Modification of Scattering Kernel for the Effective Parallel Processing in the Photon/Electron Coupled Problem

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1. Introduction

In the reactor physics calculation, solutions for the neutron transport equation are obtained mostly by the discrete ordinates method (referred as an S_N method) or Monte Carlo method. To obtain the solutions with faster speed, the parallel processing is one of the options we can have [1].

For the effective parallel processing in S_N method, transport sweep procedure can be easily considered. However, for the very anisotropic problem with up-scattering (e.g., photon/electron coupled beam problem), scattering source calculation should be considered.

In the photon/electron coupled beam problem, the Legendre expansion order is higher than that in the reactor physics calculation such as L=7 or above. In addition, photon/electron cross sections are coupled together with up/down scattering.

In this paper, the parallel processing performance with modified scattering kernel and conventional spherical harmonics scattering kernel is compared.

2. Method and results

2.1 Photon/Electron Coupled Cross Section with CEPXS Code

CEPXS [2] generates coupled photon/electron cross sections in multigroup Legendre format. There are four coupling schemes available. That are no-coupling, partial-coupling, full-coupling (no positrons), and full-coupling (positrons).

For the photon-source and full-coupling with no positrons case, global cross section matrix of 0th Legendre order is shown in Fig. 1.

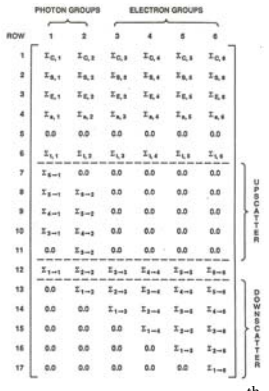

Fig. 1. A global cross section matrix of 0th Legendre order (photon-source, full-coupling, and no positrons).

As shown in Fig. 1, all groups are coupled with up/down scattering.

2.2 Scattering Kernel

Three-dimensional discrete ordinates equation is

$$\vec{\Omega}_n \bullet \nabla \psi_g(\vec{r},\vec{\Omega}_n) + \sigma_{t,g}(\vec{r})\psi_g(\vec{r},\vec{\Omega}_n) = q_{s,g}(\vec{r},\vec{\Omega}_n), \tag{1}$$

where $q_{s,g}(\vec{r},\vec{\Omega}_n)$ is scattering source as

$$q_{s,g}(\vec{r},\vec{\Omega}_n) = \sum_{g'=1}^{G}\sum_{\ell=0}^{L}\sigma_{s\ell g'\to g}(\vec{r})\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\vec{\Omega}_n)\left(\Phi^m_{\ell,g'}(\vec{r})\right), \tag{2}$$

$$\Phi^m_{\ell,g'}(\vec{r}) = \frac{1}{8}\sum_{n'=1}^{N(N+2)} \omega_{n'} Y_{\ell m}(\vec{\Omega}_{n'})\Psi_{g'}(\vec{r},\vec{\Omega}_{n'}). \tag{3}$$

With additional theorem and spherical harmonics, we have following equation as

$$\begin{aligned}
&\vec{\Omega}_n \bullet \nabla \psi_g(\vec{r},\vec{\Omega}_n) + \sigma_{t,g}(\vec{r})\psi_g(\vec{r},\vec{\Omega}_n) \\
&= \sum_{g'=1}^{G}\sum_{\ell=0}^{L}(2\ell+1)\sigma_{s\ell g'\to g}(\vec{r}) \\
&\times \left[\begin{array}{l}
P_\ell(\mu_n)\left(\frac{1}{8}\sum_{n'=1}^{N(N+2)}\omega_{n'}P_\ell(\mu_{n'})\Psi_{g'}(\vec{r},\vec{\Omega}_{n'})\right) \\
+2\sum_{m=1}^{\ell}\frac{(l-m)!}{(l+m)!}P^m_\ell(\mu_n)\cos(mw_n) \\
\quad\times\left(\frac{1}{8}\sum_{n'=1}^{N(N+2)}\omega_{n'}P^m_\ell(\mu_{n'})\cos(mw_{n'})\Psi_{g'}(\vec{r},\vec{\Omega}_{n'})\right) \\
+2\sum_{m=1}^{\ell}\frac{(l-m)!}{(l+m)!}P^m_\ell(\mu_n)\sin(mw_n) \\
\quad\times\left(\frac{1}{8}\sum_{n'=1}^{N(N+2)}\omega_{n'}P^m_\ell(\mu_{n'})\sin(mw_{n'})\Psi_{g'}(\vec{r},\vec{\Omega}_{n'})\right)
\end{array}\right].
\end{aligned} \tag{4}$$

We like to replace scattering source part in Eq. (4) simply by

$$\begin{aligned}
&\vec{\Omega}_n \bullet \nabla \psi_g(\vec{r},\vec{\Omega}_n) + \sigma_{t,g}(\vec{r})\psi_g(\vec{r},\vec{\Omega}_n) \\
&= \sum_{g'=1}^{G}\sum_{n'=1}^{N(N+2)}\omega_{n'}\,\bar{\sigma}_{n'\to n,g'\to g}(\vec{r})\,\Psi_{g'}(\vec{r},\vec{\Omega}_{n'}),
\end{aligned} \tag{5}$$

where $\bar{\sigma}_{n'\to n,g'\to g}(\vec{r})$ is pre-calculated group-to-group, ordinate-to-ordinate scattering cross section by equating Eqs. (4) and (5) [3]. The merit we can have by using this modified scattering kernel is that we can save time to calculate each do-loop for m and ℓ repeatedly.

2.3 Test and Results

To see the performance of modified scattering kernel, we devise test problem as shown in Fig. 2. 1MeV photon beam incidents on the water slab only on the 2cm x 2cm center region. The cross section data is generated by CEPXS and it consists of eight photon energy groups and eight electron groups with P_7 Legendre order. The energy groups range from 0.01MeV to 1MeV with full-coupling scheme. In the calculation, S_8 angular quadrature and 19174 tetrahedral elements are used.

The performance is tested by checking elapsed time per iteration. All procedures are the same except

scattering source calculation part. Detail locations of starting and end marks are shown with the simple diagram in Fig. 3.

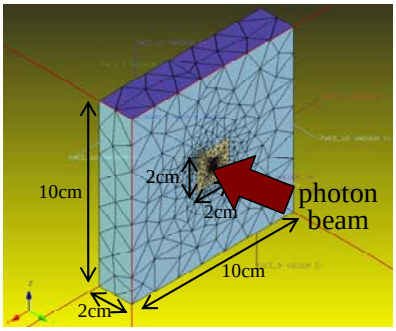

Fig. 2. Test Problem for the parallel processing performance.

All scattering sources of energy groups are being solved simultaneously using the updated fluxes through transport sweep. In the case of maximum parallelization, the user runs with one energy group per process.

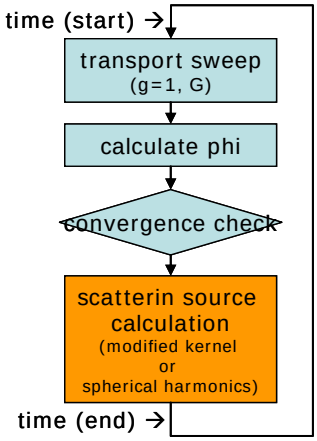

Fig. 3. The simple diagram with start/end time marks.

Table I: Elapsed time per iteration

No. of process	Average calculated energy groups/process	Modified scattering kernel (sec/iteration)	Spherical harmonics (sec/iteration)
1	16.0	1,092	98,976
2	8.0	N/A	N/A
3	5.3		
4	4.0		
5	3.2		31,917
6	2.7	254	22,835
7	2.3	253	22,887
8	2.0	181	22,788
9	1.8	181	19,098
10	1.6	181	18,999
11	1.5	182	18,830
12	1.3	181	18,676
13	1.2	181	13,460
14	1.1	182	8,877
15	1.1	169	10,013
16	1.0	110	

※ Processor: Intel Core™ 2 Quad 3.0GHz

The elapsed time per iteration is listed in the Table I. As we can see in the Table I, the maximum parallelization can be achieved as the average calculated energy groups per process is decreased to unity.

The calculated dose profile on the cutted XY plane is shown in Fig. 4.

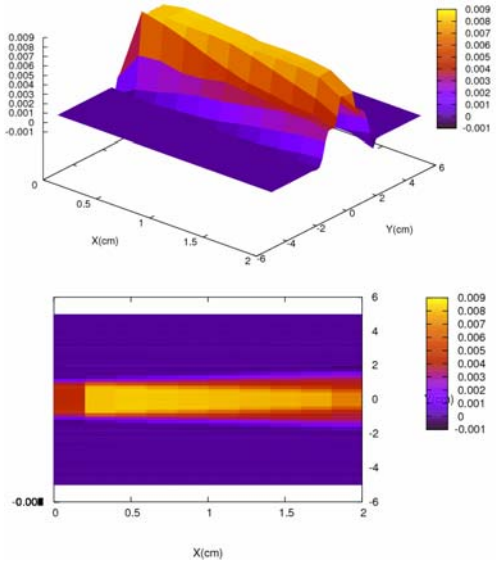

Fig. 4. The calculated dose profile (MeV/g) on X-Y plane.

3. Conclusions

The modified scattering kernel and conventional spherical harmonics kernel are tested on the parallel processing and compared their elapsed time per iteration.

The numerical tests show that the elapsed time per iteration with modified scattering kernel is much faster than that with conventional spherical harmonics kernel. This is because the modified one does not calculate mainly loop for m and ℓ including other functions (e.g., $P_\ell^m(\mu_n)$, $\sin(mw_n)$, and $\cos(mw_n)$) for a very anisotropic problem.

Acknowledgement

This work is supported by Agency for Defense Development (Contract No. UC080023GD).

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