Proceedings of the Reactor Physics Asia 2023 (RPHA2023) Conference
Gyeongju, Korea, October 24-26, 2023

Weight Window Generation Based on Forward-adjoint Coupling Calculation

Yingzhe Hu [a], Shanfang Huang [a*], Kan Wang [a]
[a]*Department of Engineering Physics, Tsinghua University, Haidian District, Beijing, China, 100086*
[*]*Corresponding author: sfhuang@tsinghua.edu.cn*

1. Introduction

Variance reduction is very important in Monte Carlo shielding calculation and certain deep penetration problem.Adjoint Monte Carlo (Adjoint MC) method is a widely used method in reactor engineering design. Previous researches show that adjoint MC calculaiton is important in variance reduction parameter generation of shielding calculation.

Reactor Monte Carlo code (RMC) is a three-dimensional particle transport Monte Carlo program developed by the Reactor Engineering and Analysis Laboratory (REAL) of the Institute of Nuclear Energy Science and Engineering Management of the Department of Engineering Physics, Tsinghua University for reactor computational analysis, which has a very powerful reactor core nuclear design capability. In order to elevate shielding calculation ability of RMC code, we developed multigroup adjoint transportation method to perform adjoint calculation and we further developed adjoint-based weight window generation based on adjoint MC calculation. In water shielding calculation we found it showed excessive efficiency elevation compared to analogue calculation.

2. Methods and Results

In shielding calculations based on Monte Carlo methods, due to the existence of the deep penetration problem, the problem of excessive variance due to the difficulty of particles to reach the counting region often occurs. In order to reduce the impact caused by the deep penetration problem, many researchers have investigated Monte Carlo variance reduction methods, including the CADIS method as well as the Becker local weight window method. Both methods use a deterministic procedure to compute the adjoint fluxes in the model region involved in the Monte Carlo computation, and use the results obtained to generate the weight window parameters for subsequent Monte Carlo computations. Thus, for programs that lack deterministic calculation ability, it becomes difficult to perform variance reduction calculations using these two methods.

On the other hand , adjoint transportation in multigruop situation is relatively easier to deal with, so we can use multigroup adjoint transportation to generate variance reduction parameters.

2.1 Adjoint Transportation in Monte Carlo code

Adjoint transportation is based on adjoint particle transportation formula:

$$-\hat{\Omega}\cdot\nabla\psi^{\dagger}(\vec{r},E,\hat{\Omega})+\Sigma_t(\vec{r},E)\psi^{\dagger}(\vec{r},E,\hat{\Omega})=$$
$$\int_{4\pi}\int_0^{\infty}\Sigma_s(E\rightarrow E',\hat{\Omega}\rightarrow\hat{\Omega}')\psi^{\dagger}(\vec{r},E',\hat{\Omega}')dE'd\hat{\Omega}'$$
$$+q_e^{\dagger}(\vec{r},E,\hat{\Omega})$$

In adjoint problem, adjoint particles travel from “detectors” to “sources” of its corresponding forward problem. This results in the fact that the researchers must find the correct mirror model to perform calculation.

2.2 Adojoint Transportation in Monte Carlo code

In the Monte Carlo computation of adjoint transport, the adjoint particles follow the same rule as in the forward computation in terms of sampling the free-fly distance and determining the geometry, but it is not the same in terms of particle scattering treatment: the "adjoint cross section" corresponding to the adjoint computation must be used to sample the type of collision of the particles and to sample the particle ejection state, and because of this problem, it is actually more difficult to compute the adjoint problem using continuous energy cross sections. Therefore, in the present Monte Carlo particle transport programs, the multi-group adjoint problems are commonly investigated, because in the multi-group computation, the energy of the particles is actually discretized, since they are divided into energy groups, and the calculation of the adjoint cross section can be simplified.

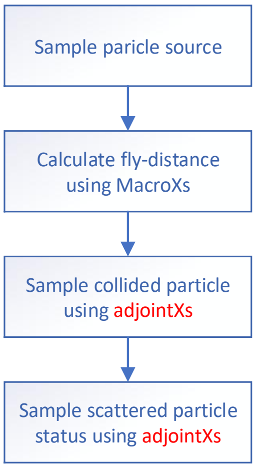

Fig.1 Calculation of Adjoint Particle Transportation

The real meaning of the adjoint particle is the value of the forward particle. For the shielding problem, it is possible to use the method of adjoint computation to solve the original problem by conjugating the original problem: the source space of the original problem is set as the detection space of the adjoint problem, and the detection region of the original problem is set as the source space of the adjoint problem, and by counting the fluxes of the adjoint particles, i.e., it is possible to solve the original problem by means of the adjoint problem solving method.

The goal of this study is not to use the adjoint computation to solve the shielding forward problem directly, but to use the results of the adjoint computation to generate the weight window parameters for the shielding forward computation problem.

2.3 Mesh-based Weight Window

The weight window is a variance reduction method commonly used in neutron Monte Carlo transport calculations, in which each weight window includes a lower limit, an upper limit, and a target weight of the weight window, and the weights of the particles are adjusted using these three weight window factors. The basic idea of this method is that when a particle enters a certain phase space with a weight window, the weight of the particle is judged: if the weight of the particle is larger than the upper limit of the weight window, the particle is split into several particles with the target weight; when the weight of the particle is smaller than the lower limit of the weight window, the roulette method is used to sample the particles with a certain probability and judge whether the particles can survive: if they survive, the weight of the particles is adjusted to the target weights. And then achieve the effect of letting the weight of the particles in a certain range of distribution, so that the statistical variance in this space is reduced.

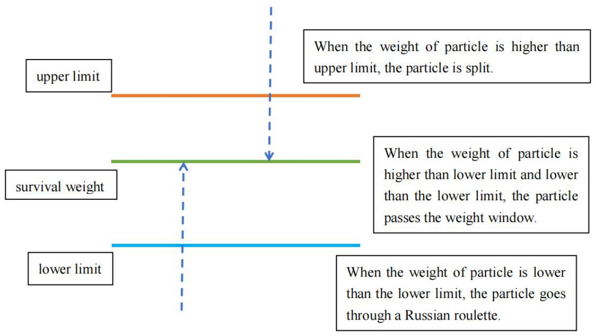

Fig. 2. Theory of Weight Window

Weight windows can be used in many variance reduction calculations, and the weight windows discussed in this study are mainly based on the meshes superimposed on cells as a partition of the space, and that’s why they are referred as “mesh-based weight window”, when particles enter certain mesh with weight window, they will go through the variance reduction process.

We further uses Becker’s local weight window to give out a set of weight window for Monte Carlo calculation, and it is introduced in the next part of this chapter.

2.4 Weight Window Generation

Many weight window generation (WWG) wethods have been proposed. In the previous studies on variance reduction, researchers proposed CADIS and FW-CADIS methods, which are based on the idea of obtaining the solution of the adojoint problem of the original deep penetration problem by deterministic computation, and then obtaining the distribution of the adjoint fluxes; and then obtaining the value of the weight window in the corresponding space by processing the value of the adjoint fluxes.

In a follow-up study, Becker et al. proposed a method to adjust the local weight window based on the response flux. The idea of this method is to adjust the calculation results using the following equation[1]:

$$\overline{w}(\vec{r},E) = \frac{B(\vec{r})}{\phi^{\dagger}(\vec{r},E)}$$

Where

$$B(\vec{r}) = \alpha(\vec{r})\tilde{\phi}^{c}(\vec{r}) + 1 - \alpha(\vec{r})$$

$$\alpha(\vec{r}) = \left[1 + \exp\left(\frac{\tilde{\phi}^{c}_{max}}{\tilde{\phi}^{c}(\vec{r})} - \frac{\tilde{\phi}^{c}(\vec{r})}{\tilde{\phi}^{c}_{max}}\right)\right]^{-1}$$

Further, we can find that if we can perform one forward computation and one adjoint computation in advance before the final Monte Carlo shielding calculation, we can obtain the weight window value of the corresponding mesh by using Becker's localized weight window method.

2.5 Development of WWG in RMC code

In previous studies, both CADIS and FW-CADIS methods first use a deterministic program to obtain the desired adjoint fluxes, on the basis of which subsequent calculations are performed. In order to reduce the dependence on the deterministic program and to improve the ability of the Monte Carlo computational methods, this study develops the function of multi-group adjoint computation in the Monte Carlo program RMC and uses the coupling of the forward and adjoint computations to generate the required weight windows for the deep penetration problem.

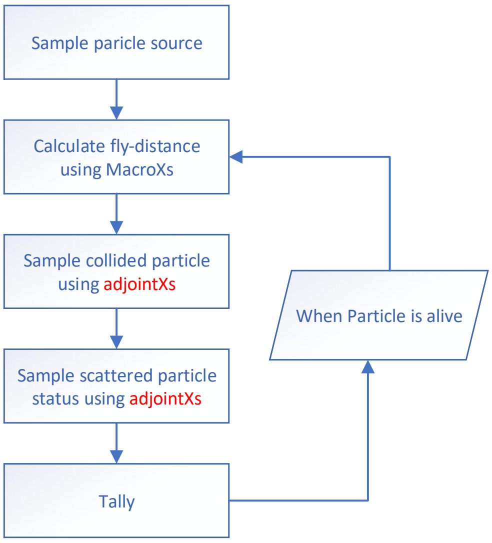

Fig.3 Adjoint particle transportation process in RMC

In the process of RMC weight window generation, the forward flux in each mesh is first obtained by forward computation; then, using the target detector as the source space of the adjoint problem, the adjoint flux in each grid body of the space is counted using the method of adjoint transport to obtain the distribution of the adjoint flux.

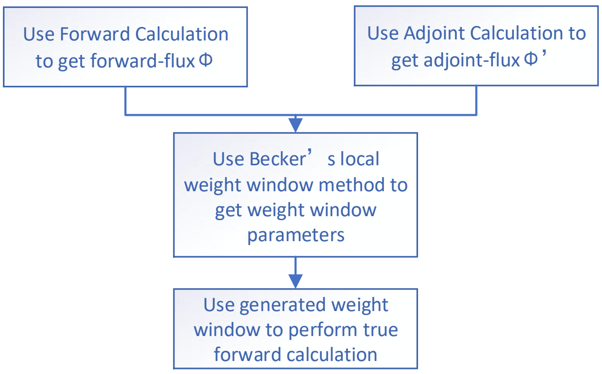

Fig.4Weight Window Generation in RMC

In this study, a newly developed adjoint computation function of RMC was used to generate a weight window for forward computation based on Becker's localized weight window method.

2.6 Numerical Results

In this study we test this new variance reduction function using two shielding problems. And the energy group used for adjoint multigroup calculation is MGXSNP[6], and they are listed as Table I and Table II:

Table I: Boundaries of Neutron Energy Groups

Energy Group	Upper Energy Bound/MeV	Energy Group	Upper Energy Bound/MeV
1	17	16	0.184
2	15	17	0.0676
3	13.5	18	0.0248
4	12	19	0.00912
5	10	20	0.00335
6	7.79	21	0.001235
7	6.07	22	4.54E-04
8	3.68	23	1.67E-04
9	2.865	24	6.14E-05
10	2.232	25	2.26E-05
11	1.738	26	8.32E-06
12	1.353	27	3.06E-06
13	0.823	28	1.13E-06
14	0.5	29	4.14E-07
15	0.303	30	1.52E-07

Table II: Boundaries of Photon Energy Groups

Energy Group	Upper Energy Bound
1	20
2	9
3	8
4	7
5	6
6	5
7	4
8	3
9	2
10	1
11	0.5
12	0.1

The first one is a thick water shielding problem, shown as below:

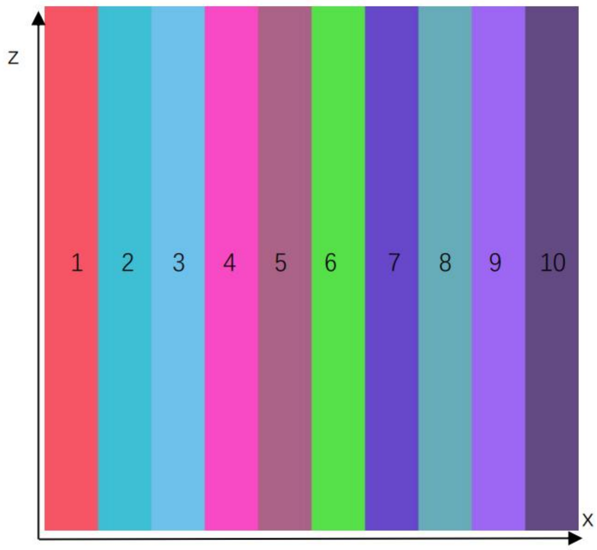

Fig.5 Model of thick water shielding problem

The example shown in the figure has a side length of 10 meters and is divided into 10 layers in the X direction, the source space is a neutron source with an energy of 2 MeV uniformly distributed in the first layer, and the counter is set to the tenth layer in the X direction. And the energy group

First, the forward calculation is used to obtain the flux results of each energy group in each layer, and then the counter is set as the source space of the accompanying neutrons, and the particle transport simulation is performed by using the newly developed adjoint transport calculation in the RMC, which in turn obtains the adjoint flux statistics of each energy group in each layer.

Using the Becker local weight window method, the two kinds of fluxes obtained above are processed and normalized to obtain the results shown in the table below, which are the weight windows results obtained from this forward-adjoint coupling calculation.

Table III Weight window results by Becker's Local Weight Wingdow Method in the thick water shielding problem

Mesh Index	**Weight Window Parameter**
1	1
2	0.393
3	0.153
4	0.0592
5	0.022406823
6	0.008179487
7	0.002814115
8	0.000848335
9	0.000150356
10	3.64193E-05

In subsequent computations, Monte Carlo forward variance reduction computations were performed on the original problem using the weight windows obtained from this coupling computation. We also performed an analog calculation without any variance reduction techniques. Both calculations were simulated with 1E8 particles and the results are shown in Table IV and V below (spatial integral values for the respective statistics):

Table IV Results of analog calculation of thick water shielding model

Mesh Index	Integrated Flux /cm	Relative Error
1	2.25E+01	8.56E-05
2	1.14E+01	1.60E-04
3	2.12E+00	3.74E-04
4	2.99E-01	9.45E-04
5	3.75E-02	2.56E-03
6	4.46E-03	7.21E-03
7	4.96E-04	2.11E-02
8	5.73E-05	6.23E-02
9	6.11E-06	1.72E-01
10	2.95E-07	6.36E-01

Table V Results of calculation with generated weight window of thick water shielding model

Mesh Index	Integrated Flux /cm	Relative Error
1	2.25E+01	1.25E-04
2	1.14E+01	2.14E-04
3	2.12E+00	3.94E-04
4	2.99E-01	7.36E-04
5	3.75E-02	1.33E-03
6	4.43E-03	2.38E-03
7	5.07E-04	4.30E-03
8	5.69E-05	7.94E-03
9	6.26E-06	1.38E-02
10	6.33E-07	1.99E-02

It can be found that compared with the results of the analog calculation, the results with the use of the generated weight window have been improved, with lower relative error. In addition, both calculations were performed under the condition of 16 core MPI parallel and the analog calculation took 5.97 min to finish while the calculation with weight window took 7.06 min to finish. Considering that the FOM of the analog one is 0.41 and the FOM of the one with weight window is 357, we can find that the efficiency of the calculation with weight window has been elevated to about 872 times of the analog calculation, which showed that this forward-adjoint coupling method can provide an effective set of weight window parameters to improve the Monte Carlo results.

The second problem is a sphere lead-water cubic shielding problem. This shielding problem consists of lead and water as photon shielding layer. The source centered evenly in the lead sphere with the radius of 20cm. The shielding consists of 6 layers of 10 cm thickness and the most internal layer is lead while all the other layers are water. The detector locates in the sixth layer, with the radius of 0.1 cm. What we want to know is the photon flux in the detector.

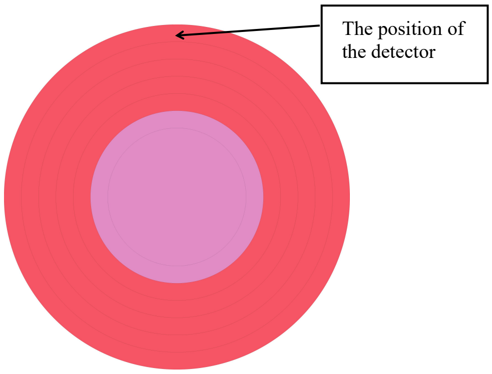

Fig.6 Model of lead-water spherical shielding problem

We used the same process to get the generated weight windows, and they are listed below (set 1E-6 as the lower bound of the weight window):

Table VI Weight window results by Becker's Local Weight Wingdow Method in the lead-water spherical shielding problem

Energy Group	Cell 1	Cell 2	Cell 3	Cell 4	Cell 5	Cell 6	Cell 7
1	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06
2	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06
3	5.00E-03	5.25E-03	7.47E-04	3.79E-04	2.24E-04	1.14E-04	7.46E-05
4	4.18E-02	1.28E-03	3.54E-04	1.97E-04	1.32E-04	8.09E-05	5.89E-05
5	1.34E-02	7.53E-04	2.54E-04	1.46E-04	1.04E-04	6.89E-05	5.24E-05
6	1.06E-02	6.49E-04	2.18E-04	1.28E-04	9.29E-05	6.37E-05	4.94E-05
7	1.05E-02	6.17E-04	2.01E-04	1.19E-04	8.69E-05	6.07E-05	4.76E-05
8	1.14E-02	6.04E-04	1.91E-04	1.13E-04	8.32E-05	5.87E-05	4.64E-05
9	1.20E-02	6.02E-04	1.83E-04	1.09E-04	8.06E-05	5.73E-05	4.55E-05
10	1.31E-02	6.04E-04	1.78E-04	1.06E-04	7.87E-05	5.63E-05	4.48E-05
11	1.51E-02	6.14E-04	1.74E-04	1.04E-04	7.72E-05	5.54E-05	4.43E-05
12	2.22E-02	6.55E-04	1.67E-04	9.98E-05	7.43E-05	5.38E-05	4.33E-05

Table VII Results of lead-water shielding model

Method	Analog	With weight window
Tally flux of the detector/cm	2.1883E-08	1.5479E-08
Relative error	9.4774E-02	5.3905E-02
Time cost	1.7146 min	1.2554 min
FOM	64.94	273.18

By comparing two results above, we can find that the calculation with weight window has more than 4 times FOM than analog calculation, which is also an obvious elevation in calculation efficiency.

The difference between thick water shielding model and lead-water shielding model lies in the material, model geometry and the particle type. The energy group that photon transportation model used is relatively rough so the generation process may not be able to give an effective weight window.

3. Conclusions

In this study, in the Monte Carlo particle simulation program RMC, the function of multi-group particle adjoint computation is developed, and the adjoint fluxes obtained from the adjoint computation are used to generate the weight window for the forward computation of the corresponding problem using the Becker local weight window method. And a more obvious variance reduction effect is obtained.

In the current RMC calculation, the coupled forward calculation-adjoint calculation can be used to generate the weight windows needed for the subsequent forward calculation. Considering the wide range of the shielding problems, in the future, we can add the method of multi-particle co-generation of weight window parameters in RMC, and test the function of RMC adjoint flux transportation and the function of generating weight windows based on the adjoint flux computation.[1]

REFERENCES

[1] MUNK M, SLAYBAUGH R N. Review of Hybrid Methods for Deep-Penetration Neutron Transport [J]. Nuclear Science and Engineering, 193(10): 1055-89, 2019.
[2]PAN Q, WANG K. Energy Biased Variance Reduction Method for Deep Penetration Problems [J]. Nuclear Power Engineering, 41(1): 1-6, 2020.
[3] SHI T, LI H, DING Q, et al. Global variance reduction method based on multi-group Monte Carlo adjoint calculation [J]. Annals of Nuclear Energy, 151, 2021.
[4] PAN Q, WANG K. An adaptive variance reduction algorithm based on RMC code for solving deep penetration problems [J]. Annals of Nuclear Energy, 128: 171-80, 2019.
[5] PAN Q, RAO J, HUANG S, et al. Improved adaptive variance reduction algorithm based on RMC code for deep penetration problems [J]. Annals of Nuclear Energy, 137, 2020.
[6] Little, R.C, Neutron and Photon Multigroup Data Tables for MCNP3B, LA-UR-98-538, 1987.