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PROGRESS ON RMC --- A MONTE CARLO NEUTRON TRANSPORT CODE FOR REACTOR ANALYSIS

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ABSTRACT

This paper presents a new 3-D Monte Carlo neutron transport code named RMC (Reactor Monte Carlo code), specifically intended for reactor physics analysis. This code is being developed by Department of Engineering Physics in Tsinghua University and written in C++ and Fortran 90 language with the latest version of RMC 2.5.0. The RMC code uses the method known as the delta-tracking method to simulate neutron transport, the advantages of which include fast simulation in complex geometries and relatively simple handling of complicated geometrical objects. Some other techniques such as computational-expense oriented method and hash-table method have been developed and implemented in RMC to speedup the calculation. To meet the requirements of reactor analysis, the RMC code has the calculational functions including criticality calculation, burnup calculation and also kinetics simulation. In this paper, comparison calculations of criticality problems, burnup problems and transient problems are carried out using RMC code and other Monte Carlo codes, and the results show that RMC performs quite well in these kinds of problems. Based on MPI, RMC succeeds in parallel computation and represents a high speed-up. This code is still under intensive development and the further work directions are mentioned at the end of this paper.

Key Words: Monte Carlo, RMC, delta-tracking method, burnup, kinetics simulation

1. INTRODUCTION

Generally there are two kinds of numerical methods to solve the neutron transport equation, one is deterministic method and the other one is Monte Carlo method. Deterministic method is quite mature and used vastly in reactor engineering and other areas, but it has considerable limitations in materials, energy spectrum and geometry. Monte Carlo Method overcomes these limitations with its capability of dealing with continuous energy cross-sections and arbitrary geometries[1]. Actually, the results of Monte Carlo method are often used as benchmark results and to test the results of deterministic method. But the calculation time of Monte Carlo method is much more expensive compared with deterministic method. With the requirement of accurate three-dimensional modeling in reactor physics and dynamics and great innovation of computer technology, Monte Carlo method is becoming an ever more powerful tool and receiving rising attention. Several countries have developed their own Monte Carlo codes, for example UK BNFL's MONK[2], France IRSN's MORET[3], Japan JAERI's MVP/GMVP[4] and Finland VTT's SERPENT[5]. Especially in US, at least 5 Monte Carlo codes have been developed, such as

LANL's MCNP[6], ANL's VIM[7], ORNL's KENO[8], LLNL's MERCURY[9] and US Navy's MC21[10].

In this paper we present a new Monte Carlo neutron transport code named RMC (Reactor Monte Carlo code)[11], which is specifically intended for reactor physics calculations. The code is being developed by Department of Engineering Physics in Tsinghua University, and the latest version is RMC2.5.0. This code is written in C++ and Fortran 90 language. To meet the requirements in reactor analysis, this code can do criticality analysis, burnup calculation and also the kinetics simulation. Compared with other Monte Carlo codes, RMC has integrated some techniques to improve calculation performance.

The following sections introduce the main features of methods and techniques used in RMC code. The results of RMC are presented in Section 3.

2. CALCULATIONAL METHODS AND TECHNIQUES IN RMC

2.1. Neutron Transport Method

The method applied in most Monte Carlo transport calculation codes is to simulate neutron histories by tracking each neutron through homogeneous material regions in the geometry and stopping at each material boundary [1][12]. The distance to next collision site, l, is randomly sampled according to the total interaction probability in the material which is exponentially distributed and depends on the macroscopic total cross section, and the l is sampled using:

$$l = -\frac{\ln(\xi)}{\Sigma_t(E,\vec{r})} \tag{1}$$

where ξ is a random number uniformly distributed between 0 and 1.

Since the geometry usually consists of various material regions, the collision distance has to be adjusted each time the neutron enters a new region. So in practice if the collision site lies beyond the material boundary, the neutron stops at the surface and the remaining part of the flight path is re-sampled or modified according to the new cross-section, this method is called ray-tracking method. The calculation of the surface distances may take a significant fraction of the computing time in complex systems, especially if the neutron mean free path is longer than the characteristic dimensions of the geometry.

Instead of using ray-tracking method, RMC uses another approach called delta-tracking method[1][13], which uses the concept of virtual collision and rejection technique. This method was developed by Woodcock et al. in the 1960's and got a detailed description in Lux and Koblinger's textbook. The main advantage of the delta-tracking method is that there is no need to calculate the surface distances, and thus it would speed-up the calculation in complex geometries. Since the total virtual collision cross-section remains unchanged throughout the geometry, non-uniform material compositions can be modeled with only minor modifications in the tracking procedure. This method has not been very popular in the modern Monte Carlo

neutron transport codes. In addition to RMC, this method is used in the SERPENT [5] and MONK[2] codes and as an optional method MCBEND [14]code.

The techniques of handling the problems with continuously varying materials have been implemented in the RMC code. In most of the Monte Carlo codes, the properties of a material in certain region are considered to be constant, but for certain cases this approximation can lead to errors which can't be ignored. Although we can treat this kind of problems using substepping method in which the region is subdivided into large amount of sub-regions, but it can bring huge increase in the calculation time. So an improved delta-tracking method is developed and implemented in RMC, and the method is proved much more efficient than the normal delta-tracking method and other methods used to solve the continuously varying material problems.

To make this method more efficient, a technique called Probability Neighbor Method (PNM) is developed to accelerate the geometry treatment instead of the traditional method. In delta-tracking method, there's no need to calculate the surface distances, but it still spends a lot of time on finding out which cell the particle is located in. When the geometry consists of a large number of cells, this procedure becomes very time-consuming. PNM searches the location of particle based on the probability that particle may enter a certain cell, and with PNM technique, the delta-tracking method can be even more efficient.

2.2. Computational-expense Oriented and Hash-table Method

In the cross-section library, the cross-section data are given as tables of energy and cross-section pairs. When incident energy is specified, the energy interval need to be searched and then cross-section at certain energy is calculated with linear interpolation. It has been found that energy search consumes a big share of time in Monte Carlo simulation, especially in the Monte Carlo burnup calculation. Accordingly, two speedup techniques are implemented into RMC.

One technique we used is computational-expense oriented (CEO) method [15] which is based on the unionized energy grid approach, but only reconstructing the computationally expensive cross-sections in the neutron transport simulation. In this method the energy grids of all nuclides are merged to form a uniform grid, then the energy search needs to be performed only once to get the macro cross-sections of all nuclides. Also the SERPENT code uses the similar technique, but the advantage of CEO method is fewer cross-section tables of unionized grid established in the calculation. As compared with the reconstructing all channels of cross-sections used in SERPENT [16], CEO method reduced the memory demand in a factor of 5~6, at the cost of only once more energy grid search for the colliding nuclide.

The other technique used in RMC is hash-table method [15]. The traditional method to search a certain energy in the energy grid is binary-search method which is implemented in MCNP and many other Monte Carlo codes, and the time complexity of binary-search method is logarithmic. Based on the hash table, we provided a more efficient search method named hash-table method. Compared with binary method, the hash-table method speeds up the energy search procedure in 3~6 times.

2.3. Burnup Calculation Method

Most Monte Carlo depletion codes explicitly couple certain MC code (e.g., MCNP) to certain independent point depletion code (e.g., CINDER or ORIGEN). However, RMC couples the depletion module in an implicit way. ORIGEN2 is incorporated as a subroutine of RMC other than linked by an interface. Data and parameters, such as reaction rates, flux, power, and nuclide densities, are transferred in the form of arrays inside the RMC, avoiding the time expense of information exchanges between input and output files.

In Monte Carlo burnup calculation, one-group reaction rates are tallied within the transport cycle. To get the one-group cross-sections and flux would become much time-consuming when there are a large number of nuclides included in burnup calculation. Instead of the conventional way of tallying one-group reaction rates, RMC employs a spectrum-based tally method (SBT) which has been previously implemented in certain coupled Monte Carlo burnup calculation codes [17][18]. By our numerical results, SBT method can improve considerably the tallying efficiency with negligible accuracy loss in a factor of 2-5. Also, RMC employs some burnup-step strategies such as middle-of-step constant flux approximation and predictor-corrector method [19], which can assure an acceptable accuracy when the burnnup step length is reasonably increased and thus improve the calculation efficiency. We are also planning to investigate the feasibility and potential of other strategies such as linear flux approximation.

2.4. Direct Simulation Method for Transient Calculation

The direct simulation method (DSM) [20] is a new method for solving short-time transient, three dimensional neutron transport problems. Different from the time-discrete approach, DSM solves the transient problem by directly simulating the dynamic behaviors of neutrons and precursors of delayed neutrons during the transient process. As we know, for reactor system without external neutron sources, neutrons always come from previous existed neutrons or precursors of delayed neutrons. The former may undergo various nuclear reactions (e.g., fission, scattering); meanwhile the latter can release neutrons by spontaneous decay. So in DSM, the transient simulation is taken out with the simulations of neutron behaviors and the simulations of precursor behaviors.

The simulations of neutron behaviors in DSM are quite similar with other Monte Carlo codes, the simulations are composed of the following sequences:
1. the collision position is identified;
2. the collision nuclide is identified;
3. the neutron thermal treatment is adopted for low-energy neutrons;
4. the collision type is identified;
5. if scattering is selected , the new energy and direction of the outgoing track are determined;
6. if fission is selected, the new neutrons and precursors are birthed.

The simulations of precursor behaviors become easier since their thermal motion can be ignored. Two main processes are involved, which are different from the existing Monte Carlo codes. One is to generate precursors based on the corresponding delayed neutron fraction when fission

occurs. The other is to produce the delayed neutron along with the decay of precursors, which follows the exponential decay rule. However, from the point reactor kinetics equations, it is estimated that, according to the difference of nuclear reactors (or neutron spectrum), the density of precursors would be more than hundreds of times of the one of neutrons, even hundreds of thousands of times. If simulating so many particles one by one, some problems (e.g. the consumption of computational time and the requirement to the random number generator) will occur. Fortunately, during the transient process, only a fraction of the precursors will decay. Therefore, before simulating them, the above fraction is estimated by the transient time and their half-life. Finally, only the concerned precursors are simulated.

3. COMPUTATIONAL RESULTS OF RMC

3.1. Results of Criticality Calculation

3.1.1. Benchmark problems calculation

The suite of criticality benchmarks [21] is provided by Los Alamos National Lab which includes a wide variety of fissile materials such as ^{233}U, ^{235}U and ^{239}PU, and more for ^{235}U, the cases of highly enriched uranium (HEU) and intermediate-enriched uranium (IEU). 8 criticality benchmarks are chosen for the calculation and simple descriptions of these benchmarks are given in Table I. The calculations using RMC and MCNP are associated with ENDF/B-VI.0 data libraries. The calculations are performed with 2,000 generations of 10,000 neutrons each, and the results from the first 400 generations are discarded. The benchmark results and MCNP's results with the same calculating conditions are given by the reference [21].

Table I. Criticality benchmark description

Benchmark Name	Benchmark Description
23umt4a	0.96" Tungsten-Reflected Sphere of U233, Planet Assembly
Pumet26	Simplified Plutonium Sphere, 11.9 cm Steel Reflector, VNIIEF
Umet1ns	Godiva, Unreflected sphere of HEU, Nested Spherical shell representation
Bigten2	BIGTEN, U(N) reflected uranium cylinder
Pumet8b	Thorium-Reflected Pu(93.59) Sphere, Thor Assembly, 2D Model
Pumet20	Depleted Uranium-Reflected Pu(~90) Sphere, VNIITF
23usl1b	ORNL-5, 1.0253g/l Unreflected Sphere of U233 nitrate solution Boron
23usl1e	ORNL-5, 1.0286g/l Unreflected Sphere of U233 nitrate solution Boron

As the results shown in Table II, keff calculated by RMC is in good agreement with the results calculated by MCNP, however, RMC costs much less time compared with MCNP. And there're differences between the codes' results and benchmark results, which we think are caused by the cross section data libraries used in RMC and MCNP[22].

Table II. Comparison of benchmark results of RMC and MCNP

Name	Benchmark k_{eff}	RMC k_{eff}	MCNP k_{eff}	RMC CPU time (min)	MCNP CPU time (min)
23umt4a	1.0000±0.0007	1.0028±0.0002	1.0031±0.0002	3.15	6.94
Pumet26	1.0000±0.0024	0.9973±0.0002	0.9973±0.0002	11.95	20.46
Umet1ns	1.000±0.001	0.9964±0.0002	0.9966±0.0002	2.88	7.09
Bigten2	0.996±0.003	1.0048±0.0002	1.0043±0.0002	24.25	47.05
Pumet8b	1.0000±0.0006	1.0061±0.0002	1.0059±0.0002	13.06	15.50
Pumet20	0.9993±0.0017	1.0004±0.0002	0.9999±0.0002	9.70	16.07
23usl1b	1.0005±0.0033	0.9972±0.0002	0.9973±0.0002	42.91	129.61
23usl1e	0.9999±0.0033	0.9964±0.0002	0.9958±0.0002	39.82	118.14

3.1.2. Constructed problems calculation

For further validation of RMC, 4 typical reactor problems are constructed and calculated. Problem 1 is a depleted PWR pin with more than 60 kinds of nuclides with the geometry shown in Fig 1, problem 2 is a SCWR assembly shown as Fig 2, problem 3 is a modified CANDU CANFLEX assembly with Th in the fuel bundles which is shown in Fig 3, and problem 4 is a homogenized fast reactor core [23] with a geometry as Fig 4. The results in Table III are calculated using MCNP and RMC with 1,000 generations of 5,000 neutrons each, and the results from the first 150 generations are discarded.

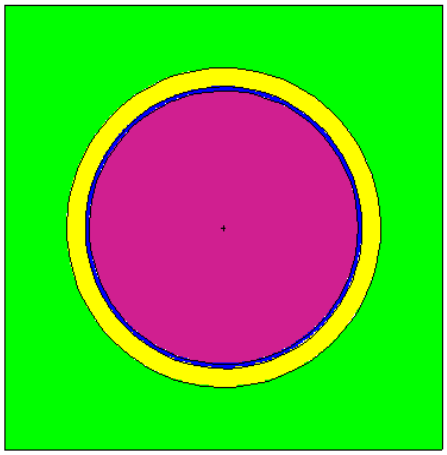


Figure 1. PWR pin.

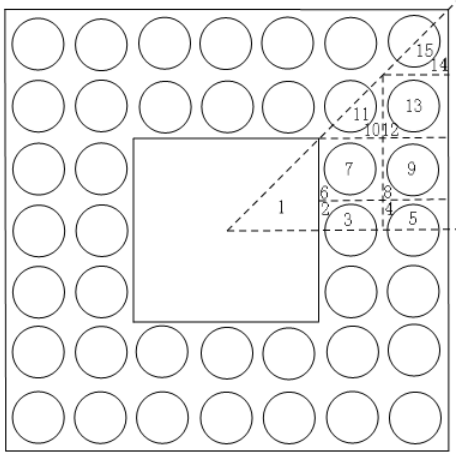


Figure 2. SCWR assembly.

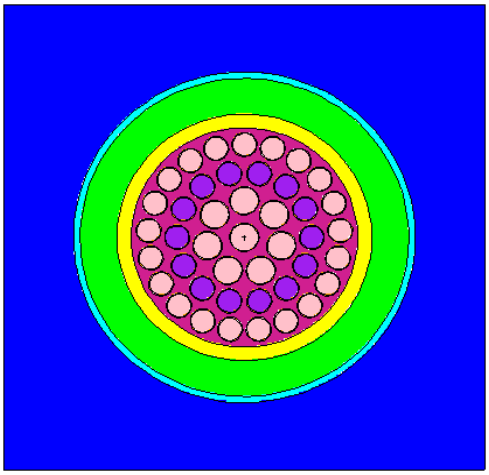


Figure 3. CANDU CANFLEX bundle.

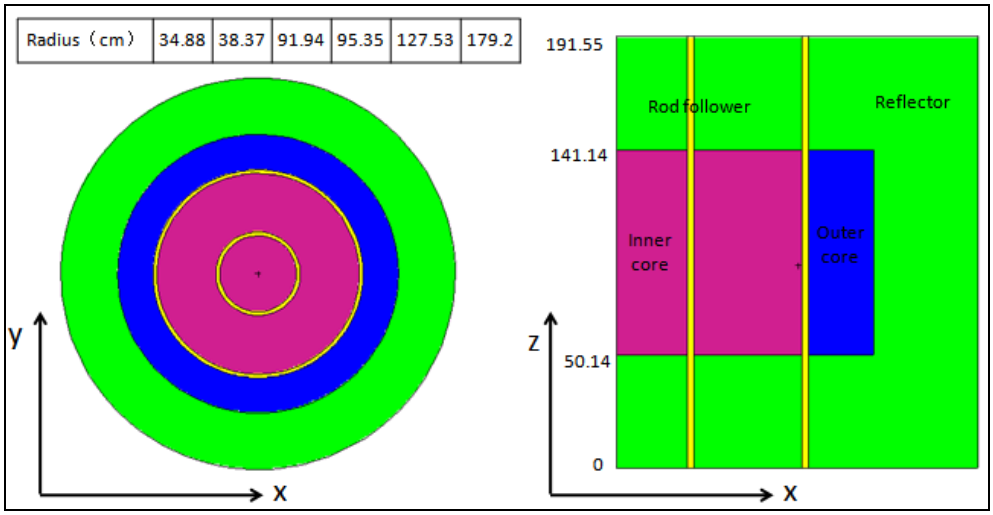


Figure 4. Fast reactor core.

Table III. Comparison of constructed problems results of RMC and MCNP

Problems	RMC k_{eff}	MCNP k_{eff}	RMC CPU time (min)	MCNP CPU time (min)
PWR Pin	1.24433±0.00034	1.24416±0.00030	15.07	48.33
SCWR assembly	1.08378±0.00028	1.08363±0.00028	16.73	28.50
CANFLEX bundle	1.06016±0.00033	1.05969±0.00025	26.25	31.10
Fast reactor core	1.13468±0.00033	1.13531±0.00025	21.78	54.13

Spectrums are also compared, as shown in Fig 5, which shows a good agreement between MCNP and RMC. The largest percent differences of spectrum results of PWR Pin, SCWR assembly, CANFLEX bundle and also fast reactor core are 0.296%, 0.419%, 0.261% and 0.373%

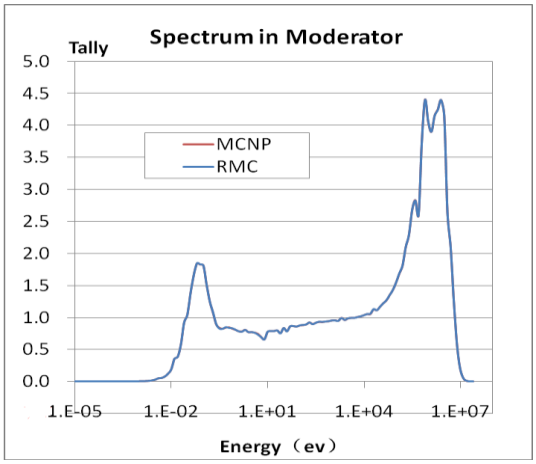


Figure 5a. Spectrum of PWR pin

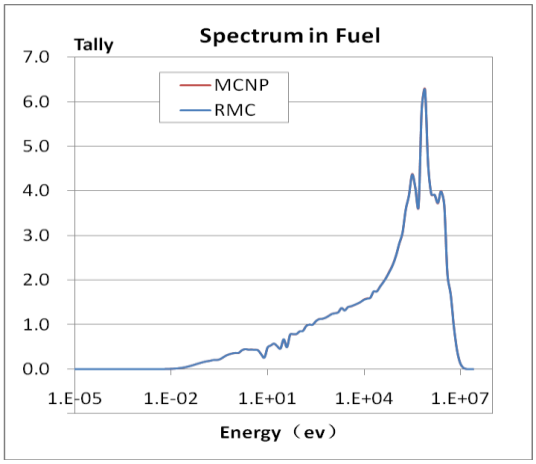


Figure 5b. Spectrum of SCWR assembly

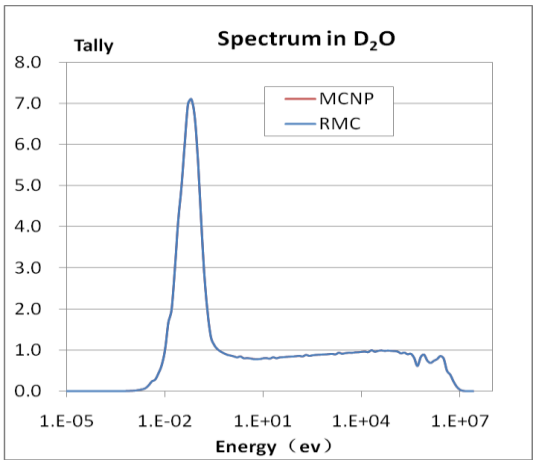


Figure 5c. Spectrum of CANFLEX bundle

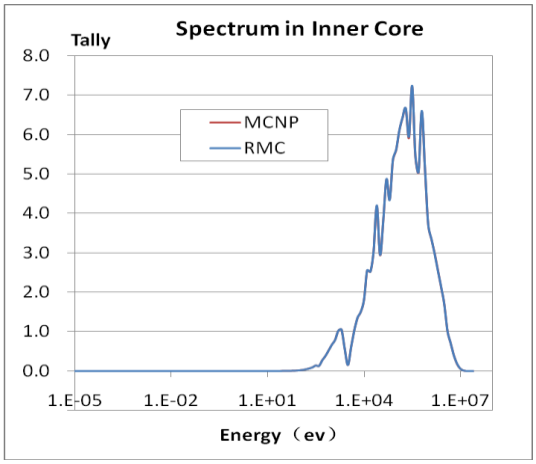


Figure 5d. Spectrum of fast reactor core

Figure 5. Spectrums of the constructed problems.

3.1.3. Parallel performance

To validate parallel performance of RMC, two examples are calculated in the condition of 1,000 generations of 5,000 neutrons each with 150 inactive cycles, results of which are shown in Table IV. According to Amdahl's Law,

$$S_N = \frac{1}{1 - F + F / N} \tag{2}$$

we can get that the parallel fraction of RMC code is more than 96%.

Table IV. Results of parallel calculation using RMC

Problems	Processors	1	2	3	4
PWR Pin	**Time (s)**	984.6	510.1	351.2	273.6
	Speedup	1.00	1.93	2.81	3.60
	Efficiency	1.00	0.97	0.94	0.90
CANFLEX Bundle	**Time (s)**	1735.2	883.8	600.0	459.6
	Speedup	1.00	1.96	2.89	3.77
	Efficiency	1.00	0.98	0.96	0.94

3.2. Results of Burnup Calculation

We choose a PWR pin-cell burnup problem for the calculation. The code McBurn [24] is chosen as the reference code which explicitly couples MCNP and ORIGEN and has been verified and validated extensively.

The problem is a single pin-cell model of a standard Westinghouse 17×17 PWR assembly[25]. Burnup calculations with 25 total steps are performed by both RMC and McBurn. Besides, different methods of tallying one-group reaction rates, namely conventional tally (CT) method and spectrum-based tally method (SBT), are also validated by RMC in this benchmark.

The curves of eigenvalue with burnup are shown in Fig 6. In addition, a comparison of some isotopes composition is presented in Table V, in which the results of CASMO and MCODE are from reference [25].

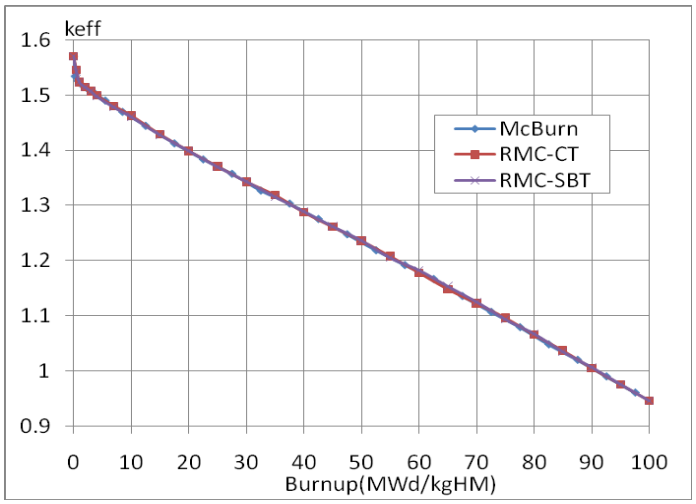


Figure 6. Eigenvalues with burnup calculated by RMC and McBurn.

Table V. Isotope composition comparisons at 100 MWD/kgHM

Isotopes	Atomic Density		Differences from MCODE		
	CASMO-4	MCODE	McBurn	RMC-CT	RMC-SBT
U-234	$6.713\ 10^{18}$	$6.793\ 10^{18}$	-0.46%	-0.67%	-0.25%
U-235	$2.595\ 10^{20}$	$2.650\ 10^{20}$	1.54%	2.01%	2.68%
U-238	$1.967\ 10^{22}$	$1.963\ 10^{22}$	-0.09%	-0.04%	-0.05%
Pu-238	$1.967\ 10^{19}$	$1.803\ 10^{19}$	4.52%	3.56%	3.05%
Pu-239	$1.477\ 10^{20}$	$1.559\ 10^{20}$	3.49%	3.51%	4.14%
Pu-240	$6.311\ 10^{19}$	$6.866\ 10^{19}$	2.37%	1.56%	2.62%
Pu-241	$4.280\ 10^{19}$	$4.498\ 10^{19}$	2.08%	2.19%	2.49%
Pu-242	$2.623\ 10^{19}$	$2.541\ 10^{19}$	-0.50%	-0.93%	-0.81%
Am-241	$2.351\ 10^{18}$	$2.586\ 10^{18}$	1.87%	2.66%	3.52%
Am-243	$6.232\ 10^{18}$	$7.678\ 10^{18}$	-0.94%	1.15%	1.29%
Np-237	$3.423\ 10^{19}$	$3.119\ 10^{19}$	1.06%	1.73%	1.05%
Cs-133	$1.145\ 10^{20}$	$1.239\ 10^{20}$	2.23%	2.13%	2.19%
Cs-135	$6.982\ 10^{19}$	$7.010\ 10^{19}$	0.55%	0.88%	1.01%
Nd-143	$7.425\ 10^{19}$	$7.447\ 10^{19}$	0.81%	0.85%	1.08%
Nd-145	$7.109\ 10^{19}$	$7.102\ 10^{19}$	0.36%	0.37%	0.32%
Sm-147	$9.572\ 10^{18}$	$1.092\ 10^{19}$	-1.28%	-1.21%	-1.11%
Sm-149	$1.246\ 10^{17}$	$1.173\ 10^{17}$	-8.19%	5.74%	6.11%
Sm-150	$2.676\ 10^{19}$	$2.892\ 10^{19}$	-9.31%	1.30%	1.24%
Sm-151	$7.682\ 10^{17}$	$6.890\ 10^{17}$	-2.01%	3.80%	4.21%
Sm-152	$9.395\ 10^{18}$	$7.873\ 10^{18}$	-5.63%	-1.52%	-1.13%
Eu-153	$1.184\ 10^{19}$	$1.049\ 10^{19}$	-1.97%	-0.12%	-0.19%

It shows that the results from RMC and McBurn, as well as other burnup codes, agree quite well. The comparison of calculation time between RMC and McBurn shows that RMC runs extremely faster than McBurn, especially when SBT method is adopted, as presented in Table VI.

Table VI. Calculation time comparison between RMC and McBurn.

Code	Time (min)
McBurn	190.2
RMC-CT	42.1
RMC-SBT	15.7

Burnup-step strategies are validated by large-step-length burnup calculation with different strategies including beginning-of-step (BOS) approximation, middle-of-step (MOS) approximation, and predictor-corrector (PC) method, which are shown in Fig 7. It is shown that middle-of-step approximation and predictor-corrector method can improve accuracy for large-step-length burnup calculation.

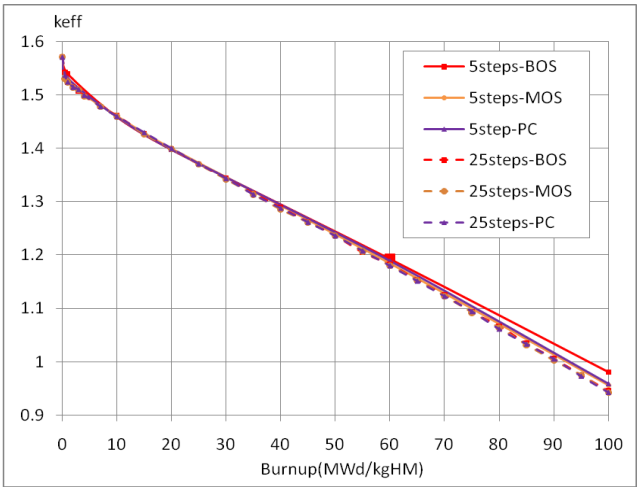


Figure 7. Eigenvalues with burnup by different burnup-step strategies in RMC

3.3. Results of Kinetics Calculation

Herein, only the results of the prompt supercritical system are presented. The continuous-energy neutron interaction data and the 6-group delayed neutron precursor data are from the ENDF/B-VI library. Fig 8 illustrates the geometry of a simplified PWR 5×5 assembly. A control rod is inserted in the central (Cell 113) of the assembly. The geometric parameters and the material compositions are listed in Table VII. At the beginning of the transient process, the control rod is ejected and the density of moderator is decreased to 56 kg/m^3, which make the k_{eff} rise to 1.00982.

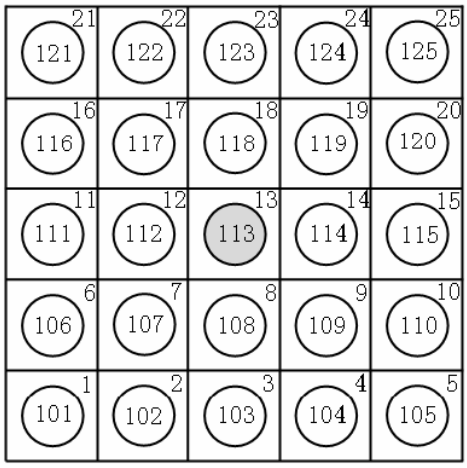


Figure 8. Geometric sketch of the 5×5 assembly.

Table VII. Geometric parameters and material composition for the 5×5 assembly

Fuel rod diameter (mm)		8.2
Gap between fuel rods (mm)		12.6
Number of fuel rods		24
Mass of fuel, UO2 (kg/m^3)		11000
Fuel enrichment		7.5%
Control rod diameter (mm)		8.2
Gap between control rod and fuel rods (mm)		12.6
Number of control rod		1
Insert depth of control rod (m)		0.99
Material of control rod (Boron carbide), nuclear density, (10^{24} cm^{-3})	^{10}**B**	0.01959
	^{11}**B**	0.08925
	C	0.02721
Density of moderator (kg/m^3)		1000
Height of the active region (m)		2.0

Considering that the moderator is water, when the flux is estimated, the neutron energy is divided into four groups, the first group (0.821MeV above), the second group (between 5.5KeV and 0.821MeV), the third group (between 0.625eV and 5.5KeV) and the fourth group (0.625eV below). The variation of neutron flux with time is presented in Fig 9. Note that this flux is the integral result over the whole assembly.

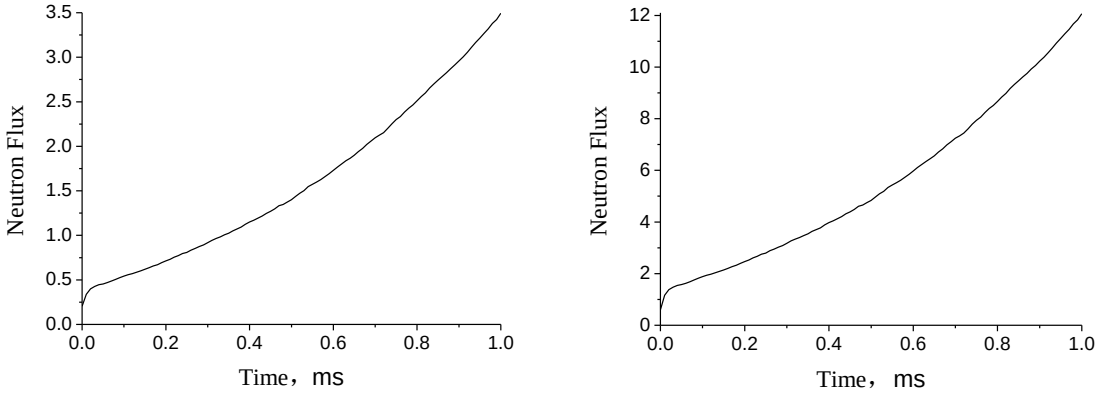


Figure 9a. Neutron flux of the first group

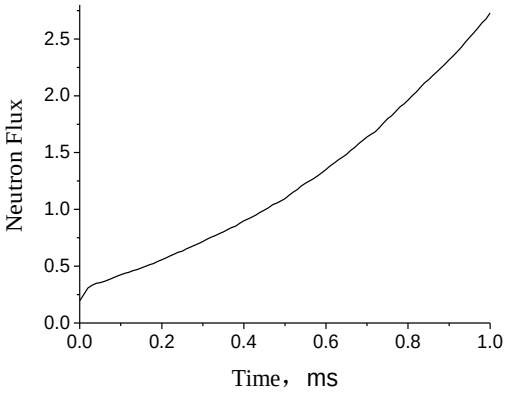


Figure 9b. Neutron flux of the second group

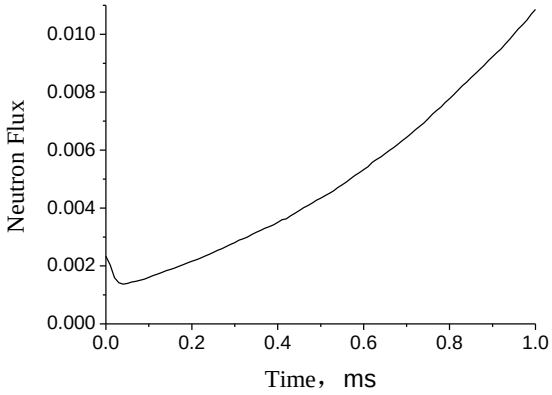


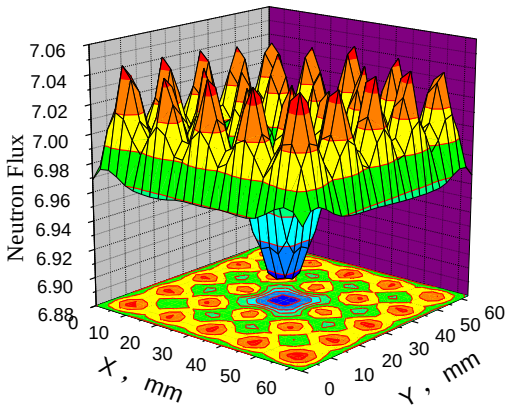
Figure 9c. Neutron flux of the third group

Figure 9d. Neutron flux of the fourth group

Figure 9. Variation of neutron flux with time.

At the beginning, the decrease of moderate diminishes the disappearance of high-energy neutron and the generation of thermal neutron, and the increment of fission reactions resulted from the ejected control rod increases the generation of fission neutron whose energy is greater than 0.625eV. So, initially, the neutron flux of the higher three groups (See Fig. (a)-(c) of the Fig. 9) is increased quickly and the fourth (See Fig. (d)) is decreased. But along with the increasing of high-energy neutron, the generation of thermal neutron is raised. Finally, its flux is increased with the time. Fig.9 shows the above process explicitly.

The spatial neutron flux distribution over the assembly at 1ms is presented in Fig.10. Although a 3-D model is calculated, the flux is the integral result along the axial direction. With the ejection of the control rod, the material of cell 113 becomes moderator. So, in the central the low-energy neutron flux (See Fig (c), (d)) is convex and others (See Fig (a), (b)) are concave.



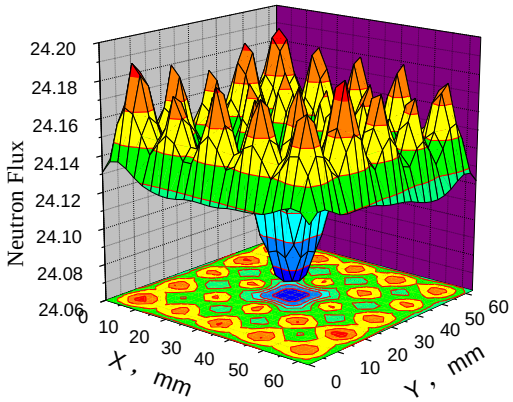


Figure 10a. Neutron flux of the first group

Figure 10b. Neutron flux of the second group

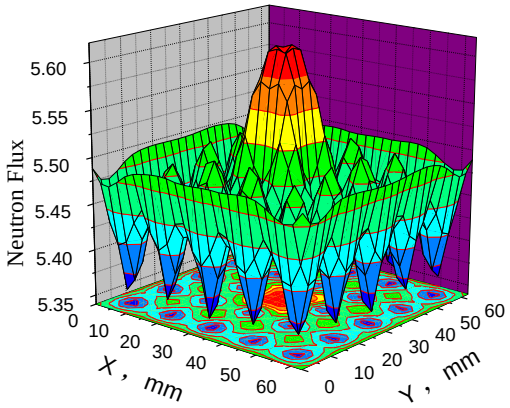


Figure 10c. Neutron flux of the third group

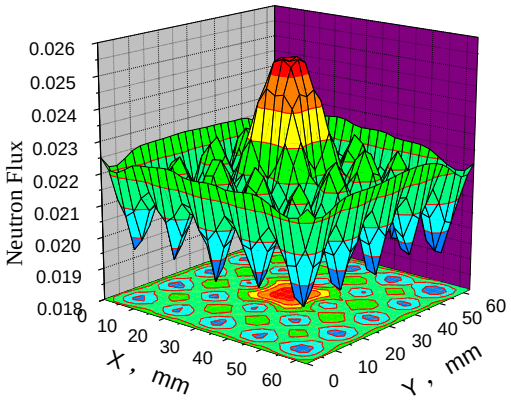


Figure 10d. Neutron flux of the fourth group

Figure 10. Spatial neutron flux distribution over the assembly at 1ms.

4. CONCLUSIONS

A new Monte Carlo neutron transport code RMC is being developed by Department of Engineering Physics, Tsinghua University. This code is specifically intended for reactor analysis, such as criticality calculation, burnup calculation and the kinetics simulation. The delta-tracking method and some other techniques such as CEO method and hash-table method are implemented to improve the performance of RMC on computational time and computer memory. The results of criticality problems, burnup problems and transient problems are presented, and the results show that RMC performs quite well in these kinds of problems.

And still some of the functions in RMC are not mature and needed for further work. Now we are focusing on these directions, such as the flux estimation method which can be used to represent the flux continuously, parallel calculation based on GPU, acceleration method of flux convergence and so on. And with these work, the RMC will be more powerful and useful in reactor physics analysis.

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