ACCELERATION OF RESPONSE MATRIX METHOD BY CROSS SECTION SCALING

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ABSTRACT

In this paper, a new acceleration scheme for the red-black response matrix iteration is proposed. The proposed method is easy to apply not only to newly developed codes but also to existing codes; cross section sets are input by multiplying by a scaling factor, without requiring code modification. The proposed method is called the cross-section scaling acceleration (CSA) method and is applicable to accelerating inner iteration of the response matrix calculation of second-order partial differential equations (e.g. diffusion, simplified Pn and Pn). An eigenvalue analysis of the proposed method was carried out for one-group homogeneous problems. The analysis showed that the maximum eigenvalue of the red-black response matrix strongly depends on the scaling factor, and that the convergence of iteration becomes faster when an appropriate scaling factor is used. The CSA method was also used for three test problems that cover a wide range of applications: a simple one-group, one-dimensional problem, a multi-group PWR assembly problem, and a more realistic multi-group PWR quarter core problem. The calculation results of the test problems showed that the number of iterations can be reduced from 30% to 80% by utilizing the CSA method. The relationship between the CSA method and the discontinuity factor is also discussed in this paper.

1. INTRODUCTION

In this paper, a new acceleration scheme for response matrix calculation is proposed. The method can be easily applied to existing calculation codes, simply by multiplying by a scaling factor to input cross sections. The proposed scheme is called the cross-section scaling acceleration (CSA) method and it can be used to accelerate the inner iteration of response matrix calculations.

In general, the coarse mesh rebalance and extrapolation method is commonly used for accelerating response matrix calculations[1]. However, the successive over relaxation (SOR) method, which is a common acceleration technique for iterative calculations, cannot be applied to response matrix calculations since sound convergence is not guaranteed and may cause divergent results[2]. Lewis and Palmiotti proposed a scheme for accelerating response matrix calculations by introducing ideal partial currents to overcome this difficulty[2]. Their method is applicable for general transport theory and is quite effective. However, application to existing codes requires some implementation work since the iteration matrix must be modified.

The CSA method proposed in this paper is effective for second order partial differential equations (e.g. diffusion, simplified Pn and Pn) and its application is much easier since no code modification is necessary. Therefore, the CSA method has extensive applicability to the existing codes.

2. BASIC CONCEPT OF THE CSA METHOD

Zika and Downar carried out a study on numerical instability that appeared during iteration of the response matrix with large discontinuity factors[3]. Their study showed that utilization of unbounded discontinuity factors might cause divergence both in the inner and the outer iterations of response matrix calculations. In other words, the spectrum property of an iteration matrix is affected by discontinuity factors. Therefore, by making use of this point, the spectrum property of an iteration matrix can be controlled by discontinuity factors; this is the underlying concept of the CSA method.

We consider two different diffusion equations for a one-group, one-region problem:

$$-D\nabla^2 f + \Sigma_a f = \frac{1}{k} n\Sigma_f f \tag{1}$$

$$-Df\nabla^2 f + \Sigma_a ff = \frac{1}{k} n\Sigma_f ff \tag{2}$$

Equation (2) is obtained by multiplying the cross sections in Eq. (1) by a scaling factor f. Note that Eq. (2) can also be derived by assuming the discontinuity factor of this region to be $1/f$.

In the mathematical sense, Eqs. (1) and (2) are equivalent; these equations provide the same eigenvalue. Actually, if the above two diffusion equations are solved with a finite-difference type diffusion code which does not treat partial current (e.g. CITATION), the iteration process and converged eivenvalue are the same if the numerical truncation error is not taken into account.

Contrary to this, if the above two equations are solved with a response matrix diffusion code, convergence processes are generally different even though converged eigenvalues are the same. In other words, the convergence property of a response matrix can be controlled by multiplying the cross sections by a scaling factor in the diffusion equation. In the previous studies (e.g. Ref.[4]) the scaling factors for cross section were used for different purposes, i.e. reduction of homogenization error. For this purpose, different scaling factors should be used for different regions. On the other hand, the same scaling factor is applied for all regions in the CSA method to accelerate convergence. Therefore, the method and purpose of applying the scaling factor are different from those of the previous studies.

2. APPLICATION OF THE CSA METHOD

Application of the CSA method can be summarized as follows:

(1) Multiply a scaling factor or scaling factors to input cross sections as follows. The scaling factor can be group dependent, but the same scaling factor should be applied to whole regions within the same group:

$$\begin{aligned} &D_g f_g \\ &\Sigma_{a,g} f_g \\ &n\Sigma_{f,g} f_g \\ &\Sigma_{s,g'\to g} f_g \end{aligned} \tag{3}$$

(2) Performs iteration calculations.

Since cross sections are multiplied by the scaling factor, power normalization should be performed carefully by taking into account the multiplied scaling factor.

If an albedo boundary condition is used, the albedo values should be modified. The relationship between incoming and outgoing partial currents at the albedo boundary is expressed as follows using diffusion theory:

$$J_g^{in} = a_g J_g^{out} = \left(\frac{1-2C_g}{1+2C_g} \right) J_g^{out} \tag{4}$$

where,

J_g^{in} : incoming partial current of group g,

J_g^{out} : outgoing partial current of group g,

a_g : albedo value

$C_g = -\frac{D_g}{f_g}\frac{df_g}{dx}$: extrapolated constant of group g.

From Eq. (4), the extrapolated constant is expressed as follows:

$$C_g = \frac{1-a_g}{2(1+a_g)} \tag{5}$$

When the scaling factor is applied to the cross sections, extrapolated value C_g should be multiplied by the scaling factor f_g since it is proportional to the diffusion coefficient. By substituting Eq. (5) multiplied by f_g into Eq. (4), the following equation is obtained:

$$a_g' = \frac{(1-f_g)+(1+f_g)a_g}{(1+f_g)+(1-f_g)a_g} \tag{6}$$

where,

a_g' : the albedo value with scaling factor f_g.

In the case of the reflective boundary condition, the value of Eq. (6) is always 1 since α_g=1. Therefore, no modification is necessary for the albedo value in the case of the reflective boundary condition.

3. EIGENVALUE ANALYSIS

In order to evaluate the basic behavior of the CSA method, eigenvalue analysis was carried out for a one-group homogeneous problem in infinite slab geometry assuming the following conditions:

- Red-black sweep
- Periodic boundary condition
- Total cross section: $\frac{1}{3D} = \Sigma_t = 2.0$ (1/cm)
- Scattering ratio: $\frac{(1-\Sigma_a)}{\Sigma_t} = c = 0.9, 0.99, 0.999$
- Mesh width: $\Delta h = 1.0$ (cm)

- Transmission and reflection probabilities for partial currents were analytically evaluated using diffusion theory.

The relationships between partial currents in the red and black node are expressed as follows (Fig. 1):

$$\begin{aligned}
J_1^+ &= r_r J_1^- + t_r J_2^- + q_r \\
J_2^+ &= r_r J_2^- + t_r J_1^- + q_r \\
J_3^+ &= r_b J_3^- + t_b J_4^- + q_b \\
J_4^+ &= r_b J_4^- + t_b J_3^- + q_b \\
J_1^- &= J_4^+ \\
J_2^- &= J_3^+ \\
J_3^- &= J_2^+ \\
J_4^- &= J_1^+
\end{aligned} \tag{7}$$

where,

r_r, r_b : reflection probability for red and black node

t_r, t_b : transmission probability for red and black node

q_r, q_b : source term for red and black node.

The reflection and transmission probabilities are given as follows:

$$\begin{aligned}
r &= \frac{\left(-1+e^{2\Delta h/L}\right)\left(-4D^2+L^2\right)}{-(-2D+L)^2+e^{2\Delta h/L}(2D+L)^2} \\
t &= \frac{8DLe^{2\Delta h/L}}{-(-2D+L)^2+e^{2\Delta h/L}(2D+L)^2}
\end{aligned} \tag{8}$$

where,

$$L = \sqrt{\frac{D}{\Sigma_a}} = \frac{1}{\Sigma_t\sqrt{3(1-c)}}.$$

Equation (7) can be written in the red-black iteration form as follows:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} J_1^+ \\ J_2^+ \\ J_3^+ \\ J_4^+ \end{bmatrix}^l = \begin{bmatrix} r_r & t_r & 0 & 0 \\ t_r & r_r & 0 & 0 \\ 0 & 0 & r_b & t_b \\ 0 & 0 & t_b & r_b \end{bmatrix} \begin{bmatrix} J_1^- \\ J_2^- \\ J_3^- \\ J_4^- \end{bmatrix}^l + \begin{bmatrix} q_r \\ q_r \\ q_b \\ q_b \end{bmatrix} \tag{9}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} J_1^- \\ J_2^- \\ J_3^- \\ J_4^- \end{bmatrix}^{l+1} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} J_1^+ \\ J_2^+ \\ J_3^+ \\ J_4^+ \end{bmatrix}^l \tag{10}$$

where,

l: number of iterations.

By substituting Eq. (9) into Eq. (10), we obtain the following equations:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} J_1^- \\ J_2^- \\ J_3^- \\ J_4^- \end{bmatrix}^{l+1} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} r_r & t_r & 0 & 0 \\ t_r & r_r & 0 & 0 \\ 0 & 0 & r_b & t_b \\ 0 & 0 & t_b & r_b \end{bmatrix} \begin{bmatrix} J_1^- \\ J_2^- \\ J_3^- \\ J_4^- \end{bmatrix}^{l} + \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} q_r \\ q_r \\ q_b \\ q_b \end{bmatrix}. \quad (11)$$

The partial in-currents in Eq.(11) can be written as $J^- = \hat{J}^- + e$, where $\hat{J}^-$ is the converged true solution and e is the residual error. By substituting it into Eq. (11), the iteration matrix for residual error of partial currents is written as follows:

$$\begin{bmatrix} 0 & 0 & t_b & r_b \\ 0 & 0 & r_b & t_b \\ t_r & r_r & 0 & 0 \\ r_r & t_r & 0 & 0 \end{bmatrix}. \quad (12)$$

Consequently, the maximum eigenvalue of Eq. (12) dominates the convergence rate of the red-black response matrix iteration.

The evaluated maximum eigenvalue (i.e. the spectrum radius) under the above condition is shown in Fig. 2. From Fig. 2, the maximum eigenvalue strongly depends on the scaling factor. In other words, the convergence of the red-black response matrix calculation can be accelerated by the scaling factor.

The optimum scaling factor under the above condition is obtained when r_r=r_b=0. By applying it into Eq.(8), we obtain the following relation.

$$\left(-4D^2 + L^2\right) = 0 \quad (13)$$

When the scaling factor f is applied to Eq.(13), Eq.(13) becomes:

$$\left(-4(Df)^2 + L^2\right) = 0 \quad (14)$$

From Eq.(14), the optimum scaling factor is derived as follows:

$$f = \sqrt{\frac{3}{4(1-c)}} \quad (15)$$

where,

$$c = \frac{(1-\Sigma_a)}{\Sigma_t}.$$

For actual application, an optimum scaling factor for multi-group, multi-dimensional problems will be desired. However, analytical derivation of an optimum scaling factor for such conditions may be too complicated; this problem is left for further investigation.

4. VERIFICATIONS

4.1 ONE-GROUP SLAB PROBLEM

The CSA method is applied to three test problems to verify its efficiency. The first one is a simple one-group homogeneous slab problem with the following calculation conditions:

- Thickness of the slab: 63cm,
- Mesh width: 1.26cm,
- Vacuum boundary condition for both sides. i.e., set incoming partial currents to be 0.0,
- Cross sections: $D = 1/3$, $\Sigma_a = 0.01$, $n\Sigma_f = 0.01$,
- Scaling factor: f=1.0, 2.0, 5.0, 8.7, 10.0, 20.0,
- Eigenvalue calculation.

From Eq. (15), the optimum scaling factor for this problem is about 8.7 since scattering ratio c is 0.99. Calculations were performed by the MOSRA-light code, which is an advanced nodal diffusion code using response matrix method[5].

Calculation results are shown in Table I. Table I shows that total number of inner iterations strongly depends on the scaling factor. The number of iterations with the optimum scaling factor becomes about one-fifth of no-acceleration case (i.e. when the scaling factor is 1.0).

4.2 MULTI-GROUP PWR ASSEMBLY PROBLEM

The second one is a multi-group PWR assembly problem with the following calculation conditions:

- Single 17x17 PWR assembly,
- Two dimensions,
- ^{235}U enrichment of 4.1wt%,
- Nine-energy group with upscattering (fast 6 groups, thermal 3 groups),
- 1x1 mesh per fuel cell,
- Scaling factor: f=1.0, 1.5, 2.0, 2.5, 3.0, 4.0, 5.0, and
- Reflective boundary condition.

Calculations were performed using the SCOPE2 code, which is a multi-dimensional, multi-group diffusion/transport code for fine mesh core calculations developed by NFI [6],[7],[8]. The SCOPE2 code utilizes red-black response matrix iterations, including feedback effects due to moderator temperature, fuel temperature, Xe density and so on. Finite-difference diffusion theory is used for this calculation.

Calculation results are shown in Table II. From Table II, a reduction in the total number of inner iterations of about 30% was found in this case.

4.3 MULTI-GROUP PWR QUARTER CORE PROBLEM

The third one is a realistic multi-group PWR quarter core problem with the following calculation conditions:

- Two-dimensional quarter core,

- Initial core without burnup,
- Three enrichment loadings (2.0wt%, 3.5wt%, 4.1wt% ^{235}U) as shown in Fig. 3,
- Nine-energy group with upscattering (fast 6 groups, thermal 3 groups),
- Pin-by-pin fine mesh calculation - 1x1 to 2x2 mesh per fuel cell,
- Scaling factor: f=1.0, 1.5, 2.33, 4.0, 9.0,
- Reflective boundary condition, and
- Consideration of feedback effects (e.g. boron concentration search, moderator and fuel temperature change).

The SCOPE2 code was also used in this problem. Finite difference diffusion theory was adopted in this calculation.

The calculation results are summarized in Table III and the behavior of the maximum residual of neutron flux during convergence is shown in Fig. 4. From Table III, the total number of outer iterations reduced as the scaling factor increased in this case. When the scaling factor is 90, the number of total outer iterations is about one third that of the non-accelerated case (i.e. the scaling factor is 1.0). When the scaling factor was larger than 9, the convergence gradually became unstable.

CONCLUSIONS

In this paper, the CSA (cross-section scaling acceleration) method, which is a scheme for accelerating the response matrix calculation, is newly proposed. Application of the CSA method to existing codes is easy since it is necessary merely to multiply the input cross sections by the scaling factor.

The effectiveness of the CSA method was verified by eigenvalue analysis of an iteration matrix and three test problems. The test problems covered a broad range of applications, from simple one-dimensional slab geometry to more realistic PWR assembly and quarter core problems.

The calculation results showed that the convergence rate of the response matrix calculation is improved by the CSA method, thus confirming the effectiveness of the proposed method.

Since the convergence rate by the CSA method greatly depends on the scaling factor, the optimum factor is important for general applications. Though the optimum scaling factor for a simple problem (e.g. one-group homogeneous problem) can be analytically derived, the factor for more complicated problems (e.g. multi-group, multi-dimensional problems) is currently obtained by sensitivity analyses. Therefore, further investigations on the optimum scaling factor for complex problems are desired.

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REFERENCES

1. K. L. Derstine, “DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite-Difference Diffusion Theory Problems," ANL-82-64 (1984).

2. E.E.Lewis and G. Palmiotti, "Red-Black Response Matrix Acceleration by Transformation of Interface Variables," Nucl. Sci. Eng., **130**, 181 (1998).
3. M.Zika and T. Downar, "Numerical Divergence Effects of Equivalence Theory in the Nodal Expansion Method," Nucl. Sci. Eng. **115**, 219 (1993).
4. K. Koebke, H. Haase, L. Hetzelt and H.-J. Winter, "Application and Verification of the Simplified Equivalence Theory for Burnup States," Nucl. Sci. Eng., **92**, 56, (1986).
5. K. Okumura, "MOSRA-Light; High-Spped Three Dimensional Nodal Diffusion Code for Vector Computers," JAERI-Data/Code 98-025, JAERI, (1998) [in Japanese].
6. M. Tatsumi and A. Yamamoto, "Advanced Reactor Core Analysis by the Object-oriented 3-D Fine Mesh Transport Calculation on Parallel/Distributed Environment," Proc. Int. Conf. Mathematical and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications (M&C '99), Madrid, Spain, Sep. 1999, **Vol. 2**, p.1288 (1999).
7. M. Tatsumi and A. Yamamoto, "Object-Oriented Three-Dimensional Fine-Mesh Transport Calculation on Parallel/Distributed Environments for Advanced Reactor Core Analyses," Nucl. Sci. Eng. **141**, p.1 (2002).
8. M. Tatsumi and A. Yamamoto, "SCOPE2: Object-Oriented Parallel Code for Multi-Group Diffusion/Transport Calculations in Three-dimensional Fine-Mesh Reactor Core Geometry," submitted to Physor2002, (2002).

Table I. Calculation results of the MOSRA-light code for the one-group slab problem

Scaling factor	1 (no-accel.)	2	5	8.7 (opt. accel.)	10	20
K-effective	0.9263	0.9263	0.9263	0.9263	0.9263	0.9263
Total number of inner iterations	1254	586	289	264	269	271

Table II. Calculation results of the SCOPE2 code for the multigroup PWR assembly problem

Scaling factor	1 (no accel.)	1.5	2	2.5	3	4	5
K-effective	1.2726	1.2726	1.2726	1.2726	1.2726	1.2726	1.2726
Total number of inner iterations	51	38	37	44	51	60	71

Table III. Calculation results of the SCOPE2 code for the two-dimensional PWR quarter core problem

Scaling factor	1 (no-accel.)	2	2.33	4	9
Total number of outer iterations	432	345	281	230	164
Critical boron concentration(ppm)	1711.6	1711.6	1711.6	1711.6	1711.6

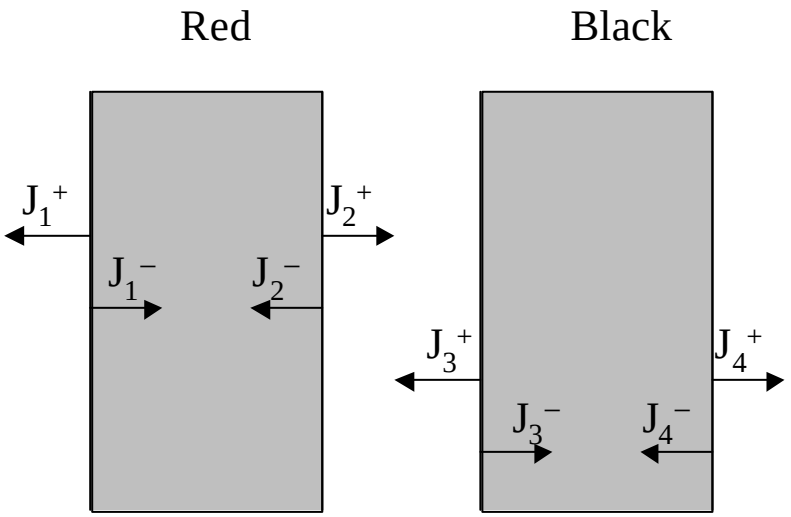

Figure 1. Configuration for eigenvalue analysis

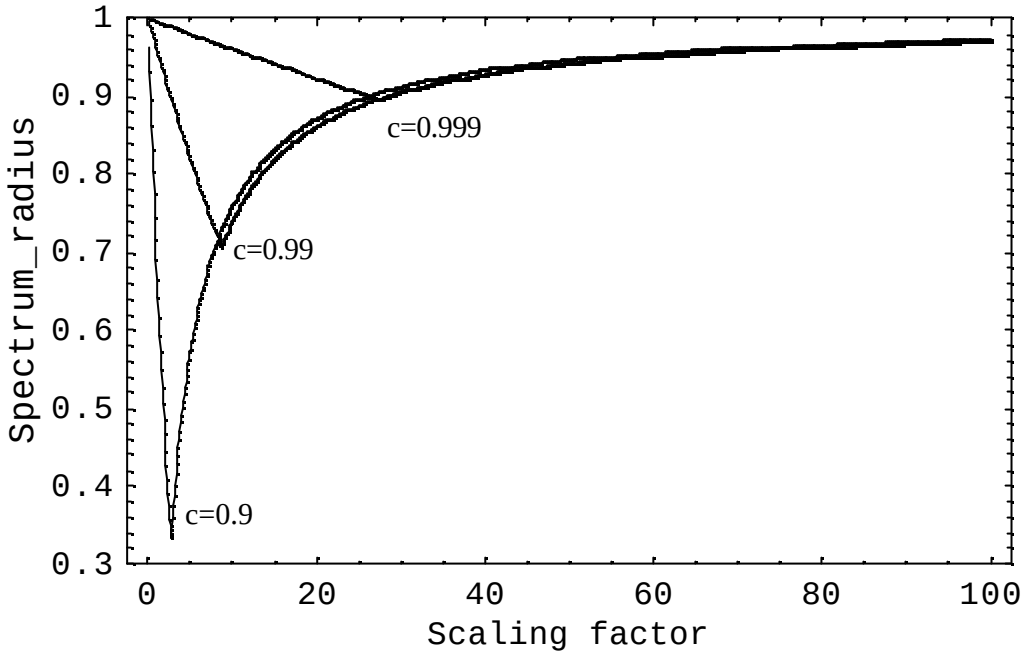

Figure 2. Scaling factor versus spectrum radius in one-group homogeneous slab geometry

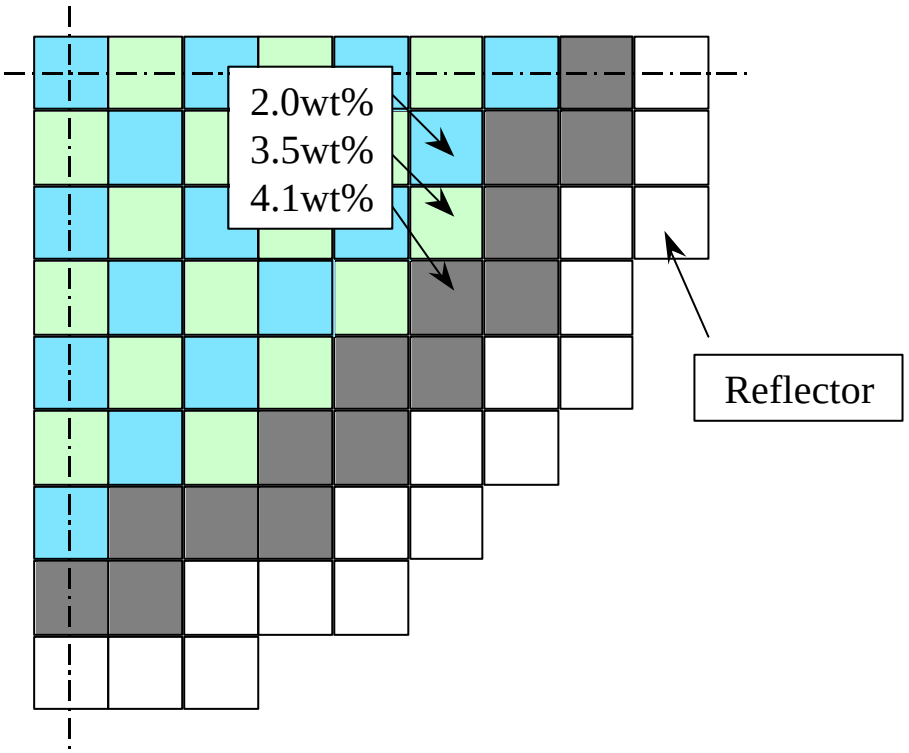

Figure 3. Geometry of multi-group two-dimensional PWR quarter-core problem

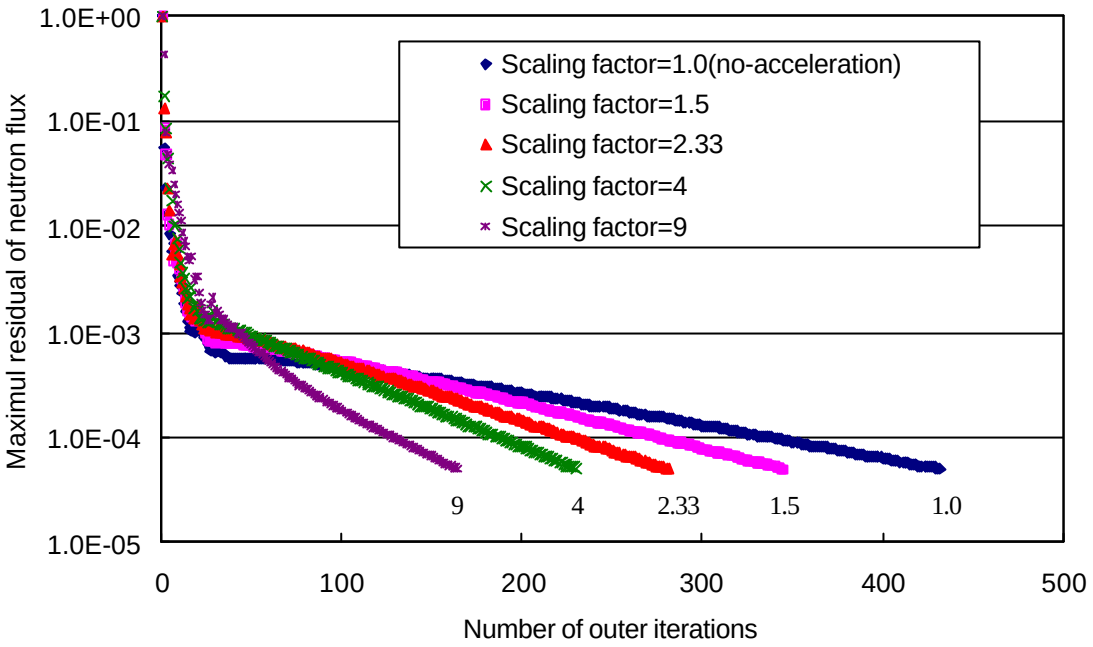

Figure 4. Convergence status of the PWR quarter-core problem