

Table I. Eigenvalue summary

The eigenvlaues of five different calculations are summarized in Table I: two MC solutions, one MOC solution, and two hybrid solutions. The first MC solution is the reference solution for comparison. The numbers of inactive cycles, active cycles, and histories per cycle are 50, 1600, and 20000, respectively as shown in the second column. The second MC result with less number of neutron histories matches the reference solution within the statistical uncertainty. MOC solution is also within the uncertainty. In case of the hybrid method, there is no need of inactive cycle since the MC source neutrons are sampled from the source term obtained in the upper group MOC calculation. Two hybrid cases use 10 and 100 active cycles each and the standard deviation reflects the different number of neutron histories. Two eigenvalues match the reference solution within uncertainties. It can be noted that MC-only, MOC-only, and the hybrid methods produce consistent solutions.

4. Conclusions

A new hybrid method that combines the deterministic MOC and the probabilistic MC method is proposed to solve the Boltzmann transport equation more accurately especially for the continuous energy problems. This paper presented the methodology of the multigroup version and the results of its application to a model problem. From the comparison with the reference MC calculation and the conventional MOC calculation, it was confirmed that the new method produces consistent solutions with the MC-only and MOC-only methods. Further study of the application of this hybrid method to the continuous energy Boltzmann transport equation is underway.

Acknowledgements

This research was supported by National Nuclear R&D Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology.

REFERENCES

[1] Joel Rhodes, Kord Smith, and Deokjung Lee, "CAS MO-5 Development and Applications," *PHYSOR 2006*, Vancouver, Canada (2006)

[2] H. G. Joo, et al., "Methods and Performance of a Th ree-Dimensional Whole-Core Transport Code DeCAR

T," *Proc. PHYSOR 2004*, April 25-29, 2004, Chicago, I llinois, USA (2004)

[3] R. J. Stamml'er, et al., "HELIOS Methods," Studsvi k Scandpower (1998)

[4] J. F. Breismeister, et al., "MCNP – A General Mont e Carlo N-Particle Transport Code, Version 4B," LA-12 625-M (1997)

[5] Deokjung Lee, Kord Smith, and Joel Rhodes, "The i mpact of $238\overline{U}$ resonance elastic scattering approximatio ns on thermal reactor Doppler reactivity," *Annals of Nu clear Energy*, **36**, pp. 274-280 (2009)

[6] Kang-Seog Kim, et al., "Monte Carlo Resonance Tre atment for the Deterministic Transport Lattice Codes," *J ournal of the Korean Nuclear Society*, **35**, pp. 581-595 (2003)

[7] E. W. Larsen and J. Yang, " A Functional Monte Carlo Method for k-Eigenvalue Problems," *Nucl. Sci. Eng.*, **159**, 107 (2008)

[8] Min Jae Lee, Han Gyu Joo, Deokjung Lee, and Kord Smith, "Multigroup Monte Carlo Reactor Calculation wi th Coarse Mesh Finite Difference Formulation for Real Variance Reduction," *Proc. SNA+MC2010*, October 17 -21, Tokyo, Japan (2010)

[9] Deokjung Lee, "Hybrid Method of Deterministic and Probabilistic Approaches for Multigroup Neutron Transport Problem," *PHYSOR 2012*, Knoxville, USA (2012)

[10] SCALE: *A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluati on*, ORNL/TM-2005/39, Version 6, Vols. I-III, January 2009. Available from Radiation Safety Information Co mputational Center at Oak Ridge National Laboratory a s CCC-750

[11] M. L. Williams, M. Asgari, D. F. Hollenbach, "CE NTRM: A ONE-DIMENSIONAL NEUTRON TRANS PORT CODE FOR COMPUTING POINTWISE ENER GY SPECTRA," ORNL/TM-2005/39 , Version 6, Vol. II, Sect. F18

[12] Forrest B. Brown, "Fundamentals of Monte Carlo Particle Transport," LA-UR-05-4983