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A High-Order Nonlinear Diffusion Acceleration for the S_N Equations Discretized with the Discontinuous FEM I: Theory and Numerical Results

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INTRODUCTION

The solution of the radiation transport equation in multiphysics simulations is usually extremely resource intensive and hence requires powerful acceleration methods regardless of whether Monte Carlo [1] or deterministic solvers are used. Recently, nonlinear diffusion acceleration (NDA) methods have received widespread attention in the radiation transport community because of their inherent efficiency [2], [3], [4]. However, NDA is in general only conditionally stable [5], while diffusion synthetic acceleration methods (DSA) are unconditionally stable if suitable discretization methods for the transport and diffusion systems are chosen [6]. The presented work introduces a new generalized NDA method for solving the transport equation discretized with S_N (discrete ordinates) and discontinuous Finite Elements. In contrast to common coarse-mesh finite difference methods (CMFD), where the diffusion system is discretized using constant shape functions, the presented NDA method discretizes the diffusion system using the same (higher order) finite element basis functions as those used for the transport system. This paper focuses on the solution of the steady-state transport equation with the low-order diffusion equation employing the same mesh and the same spatial shape functions, but the NDA method currently under development for the Rattlesnake radiation transport solver [7] based on the MOOSE [8] framework is more general: it allows for the diffusion system to be discretized using an arbitrary group structure and arbitrary mesh nested in their S_N system counterparts, and arbitrary combinations of FEM basis functions.

The purpose of this paper is to demonstrate that using higher order FEM shape functions for the discretization of the diffusion system restores stability where CMFD is unstable. This paper demonstrates this by numerical experiments for two problems discretized with well-shaped quadrilateral cells: (1) a simple, homogeneous source driven problem, and (2) the two-group IAEA-2D PWR benchmark (eigenvalue problem) [9]. Fourier analysis (FA) of the linearized NDA equations can be found in a companion summary [10]. Results indicate that the developed method is unconditionally stable for the selected test problems. Future work will investigate stability on unstructured and/or ill-shaped meshes and in the presence of strong material heterogeneities in the light of previous findings that DSA's performance can degrade under these conditions [11], [12]. This work is related to [11] in that it applies linear shape functions for the discretization of the transport and diffusion systems, but [11] focuses on DSA while this work focuses on NDA. Furthermore, [13] describes an unconditionally stable nonlinear diffusion acceleration scheme for the k-eigenvalue problem that is not based on the drift-diffusion form that this work is focused on. The main novelty of the presented work is the focus on the application of consistent shape function discretization for the drift-diffusion form of NDA.

THEORETICAL DEVELOPMENT

The weak form of the mono-energetic, isotropic scattering S_N equations is given by:

$$\sum_{m=1}^{M} w_m \left((\Psi_m^{l+1/2}, (-\mathbf{\Omega}_m \cdot \boldsymbol{\nabla} + \Sigma_t)\Psi_m^*)_{\mathcal{D}} - \left\langle \Psi_m^{l+1/2,-}, [\![\Psi_m^*]\!] \right\rangle_{\Gamma_i} \right) - \sum_{E \in \partial\mathcal{D}^r} \sum_{\mathbf{\Omega}_m \cdot \boldsymbol{n}_b > 0} w_m \left\langle \Psi_m^l, \Psi_{m_r}^* \right\rangle_E - \left(\phi^l, \frac{\Sigma_s}{4\pi}\Phi^* \right)_{\mathcal{D}} = \left(\frac{S}{4\pi}, \Phi^* \right)_{\mathcal{D}} + \sum_{E \in \partial\mathcal{D}^s} \sum_{\mathbf{\Omega}_m \cdot \boldsymbol{n}_b < 0} w_m \left\langle \Psi_m^{inc}, \Psi_m^* \right\rangle_E \quad (1)$$

where standard radiation transport notation is used. In addition, the superscript l is the iteration index; the $*$ denotes an arbitrary test function within the FEM space; $[\![f]\!]_m = f^+ - f^-$ is the difference of the down and upwind side across faces with respect to the streaming direction $\mathbf{\Omega}_m$; $(\cdot,\cdot)_{\mathcal{D}}$ denotes an integral over the domain $\mathcal{D}$; and $\langle\cdot,\cdot\rangle_E$ denotes the integration over the side set E weighted with $|\mathbf{\Omega}\cdot\boldsymbol{n}|$ where $\boldsymbol{n}$ is the side set's normal vector; m_r is the index of the reflected angular direction associated with m. The set of interior faces is denoted by Γ_i, while the boundary $\partial\mathcal{D}$ is composed of the inflow boundary $\partial\mathcal{D}^s$ and the reflective boundary $\partial\mathcal{D}^r$. Extension of Eq. 1 to more general cases, multigroup S_N equations and eigenvalue problems, is straight-forward and is hence omitted for the sake of brevity. Furthermore, the associated discontinuous diffusion weak form is:

$$(D\boldsymbol{\nabla}\phi^{l+1}, \boldsymbol{\nabla}\phi^*)_{\mathcal{D}} + (\Sigma_a\phi^{l+1}, \phi^*)_{\mathcal{D}} - (\kappa[\![\phi^{l+1}]\!], [\![\phi^*]\!])_{\Gamma_i} + (\{D\boldsymbol{\nabla}\phi^{l+1}\cdot\boldsymbol{n}\}, [\![\phi^*]\!])_{\Gamma_i} + \left(\frac{\alpha}{4}\phi^{l+1}, \phi^*\right)_{\partial\mathcal{D}^s} + \left(\mathbf{D}\phi^{l+1}, \boldsymbol{\nabla}\phi^*\right)_{\mathcal{D}} + \left([\![\hat{\kappa}\phi^{l+1}]\!], [\![\phi^*]\!]\right)_{\Gamma_i} = (S, \phi^*)_{\mathcal{D}} + \left(J^{inc}, \phi^*\right)_{\partial\mathcal{D}^s}, \quad (2)$$

where $(\cdot,\cdot)_{\Gamma_i}$ denotes integration over the interior sides of the domain , $[\![f]\!]$ is the difference of the down and upwind side across faces with respect to the face's normal vector, $\{f\} = \frac{1}{2}(f^+ + f^-)$ and κ is defined based on the order of the FEM basis of the diffusion discretization and the cell's half-width h:

$$\kappa = \max\left(\frac{1}{4}, \kappa^{IP}\right)$$
$$\kappa^{IP} = \begin{cases} 2\left(\frac{D^+}{h^+} + \frac{D^-}{h^-}\right) & \text{Linear;} \\ \frac{1}{\frac{h^+}{D^+} + \frac{h^-}{D^-}} & \text{Constant.} \end{cases} \quad (3)$$

The drift vector $\mathbf{D}$ and surface-source boundary coefficient α are given by

$$\mathbf{D} \equiv -\frac{D\nabla\Phi^{l+1/2} + \boldsymbol{J}^{l+1/2}}{\Phi^{l+1/2}}, \tag{4}$$

$$\alpha \equiv \frac{4J^{l+1/2,out}}{\Phi^{l+1/2}}. \tag{5}$$

Various options exist for the definition of the face closure coefficient $\hat{\kappa}$, but in this work we focus on the generalization of the partial current CMFD closure labelled pNDA:

$$\hat{\kappa}^{\pm} \equiv \frac{J^{l+1/2,out} + \frac{\phi_s}{4} \mp [\![\frac{1}{2}\kappa\phi^{l+1/2} - \frac{1}{4}D\boldsymbol{n}\cdot\nabla\Phi^{l+1/2}]\!]}{\Phi^{l+1/2}}, \tag{6}$$

where $\phi_s = \frac{\{\Phi^{l+1/2}D/h\}}{\{D/h\}}$. We can prove the transport scalar flux satisfies the diffusion weak form Eq. 2 by applying isotropic test functions $\Psi_m^* = \Phi^*$ in Eq. 1. The NDA system of equations is solved using Picard iterations alternating between transport updates, i.e. inversion of the transport operator, and solution of the low order diffusion system using MOOSE's PJFNK solver. For fixed source problems the diffusion equation is linear and hence the PJFNK solver only requires a single nonlinear iteration.

NUMERICAL RESULTS

Homogeneous fixed source problem

A two-dimensional, mono-energetic, homogeneous, source-driven problem is used for assessing the stability and effectiveness of the developed NDA method. The problem is set up with vacuum boundary conditions on all boundaries and features various scattering ratios $c = \Sigma_s/\Sigma_t = 0.9, 0.99, 0.9999$. The domain thickness varies depending on the optical thickness of the cells between 10 mfp and 4000 mfp. For simplicity, the domain is discretized using regular, quadrilateral elements, but it should be pointed out that the NDA method is designed for general unstructured meshes. The transport S_N system uses an S_8 level-symmetric quadrature. In addition, a FA of the linearized NDA iteration algorithm for a single two-dimensional rectangular cell configuration with periodic boundary conditions is performed using the same set of scattering ratios. For each case, the element's optical thickness is varied between $\Delta\Sigma_t = 0.001$ and 1000 and the spectral radius ρ is obtained either from the FA or computed as $\rho = \|\Psi_m^{l+1/2} - \Psi_m^{l-1/2}\|/\|\Psi_m^{l-1/2} - \Psi_m^{l-3/2}\|$. Numerical experiments are not performed with periodic boundary conditions for two reasons: (1) periodic boundary conditions are currently not implemented in Rattlesnake's first order S_N solver, and (2) implicit boundary conditions inherently change the underlying iteration scheme because they require using lagged angular inflow fluxes in Eq. 1.

The spectral radii computed via numerical experiment and FA are plotted in Fig. 1 versus the optical cell thickness. For all curves, the S_N equations are discretized using linear shape functions, while the diffusion system is discretized using either linear shape functions (L) or constant shape functions (C); the latter cases are referred to as CMFD scheme. First,

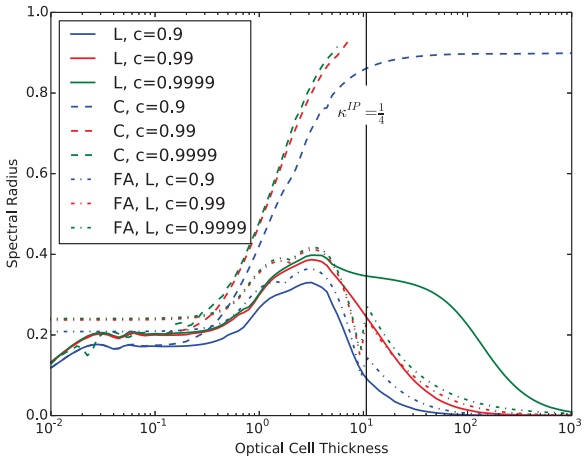

Fig. 1. Spectral radius of the NDA method using constant (C) and linear (L) shape functions for discretizing the diffusion system for homogeneous fixed source problem.

the FA matches the numerical results quite well with the exception of the $c = 0.9999$ case for optical cell thicknesses above 10 mfp. However, these differences indicate merely a quantitative difference between numerical experiment and FA while their qualitative behavior is still consistent. Differences between numerical experiments and FA are expected in light of the assumption made when conducting the FA: converged solutions are uniform in space and second order iterative error terms can be neglected. Therefore, the comparison of numerical experiments and FA gives us confidence in the correct implementation and spectral properties of the presented NDA method. Most importantly, when increasing the optical cell thickness, the CMFD scheme (C) becomes unstable for optical thicknesses between 1 and 10, while the linear (L) NDA method is unconditionally stable.

IAEA-2D two-group eigenvalue problem

The IAEA-2D two-group benchmark models the center plane of an assembly-homogenized PWR core measuring 340 by 340 cm and featuring 17 by 17 rectangular assemblies made up of three fuel types or reflector. Since the IAEA-2D benchmark was conceived as a neutron diffusion benchmark with large homogenized cells, the typical cell thicknesses are large (> 20 mfp) posing challenges to CMFD methods and further the problem has a dominance ratio close enough to unity to be challenging for an iterative solution with power iterations.

The iterative error ϵ, defined as the L_2 difference of two successive fission sources, is plotted versus the iteration count using pNDA and the inverse power method (PI) in Fig. 2. While the cases using a constant discretization of the diffusion system are unstable because of the optically thick cells, NDA using linear shape functions for the discretization of the diffusion system converges to a tolerance of 10^{-8} within 5 Picard iterations. For comparison, accelerated PI and unaccelerated PI require in excess of 30 and 100 iterations, respectively, to

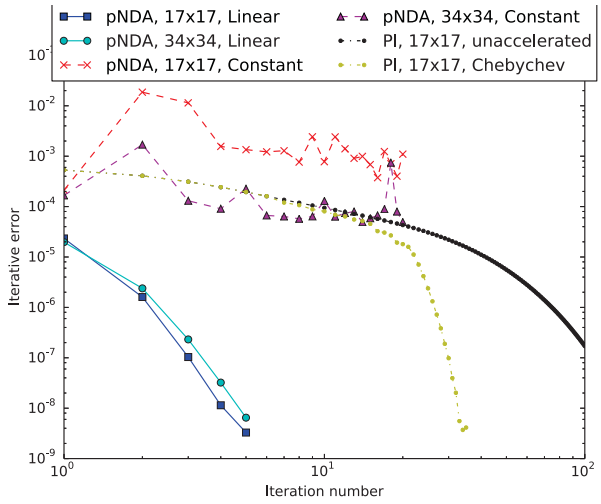

Fig. 2. Convergence behavior of NDA (linear and constant) and power iterations for the IAEA-2D benchmark.

converge to this tolerance.

CONCLUSIONS

In this work, we presented a new NDA method for the first order S_N equations discretized with discontinuous FEM that differs from the commonly used CMFD methods by discretizing the diffusion equations with high-order shape functions; in particular, this work focused on diffusion FEM bases matching the S_N system's counterparts. We demonstrated via Fourier analysis and numerical experiment for a fixed source homogeneous problem and the IAEA-2D two-group benchmark that the presented NDA method, unlike CMFD, is unconditionally stable on quadrilaterial, well-shaped meshes. Efficient solution methods for the S_N transport equation remain an active field of study despite the development of powerful surrogate models for large-scale radiation transport problems [14] .

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