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A Multilevel in Space and Energy Solver for Multigroup Diffusion Eigenvalue Problems

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Abstract - *In this paper, we present the newly developed Multilevel in Space and Energy Diffusion (MSED) method for solving multigroup diffusion eigenvalue problems. The MSED method can be described as a power iteration scheme with three additional features: (1) a grey (1-group) diffusion equation used to efficiently converge the fission source and eigenvalue, (2) a space-dependent Wielandt shift technique [1] used to reduce the number of power iterations required, and (3) a multigrid in space linear solver for the linear solves required by each power iteration step. It is a method in which the convergence of the solution on the full multigroup diffusion eigenvalue problem is accelerated by performing work on lower-order equations with only 1 group and/or coarser spatial grids. Results from several Fourier analyses and a 1-D Python code are provided to verify the efficiency of the MSED method and to justify the incorporation of the grey diffusion equation and the multigrid linear solver. These results highlight the potential efficiency of the MSED method as a solver for large multigroup diffusion eigenvalue problems, and serve as a proof of principle for our future work going forward. Ultimately, our goal is to implement the MSED method as an efficient solver for the 2-D/3-D Coarse Mesh Finite Difference (CMFD) diffusion system in the Michigan Parallel Characteristics Transport (MPACT) code [2]. The work in this paper represents an important step towards that goal.*

I. INTRODUCTION

The multigroup (MG) diffusion eigenvalue equation is an approximation to the neutron transport equation that is widely used for reactor physics simulations. Its solution can also be used to accelerate the source iteration procedure for solving neutron transport problems via methods such as Coarse Mesh Finite Difference (CMFD) [3]. Although a diffusion problem requires significantly fewer computational resources to solve than a transport problem, the computational cost of solving a diffusion problem is still not trivial. In many transport codes that use CMFD-like procedures (e.g., the Michigan Parallel Characteristics Transport (MPACT) code [2]), obtaining solutions to the CMFD diffusion eigenvalue problem constitutes a large portion of the computational effort.

In this work, we introduce a new method, which we have named Multilevel in Space and Energy Diffusion (MSED), for solving the multigroup diffusion eigenvalue problem. It is a multi-component method that draws from existing ideas (multigrid in space [4] and two-grid in energy [5]) as well as new ideas (space-dependent Wielandt shift [1]). The three primary components of MSED are: (1) a "grey" (1-group) diffusion equation that is used to converge the eigenvalue and fission source, (2) a space-dependent Wielandt shift that is used to reduce the number of power iterations required for convergence, and (3) a multigrid in space solver that is used to solve the fixed-source grey and multigroup diffusion linear systems. A visual overview of MSED is provided in Figure 1 and will be further explained in Sections II and III. From Figure 1, we see that the MSED method can be viewed as either an extension of the CMFD method in which the multigroup diffusion equation is accelerated by lower-order (fewer variables or coarser grid) diffusion equations, or an extension of the multigrid method to non-spatial variables.

In the following sections, we provide an overview of the theory for the three components, describe the full algorithm, and present results from our Fourier analysis and 1-D code. This paper should be viewed as a progress report for the development of the MSED method, and the work presented in this paper represents important initial steps towards our eventual goal of implementing MSED as a solver for the CMFD equations in MPACT. As this development progresses and as we learn more about the performance of the MSED method, it is likely that changes will need to be made to the algorithm so that it performs optimally in parallel on 2-D and 3-D problems in the MPACT code.

II. THEORY

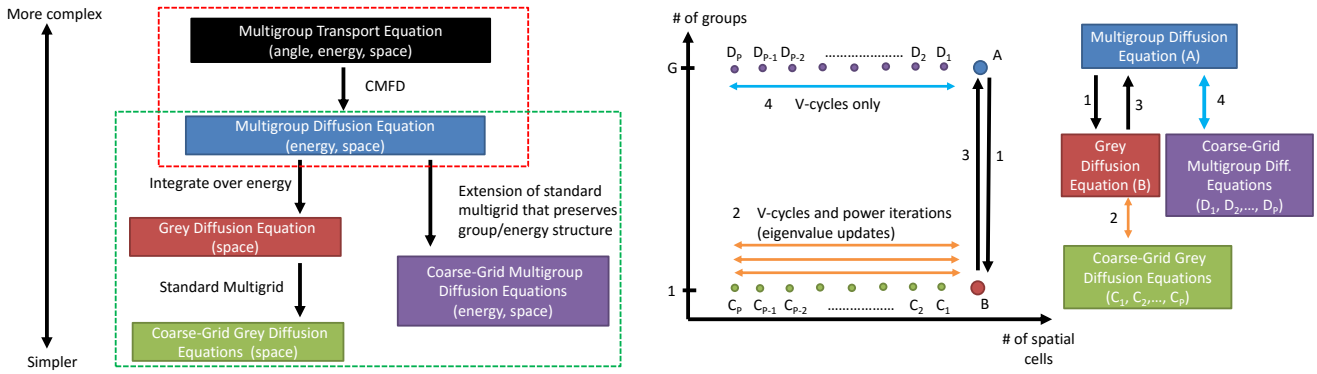
The 1-D multigroup diffusion equation (blue box in Figure 1a), discretized using finite-difference, is given by:

$$\frac{1}{\Delta x_j}\left[D_{j+\frac{1}{2},g}\frac{\phi_{j+1,g}-\phi_{j,g}}{\Delta x_{j+\frac{1}{2}}}-D_{j-\frac{1}{2},g}\frac{\phi_{j,g}-\phi_{j-1,g}}{\Delta x_{j-\frac{1}{2}}}\right]+\Sigma_{,j,g}\phi_{j,g}-\sum_{g'=1}^{G}\Sigma_{s0,j,g'\rightarrow g}\phi_{j,g'}=\lambda\chi_{j,g}\sum_{g'=1}^{G}\nu\Sigma_{f,j,g'}\phi_{j,g'}\,. \quad (1)$$

Here, j is the spatial index, g is the group index, G is the number of groups, $D_{j+\frac{1}{2},g}$ is the diffusion coefficient, $\Sigma_{t,j,g}$ is the total cross section, $\Sigma_{s0,j,g'\rightarrow g}$ is the differential scattering cross section, $\nu\Sigma_{f,j,g}$ is the neutron multiplicity times the fission cross section, $\chi_{j,g}$ is the fission spectrum, $\phi_{j,g}$ is the multigroup scalar flux (spatially averaged over cell j), Δx_j is the width of cell j, and

$$\Delta x_{j+\frac{1}{2}} \equiv \frac{1}{2}\left[\Delta x_j + \Delta x_{j+1}\right]. \quad (2)$$

Eq. (1) can represent either a standard diffusion system or a CMFD system. Although a CMFD system will have correction



(a) (b)

Fig. 1: Each figure provides an overview of the MSED iteration procedure. In (a), the hierachy of equations in MSED is shown, with a scale on the left describing the relative complexity of these equations (i.e., the number of unknowns). The red dashed box encloses the equations used in the CMFD method, while the green dashed box encloses the equations used in the MSED method. In (b), an MSED iteration is broken up into 4 steps, and the changes in the energy and spatial grid sizes at each step are visualized.

factors from the transport system, we can account for these factors by redefining the diffusion coefficients $D_{j+\frac{1}{2},g}$ in Eq. (1) so that it is equivalent to the CMFD system of interest.

Moreover, we note that Eq. (1) is often represented using matrix or operator notation as

$$\underline{\underline{M}}\underline{\phi} = \lambda \underline{\underline{F}}\underline{\phi}\,. \tag{3}$$

Throughout this paper, a double underscore will denote a matrix while a single underscore will denote a column vector.

As a starting point, we define the standard power iteration (PI) scheme for solving diffusion eigenvalue problems:

$$\frac{1}{\Delta x_j}\left[D_{j+\frac{1}{2},g}\frac{\phi^{(l+\frac{1}{2})}_{j+1,g}-\phi^{(l+\frac{1}{2})}_{j,g}}{\Delta x_{j+\frac{1}{2}}} - D_{j-\frac{1}{2},g}\frac{\phi^{(l+\frac{1}{2})}_{j,g}-\phi^{(l+\frac{1}{2})}_{j-1,g}}{\Delta x_{j-\frac{1}{2}}}\right] + \Sigma_{t,j,g}\phi^{(l+\frac{1}{2})}_{j,g} - \sum_{g'=1}^{G}\Sigma_{s0,j,g'\to g}\phi^{(l+\frac{1}{2})}_{j,g'} = \lambda^{(l)}\chi_{j,g}\sum_{g'=1}^{G}\nu\Sigma_{f,j,g'}\phi^{(l)}_{j,g'}\,, \tag{4a}$$

$$\lambda^{(l+1)} = \lambda^{(l)}\frac{\sum_{g'=1}^{G}\sum_{j}\nu\Sigma_{f,j,g'}\phi^{(l)}_{j,g'}}{\sum_{g'=1}^{G}\sum_{j}\nu\Sigma_{f,g'}\phi^{(l+\frac{1}{2})}_{j,g'}}\,, \tag{4b}$$

$$\phi^{(l+1)}_{j,g} = \left\|\underline{\phi}^{(l+\frac{1}{2})}\right\|^{-1}\phi^{(l+\frac{1}{2})}_{j,g}\,. \tag{4c}$$

Here, l is the iteration index for power iteration. In the following subsections, three modifications will be made to the PI scheme in order to establish the MSED method illustrated in Fig. 1. Each subsection will describe a modification, the motivation for that modification, and its effect on accelerating the PI scheme.

Algorithm 1: A standard power iteration step

Input: $\phi^{(l)}_{j,g}$, $\lambda^{(l)}$

Result: $\phi^{(l+1)}_{j,g}$, $\lambda^{(l+1)}$

1. Update the scalar flux using Eq. (4a).
2. Update the eigenvalue using Eq. (4b).
3. Renormalize the scalar flux using Eq. (4c).

For simplicity and brevity, we only present the theory for the MSED method in 1-D for a finite-difference spatial discretization. The generalization of the theory to 2-D and 3-D is straightforward; we would only need to add spatial indices to the subscripts and additional leakage terms. The generalization of the method to other spatial discretizations is less straightforward, but can be done if one carefully modifies the definitions of the grey diffusion coefficients (Eq. (6d)) and the spatial interpolation and restriction operators (Eqs. (15)).

1. Grey Diffusion Equation

The first and perhaps most important component of the MSED method is the grey (1-group) diffusion equation (red box in Figure 1a), which is derived by summing Eq. (1) over the groups g. The collapse is straightforward for all of the terms except the leakage term. Performing the collapse yields the following grey equation:

$$\left[\frac{\left\langle D_{j+\frac{1}{2},j+1}\right\rangle}{\Delta x_j\Delta x_{j+\frac{1}{2}}}\right]\Phi_{j+1} + \left[\frac{\left\langle D_{j-\frac{1}{2},j-1}\right\rangle}{\Delta x_j\Delta x_{j-\frac{1}{2}}}\right]\Phi_{j-1} + \left[\frac{\left\langle D_{j+\frac{1}{2},j}\right\rangle}{\Delta x_j\Delta x_{j+\frac{1}{2}}} + \frac{\left\langle D_{j-\frac{1}{2},j}\right\rangle}{\Delta x_j\Delta x_{j-\frac{1}{2}}} + \left\langle\Sigma_{a,j}\right\rangle\right]\Phi_j = \lambda\left\langle\nu\Sigma_{f,j}\right\rangle\Phi_j\,. \tag{5}$$

In this equation, the grey scalar flux and the bracketed grey quantities are given by:

$$\Phi_j \equiv \sum_{g=1}^{G} \phi_{j,g} \,, \tag{6a}$$

$$\left\langle \Sigma_{a,j} \right\rangle \equiv \frac{1}{\Phi_j} \sum_{g=1}^{G} \Sigma_{a,j,g} \phi_{j,g} \,, \tag{6b}$$

$$\left\langle \nu\Sigma_{f,j} \right\rangle \equiv \frac{1}{\Phi_j} \sum_{g=1}^{G} \nu\Sigma_{f,j,g} \phi_{j,g} \,, \tag{6c}$$

$$\left\langle D_{j_1,j_2} \right\rangle \equiv \frac{1}{\Phi_{j_2}} \sum_{g=1}^{G} D_{j_1,g} \phi_{j_2,g} \,. \tag{6d}$$

Here, $\Sigma_{a,j,g}$ is the absorption cross section, defined by

$$\Sigma_{a,j,g} = \Sigma_{t,j,g} - \sum_{g'=1}^{G} \Sigma_{s0,j,g\to g'} \,. \tag{7}$$

The careful collapse of the diffusion coefficient via Eq. (6d) is necessary to ensure that the grey diffusion coefficients are positive and well-defined when $(\Phi_{j+1} - \Phi_j) \to 0$. If a different spatial discretization is used, the collapse of the diffusion coefficients may require modification to ensure consistency and positivity.

We note that the term "grey" is not typically used in reactor physics. The history of this term stems from the study of the radiative transfer equations and, in particular, this term is frequently used when describing the numerical simulation of these equations for astrophysics and atmospheric applications. Despite its origins, we feel that it is appropriate to use the term "grey" in this paper, as the development of Eq. (5) was strongly motivated by our knowledge of similar concepts in radiative transfer. When numerically simulating radiative transfer, a grey diffusion or transport equation is often used to accelerate the convergence of the more complex, multifrequency (i.e., energy-dependent or multigroup) radiative transfer problems through some scale-bridging algorithm [6, 7]. In our work, the motivation for using the grey diffusion equation is more or less the same; we intend to use the grey diffusion system to accelerate the convergence of the more complex multigroup diffusion system.

Algorithm 2 briefly describes how the grey diffusion equation can be incorporated into the standard power iteration scheme. Unlike Algorithm 1, iterations are performed on both a grey diffusion system and a multigroup diffusion system. By using a grey equation, Algorithm 2 is able to efficiently converge the eigenvalue and fission source. The basic reason for this efficiency is that the right side of Eq. (1) is separable in the indices g and g' – a mathematical representation of the fact that the energy of an outgoing neutron born from fission is independent of the energy of the incoming neutron that induced the fission. Because of this property, the fission source ($\sum_{g'=1}^{G} \nu\Sigma_{f,j,g'} \phi_{j,g'}$) in a multigroup diffusion eigenvalue problem is naturally a grey quantity, and is the same for both the grey and multigroup systems upon convergence.

With the grey diffusion equation providing an efficient means of converging the fission source and eigenvalue, iterations on the multigroup system (step 4 in Algorithm 2) are only needed to converge the energy-dependence of the scalar flux (and, consequently, the scattering source). As a result, the required number of multigroup power iterations is 1-2 orders of magnitude smaller than that of standard power iteration. While it is true that Algorithm 2 requires power iterations on the grey diffusion system in addition to power iterations on the multigroup diffusion system, these new grey iterations are significantly cheaper than those on the larger multigroup system. In short, the incorporation of the grey diffusion system allows us to shift the bulk of the work in the iteration scheme from the multigroup diffusion system to a smaller grey system.

Algorithm 2: A power iteration step accelerated by a grey diffusion equation.

Input: $\phi_{j,g}^{(l)}$, $\lambda^{(l)}$

Result: $\phi_{j,g}^{(l+1)}$, $\lambda^{(l+1)}$

1. Compute $\Phi^{(l,0)}$ and the grey cross sections from $\phi_{j,g}^{(l)}$ using Eqs. (6).

2. Perform M power iterations (Algorithm 1 with $G = 1$) on the grey diffusion eigenvalue problem (Eq. (5)) to obtain the normalized grey scalar flux $\Phi^{(l,M)}$ and its corresponding eigenvalue $\lambda^{(l,M)}$.

   M can be either a fixed number or the number of PIs required to converge the grey diffusion solution to a certain tolerance.

3. Update the multigroup scalar flux and eigenvalue:

$$\phi_{j,g}^{(l+\frac{1}{2})} = \phi_{j,g}^{(l)} \frac{\Phi_j^{(l,M)}}{\Phi_j^{(l,0)}} \,, \tag{8a}$$

$$\lambda^{(l+1)} = \lambda^{(l,M)} \,. \tag{8b}$$

4. Consider Eq. (4a), except with the iteration indices on ϕ incremented by 1/2 and with $\lambda^{(l+1)}$ instead of $\lambda^{(l)}$. Solve this equation to obtain $\phi_{j,g}^{(l+1)}$. An optional update of the eigenvalue using Eq. (4b) may also be performed here.

In our work, we have also explored the use of an alternate grey diffusion equation, derived by performing a weighted sum over g. This alternate grey diffusion equation is obtained by multiplying Eq. (1) by a space- and group-dependent function $f_{j,g}$ and then summing over g. (In Eq. (5), $f_{j,g} = 1$.) From our Fourier analysis, we have found that choosing $f_{j,g}$ to be an estimate of the multigroup adjoint eigenfunction (e.g., $f_{j,g}$ could be the infinite-medium adjoint eigenfunction in each spatial cell) leads to an iteration scheme with an improved spectral radius and a reduced likelihood of instability. However, we have not yet encountered any physically relevant examples for which the MSED method is unstable with $f_{j,g} = 1$ or for which the convergence rate is significantly improved by some choice of $f_{j,g} \neq 1$. Nonetheless, this alternate grey diffusion

equation should be considered if one encounters a problem in which the use of the standard grey diffusion equation results in instability.

Lastly, we acknowledge recent work by Cornejo and Anistratov, in which an additional energy grid between 1 group and G groups is introduced [8]. Their results have shown that the use of an intermediate energy grid can provide tangible improvements in the runtime, and it may be possible to use a similar strategy to improve the MSED algorithm.

2. Space-Dependent Wielandt Shift

The second component of the MSED method is the space-dependent Wielandt shift (SDWS). The spectral radius for the power iteration scheme for solving eigenvalue problems is determined by the dominance ratio – the ratio of the second largest eigenvalue (in magnitude) to the largest eigenvalue. When problems are optically thick (i.e., realistic reactor problems), this dominance ratio approaches 1 and power iteration is slowly converging. In the previous section, we noted that the number of multigroup power iterations required to solve Eq. (1) may be significantly reduced by leveraging the solution of the grey diffusion system. However, obtaining this grey solution still requires computational effort and, if power iteration is used, many iterations may be required to converge the grey diffusion system. Thus, even when the grey diffusion equation is used, a technique for reducing the dominance ratio of diffusion systems is still needed.

Before we introduce the space-dependent Wielandt shift, we first introduce the standard Wielandt shift (WS). The Wielandt shift is a well-established acceleration technique for the PI scheme that shifts the eigenvalue spectrum of a diffusion system by some estimate of the true eigenvalue, λ', in order to reduce the dominance ratio of the system [9]. The PI scheme with Wielandt shift can be described by the following equations:

$$\frac{1}{\Delta x_j}\left[D_{j+\frac{1}{2},g}\frac{\phi^{(l+\frac{1}{2})}_{j+1,g}-\phi^{(l+\frac{1}{2})}_{j,g}}{\Delta x_{j+\frac{1}{2}}}-D_{j-\frac{1}{2},g}\frac{\phi^{(l+\frac{1}{2})}_{j,g}-\phi^{(l+\frac{1}{2})}_{j-1,g}}{\Delta x_{j-\frac{1}{2}}}\right] + \Sigma_{t,j,g}\phi^{(l+\frac{1}{2})}_{j,g}-\sum_{g'=1}^{G}\left[\Sigma_{s0,j,g'\to g}+\lambda'^{(l)}_{j}\chi_{j,g}\nu\Sigma_{f,j,g'}\right]\phi^{(l+\frac{1}{2})}_{j,g'} = \left[\lambda^{(l)}-\lambda'^{(l)}_{j}\right]\chi_{j,g}\sum_{g'=1}^{G}\nu\Sigma_{f,j,g'}\phi^{(l)}_{j,g'}, \quad (9a)$$

$$\lambda^{(l+1)}=\frac{\sum_{g'=1}^{G}\sum_{j}\nu\Sigma_{f,j,g'}\left\{\lambda'^{(l)}_{j}\phi^{(l+\frac{1}{2})}_{j,g'}+\left[\lambda^{(l)}-\lambda'^{(l)}_{j}\right]\phi^{(l)}_{j,g'}\right\}}{\sum_{g'=1}^{G}\sum_{j}\nu\Sigma_{f,g'}\phi^{(l+\frac{1}{2})}_{j,g'}}, \quad (9b)$$

$$\phi^{(l+1)}_{j,g}=\left\|\underline{\phi}^{(l+\frac{1}{2})}\right\|^{-1}\phi^{(l+\frac{1}{2})}_{j,g}. \quad (9c)$$

Eqs. (9) and Algorithm 3 describe the Wielandt shift technique for both multigroup and grey diffusion systems. Although λ' does not have space-dependence in the case of a standard Wielandt shift, we have included spatial indices on λ' so that Eqs. (9) can be used to describe both SDWS and standard WS.

Algorithm 3: A power iteration step accelerated by (Space-Dependent) Wielandt Shift

Input: $\phi^{(l)}_{j,g}$, $\lambda^{(l)}$

Result: $\phi^{(l+1)}_{j,g}$, $\lambda^{(l+1)}$

1. Compute the Wielandt shift parameter $\lambda'^{(l)}_{j}$.
2. Update the scalar flux using Eq. (9a).
3. Update the eigenvalue using Eq. (9b).
4. Renormalize the scalar flux using Eq. (9c).

Typically, one determines the Wielandt shift from the most recent iterates of the eigenvalue. In the 3-D multigroup diffusion code PARCS (Purdue Advanced Reactor Core Simulator) [10], the Wielandt shift is an iteration-dependent quantity that determines the shift at each iteration from the two most recent estimates of the eigenvalue:

$$\lambda'^{(l)}_{P}\equiv\max\left\{\lambda^{(l)}-c_1\left|\lambda^{(l)}-\lambda^{(l-1)}\right|-c_0,\lambda_{\min}\right\}. \quad (10)$$

Here, c_1 and c_0 are user-defined constants (with typical values of 10 and 0.02, respectively) while $\lambda_{\min}$ is chosen such that it is physically impossible for λ to be less than $\lambda_{\min}$ (typically, $\lambda_{min}\approx 1/3$). This type of shift works well if one has a good estimate of the true eigenvalue and the eigenvalue is not changing significantly from iteration to iteration (i.e., when we are near convergence).

The recently developed space-dependent Wielandt shift improves upon traditional Wielandt shifts by providing a physically-motivated shift that is more effective at the beginning of the iteration scheme, when one does not necessarily have a good estimate of the true eigenvalue [1]. Briefly, SDWS is a class of shift techniques in which the shift λ' in Eq. (9a) is allowed to have space-dependence. Several variants of SDWS are described in [1], but, in this summary, we will focus on the Improved Local Eigenvalue Positive Source (ILEPS) shift $\lambda'^{(l)}_{ILEPS,j}$:

$$\lambda'^{(l)}_{ILEPS,j}=\max\left\{\lambda'^{(l)}_{P},\min\left\{\lambda_{\infty,j},\lambda^{(l)}\right\}\right\}. \quad (11)$$

We note that the ILEPS shift was denoted the IPS shift in [1]; we have since renamed the shift in order to improve the notational consistency between this shift and other recently developed space-dependent Wielandt shifts. In Eq. (11), $\lambda'^{(l)}_{P}$ is the shift used in the PARCS code (Eq. (10)) and $\lambda_{\infty,j}$ is the infinite-medium eigenvalue in spatial cell j, defined by the following equation:

$$\Sigma_{t,j,g}\phi_{\infty,j,g}-\sum_{g'=1}^{G}\Sigma_{s0,j,g'\to g}\,\phi_{\infty,j,g'} = \lambda_{\infty,j}\,\chi_{j,g}\sum_{g'=1}^{G}\nu\Sigma_{f,j,g'}\phi_{\infty,j,g'}. \quad (12)$$

Eq. (12) can be rewritten as a $G \times G$ linear system using matrix/vector notation as follows:

$$\left[\underline{\underline{\Sigma}}_{t,j} - \underline{\underline{\Sigma}}_{s0,j}\right] \underline{\phi}_{\infty,j} = \lambda_{\infty,j}\, \underline{\chi}_j\, \underline{\nu\Sigma}_{f,j}^T\, \underline{\phi}_{\infty,j}\,. \tag{13}$$

Here, $\underline{\underline{\Sigma}}_{t,j}$ is a $G \times G$ diagonal matrix, $\underline{\underline{\Sigma}}_{s0,j}$ is a $G \times G$ matrix, $\underline{\phi}_{\infty,j}$, $\underline{\chi}_j$, and $\underline{\nu\Sigma}_{f,j}$ are length-G column vectors, and the superscript T represents the transpose operator. The structure of the fission source allows us to deduce that there is only one nonzero eigenvalue solution to this infinite-medium problem, and it can be computed directly using the following expression:

$$\lambda_{\infty,j} = \left\{ \underline{\nu\Sigma}_{f,j}^T \left[\underline{\underline{\Sigma}}_{t,j} - \underline{\underline{\Sigma}}_{s0,j}\right]^{-1} \underline{\chi}_j \right\}^{-1}. \tag{14}$$

From Eq. (14), we see that a major drawback of the ILEPS shift is that it requires the computation of $\lambda_{\infty,j}$ in each spatial cell. Each of these computations requires solving a $G \times G$ linear system. This is a trivial burden for the grey diffusion system, but not for the multigroup diffusion system. Because of this, our current version of the MSED method only uses the ILEPS shift for the grey diffusion system. In the MSED method, the grey diffusion system has already significantly reduced the number of multigroup power iterations required and, as a result, the application of the ILEPS shift on the multigroup diffusion system can only save a few iterations at best. This makes it difficult to justify the cost of computing $\lambda_{\infty,j}$.

More details regarding the advantages and disadvantages of all the variants of SDWS can be found in a recent conference summary [1]. We note that the development and theory for SDWS is entirely independent of that of the grey diffusion system derived in the previous section. SDWS is simply a technique by which one can effectively reduce the dominance ratio of a (multigroup or grey) diffusion system, and its applications can extend beyond its use in the MSED method. Moreover, we are currently developing additional variants of SDWS not found in [1]; these new variants do not require solving a $G \times G$ linear system in each spatial cell and would be more feasible for the multigroup diffusion system in the MSED method.

3. Multigrid in Space

Thus far, we have ignored an important question in the power iteration schemes in Algorithms 1, 2, and 3: how do we solve for $\phi^{(l+\frac{1}{2})}$ in Eqs. (4a) and (9a), or for $\Phi^{(l,m+\frac{1}{2})}$ in Eq. (5)? In order for algorithms such as Algorithms 3 and 2 to solve problems efficiently, Eqs. (4a) and (9a) must be solved in an efficient manner. For typical full-core reactor simulations, the large size of the linear systems defined by Eqs. (4a) and (9a) prevent the use of direct linear solvers such as Gaussian elimination or LU factorization. As such, iterative solvers are needed. However, when a Wielandt shift such as the PARCS or ILEPS shift is used, Eq. (9a) is a nearly singular system whose condition number can be orders of magnitude greater than its unshifted counterpart. This can cause many standard iterative solvers such as GMRES, BiCGSTAB, or SOR, whose convergence rates depend heavily on the condition number and the diagonal dominance of the system, to converge extremely slowly or even diverge. Thus, the MSED method requires an efficient, iterative linear solver that is insensitive to the ill-conditioning caused by Wielandt shift. We have found that a multigrid (in space) linear solver fits this description.

The multigrid method is an acceleration technique for (generally simple) iterative linear solvers [4, 11]. Many iterative linear solvers, often referred to as "smoothers," rapidly dampen and remove high-frequency error components, but are inefficient at reducing low-frequency error components. The multigrid method remedies this deficiency by mapping the linear system to a coarser spatial grid. When low-frequency error components are mapped onto coarser grids, their frequency is artificially increased by the coarser grid size. As a result, these error components can be more easily removed by the iterative linear solver. A "V-cycle" is generally performed in which one repeatedly generates an error equation from the current residual, maps this error equation to a coarser grid ("restriction"), and performs linear solver iteration(s) on the error equation on the coarser grid. At the bottom of the V-cycle is generally a grid on which the system is small enough to be solved directly. Once this is done, one traverses up the V-cycle by successively interpolating errors onto finer grids until the original fine-grid is reached and the solution on that grid updated.

Although the multigrid method has existed for decades, its use in reactor physics has been rather limited. Many reactor physics codes, such as MPACT, have preferred to use either Krylov solvers or even simpler iterative solvers such as SOR. However, the diffusion equation in this work can be viewed as a variation of the standard Laplace problem ($\triangle u = f$), which serves as the primary example in many introductory texts for the multigrid method. Moreover, the multigrid method has an extensive history as a solver or preconditioner for diffusion-like problems, especially in the field of radiative transfer [12, 13]. Because of this, we feel that the multigrid method is a natural and logical choice for the linear solver in MSED.

As suggested by Alcouffe [12], we choose the interpolation and restriction operators so that the leakage $D\frac{d}{dx}\phi$ is represented as a linear operator. The interpolation operators for the grey diffusion system are given by:

$$x_{(p),2j-1} = x_{(p+1),j}\,, \tag{15a}$$

$$x_{(p),2j} = i_{(p+1),j}^{(p),2j}\, x_{(p+1),j} + i_{(p+1),j+1}^{(p),2j}\, x_{(p+1),j+1}\,, \tag{15b}$$

$$i_{(p+1),j}^{(p),2j} \equiv \left[\frac{\left\langle D_{2j+\frac{1}{2}}, 2j+1 \right\rangle}{\Delta x_{2j+\frac{1}{2}}} + \frac{\left\langle D_{2j-\frac{1}{2}}, 2j-1 \right\rangle}{\Delta x_{2j-\frac{1}{2}}} \right]^{-1} \frac{\left\langle D_{2j+\frac{1}{2}}, 2j+1 \right\rangle}{\Delta x_{2j+\frac{1}{2}}}\,, \tag{15c}$$

$$i_{(p+1),j+1}^{(p),2j} \equiv 1 - i_{(p+1),j}^{(p),2j}\,. \tag{15d}$$

Here, p is an index representing the grid size – higher values of p correspond to coarser grids – and x is a quantity being mapped between the coarse and fine grids. In matrix notation, Eqs. (15) can be written as:

$$\underline{\underline{I}}_{(p+1)}^{(p)}\, \underline{x}_{(p+1)} = \underline{x}_{(p)}\,. \tag{16}$$

In the MSED method, we define the restriction operator to be the transpose of the interpolation operator multiplied by

a diagonal matrix $\underline{\underline{\mathcal{D}}}_{(p)}^{(p+1)}$:

$$\underline{\underline{I}}_{(p)}^{(p+1)} \underline{x}_{(p)} \equiv \underline{\underline{\mathcal{D}}}_{(p)}^{(p+1)} \left(\underline{\underline{I}}_{(p)}^{(p+1)} \right)^T \underline{x}_{(p)} = \underline{x}_{(p+1)} . \tag{17}$$

In this definition, $\underline{\underline{\mathcal{D}}}_{(p)}^{(p+1)}$ is used to normalize the sum of the weights in each row to 1. This restriction operator is a common choice for multigrid methods and leads to several desirable properties for the multigrid scheme [4]. With the interpolation and restriction operators defined as matrices, the coarse grid operators can be obtained using the following matrix expression:

$$\underline{\underline{M}}_{(p+1)} = \underline{\underline{I}}_{(p)}^{(p+1)} \underline{\underline{M}}_{(p)} \underline{\underline{I}}_{(p+1)}^{(p)} . \tag{18}$$

Algorithm 4 describes the steps in a single V-cycle in the multigrid linear solver used in MSED. For the grey system in the MSED method, multigrid is paired with a red-black Jacobi smoother. The "red-black" aspect refers to the classification of spatial cells into red and black cells in a checkerboard pattern. Because of the checkerboard pattern, the update of the black cells only depends on the solution in the red cells, and vice versa. Thus, one can reduce the amount of computational effort required for convergence by updating the red and black cells successively rather than simultaneously. That is, we can first iterate on the red cells and then use the updated solutions in the red cell for the iterations on the black cells.

For the multigroup system, we pair multigrid with a red-black block Jacobi method with blocks of size G. Despite the multigroup nature of the equations, the multigrid interpolation and restriction operators described in Eqs. (15) can still be used to transition between the spatial grids while leaving the group structure mostly in tact. The quantities x and i in Eqs. (15) are group-dependent quantities in the multigroup system, but the interpolation/restriction process is still more or less the same as that of the grey system. The interpolation and restriction operators are group-dependent and treat each group separately, while the block Jacobi smoother helps resolve the group-dependence of the flux.

We suspect that the Jacobi smoother, though simple, may not be the optimal choice. In future work, we will study the performance of the multigrid method with other smoothers (e.g., under-relaxed Jacobi) and select the optimal smoother for the MSED method.

III. THE MSED ALGORITHM

In Algorithm 5, we assemble the components described in the previous section and describe the steps required for one complete MSED iteration. We remind the reader that the steps in Algorithm 5 are illustrated in Figure 1b. Step 2 of the MSED iteration is represented in Figure 1b by multiple orange arrows to indicate the two layers of nested iterations (V-cycles and power iterations) that are required. In step 2, M power iterations are performed and each power iteration requires some number of multigrid V-cycles to solve the fixed-source grey diffusion problem. In step 4, we do not perform a power iteration; rather, we simply update the multigroup scalar flux once by performing two V-cycles. As noted earlier, the purpose of step 2 is to converge the eigenvalue and the fission source, while

Algorithm 4: V-cycle with a red-black block Jacobi smoother for solving the fixed-source diffusion problem $\underline{\underline{M}}\underline{\phi} = \underline{g}$.

Input: $\underline{\phi}^{(q)}$
Result: $\underline{\phi}^{(q+1)}$

1. Perform one red-black block Jacobi iteration on the linear system on the original grid ($p = 0$) to obtain $\underline{\phi}^{(q+\frac{1}{2})}$.
2. Compute the residual on the original grid:
$$\underline{r}_{(0)}^{(q+\frac{1}{2})} \equiv \underline{g} - \underline{\underline{M}}\underline{\phi}^{(q+\frac{1}{2})} . \tag{19}$$
3. Traverse down the V-cycle. That is, for $p = 1, \ldots, P-1$:
   (a) Restrict the residual from grid $p-1$ to grid p:
   $$\underline{r}_{(p)}^{(q)} = \underline{\underline{I}}_{(p-1)}^{(p)} \underline{r}_{(p-1)}^{(q+\frac{1}{2})} . \tag{20}$$
   (b) Perform one red-black block Jacobi iteration on the grid p error equation,
   $$\underline{\underline{M}}_{(p)} \underline{\varepsilon}_{(p)} = \underline{r}_{(p)} , \tag{21}$$
   to obtain $\underline{\varepsilon}_{(p)}^{(q+\frac{1}{2})}$, an estimate of $\underline{\varepsilon}_{(p)}$. Here, $\underline{\varepsilon}_{(p)}$ is the coarse version of the error $\underline{\varepsilon}_{(p-1)} - \underline{\varepsilon}_{(p-1)}^{(q+\frac{1}{2})}$.
   (c) Compute the residual of the grid p error equation:
   $$\underline{r}_{(p)}^{(q+\frac{1}{2})} \equiv \underline{r}_{(p)}^{(q)} - \underline{\underline{M}}\underline{\phi}^{(q+\frac{1}{2})} . \tag{22}$$
   We note that traversing down the V-cycle is a process by which errors of errors and residuals of error equations are computed/estimated recursively.
4. Restrict the residual from grid $P-1$ to the final grid, P. Solve the error equation exactly on this grid to obtain $\underline{\varepsilon}_{(P)}^{(q+1)}$.
5. Traverse up the V-cycle. That is, for $p = P-1, \ldots, 1$, interpolate the estimate of the error from grid $p+1$ to grid p, and use this result to update the error estimate on grid p and obtain $\underline{\varepsilon}_{(p)}^{(q+1)}$:
$$\underline{\varepsilon}_{(p)}^{(q+1)} = \underline{\varepsilon}_{(p)}^{(q+\frac{1}{2})} + \underline{\underline{I}}_{(p+1)}^{(p)} \underline{\varepsilon}_{(p+1)}^{(q+1)} . \tag{23}$$
6. Interpolate $\underline{\varepsilon}_{(1)}^{(q+1)}$ to the original grid and update $\underline{\phi}^{(q+\frac{1}{2})}$:
$$\underline{\phi}^{(q+1)} = \underline{\phi}^{(q+\frac{1}{2})} + \underline{\underline{I}}_{(1)}^{(0)} \underline{\varepsilon}_{(1)}^{(q+1)} . \tag{24}$$

Algorithm 5: An MSED Iteration Step

Input: $\phi_{j,g}^{(l)}$, $\lambda^{(l)}$

Result: $\phi_{j,g}^{(l+1)}$, $\lambda^{(l+1)}$

1. Compute the grey quantities given by Eqs. (6) using the current multigroup scalar flux $\phi_{j,g}^{(l)}$ in order to construct the grey diffusion system (Eq. (5)).
2. Perform M power iterations with a space-dependent Wielandt shift on the grey diffusion equation (see Eq. (11) and Algorithm 3) to obtain the normalized grey scalar flux $\Phi_j^{(l,M)}$ and its corresponding eigenvalue $\lambda^{(l,M)}$.

   Within each PI step, the grey diffusion linear system (Eq. (5) with the ILEPS shift applied and the fission source fixed) using Q V-cycles. These V-cycles are described by Algorithm 4 and Q is the dynamically determined number of V-cycles required to converge the residual of the grey linear system to some specified tolerance.
3. Update the multigroup flux and eigenvalue using the grey diffusion results via Eqs. (8).
4. Consider the linear system in Eq. (4a), except with the iteration indices incremented by $1/2$. Perform two V-cycles on this system to obtain $\phi_{j,g}^{(l+1)}$.
5. An optional update of the eigenvalue λ may be performed here using the ratio of the magnitudes of the $(l+\frac{1}{2})$ and $(l+1)$ multigroup fission sources.

the purpose of step 4 is to converge the energy-dependence of the scattering source and, consequently, the multigroup scalar flux. The decision to use two V-cycles in step 4 will be justified by the Fourier analysis in the next section.

IV. FOURIER ANALYSIS

For each component of the MSED method, we used Fourier analysis to assess the decay rate of error modes on homogeneous problems with periodic boundary conditions. Due to the length constraints, we omit the algebraically intensive derivations from our Fourier analysis and only present a summary of the relevant results.

In a homogeneous setting with periodic boundary conditions, the ILEPS shift is equivalent to setting λ' equal to the true eigenvalue, λ_∞. The Fourier analysis in this case indicates that a power iteration with such a shift would have a spectral radius of zero [1]. This is a rather trivial result – λ_∞ is the true eigenvalue, and it should not be a surprise that it only takes one iteration to converge the problem if we already know the eigenvalue (and are able to solve a singular linear system). In real problems, however, the spectral radius is not zero due to space-dependence, heterogeneity, and/or boundary conditions. Nonetheless, as indicated in [1], it generally only takes $O(10)$ PIs to converge when the SDWS-ILEPS shift is used.

Secondly, we performed a Fourier analysis of the multigrid V-cycle on two homogeneous, multigroup, fixed-source diffusion problems with different cross sections. One set of cross sections is obtained by homogenizing the UO_2 pin cell from the C5G7 problem [14], while the other set is obtained by homogenizing the center fuel pin in the Watts Bar problem [15] with the 47-group MPACT library [2]. The results of this Fourier analysis are shown in Figure 2, where the magnitude of the decay factor $|\omega_0|$ is plotted against the spatial frequency (ξ) of the error mode. The spectral radius ρ is given by

$$\rho = \max_{\xi} |\omega_0| \tag{25}$$

and is approximately 0.1249 and 0.1250 for the C5G7 and Watts Bar cross sections, respectively. The two plots in Figure 2 are nearly identical, indicating that the multigrid V-cycles are relatively insensitive to the number of groups or the cross sections values. In the grey setting, we have found through our Fourier analysis that the spectral radius is bounded by approximately $1/8$, regardless of the values of the diffusion coefficient, cross sections, grid size, and Wielandt shift. It is more difficult to properly verify this bound in the multigroup Fourier analysis as the equations become more complex. However, we have seen in practice (i.e., in our 1-D Python code for simulating heterogeneous, multigroup problems) that the convergence of the multigrid V-cycle is approximately the same in both the multigroup and 1-group settings for all of the problems we have considered.

Next, we performed a Fourier analysis of the iteration between the MG and grey systems. Here, we assume that the grey and MG systems (steps 2 and 4) are solved exactly. Effectively, this analysis computes the spectral radius of an MSED iteration scheme in which the nested inner iterations (multigrid and PI) are converged perfectly. The analysis yields the following formula for the spectral radius:

$$\rho_{MSED} = \max_{\xi} \left[\lambda_\infty \frac{\overline{\nu\Sigma}_f}{\xi^2 \overline{D}} \left(\lambda_0 \underline{\nu\Sigma}_f - \underline{\Sigma}_a \right) + \underline{\nu\Sigma}_f - \frac{\overline{\nu\Sigma}_f}{\overline{D}} \underline{D} \right]^T \left[\underline{\underline{\Sigma}}_r + \xi^2 \underline{\underline{D}} \right]^{-1} \underline{\chi} \,. \tag{26}$$

Here, underlined quantities are $G \times 1$ column vectors, quantities with overbars (e.g., $\overline{\nu\Sigma}_f$) are scalars obtained by dotting the corresponding column vector with the infinite-medium spectrum, ξ is the spatial frequency of the error mode, $\underline{\underline{D}}$ is a diagonal matrix whose entries are the diffusion coefficients, and $\underline{\underline{\Sigma}}_r$ is a matrix whose g-th row and g'-th column is given by:

$$\Sigma_{r,g'\to g} \equiv \Sigma_{t,g}\delta_{gg'} - \Sigma_{s0,g'\to g} \,. \tag{27}$$

Because of the presence of the ξ^2 in the denominator of the first term, it is technically possible for ρ to be unbounded as $\xi \to 0$. As noted earlier, however, we have found no realistic problems for which slow convergence or divergence is an issue. In practice, we have found that most problems (such as the 1-D Watts Bar problem) converge to a tolerance of 10^{-6} in fewer than 10 MSED iterations. This is supported by the spectral radius predicted by our Fourier analysis; when we substitute

either the C5G7 or Watts Bar cross sections into Eq. (26), we obtain a spectral radius of approximately 0.1.

Lastly, we performed a Fourier analysis that allowed us to optimize the number of V-cycles performed on the multigroup diffusion system per MSED iteration. This is an important parameter since the V-cycles on the multigroup diffusion system are computationally expensive relative to the other steps in the MSED iteration scheme. In our Fourier analysis, we allowed N, the number of multigroup V-cycles per MSED iteration, to vary and computed the spectral radius for several values of N. The results, shown in Figure 3, show that the spectral radius is nearly unchanged by increasing N beyond 2. Thus, there is essentially no additional benefit from performing more than 2 multigroup V-cycles per MSED iteration, and our choice of $N = 2$ in step 4 of Algorithm 5 is justified.

V. 1-D RESULTS

To test the MSED method, we have developed a Python code for solving heterogeneous, multigroup diffusion eigenvalue problems in 1-D. Results from the code are shown in Table I for a 1-D Watts Bar problem using the MPACT 47-group library. This 1-D Watts Bar problem is generated from the center row of pin cells in the 2-D Watts bar problem described in [15]. In our simulation, Δx is equal to the width of a pin cell and the cross sections are homogenized over each pin cell.

Overall, the results in Table I demonstrate the efficiency of the MSED method in solving 1-D diffusion eigenvalue problems. More specifically, these results provide a sense of the benefit introduced by (1) leveraging the grey diffusion system in the power iteration scheme and (2) using a multigrid linear solver instead of other iterative linear solvers such as BiCGSTAB. When the grey diffusion system is used, the number of inner linear solver iterations required is reduced by an order of magnitude and the runtime is reduced by a factor of approximately 4. Moreover, the runtime is also reduced by a factor of 5-6 when a multigrid linear solver is used instead of BiCGSTAB (with a block Jacobi preconditioner). The benefit of using SDWS-ILEPS is not explicitly shown in these results; the acceleration provided by SDWS-ILEPS has already been discussed in [1] and will be discussed in greater detail in future work.

The ultimate goal of our work on the MSED method is to develop a method that efficiently solves large, multigroup, 2-D/3-D diffusion eigenvalue problems. Although a method that is efficient in 1-D is not necessarily efficient in 2-D or 3-D, the results in this section serve as a proof of principle and show the potential of the MSED method. The bulk of our immediate future work will consist of implementing the MSED method as a solver for the CMFD problem in MPACT. This is not a trivial task and many challenges will have to be overcome in order for MSED to perform as efficiently as possible in MPACT. These challenges include implementing the multigrid linear solver in parallel, finding the most efficient smoother for multigrid, and optimizing P in Algorithm 5. As we implement and test the MSED method in MPACT, we will likely need to make small changes to the MSED method, and the final details of the MSED algorithm will likely differ from that presented in this paper. Future work will also include comparison of MSED to other methods such as the Generalized Davidson method [16], testing MSED on boiling water reactor problems and fast reactor problems, and possibly extending the MSED method so that it can work for unstructured grids and/or other spatial discretizations.

VI. CONCLUSION

We have developed a new method – the MSED method – for efficiently solving multigroup diffusion eigenvalue problems. The MSED method can be thought of as a power iteration scheme with three additional features: (1) acceleration of power iteration on the multigroup diffusion system via the solution of a grey diffusion system, (2) acceleration of power iteration via a space-dependent Wielandt shift, and (3) the use of a multigrid in space linear solver for the linear solves required by each power iteration step. Alternatively, the MSED method can also be viewed as an extension of the multigrid method to non-spatial variables (see Figure 1b) or a multilevel extension of the CMFD method (see Figure 1a). Results from our Fourier analysis and 1-D code indicate that our new MSED method can efficiently solve the multigroup diffusion eigenvalue problem. We recognize that the specific 1-D performance results may not necessarily carry over to 2-D/3-D problems in parallel. In future work, we will implement the MSED method into MPACT as a solver for the CMFD system, and adjust the MSED method as necessary so that it is optimized for our particular application.

VII. ACKNOWLEDGMENTS

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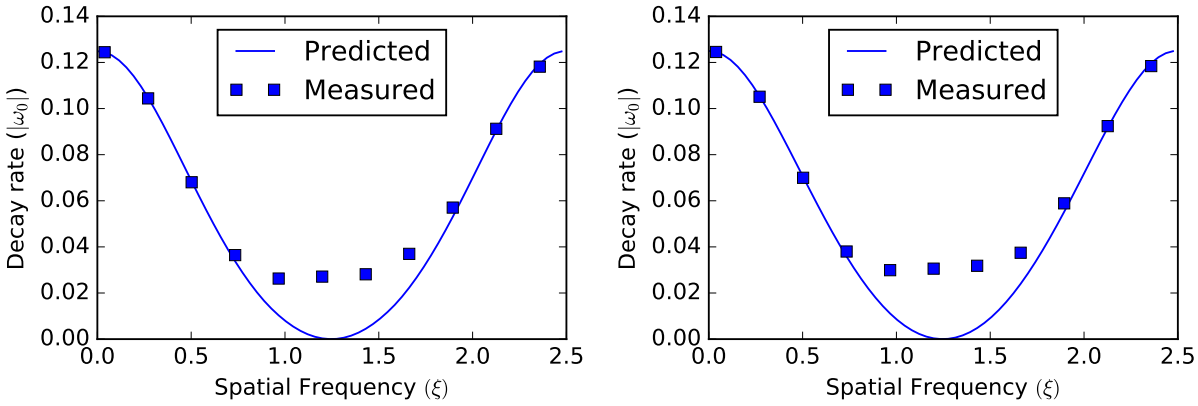
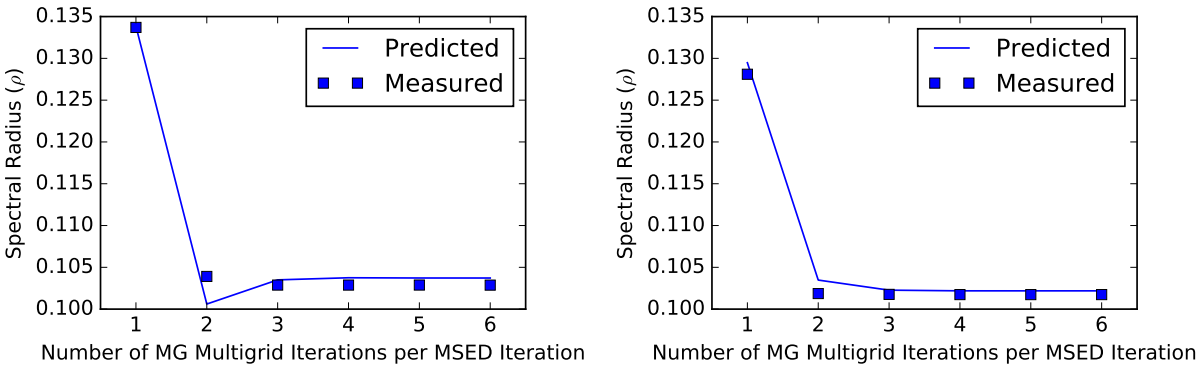


(a) C5G7 UO_2 fuel pin, $\rho = 0.1249$.

(b) Watts Bar center pin, 47G MPACT lib, $\rho \approx 0.1250$.

Fig. 2: Results of our Fourier analysis of a V-cycle (Algorithm 4) for two sets of cross sections. The solid line is the decay factor predicted by our Fourier analysis, while the square symbols represent numerical results. The disagreement in the measured and predicted values for very low decay rates is due to the numerical precision limits in the code used to verify the Fourier analysis; the toy problems converge so rapidly in these cases that it is difficult to measure the spectral radius.



(a) C5G7 UO_2 fuel pin.

(b) Watts Bar center pin, 47G MPACT lib.

Fig. 3: Spectral radius of an MSED iteration versus the number of multigroup V-cycles performed per MSED iteration. The solid line is the spectral radius predicted by the Fourier analysis, while the square symbols represent numerical results.

TABLE I: Results for a 1-D Watts Bar problem [15] using a 1-D Python test code and the MPACT 47G library. "Solves" refer to the number of times the method attempts to solve (partially or fully) the grey or MG system, while "inners" refer to the number of linear solver iterations (i.e., the number of V-cycles or BiCGSTAB iterations). Serial runtimes are provided in the final column. For the BiCGSTAB results, a block-Jacobi preconditioner was used.

Method	Grey Solves	Grey Inners	MG Solves	MG Inners	Runtime [s]
Alg. 5 (MSED)	69	469	7	12	9.0
Alg. 5 w/ multigrid replaced by BiCGSTAB	70	6726	7	448	46.8
Alg. 3 w/ ILEPS shift and Multigrid	–	–	17	175	34.6
Alg. 3 w/ ILEPS shift and BiCGSTAB	–	–	17	2184	185.8

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