Simulated Annealing Approach to Relaxation Optimization for Partial Current based Coarse Mesh Finite Difference Method (p-CMFD)

Chang Je Park^{a*}, Moon Ghu Park^a

^aNuclear Engineering Dept., Sejong Univ., 209 Neungdong-ro, Gwangjin-gu, Seoul 143-747, Korea *Corresponding author: parkcj@sejong.ac.kr

1. Introduction

Partial current based coarse mesh finite difference acceleration method (p-CMFD) has been widely used to accelerate the solution of neutron transport equation.[1]-[3] Relaxation of diffusion coefficient was proposed to get stable solutions of coarse mesh finite difference method (CMFD).[4][5] Relaxation parameter plays role in stabilization through over-relaxation and fast convergence through under-relaxation. In this paper, p-CMFD with the previous relaxation approach was combined and the optimal relaxation parameter approach is suggested. In the previous results, it is mostly assumed that the relaxation parameter is varied smoothly as a function of optical thickness and a simple steepest decent method is applied to get an optimal relaxation parameter. In this study, in order to obtain optimal relaxation parameter in p-CMFD relaxation method, a simple simulated annealing method[6][7] is adapted. This approach is well known to get the global optimum by jumping out local optimums quickly through iterative cooling and search steps. Thus the simulated annealing optimization has been widely used around various engineering applications and lots of tools are developed and it is easily obtained and applicable, too. In this study, a simple MATLAB tool is used and the minimal relaxation parameter is expressed as a function of independent parameter of optical thickness. And the simple slab test problem is chosen of which the scattering ratio is fixed as 0.99.

2. p-CMFD Formula with Relaxation

The high order discrete equation of a slab geometry with diamond differencing method is given as follows.

$$\mu_n \frac{\psi_{k+1/2}^{(+1/2)} - \psi_{k-1/2}^{(+1/2)}}{h} + \sigma \frac{\psi_{k+1/2}^{(+1/2)} + \psi_{k-1/2}^{(+1/2)}}{2} = \sigma_s \phi_k^l + Q, \tag{1}$$

$$\phi_k^{l+1/2} = \frac{1}{2} \sum_{n=1}^N w_n \frac{\psi_{k+1/2}^{l+1/2} + \psi_{k-1/2}^{l+1/2}}{2}.$$
 (2)

Where l is an iteration index and others are typical notations are used. The low order partial current based coarse mesh finite difference equation is given as

$$J_{i+1/2}^{l+1/2} = \frac{1}{2} \sum_{n=1}^{N} w_n \ \mu_n \ \psi_{n,i+1/2}^{l+1/2} \ . \tag{3}$$

$$J_{i+1/2}^{+,l+1/2} = \frac{1}{2} \sum_{n=1}^{N/2} w_n \mid \mu_n \mid \psi_{n,i+1/2}^{l+1/2} .$$
⁽⁴⁾

$$J_{i+1/2}^{-l+1/2} = \frac{1}{2} \sum_{n=N/2+1}^{N} w_n \mid \mu_n \mid \psi_{n,i+1/2}^{l+1/2}$$
 (5)

$$J_{i+1/2}^{+,l+1/2} = \frac{-\widetilde{D}_{i+1/2} \left(\phi_{i+1}^{l+1/2} - \phi_{i}^{l+1/2} \right) + 2 \hat{D}_{i+1/2}^{l+1/2,+} \phi_{i}^{l+1/2,+}}{2}$$
(6)

$$J_{i+1/2}^{-,i+1/2} = \frac{\widetilde{D}_{i+1/2}\left(\phi_{i+1}^{i+1/2} - \phi_{i}^{i+1/2}\right) + 2\hat{D}_{i+1/2}^{i+1/2} - \phi_{i+1}^{i+1/2}}{2}$$
(7)

$$\hat{D}_{i+1/2,+}^{l+1/2,+} = \frac{2J_{i+1/2}^{+,l+1/2} + \widetilde{D}_{i+1/2}(\phi_{i+1}^{l+1/2} - \phi_{i}^{l+1/2})}{2\phi_{i}^{l+1/2}},$$
(8)

$$\hat{D}_{i+1/2}^{l+1/2,-} = \frac{2J_{i+1/2}^{-,l+1/2} - \widetilde{D}_{i+1/2}(\phi_{i+1}^{l+1/2} - \phi_i^{l+1/2})}{2\phi_{i+1/2}^{l+1/2}},$$
(9)

The relaxations applied to diffusion coefficients are provided such as

$$\hat{D}_{i+1/2}^{l+1,+} = \theta \; \hat{D}_{i+1/2}^{l+1/2,+} + (1-\theta) \hat{D}_{i+1/2}^{l,+}, \tag{10}$$

$$\hat{D}_{i+1/2}^{l+1,-} = \theta \, \hat{D}_{i+1/2}^{l+1/2,-} + (1-\theta) \hat{D}_{i+1/2}^{l,-}, \tag{11}$$

The final form of p-CMFD equation with relaxation is

$$\begin{split} &-\widetilde{D}_{i+1/2} \left(\phi_{i+1}^{l+1} - \phi_{i}^{l+1} \right) - (\hat{D}_{i+1/2}^{l+1} - \phi_{i+1}^{l+1} - \hat{D}_{i+1/2}^{l+1} + \phi_{i}^{l+1}) \\ &+ \widetilde{D}_{i-1/2} \left(\phi_{i}^{l+1} - \phi_{i-1}^{l+1} \right) + (\hat{D}_{i-1/2}^{l+1} - \phi_{i}^{l+1} - \hat{D}_{i-1/2}^{l+1} + \phi_{i-1}^{l+1}) \\ &+ h_{i} (\sigma_{i} - \sigma_{si}) \phi_{i}^{l+1} = h_{i} q_{i} . \end{split}$$
(12)

Our main concern is to optimize the relaxation parameter θ in Eqs. (10) and (11).

3. Parameter Optimization with Simulated Annealing for p-CMFD relaxation

The proposed test problem is a slab problem with vacuum boundary conditions on both sides. The scattering ratio is fixed and the description is given in Fig. 1.

Vacuum
$$Q=1.0 \ \#/cm^3 \ sec$$
 Vacuum $\sigma=1 \ cm^{-1} \ c = \sigma_s/\sigma$ Vacuum

Fig. 1. Description of a test problem.

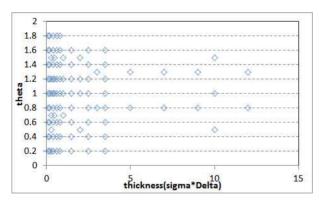
Diamond differencing (DD) scheme is used for spatial discretization and S-16 Gauss-Legendre quadrature set is chosen. The convergence criterion of 1E-9 for the maximum point-wise scalar flux is given.

Table I shows the numerical spectral radius and number of iterations for various optical thickness and relaxation parameters when the coarse mesh ratio (p) is 4. Various cases are tested relaxation data and optic thicknesses are provided in Fig. 2. By utilizing these data, a typical simulated annealing approached is applied and around 30 simulated results are obtained when optical thickness is fixed between 0.1 and 1.0 for simplicity. The minimum valued of relaxation parameter is obtained around 1.2 when the optical thickness lies around 0.1. If the optical thickness range is extended to whole range, the optimal value of relaxation parameter is about 1.19 and its spectral radius is obtained about 0.04 for sufficiently small optical thickness. This trend goes well with natural behaviors in the numerical simulation as shown in Fig.2 (d). However, the simulated annealing results are significantly dependent of the collecting data. More reliable and randomly distributed data will provide more confident results through simulated annealing tests. The various results of simulated annealing test are tabulated in Table II.

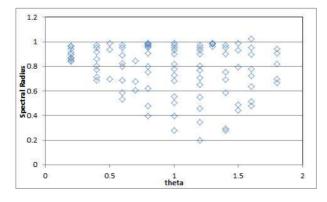
Table I: Number of Iterations and Numerical Spectral
Radius for Various Optical Thicknesses (p=4)

- 1	Scattering ratio(c) = 0.9				
σΔ	SI ^a	θ=0.8	θ=1	θ=1.2	
0.1	12 ^b (0.168) ^c	20(0.367)	15(0.243)	12(0.177)	
1	11(0.179)	55(0.737)	54(0.735)	54(0.736)	
10	10(0.171)	132 (0.928)	132 (0.892)	132 (0.892)	
- 1	Scattering ratio(c) = 0.99				
σΔ	SI	θ=0.8	$\theta = 1$	θ=1.2	
0.1	126(0.861)	22(0.395)	16(0.276)	13(0.197)	
1	1269 (0.987)	92(0.836)	85(0.821)	80(0.805)	
10	1604 (0.989)	983 (0.987)	983 (0.987)	983 (0.987)	

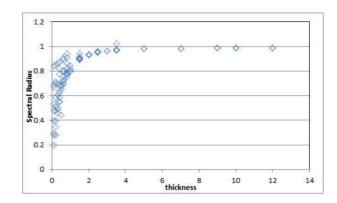
^a Source iteration, ^b Number of iteration, ^cNumerical spectral radius



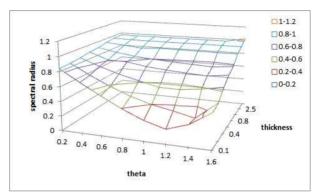
(a) Data set of optical thickness and relaxation parameter



(b) Data set of relaxation parameter and spectral radius



(c) Data set of optical thickness and spectral radius.



- (d) Spectral radius behavior for various optical thicknesses and relaxation parameters
- Fig. 2. Convergence data for p-CMFD relaxation for various relaxation parameters and optical thicknesses.

Table II: Simulated Results of Annealing Method for Various Relaxation Data and Optical Thickness

Index	Optical Thickness	theta	Spectral radius
1	0.100239	1.19198	0.241487
2	0.101106	1.20676	0.241766
3	0.100103	1.20922	0.241169
4	0.100885	1.21105	0.241686
5	0.100158	1.18711	0.241692
6	0.100179	1.20255	0.241188
7	0.1009	1.20233	0.24164
8	0.100366	1.20083	0.241321
9	0.100342	1.20292	0.241287
10	0.1004	1.19538	0.241461
11	0.10057	1.19006	0.241785
12	0.100058	1.20494	0.241106
13	0.10009	1.21017	0.241177
14	0.100659	1.21163	0.241559
15	0.100086	1.21058	0.241182
16	0.100212	1.20244	0.241209
17	0.100049	1.20919	0.241135
18	0.100377	1.19253	0.24155
19	0.100697	1.21481	0.241672
20	0.100292	1.20803	0.24127
21	0.101272	1.21063	0.241919
22	0.10032	1.21742	0.241541

23	0.100192	1.20326	0.241192
24	0.100042	1.19714	0.241189
25	0.100929	1.21619	0.241865
26	0.100751	1.20679	0.241544
27	0.101098	1.20492	0.241754
28	0.101313	1.20248	0.241898
29	0.101129	1.21655	0.242003
30	0.100472	1.21584	0.24157
min	0.100058	1.20405	0.241106
Global min	1.841E-05	1.19845	0.043158

4. Conclusions

The partial current based coarse mesh finite differencing rebalancing method (p-CMFD) with relaxation approach is applied in this study. In order to optimize the relaxation parameter in a slab geometry problem, the typical simulated annealing method is taken into consideration. The general convergence trend is obtained from the analysis results based on various optical sizes and relaxation parameters. The optimum of relaxation parameter for the optical thickness of 0.1 is about 1.2 from the simulated annealing analysis, which is very consistent with the numerical test results.

For the further analysis, the linearization and Fourier convergence analysis will be carried out. The analytical form of spectral radius will be expressed in a matrix form and its results will verify the simulated results in this study soon.

The relaxed p-CMFD method will be extended scalar flux, too. Although the optimal value is sensitively depending on the scattering ratio and problem geometry, it is of interest to reduce tedious computing work based on the advanced computational tool such as the simulated annealing method.

REFERENCES

[1] N.Z. Cho, C.J. Park., "A Comparison of Coarse Mesh Rebalance and Coarse Mesh Finite Difference Accelerations for the Neutron Transport Calculations," *Int. Conf. Nuclear Mathematical and Computational Sciences (M&C 2003)*, (2003).

[2] N.Z. Cho, G.S. Lee, C.J. Park, "Partial Current-Based CMFD Acceleration of the 2D/1D Fusion method for 3D Whole-Core Transport Calculations," *Trans. Am. Nucl. Soc.* (2003, submitted); see also "On a New Acceleration Method for 3D Whole-Core Transport Calculations," *Proceedings of* 2003 Annual Meeting of the Atomic Energy Society of Japan, Volume II, pp. 14-15, March 27-29, 2003, Sasebo, Japan.
[3] N.Z. Cho, "The Partial Current-based CMFD (p-CMFD) Method Revisited", *Transactions of the Korean Nuclear* Society Autumn Meeting Gyeongju, Korea, October 25-26, 2012

[4] M. Jarrett, B. Kelly, B. Kohunas, T. Downar, E. Larsen, "Stabilization Methods for CMFD Acceleration", *M&C and SNA Joint Conf. 2015, Nashville, TN, April 19-23 (2015).*[5] M. Jarrett, B. Kelly, B. Kohunas, T. Downar, E. Larsen, "Stabilization Methods for CMFD Acceleration", *M&C and SNA Joint Conf. 2015, Nashville, TN, April 19-23 (2015).* [6] D.J. Lee, T.J. Downar, Y.H. Kim, "Convergence Analysis of the Nonlinear Coarse Mesh Finite Difference Method for One dimensional Fixed Source Neutron Diffusion Problem," Nucl. Sci. Eng., Vol. 147, No.2, June, 2004.

[7] W.L. Goffe, "Global Optimization of Statistical Functions with Simulated Annealing," J. Econometrics. p.60,1994.
[8] H.C. Shin, M.G. Park, S.T. Yang, K.H. Rho, S.R. Moon,

S.K. Hong, "Locally Optimal Solution of Robust Ex-core Detector Response using Constrained Simulated Annealing," Nucl. Eng. Des. Vol. 239, No.1, p.51, January, 2009.