A Local Adaptive Coarse-Mesh Nonlinear Diffusion Acceleration Scheme for Neutron Transport Calculations

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Abstract — In order to improve the effectiveness and stability of the coarse-mesh finite difference method (CMFD), we developed a new nonlinear diffusion acceleration scheme for solving neutron transport equations. This scheme, called LR-NDA, employs a local refinement approach on the framework of CMFD by solving a local boundary value problem of the scalar flux on the coarse-mesh structure to replace the piecewise constant scalar flux obtained by CMFD. The refined flux is then used to update the scalar flux in the neutron transport source iteration. In this paper, a detailed convergence study of LR-NDA is carried out based on a two-dimensional fixed-source problem, and it shows that LR-NDA is much more effective and stable than CMFD for a wide range of optical thicknesses. In addition, we demonstrate that LR-NDA is a local adaptive method. LR-NDA does not necessarily require local refinement for all the coarse-mesh cells on the problem domain, i.e., it can be used only for relatively optically thick regions where the standard CMFD scheme would encounter the convergence problem.

Keywords — Neutron transport, CMFD, LR-NDA.

Note — Some figures may be in color only in the electronic version.

I. INTRODUCTION

The numerical solution of the neutron transport equation often requires acceleration techniques to improve its computational efficiency. Various acceleration methods have been developed in the last two decades.1–5 Of these methods, the coarse-mesh finite difference (CMFD) has become one of the most popular methods due to its efficiency and simplicity. However, various numerical and theoretical results show that CMFD will become unstable for problems with large optical thickness.

There exist a number of stabilization techniques to improve the stability of CMFD. For example, an ad-hoc technique5 with an underrelaxation factor applied on the drift flux term is used to stabilize CMFD. However, an issue with this technique is that the convergence will deteriorate or even fail if a nonoptimal underrelaxation factor is used. Reference 4 introduced a linear prolongation from two neighboring coarse-mesh cells instead of the flat prolongation approach utilized in the standard CMFD calculation to update the scalar flux for neutron transport iteration. It was shown that the linear prolongation technique is more effective than the underrelaxation factor applied on the drift flux term. Reference 5 proposed a variant of the CMFD method, called partial-current-based CMFD (pCMFD), which was found to be unconditionally stable for monoenergetic infinite homogenous problems, but it becomes slower than CMFD for intermediate and smaller coarse-mesh sizes.6 Most recently, Ref. 7 proposed a new optimally diffusive coarse-mesh finite difference (odCMFD) method, which generalizes pCMFD by adding an artificial term to the diffusion coefficient. The coefficient of the artificially diffusive term is a function of optical thickness, which is optimized using Fourier analysis. It was found that odCMFD is unconditionally stable and can slightly improve the convergence of pCMFD. Reference 8 introduced a two-level pCMFD
acceleration scheme to overcome the slow convergence problem of pCMFD for optically thick coarse-mesh cells. In this scheme, a fine-mesh-based acceleration with a fixed-source is coupled with a coarse-mesh-based acceleration with power iteration. It was found that the two-level pCMFD scheme enhances the convergence speed of pCMFD for optically thick coarse-mesh cells.

Recently, we developed a new nonlinear diffusion acceleration scheme, called LR-NDA, which not only can stabilize CMFD, but also can greatly improve its effectiveness. Based on the framework of CMFD, this scheme employs an additional computational level which solves a local boundary value problem (BVP) of the scalar flux on the coarse-mesh structure of CMFD and uses the refined flux to update the source term of the neutron transport iteration. As compared with the two-level pCMFD scheme, it should be noted that LR-NDA does not need to solve a global fine-mesh nonlinear diffusion equation for the CMFD calculations. This paper extends our study of LR-NDA by focusing on its acceleration effectiveness for two-dimensional (2-D) problems and local adaptivity.

The paper is organized as follows. A brief overview of the formulation and algorithm of LR-NDA is given in Sec. II. Section III is devoted to a detailed study of the convergence performance of LR-NDA and its comparison with CMFD based on a 2-D fixed-source problem. Section IV discusses local adaptivity of LR-NDA with a simple 2-D k-eigenvalue problem. A brief summary and discussion is given in Sec. V.

II. LR-NDA FORMULATION AND ALGORITHM

In our previous study, a monoenergetic $S_N$ fixed-source neutron transport problem in slab geometry was used to study the convergence behavior of LR-NDA. In this paper, we extend our study of the convergence behavior of LR-NDA for 2-D problems by using a monoenergetic $S_N$ fixed-source neutron transport equation with isotropic scattering and neutron source. The flow chart of the LR-NDA algorithm is shown in Fig. 1. There are three levels of mesh structures employed in LR-NDA. The $S_N$ transport equation is first solved on the fine-mesh grid, and the CMFD equation is then solved on the coarse mesh. Finally, local refinement, solving a local BVP of the scalar flux, is carried out on the local refined mesh.

The $l$'th iteration cycle, which begins with the $S_N$ transport equation with iteration indices, is expressed as

\[
\frac{\partial}{\partial x} \psi^{l+1/2}(x,y;\mu,\eta) + \eta \frac{\partial}{\partial y} \psi^{l+1/2}(x,y;\mu,\eta) + \Sigma \psi^{l+1/2}(x,y;\mu,\eta) = \frac{\Sigma}{4} \phi(x,y) + \frac{Q(x,y)}{4},
\]

where

- $\phi$ = scalar flux
- $\psi$ = angular flux
- $\Sigma_s$ = scattering cross section
- $\Sigma_t$ = total cross section
- $\mu, \eta$ = neutron angular directions
- $x, y$ = spatial positions
- $Q$ = external neutron source
- $l$ = source iteration index
- $l+1/2$ = intermediate step.

During each $S_N$ source iteration, the coarse-mesh flux is obtained by solving the CMFD equation

\[
\nabla \cdot \left( \frac{-1}{3\Sigma_{CM}} \nabla + \hat{D}_{CM}^{l+1/2} \right) \Phi^{l+1} + (\Sigma_{i,CM} - \Sigma_s,CM) \Phi^{l+1} = Q,
\]

where

- $\Phi^{l+1}$ = coarse-mesh scalar flux
- $Q$ = external neutron source
- $\Sigma_{i,CM}$ = total cross section defined on the coarse mesh
- $\Sigma_s, CM$ = scattering cross section defined on the coarse mesh
- $\hat{D}_{CM}^{l+1/2}$ = drift coefficient which is calculated using the information from the $l + 1/2$ step $S_N$ source iteration.

For the 2-D coarse mesh, we define $\hat{D}_{CM}^{l+1/2}$ in $x$- and $y$-directions on the coarse-mesh edge as

\[
\hat{D}_{CM,x}^{l+1/2} = \int_{-1}^{1} \mu \psi^{l+1/2}(x,y;\mu,\eta)d\mu + \frac{1}{3\Sigma_{i,CM}} \frac{\partial \Phi^{l+1/2}}{\partial x}
\]

and
where the denominator in Eqs. (3) and (4) is the averaged value of the scalar flux of two neighboring coarse meshes relative to the coarse-mesh edge. After solving Eq. (2), we employ two types of flux update. For coarse-mesh cells with small optical thickness, the $S_N$ source iteration scalar flux for the $l+1$ cycle is updated using the same scaling approach as in the standard CMFD:

$$\phi^{l+1} = \phi^{l+1/2} \frac{\phi^{l+1}}{\phi^{l+1/2}},$$

(5)
where $\phi_{l+1/2}$ is obtained by averaging the calculated transport scalar flux on the coarse mesh.

For coarse-mesh cells with large optical thickness, a local refinement calculation is performed on these coarse-mesh cells by solving the local neutron diffusion in Eq. (6) with the fixed boundary conditions on the local mesh:

$$\nabla \cdot \left( \frac{-1}{\Sigma_t} \nabla + D_{FM}^{l+1/2} \right) \phi_{local}^{l+1} + (\Sigma_i - \Sigma_t) \phi_{local}^{l+1} = Q ,$$

(6)

where $\phi_{local}^{l+1}$ is the scalar flux on the local mesh, and $D_{FM}^{l+1/2}$ is the drift coefficient which is defined on the local mesh and calculated using the information from the $l+1/2$ step $S_N$ source iteration. $\phi_{local}^{l+1}$ in Eq. (6) is the scalar flux on the local refinement mesh point, marked as green points in Fig. 2.

The $D_{FM}^{l+1/2}$ in Eq. (6) is defined on the fine-mesh edges, including $D_{FM,x}^{l+1/2}$ and $D_{FM,y}^{l+1/2}$:

$$D_{FM,x}^{l+1/2} = \int_{-1}^{1} \mu \psi^{l+1/2}(x, y, \mu, \eta) d\mu + \frac{1}{3 \Sigma_t} \frac{\partial \phi^{l+1/2}}{\partial x} ,$$

(7)

and

$$D_{FM,y}^{l+1/2} = \int_{-1}^{1} \eta \psi^{l+1/2}(x, y, \mu, \eta) d\eta + \frac{1}{3 \Sigma_t} \frac{\partial \phi^{l+1/2}}{\partial y} ,$$

(8)

where the denominator in Eqs. (7) and (8) is the averaged value of the scalar flux of two neighboring fine meshes relative to the fine-mesh edge. The boundary scalar fluxes (marked as the red points in Fig. 2) for the local BVP are obtained by weighting the transport flux values at the mesh points on the coarse-mesh edges with the coarse-mesh flux ratio between the CMFD and $S_N$ transport results. There are two types of mesh points, i.e., coarse-mesh corner points and coarse-mesh side points. The boundary flux at each corner-mesh point is defined in Eq. (9):

$$\phi_{BC, \; corner}^{l+1} = \frac{1}{4} \left( \phi^{l+1}_{L_B} + \phi^{l+1}_{R_B} + \phi^{l+1}_{L_T} + \phi^{l+1}_{R_T} \right) \phi^{l+1/2} ,$$

(9)

and the boundary flux at each side-mesh point is defined in Eq. (10):

$$\phi_{BC, \; side}^{l+1} = \frac{1}{2} \left( \phi^{l+1}_{+} + \phi^{l+1}_{-} \right) \phi^{l+1/2} ,$$

(10)

where $\phi_{corner}^{l+1/2}$ and $\phi_{side}^{l+1/2}$ are the transport flux at the corner- and side-mesh point, respectively. The subscripts $L_B$, $R_B$, $L_T$, and $R_T$ denote the left-bottom, right-bottom, left-top, and right-top coarse-mesh cells surrounding the corner-mesh point, respectively. The subscripts $+$ and $-$ denote the right and left sides of the coarse-mesh cell edge in the $x$-direction or the top and bottom sides of the coarse-mesh cell edge in the $y$-direction. If local refinement is applied for coarse-mesh cells which share the boundary with the problem domain, Eqs. (9) and (10) can be used to calculate the

![Fig. 2. Local refinement mesh for 2-D problem.](image-url)
boundary conditions for local refinement calculations with appropriate simplification for the corner- or side-mesh points.

After solving Eq. (6), the calculated local mesh point scalar flux along with the BVP boundary mesh point flux are averaged to obtain the center flux of each fine-mesh cell which is used to update the scalar flux in the next transport sweeping:

\[
\phi_{i,j+1}^{l+1} = \frac{1}{4} \left( \phi_{i,j}^{l+1} + \phi_{i+1,j}^{l+1} + \phi_{i,j+1}^{l+1} + \phi_{i+1,j+1}^{l+1} \right),
\]  

(11)

where \( i \) and \( j \) are the indices of the mesh point in the local refinement mesh as shown in Fig. 2.

The source iteration will continue until the convergence criterion is satisfied.

The flowchart in Fig. 3 illustrates the LR-NDA scheme used for \( k \)-eigenvalue problems.

In Fig. 3, \( m \) stands for the power iteration index, \( \varepsilon_1 \) is the convergence criterion for the power iteration in the CMFD calculation, and \( \varepsilon_2 \) is the convergence criterion for the \( k \)-eigenvalue. A local refinement calculation level is added into the two-level Transport/CMFD algorithm. After the CMFD power iteration is done, the new coarse-mesh flux and \( k_{\text{eff}} \) are obtained. For coarse-mesh cells with small optical thickness, Eq. (5) is still used to update the \( S_N \) transport sweep scalar flux for the \( l + 1 \) cycle. For coarse-mesh cells with large optical thickness, a local refinement calculation is performed on these coarse-mesh cells by solving the local neutron diffusion in Eq. (12) with the fixed boundary conditions for local refinement calculations on the local mesh obtained with Eqs. (9) and (10):

\[
\nabla \cdot \left( \frac{-1}{3\Sigma_f} \nabla + \vec{D}_{FM}^{l+1/2} \right) \phi_{\text{local}}^{l+1} + (\Sigma_f - \Sigma_t)\phi_{\text{local}}^{l+1} = \nu\Sigma_f \phi_{\text{local}}^{l+1} / k_{\text{eff}},
\]  

(12)

where

\[
\nu = \text{mean number of neutrons produced per fission}
\]

\[
\Sigma_f = \text{fission cross section}
\]

\[
k_{\text{eff}} = \text{eigenvalue calculated from CMFD.}
\]

Similarly, after solving Eq. (12), the \( S_N \) transport sweep scalar flux for the \( l + 1 \) cycle is updated with Eq. (11).

In addition, it is worthwhile to mention that the LR-NDA method can be utilized to accelerate other transport solvers, such as the Method of Characteristics and Monte Carlo methods.

### III. NUMERICAL CONVERGENCE STUDY

A numerical study of the LR-NDA convergence performance was carried out based on a 2-D model problem, which is a homogeneous \( 10 \times 10 \)-cm square with the vacuum boundary condition for four sides. The domain is discretized into \( 10 \times 10 \) uniform coarse-mesh cells. The fine-mesh number in each coarse-mesh cell is \( 10 \times 10 \). The numerical solutions were obtained using the Gauss-Legendre \( S_{1,2} \) quadrature set for angular discretization and the diamond difference (DD) method for spatial discretization. Both CMFD and LR-NDA acceleration schemes were implemented in the MATLAB code for the problem.

In order to characterize the convergence behavior, we calculated the spectral radius numerically as defined by

\[
\rho = \frac{||\phi^{l+1} - \phi||}{||\phi^l - \phi^{l-1}||}.
\]  

(13)

Figure 4 presents the spectral radius results for CMFD and LR-NDA as a function of coarse-mesh optical thickness (i.e., \( \Sigma_tCM\Delta \), where \( \Delta \) is the coarse-mesh size), for the scattering ratios of 0.6, 0.8, 0.9, and 0.99.

Similar to our previous one-dimensional findings, the following observations can be drawn from the 2-D results:

1. For small scattering ratio, i.e., \( c = 0.6 \) or 0.8, CMFD is stable for the whole range of the optical thickness.

2. When the scattering ratio increases to 0.99, CMFD is only effective for the optical thickness < 1. It becomes unstable and fails to converge when the optical thickness is > 2.

3. The convergence performance of LR-NDA is almost the same with CMFD for the optical thickness < 1, and is more effective and stable than CMFD for the optical thickness > 1.

4. In addition, it is interesting to note that the spectral radius of LR-NDA first increases with the optical thickness up to 10 and thereafter tends to decrease. The improved performance of LR-NDA at high optical thickness is due to the fact that the diffusion solution becomes a better approximation to the \( S_N \) solution at high optical thickness.
IV. LOCAL ADAPTATION OF LR-NDA

In this section, we study the local adaptivity of the LR-NDA scheme based on a 2-D monoenergetic \( k \)-eigenvalue problem with large cross-section variations in the domain. The model problem considered is a 5 × 5-cm square with the reflective boundary condition on the four sides. The domain is divided into 25 uniform coarse-mesh cells. The fine-mesh number in each coarse mesh is 10 × 10 as shown in Fig. 5. Similar to the 2-D fixed-source problem in Sec. III, the numerical solutions for the \( S_N \) neutron transport are obtained using the DD method for spatial discretization and the Gauss-Legendre \( S_{12} \) quadrature set for angular discretization.

![Flowchart of the LR-NDA algorithm for \( k \)-eigenvalue problems.](image)

Fig. 3. Flowchart of the LR-NDA algorithm for \( k \)-eigenvalue problems.
In this problem, there are three local regions shown in color in Fig. 5, which have very large total cross sections, i.e., the local optical thickness is very large. It should be pointed out that the cross sections are arbitrarily given to make it a very challenging problem for numerical solution. For this problem, the standard CMFD scheme fails to converge the $S_N$ iteration.

To study the local adaptivity of LR-NDA, we consider three types of local refinement in Fig. 6. The first case is that local refinement is only applied for the three diagonal coarse-mesh cells. In the second case, the local refinement calculation is applied for the 3 × 3 coarse-mesh cells containing the three optically thick cells. The last case is that local refinement is applied for all the coarse-mesh cells in the domain (i.e., 5 × 5).

Figure 6a shows the normalized converged scalar flux. The flux changes significantly in the three optically thick regions. The $k_{ef}$ relative error is used as the convergence performance index in Fig. 6b. The error criterion $\varepsilon_2$ is $10^{-8}$ (Fig. 3). The error criterion $\varepsilon_1$ for the power iteration in CMFD is $10^{-12}$. It is shown that the second case with local refinement for the 3 × 3 cells is similar to the case where local refinement is applied for the whole domain (5 × 5).

It is noteworthy to point out that the first case, where
local refinement is only applied on the three diagonal coarse-mesh cells, is still very effective, although requires more iterations. This study demonstrates that LR-NDA is a local adaptive method and can be easily implemented for any region of the problem domain, which means that it can be used only for optically thick regions where CMFD could have a convergence problem.

The computing time for each case is summarized in Table I. It is shown that LR-NDA can significantly reduce the number of transport sweeps. Compared to the CPU time spent on the transport sweeps and CMFD calculations, the time spent on the local refinement calculation is much less. In addition, local refinement calculations for each coarse-mesh cell can be parallelized to make the computational cost negligible.
TABLE I

Computational Performance Comparison of the 2-D $k$-Eigenvalue Problem

<table>
<thead>
<tr>
<th></th>
<th>No Acceleration (Transport Sweep)</th>
<th>LR-NDA (3)</th>
<th>LR-NDA (3 × 3)</th>
<th>LR-NDA (5 × 5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of unknowns(^a)</td>
<td>$M^2 \times P^2 \times (N + 2)N/2$</td>
<td>$(P - 1)^2 \times 3$</td>
<td>$(P - 1)^2 \times 3^2$</td>
<td>$(P - 1)^2 \times 5^2$</td>
</tr>
<tr>
<td>(5(^2) × 10(^2) × 84)</td>
<td>(9(^2) × 3)</td>
<td>(9(^2) × 3(^2))</td>
<td>(9(^2) × 5(^2))</td>
<td></td>
</tr>
<tr>
<td>Number of transport sweep</td>
<td>1483</td>
<td>51</td>
<td>36</td>
<td>32</td>
</tr>
<tr>
<td>Transport calculation time (s)</td>
<td>1895.6</td>
<td>64.5</td>
<td>45.2</td>
<td>40.4</td>
</tr>
<tr>
<td>CMFD power iteration number</td>
<td>0</td>
<td>6495</td>
<td>4597</td>
<td>4078</td>
</tr>
<tr>
<td>CMFD calculation time (s)</td>
<td>0</td>
<td>2.2</td>
<td>1.5</td>
<td>1.4</td>
</tr>
<tr>
<td>Total local refinement calculation time (s)</td>
<td>6.9 × 10(^{-2})</td>
<td>1.8 × 10(^{-1})</td>
<td>3.2 × 10(^{-1})</td>
<td></td>
</tr>
<tr>
<td>Local refinement calculation time for one coarse mesh (s)</td>
<td>2.3 × 10(^{-2})</td>
<td>2.0 × 10(^{-2})</td>
<td>1.3 × 10(^{-2})</td>
<td></td>
</tr>
<tr>
<td>Total calculation time (s)</td>
<td>1895.6</td>
<td>66.8</td>
<td>46.9</td>
<td>42.1</td>
</tr>
<tr>
<td>Speedup</td>
<td>1</td>
<td>28.4</td>
<td>40.4</td>
<td>45.0</td>
</tr>
</tbody>
</table>

\(^a\)Computation with a single CPU [Intel (R) Xeon (R) E5-2630 v3 at 2.40 GHz].
\(^b\)$M = 5$ (coarse-mesh number in the x- or y-direction in the problem domain); $P = 10$ (fine-mesh number in the x- or y-direction in each coarse-mesh); and $N = 12$ (the $S_{12}$ quadrature set).

V. CONCLUSIONS

This paper presents our latest work on the development and assessment of the nonlinear LR-NDA acceleration scheme for neutron transport calculations. LR-NDA incorporates a local refinement solution on the coarse-mesh structure based on the CMFD framework. The convergence study of LR-NDA based on the 2-D $S_N$ fixed-source problem demonstrates that LR-NDA can greatly improve the stability and effectiveness of CMFD.

In addition, we demonstrate in this paper that LR-NDA is a local adaptive method and that it can be easily implemented for any region of the problem domain where the standard CMFD method would become ineffective or unstable. It should be pointed out that the computational cost of local refinement is negligible as compared with the CMFD cost because of its local compactness and efficient parallel implementation. This novel feature will make it very computationally attractive for large 2-D/three-dimensional neutron transport problems.

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