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Domain Decomposition Strategy for Large Scale Whole Core Burnup Calculation Based on RMC Code

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1. Introduction

With the higher requirements for the safety and economy of nuclear reactors as well as the developments of new types of nuclear systems, traditional methods and tools for reactor analysis are challenged. The Monte Carlo (MC) method is becoming an important research direction as next generation methods for reactor physics calculations. The expectation of MC being applied in nuclear reactor engineering design warms up especially with the development of parallel computing technology [1]. However, prohibitive data are required to be stored in large-scale calculations in MC codes and excessive memory demand turns into a key obstacle for MC method to accomplish pin-wise three-dimensional full core calculations. Particularly for whole core burnup calculations with millions of burnup regions, the data storage of reaches up to hundreds of gigabytes or even terabytes, which far exceeds the capacity of current computers.

Data decomposition and domain decomposition are two feasible ways to solve the memory problem of MC. Through the former method, specific types of data are decomposed and distributed on different processors and parallel communications are called for data operation in neutron simulating process. For the latter method, the idea is to divide the problem model into smaller geometry domains which are assigned to different processors. The domain related data is decomposed meanwhile. The particles are communicated between processors in domain decomposition method as the tracks of particle are cut into pieces.

In the previous studies, tally data decomposition (TDD) algorithms [2] are designed and implemented based in Reactor Monte Carlo code RMC [3]. Thereafter combination of TDD and depletion isotope data decomposition [4] is utilized to alleviate memory problem, enabling simple 3D whole core MC burnup calculations with hundreds of thousands of depletion regions [5]. However, memory problem still exists for larger scale or fine 3D whole core burnup because the material data is not decomposed. In this paper, domain decomposition method is investigated to solve the memory problem thoroughly. Further on, fine 3D whole core burnup calculation with millions of depletion region is achieved.

2. Memory evaluation of Monte Carlo codes

For the in-depth knowledge of memory problem of MC, it is necessary to classify data and analyze each data class quantitatively. In the reference of RMC, normally suitable to other codes, the data can be classified into 6 categories: geometry, material, nuclear data, particles, tallies and burnup. The memory model can be constructed by going deep into each data type and evaluating their memory sizes in detail, as shown in equation (1) and (2).

$$M = M_{\text{geo}} + M_{\text{mat}} + M_{\text{cs}} + M_{\text{part}} + M_{\text{tally}} + M_{\text{burn}} + M_{\text{temp}} \tag{1}$$

$$M \approx N_{\text{cell}}\bar{m}_{\text{cell}} + N_{\text{mat}}\bar{m}_{\text{mat}} + N_{\text{tot\_nuc}}\bar{m}_{\text{nuc\_cs}} + N_{\text{part}}m_{\text{part}} + N_{\text{tally}}\bar{m}_{\text{tally}} + N_{\text{burncell}}m_{\text{burncell}} \tag{2}$$

Specially, the equation (3) describes the memory consumption of RMC.

$$M_{\text{RMC}} \approx (100N_{\text{cell}} + 4.8N_{\text{mat}} \times 10^3 + 2N_{\text{tot\_nuc}} \times 10^6 + 64N_{\text{part}} + 70N_{\text{tally}} + 3.6N_{\text{burncell}} \times 10^4)\ \text{Bytes} \tag{3}$$

Table I shows unit storage, scale of unit and maximum storage of each data type. It can be seen that 3 types of data, i.e. tally, burnup and material, are the main source of memory problem.

Table I. Memory storage evaluation of data type

Data types	Unit storage	Scale	Maximum storage
Geometry	100 Bytes	10^0~10^6	0.1 Gbytes
Material	4.8 KBytes	10^0~10^7	10 Gbytes
Nuclear data*	2 MBytes	10^0~10^2	1 Gbytes
Particle	64 Bytes	10^4~10^6	0.1 GBytes
Tally	70 Bytes	0~10^{10}	100 GBytes
Burnup	36 KBytes	0~10^7	100 GBytes

* assuming nuclides are in one-temperature

Hoogenboom-Martin whole core [6] is chosen for case study of large scale MC burnup calculation. There are totally 241 assemblies and 63624 fuel rods in H-M core. It is modeled each rod contains 24 burnup regions (12 axially by 2 radially) to perform depletion calculation. Table II predicts the memory storage.

Table II. Memory storage of H-M whole core burnup

Data types	Memory storage

Material	7.3 GBytes
Nuclear data	400 MBytes
Particle	64 MBytes
Tally	64.1 GBytes
Burnup	55.0 GBytes
Total	126.9 GBytes

3. Domain decomposition method

Different from data decomposition method, spatial domain decomposition (SDD) divides spatial geometry into domains, which are simulated separately by parallel processors, and particles crossing domains are communicated.

As indicated in Fig. 1, main steps of implementing SDD in particle transport Monte Carlo code includes: (1) dividing model geometry and decomposing data of tallies and materials simultaneously; (2) tracking particle histories by means of "stages" which are bounded with particle communications; (3) finishing simulation by checking all particles stages and communications.

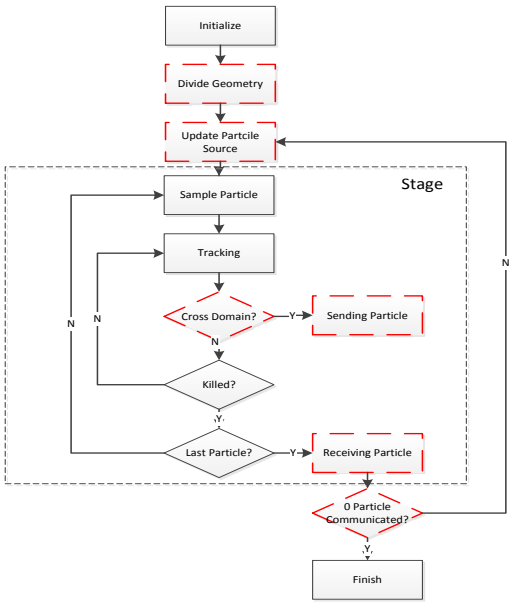


Fig. 1. Flow chart of domain decomposition method

It should be noted that except for domain partition strategy, particle communication algorithm is a key part for SDD. Asynchronous particle communication algorithm is designed using MPI (message passing interface [7]), as shown in Fig. 2. In the algorithm, particles flying out of current domains are buffered in local processor and one buffer is sent to the remote processor when it is full. MPI non-blocking functions (MPI_Isend/MPI_Irecv) are used for overlap of computing and passing messages, to shorten total communication costs as low as possible.

```
1:  decompose Geometry to all processes
2:  for cycle = 1 to CycleNum
3:  |  do // stages
4:  |  |  post non-blocking receives to all other processes(MPI_Irecv)
5:  |  |  for neutron = 1 to NeutronNum
6:  |  |  |  tracking history
7:  |  |  |  |  test all receives(MPI_Test)
8:  |  |  |  |  |  while(one receive success)
9:  |  |  |  |  |  |  add received particle to local bank
10: |  |  |  |  |  |  if(not last recv)post receive to the same target (MPI_Irecv)
11: |  |  |  |  end while loop
12: |  |  |  |  if(cross domain)
13: |  |  |  |     save it to particle buffer
14: |  |  |  |     if(buffer is full)send this buffer to target(MPI_Isend)
15: |  |  |  end one history
16: |  |  end for loop
17: |  |  send all buffer out(MPI_Isend)
18: |  |  wait all send and receive success(MPI_Wait)
19: |  |  reduce all received particles number(MPI_Allreduce)
20: |  while(received particle exist)
21: |  process cycle end
22: end for loop
```

Fig. 2. Asynchronous particle communication algorithm in domain decomposition method

4. Coupling domain decomposition with MC burnup

4.1 Coupling strategy and memory estimation

It is known that MC burnup calculation process is a combination of MC neutron transport simulation and depletion equation computation. The basic calculation unit in depletion, i.e. burnup cell, is geometrical region as well. Therefore, it is possible to couple domain decomposition with MC burnup by utilizing consistent domain partition in transport process and depletion process. In other words, burnup regions can be decomposed automatically according to geometry decomposition in transport.

Through the coupling, geometry-based data including data of tally, material and isotope densities, i.e. main memory-consuming data types are all decomposed.

From the memory model in section 2, assuming geometry are evenly decomposed into P domains, the memory size of one domain can be estimated as equation (4).

$$M_{\text{Domain}} \approx M_{\text{geo}} + M_{\text{cs}} + M_{\text{part\_Domain}} + \frac{M_{\text{mat}} + M_{\text{tally}} + M_{\text{burn}}}{P} \quad (4)$$

Actually, three major data types are all proportional to number of burnup cells, as shown in equation (5). Note that it is assumed there are about 150 isotopes in every burnable cell or material for transport simulation. Totally 4 types of one-group cross section for every isotope in every material should be enabled for depletion calculation [8].

$$\begin{aligned} M_{\text{mat}} + M_{\text{tally}} + M_{\text{burn}} &\cong N_{\text{burncell}} (4.8\times10^{3} + 70\times600 + 3.6\times10^{4}) \text{ Bytes} \\ &\approx 0.08 N_{\text{burncell}} \text{ MBytes} \end{aligned} \quad (5)$$

Therefore, the necessary number of domain decomposition can be figured out according to the capacity of computer RAM. For example, in order to carry out MC burnup calculation on 4 GBytes RAM

computers, assuming that memory size of data not decomposed is no more than 2 GBytes, the condition and result can be derived as (6) and (7), which mean no less than 42 domain partitions is adequate for one-million-region burnup calculation.

$$\frac{M_{mat}+M_{tally}+M_{burn}}{P} \le 2\,\text{GBytes} \quad (6)$$

$$P \ge 4.14 N_{burncell} \times 10^{-5} \quad (7)$$

4.2 Implementation of coupled domain decomposition

Coupled domain decomposition is implemented in RMC based on the above coupling strategy, as shown in Fig.3. It can be seen that depletion regions are grouped according to domain partition in transport process.

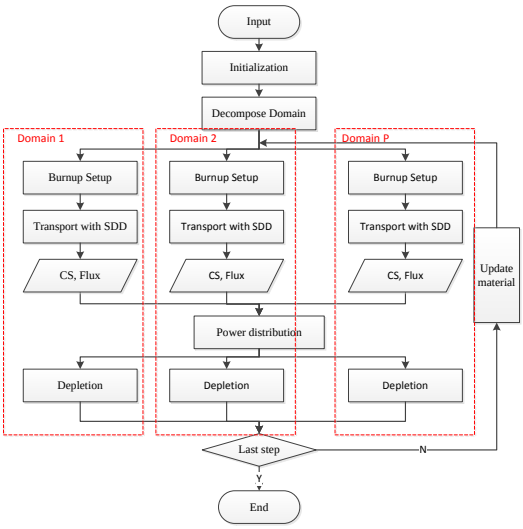


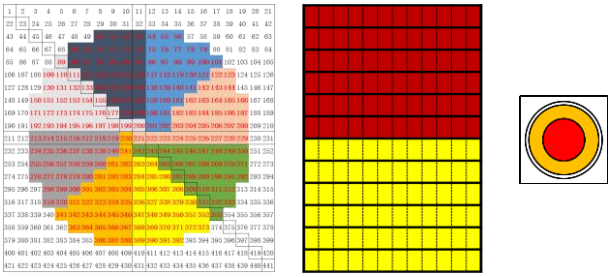
Fig. 3. Frame of coupled domain decomposition

5. Numerical test of 3D full core burnup calculation

Hoogenboom-Martin core is used to do 3D full core burnup calculation test. Table III shows the main calculation parameters used in the calculation. Totally 1.5 million burnup regions are set up with 24 burnup regions (12 axially by 2 radially) per rod, illustrated by Fig. 4. This full core is decamped into 96 domains with 8 pieces radially and 12 slices axially. The partitions in radial planes are performed in a way to make every assembly fully belonging to only one domain while balancing the loads of domains as far as possible.

Table III. Main calculation parameters used

Parameters	Data
Number of histories in MC transport	1,000,000 particle/cycle 750 cycles(250 inactive)
Number of burnup regions	1,526,976
Number of isotopes per burnup region	1487
Number of time steps	14
Step length (ΔMWD/kgU)	0.1, 0.4, 0.5, 1×11
Number of inner steps in depletion	10
Burnup strategy	predictor-corrector
Power density (W/gU)	30
Total burnup (MWD/kgU)	12
Number of parallel processors	96



8 domains radially 12 segments axially 2 rings/rod

Fig. 4. Domain and depletion region partition in 3D full core burnup

"Inspur TS10000" cluster at Tsinghua University is used to run the 96-domain parallel calculation.

As estimated in Section 2, total memory storage consumed in this calculation is up to 127 GBytes, which exceeds memory capacity for normal MC code. Nevertheless, it is demonstrated that RMC code integrated with domain decomposition method is capable to complete the calculation.

Fig. 5 to Fig. 8 show the results of calculation.

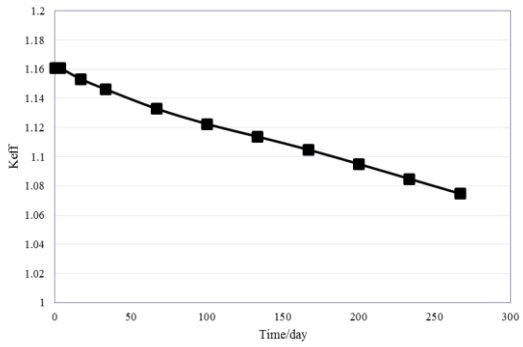


Fig. 5. Variation of core K-effective with burnup

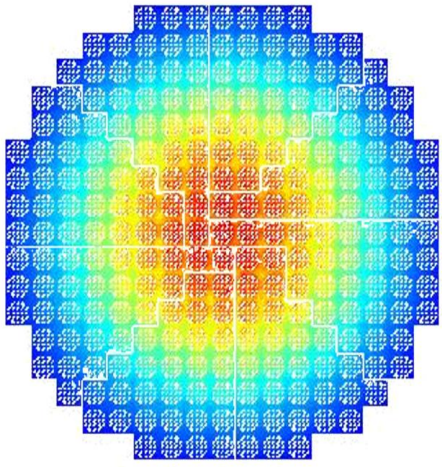


Fig. 6. Core radial power distribution at 0 MWD/kgU

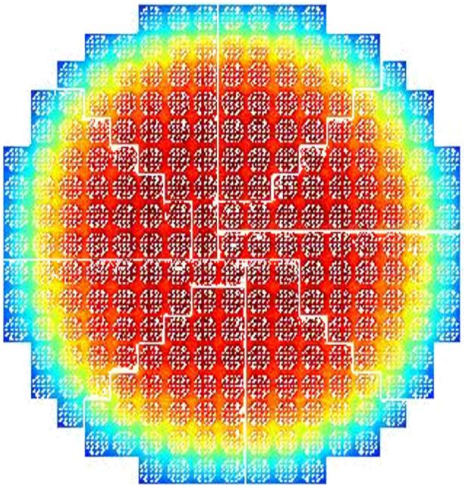


Fig. 6. Core radial power distribution at 5 MWD/kgU

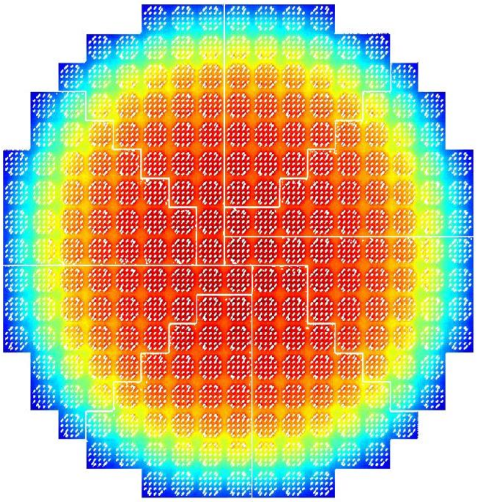


Fig. 7. Core radial burnup distribution at 8 MWD/kgU

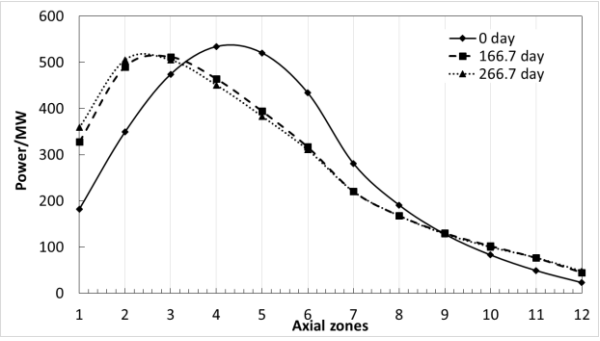


Fig. 8. Axial power distributions

This test is to show the capability of domain decomposition method in large-scale burnup calculation. Only one way of domain partition is used and performances are not tested. Actually, the pattern of decomposition determines source load imbalances level which influences computing performance significantly. Siegel et al have studied the impact of particle load imbalances [9].

6. Conclusions

The successful running of the H-M benchmark with the assumed burnup cases demonstrates the effectiveness of domain decomposition methods for solving memory problems with Monte Carlo codes. It can be indicated that domain decomposed MC codes are capable of pin-wise full core burnup calculations with millions of depletion regions.

Acknowledgements

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