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# Fission and Surface Source Iteration Scheme with Source Splitting in Domain Decomposition Monte Carlo Calculation

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## 1. Introduction

There are several challenges for whole-core continuous-energy Monte Carlo (MC) calculation, such as slow source convergence, excessive memory demand for massive tallies, under-estimation of apparent variance, and variance reduction, etc., as noted in Ref. [1].

As a domain decomposition method, the overlapping local/global (OLG) iteration scheme [2,3] using MC/p-CMFD was proposed as an alternative to the direct whole-core transport calculation. The OLG iteration scheme uses overlapping regions for each local problem solved by continuous-energy MC calculation to reduce errors in inaccurate boundary conditions (BCs) that are caused by discretization in space, energy, and angle. However, the overlapping region increases computational burdens and the discretized BCs for continuous-energy MC calculation result in an inaccurate global p-CMFD solution.

On the other hand, there also have been several studies [4-6] on the direct domain decomposed MC calculation where each processor simulates particles within its own domain and exchanges the particles crossing the domain boundary between processors with certain frequency. The efficiency of this method depends on the message checking frequency and the buffer size. Furthermore, it should overcome the load-imbalance problem for better parallel efficiency.

Recently, fission and surface source (FSS) iteration method [7] based on banking both fission and surface sources for the next iteration (i.e., cycle) was proposed to give exact BCs for nonoverlapping local problems in domain decomposition and tested in one-dimensional continuous-energy reactor problems.

In this paper, the FSS iteration method is combined with a source splitting scheme to reduce the load-imbalance problem and achieve global variance reduction. The performances are tested on a two-dimensional continuous-energy reactor problem with domain-based parallelism and compared with the FSS iteration without source splitting. Numerical results show the improvements of the FSS iteration with source splitting.

## 2. Methodology

### *2.1 Fission and Surface Source (FSS) Iteration Method*

When the whole-core geometry is decomposed into $I$ local domains, the local problem for domain $D_i$ ($i$=1 to $I$) is given by the following fixed-$k$ (also known as fixed-source) problem [2]:

$$L\psi_i + T\psi_i - S\psi_i = \frac{1}{k_{global}} F\psi_i \ , \qquad (1)$$

with surface source BC at the local domain boundary $\partial D_i$:

$$\psi_i^-(\vec{r}_s, E, \vec{\Omega}) \text{ given for } \vec{r}_s \in \partial D_i \text{ and } \vec{\Omega} \in \{\vec{n}_i \cdot \vec{\Omega} < 0\} \ ,$$

where $\psi_i$, and $L$, $T$, $S$, and $F$ are defined as

$$\psi_i = \psi(\vec{r}, E, \vec{\Omega}) \text{ for } \vec{r} \in D_i \ ,$$

$$L\psi = \vec{\Omega} \cdot \nabla \psi(\vec{r}, E, \vec{\Omega}) \ ,$$

$$T\psi = \sigma_t(\vec{r}, E)\psi(\vec{r}, E, \vec{\Omega}) \ ,$$

$$S\psi = \int dE' \int d\Omega' \sigma_s(\vec{r}, E' \to E, \vec{\Omega}' \cdot \vec{\Omega})\psi(\vec{r}, E', \vec{\Omega}') \ ,$$

$$F\psi = \frac{\chi(E)}{4\pi} \int dE' \int d\Omega' \nu\sigma_f(\vec{r}, E')\psi(\vec{r}, E', \vec{\Omega}') \ ,$$

and $k_{global}$ is the global multiplication factor, $\vec{n}_i$ is the out-normal direction on $\partial D_i$. The way to calculate $k_{global}$ is described later in Eq. (6).

Eq. (1) can be iteratively solved by

$$L\psi_i^t + T\psi_i^t - S\psi_i^t = \frac{1}{k_{global}^{t-1}} F\psi_i^{t-1} \ , \qquad (2)$$

with BC given as surface source:

$\psi_i^{-,t}(\vec{r}_s, E, \vec{\Omega}) =$ neutron angular flux entering local problem $i$ in iteration (or cycle) $t$-1 from neighboring local problems for $\vec{r}_s \in \partial D_i$ and $\vec{\Omega} \in \{\vec{n}_i \cdot \vec{\Omega} < 0\}$.

The fission source for the next iteration is updated by banking position and energy of new fission particles as usual. The number of fission particles banked within $D_i$ is given by

$$N_{i,f}^t = \sum_{n=1}^{N_i^{t-1}} \sum_c \left\lfloor \frac{1}{k_{global}^{t-1}} \frac{\nu\sigma_f}{\sigma_t} W_{n,c} + \xi \right\rfloor , \qquad (3)$$

where $N_i^{t-1}$ is the number of both fission and surface sources for $\vec{r} \in D_i$ produced in iteration $t$-1, $c$ is summation index over all collisions of the $n$-th source, $n$ is the source index, $W_{n,c}$ is a weight of the $n$-th source entering collision, and $\xi$ is a random number in the interval (0, 1).

When a particle crosses $\partial D_i$ from neighboring local problem $j$, position, energy, and angle of the particle are

banked to update the surface source for local problem $i$. The number of banked particles crossing $\partial D_i$ is given by

$$N_{i,s}^{t} = \sum_{j} \sum_{n=1}^{N_j^{t-1}} \left\lfloor W_{n,j\to i} + \xi \right\rfloor , \quad (4)$$

where $W_{n,j\to i}$ is a weight of the $n$-th source crossing $\partial D_i$ from neighboring local problem $j$. Note that the discretization errors of BCs having occurred in the previous studies [2,3] are removed in this FSS iteration method.

The initial weight of either fission or surface source for the next iteration is determined as

$$W^{t} = \frac{N}{\sum_{i=1}^{I} \left( N_{i,f}^{t} + N_{i,s}^{t} \right)} , \quad (5)$$

where $N$ is the nominal source size of each iteration.

The global multiplication factor is updated as

$$k_{global}^{t} = \frac{\sum_{i=1}^{I} \left\langle F\psi_i^{t} \right\rangle}{\sum_{i=1}^{I} \left\langle (T-S)\psi_i^{t} \right\rangle + J_{global}^{t}} , \quad (6)$$

where $\langle\ \rangle$ denotes integration over space, energy, and angle. $J_{global}^{t}$ is leakage rate at the global problem boundary in iteration $t$. Note that while collision, track-length, and absorption estimators are available for production rate and total reaction rate, scattering reaction rate is tallied by absorption estimator and leakage rate is tallied based on surface crossing estimator.

### *2.2 Several Features of FSS Iteration Method*

First, during an iteration, each local problem can be solved independently, due to banked surface source, as shown in Fig. 1.

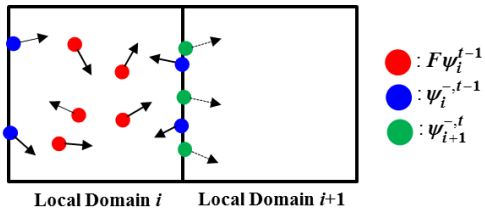


Fig. 1. Sources in local problem $i$ at iteration $t$

Second, since outgoing particles from local domain boundaries become surface source of neighboring local problems in the next iteration, apparent variances of flux distributions would be more under-estimated, especially near local domain boundaries, than those of the conventional power iteration.

Third, the new iteration method requires converged fission and surface sources through inactive cycles. To obtain converged source distributions, there are two options. One option is to obtain both fission and surface sources for each local problem by using the FSS iteration based on the same domain decomposition. The other option is to obtain converged fission source by using the conventional power iteration. After that, using the converged fission source, another cycle ("switch" cycle) will provide both fission and surface sources for each local problem. In both options, the inactive cycles can be effectively accelerated by p-CMFD acceleration method [8, 9], including its variations suggested in [10].

Fourth, FSS iteration method can perform calculation and communication simultaneously. During simulating histories starting from fission sources, surface source data can be transmitted by asynchronous, non-blocking communication with MPI message-passage parallelism.

### *2.3 FSS Iteration Method with Source Splitting*

For active cycles, when the fission and surface sources for local problem $i$ are sampled with weight $W^{t}$, these sources are split with weight $W_i^{t}$ which is set as $N_i^{t} / \max_i(N_i^{t})$ and weight cutoff threshold is set as $W_i^{t} / 4$. Then the numbers of split sources of local problems are expected to be equal over all the local problems as shown in Fig. 2. This source splitting scheme is expected to reduce the load-imbalance problem. Furthermore, by equating the numbers of sources of local problems with source splitting, the number density of MC particles would become much more uniform over local domains than the number density without source splitting. Thus, similarly to the Global Flux Weight Window (GFWW) [11], the FSS iteration with source splitting would achieve global variance reduction.

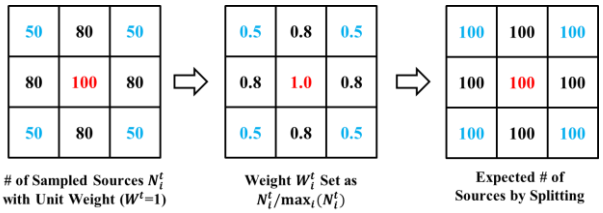


Fig. 2. Example of source splitting in a problem consisting of 9 local domains with vacuum boundary condition

## 3. Numerical Results

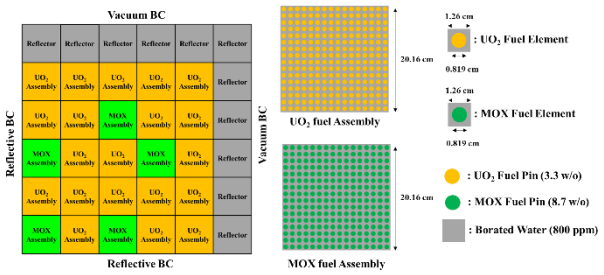


Fig. 3. Two-dimensional continuous-energy thermal reactor test problem

For a two-dimensional continuous-energy reactor problem shown in Fig. 3, sample standard deviations of

keff and pin-power distributions obtained by following two cases:

Case 1: FSS iteration without source splitting

Case 2: FSS iteration with source splitting

are compared. In Case 2, the source splitting is not applied in a local problem which does not contain fuel material.

For the FSS iteration method, the whole-core problem is divided into 6x6 local problems based on unit assembly, in which each local problem is assigned to a processor in a Beowulf system consisting of 9 Quad-core processors.

To accelerate source convergence, fission and surface sources are adjusted by the coarse-mesh flux from p-CMFD calculation, where the p-CMFD parameters are accumulated after the first 10 iterations to stabilize the source fluctuations. Table I shows calculational conditions for MC calculations, where MC calculations are performed by the in-house research code McBOX [12] with ENDF/B-VII.0 continuous-energy cross section library.

Table II compares multiplication factors of the two cases. Case 2 which uses source splitting shows smaller sample standard deviation than Case 1, where the computing times for active iterations are almost same.

Table I. Monte Carlo calculational conditions in FSS iteration

| | |
|---|---|
| # of Inactive Iterations | 20 |
| # of Active Iterations | 100 |
| # of Fiss. Src./Iteration | ~1,000,000 |
| # of Surf..Src./Iteration | ~1,480,000 |

Table II. Comparison of multiplication factors of FSS iteration method without and with source splitting

| | Case 1 | Case 2 |
|---|---|---|
| $k_{eff}$ | 1.26683 | 1.26686 |
| $\sigma_{sample}$ | 0.000077 | 0.000056 |
| Time for Active Iteration | 1840 [sec] | 1834 [sec] |

Fig. 4 shows pin-power distributions in Case 1. Case 2 shows same pin-power distributions within one sample standard deviation of the sample mean. Figs. 5 and 6 show relative sample standard deviations of pin-power distributions in Cases 1 and 2, respectively.

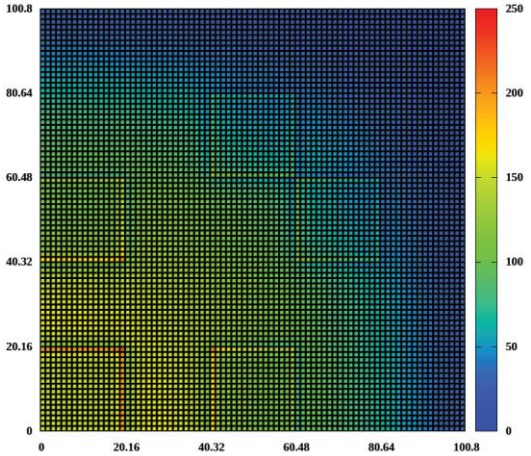


Fig. 4. Pin-power distributions of two-dimensional thermal reactor test problem

In Case 1, relative standard deviations depends quite sensitively on the location of the local problem. When the local problem is located near the reflector, it shows larger relative standard deviations than the local problem located at the center. On the other hand, Case 2 shows small relative standard deviations over all fuel assemblies.

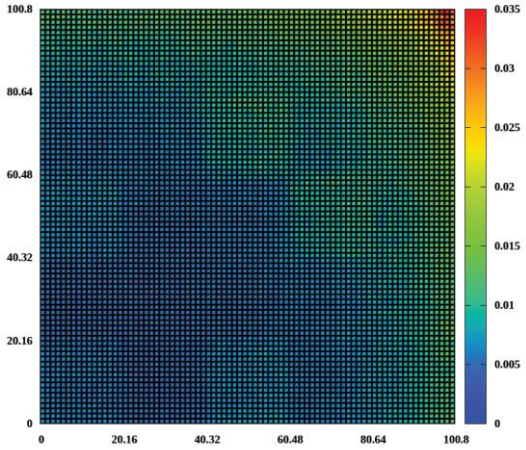


Fig. 5. Relative sample standard deviation of pin-power distributions in Case 1

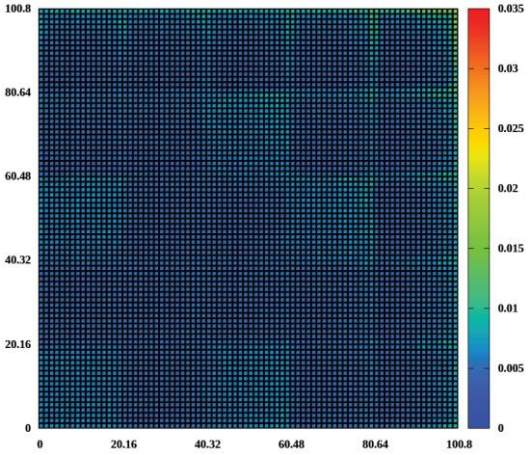


Fig. 6. Relative sample standard deviation of pin-power distributions in Case 2

Figs. 7 and 8 show elapsed times of local problems for particle tracking in Cases 1 and 2, respectively, at Cycle 21. Compared to Case 1, Case 2 shows much more uniform computing times over local problems. It means that the source splitting scheme effectively reduces idle times of the processors to wait for the results from other local problems. However, Case 2 still shows load-imbalance, in that the computing times for MOX assemblies are longer than those for $UO_2$ assemblies. Since the MOX fuel contains more nuclides than the $UO_2$ fuel, it is more time-consuming for energy grid search for point-wise reaction cross sections in the MOX fuel.

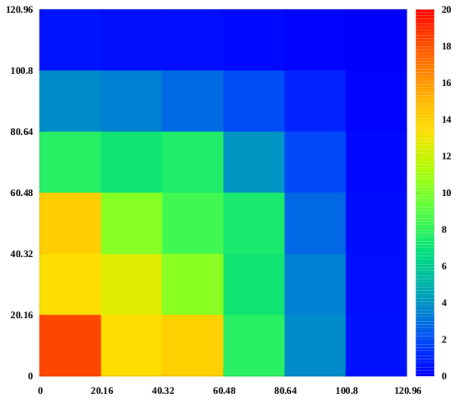


Fig. 7. Elapsed times [sec] of local problems for particle tracking in Case 1 at Cycle 21.

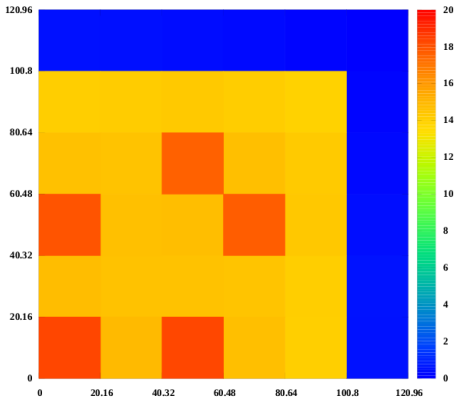


Fig. 8. Elapsed times [sec] of local problems for particle tracking in Case 2 at Cycle 21.

## 4. Summary and Conclusions

This paper describes the FSS iteration scheme in the domain decomposition method and proposes the FSS iteration combined with the source splitting based on the number of sampled sources, reducing the load-imbalance problem in domain-based parallelism and achieving global variance reduction.

Numerical results on a two-dimensional continuous-energy thermal reactor test problem show that Case 2 which uses source splitting reduces load-imbalance and sample variances of the multiplication factor and pin-power distributions without additional computing time. However, depending on local problems, the average computing time for a particle is different, which should be considered in setting weight for source splitting. Thus, investigations of source splitting in more test problems would be worthwhile as further studies.

## Acknowledgement

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