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Monte Carlo Region Isolation Method Used for Geometrical Perturbation

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Abstract – *This paper proposes a new method used for geometrical perturbation, namely region isolation method. The whole model is divided into perturbed region and unperturbed region. Transportation in two parts are divided to save total computation time. Basic principle of this method is introduced and it is found that the problem lies in the destruction of source convergence process. Fixed sampling number method is researched, and it is found that this method can only partially eliminate the error.*

I. INTRODUCTION

Monte Carlo method has been widely used in the calculation of reactor eigenvalue due to the advantages of continuous energy and geometry fine modeling, but the problems of geometric perturbation such as control rod movement and reflection layer movement still exist. Besides, the inverse problem of geometrical perturbation is geometrical criticality search problem.

Nowadays there has been direct differential method and random sampling method [1] used for geometrical perturbation, and direct differential method can be achieved by two independent criticality calculations or one criticality calculation with two simultaneous material perturbation calculations [2,3]. These two methods are time-consuming. An intuitive idea is to divide the whole computational region into perturbed region (such as moveable control rod) and non-perturbed regions. In bisection, regula falsi or other iteration-based methods [4,5] for geometrical eigenvalue search, to save time in multiple criticality calculation, the transportation process of non-perturbed region is reused and only perturbed region is calculated many times. In this paper, this method is temporarily named "region isolation method", and we try to explore the basic principle of the regional isolation method, source convergence correction problem and so on.

This chapter is divided into four parts: introduction, method, result and conclusion. In method part, firstly it is showed that how the region isolation method works; secondly, as the region is isolated, the source convergence process is destructed and fixed sampling number method is currently used to correct this effect; finally the region isolation method adapts to MPI parallel mode naturally. In result part, the effect of correction is shown by modeling Beavrs [6] hot zero power benchmark in reactor Monte Carlo code RMC [7].

II. METHOD

1. Region Isolation Method

In Monte Carlo criticality computation, the initial total weight is equally distributed to the source particles (the initial source particles are specified by input file, and the subsequent source particles are determined by the previous generation fission neutrons), which are transported until they are absorbed or out of boundary. The number of fission neutrons generated at a certain fission point is determined according to Equation (1). k is estimated by all previous generations. Dividing k can ensure that the number of particles simulated per generation is relatively stable both in supercritical and subcritical systems and the starting weight of all generations is nearly 1.

$$n = \omega \frac{\nu\Sigma_f}{\Sigma_t} \frac{1}{k} \tag{1}$$

According to the above process, the region isolation method is as follows: the region where the parameter will change is defined as the “region”. When the particle arrives at the boundary of “region” from the outside, the code stores the particle’s generation, weight, position, energy and direction. These particles are marked as "region surface particles", and are treated to be “killed” after they are stored. After all the particles outside the “region” finish transportation, “region surface particles” begin normal transportation, as shown in Fig. 1. Normal transportation means no difference between “region” and out of “region”.

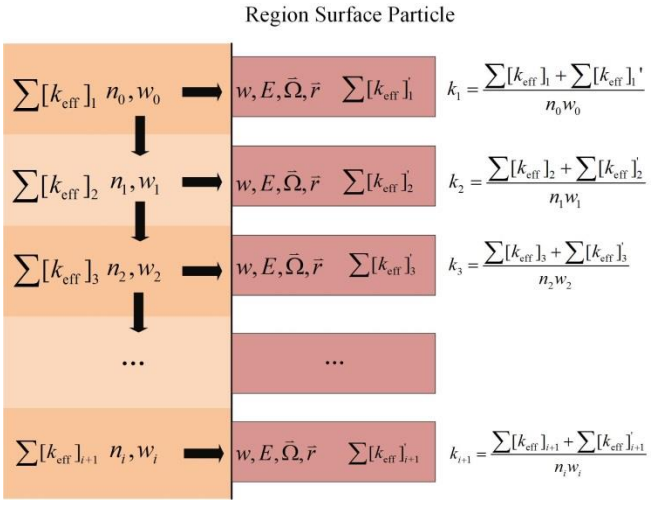

Fig. 1. Basic flow of region isolation method.

In Fig. 1, there is no fissionable element in "region". Therefore, there is no source particle in "region" that is generated from fission in previous generation. Besides, it is assumed that "region surface particles" do not produce fission neutrons. Strong absorption material in "region" or long distance between "region" and fissile material will meet this requirement. If not, the next part will discuss this problem.

Assuming the original system is nearly critical and the eigenvalue is k_0, then system out of "region" is a subcritical system whose eigenvalue is k'. When transporting outside the "region", as k_0 is unknown, Equation (1) is replaced by Equation (2). This will decrease the number of source particle but increase the starting weight, when total starting weight keeps the same. After the "region surface particles" are released, the k_{eff} estimator $\Sigma[k_{eff}]'_{i+1}$ is added to corresponding estimator outside the "region" $\Sigma[k_{eff}]_{i+1}$, and normalization is shown in Equation (3) to get k_0 in every generation.

$$n = \omega \frac{\nu \Sigma_f}{\Sigma_t} \tag{2}$$

$$k_{i+1} = \frac{\Sigma[k_{eff}]_{i+1} + \Sigma[k_{eff}]'_{i+1}}{n_i w_i} \tag{3}$$

2. Source Iteration Correction

If the "region" doesn't include fissile material, and the absorption cross section is very large or the "region" is far away from the fission region, the result of region isolation method will be the unbiased estimation of original system. The algorithm above is simply dividing normal k_{eff} estimator into two parts.

If not, the region isolation method will destroy the normal source convergence process, that is, the distribution of the fission source after convergence outside the region will be different from the original fission source distribution. In order to correct this effect, it is necessary to transport the "region surface particles" (RSP) of the i_{th} generation together with the fission neutrons generated from RSP of the $(i-1)_{th}$ generation, as shown in Fig. 2 and Fig. 3.

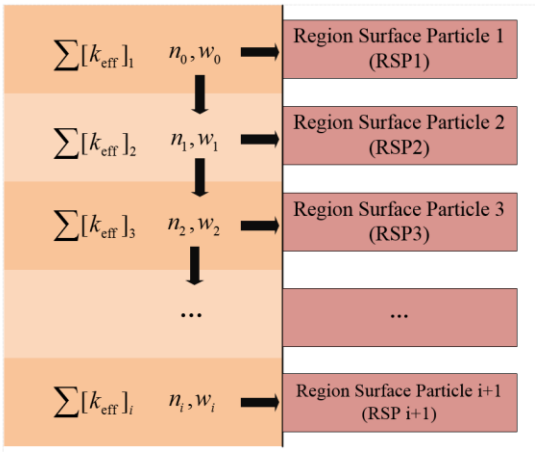

Fig. 2. The transportation of particles outside the "region".

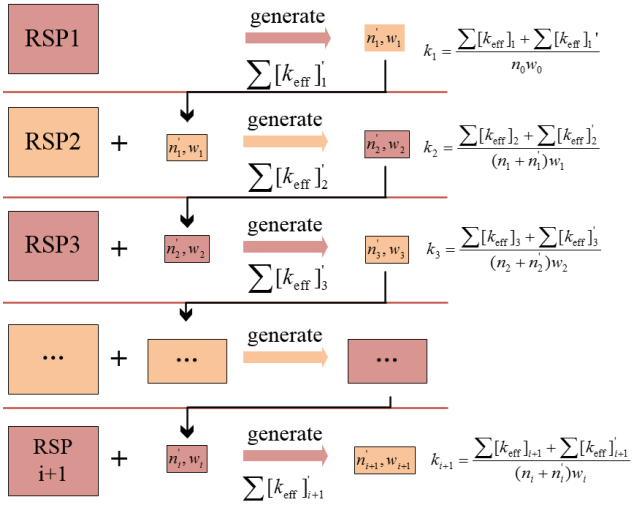

Fig. 3. The transportation in the "region".

In the first active generation in Fig.3, "region surface particles" of generation 1 (RSP1) will generated fission neutrons whose number is n_1'. To avoid biasness, n_1 should also determined by Equation (2) and their weights are same as w_1 in Fig.2. These neutrons (n_1',w_1) are transported together with RSP2. This process is repeated every generation and Equation (3) is therefore replaced by Equation (4).

$$k_{i+1} = \frac{\Sigma[k_{eff}]_{i+1} + \Sigma[k_{eff}]'_{i+1}}{(n_i + n_i')w_i} \tag{4}$$

As total weight per generation outside the "region" is constant, a fixed share of total weight will be allocated to the "region surface particles" every generation. This can guarantee the computational time of "region surface particles" is stable. The problem lies in the fission neutrons generated by "region surface particles". In order to ensure the unbiasedness of fission source in the $(i+1)_{th}$ generation, the fission neutrons generated by the i_{th} "region surface particle" should be included in the fission source of the

$(i+1)_{th}$ generation, and the weight should be equal to the initial weight of the $(i+1)_{th}$ generation. Thus more and more fission neutrons are generated, namely $n_1' < n_2' < \ldots < n_i'$.

In order to ensure the unbiased correction and control the computation time, fixed sampling number method is tried. The fixed number is marked as N. When $n_i' \leqslant N$, n_i' source neutrons are transported. When $n_i' > N$, N source neutrons sampled from n_i' neutrons are transported. That means that each generation will lost part of information, but the number of particles simulated per generation is stable. The following results will show that when the fixed number is small, it will result in a low estimation of K_{eff}, similar to the traditional Monte Carlo undersampling problem [8]. The low estimation problem can be further diagnosed by Shannon entropy, which is beyond the scope of this paper. However, when the fixed number is large enough, it seems that the low estimation error can be decreased, but cannot be canceled.

3. Natural Parallelism

In MPI parallelism mode, for load balance, the fission source of the i_{th} generation outside the "region" is rearranged. Therefore the "region surface particles" of the $(i+1)_{th}$ generation are also distributed uniformly, as well as the fission neutrons generated by "region surface particles". Therefore, for MPI parallel mode, the region isolation method has natural parallelism, which can directly inherit the critical fission source rearrangement algorithm. When sum of the fixed sampling numbers of different cores in MPI mode equals that of serial mode, the expectations of Monte Carlo result are the same, while the random number algorithm can't guarantee the repeatability. The following results will verify this conclusion.

III. RESULT

The algorithm is implemented on reactor Monte Carlo code RMC, and the Beavrs benchmark in HZP condition is used for verification. There are two computing platforms. In Intel(R) Xenon(R) CPU E5-2690 v3 @ 2.60GHz with 48 cores, 100,000 particles per generation with 200 inactive generation and 200 active generation are used. In Milkyway-2 supercomputer with 1000 cores, 1,000,000 particles per generation with 100 inactive generation and 200 active generation are used. Both use MPI parallel mode.

In all control rod out status, D bank is chosen for verification, namely 5(assembly)* 25(pin) * 2(layer) = 250 cells are marked as "region", the materials of which is Ag-In-Cd or boron water, shown in Fig. 4 and Fig. 5. In Fig. 5, stainless 304 (blue part) is exclude from the "region" for simplification. Purple and green parts are the same boron water, but are marked as two different materials in input file. This is because in repeated model, using material rather than cell or surface as the indicator of entering the "region" is easier.

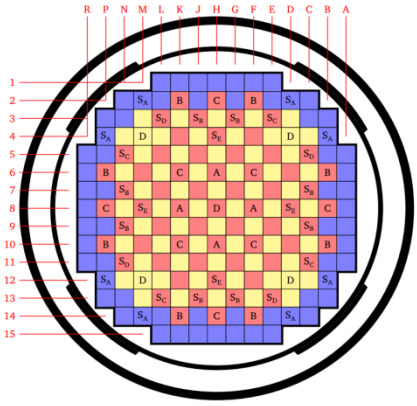

Fig. 4. Beavrs control rod bank distribution.

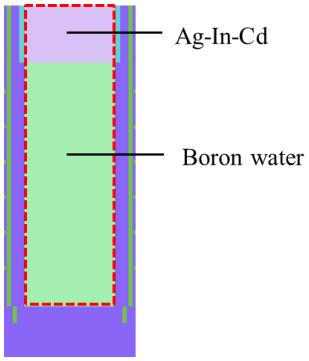

Fig. 5. "Region" of a single pin marked as red dotted box.

Firstly, the correctness of MPI parallel algorithm is verified in Table I. The total fixed sampling numbers of three cases are all 10,000. It can be seen the k_{eff} differences are in the range of relative standard error.

Table I. Comparison of serial and parallel results

	serial	100 cores	1000 cores
N/core	10,000	100	10
k_{eff}	0.99666±20	0.99666±20	0.99657±20
Time/min	221.2558	2.4880	0.3914

Secondly, the result of region isolation method in Windows platform is shown in Table II. 100,000 particles per generation with 200 inactive generation and 200 active generation are run in 48 cores. The computation time outside the "region" is t_1 and total computation time is t_2. For reference, the K_{eff} without region isolation method is 0.99889±14, and the total transportation time t_0 is 20.3222 min. If there are n geometric perturbation calculations, the total transport time will be $t_1+n(t_2-t_1)$, while the time of direct calculation is nt_0. When n increase to infinity, the time ratio $[t_1+n(t_2-t_1)]/\ nt_0$ will converge to $(t_2-t_1)/t_0$. Thus we define the acceleration ratio as:

$$\mathrm{AR} = \frac{t_0}{t_2 - t_1}$$

Table II. Results of region isolation method

Number/core	K_{eff}	t_1/min	t_2/min	AR
10	0.99677±14	19.6922	19.8636	118.6
50	0.99719±14	19.9367	20.3644	47.5
100	0.99739±14	19.959	20.6517	29.3
200	0.99766±14	19.626	20.8129	17.1
300	0.99782±14	19.7825	21.4113	12.5
400	0.99812±14	19.5157	21.6522	9.5
500	0.99817±13	19.6347	22.2576	7.7
600	0.99827±13	19.7965	22.9006	6.5
700	0.99831±13	19.6006	23.1712	5.7
800	0.99843±14	20.0137	24.0759	5.0
900	0.99855±13	19.5889	24.1495	4.5
1000	0.99838±13	19.6584	24.6719	4.1
1200	0.99858±14	19.8176	25.8569	3.4

The K_{eff} and acceleration ratio curves over fixed sampling number per core are shown in Fig. 6. The meaning of fixed sampling number has been explained in Method chapter. It can be seen that with the increase of sampling number, the K_{eff} is getting closer to the reference value, but the corresponding acceleration ratio gets lower and lower.

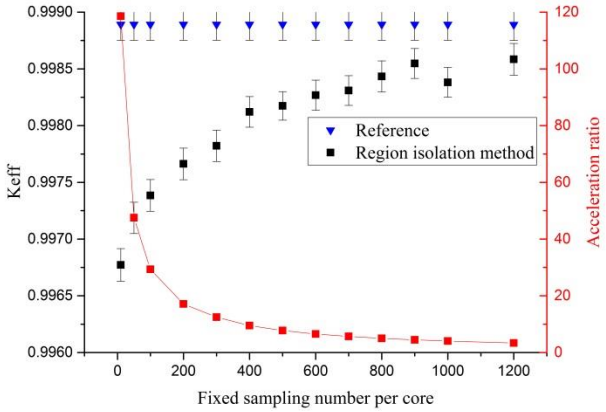

Fig. 6. Keff and acceleration ration curve.

It seems that there is a gap between k_{eff} of region isolation method and reference k_{eff}. To avoid the effect of statistic fluctuation, larger population is used in Milkyway-2 supercomputer with 1000 cores. The reference k_{eff} is 0.998581±15, calculated with 10,000,000 particles per core, 200 inactive cycles and 200 active cycles. Then using fixed sampling number method, 1,000,000 particles per generation with 100 inactive generation and 200 active generation are run again. The results are shown in Table III and Fig. 7.

Table III. Results of region isolation method with larger population

Number/core	Keff	Time/min
0	0.996300±48	4.3705
50	0.997120±50	4.4500
100	0.997403±48	4.6136
200	0.997675±49	4.8787
500	0.997917±50	5.6189
1000	0.998051±49	6.8261

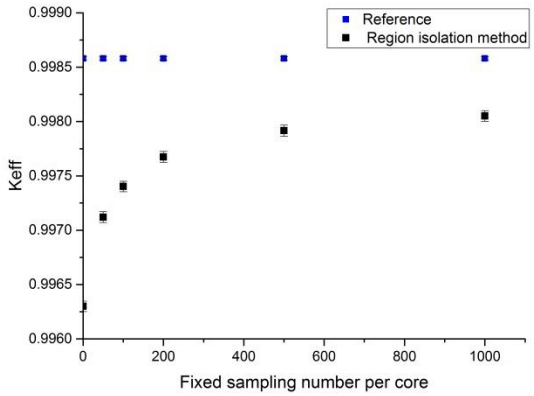

Fig. 7. Correction effect of fixed sampling number method

It is shown that even using large number of particles, k_{eff} of region isolation method is still lower than the reference k_{eff}. This is probably caused by Monte Carlo undersampling problem, which needs more research.

IV. CONCLUSION

Region isolation method can save multiple geometrical perturbation calculation time. The accelerating effect depends on the region isolation effect on fission source distribution. The fixed sampling number method can reduce the influence of fission neutrons generated by "region surface particles", but cannot totally cancel this effect. Other more effective methods need to researched to eliminate the gap between k_{eff} of region isolation method and reference k_{eff} . If so, the computation time of geometric perturbation will be shortened greatly, and the efficiency of geometric search will also be improved greatly.

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