Solving Eigenvalue Response Matrix Equations with Nonlinear Techniques

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Abstract

This paper presents new algorithms for use in the eigenvalue response matrix method (ERMM) for reactor eigenvalue problems. ERMM spatially decomposes a domain into independent nodes linked via boundary conditions approximated as truncated orthogonal expansions, the coefficients of which are response functions. In its simplest form, ERMM consists of a two-level eigenproblem: an outer Picard iteration updates the k-eigenvalue via balance, while the inner λ-eigenproblem imposes neutron balance between nodes. Efficient methods are developed for solving the inner λ-eigenvalue problem within the outer Picard iteration. Based on results from several diffusion and transport benchmark models, it was found that the Krylov-Schur method applied to the λ-eigenvalue problem reduces Picard solver times (excluding response generation) by a factor of 2–5. Furthermore, alternative methods including Picard acceleration schemes, Steffensen's method, and Newton's method are developed. These approaches can yield faster k convergence and a need for fewer k-dependent response function evaluations, important because response computation is the largest cost for many problems. It was found that accelerating Picard iteration yields a reduction of 2–3 in total time compared to the unaccelerated case for problems dominated by response generation but that Newton's method may provide nearly the same performance with improved robustness.

Keywords:
response matrix, reactor physics, neutron transport, eigenvalue

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1. Introduction and Background

Fundamental to reactor modeling is analysis of the steady-state balance of neutrons, described concisely as

$$\mathbf{T}\phi(\vec{\rho}) = \frac{1}{k}\mathbf{F}\phi(\vec{\rho}), \tag{1}$$

where the operator **T** describes transport processes, **F** describes neutron generation, ϕ is the neutron flux, $\vec{\rho}$ represents the relevant phase space, and k is the eigenvalue, the ratio of the number of neutrons in successive generations.

For the past several decades, full core analyses for light water reactors (LWR) have been performed using relatively low fidelity nodal methods based on clever homogenization of phase-space with proven success. However, for more aggressive fuel loadings (including MOX) and longer cycle lengths in existing LWR's, these methods are becoming less applicable, and for new, highly heterogeneous reactor designs, even less so. While advances in production nodal codes including use of generalized multigroup SP_3 transport with subassembly resolution address several important issues [1], there likely is limited room for further improvement of the underlying approach.

Consequently, a move toward full core analysis techniques that can leverage the high fidelity methods typically used for smaller problems is desired. One such approach is the response matrix method, which is based on a spatial decomposition of the global problem of Eq. 1 into local fixed source problems connected by approximate boundary conditions.

1.1. The Eigenvalue Response Matrix Method

The response matrix method (RMM) has been used in various forms since the early 1960's [2]. Using the terminology of Lindahl and Weiss [3], the method can be formulated using explicit volume flux responses, called the "source" RMM, or by using current responses that include fission implicitly and hence are functions of k, known as the "direct" RMM. While both methods are used in various nodal methods, the former is more widespread; the focus of this work is on the latter, which shall be referred to as the *eigenvalue* response matrix method (ERMM) for clarity.

Various formulations of ERMM have been proposed since its first use. Here, a rather general approach is described that is based on expansions of the boundary conditions that couple subvolumes of the global problem, a formalism introduced as early as the work of Lindahl [4] and studied more recently by several authors [5, 6, 7].

Suppose the global problem of Eq. 1 is defined over a volume V. Then a local homogeneous problem can be defined over a subvolume V_i subject to

$$\mathbf{T}\phi(\vec{\rho}_i) = \frac{1}{k}\mathbf{F}\phi(\vec{\rho}_i), \tag{2}$$

and

$$J_-^{\text{local}}(\vec{\rho}_{is}) = J_-^{\text{global}}(\vec{\rho}_{is}), \tag{3}$$

where $J_-^{\text{local}}(\vec{\rho}_{is})$ is a function of the incident boundary flux, typically the partial current, which quantifies net flows through a surface.

To represent the local problem numerically, an orthogonal basis, P_n, over the relevant phase space is defined

$$P_n(\vec{\rho}_{is}),\ \ n = 0, 1, \ldots N \tag{4}$$

subject to

$$\int P_m(\vec{\rho}_{is})P_n(\vec{\rho}_{is}) = \delta_{mn} d\rho_{is}\,. \tag{5}$$

A response equation is defined

$$\mathbf{T}\phi_i^{ms}(\vec{\rho}_i) = \frac{1}{k}\mathbf{F}\phi_i^{ms}(\vec{\rho}_i) \tag{6}$$

subject to

$$J_-^{\text{local}}(\vec{\rho}_{is}) = P_m(\vec{\rho}_{is})\,. \tag{7}$$

The resulting outgoing currents $J_-(\vec{\rho}_{is})$ are used to define response functions

$$r_{im's'}^{ms} = \int P_n(\vec{\rho}_{is})J_{i+}^m(\vec{\rho}_{is'})d\rho_{is}\,. \tag{8}$$

The quantity $r_{im's'}^{ms}$ has a simple physical interpretation: it is the m'th order response out of surface s' due to a unit incident mth order condition on surface s of subvolume i.

The incident and outgoing currents are expressed as truncated expansions using the same basis

$$J_{is\pm}(\vec{\rho}_{it}) \approx \sum_{n=0}^{N} j_{is_\pm}^n P_n(\vec{\rho}_{is}) \tag{9}$$

where

$$j_{is_\pm}^n = \int P_n(\vec{\rho}_{is})J_\pm(\rho_{is})d\rho_{is}\,. \tag{10}$$

These coefficients are then represented in vector form as

$$\mathbf{J}_{i\pm} = (j^0_{i1_\pm}\, j^1_{i1_\pm} \cdots j^0_{i2_\pm}\, j^1_{i2_\pm} \cdots j^N_{iS_\pm})^\mathsf{T}\,, \tag{11}$$

and using these together with Eq. 8 yields the nodal balance equation

$$\mathbf{J}_{i+} = \begin{bmatrix} j^0_{i1_+} \\ j^1_{i1_+} \\ \vdots \end{bmatrix} = \begin{bmatrix} r^{01}_{i01} & r^{11}_{i01} & \cdots \\ r^{01}_{i11} & r^{11}_{i11} & \cdots \\ & & \ddots \end{bmatrix} \begin{bmatrix} j^0_{i1_-} \\ j^1_{i1_-} \\ \vdots \end{bmatrix} = \mathbf{R}_i \mathbf{J}_{i-}\,. \tag{12}$$

Global balance is defined by the eigenvalue response matrix equation

$$\mathbf{MR}(k)\mathbf{J}_- = \lambda \mathbf{J}_-\,, \tag{13}$$

where $\mathbf{R}$ is the block diagonal response matrix of $\mathbf{R}_i$, $\mathbf{J}_-$ are vectors containing all incident current coefficients, $\mathbf{M} = \mathbf{M}^\mathsf{T}$ is the connectivity matrix that redirects outgoing responses as incident responses of neighbors, superscript T represents the matrix transpose, and λ is the current eigenvalue. If the response matrix $\mathbf{R}$ is conservative (i.e. it strictly maintains neutron balance),

$$\lim_{k \to k^*} \lambda = 1\,, \tag{14}$$

where k^* is the true eigenvalue. For nonconservative response expansions, the deviation of λ from unity measures the discontinuities introduced across node boundaries and may be used to evaluate the accuracy of the expansions used (with respect to an infinite expansion).

1.2. Survey of ERMM Implementations

The method defined by Eqs. 2-12 has its roots in the work of Shimizu et al. [8, 2], which represents what appears to be the first work on response matrix methods. While independent from it, those authors acknowledge a connection between their work and the earlier and more general theory of invariant imbedding as developed by Bellman *et al.* [9]. This initial work was based on 1-D diffusion in slab geometry. Aoki and Shimizu extended the approach to two dimensions, using a linear approximation in space to represent boundary currents [10]. A fundamental shortcoming of this early work is what seems to be an assumed value (unity) of the k-eigenvalue when evaluating responses. Since k is typically around unity for nuclear reactors, the errors observed are only tens of pcm, which in general is pretty good, but in their case may be deceptively small. In the later 2-D analysis, the results observed compared favorably to fine mesh diffusion calculations.

Weiss and Lindahl generalized the method by considering arbitrarily high order expansions of the boundary currents in Legendre polynomials [11], while also accounting for k explicitly. Lindahl further studied expansions of the current, comparing Legendre expansions to an approach that divides the boundary in several segments in which the current is taken to be flat [4]. A more complete overview of these approaches can be found in the review by Lindahl and Weiss [3].

These diffusion-based methods all rely on semi-analytic solutions to the diffusion equation and hence require homogeneous nodes. In the initial scoping studies performed in support of the present paper, diffusion-based responses using discretized operators were examined [6]. By numerically integrating the diffusion equation, heterogeneous nodes are treated naturally, though no diffusion models having heterogeneous nodes were studied.

In addition to methods based on diffusion theory, work was also done to use transport theory in generating responses. Pryor *et al.* used what might be now called a hybrid approach, employing Monte Carlo coupled with the collision probability method to generate responses [12, 13, 14]. That work is unique in its definition of the response matrix $\mathbf{R}(k)$. Considering again Eq. 2, the solution ϕ (omitting indices) can be expressed as

$$\phi = \phi_0 + \frac{1}{k}\phi_1 + \frac{1}{k^2}\phi_2 + \dots , \tag{15}$$

where ϕ_i is the flux for the ith neutron generation due to fission. The associated responses can be similarly defined

$$\mathbf{R}(k) = \mathbf{R}_0 + \frac{1}{k}\mathbf{R}_1 + \frac{1}{k^2}\mathbf{R}_2 + \dots . \tag{16}$$

The authors claim this series can be truncated in as few as three terms by estimating the analytical sum, though it is not clear with what accuracy [14]. Note that when no fissile material is present, $\phi_i = 0$ for $i > 0$, and so $\mathbf{R}(k) = \mathbf{R}_0$.

A somewhat similar approach was taken by Moriwaki et al. [15] in which Monte Carlo was used to generate responses, nominally for application to full assemblies for full core analyses. Their method decomposes the response matrix into four physically distinct components: transmission of incident neutrons from one surface to another surface (T), escape of neutrons born in the volume out of a surface (L), production of neutrons in the volume due to neutrons born in the volume (A), and production of neutrons in the volume due to neutrons entering a surface (S). If all indices but the surface are neglected, a current response can be expressed as

$$r_t^s = T_t^s + \frac{1}{k}S^s(L_t + \frac{1}{k}A(L_t + \frac{1}{k}A(L_t + \cdots)) + \cdots) . \tag{17}$$

Like Eq. 16, this infinite sum represents the contributions of each generation to the total response. The matrices **T**, **L**, **A**, and **S** are precomputed, and the full matrix **R** is computed on-the-fly by iteration. In the actual implementation, the volume-dependent responses are unique for each pin in an assembly. Additionally, spatial segmentation was used on boundaries, but angular dependence was neglected.

The more recent extension of Ishii *et al.* addressed this latter limitation by including angular segmentation, increasing the achievable fidelity. However, the resulting amount of data required is quite significant, since the responses are then dependent on spatial segment, angular segment, energy group, and for volume responses, unique pins. For this reason, it seems as though the approach contained in Eq. 16 might be more economical, as no volume-dependent responses are required. Of course, obtaining pin reaction rates would require such responses to be available but would preclude their use in solving Eq. 13.

Other related work has been development of the incident flux expansion method [16, 5]. The initial work by Ilas and Rahnema focused on a variational approach using a basis consisting of Green's functions for each variable using one-dimensional discrete ordinates [16]. Mosher and Rahnema extended the method to two dimensions, again using discrete ordinates, and used discrete Legendre polynomials for space and angle expansions. Additionally, they introduced a nonvariational variant that is equivalent to ERMM, though without explicit construction of matrices. Forget and Rahnema further extended this nonvariational approach to three dimensions using Monte Carlo, with continuous Legendre polynomials in space and angle [17]. In all cases, the responses were precomputed as functions of the k-eigenvalue, and linear interpolation was used to compute responses during global analysis.

1.3. Major Challenge

To apply ERMM even to realistic steady state analyses including feedback effects entails several challenges, the chief of which is the shear number of responses functions and hence transport solves required. Of course, these response functions are entirely independent for a given state and k, and so parallelization is a natural part of the solution.

In much recent work, responses were pre-computed as a function of k and interpolated as needed. In many cases, clever use of symmetry can further minimize the required data. For benchmark problems, this is sensible, but as the effects of thermal feedback are included, each node becomes unique. As such, precomputation of responses would require dependence on several variables, in addition to k, be included in some manner. There seems at this time no completely satisfactory way to parameterize a response function database for

accurate steady state analyses. The problem is further exacerbated if burnup is included for cycle analyses. Recent work has attempted to parameterize the responses for steady state analysis of cold critical experiments [18]. While the results are promising (sub-percent errors on pin fission rates—though which error and what norm used are not clearly noted), the problem assessed is not entirely representative of the problems of interest here.

Consequently, this paper focuses on ERMM implementations suitable for on-the-fly generation of response functions, as this seems at present to be the only meaningful manner in which to apply ERMM. Of course, any successes achieved in this context would be readily applicable for generation of response databases, should an adequate parameterization scheme be developed in the future.

1.4. Goals

The primary goal of this work is to develop a response matrix method that can efficiently leverage high fidelity deterministic transport methods for solving large scale reactor eigenvalue problems on a variety of computer architectures. Several solvers that support this goal are developed in this paper, the remainder of which is organized as follows. Section 2 discusses solution of the response matrix equations via fixed point iteration and methods for solving the resulting eigenvalue problem for λ efficiently. Section 3 presents schemes that provide faster convergence in k than standard fixed-point iteration, which is important since the number of k-evaluations defines the number of responses evaluated. A numerical study of the methods using several benchmark problems is provided in Section 4 followed by concluding remarks in Section 5.

2. Solving the λ-Eigenvalue Problem

The k-eigenvalue can be interpreted physically as the ratio of neutrons produced in one generation to the previous generation. This can alternatively be viewed as the ratio of gains to losses in a given generation. Applying this interpretation to the response matrix formalism, k can be updated via the process

$$f(k) = k_{n+1} = \frac{\mathbf{F}(k_n)\mathbf{J}_-}{\mathbf{A}(k_n)\mathbf{J}_- + \mathbf{L}(k_n)\mathbf{J}_-}, \tag{18}$$

where $\mathbf{F}(k)\mathbf{J}_-$ is the global fission rate, $\mathbf{A}(k)\mathbf{J}_-$ is the global absorption rate, and $\mathbf{L}(k)\mathbf{J}_-$ is the total leakage rate from global boundaries.

Equations 13 and 18 represent a Picard (fixed point) iteration for the k-eigenvalue. For each new k value, however, the λ-eigenvalue problem defined by Eq. 13 must be solved.

Historically, the method to solve Equation 13 amounts to simple power iteration. For a given $k^{(n)}$, the current vector is guessed and normalized, $\mathbf{MR}(k^n)$ is applied to the guess, and the resulting vector points closer to the dominant eigenvector of interest. The result is normalized, and the process repeats until converged.

Unfortunately, the asymptotic convergence rate to the dominant mode is equal to $\ln(1/\rho)$, where the dominance ratio ρ is defined

$$\rho = |\lambda_2|/|\lambda|, \tag{19}$$

and the eigenvalues of **MR** satisfy $\lambda > |\lambda_2| \geq |\lambda_i|, \ \forall\, i > 2$. For many problem, ρ typically falls above 0.99, significantly larger than the dominance ratio associated with k.

Due to the large ρ, 1000's of iterations are required to reduce residual norms $||\mathbf{MRJ}_- - \lambda \mathbf{J}_-||$ to within the tolerances used in the analysis below. Chebyshev acceleration was considered for accelerating convergence, but its utility is severely limited due to the nature of the eigenspectrum of **MR**, a significant portion of which sits away from the real axis . For a typical problem, previous work showed that the expected (theoretical) speedup is limited to about 2, as opposed to the factor of 20 gained were the spectrum completely real [7]. Despite these theoretical limitations, Chebyshev acceleration was recently used successfully for solving the inner problem [19]. However, it seems likely its success would be highly problem-dependent and subject to significant tuning, two features worth avoiding if possible.

More efficient eigenvalue solvers such as Krylov subspace methods can be used. Krylov methods are based on generation of a Krylov subspace of dimension n, defined for an $m \times m$ operator **A** as

$$\mathscr{K}(n, x_0) \equiv \text{span}\{x_0, \mathbf{A}x_0, \mathbf{A}^2 x_0, , \ldots, , \mathbf{A}^{m-1} x_0\}, \tag{20}$$

for some initial, possibly random, vector x_0. The main idea of any Krylov subspace method is to find $x \in \mathscr{K}(m, x_0)$ that "best" solves the system of interest, be it an eigenproblem or linear system, where it is assumed that $m \ll n$.

Working with $\mathscr{K}(n, x_0)$ directly is difficult numerically, since repeated application of **A** sends the initial vector x_0 into the same direction, namely that of the dominant eigenvector of **A**. Hence, the basis must be orthogonalized. The canonical approach for nonsymmetric operators is Arnoldi's method, which by successive application of the modified Gram-Schmidt process yields the Arnoldi decomposition

$$\mathbf{AV} = \mathbf{VH} + f e_m^{\mathsf{T}}, \tag{21}$$

where $\mathbf{V} \in \mathbb{R}^{m \times n}$ consists of orthonormal columns, $\mathbf{H} \in \mathbb{R}^{n \times n}$ is an upper Hessenberg matrix, e_n is the n-vector of all zeros except a one in the nth location, and f is the residual, which is orthogonal to the columns of $\mathbf{V}$.

It turns out that the eigenvalues of $\mathbf{H}$, called "Ritz values", tend to be good estimates of eigenvalues of $\mathbf{A}$, and given an eigenpair $(\tilde{\lambda}, y)$ of $\mathbf{H}_m$, the Rayleigh-Ritz estimate of the corresponding eigenvector of $\mathbf{A}$ is defined $x = \mathbf{V}_m y$, and is called a "Ritz vector". This is the basis of Arnoldi's method for eigenvalue problems.

The eigenpairs of $\mathbf{H}$ are found via a dense eigensolver, such as the QR method. While this is done on a small system (since $m \ll n$), it is done repeatedly for increasing m until some criterion is met. If m becomes too large, the dense methods become too expensive. To circumvent this issue, the Arnoldi method must be restarted. In the *explicitly* restarted Arnoldi method (ERAM), some combination of the existing m Ritz vectors is used to choose a single starting guess, from which a new Arnoldi factorization is generated [20]. An alternative to explicit restart is *implicit* restart, where the desired portion of the spectrum is retained continuously by contracting from a subspace of dimension m to a smaller space of size p and mapping back to the larger space. Several methods implement this idea, and the one used here is the Krylov-Schur (KS) method [21], which transforms a general Krylov decomposition (of which the Arnoldi decomposition is a special case) into a Krylov-Schur decomposition, where the upper Hessenberg matrix $\mathbf{H}$ above becomes a strictly upper triangle matrix $\mathbf{T}$. Using this decomposition, it is comparatively easier numerically to keep the desired spectral information, and the method can be more efficient than other implicitly-restarted algorithms [20].

3. Acceleration k-convergence

The convergence properties of the fixed-point iteration are generally favorable [22], but in many cases, better convergence in k is desirable. Because responses must be recomputed for each new value of k, methods that minimize the number of unique k values are critical for efficient application of ERMM.

3.1. Accelerating Fixed Point Iteration

In this section, several techniques are studied for accelerating the fixed point iteration in k. All the methods are based on some form of extrapolation with respect to k, and hence no machinery beyond that needed for the fixed point iteration is required for their use.

3.1.1. Regula Falsi and Related Methods

Recall that the current eigenvalue λ approaches unity in the limit $k \to k^*$. For conservative responses with negligible iteration error, λ tends to *exactly* unity. Various schemes have been used to capitalize on this relationship. In each case, an initial guess k_0 is made for which the corresponding λ_0 is found. Subsequently, k_1 is selected, potentially via balance, and λ_1 is computed. All successive values k_n are selected so that $\lambda_n \approx 1$. Such a scheme is often called *regula falsi* or the *method of false points* [4].

Lindahl studied the relationship between λ and k and found that $\tilde{k} = 1/k$ varies quite linearly with $\tilde{\lambda} \propto 1/\lambda$. Lindahl extended the concept by storing three or more pairs for interpolation via higher order polynomials [4].

Anghel and Gheorghu [23] modified the approach of Lindahl by assuming the exponential relation

$$\lambda \propto a e^{b/k}. \tag{22}$$

Because response functions tend to have exponential dependence on k, they assumed that would also apply to the current eigenvalue. As the results below will indicate, this form compares favorably with Lindahl's.

A more recent study by Forget and Rahnema [24] rediscovered the relationship between k and λ, the latter of which they denoted the "normalization constant." Moving from a k-update via balance, they assumed the relation $k \propto 1/\lambda$ and found good results. In theory, it is reasonable to expect this to be the case. Previous work [22] showed using one group diffusion theory that

$$\frac{d\lambda}{dB} \propto B \tag{23}$$

for small buckling $B = \sqrt{\nu\Sigma_f/k - \Sigma_a}$, which suggests

$$\lambda \approx aB^2 + b \approx \frac{a'}{k} + b'. \tag{24}$$

Interestingly, Lindahl found that $k^{-1} \propto \lambda^{-1}$ produced better results, having compared to both $k \propto \lambda^{-1}$ and $k \propto \lambda$ (though without giving numerical results) [4].

All four two-term schemes have been implemented and are assessed in the results to follow. A key limitation of these schemes is that they depend on λ getting to unity, or at least close enough so that its departure from unity is within the convergence criteria used. If either the responses or the inner iterations are poorly converged, or the response expansions are not conservative, the schemes can become unstable.

3.1.2. Steffensen's Method

A similar approach is Steffensen's method, which like the extrapolation schemes, relies on a sequence of evaluations of the fixed point. Steffensen's method can be written as the one step fixed point iteration

$$k_{n+1} = g(k_n) = k_n - \frac{(f(k_n) - k_n)^2}{f(f(k_n)) - 2f(k_n) + k_n}. \tag{25}$$

This process has second order convergence, meaning the error diminishes with the square of n. This can be demonstrated by expanding $g(k)$ about the fixed point $g(k^*) = k^*$, yielding

$$g(k) = k^* + \Delta g'(k^*) + \frac{\Delta^2}{2} g''(k^*) + \mathcal{O}(\Delta^3). \tag{26}$$

To be (at least) second order, $g'(k^*)$ must vanish. Here,

$$\begin{aligned} \lim_{k \to k^*} g'(k) &= 1 - \frac{2(k - f(k))(1 - f'(k))}{f(f(k)) - 2f(k) + k} \\ &\quad + \frac{(k - f(k))^2 (f'(f(k))f'(k) - 2f'(k) + 1)}{(f(f(k)) - 2f(k) + k)^2} \\ &= 1 - (2) + (1) \\ &= 0, \end{aligned} \tag{27}$$

where the second two terms are reduced via L'Hôpital's rule. Hence, $k_{n+1} - k^* = \mathcal{O}(\Delta^2)$, so the method is second order as stated.

In practice, Steffensen's method is highly sensitive to the accuracy of the sequence estimates. Within ERMM, it has been observed that Steffensen's method becomes unstable unless very small tolerances ($\approx 10^{-9}$) are used for solving the λ-eigenvalue problem [7]. Furthermore, once the responses are evaluated for the initial guess, each successive Steffensen iteration requires two response evaluations. In general, the savings gained by second order convergence may or may not outweigh the cost of additional evaluations depending on the problem.

3.2. Newton Methods

The eigenvalue response matrix problem has been recognized as being nonlinear since it was first solved, but it does not appear to have been cast in a form for solution directly by Newton-based methods until quite recently [6, 25].

The eigenvalue response matrix equation, k update equation, and L_2 normalization of J_- can be written as the nonlinear residual

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} (\mathbf{MR}(k) - \lambda\mathbf{I})\mathbf{J}_- \\ \mathbf{F}(k)\mathbf{J}_- - (k\mathbf{L}(k)\mathbf{J}_-) \\ \frac{1}{2} - \frac{1}{2}\mathbf{J}_-^{\mathbf{T}}\mathbf{J}_- \end{bmatrix} = \mathbf{0}, \tag{28}$$

and the associated Jacobian is defined

$$\mathbf{f}'(\mathbf{x}) = \begin{bmatrix} (\mathbf{MR} - \lambda\mathbf{I}) & \mathbf{MR_k}\mathbf{J}_- & -\mathbf{J}_- \\ (\mathbf{F} - k\mathbf{L}) & (\mathbf{F_k} - k\mathbf{L_k} - \mathbf{L})\mathbf{J}_- & 0 \\ -\mathbf{J}_-^{\mathbf{T}} & 0 & 0 \end{bmatrix}, \tag{29}$$

where the k subscripts indicate partial differentiation. For $\mathbf{R}(k)$ of size $m \times m$, the Jacobian is of size $(m+2)\times(m+2)$. Moreover, after one evaluation of the response quantities, only the first $m+1$ rows of the $(m+1)$th column of $\mathbf{f}'$ are not known *a priori*, and that unknown column requires only one additional evaluation of the response quantities to allow for a finite difference approximation of the partial derivatives with respect to k. Hence, like Steffensen's method, Newton's method requires two evaluations of k per iteration, if the latter approximates the derivative via functions evaluated at k and $k + \delta k$. Typically, a value of $\delta k \approx \sqrt{\epsilon_{\text{machine}}} \approx 10^{-8}$ is close to optimal. However, at potentially reduced performance, the finite difference can use previous values of k; in this case, convergence would likely improve every iteration as successive k values approach the solution.

3.2.1. Newton's Method

Newton's method [26] solves a nonlinear system via the sequence

$$\mathbf{s} = -\mathbf{f}'(\mathbf{x}^{(n)})^{-1}\mathbf{f}(\mathbf{x}^{(n)}) \tag{30}$$

where $\mathbf{s}$ is the Newton step, and the Newton update is

$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} + l\mathbf{s}, \tag{31}$$

with a step length l defined to guarantee a decrease in $||\mathbf{f}(\mathbf{x})||_2$. If a solution $\mathbf{x}^*$ exists, and $\mathbf{f}'$ is Lipschitz continuous near and nonsingular at $\mathbf{x}^*$, then Newton's method is known to exhibit quadratic convergence [26].

For the nonlinear residual of Eq. 28 and Jacobian of Eq. 29, these constraints appear to be true in practice. For a standard, non-parameterized eigenvalue problem $Ax = \lambda x$, Peters and Wilkinson [27] have shown the associated

Jacobian (akin to Eq. 29 without the the $(m+1)$th column and row) is non-singular at the solution if λ is simple (which is true for the dominant mode of interest [3]); however, it does not appear this is always true for the full Jacobian in Eq. 29, though in practice the conditions for singularity have not been encountered.

3.2.2. Inexact Newton and JFNK

An *inexact* Newton method uses an approximate linear solve for the Newton step satisfying

$$||\mathbf{f}'(x^{(n)})\mathbf{s} + \mathbf{f}(\mathbf{x}^{(n)})||_2 \leq \eta ||\mathbf{x}^{(n)}||_2 \,, \tag{32}$$

where η is the "forcing term" that may vary at each iteration [26]. The inexact solution of the Newton step necessarily impacts convergence of Newton's method, but typically convergence remains superlinear. While any iterative linear solver could be used, the focus here is on Krylov solvers, leading to Newton-Krylov methods.

Since solving for $\mathbf{s}$ involves only the action of the Jacobian, the Jacobian need not be explicitly formed. Then Newton-Krylov methods become Jacobian-Free Newton-Krylov (JFNK) methods, for which Knoll and Keyes provide an extensive survey [28]. If the action of $\mathbf{MR}$ were performed in a matrix-free manner, the same algorithm could be used in evaluating the action of $\mathbf{f}'$ for a fully matrix-free approach.

Often in the context of JFNK, the action of the Jacobian is approximated as a finite difference approximation; however, since the Jacobian in Eq. 29 is defined almost entirely *a priori*, only a relatively small portion of the action need be approximated via finite differences. This is critical for on-the-fly response generation, for which evaluation of k-dependent responses is the dominant cost, since each Krylov vector generally represents a perturbed k.

3.2.3. Preconditioning JFNK

The key to effective use of Krylov-based linear solvers is often adequate preconditioning. For JFNK, a preconditioner $\mathbf{M}$ is in some way "close" to the Jacobian $\mathbf{f}'$ but is easier to construct or apply. Moreover, $\mathbf{M}$ can be applied either to the left, yielding the system $\mathbf{M}^{-1}\mathbf{f}'\mathbf{s} = -\mathbf{M}^{-1}\mathbf{f}$, or to the right by solving $\mathbf{f}'\mathbf{M}^{-1}\tilde{\mathbf{s}} = -\mathbf{f}$ and setting $\mathbf{s} = \mathbf{M}^{-1}\tilde{\mathbf{s}}$.

4. Numerical Results

In this section, the solvers developed in Section 3 are applied to several benchmark problems. The goal is to determine which of the various algorithms

is best suited for solving response matrix equations. All response matrix calculations are performed using `Serment`, a parallel eigenvalue response matrix code, while all responses by linking to libraries of `Detran`, a deterministic transport code based on the discrete ordinates, method of characteristics, and diffusion approximations, and having implementations of several modern transport solvers developed specifically for the fixed-source problems characteristic of response generation [29]. `Serment` and `Detran` use several external packages, including PETSc [30] and SLEPc [20] for various linear and nonlinear solvers.

Several diffusion and transport benchmarks were studied. These include the 2-D and 3-D IAEA [31], the 2-D Biblis [32], and 2-D Koeberg diffusion benchmarks as well as the 2-D C5G7 [33] and 3-D Takeda [34] transport benchmarks. For all problems, the multigroup dependence is exactly treated while the spatial dependence is expanded in discrete Legendre polynomials [5, 35] DLPs.

For the diffusion problems, each 2-D assembly is discretized using a uniform 20×20 spatial mesh, corresponding roughly to 1 cm square cells. For the 3-D IAEA problem, 20 cm cubes are represented by a $10 \times 10 \times 10$ spatial mesh to reduce the size of the reference calculation. A mesh-centered finite volume discretization is used throughout.

For the 2-D C5G7 problem, pin cells are represented with a non-uniform, volume-conserving 7×7 mesh. The DLP basis on non-uniform meshes is *not* conservative, meaning λ does not approach unity. For the 3-D Takeda benchmark, 5 cm cubes are represented using a uniform 0.25 cm spatial mesh in all directions. Both problems are modeled using the discrete ordinates method in angle with the diamond difference approximation in space.

For the transport benchmarks, the angular dependence is expanded in DLPs for the angular flux or angular current, or a conservative basis based on Chebyshev, Legendre, and/or Jacobi polynomials [35, 19] for the angular flux. For all cases, a product quadrature is employed that exactly integrates the conservative basis moments [35].

When computing responses, no symmetry is considered. For homogeneous problems, exploiting symmetry would reduce the number of responses by a factor of 4 in 2-D or a factor of 6 in 3-D. Such tricks are of course handy for benchmarking, but in reality, reactor assemblies are only symmetric at beginning-of-life (and that is on the order of 1/3 of the core fuel), and even then, only at cold zero power. Once any realistic treatment of temperature feedback is considered, all symmetry is lost, and hence there is essentially no insight to be gained from artificially reducing the problem size.

Unless stated otherwise, convergence is defined by $||\mathbf{f}||_2 \leq 10^{-7}$, where $\mathbf{f}$

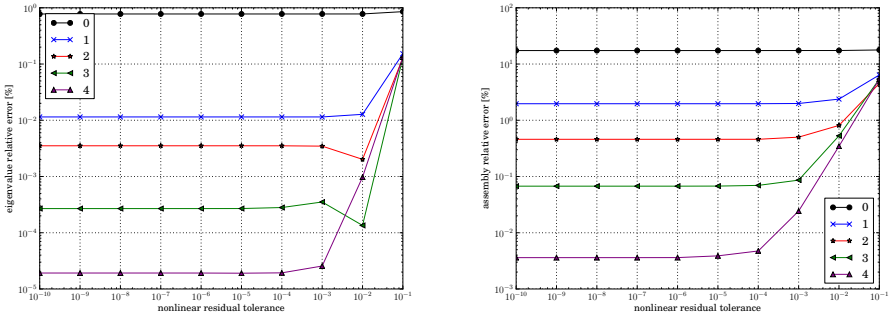
is the nonlinear residual defined by Eq. 28. Using this criterion makes comparison of Picard and Newton methods much more straightforward. For the diffusion and Takeda transport benchmarks, `Detran` was used to compute the reference solution, while for the 2-D C5G7, the reference results from the original documentation were used.

4.1. Diffusion Benchmarks

All the diffusion benchmarks studied are based on homogeneous assemblies using two (IAEA, Biblis) or four (Koeberg) group data. Certainly not challenging by today's standards, these benchmarks are useful for probing the response matrix solvers as functions of tolerance, expansion order, and other parameters.

4.1.1. Tolerances and Errors

A convergence criterion based on one quantity may not be an accurate measure of the error in some other quantity. To illustrate, the assembly powers for the 2-D IAEA problem were computed for spatial orders of 0 through 4 subject to a tolerance on the residual norm ranging from 10^{-1} down to 10^{-12}. The relative eigenvalue error and maximum relative assembly error for each order as functions of tolerance are shown in Figure 1. The results indicate that the *convergence* error in assembly powers for a given order is vanishingly small compared to the *truncation* error due to the order for tolerances below about 10^{-6}. A similar trend appears for the eigenvalue error, but for even looser tolerances. For all subsequent analyses, a tolerance of 10^{-7} was selected to ensure only truncation errors affect the solutions observed.



(a) Eigenvalue error.

(b) Assembly power error.

Figure 1: Absolute relative eigenvalue (1a) and absolute maximum relative assembly power (1b) errors for the 2-D IAEA problem as functions of the residual norm tolerance for several spatial orders.

4.1.2. Orders and Accuracy

While a detailed discussion of basis accuracies is outside the present scope, it is illustrative to assess convergence of the DLP spatial basis applied to the diffusion benchmarks. Figure 2 shows the maximum relative error in the assembly powers and absolute relative eigenvalue error as functions of spatial order. For the 3-D IAEA problem, two cases are performed. The first uses a full expansion of order m in both spatial variables. That means on a given side the two-dimensional expansion is equivalent to the form

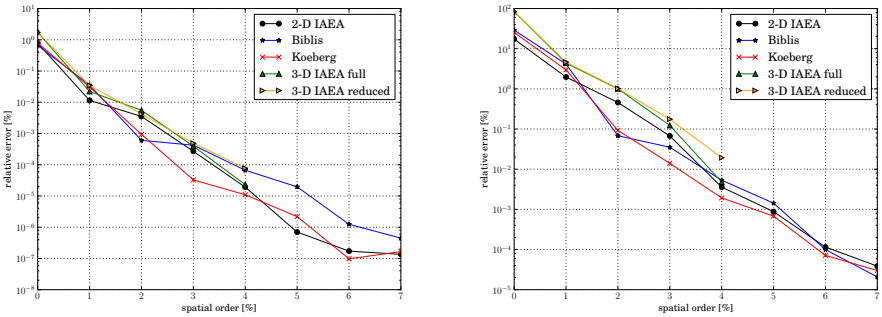
$$F(x,y) \approx a + bx + cy + dx^2 + exy + fy^2 + \dots . \tag{33}$$

The second case uses an order reduction scheme that limits the sum of the x and y orders [17]. In this case,

$$F(x,y) \approx a + bx + cy + dx^2 + fy^2 + \dots , \tag{34}$$

where the cross term exy has been omitted. Previous experience has demonstrated these cross terms, particularly at high order, have little value, and this is demonstrated quite strongly in the results of Figure 2.

For all the problems, a fourth order expansion yields assembly (or nodal, for the IAEA-3D problem) errors below a tenth of a percent and eigenvalue errors on the range of a few pcm. Consequently, a fourth order expansion was selected for use in comparing the solvers in subsequent performance analyses.



(a) Eigenvalue error.

(b) Assembly power error.

Figure 2: Absolute relative eigenvalue (2a) and absolute maximum relative assembly power (2b) errors as functions of spatial order.

4.1.3. Inner Solver Comparison

For use in the Picard solver, several eigenvalue solvers were investigated to solve the inner λ-eigenvalue problem, including the power (PI), Krylov-Schur

(KS), and explicitly-restarted Arnoldi methods (ERAM), each of which is implemented in SLEPc [20]. Because convergence of the outer Picard iteration is sensitive to the inner convergence, the tolerance τ_λ of the inner problem was set more tightly at 10^{-10}.

Table 1 provides the number of inner and outer iterations, total computational time, and response generation time for each method for each of the diffusion problems. For all problems, KS outperforms ERAM by a small margin and PI by a factor of two or three. Initial studies demonstrated that IRAM (not included by default with SLEPc) performs at about the same level as KS [7]. Were the tolerance smaller, the improvement of KS over PI would likely diminish, and contrarily were the tolerance greater.

For the three 2-D problems, the response time constitutes a significant portion of the total computational time, ranging from about a third to half depending on the solver. For the 3-D IAEA problem, the global solver becomes the dominant cost. This makes some sense, as the diffusion problems underlying the response generation are quite cheap compared to the much larger global problem.

4.1.4. Outer Solver Comparison

Because KS was the best of the inner solvers investigated, it was selected for studies of the Picard-based outer iteration schemes. For this study, Picard iteration along with the accelerated variant based on the *regula falsi* method was compared to Steffensen's method and Newton's method.

4.1.5. Picard Acceleration

The four Picard acceleration schemes were applied to the 2-D IAEA and Koeberg problems using a fourth order expansion. Figure 3 shows the nonlinear residual as a function of outer iteration for the unaccelerated case along with the four accelerated cases.

As the numerical results of the last section show, the Picard iteration by itself is a quickly converging process. However, the acceleration schemes can offer some improvement. Here, exponential and inverse-inverse extrapolation provide the most robust improvement, though they actually provide no reduction in iterations for the Koeberg problem. Recall that all the schemes depend critically on the limit $\lambda \to 1$, and this only occurs if the responses are computed very accurately and the responses are conservative. Here, the diffusion responses are computed essentially by LU factorization since they are such small problems and are conservative based on the uniform mesh and DLP expansion. Even so, the linear-inverse and linear-linear suffer from their sensitivity

solver	time [a]	r. time [b]	inners	outers
		2-D IAEA		
PI	1.87	0.37	3416	6
KS	0.69	0.41	33	6
ERAM	0.77	0.40	36	6
		Biblis		
PI	2.16	0.68	3437	5
KS	0.97	0.68	31	5
ERAM	1.05	0.69	34	5
		Koeberg		
PI	5.83	1.62	2012	3
KS	2.38	1.66	21	3
ERAM	2.63	1.67	21	3
		3-D IAEA		
PI	910.63	18.77	4427	6
KS	210.91	19.47	75	6
ERAM	294.48	19.75	70	6

[a] Total time [s]
[a] Response generation time [s]

Table 1: Picard inner solver comparison for diffusion problems.

to round-off errors, and while care was taken when implementing the coefficients, the convergence tolerances used are apparently not tight enough to ensure stability. Because the exponential scheme yields a slightly smaller final residual norm, it was included for study with the remaining algorithms.

4.1.6. Newton Variants

For Newton's method, both an unpreconditioned and ILU-preconditioned variant were studied. The ILU preconditioner is based on an explicit Jacobian constructed either once, using the initial responses, or every iteration, using the updated responses. In all cases, the underlying linear solves were performed with GMRES(30), and the ILU preconditioner was applied with 0 through 2 levels.

Table 2 provides results for the 2-D IAEA and Koeberg problems using a

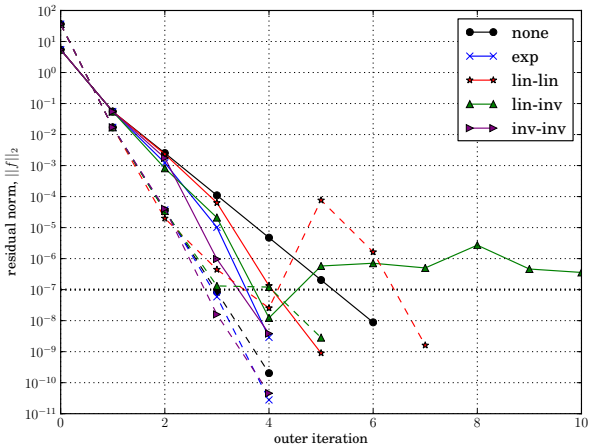


Figure 3: Comparison of Picard acceleration schemes for the 2-D IAEA problem (solid lines) and Koeberg problem (dashed lines).

fourth order spatial expansion and 4×4 nodes per assembly. This yields a somewhat larger problem that better illustrates differences in the preconditioner; the preconditioners offer no benefit for the single node case. The problems have 184962 and 369922 unknowns, respectively.

For both problems, ILU(0) preconditioning offers the best performance with respect to time despite higher levels yielding lower numbers of inner iterations. Interestingly, not updating the preconditioner has no discernible effect on the iteration count and yields lower computational times than when the preconditioner is updated at every iteration. This can be explained by noting that the majority of the Jacobian is relatively insensitive to small changes in k. Given the initial guess (unity in these cases) is expected to be pretty close to the final answer, the original Jacobian should be pretty close to its final value.

4.1.7. Comparing Picard, Steffensen, and Newton

To compare the methods, several metrics are of interest. Ultimately, the wall clock time is of most importance. However, the number of iterations of each method, both outer and inner, is also indicative of the algorithm performance independent of any particular implementation. These data are provided in Table 3 for each of the benchmarks. A fourth order spatial expansion was used throughout, with order reduction being applied to the 3-D IAEA problem. For the 2-D problems, a 4 × 4 node-per-assembly model is used, while for the 3-D IAEA problem, a single node is used. This corresponds to 184962 unknowns

preconditioner	time[a]	r. time[b]	inners	outers
		2-D IAEA		
none	12.62	0.46	477	4
no update ILU(0)	10.43	0.46	144	4
no update ILU(1)	11.68	0.46	118	4
no update ILU(2)	12.37	0.46	86	4
ILU(0)	10.69	0.46	144	4
ILU(1)	14.07	0.45	118	4
ILU(2)	17.12	0.45	86	4
		Koeberg		
none	45.82	3.29	403	4
no update ILU(0)	43.18	3.34	157	4
no update ILU(1)	52.18	3.35	136	4
no update ILU(2)	58.26	3.35	91	4
ILU(0)	45.61	3.35	157	4
ILU(1)	67.44	3.38	136	4
ILU(2)	89.90	3.35	91	4

[a] Total time [s]
[b] Response generation time [s]

Table 2: Newton solver ILU preconditioner comparison for diffusion problems.

for the 2-D IAEA and Biblis problems, 369922 for the Koeberg problem, and 988382 for the 3-D IAEA problem.

The solvers tested included Picard (P) with and without exponential extrapolation (exp), Steffensen's method (S), and Newton's method (N). For Newton's method, two schemes were examined. The first is the same as used for testing the preconditioning and is based on a Jacobian with k-derivatives computed using a finite difference with a $\Delta k = 10^{-8}$. The second scheme uses the two most recent k values for computing Δk. This results in a larger Δk and hence less accurate finite difference. However, the accuracy of the finite difference has no observable effect on the convergence, and for all four problems, this approach yields the same number of outer iterations as the regular approach but reduces the number of k evaluations by nearly half.

Steffensen's method provides the fastest convergence with respect to outer iterations, but it relies on two k evaluations per outer iteration. Picard with

solver	time[f]	r. time[g]	inners	outers	k-evals.
			2-D IAEA		
P[a]	10.26	0.32	76	5	6
P+exp[b]	9.09	0.27	65	4	5
S[c]	11.20	0.39	80	3	7
N+δk[d]	10.35	0.44	144	4	8
N+Δk[e]	10.22	0.28	146	4	5
			Koeberg		
P	9.26	0.56	64	4	5
P+exp	9.06	0.56	62	4	5
S	9.36	0.56	64	2	5
N+δk	10.89	0.92	140	4	8
N+Δk	10.49	0.57	140	4	5
			Biblis		
P	25.65	1.61	54	3	4
P+exp	25.76	1.62	54	3	4
S	29.61	2.02	60	2	5
N+δk	43.10	3.26	157	4	8
N+Δk	42.07	2.05	157	4	5
			3-D IAEA		
P	213.51	17.93	75	6	7
P+exp	167.93	12.79	62	4	5
S	214.07	17.98	75	3	7
N+δk	269.36	20.93	129	4	8
N+Δk	261.27	13.02	129	4	5

[a] Picard
[b] Picard with exponential extrapolation
[c] Steffensen
[d] Newton with fine k difference
[e] Newton with coarse k difference
[f] Total time [s]
[g] Response generation time [s]

Table 3: Outer solver comparison for diffusion problems.

exponential extrapolation yields the lowest computational time and the fewest k evaluations. While Newton's method with a coarse Δk is competitive with respect to k evaluations, the overhead of solving the linear systems is higher than the cost of the λ-eigenvalue problem in the Picard iteration.

4.1.8. Comments

From the diffusion analyses, it appears that Picard iteration using KS for the inners and the exponential extrapolation for accelerating the outers yields the best performance. The Newton methods perform about as well with respect to k evaluations, but the cost of applying the method is higher per iteration than the Picard variants, implying further work on preconditioning the inner solves is warranted.

4.2. 2-D C5G7

The 2-D C5G7 transport benchmark is a small quarter core model consisting of two UO_2 assemblies and two MOX assemblies, all surrounded by an assembly-width reflector. The model is based on 7 group data.

4.2.1. Orders and Accuracy

To assess the accuracy of the response schemes available for transport problems, the C5G7 benchmark was solved using a variety of angular bases. Because the spatial mesh is not exactly uniform, the DLP spatial expansion does not converge as quickly for the C5G7 problem as for the uniformly-meshed diffusion problems. For all cases, the response transport calculations were converged to a relative residual norm of 10^{-8}, and the outer calculation was converged to a nonlinear residual norm of 10^{-7}.

Figure 4 shows the convergence of the eigenvalue and pin power errors as a function of space-angle order. By third order, the conservative basis appears to approach a very limited improvement. This is most likely due to the DLP spatial basis used; since the mesh is not uniform, a DLP expansion is not conservative, and low order expansions cannot be expected to yield good results. Since both the DLP and Chebyshev bases yield maximum relative pin power errors of just over 2%, it appears the spatial expansion becomes the dominant source of error. These results are in contrast to those cited in Ref. [36], for which a full order spatial basis helped isolate just the error due to expanding in angle. This indicates that a full implementation and systematic study of the new spatial bases would potentially be of great value.

basis	order	e_k [a]	$\max\|e_i\|$ [b]	$\frac{\max\|e_i\|}{p_i^{\text{ref}}}$	$\frac{\sum_i \|e_i\|}{N}$	$\frac{\sqrt{\sum_i e_i^2}}{N}$	$\frac{\sum_i \|e_i\| p_i^{\text{ref}}}{N} \bar{p}^{\text{ref}}$
DLP-ψ	0	1.00	33.35	108.87	9.49	0.36	11.11
DLP-ψ	1	0.72	37.78	18.52	2.63	0.12	3.07
DLP-ψ	2	0.13	4.67	7.74	0.92	0.04	1.25
DLP-ψ	3	0.01	2.35	6.24	0.35	0.02	0.37
Chebyshev-ψ	0	2.61	40.73	107.01	9.57	0.37	11.03
Chebyshev-ψ	1	0.07	19.54	11.09	1.01	0.06	1.26
Chebyshev-ψ	2	0.04	2.95	6.70	0.39	0.02	0.37
Chebyshev-ψ	3	0.04	2.42	6.43	0.35	0.02	0.35

[a] $e_k = |k - k^{\text{ref}}|/k^{\text{ref}}$
[b] $e_i = p_i - p_i^{\text{ref}}$, for ith pin

Table 4: 2-D C5G7 order convergence. All errors in %, with reference results from `Detran` on same mesh.

4.2.2. Solver Comparison

The same set of global solvers used in Section 4.1.7 were also applied to the 2-D C5G7 problem. In this case, 64 processes were used for response generation while a single process was used for the outer (λ-eigenvalue) problem.

Table 5 provides the wall time as well as the total and response time summed over all processes. Included also are the number of inner iterations, outer iterations, and k evaluations. Newton's method with the coarse k derivative yields the best performance. Surprisingly, using the fine k derivative requires more outer iterations and hence significantly greater time. Steffensen's method, as for the diffusion problems, requires the fewest outer iterations but at the cost of more k evaluations. Standard Picard iteration performs reasonably well, but the extrapolated Picard iteration fails miserably. However, this is *completely expected*: since the spatial basis is not conservative, λ does not tend toward unity, and hence extrapolation does not apply. This highlights a significant value in selecting a conservative basis, since the extrapolated Picard iteration was the best performing method for the diffusion problems.

4.3. 3-D Takeda

The 3-D Takeda benchmark is a rather simple benchmark, but it allows us to examine in more depth the convergence properties of the basis sets. The model consists of three homogeneous regions using a two group approximation. For this study, the model in the "rods in" configureation was used.

solver	w. time[f]	time[g]	r. time[h]	inners	outers	k-evals.
P[a]	$1.67 \cdot 10^3$	$1.07 \cdot 10^5$	$1.07 \cdot 10^5$	16	6	7
P+exp[b]	$6.26 \cdot 10^3$	$4.00 \cdot 10^5$	$4.00 \cdot 10^5$	36	21	21
S[c]	$1.73 \cdot 10^3$	$1.11 \cdot 10^5$	$1.11 \cdot 10^5$	16	3	7
N+δk[d]	$4.60 \cdot 10^3$	$2.94 \cdot 10^5$	$2.94 \cdot 10^5$	76	8	16
N+Δk[e]	$1.09 \cdot 10^3$	$6.97 \cdot 10^4$	$6.96 \cdot 10^4$	33	4	5

[a] Picard
[b] Picard with exponential extrapolation
[c] Steffensen
[d] Newton with fine k difference
[e] Newton with coarse k difference
[f] Wall time [s]
[g] Total time summed over all processes [s]
[h] Total response generation time summed over all processes [s]

Table 5: Outer solver comparison for 2-D C5G7 problem with first order expansion. Picard with exponential extrapolation fails due to the nonconservative spatial basis, *i.e.* $\lambda \neq 1$.

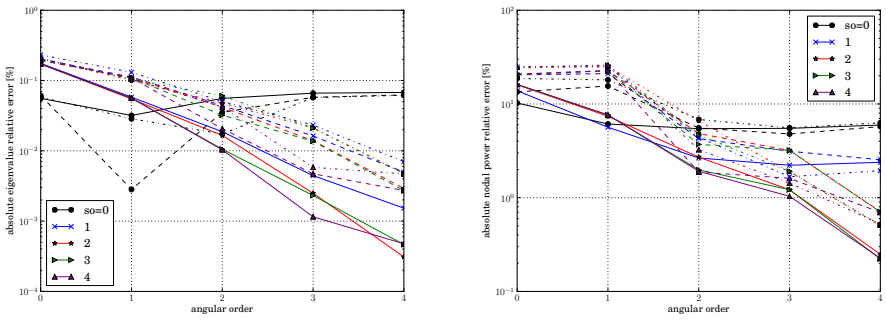
4.3.1. Order Convergence

Figures 4a and 4b provide the absolute relative error in the eigenvalue and the maximum absolute relative error in the nodal powers as a function of angular order for several spatial orders. Order reduction was used in both space and angle. It is readily apparent little is gained with increasing angular order when the spatial order is limited to zero. For higher spatial orders, an increasing angular order yields a monotonically decreasing error for both k and the nodal powers. The conservative basis outperforms the DLP variants, yielding nearly sub-1% nodal errors for a third order angular expansion and spatial orders greater than 1. DLP-J yields slightly better nodal powers than DLP-ψ at higher orders but yields higher k errors for all orders.

For all the bases, a significant trend is that spatial orders above 2 yield diminishing returns; that is, the most consistent improvement over all angular orders and bases is a shift from first to second order in space. This is reasonable because the nodes are homogeneous and boundary quantities should therefore be relatively smooth functions of space.

4.3.2. Solver Comparison

The same set of solvers as used for the diffusion problems and the 2-D C5G7 problem were applied to the Takeda problem. A second order spatial expansion



(a) Eigenvalue error.

(b) Nodal power error.

Figure 4: Takeda problem absolute relative eigenvalue (4a) and nodal power (4b) errors as a function of angular order for several spatial orders. The solid lines indicate the conservative basis, while the dashed and dashed-dot lines indicate the DLP basis used to expand the angular flux ψ and current J, respectively.

with a third order angular expansion in the azimuth and polar variables was used. Order reduction was applied to both the spatial and angular terms. The problem was run on 64 processors, with one process for the global problem. Table 6 provides the wall time, total time summed over all processors, and the total response function time summed over all processors.

Similar to the diffusion results, the extrapolated Picard iteration proves to be the most efficient of the solvers studied. Newton's method with the coarse k finite difference yielded just as few k evaluations but with a slightly higher overall cost.

5. Conclusion

Based on the results for both the diffusion and transport problems, Picard iteration with exponential extrapolation appears to be the most efficient of the methods, yielding minimum numbers of k evaluations while providing the lowest global solver overhead. However, the extrapolation is based on λ converging to unity, and because this is not always guaranteed, Newton's method with the coarse finite difference provides a more consistently robust solver, with nearly as few k evaluations and only relatively small overhead due to the inner linear solves.

It is anticipated further work on preconditioners for Newton's method would put the corresponding (global) computation time more in line with that of the

solver	w. time[f]	time[g]	r. time[h]	inners	outers	k-evals.
P[a]	$9.76 \cdot 10^2$	$6.25 \cdot 10^4$	$5.91 \cdot 10^4$	56	13	14
P+exp[b]	$3.51 \cdot 10^2$	$2.24 \cdot 10^4$	$2.12 \cdot 10^4$	23	4	5
S[c]	$1.05 \cdot 10^3$	$6.72 \cdot 10^4$	$6.36 \cdot 10^4$	58	7	15
N+δk[d]	$7.30 \cdot 10^2$	$4.67 \cdot 10^4$	$4.26 \cdot 10^4$	57	5	10
N+Δk[e]	$3.87 \cdot 10^2$	$2.48 \cdot 10^4$	$2.14 \cdot 10^4$	44	4	5

[a] Picard
[b] Picard with exponential extrapolation
[c] Steffensen
[d] Newton with fine k difference
[e] Newton with coarse k difference
[f] Wall time [s]
[g] Total time summed over all processes [s]
[h] Total response generation time summed over all processes [s]

Table 6: Outer solver comparison for 3-D Takeda problem with second order spatial expansion and third order polar and azimuthal angle expansions.

extrapolated Picard iteration. Even so, the efficacy and simplicity of the Picard iteration suggests that care should be taken to select a conservative basis leading to $\lambda = 1$ upon convergence.

Ultimately, the goal is to use ERMM in production level analyses, and to get there, significant challenges remain. Chief among these remains the shear number of responses required for realistic modeling. The solvers studied that reduce the number of k evaluations required go a long way to minimize the time spent generating responses, while related recent work successfully developed diffusion-based transport preconditioners that significantly reduce the time of individual response calculations [29]. Because responses are independent, parallel computation will be a natural component of any future ERMM implementation. Scoping studies have demonstrated good scaling of `Serment` on a small research cluster [35], and ongoing work aims to test `Serment` on leadership-class machines.

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