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An optimally diffusive Coarse Mesh Finite Difference method to accelerate neutron transport calculations

Ang Zhu *, Michael Jarrett, Yunlin Xu, Brendan Kochunas, Edward Larsen, Thomas Downar

Department of Nuclear Engineering & Radiological Science, University of Michigan, Ann Arbor 48105, USA

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ABSTRACT

A new optimally diffusive Coarse Mesh Finite Difference (odCMFD) method is proposed. The new method generalizes the Coarse Mesh Finite Difference (CMFD) and partial current-based CMFD (pCMFD) methods by adding an artificial term to the diffusion coefficient. The standard CMFD and pCMFD methods preserve the net current and partial currents respectively and can greatly reduce the spectral radius for solving neutron transport problems. Linearized Fourier analysis shows that these methods essentially differ only by the definition of the diffusion coefficient – the pCMFD diffusion coefficient contains an additional "artificial" term, usually taken to be ¼ the coarse mesh size. In this paper, the magnitude of the artificially diffusive term is numerically investigated and optimized using Fourier analysis. The results show that the optimal coefficient increases as the coarse cell optical thickness increases. Also, the optimal value is always smaller than the pCMFD value. This indicates that the pCMFD method overcorrects the diffusion coefficient which increases the spectral radius. A simple polynomial fitting was found for implementing the odCMFD in the MPACT code to perform calculations for realistic problems. Numerical MPACT results for a two-region homogeneous problem, a 2D C5G7 problem, a VERA problem 5 and a 2D BWR Peach Bottom Unit 2 core problem agree well with the Fourier analysis and confirm previous research results that: (1) CMFD converges faster than pCMFD for optically thin coarse grids, but CMFD diverges for optically thick coarse grids; (2) pCMFD is unconditionally stable for all coarse grids; and show that the newly proposed odCMFD is the most efficient among these three methods for all cases. The new method has a similar convergence rate as CMFD for optically thin coarse grids, is faster than both CMFD and pCMFD for coarse grids with intermediate optical thickness, and is unconditionally stable and faster than pCMFD for optically thick coarse grids.

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1. Introduction

Three-dimensional, full-core modeling with pin-resolved detail has become the state of the art for computational simulations of neutron transport for nuclear reactors. However, the computational intensiveness of these problems is challenging, especially for cycle depletion (Kochunas et al., submitted for publication) and time-dependent transient analysis (Zhu et al., 2016a,b) which requires the solution of multiple steady state eigenvalue/transient fixed source problems.

Extensive studies of various acceleration methods for neutron transport have been performed, and their convergence and stability have been analyzed both theoretically and numerically (Adams and Larsen, 2002; Li, 2013). Of these methods, the Coarse Mesh Finite Difference (CMFD) method, which originates from the early 1980's (Smith, 1983) for diffusion problems has gained popularity in recent decades for its simplicity and efficiency in accelerating the steady state (Downar et al., 2009; MPACT Team, 2013) and transient neutron transport calculations (Zhu et al., 2015; Cho et al., 2005; Shaner et al., 2013). However, numerical and theoretical results show that for realistic whole-core calculations, the CMFD method becomes unstable for problems with large coarse mesh cells (Jarrett et al., 2015; Keady and Larsen, 2015; Lee et al., 2004; Hong et al., 2010).

More recently, a variant of the CMFD method, called partial current-based CMFD (pCMFD), was developed by Cho (Cho et al., 2003) and found to be unconditionally stable for monoenergetic infinite homogeneous medium problems (Hong et al., 2010; Cho, 2012). A linearized Fourier analysis (Jarrett et al., 2015; Jarrett, submitted for publication) demonstrated that the pCMFD is theoretically and algebraically "equivalent" to the CMFD method if an additional term $\theta\Delta$ – shown in Eq. (1) – is added to the diffusion coefficient (referred as artificially diffusive CMFD method), where

* Corresponding author.
E-mail address: angzhu@umich.edu (A. Zhu).

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Δ denotes the coarse mesh size. This extra term effectively suppresses the spectral radius for large coarse mesh sizes, for which the CMFD method can be unstable. However, the Fourier analysis of pCMFD, along with numerical results has shown that pCMFD will be slower than CMFD for intermediate and smaller coarse mesh sizes (Cho, 2012). This may explain in part why the pCMFD has not been more widely adopted.

$$D_{pCMFD} = \frac{1}{3\Sigma_{tr}} + \theta\Delta, \quad \theta_{pCMFD} = \frac{1}{4} \tag{1}$$

The idea of optimally diffusive CMFD originates from Larsen (2003), where an "exact" diffusion coefficient is developed for discrete transport solutions in planar geometry with a quadratic source and equal sizes of the fine and coarse meshes. The "exact" diffusion coefficient differs from the standard diffusion coefficient shown in Eq. (1) by adding different coefficients. These are shown in Eq. (2), in which μ_n and ω_n are the 1-D discrete ordinates and weights, and α_n is the step characteristics auxiliary equation coefficient defined in Eq. (3).

$$\theta_{od} = \frac{1}{4}\sum_{n=1}^{N}\mu_n\alpha_n\omega_n \tag{2}$$

$$\alpha_p = \frac{1 + e^{-\Sigma_t\Delta/\mu_n}}{1 - e^{-\Sigma_t\Delta/\mu_n}} - \frac{2\mu_n}{\Sigma_t\Delta} \tag{3}$$

The θ value as a function of optical thickness $\Sigma_t\Delta$ based on Eq. (2) is shown in Fig. 1. The value of θ changes dramatically as a function of the coarse cell optical thickness, ranging from the (CMFD) value of 0 for optically thin coarse grids, to the pCMFD value of 1/4 for optically thick coarse grids. The previous work (Larsen, 2003) investigated the optimal θ value from the viewpoint of accuracy, but it is straightforward to demonstrate that the "exact" diffusion solver can efficiently accelerate the discrete transport calculation in planar geometry with a quadratic source and equal sizes of the fine and coarse meshes by one iteration since the accelerator calculates the same result as the high order solver. Furthermore, such an "exact" approximation of the diffusion equation to the transport equation may not be possible for a complicated geometry especially with multiple fines cells per coarse cell. However, this motivates the research here to develop an optimal set of optical thickness dependent θ rather than directly using 0 for CMFD and ¼ for pCMFD.

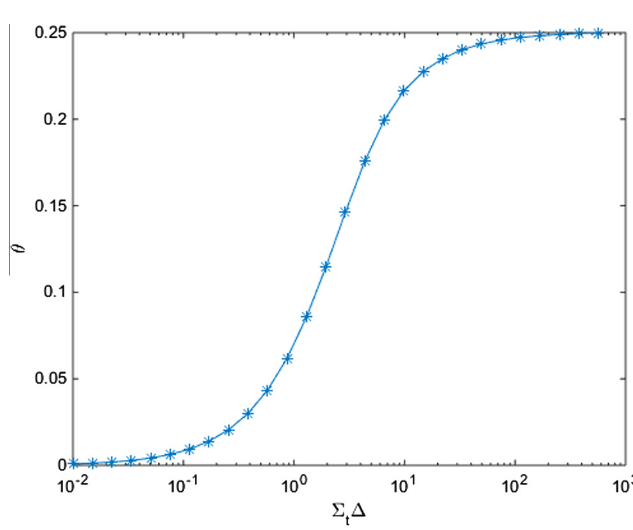

Fig. 1. Value of θ based on Eq. (2).

A similar idea, referred to as generalized coarse-mesh rebalance (GCMR), was proposed by Yamamoto (Yamamoto, 2005), in which a Fourier analysis was used to obtain an optimal multiplication factor that was applied to diffusion coefficients for the coarse mesh rebalance (CMR) and CMFD methods for solving fixed source problems. The GCMR method showed improvement in the spectral radius over the traditional CMR and CMFD methods for monoenergetic infinite homogeneous problems. However, the analysis stopped at the theoretical analysis, when the author argued that the optimal multiplication factor would be too difficult to be determined for complex geometries.

Recently, an under-relaxation factor (Kelley and Larsen, 2015) to resolve 2D/1D stability issues was successfully implemented into MPACT (Michigan Parallel Characteristic Transport) (Zhu et al., 2015). This work demonstrated that "optimized" coefficients derived from the Fourier analysis of the model problem can improve the convergence of complicated complex realistic heterogeneous calculations.

In the work here, an optimally diffusive CMFD (odCMFD) method is proposed and demonstrated in MPACT. The optimal "artificially diffusive" θ value is investigated which minimizes the spectral radius of the coupled high-order transport and low-order CMFD calculations for the steady state eigenvalue problems of a variety of cases.

The remainder of this paper is organized as follows. Section 2 presents a detailed overview of the steady state neutron transport equation and the various CMFD methods, including: the standard CMFD method, the pCMFD method, and the newly-proposed odCMFD method. Section 3 is devoted to a Fourier analysis to determine the optimal θ value required for the odCMFD method. Numerical comparisons of the CMFD, pCMFD and the odCMFD methods are also provided. Section 4 presents numerical results for the CMFD method and two of its variants for a two-region homogeneous problem, a 2D C5G7 problem, a VERA problem 5 and a 2D BWR Peach Bottom Unit 2 core problem using the MPACT code (MPACT Team, 2013). A summary and final conclusions are given in Section 5.

2. CMFD accelerated neutron transport methods

2.1. The neutron transport equation

We consider the multi-group steady state neutron transport equations shown in Eq. (4), where the solution can be obtained by the Method of Characteristics (MOC), Discrete Ordinates (S_N) methods, etc.

$$\begin{aligned}\mathbf{\Omega}\nabla\varphi_g(\mathbf{r},\mathbf{\Omega}) = & -\Sigma_{t,g}(\mathbf{r})\varphi_g(\mathbf{r},\mathbf{\Omega}) \\ & + \sum_{g'=1}^{G}\int_0^{4\pi}\Sigma_{s,g'\to g}(\mathbf{r},\mathbf{\Omega}\mathbf{\Omega}')\varphi_{g'}(\mathbf{r},\mathbf{\Omega}')d\Omega' \\ & + \frac{1}{4\pi}\chi_g(\mathbf{r})\frac{1}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r}).\end{aligned} \tag{4}$$

Using standard notation, the terms in this equation are defined as:

φ_g: group g angular flux;
ϕ_g: group g scalar flux;
χ_g: fission spectrum for group g;
$\Sigma_{s,g'\to g}$: scattering cross-section from group g' to group g;
$\Sigma_{t,g}$: total cross-section for group g;
ν: averaged neutron emitted per fission reaction;
$\Sigma_{f,g}$: fission cross-section for group g;
k_{eff}: steady state eigenvalue.