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A FLEXIBLE NONLINEAR DIFFUSION ACCELERATION METHOD FOR THE FIRST ORDER EIGENVALUE S_N EQUATIONS DISCRETIZED WITH DISCONTINUOUS FEM

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Abstract

This work describes a nonlinear diffusion acceleration (NDA) method for the first order S_N equations that discretizes both the transport equation and the associated diffusion system using discontinuous finite elements; the diffusion system is solved on a potentially coarser mesh and with a coarser energy group structure than the S_N equations. The developed method differs from current methods by allowing the S_N and diffusion system to be discretized with arbitrary FEM bases and by using an additive update of the S_N system. The benefit of this capability is extension of the stability region to optically thicker mesh cells without underrelaxing the iterative algorithm. The presented method introduces the notion of *consistency* of the S_N and diffusion solutions and derives suitable definitions of the cross sections, drift vectors, and element face closures. The NDA equations are solved using a Picard iteration scheme. Numerical results are presented for the C5G7 benchmark problem highlighting the effectiveness of the methods when deployed with the diffusion system discretized on the same mesh as the S_N system. Additional results are presented for cases where the diffusion system features a coarser mesh, coarser energy group structure, or both, demonstrating its stability and effectiveness in these cases. It is observed that the effectiveness of the NDA method reduces when reducing the resolution of the associated diffusion system.

Key Words: **NDA, Rattlesnake, C5G7**

1. Introduction

This work focuses on acceleration of Rattlesnake's first order S_N solver for multigroup eigenvalue S_N equations via nonlinear diffusion acceleration (NDA) of the drift diffusion type. Recently, drift-diffusion NDA has received widespread attention in the radiation transport community for reactor physics applications because of its inherent effectiveness [1], [2], [3]. Drift diffusion NDA uses the solution of a modified diffusion equation for accelerating the iterative convergence of the S_N equations;

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the modifications, referred to as closures in the remainder of this work, of the diffusion equation are chosen so that its solution is *consistent* with the S_N solution at convergence.

Typically, NDA has been implemented as coarse mesh finite difference method (CMFD) discretizing the diffusion equation with a piecewise constant approximation, [4], [5]. However, CMFD has been demonstrated to be only conditionally stable even when discretizing transport and diffusion equations on the same well-shaped mesh and in the absence of material discontinuites [6]. Embedding the NDA method into a discontinuous FEM framework and using identical shape functions in the transport and diffusion system can restore stability where CMFD is unstable for homogeneous problems discretized with well-shaped quadrilateral elements, [7], [8]. The NDA system of equations is solved using Picard iterations, i.e. alternating between solving the multigroup diffusion equations and performing one or more transport updates. Reference [5] pointed out that Picard iterations may exhibit lack of convergence for CMFD that are typically mitigated by underrelaxation. In this work, convergence properties of the presented NDA method are investigated for the two-dimensional version of the C5G7 benchmark [9]. It is found that the presented NDA algorithm does not require underrelaxation for convergence. It should be pointed out that Ref. [5]'s focus is mitigating the described convergence issues observed for CMFD acceleration and that promising results are obtained using a higher order prolongation strategy when updating the transport source term. This work naturally incorporates consistent projection and prolongation operations derived within the discontinuous FEM framework.

Within this paper, the NDA method implemented for Rattlesnake's first order S_N solver [7] is extended to multigroup eigenvalue problems accelerated with a coarse mesh and coarse group diffusion calculation. For this purpose we define the notion of *consistency* of the transport and diffusion solutions within the FEM framework. From this definition, projection and prolongation operators are derived that allow us to define closures and cross sections in the diffusion equation, and transport scalar flux updates that lead to a system of NDA equations featuring the following properties: (1) the transport and diffusion solutions are *consistent* in the low-order solution space, (2) the solution is equal to the solution of the stand-alone transport equation without acceleration.

In section 2 the FEM weak forms, the notion of *consistency* and the NDA algorithm are introduced, in section 3 numerical results based on the C5G7 problem are presented, and in section 4 the presented work is summarized and conclusions are drawn.

2. Consistent Weak Forms of the S_N and Diffusion Equation

NDA uses a *consistent* diffusion equation for accelerating the iterative convergence of the multigroup, eigenvalue S_N equations' solution. Without modification of the diffusion equation, S_N and diffusion solutions will be different at convergence even when obtained on the same mesh and using the same FEM bases. Therefore, closure terms evaluated from S_N computed quantities are added to the discretized diffusion equation that ensure that at convergence the solution of the diffusion equation is *consistent* to the S_N solution.

2.1. Weak Form of the S_N Equations

This work focuses on accelerating the iterative solution of the first order, multigroup S_N eigenvalue equations with isotropic scattering. In its original form it is given by:

$$\vec{\Omega}_m \cdot \nabla \Psi_{g,m} + \Sigma_{t,g}(\vec{r})\Psi_{g,m}(\vec{r}) = \frac{1}{4\pi}\sum_{g'=1}^{G}\Sigma_s^{g'\to g}\Phi_{g'} + \frac{K_g(\vec{r})}{4\pi k}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\vec{r})\Phi_{g'}(\vec{r}), \text{ on } \mathcal{D}, \quad (1)$$

$$\Psi_{g,m} = 0 \text{ on } \partial\mathcal{D}^s : \vec{n}\cdot\vec{\Omega}_m < 0, \quad (2)$$

$$\Psi_{g,m} = \Psi_{g,m^r} \text{ on } \partial\mathcal{D}^r : \vec{n}\cdot\vec{\Omega}_m < 0, \quad (3)$$

where g is the group index, $\vec{\Omega}_m$ is the m-th angular direction, $\Psi_{g,m}$ is the angular flux and Φ_g is the scalar flux. Further, $\mathcal{D}$ is the spatial domain, $\partial\mathcal{D}^s$ and $\partial\mathcal{D}^r$ are the fixed inflow and reflective boundaries, respectively, $\vec{n}$ is an outward normal vector on the boundary, m_r is the reflected direction associated with $\vec{\Omega}_m$, $\Sigma_{t,g}$ is total interaction cross section in group g, $\Sigma_s^{g'\to g}$ is the scattering transfer cross section from group g' to group g, K_g is the fission spectrum, $\nu\Sigma_{f,g}$ is the neutron production cross section, and k is the multiplication factor. We intentionally use the capitalized notation for cross sections in Eq. 1 to distinguish the S_N cross sections from the diffusion system cross sections.

For obtaining the weak form of Eq. 1 we multiply it with the arbitrary test function $\Psi^*_{g,m}$, integrate over the domain $\mathcal{D}$ and sum over all groups and angular direction, and finally apply Green's identity and the upwind scheme:

$$\sum_{g=1}^{G}\sum_{m=1}^{M} w_m \left(\left(\Psi_{g,m}, \left(\vec{\Omega}_m \cdot \nabla + \Sigma_{t,g} \right) \Psi^*_{g,m} \right)_{\mathcal{D}} - \left\langle \Psi^-_{g,m}, [\![\Psi^*_{g,m}]\!] \right\rangle_{\Gamma} \right)$$

$$-\sum_{g=1}^{G}\sum_{E\in\partial D^r}\sum_{\vec{\Omega}\cdot\vec{n}>0} w_m \left\langle \Psi_{g,m}, \Psi^*_{g,m^r} \right\rangle_E = \frac{1}{4\pi}\sum_{g=1}^{G}\sum_{g'=1}^{G}\left(Q_{s,g',g}, \Phi^*_g\right)_{\mathcal{D}} + \frac{1}{4\pi k}\sum_{g=1}^{G}\sum_{g'=1}^{G}\left(Q_{f,g',g}, \Phi^*_g\right)_{\mathcal{D}}, \quad (4)$$

where E is an FEM element's face, $\vec{n}$ is an arbitrarily oriented normal vector on E (outward normal vector on $\partial\mathcal{D}$), f^+ and f^- are upwind and downwind values of f, respectively, $\Gamma = \cup E \setminus \partial\mathcal{D}$ is the set of all interior faces, $[\![f]\!] = f^+ - f^-$ is the jump across an element's face with the upwind and downwind sides being defined by $\vec{\Omega}_m$, and

$$(f,g)_{\mathcal{D}} = \int_{\mathcal{D}} dV f g, \quad (5)$$

$$\langle f,g\rangle_E = \int_E dA \left|\vec{\Omega}_m\cdot\vec{n}\right| f g. \quad (6)$$

In Eq. 4, the scattering and fission sources $Q_{s,g',g}$ and $Q_{f,g',g}$ are defined for convenience when defining the NDA system of equations. For the unaccelerated S_N equations, Eq. 1, they are given by

$Q_{s,g',g} = \Sigma_s^{g'\to g}\Phi_{g'}$ and $Q_{f,g',g} = K_g\nu\Sigma_{f,g'}\Phi_{g'}$. For convenience the lumped source Q_g is defined as:

$$Q_g = \frac{1}{4\pi}\sum_{g'=1}^{G} Q_{s,g',g} + \frac{1}{4\pi k}\sum_{g'=1}^{G} Q_{f,g',g}. \tag{7}$$

2.2. Definition of Consistency of S_N and Diffusion Solution

The S_N equations are potentially discretized on a finer mesh and using more energy groups than the diffusion equation with the only restriction that the fine spatial mesh and energy group structure is nested within the coarse mesh and coarse energy group structure. In addition, the choice of the FEM function spaces used for discretizing the S_N and diffusion systems is arbitrary. To establish the definition of *consistency* a projection operator Π is introduced:

$$\phi_p = \Pi\left[\Phi_g\right], \tag{8}$$

where ϕ_p is the scalar flux in coarse energy group p obtained from the solution of the diffusion system. Within the FEM framework, the projection can be defined by requiring

$$\left(\phi_p^*, \phi_p\right)_{\mathcal{D}} = \sum_{g\in p}\left(\phi_p^*, \Phi_g\right)_{\mathcal{D}}. \tag{9}$$

Similarly, a prolongation operation Π^{-1} can be defined by:

$$\left(\Phi_g^*, \Phi_g\right)_{\mathcal{D}} = \left(\Phi_g^*, \phi_p\right)_{\mathcal{D}}. \tag{10}$$

The low-order diffusion system could use shape functions with higher polynomial order than the S_N discretization; in such cases, the low-order space is not completely embedded in the high-order space and complete consistency is usually lost.

2.3. Consistent Weak Form of the Diffusion Equation

NDA uses a *consistent* diffusion weak form that is solved along with the S_N equations. In addition to the interior-penalty discontinuous FEM diffusion weak form outlined in [10] closures are added which are evaluated from S_N computed quantities. The consistent diffusion weak form can be obtained by a P_0 projection of Eq. 4 but for the sake of brevity is simply stated here:

$$\begin{aligned}
&\sum_{p=1}^{P}\left(D_p\vec{\nabla}\phi_p, \vec{\nabla}\phi_p^*\right)_{\mathcal{D}} + \sum_{p=1}^{P}\left(\sigma_{r,p}\phi_p, \phi_p^*\right)_{\mathcal{D}} - \sum_{p=1}^{P}\sum_{p'\neq p}\left(\sigma_s^{p'\to p}\phi_{p'}, \phi_p^*\right)_{\mathcal{D}} \\
+\frac{1}{k}\sum_{p=1}^{P}\sum_{p'=1}^{P}&\left(\chi_p\nu\sigma_{f,p'}\phi_{p'}, \phi_p^*\right)_{\mathcal{D}} + \underline{\sum_{p=1}^{P}\left(\widehat{D}_p\phi_p, \vec{\nabla}\phi_p^*\right)_{\mathcal{D}}} + \sum_{p=1}^{P}\left(\left\{\!\!\left\{D_p\vec{\nabla}\phi_p\cdot\vec{n}\right\}\!\!\right\}, \left[\!\left[\phi_p^*\right]\!\right]\right)_{\Gamma} \\
&+\sum_{p=1}^{P}\left(\kappa_p\left[\!\left[\phi_p\right]\!\right], \left[\!\left[\phi_p^*\right]\!\right]\right)_{\Gamma} + \underline{\sum_{p=1}^{P}\left(\left[\!\left[\widehat{\kappa}_p\phi_p\right]\!\right], \left[\!\left[\phi_p^*\right]\!\right]\right)_{\Gamma}} = 0,
\end{aligned} \tag{11}$$

where the closure terms are underlined and $\{\!\{f\}\!\} = \frac{1}{2}(f^+ + f^-)$ and $[\![f]\!] = f^+ - f^-$ with the upwind and downwind side being defined by the global face normal vector $\vec{n}$. For achieving a consistent diffusion weak form the material properties in Eq. 11 must be evaluated from the S_N computed quantitites:

- Diffusion coefficient: $D_p = \frac{\Pi\left[\frac{1}{3\Sigma_{t,g}}\Phi_g\right]}{\Pi[\Phi_g]}$. It needs to be pointed out that the definition of the diffusion coefficient does not affect the consistency of the method and it therefore is a free parameter. The described choice is the most straight-forward definition, but might not be optimal in terms of the convergence properties.
- Removal cross section: $\sigma_{r,p} = \frac{\Pi\left[\left(\Sigma_{t,g} - \Sigma_s^{g\to g}\right)\Phi_g\right]}{\Pi[\Phi_g]}$.
- Scattering cross section: $\sigma_s^{p'\to p} = \frac{\Pi\left[\left(\sum\limits_{g\in p}\Sigma_s^{g'\to g}\right)\Phi_{g'}\right]}{\Pi\left[\Phi_{g'}\right]}$.
- Fission production cross section: $\nu\sigma_{f,p'} = \frac{\Pi\left[\nu\Sigma_{f,g'}\Phi_{g'}\right]}{\Pi\left[\Phi_{g'}\right]}$.
- Fission spectrum: $\chi_p = \frac{\Pi\left[K_g\left(\sum\limits_{g'}\nu\Sigma_{f,g'}\Phi_{g'}\right)\right]}{\Pi\left[\left(\sum\limits_{g'}\nu\Sigma_{f,g'}\Phi_{g'}\right)\right]}$.

In addition to defining the material properties, the drift vector $\widehat{D}_p$ is defined as:

$$\widehat{D}_p = -\frac{D_p\nabla\Pi\left[\Phi_g\right] + \Pi\left[\vec{J}_g\right]}{\Pi\Phi_g}, \tag{12}$$

where $\vec{J}_g$ is the current evaluated from the S_N solution, and the face closure $\widehat{\kappa}_p$ is given by:

$$\widehat{\kappa}_p = \frac{\Pi\left[J_g^{out}\right] - \frac{1}{4}\phi_{s,p} + \vec{n}\cdot\vec{n}_e[\![\frac{1}{2}\kappa_p\Pi\left[\Phi_g\right] - \frac{1}{4}D_p\vec{n}_e\cdot\vec{\nabla}\Pi\left[\Phi_g\right]]\!]}{\Pi\left[\Phi_g\right]}, \tag{13}$$

where J_g^{out} is the partial outflow current, $\vec{n}_e$ is the element outward normal vector and $\phi_{s,p}$ is the scalar face flux [7] defined as:

$$\phi_{s,p} = \frac{\{\!\{\Pi\left[\Phi_g\right]\frac{D_p}{h}\}\!\}}{\{\!\{\frac{D_p}{h}\}\!\}}, \tag{14}$$

where h denotes the effective half-width of a mesh element. Finally, the penalty coefficient κ_p is given by:

$$\begin{aligned}\kappa_p &= \max\left(\frac{1}{4}, \kappa_p^{IP}\right)\\ \kappa_p^{IP} &= \begin{cases} 2\left(\frac{D_p^+}{h^+} + \frac{D_p^-}{h^-}\right) & \text{Linear;}\\ \frac{1}{\frac{h^+}{D_p^+} + \frac{h^-}{D_p^-}} & \text{Constant.}\end{cases}\end{aligned}. \tag{15}$$

For completing the NDA system of equations the scattering and fission sources $Q_{s,g',g}$ and $Q_{f,g',g}$ are evaluated using the diffusion scalar flux:

$$\begin{aligned} Q_{s,g',g} &= \Sigma_s^{g'\to g}\left(\Phi_{g'} + \Pi^{-1}\left[\phi_{p'} - \Pi\left[\Phi_{g'}\right]\right]\right) \\ Q_{f,g',g} &= K_g \nu\Sigma_{f,g'}\left(\Phi_{g'} + \Pi^{-1}\left[\phi_{p'} - \Pi\left[\Phi_{g'}\right]\right]\right). \end{aligned} \tag{16}$$

The particular form of Eq. 16 ensures that only the fraction of the S_N solution is modified that is within the span of the diffusion FEM space. This is important to not introduce spurious modes into the high order solution. This particular additive update of the S_N system is different than the standard multiplicative update [5].

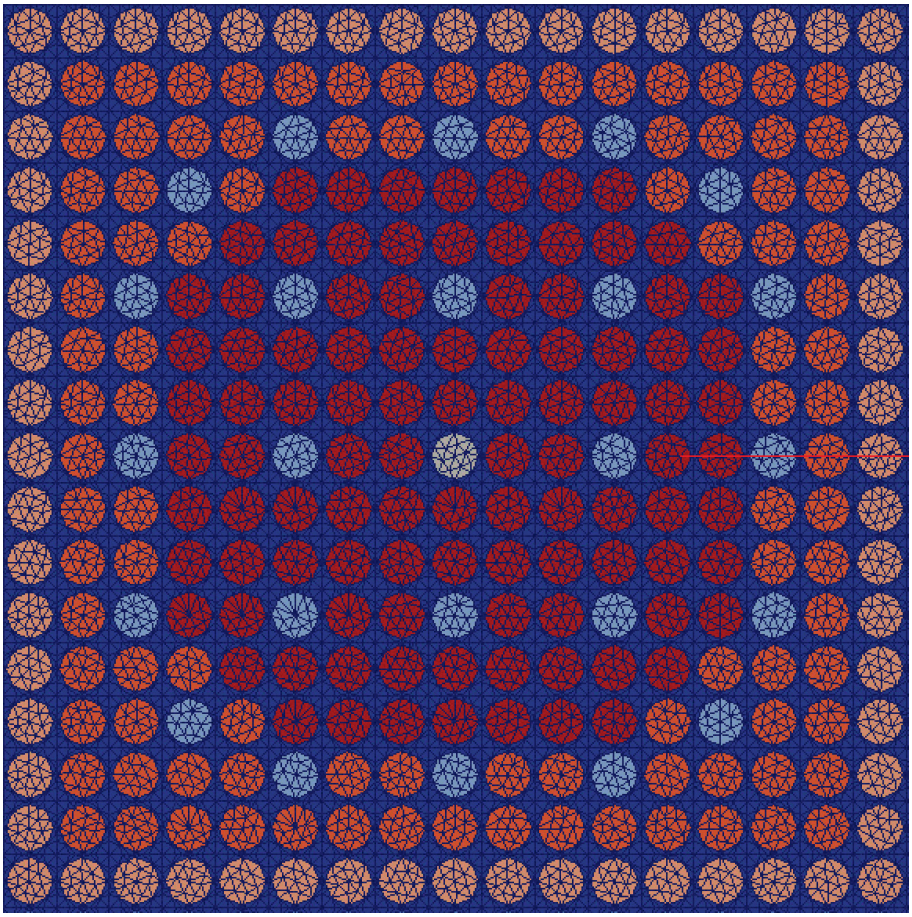

Figure 1. Triangular mesh for a single C5G7 MOX assembly.

2.4. Solution of the NDA Equations via Picard Iterations

The S_N and diffusion weak forms constitute a nonlinear system of equations that is solved via Picard iterations. The solution proceeds by alternating between the solution of the diffusion system using MOOSE's PJFNK solver, [11], and a single transport update on the sources defined in Eq. 16. It should be stressed that no under-relaxation as described in [5] is required for achieving convergence. The algorithm is described in detail in Alg. 1.

Algorithm 1 Nonlinear diffusion acceleration algorithm.

1: Set $l = 0$, $\Phi_g^l = 1$, $J^{out} = 0$, $\epsilon = 10$tol.
2: **while** $\epsilon > tol$ **do**
3: Project reaction rates, currents, and partial outflow currents.
4: Evaluate diffusion cross sections, $\hat{D}_p^l$, and $\hat{\kappa}_p^l$.
5: Solve low order eigenvalue problem using PJFNK solver capability.
6: Prolongation for evaluating $Q_{s,g',g}$ and $Q_{f,g',g}$. Transfer eigenvalue and compute Q_g
7: Obtain $\Psi_{g,m}^{l+1}$ by performing a single transport sweep on Q_g.
8: Compute Φ_g^{l+1}.
9: $\epsilon = \| \sum_{g=1}^{G} \nu\Sigma_{f,g} \left(\Phi_g^{l+1} - \Phi_g^l\right) \|_2$, $l = l + 1$.
10: **end while**

3. Numerical Results

Numerical results are presented for the C5G7 benchmark problem[9]. The S_8 level symmetric quadrature is utilized throughout. For discretizing the S_N problem a triangular mesh depicted for a single MOX assembly in Fig. 1 is used featuring roughly $120,000$ elements. In contrast, the diffusion equation is discretized either on the same mesh or on a rectangular mesh coincident with the pin cell boundaries. Further, seven energy groups are used for the S_N problem, while the diffusion system employs either the same energy group structure or a two group structure collapsing the first three groups (fast groups) into coarse group one and the last four groups (thermal groups with upscattering) into coarse group two. It is important to split the groups such that no upscattering occurs across the coarse energy group boundary. Initial tests use an incorrect splitting of four groups and three groups leading to slower convergence overall and even stalling convergence at an iterative error of 10^{-5}. At each Picard iteration, the diffusion eigenvalue problem is solved using MOOSE's PJFNK solver. For circumventing problems with selecting correct preconditioner settings for the linear GMRES iterations, an exact LU inversion is performed such that linear iterations converge after one iteration. The nonlinear relative and absolute iterative tolerances are set to 10^{-6} and 10^{-9}, respectively. It needs to be stressed that all presented results are obtained for a single processor and therefore solver asynchronicity is not an issue in the presented work. The S_N system uses linear shape functions, while the diffusion system uses either constant shape functions (CMFD), or linear shape functions (NDA). Convergence of the fission source

is measured as the absolute L_2 difference between subsequent Picard iterates. The fission source error is plotted versus the iteration number in Fig. 2. Table I summarizes the total number of Picard iterations required for convergence depending on the solver settings.

CMFD and NDA appear to be stable for all combinations of diffusion meshes and energy group structures. In general, reducing the complexity of the diffusion system reduces the effectiveness of the NDA method. When using a fine mesh and seven energy groups for the diffusion system, the NDA and CMFD methods are stable and effective (8 iterations for convergence to 10^{-6} fission source difference) and virtually no advantage is gained when the diffusion system is discretized using linear shape functions. However, when coarsening the diffusion mesh, NDA exhibits only a moderate increase in number of Picard iterations, while CMFD's iteration count doubles. This result is of great importance because coarse diffusion acceleration is the target application of the presented NDA method. Coarsening the group structure affects both methods' effectiveness equally as the iteration count more than doubles revealing that reducing the complexity in energy has a larger effect on the Picard iteration count. Finally, using a coarse mesh in conjunction with two energy groups increases the iteration count only marginally when compared to the coarse energy group structure only case. Again, NDA requires fewer iterations than CMFD but the difference is not as pronounced as when seven groups are used for the diffusion system.

The immediate conclusion from the numerical experiment is that NDA with a fine group and coarse mesh diffusion system should be the algorithm of choice, because the Picard iteration count increases only slightly while the cost for solving the low order diffusion problem reduces significantly: 25% increase in Picard iteration count but a reduction of DOFs in the diffusion system by roughly a factor of 50.

	CMFD		NDA	
	Fine mesh	Coarse Mesh	Fine Mesh	Coarse Mesh
Fine group	8	16	8	10
Coarse group	18	21	18	19

Table I. Picard iterations required for convergence.

4. Conclusions

This work describes a flexible NDA method implemented in the Rattlesnake radiation transport code that uses discontinuous FEM for discretizing the S_N and diffusion systems. It is flexible because it allows the diffusion system to be solved on a coarser mesh and with a coarser energy group structure as long as they are nested in the S_N mesh or energy group structure, respectively. Moreover, arbitrary FEM bases can be used for the S_N and diffusion systems which, to the best of our knowledge, is a novel concept in drift-diffusion NDA methods discretized with discontinuous FEM. In contrast to standard CMFD methods, the presented NDA method uses an additive update of the transport source. Numerical results

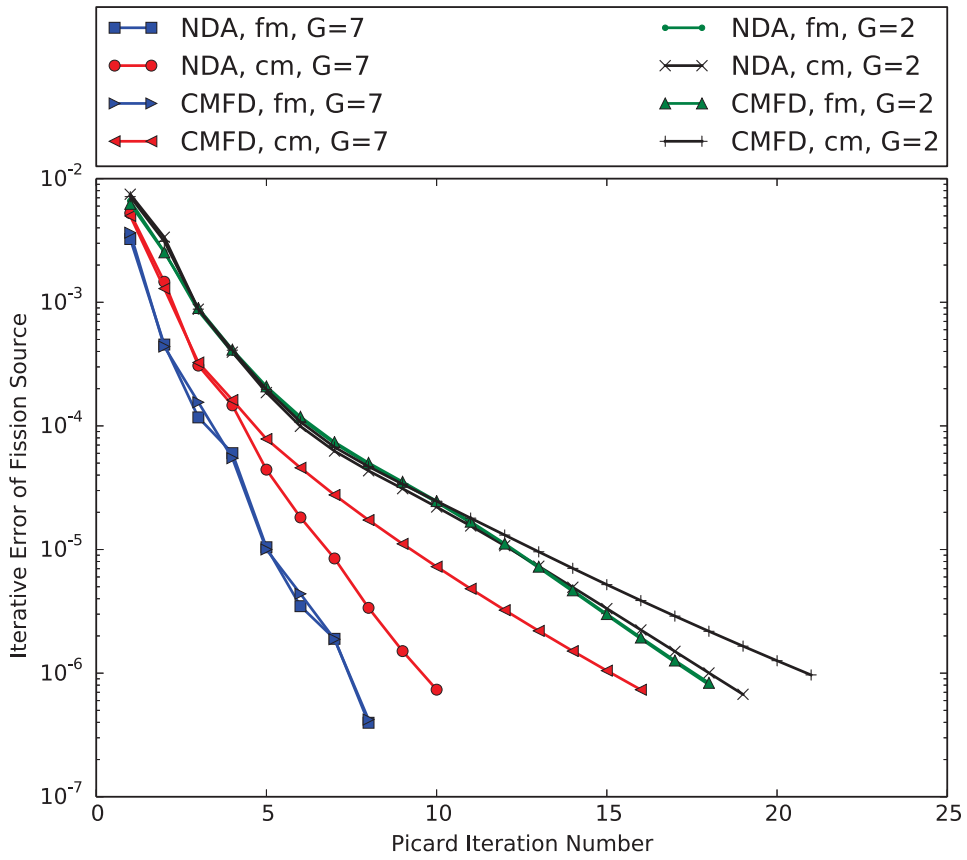

Figure 2. Fission source error plotted versus iteration number for C5G7-2D. The diffusion system's discretization is varied using fine/coarse meshes (fm, cm) and fine/coarse energy group structures (G=7, G=2) and various combinations thereof.

are presented for the C5G7 test problem, a representative LWR geometry, using fine and coarse meshes and energy group structures for the discretization of the diffusion system. The results indicate that the presented method is stable for all combinations of diffusion shape functions, meshes, and energy group structures. In addition, no underrelaxation of the Picard iteration strategy is required for convergence. A reduction of effectiveness ranging from moderate (+25% Picard iteration count) to significant (+165% Picard iteration count) is observed when the diffusion system's fidelity is reduced. Using identical FEM bases for the S_N and diffusion equation, the increase in iteration count is moderate when coarsening the diffusion mesh, but for CMFD the iteration count doubles. Reduction of the number of energy groups in the diffusion system has a similar effect on the NDA and CMFD iteration count leading to an increase in excess of 100%. NDA with a fine group and coarse mesh diffusion system should be the algorithm of choice as it only increases the Picard iteration count by 25% while reducing the DOFs of the diffusion system by a factor of 50.

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