PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)

An Approach of Super-Element Sweeping for the Solution of Neutron Transport Equation in Heterogeneous Geometry

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We describe a new solution method for the discrete ordinates equations based on super-element sweeping for 2-D and 3-D neutron transport calculations. A super-element is a unit of sweeping calculation and may consist of several heterogeneous meshes. Unlike existing S_N sweeping methods, super-element sweeping method performs sweeping calculation with point value angular fluxes of a super-element. This super-element sweeping method can treat heterogeneous geometries and it costs less computation time compared with other transport methods for heterogeneous geometry such as the method of characteristics and collision probability method. The paper provides the results of the method's applications to homogeneous and heterogeneous problems.

KEYWORDS : heterogeneous geometry, super-element sweeping

1. Introduction

In neutron transport calculations, the S_N method has been widely used with its simplicity. But its application areas are limited to the problems whose computational meshes are rectangular or triangular. For complex geometry problems including circular meshes, the method of characteristics (MOC)[1−3] and collision probability method (CPM)[4] are popular, but they take long computing times and have difficulties in directly extending to three-dimensional problems. In the even-parity transport finite element method[8] for complex geometry problems, the geometries are approximated with triangles or rectangles.

In this paper, we propose a new sweeping method which can treat heterogeneous problems while preserving simplicity of S_N. This method is different from existing S_N sweeping methods in the following viewpoints : 1) it represents angular flux in a distribution form on a super-element, which is allowed to consist of heterogeneous meshes, instead of average angular flux on a computational mesh in existing methods, 2) it works with angular fluxes at corner points instead of edge average fluxes in existing methods, 3) it marches from a super-element to an adjacent super-element in a sweeping manner similarly to the existing S_N methods.

Because we assume distributions on a super-element with heterogeneous geometry, accuracy of the solution may be lower than MOC and CPM. But calculation is much simpler than those methods and we can obtain continuous flux distributions in the entire problem domain.

In this paper, we assumed flux distribution is in bilinear form of trial functions of the finite element method (FEM)[5] type. Thus it is expected that the solution can be acceptable if flux shape is monotonic in a super-element. We also expect that use of small size super-elements and high order trial functions would provide better solution. To demonstrate efficiency and accuracy, we tested the method on a small test problem with homogeneous geometry and also on 2-D and 3-D configurations of the OECD benchmark problem C5G7 MOX[6] which has heterogeneous geometry.

2. Method

2.1 2-D Formulation

The two-dimensional within-group transport equation is given as follows :

$$\mu_n \frac{\partial \psi_{g,n}(x,y)}{\partial x} + \eta_n \frac{\partial \psi_{g,n}(x,y)}{\partial y} + \sigma_g \psi_{g,n}(x,y) = q_{g,n}(x,y), \tag{1}$$

where standard notations[7] are used. Let us consider super-element in Fig. 1 which is a unit of sweeping calculation, that as an example, consists of heterogeneous three (mixed-shape) computational meshes.

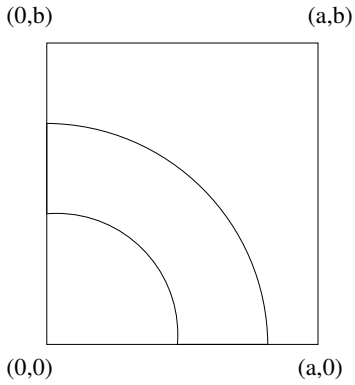

Fig. 1 Rectangular super-element with heterogeneous geometry

In this super-element, we assume angular flux distribution as follows, dropping direction and energy group indices, n and g :

$$\psi(x,y) = \sum_{i=1}^{4} f_i(x,y) p_i, \tag{2}$$

where

$$\begin{aligned} p_1 &= \psi(0,b), \\ p_2 &= \psi(0,0), \\ p_3 &= \psi(a,0), \\ p_4 &= \psi(a,b), \end{aligned} \tag{3}$$

$$\begin{aligned} f_1(x,y) &= \frac{1}{ab}(a-x)y, \\ f_2(x,y) &= \frac{1}{ab}(a-x)(b-y), \\ f_3(x,y) &= \frac{1}{ab}x(b-y), \\ f_4(x,y) &= \frac{1}{ab}xy. \end{aligned} \tag{4}$$

Eq.(2) consists of bi-linear trial functions of finite element method type in rectangular geometry. By integrating Eq.(1) over a super-element which contains N computational meshes, we obtain

$$\int_0^b dy \int_0^a dx \left(\mu \frac{\partial \psi(x,y)}{\partial x} + \eta \frac{\partial \psi(x,y)}{\partial y} + \sigma(x,y)\psi(x,y) \right) = \int_0^b dy \int_0^a dx q(x,y), \tag{5a}$$

or

$$\int_0^b dy \int_0^a dx \left(\mu \frac{\partial \psi(x,y)}{\partial x} + \eta \frac{\partial \psi(x,y)}{\partial y} \right) + \sum_{m=1}^{N} \int_{V_m} dA \sigma_m \psi(x,y) = \sum_{m=1}^{N} \int_{V_m} dA q(x,y), \tag{5b}$$

where material properties are constant in a computational mesh. Eq.(5b) can be rewritten as follows using Eq.(2) :

$$\sum_{i=1}^{4} F_i p_i = Q, \tag{6}$$

where

$$F_i = \int_0^b dy \int_0^a dx \left(\mu \frac{\partial f_i(x,y)}{\partial x} + \eta \frac{\partial f_i(x,y)}{\partial y} \right) + \sum_{m=1}^{N} \int_{V_m} dA \sigma_m f_i(x,y), \tag{7}$$

and

$$Q = \sum_{m=1}^{N} \int_{V_m} dA q(x,y). \tag{8}$$

These F values can be pre-calculated before iteration. Now sweeping calculation is possible with Eq.(6). Fig. 2 shows a schematic of the sweeping calculation for $\mu > 0, \eta > 0$.

In existing S_N sweep methods, they calculate two unknowns with two knowns, using auxiliary equations (approximate) such as diamond difference scheme (DD). In the case of DD, unknowns are obtained as follows :

$$\begin{aligned} \psi_{i+1/2,j} &= 2\psi_{ij} - \psi_{i-1/2,j}, \\ \psi_{i,j+1/2} &= 2\psi_{ij} - \psi_{i,j-1/2}, \end{aligned} \tag{9}$$

where

$$\psi_{ij} = \frac{\frac{2\mu}{\Delta x_i}\psi_{i-1/2,j} + \frac{2\eta}{\Delta y_j}\psi_{i,j-1/2} + q_{ij}}{\sigma_{ij} + \frac{2\mu}{\Delta x_i} + \frac{2\eta}{\Delta y_j}}. \tag{10}$$

In the super-element sweeping method, there are one unknown (p_4) and three knowns ($p_1,\ p_2$ and p_3). We can calculate unknown p_4 with Eq.(6) :

$$p_4 = (Q - F_1 p_1 - F_2 p_2 - F_3 p_3)/F_4. \tag{11}$$

The average angular flux of a computational mesh can then be written as follows :

$$\psi_m = \sum_{i=1}^{4} \int_{V_m} dA f_i(x,y) p_i. \tag{12}$$

This method may describe heterogeneous geometry more closely considering additional unknowns inside a geometrically complex super-element. These unknowns can be obtained by simple algebraic relations. Such a super-element may consist of several sub-elements, each "supported" by local trial functions. Fig. 3 shows a rectangular super-element that consists of four triangular sub-elements.

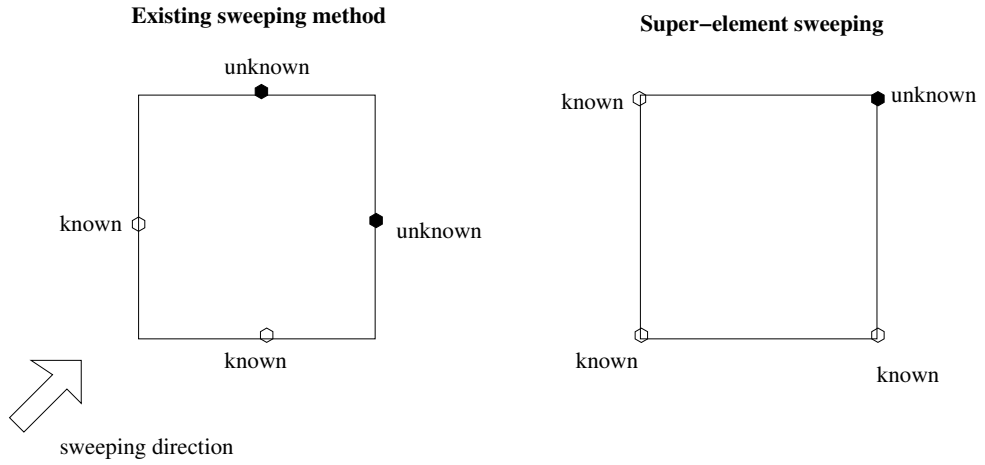

Fig. 2 Sweeping schemes of existing and super-element sweeping methods

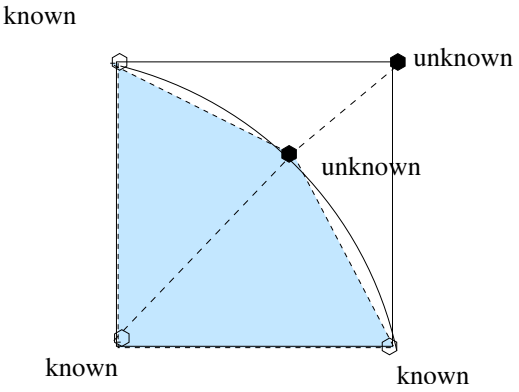

Fig. 3 Super-element with four sub-elements

2.2 3-D Formulation

In 3-D sweeping calculation, cubic form of super-element is used. The sweeping scheme is described in Fig. 4. There are 8 corner points and the angular fluxes at 7 points of them are given as incoming angular fluxes.

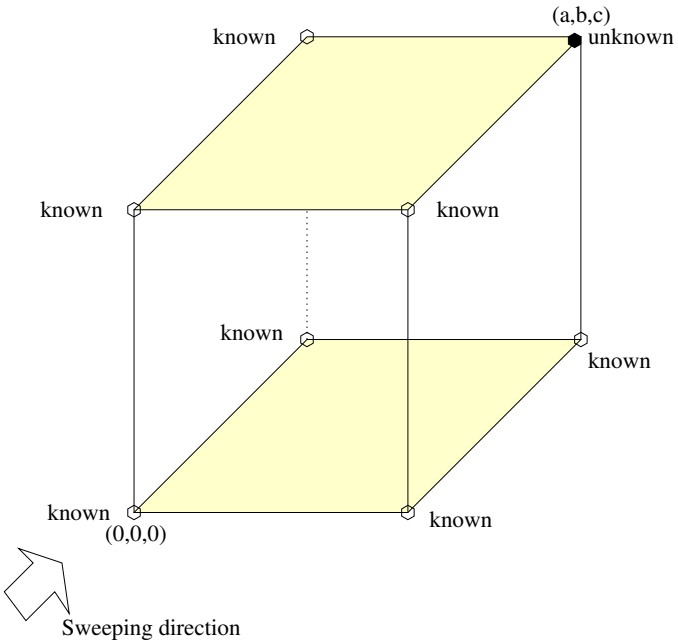

Fig. 4 Sweeping scheme for 3-D problems when $\mu,\ \eta,\ \xi\ >\ 0$
(7 knowns and 1 unknown)

We assume angular flux distribution on a super-element as follows :

$$\psi(x,y,z) = \sum_{i=1}^{8} g_i(x,y,z)p_i, \tag{13}$$

where

$$\begin{array}{c} p_1 = \psi(0,b,0),\ p_2 = \psi(0,0,0),\ p_3 = \psi(a,0,0),\ p_4 = \psi(a,b,0), \\ p_5 = \psi(0,b,c),\ p_6 = \psi(0,0,c),\ p_7 = \psi(a,0,c),\ p_8 = \psi(a,b,c), \end{array} \tag{14}$$

$$g_i(x,y,z) = \begin{cases} f_i(x,y)\dfrac{c-z}{c} & \text{if } 1 \le i \le 4 \\ \\ f_{i-4}(x,y)\dfrac{z}{c} & \text{if } 5 \le i \le 8 \end{cases} \tag{15}$$

where c is axial height of a super-element. Integrating three-dimensional within-group transport equation over super-element, we obtain the following equation by a similar procedure used in 2-D :

$$\sum_{i=1}^{8} G_i p_i = Q, \tag{16}$$

where

$$\begin{aligned} G_i = \int_0^c dz \int_0^b dy \int_0^a dx \left(\mu \frac{\partial g_i(x,y,z)}{\partial x} + \eta \frac{\partial g_i(x,y,z)}{\partial y} + \xi \frac{\partial g_i(x,y,z)}{\partial z} \right) \\ + \sum_{m=1}^{N} \int_{V_m} dV \sigma_m g_i(x,y,z), \end{aligned} \tag{17}$$

and

$$Q = \sum_{m=1}^{N} \int_{V_m} dV q(x,y,z). \tag{18}$$

Then unknown p_8 can be calculated as follows :

$$p_8 = (Q - \sum_{i=1}^{7} G_i p_i)/G_8. \tag{19}$$

The average angular flux of a computational mesh can then be written as follows :

$$\psi_m = \sum_{i=1}^{8} \int_{V_m} dV g_i(x,y,z)p_i. \tag{20}$$

3. Numerical Results

First we tested the method on a small test problem with two energy groups described in Fig. 5. Each cell has size of 1.0cm $\times$ 1.0cm. There are two types of cells and material properties are homogeneous in a cell. The material properties are listed in Table I.

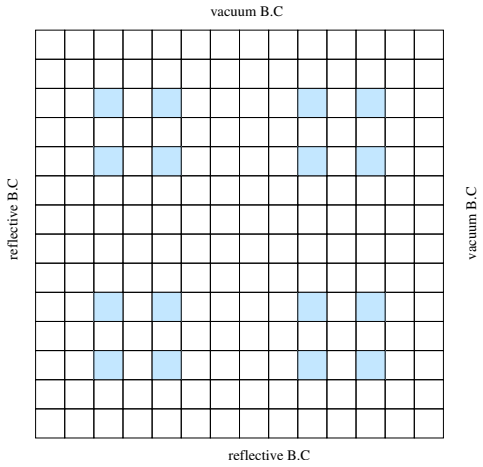

Fig. 5 Configuration of the test problem

Table 1 Material properties [cm^{-1}]

material	g	σ_t	$\nu\sigma_f$	$\sigma_{s,1\to g}$	$\sigma_{s,2\to g}$
1 (white)	1	0.2531	0.005925	0.233427	0.0000
	2	0.5732	0.098170	0.010690	0.514280
2 (shaded)	1	0.2535	0.004820	0.233793	0.0000
	2	0.5797	0.08228	0.010950	0.524960

The results are compared with those of the TWODANT code. S_{10} quadrature was selected for both calculations and each computational mesh (super-element) size is 0.5cm $\times$ 0.5cm and iteration criteria were 10^{-6} for eigenvalue and scalar flux. The results are very similar. The eigenvalues are 0.4896750 from the super-element sweeping method and 0.4896751 from the TWODANT code.

To test performance on heterogeneous problems, we chose the 2-D OECD benchmark problem C5G7 MOX (Fig. 6) that is specified in seven energy group cross sections. S_{10} quadrature was used and iteration criteria were 10^{-6} for eigenvalue and scalar fluxes. Table II shows the results.

We tested this benchmark problem in two cases as in Fig. 7. The dotted lines are boundaries of super-elements. The number of computational meshes in each cell are 8 and 24, respectively.

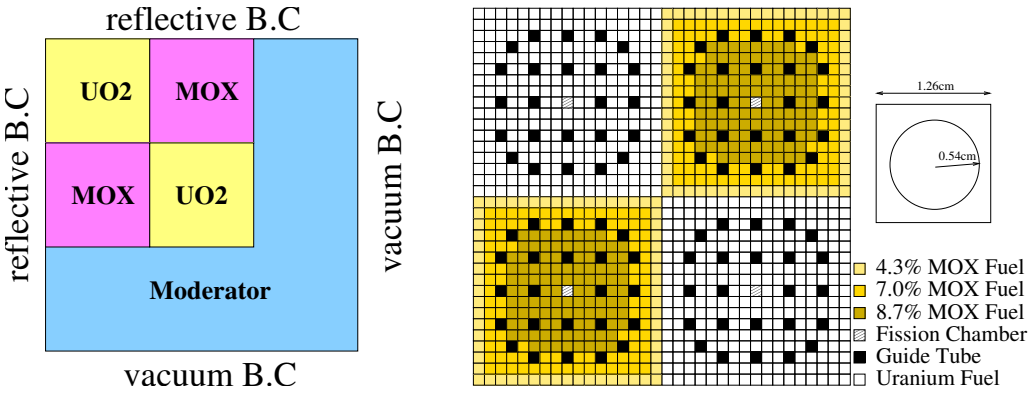

Fig. 6 Configuration of the 2-D OECD benchmark problem

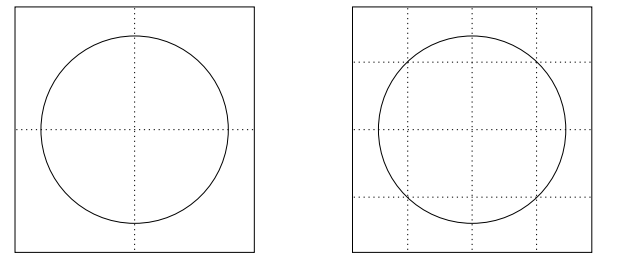

Fig. 7 Super-element configuration in a fuel cell

Table 2 Results of the OECD benchmark problem

	k_{eff}	Max./Min. pinpower	RMS error(%)
4 super-elements/cell	1.18858	2.579/0.230	1.99
16 super-elements/cell	1.18511	2.530/0.231	0.87
Reference[a]	1.18655	2.498/0.232	-

[a] Monte Carlo calculation

We found that the refined calculation provides more accurate solution as expected. But its accuracy should improve further with more refined calculation or higher order trial functions.

We also solved the 3-D OECD benchmark problem C5G7 MOX with Rodded A configuration described in Fig. 8. The detailed configurations are listed in the Ref.[6].

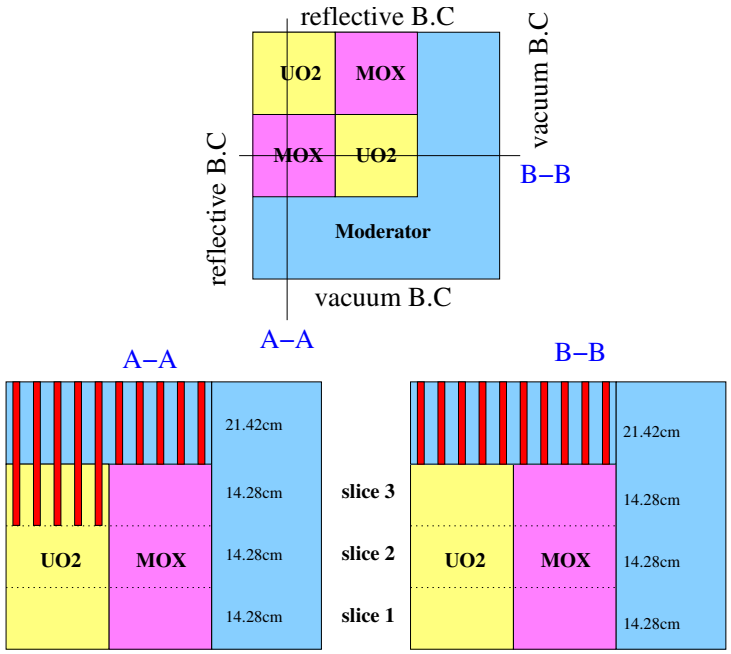

Fig. 8 Rodded A Configuration of the 3-D OECD Benchmark Problem

Table 3 shows the results of the calculation. In this calculation, we used 10^{-6} for eigenvalue and 10^{-4} for scalar flux error criteria. Super-element used has 0.63 cm $\times$ 0.63 cm radial size (4 super-elements in a cell of Fig. 7) and the height of super-element is 4.76 cm and 7.14 cm for fuel and reflector, respectively. S_8 angular quadrature was selected for this calculation.

Table 3 Results of the 3-D OECD benchmark problem

k_{eff}	1.129162 (+0.098%)			
Pin power error	slice 1	slice 2	slice 3	overall
AVG error(%)	1.651	1.735	2.430	1.552
RMS error(%)	2.000	2.071	2.868	1.865

The reference solution provided by OECD was obtained by Monte Carlo calculation. In this calculation, there are about 0.1% and 2-3% errors in k_{eff} and pinpower RMS, respectively. The order of errors are similar to those of 2-D calculation with the same radial super-element divisions. It is expected that these errors would be reduced further with more refined calculations.

4. Conclusions

A new sweeping scheme of S_N methods was developed and described in this paper. It performs sweeping calculation with angular fluxes at corner points and with a super-element which is allowed to consist of heterogeneous meshes as a unit of sweeping calculation. It assumes flux distribution in a super-element and we can obtain continuous flux distribution in the entire problem as a result of the sweeping calculation.

For the test problem with homogeneous geometry, super-element sweeping provides almost the same results compared with DD calculation. For the OECD benchmark problem of 2-D configuration with heterogeneous geometry, there are -0.12% errors for eigenvalue and 0.87% RMS errors for power distribution compared with the reference values provided by Monte Carlo calculation, when 16 super-elements per cell are used. The order of errors in 3-D calculation are similar to those of 2-D calculation.

The super-element sweeping method shows good performance in computation time, but it needs to improve accuracy. To improve accuracy, several methods are being considered. As one, we are now investigating the way to allow discontinuity at material (computational mesh) interfaces and increase the order of trial functions.

Acknowledgment

The work was supported in part by the Ministry of Science and Technology of Korea through the National Research Laboratory (NRL) Program.

References

1) N. Z. Cho and S. G. Hong, "CRX : A Transport Theory Code for Cell and Assembly Calculations Based on Characteristic Method," *Proc. International Conf. on the Physics of Reactors*, September 16-20, Mito, Japan, Vol. 1A, p.250, (1996).

2) G. S. Lee, N. Z. Cho, and S. G. Hong, "Acceleration and Parallelization of the Method of Characteristics for Lattice and Whole-Core Heterogeneous Calculations," *Proc. PHYSOR 2000*, Session II-C, May 7-11, 2000, Pittsburgh, USA (2000).

3) M. J. Halsall, "CACTUS, A Characteristics Solutions to the Neutron Transport Equations in Complicated Geometries," AEEW-R-1291, U.K. Atomic Energy Authority, (1980).

4) R. Stamm'ler, J. Casal, A. Ferri and E. Villarino., "User's Manual for HELIOS," 05DEC94, Studsvik, (1994).

5) E.B. Becker, G.F. Carey, and J.T. Oden, Finite Elements An Introduction, Volume 1, Prentice-Hall, (1981)

6) E. E. Lewis, et. al., "Expert Group on 3-D Radiation Transport Benchmarks Summary of Meeting on C5G7 MOX Benchmark," NEA/NSC/DOC (2001)17, (2001).

7) E.E. Lewis and W.F. Miller, Jr., Computational Methods of Neutron Transport, John Wiley & Sons, (1984)

8) M. A. Smith, N. Tsoulfanidis *et. al.*, "Whole-Core Neutron Transport Calculations without Fuel-Coolant Homogenization," *Proc. PHYSOR 2000*, Session II-C, May 7-11, 2000, Pittsburgh, USA, (2000).