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Optimal Monte Carlo particle splitting for neutron transport equation

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Abstract. Global tallying problem is hard to be solved efficiently when using Monte carlo method to simulate neutron transport equation, especially for system with big scale and/or strong imbalanced characteristics. Among numerous global variance reduction methods, particle splitting is an easy-to-implement method, but the efficiency is hard to be satisfying for practical problems. The essential challenge lies in the fact there are too many parameters to be optimized. In this paper, a systematic approach for setting all splitting parameters is proposed based on maximization of some global efficiency indicator. Results of two models show this approach can increase the global efficiency indicator up to two orders of magnitude while keeping the results unbiased.

1 Introduction

Monte Carlo method is an important candidate for solving neutron transport problem. Its advantages in exact geometric and physical modeling, high parallel efficiency make it be an powerful tool for difficult neutron transport problem. But analogous Monte Carlo, that is, simulating the movement of neutron according to true physical laws is seldom efficient. So, many algorithms are proposed to increase the efficiency by modifying one or more distribution density functions which control the stochastic behavior of neutrons. The unbiased results are contained by correcting weights of neutrons.

According to some kind of rough standard, Monte Carlo variance reduction algorithms can be divided into two types. The one is for single target tally, the other is for multiple target tallies (global tallying problem is a special case, which means the same kind of tallies in all meshes of geometric space or phase space are to be solved). For the former, if each history contributes same result for target tally, a perfect simulation (zero variance simulation [1]) will be achieved. This case seldom happens, even if it's not impossible. But theoretically, a zero variance schedule is present, not like the latter. For the latter, the situation is more challenging. Considering the fact that geometric models contain much more meshes than before, there are two key challenges for getting high efficiency(in here, high efficiency means getting precise results for most meshes within small enough time, such as the 95/95 rule [2]. This rule means in some limited time, at least 95% fraction of regions will get tallies with relative errors less than 1% at the 95% confidence level). One challenge is, because of strong imbalanced characteristic in different regions(this means one region may get ample neutron tracks but another region can only get insufficient tracks because of different characteristics of these

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regions), even with huge number of histories, some meshes can only get very small number of tracks. This fact makes the global efficiency is low and can hardly be increased obviously by merely increasing number of histories [3–5]. Another challenge is, because meshes in some regions may be far from source region, deep penetration problem [6] may exist, which is one of the most difficult problem for Monte Carlo simulation of neutron transport problem for many years.

For global tallying problem mentioned above, which is the main concern of this paper, some algorithms are proposed to increase the efficiency. Implicit capture [1], although simple, is a global variance reduction method. But using this method alone can not get satisfying results for most problems. Weight window method [1, 7] is also thought as a global variance reduction method. This method is powerful if its parameters are suitable. Above mentioned methods are traditional global variance reduction method. In recent years, some advance global variance reduction method are proposed to solve difficult global tallying problem. These methods can be mainly classified into two types. One is based on forward transport calculation and another is based on adjoint transport calculation. The representative of the former are Wijk method [8, 9] and MAGIC method [10]. They use forward transport calculation and iteration process to make neutrons more evenly distributed in whole region. But in general, these methods are time consuming. The representative of the latter is FW-CADIS method [11]. It uses adjoint transport calculation to get global adjoint flux and uses this global adjoint flux as importance function. This method has many applications in engineering problems. Except algorithms mentioned above, there are also other researches [12–14] which can not be classified into these two types.

In this paper, the focus is particle splitting algorithm [1] which only considers splitting particle when this particle crosses the boundary of a geometry mesh. Suppose the weight is w, when it flies into another mesh, this algorithm will split this particle into M particles and each particle has the same position, energy and direction as the original one, but with a weight equals to w/M. The M is called splitting number and each mesh should has different M. It is obvious that when the splitting number increases, the variance of tally in each mesh will decrease while the simulation time will increase, so, global efficiency will increase firstly and decrease then. For each mesh, the splitting number when a particle flies into this mesh is one of all parameters of this algorithm. So, this algorithm has as many parameters as the number of meshes. For many years, a strategy for setting all these parameters aiming to maximize some kind of global efficiency indicator is absent. This paper will fills in this gap by proposing a strategy based on strict theoretical analysis. The necessary data of this strategy will comes from an inexpensive trial calculation.

In next section, this strategy will be described in detail. The third section will contains some active numerical results. The last section gives some conclusions and prospects.

2 Setting particle splitting parameters based on maximization of some global efficiency indicator

Suppose there are N geometry meshes in total. The aim is setting all N parameters to maximize the global efficiency indicator [15]

$$E_g = \frac{N}{T \sum_{i=1}^{N} R_i^2}, \tag{1}$$

here, T is the calculation time and $R_i (i = 1, \cdots, N)$ are calculated relative standard deviations of tallies in all meshes.

For any theoretical analysis be possible, two hypotheses are necessary. The first one is, when number of histories is large enough, the total number of tracks in each mesh will be proportional to this number. This assumption is reasonable because the total number of tracks in each mesh produced by one sample is almost a fixed quantity when number of histories is large enough. The second one is, total calculation time will be proportional to the sum of number of tracks in all meshes. This point can be explained by the fact that the total calculation time is considered commonly to be proportional to number of histories. According to the first assumption, total number of tracks in each mesh is proportional to number of histories. So, the total calculation time can be considered to be proportional to the sum of all number of tracks in all meshes.

Based on these two assumptions mentioned above, some kind of theoretical analysis about how to set all splitting parameters to maximize global efficiency indicator E_g can be described as follows. Let N_h be the number of histories. It is well known for each mesh i, its tally's relative standard deviation can be written as [1]

$$R_i = \frac{c_i}{\sqrt{N_h}}, \tag{2}$$

here c_i is a constant which is dependent on the algorithms used. From the two assumptions mentioned above, two equalities will be satisfied. The one is

$$J_i = g_i N_h, \tag{3}$$

here J_i is the number of tracks in mesh i and g_i is a constant which is not dependent on N_h. The other is

$$T = c \sum_{i=1}^{N} J_i. \tag{4}$$

From Equation (2) and Equation (3), we have

$$R_i = \frac{h_i}{\sqrt{J_i}}, h_i = c_i \sqrt{g_i}. \tag{5}$$

Note that whatever other algorithms are used, the target is maximizing global efficiency indicator in Equation (1) when implementing the splitting algorithm additionally. Because of the character of splitting algorithm, h_i can be considered unchanged approximately when implementing this algorithm. This point will be clear when considering c_i will be decreased while g_i will be increased when executing the splitting algorithm. So, using the Cauchy inequality, we have

$$E_g = \frac{N}{T \sum_{i=1}^{N} R_i^2} = \frac{N}{c(\sum_{i=1}^{N} J_i)(\sum_{i=1}^{N} (\frac{h_i^2}{J_i}))} \leq \frac{N}{c} \frac{1}{(\sum_{i=1}^{N} h_i)^2}. \tag{6}$$

Only when $J_{i,best} = \lambda h_i, i = 1, \cdots, N$, E_g can achieve the maximum value. So, it will be clear $\lambda = \frac{\sum_i^N J_i}{\sum_i^N h_i}$. For the formal calculation with splitting algorithm, in average, particles in grid j flying into grid i should be split into $J_{i,best}/J_i = \lambda \frac{h_i}{J_i}$ copies. But in grid j, the number of tracks has been enlarged by a factor $\lambda \frac{h_j}{J_j}$, so the actual splitting number when particle flying from grid j into grid i should be $\frac{h_i}{J_i} / \frac{h_j}{J_j}$. Note that this splitting number is irrelevant with the number of histories. Clearly, all the data needed must be gotten by a trial calculation.

Note that if after the trial calculation, some h_i or J_i are zero because no neutron crosses these meshes, then, these h_i or J_i can be set with the minimum of all h_i or J_i which are not zero. For avoiding excessive splitting in some special cases, a maximum number of branches of one particle history can be set in advance. If some particle's branch number exceeds this number, this particle and all branches it produced will no be split again.

3 Numerical results

3.1 Problem one of Kobayashi benchmark model

Problem one of Kobayashi benchmark model is the first one of all three cases [16]. Kobayashi benchmark model consists of three nested cubic regions with dimensions of 10cm, 50cm, and 100cm, and the layout of the problem is shown in Figure (1). This problem has only one energy group. The total cross sections of three regions are $0.1cm^{-1}, 0.0001cm^{-1}$ and $0.1cm^{-1}$. The scattering cross section has two cases. The first case is pure absorption which means the scattering cross section is zero, and the second case is half-scattering which means the scattering cross section is half of the total cross section. An isotropic source is uniformly distributed over the smallest cubic region. The whole region is divided into a cubic mesh with a step size of 2cm, which means the number of meshes is 125000.

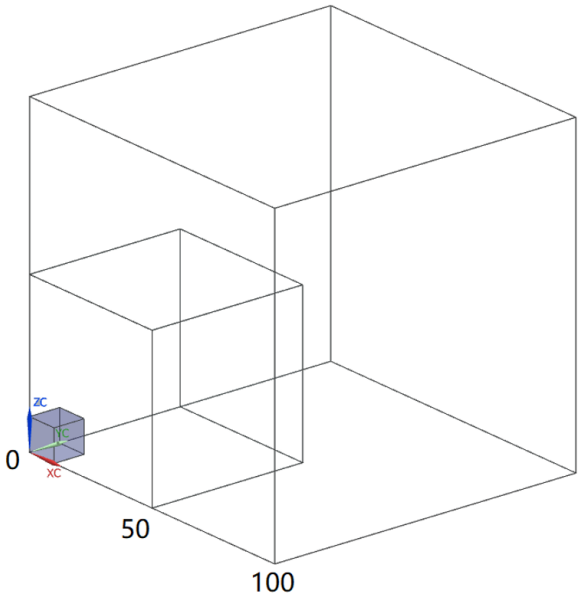

Figure 1: The layout of problem one of Kobayashi benchmark model

For this model, $2.4E+9$ particles are simulated using 240 processors. Firstly, splitting algorithm is not invoked for calculating fluxes of key points. Then, all splitting algorithm parameters are generated. Finally, splitting algorithm is invoked with the same number of histories to obtain fluxes of key points again. The results are listed in Tables 1 and 2 . The calculated relative standard deviation of flux is listed in parentheses below the mean. A positive relative error compared to reference value means the calculated flux is larger than reference value and a negative relative error means the calculated flux is smaller than reference value. The referenced values of these fluxes are calculated by GMVP code [16]. It is worthy to point out that although the reference values are obtained by point detector estimator while we use track length estimator, for the reason that the mean free path in this problem is significantly larger than mesh size, it will has negligible error between point flux and track length flux.

It can be seen from Table 1 that for positions far from source region, such as (85, 85, 85), (95, 95, 95), the error without splitting is much more large, especially in pure absorption case.

Table 1: Results of pure absorption

position	reference value	without splitting		with splitting	
		flux	relative error compared to reference(%)	flux	relative error compared to reference(%)
5,5,5	5.95332E+0	5.93094E+0 (0.00038)	-0.38	5.93578E+0 (0.00041)	-0.29
85,85,85	2.24543E-5	2.97004E-5 (0.17216)	32.27	2.24498E-5 (0.00990)	-0.02
95,95,95	3.00945E-6	8.83913E-7 (0.74042)	-70.63	2.99086E-6 (0.01139)	-0.62
95,55,5	1.37060E-4	1.35381E-4 (0.08325)	-1.23	1.37817E-4 (0.00713)	0.55

Table 2: Results of half-scattering

position	reference value	without splitting		with splitting	
		flux	relative error compared to reference(%)	flux	relative error compared to reference(%)
5,5,5	8.29260E+0	8.25490E+0 (0.00010)	-0.45	8.24798E+0 (0.00038)	-0.54
85,85,85	8.66059E-5	8.37085E-5 (0.02657)	-3.35	8.66524E-5 (0.00348)	0.05
95,95,95	1.12892E-5	1.15719E-5 (0.07179)	2.50	1.12520E-5 (0.00405)	-0.33
95,55,5	7.93924E-4	7.89601E-4 (0.00854)	-0.54	7.96880E-4 (0.00202)	-0.37

Table 3: Comparison of global efficiency

Scattering ratio	without splitting	with splitting	relative increasing
0.0	43.429	49.713	14.5%
0.1	50.123	58.404	16.5%
0.5	131.158	219.99	67.7%
0.9	1307.284	1738.246	34.0%

It can be found that the relative error without splitting becomes notably larger as the point is far from source region. This is not surprising because the number of particle tracks in the regions near source is much more higher than that in regions far from source. But the relative error with splitting algorithm does not significantly increase in regions far from source region because the splitting generates more particle tracks in these regions. Furthermore, global efficiencies(the indicator in Equation(1) is used) in all cases with different scattering ratios (the scattering ratio is defined as the ratio of the scattering cross section to the total cross section) are calculated with or without splitting . When calculating global efficiency of case with splitting, the total time is taken as the sum of time spent on generating parameters and

time spent on simulation with splitting, which means the extra time to get parameters is also taken into account although it is not necessary because parameters generated can be reused in all calculations that followed. Note that if tally in a grid is zero, then relative error is set to be one, which is the common practices. Comparison of global efficiencies are listed in Table 3.

From Table 3, firstly, it can be seen that global efficiency increases as the scattering ratio increases. This is because a low scattering ratio means stronger absorption. In this case the number of tracks that a single particle can generate is smaller, causing the statistical error to be larger. Secondly, it can be seen that splitting does not improve efficiency significantly in cases with low scattering ratio, this is because particles in low scattering ratio cases are quickly absorbed, making simulation without splitting takes very short time, which compensates the disadvantage of high relative standard deviations.

3.2 Problem based on two-dimensional C5G7 benchmark model

The two-dimensional C5G7 benchmark [17] model is originally a model designed for verifying deterministic methods. It contains 2×2 fuel assemblies and reflector, each assembly contains 17×17 rod meshes, each rod pin cell consists of moderator and cylinder rod, and thickness of the reflector is the width of one assembly. To validate our algorithm, a test case is constructed based on this model, as shown in Figure (2). The seven group cross sections, the assembly layout and the pin-by-pin layout of each assembly remain unchanged, but thickness of the reflector extends to three times of the width of one assembly to make particles undergo sufficient attenuation.

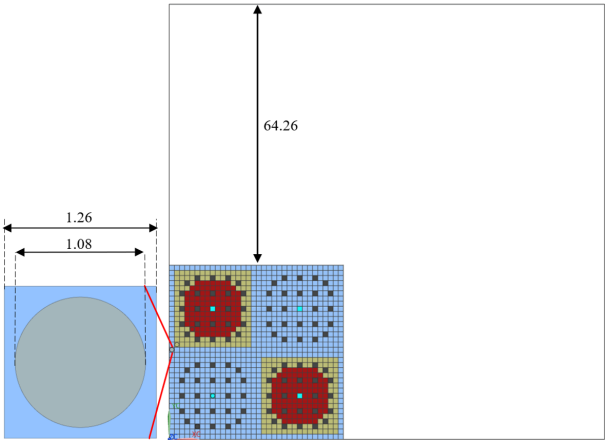

Figure 2: Constructed test case based on C5G7

The k_{eff} eigenvalue case is changed to fixed source case with fission is turned off, and the source distribution comes from the convergent distribution formed by k_{eff} eigenvalue calculation. The reflector layer is divided into square mesh with size $1.26cm \times 1.26cm$, so it has $85 \times 85 - 34 \times 34 = 6069$ meshes in total. The 2×2 assemblies have $2 \times 34 \times 34 = 2312$ meshes. The track length estimator is used for flux in each mesh without energy bin.

We firstly use 120 processors to simulate $2.4E + 7$ particles to generate splitting parameters. Then, we simulate $5E + 6$ particles using one processor without or with splitting, fluxes are shown in Figure (3). Corresponding relative standard deviations are shown in Figure (4).

Table 4: Comparison of global efficiency

history number	processor number	with splitting or not	zero tally mesh number	global efficiency
5E6	1	No	1771	0.130948
5E6	1	Yes	0	1.716844
2.4E8	120	No	299	1.112897
2.4E8	120	Yes	0	161.3294

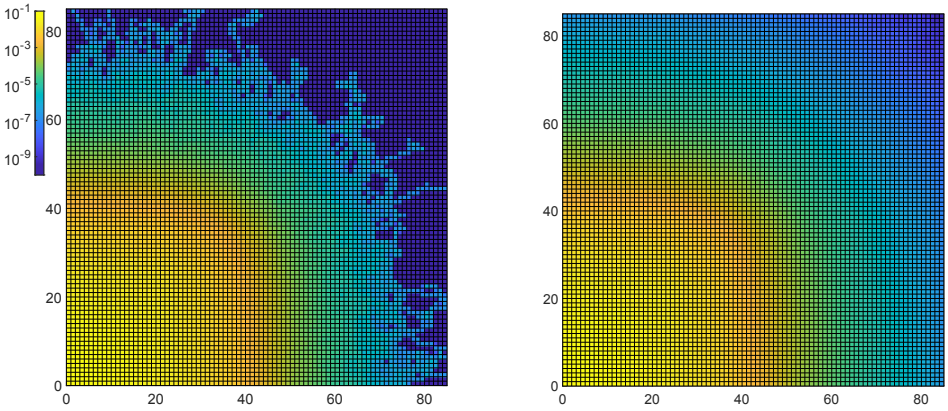

Figure 3: Fluxes with $5e + 6$ particles by one processor.(a)without splitting;(b)with splitting

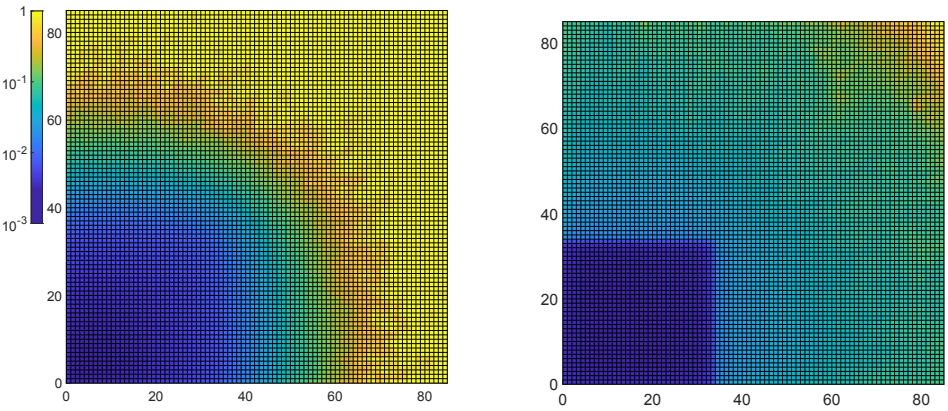

Figure 4: Relative standard deviations with $5e + 6$ particles by one processor.(a)without splitting;(b)with splitting

After that, $2.4E + 8$ particles are simulated using 120 processors, fluxes and relative standard deviations with or without splitting are shown in Figure (5) and Figure (6).

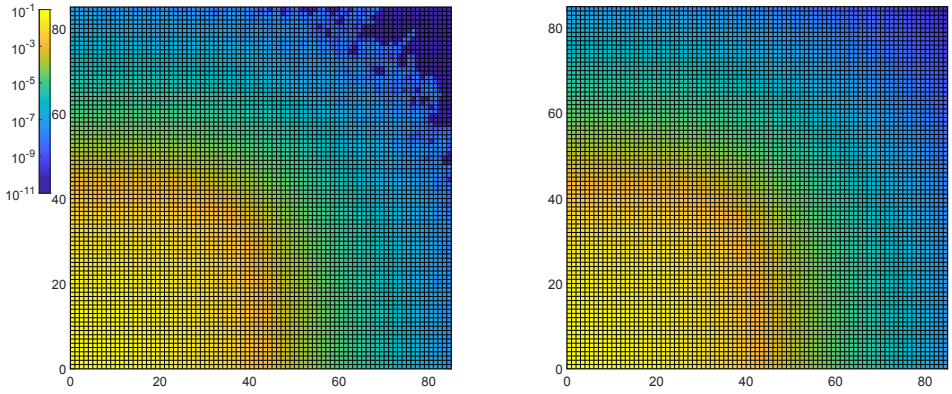

Figure 5: Fluxes with $2.4e+8$ particles by 120 processors.(a)without splitting;(b)with splitting

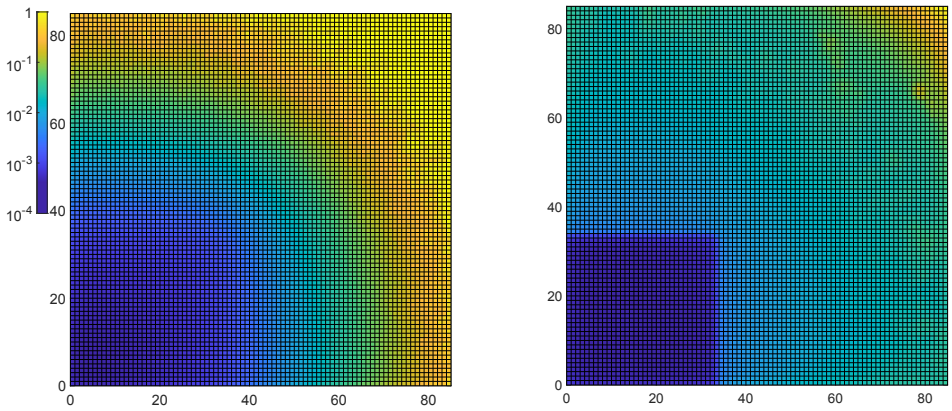

Figure 6: Relative standard deviations with $2.4e+8$ particles by 120 processors.(a)without splitting;(b)with splitting

From Figure (3) and Figure (4), it can be seen in case without splitting, it is difficult for neutrons to reach regions far away from fuel assembly, leading to large relative standard deviations in such regions. But using splitting, more particles can arrive in regions far away from the fuel, leading to smoother flux distribution and smaller relative standard deviations. Comparing Figure (5)(a) and Figure (3)(a), it can be seen when more particles are used, more tracks tend to reach regions far from fuel, but still the corner region cannot get enough tracks without splitting. The situation improves significantly when splitting is used. For further study, global efficiency of each case are calculated. Again for meshes with zero tally, the relative standard deviations are set to one. Also, we count the number of meshes with zero tally. The results are listed in Table (4). It can be seen splitting with parameters generated by our strategy has produced a significant variance reduction. Even in case with $5E+6$ particles,

using splitting can also ensure all meshes have tracks. By using splitting algorithm, global efficiency improves significantly, which can be increased by about 13 times under $5E + 6$ particles, and by about 145 times under $2.4E + 8$ particles.

4 Conclusions

Using strict theoretical analysis and inexpensive trial calculation to get necessary data, this paper proposes a whole strategy to set all parameters of particle splitting algorithms aiming to maximize some global efficiency indicator. Although this objective can only been reached approximately because of the inevitable error, two models' results show this strategy can increase the global efficiency indicator greatly. In future, we will continue to apply the same analysis framework to set all parameters of weight window method and hope to extricate this powerful method from difficult parameter-setting problem.

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References

1. I. Lux, L. Koblinger, *Monte Carlo Particle Transport Methods: Neutron and Photon Calculations* (CRC press, 1991) 332
2. Daniel. J. K, Thomas. M. S, and Stephen. C. W, Proceeding of PHYSOR 2012 (2012)
3. ShangGuan. D. H, Ji. Z. C, Deng. L, et al, Acta. Phys. Sin **68**, 122801 (2019)
4. ShangGuan. D. H, Li. G, Zhang. B. Y, et al, Nuclear Science and Engineering **182**, 555 (2016)
5. D. J. Kelly, B. N. Aviles, and B. R. Herman, Proc. Int. Conf. Mathematics and Computational Methods Applied to Nuclear Science and Engineering (2013)
6. M. Munk, R. N. Slaybaugh, Nuclear Science and Engineering **193**, 1055 (2019)
7. X-5 Monte Carlo Team, LA-UR-03-1987 (2003)
8. Wijk. A. J, Eynde. A, J, Hoogenboom. J. E, Annals of Nuclear Energy **38**,2496 (2011)
9. Wijk. A. J, Master thesis of Delft University of Technology (2010)
10. Davis. A, Turner. A, Fusion Engineering and Design **86**,2698 (2011)
11. Zheng. Z, Wang. M, Li. H, et al, Nuclear Engineering and Design **326**,87 (2018)
12. Simakov. S. P, Li. J, Fischer. U, Fusion Engineering and Design **85**,1924 (2010)
13. Wu. Z, Hany. S, Applied Radiation and Isotopes **72**,83 (2013)
14. Q. Q. Pan, H. W. Lv, S. Q. Tang, J. B. Xiong, X. J. Liu, Computer Physics Communications **291**,108850 (2023)
15. Q. Q. Pan, Ph.D thesis, Tsinghua University (2020)
16. K. Kobayashi, N. Sugimura, Y. Nagaya, Progress in Nuclear Energy **39**,119 (2001)
17. M. A. Smith, E. E. Lewis, Byung-Chan Na, Progress in Nuclear Energy **48**,383 (2006)