A Review and Critique of "Jacobian-Free Newton-Krylov Nodal Expansion Methods with Physics-Based Preconditioner and Local Elimination for Three-Dimensional and Multigroup k-Eigenvalue Problems"

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Abstract

Jacobi-Free Newton-Krylov (JFNK) methods promise a robust framework for solving nonlinear equations. The JFNK methods converge q-quadratically and only require a finite difference Jacobian-vector product rather than a full Jacobian. However, the adoption of the JFNK method in the simulation of nuclear reactors has proven difficult due to computational complexity. As such, the traditional Power Iteration (PI) method is typically preferred to solve for the fundamental eigenmode of a nuclear reactor system.

In "Jacobian-Free Newton-Krylov Nodal Expansion Methods with Physics-Based Preconditioner and Local Elimination for Three-Dimensional and Multigroup k-Eigenvalue Problems," authors Zhou and Li present an implementation of the JFNK method to solve the Nodal Expansion Method (NEM) equations. In their implementation, the authors reduce the number of solution variables by employing local-elimination and improve the efficiency of the Krylov solver by preconditioning with a specially designed, physics-based, preconditioner. This implementation of the JFNK method is compared to a PI method and the authors conclude that "the NEM_JFNK methods can greatly improve the convergence rate and the computational efficiency" [Zho+18].

The claims by the authors are exaggerated and insufficient results are provided to justify such claims. The claim of improved computational efficiency is based on comparing the proposed JFNK method to a suboptimal implementation of the PI method. Notably, the authors do not properly consider the importance of the Wielandt Shift (WS) and do not use a Coarse Mesh Finite Difference (CMFD) formulation of the NEM equations. In their closing remarks, Zhou and Li also claim that the proposed methods can be extended to multiphysics simulations though other work suggests this is challenging, if at all feasible [Ham+16].

Ultimately, Zhou and Li present a comparison of suboptimal codes and suggest that the JFNK method is preferable because it had reduced execution time. Such claims cannot be substantiated by the results presented. It is essential to compare optimized codes before making conclusions regarding an improvement in methods.

1 Introduction

The multigroup neutron diffusion equation has proven to be a useful tool for modeling the neutron distribution in a typical nuclear reactor. With the development of the Nodal Expansion Method (NEM), the model was made more accurate and computational time was significantly decreased. The typical quantity of interest in these reactor simulations is the fundamental mode of the eigenvalue problem; that is, the largest eigenvalue and associated eigenvector which represent the effective neutron multiplication factor and scalar neutron flux distribution respectively.

Traditionally, the multigroup neutron diffusion equation and NEM equations have been solved using the Power Iteration (PI) method. The PI method is a fixed-point method useful for solving eigenvalue problems. It is a linear iteration method and converges to the fundamental eigenmode at a linear rate. Recently, the use of Jacobi-Free Newton-Krylov (JFNK) methods has been investigated in an attempt to reduce the computing time required to solve the NEM equations. JFNK methods are attractive because when the iteration terminates, the method converges q-quadratically. However, JFNK methods require the computation of quantities not required by the PI method including the finite difference Jacobian-vector product. Due to the challenges of computing these quantities, the implementation of JFNK methods for computing the fundamental mode to the multigroup neutron diffusion equation and NEM equations remains an active area of research.

In "Jacobian-Free Newton-Krylov Nodal Expansion Methods with Physics-Based Preconditioner and Local Elimination for Three-Dimensional and Multigroup k-Eigenvalue Problems," Zhou and Li explore an implementation of the JFNK method that seeks to efficiently solve the NEM equations for the fundamental eigenmode. §2 briefly summarizes this work and a few considerations for solving the NEM equations using the JFNK method are provided. Then, §3 critiques the authors' implementation with a focus on the applicability of the proposed method to realistic nuclear reactor simulations. Finally, §4 provides a few conclusions based on the work by Zhou and Li and some considerations for future implementations of the JFNK method to solve the NEM equations in nuclear reactor simulations.

2 Summary and Background

A brief summary of "Jacobian-Free Newton-Krylov Nodal Expansion Methods with Physics-Based Preconditioner and Local Elimination for Three-Dimensional and Multigroup k-Eigenvalue Problems" follows. Supporting information and commentary on the methods presented is included as applicable.

2.1 Multigroup Neutron Diffusion and Nodal Expansion Method

In its conventional form, the multigroup neutron diffusion equation for a problem domain $\mathbf{r} \in \Omega$ can be written

$$\nabla \cdot \mathbf{J}_g(\mathbf{r}) + \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r}) = \frac{\chi_g(\mathbf{r})}{\lambda} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \Sigma_{s,g' \to g}(\mathbf{r})\phi_{g'}(\mathbf{r}) \tag{1}$$

where

$\mathbf{r}$ = spatial position vector,
$\mathbf{J}_g(\mathbf{r})$ = net neutron current for energy group g $\left[\frac{1}{\text{cm}^2\ \text{s}}\right]$,
$\phi_g(\mathbf{r})$ = fundamental eigenvector, scalar neutron flux for energy group g $\left[\frac{1}{\text{cm}^2\ \text{s}}\right]$,
$\Sigma_{r,g}(\mathbf{r})$ = macroscopic removal cross section for energy group g $\left[\frac{1}{\text{cm}}\right]$,
$\chi_g(\mathbf{r})$ = fission spectrum for energy group g,
λ = fundamental eigenvalue, effective neutron multiplication factor,
$\nu\Sigma_{f,g}(\mathbf{r})$ = number of fission neutrons times macroscopic fission cross section in energy group g $\left[\frac{1}{\text{cm}}\right]$,
$\Sigma_{s,g'\to g}(\mathbf{r})$ = macroscopic scatter cross section from energy group g' to energy group g $\left[\frac{1}{\text{cm}}\right]$,
G = total number of energy groups.

The three-dimensional domain, Ω, can then be discretized into a structured grid of nodes. Next, the NEM is introduced. Fundamentally, the NEM projects the transverse integrated flux onto a set of basis functions. The transverse integrated multigroup neutron equation is given as

$$\frac{d\mathbf{J}_{g,u}(u)}{du} + \overline{\Sigma_{r,g}}\phi_{g,u}(u) = Q_{g,u}(u) - L_{g,u}(u) \tag{2}$$

where $u = x,\ y,\ z$ is a coordinate direction [Zho+18]. The terms $Q_{g,u}(u)$ and $L_{g,u}(u)$ represent the transverse integrated neutron source and transverse leakage respectively. Note that in Eq. (2), the node indices (i.e. i, j, k) have been omitted and $\overline{\Sigma_{r,g}}$ represents the average value of $\Sigma_{r,g}(\mathbf{r})$ in the node. The transverse integrated current $\mathbf{J}_{g,u}$ is then approximated

$$\mathbf{J}_{g,u}(u) = -\overline{D_g}\,\frac{d\phi_{g,u}(u)}{du} \tag{3}$$

where $\overline{D_g}$ is the average value of the diffusion coefficient in the node.

NEM basis functions are typically polynomials and Zhou and Li select the Legendre polynomials. In their work, the scalar flux is projected onto quartic polynomials and the transverse integrated neutron source and transverse leakage terms are projected onto quadratic polynomials. The selection of quartic and quadratic polynomials respectively is consistent as the second derivative of the scalar flux is related to the source and leakage terms [Geh92]. This projection can be written

$$\phi_{g,u}(u) = \sum_{n=0}^{N_\phi=4} a_{g,u,n}\, f_{u,n}(u), \tag{4}$$

$$Q_{g,u}(u) = \sum_{n=0}^{N_Q=2} q_{g,u,n}\, f_{u,n}(u), \tag{5}$$

$$L_{g,u}(u) = \sum_{n=0}^{N_L=2} l_{g,u,n}\, f_{u,n}(u), \tag{6}$$

where $a_{g,u,n}$, $q_{g,u,n}$, and $l_{g,u,n}$ are the expansion coefficients of $\phi_{g,u}(u)$, $Q_{g,u}(u)$, and $L_{g,u}(u)$ respectively and $f_{u,n}(u)$ is the n^{th} Legendre polynomial [Zho+18]. To solve for the coefficients of the expansions in Eq. (4), Eq. (5), and Eq. (6), five equations are required. The selected equations are:

1. flux continuity condition,
2. current continuity condition,
3. nodal neutron balance (f_0 weighted residual),
4. f_1 weighted residual, and
5. f_2 weighted residual.

Special attention is paid to boundary conditions and these conditions replace the flux and current continuity equations on the problem boundary.

2.2 Local Elimination

Recall the quantity of interest for this calculation is the fundamental eigenmode composed of eigenvalue, λ, and eigenvector, $\phi_g(\mathbf{r})$. The coefficients in Eq. (4), Eq. (5), and Eq. (6) are not desired directly, but must be solved in order to obtain the quantity of interest. It has been previously demonstrated that all coefficients need not be solved simultaneously which allows for the reduction of the dimensionality of the problem. The odd and even coefficients can be solved separately as a result of the five solution equations selected [Geh92].

Zhou and Li then show that the number of coefficients can be further reduced as the odd coefficients can be expressed in terms of each other with similar results for the even coefficients. That is, instead of solving for $a_{g,u,1}$ and $a_{g,u,3}$, a new coefficient is introduced: $a_{g,u,1-3}$. Similarly, $a_{g,u,2-4}$ becomes a solution variable. This is an important and novel step of the reviewed work as the solution of NEM coefficients represents the bulk of the computational time and the number of coefficients required for solving the NEM equations has been reduced [Zho+18].

Finally, the NEM equations are solved to obtain currents, scalar fluxes, $a_{g,u,1-3}$, and $a_{g,u,2-4}$. The resulting solution vector, $\mathbf{\Phi}_g$, can be written

$$\mathbf{\Phi}_g = \begin{pmatrix} \mathbf{J}_{g,x,+} \\ \mathbf{J}_{g,y,+} \\ \mathbf{J}_{g,z,+} \\ \overline{\phi_g} \\ a_{g,x,1-3} \\ a_{g,y,1-3} \\ a_{g,z,1-3} \\ a_{g,x,2-4} \\ a_{g,y,2-4} \\ a_{g,z,2-4} \end{pmatrix} \tag{7}$$

and the total number of solving variables is $10 \times N \times G$ where N is the total number of nodes and G is the total number of energy groups. Note that the NEM coefficients and neutron current must be solved in each spatial direction. Typically, solving for the NEM coefficients themselves is not preferred as the values themselves are

not quantities of interest. The preferred Coarse Mesh Finite Difference (CMFD) implementation computes a modified diffusion coefficient, $\widetilde{D}$, and will be discussed in §3.3.

2.3 Jacobi-Free Newton-Krylov Theory and Inexact Newton Condition

The JFNK method begins with Newton's method. Newton's method provides a framework to find the root of a residual function as $\mathbf{R}(\mathbf{x}^*) = \mathbf{0}$ where $\mathbf{x}^*$ is a root of the residual function. It is first necessary to construct a residual function based on the NEM equations. Zhou and Li propose a residual function that contains the residual of the NEM solution, $\mathbf{\Phi}_g$, and the absolute change in the fundamental eigenvalue, λ, during the Newton iteration. This differs from the residual function proposed by Gill and Azmy but the new form may be preferable as it directly contains information about the fundamental eigenvalue, λ.

The m^{th} Newton step can be described

$$\mathbf{Ja}(\mathbf{x}^m) \cdot \delta\mathbf{x}^m = -\mathbf{R}(\mathbf{x}^m) \tag{8}$$

where $\mathbf{Ja}(\mathbf{x}^m)$ is the Jacobian of $\mathbf{R}(\mathbf{x}^m)$ and $\delta\mathbf{x}^m$ is the Newton step. Then, the Newton step proceeds as

$$\mathbf{x}^{m+1} = \mathbf{x}^m + \delta\mathbf{x}^m. \tag{9}$$

For the choice of residual function made by Zhou and Li, an analytic Jacobian is not simple to compute. Therefore, a finite difference approximation is used to estimate the Jacobian. In fact, the Jacobian itself is not needed as the Newton step in Eq. (8) will be solved with a Krylov method. All that is needed is the finite difference Jacobian-vector product which is equivalent to a directional derivative. The directional derivative can be written

$$\mathbf{Ja}(\mathbf{x}^m) \cdot \mathbf{v} \approx \frac{\mathbf{R}(\mathbf{x}^m + \varepsilon\mathbf{v}) - \mathbf{R}(\mathbf{x}^m)}{\varepsilon} \tag{10}$$

where $\mathbf{v}$ is the direction and ε is the finite difference step size. Typically, ε is on the order of the square-root of machine precision, $\sqrt{\varepsilon_{mach}} \approx 10^{-8}$ [Gil+11; Kel95; Zho+18]. Since the Jacobian has been replaced by a directional derivative, the method is termed Jacobian-Free.

As previously mentioned, the Newton step in Eq. (8) is solved using a Krylov method as

$$\|\mathbf{R}(\mathbf{x}^m) + \mathbf{Ja}(\mathbf{x}^m) \cdot \delta\mathbf{x}^m\| \leq \eta_m \|\mathbf{R}(\mathbf{x}^m)\| \tag{11}$$

where the tolerance η_m is referred to as the forcing term. Zhou and Li investigated solving Eq. (11) using Generalized Minimal Residual (GMRES) and BiConjugate Gradient STABilized (BiCGSTAB) Krylov methods and determined that BiCGSTAB performed preferably. Eq. (11) is termed the inexact Newton condition. It is known that the choice of forcing term, η_m, can significantly effect the convergence rate of the JFNK method [Kel95]. Essentially, it is undesirable to "over-solve" Eq. (11), especially during the initial Newton iterations.

The Eisenstat-Walker forcing term is a standard choice for η_m and has been shown to work well [Gil+11; Zho+18]. In both the work by Zhou and Li and the work by Gill and Azmy, the authors perform a study to determine a preferable choice of forcing term. The authors all determine that the Eisenstat-Walker forcing

term is ideal. However, $\eta_m = 10^{-1}$ provides equally well and sometimes better results [Gil+11; Kel19; Kno+11; Zho+18]. These results indicate that both the Eisenstat-Walker forcing term and $\eta_m = 10^{-1}$ perform similarly and such a study is unnecessary in the future.

2.4 Choice of Physics-Based Preconditioner

The inexact Newton condition (discussed in §2.3) is solved iteratively with a Krylov solver. The wise choice of preconditioner can significantly reduce the number of Krylov iterations required to solve a linear system. It can be shown that if one preconditions a matrix with its inverse, the Krylov method will converge in one iteration [Kel95]. While computing the matrix inverse would defeat the purpose of the Krylov method, this result indicates that the preconditioning operator is selected to approximate the matrix inverse.

Zhou and Li investigate only left-preconditioning. The left-preconditioned form of the inexact Newton condition can be written

$$\|\mathbf{M}_L^{-1}\mathbf{R}(\mathbf{x}^m) + \mathbf{M}_L^{-1}\left(\mathbf{Ja}(\mathbf{x}^m)\cdot\delta\mathbf{x}^m\right)\| \leq \eta_m\|\mathbf{M}_L^{-1}\mathbf{R}(\mathbf{x}^m)\| \tag{12}$$

where $\mathbf{M}_L$ is the left-preconditioning operator. Note that in Eq. (12), the residual that is reduced during a Krylov iteration is not directly related to the residual $\mathbf{R}(\mathbf{x}^m)$. Typically, this is not a problem. Right-preconditioning can also be considered but is not investigated in the proposed implementation. Gill and Azmy investigate both left- and right-preconditioning.

An extensive review of the choice of preconditioner in JFNK solutions to the multigroup neutron diffusion equation has been presented elsewhere [Gil+11]. It is expected that the results of the preconditioner study for the multigroup neutron diffusion equation should be applicable to the NEM equations. Preconditioners investigated include the diffusion operator, incomplete Cholesky factorization, the diffusion-fission operator, and preconditioning with a few PIs. The results of the preconditioner study indicates that preconditioning with approximately five PIs provided the fastest convergence of the JFNK iterations. The incomplete Cholesky preconditioner provided similar convergence rate but requires additional and expensive matrix calculations. A PI preconditioner was also investigated in work by Knoll et al. and similar performance was reported [Kno+11].

The use of a PI preconditioner was not investigated by Zhou and Li. Instead, the authors designed a new preconditioner based on the data available during the NEM iterations. Special attention is also paid to ensure the preconditioner can be solved using the TriDiagonal Matrix Algorithm (TDMA) and Alternating Direction Iterative (ADI) methods. These methods are among the fastest numerical matrix solution techniques available. The authors incorporate information in the preconditioner from the NEM equations, group-to-group scattering, and transverse leakage contributions. The construction of the preconditioner appears to be computationally expensive. Unfortunately, Zhou and Li do not compare their preconditioner to any other preconditioner or even a case without a preconditioner. Therefore, it is impossible to determine the relative computational efficiency of this preconditioning method.

2.5 Convergence Rate Consideration

The q-quadratic convergence rate of the JFNK method is what makes it desirable to implement. Therefore, it is important to compare the convergence behavior of the JFNK method to the traditional PI method.

2.5.1 Convergence of Power Iteration Method

The convergence behavior of the PI method is known and studied well [Daw19; Geh92; Nak77]. The convergence rate of the PI method is determined by the first and second largest eigenvalues of the equations of interest (either the multigroup neutron diffusion equation or NEM equations). It can be shown that each iteration of the PI method reduces the error by a multiple termed the dominance ratio, d, defined as

$$d = \frac{\lambda_1}{\lambda_0} \tag{13}$$

where $\lambda_0 = \lambda$ is the fundamental eigenvalue and λ_1 is the next largest eigenvalue [Daw19]. The PI method converges linearly and the dominance ratio is the leading coefficient in the convergence behavior. For the multigroup neutron diffusion and NEM equations, d is guaranteed to be less than one and smaller values of d result in faster convergence [Nak77]. For typical reactor simulations, $d > 0.9$ and often $d > 0.95$ implying convergence is slow, often requiring hundreds of iterations.

The typical approach to address the challenge of large dominance ratios is the Wielandt Shift (WS) [Geh92]. Briefly, the WS subtracts a portion of the fission source from both sides of the equation. It can be shown that the dominance ratio is decreased *significantly* such that $d \approx 0.5$ may be expected. It is common for the WS to speedup the solution PI method by a factor of three or more. This will be discussed more in §3.4.2.

2.5.2 Convergence of Newton Method

When the iterate in the JFNK method, $\mathbf{x}^m$, is far from the solution, $\mathbf{x}^*$, the method converges q-superlinearly. As the iteration approaches the solution, it achieves q-quadratic convergence [Kel95].

It has been demonstrated that the dominance ratio of the multigroup neutron diffusion equation has little effect on the convergence rate when the equations are solved using the JFNK method [Gil+11]. This is expected as the convergence rate of the JFNK method is not related to the eigenvalues of the operator but is related to the properties of the Jacobian including its Lipschitz continuity [Kel95]. These results indicate that the WS would have little to no effect on the JFNK method. However, Zhou and Li indicate in their concluding remarks that they expect the WS to "improve the efficiency further" and this is inaccurate [Zho+18].

3 Critique

The primary motivation for this work is to critique the article by Zhou and Li. While there may be more to critique, the discussion here focuses on the application of proposed the JFNK method to realistic reactor simulation problems.

3.1 Verification and Validation

Had the authors provided additional results, the implications of the work may be more significant. To demonstrate the implementation of their method, the authors compare their converged eigenvalue and scalar flux distribution to a single benchmark problem: the International Atomic Energy Agency (IAEA) 3D Pressurized Water Reactor (PWR) benchmark. While results are presented for a second pebble bed reactor, these results have not been previously verified. The authors do not demonstrate the spatial convergence order of their method. Typically spatial convergence is demonstrated with the solution to an analytic problem and a mesh convergence study. Additionally, the fundamental eigenvalue, λ, is not directly related to the norm of the residual, $\|\mathbf{R}(\mathbf{x}^m)\|$, so no conclusion can be made regarding the behavior of λ during the JFNK iterations [Ham+16].

3.2 Critical Boron Concentration Search

For the simulation of PWRs, one is typically not interested in the value of λ. Instead, the critical boron concentration is desired such that $\lambda = 1.0$. While this may be a simple feature, the authors have not demonstrated the ability of this new method to solve for the critical boron concentration. In similar studies, the calculation of a critical boron concentration has been performed using a JFNK-like method but it required special tuning and consideration [Ham+16]. The typical method for calculating the critical boron concentration is related to the PI method. The JFNK method presented by Zhou and Li will have different convergence behavior compared to the conventional PI method so the standard calculation technique may not be applicable.

3.3 Coarse Mesh Finite Difference Formulation

A significant challenge of the JFNK method presented by Zhou and Li is the solution of the NEM coefficients. Typically, the NEM coefficients, $a_{g,u,n}$, are not solved directly and, instead, a modified diffusion coefficient, $\widetilde{D}$, term is calculated. Consider two neighboring nodes, indexed ℓ and $\ell+1$. Then, using the NEM coefficients calculated in only these two nodes, the current across the intervening surface, $\mathbf{J}_{g,u}(u)$, can be calculated. A $\widetilde{D}$ can be calculated as

$$\mathbf{J}_{g,u}(u) = -2\left(\frac{h_{\ell+1}}{\overline{D}_{g,\ell+1}} + \frac{h_\ell}{\overline{D}_{g,\ell}}\right)^{-1}\left(\overline{\phi}_{g,u,\ell+1} - \overline{\phi}_{g,u,\ell}\right) + \widetilde{D}_{g,u}\left(\overline{\phi}_{g,u,\ell+1} + \overline{\phi}_{g,u,\ell}\right) \tag{14}$$

where $\mathbf{J}_{g,u}(u)$ is the current on the surface between the nodes, $\overline{\phi}_{g,u,\ell}$ is the node average scalar flux in node ℓ, and $\widetilde{D}$ is dimensionless. $\widetilde{D}$ is now unique to a particular surface and must be solved during every outer iteration as a nonlinear update. The implementation of $\widetilde{D}$ as in Eq. (14) has been demonstrated previously [Pal97; Smi83]. Note that all demonstrations of the CMFD formulation and proofs relating to the nonlinear iteration process are related to the PI method. Implementing the CMFD formulation with the JFNK method may present additional challenges.

Calculation of $\widetilde{D}$ has several benefits compared to directly solving for the NEM coefficients. Originally, the form of Eq. (14) and the nonlinear iteration method was proposed by Smith to save on storage. In the nonlinear

iteration method, the NEM coefficients need not be stored. This CMFD formulation would reduce the number of solution variables from $10 \times N \times G$ to $N \times G$. The bulk of the computation in each Newton iteration is spent in the Krylov solver to solve the inexact Newton condition from Eq. (11). Reducing the dimension of the linear operator by implementing a CMFD formulation will therefore reduce the computational expense of the matrix-vector products required by the Krylov solver.

A final consideration for the CMFD formulation is the incorporation into existing reactor simulation computer programs. A majority of computer programs developed to simulate nuclear reactors use a $\widetilde{D}$ term whether it be calculated using the NEM or another, higher-order, method such as Diffusion Synthetic Acceleration (DSA) [Col+15; Stu09a; Stu09b]. By solving for the NEM coefficients themselves, the method proposed by Zhou and Li requires the development of an entirely new computer program.

3.4 Comparison to Production-Quality Computer Programs

The most significant challenge to analyzing the results presented by Zhou and Li is that the results of the JFNK method are not compared to "production-quality" computer programs.

3.4.1 Ragged Core

It almost goes without saying that solution time can be expected to be directly related to the number of solving variables. However, Zhou and Li include unnecessary nodes in their simulation. The simulations presented are in the domain of a rectangular prism but standard reactor simulations are performed on a "ragged core" domain. In order to simplify the boundary description, the authors introduce new nodes at the periphery of the problem. Consider the IAEA 3D PWR benchmark. The introduction of new nodes does not significantly affect the result as the simulation agrees to the benchmark within 4 [pcm]. However, the benchmark geometry can be described exactly by 245, $10\,[\text{cm}] \times 10\,[\text{cm}]$ nodes at each axial elevation and the authors simulate 289 nodes at each axial elevation. The authors went to great lengths to reduce the number of solution variables (see §2.2), but approximately 18% of the nodes solved are absolutely unnecessary for the problem.

It may seem that simulating a ragged core would only further improve the relative speedup of the JFNK method compared to the PI method, but such a conclusion is not straightforward. It is known that in reactor simulations using the PI method, the method may spend many iterations unnecessarily solving for the flux in cells with little or no fissile material [Geh92]. In the work by Zhou and Li, the convergence of the quantities of interest, λ and $\overline{\phi}$, cannot be inferred. Therefore, it is possible that the PI method may be spending many iterations solving for the scalar flux in these unnecessary nodes whereas the JFNK method would not experience such behavior.

3.4.2 Wielandt Shift

The final shortcoming of the comparison of the JFNK and PI methods presented by Zhou and Li is the improper consideration of the WS. The authors claim that integrating the WS method into the JFNK method will "improve efficiency further" [Zho+18]. However, both the work by Gill and Azmy and the discussion of

the PI dominance ratio in §2.5.1 indicate that this claim is misguided. It is not expected that implementing the WS will improve the efficiency of the JFNK method.

The greatest difficulty of the results presented by Zhou and Li is that the PI method to which the results were compared did not implement the WS. It is expected that the WS can speedup results of the PI method for these problems by a factor of three or more. This would invalidate some of the conclusions by Zhou and Li because the PI method would then be faster than the JFNK method for some cases.

Results by Knoll et al. indicate that even with the WS, the JFNK method may still provide speedup for the multigroup neutron diffusion equation solution to the IAEA benchmark in two spatial dimensions compared to the PI method [Kno+11]. However, these results do not directly extend to the work by Zhou and Li as the solution is presented for the NEM and a heavily modified and specially preconditioned form at that.

Including the WS in the JFNK method has also been shown to be useful for preconditioning the Krylov solver with a series of PIs [Kno+11]. Unlike Gill and Azmy and Knoll et al., Zhou and Li do not investigate PI preconditioning but such a preconditioner warrants investigation.

4 Conclusions and Implications

In "Jacobian-Free Newton-Krylov Nodal Expansion Methods with Physics-Based Preconditioner and Local Elimination for Three-Dimensional and Multigroup k-Eigenvalue Problems," Zhou and Li conclude that the proposed implementation of solving the NEM equations with the JFNK method after performing local elimination and using the physics-based preconditioner provides improved convergence rate and reduced computation time compared to their implementation of the PI method. It is difficult to argue with these results as presented. However, §3 has shown that it is the data omitted from the results that merits consideration. Without additional data, it is difficult to extend the results of Zhou and Li to broader applications of the JFNK method for solving the NEM equations.

A first step for better interpreting the results presented is to compare the JFNK method to a PI method using the WS as in the work by Knoll et al. It would also be useful to investigate preconditioning with a few PIs as this has been demonstrated to be the preferable preconditioning by others [Gil+11; Kno+11]. Additionally, the NEM should be implemented in the CMFD formulation to investigate improved computational efficiency and allow for compatibility with existing production-quality computer programs [Pal97; Smi83].

In their concluding remarks, Zhou and Li claim that their method will be extended to "improve the computational efficiency for large-scale complicated multiphysics coupled problems in nuclear reactor analysis" [Zho+18]. This may seem like a straightforward extension, but a new residual function and Jacobian approximation will likely be required.

The authors' claim of incorporating multiphysics effects is extremely bold given both the omission of important results and other publications in the field. Specifically, Hamilton et al. investigated this exact application of JFNK to large-scale multiphysics simulations. Such an application required significant work in the formation of the Jacobian including constructing approximations of temperature derivatives of cross sections. These cross section derivatives were specific to a particular type of reactor (PWRs) but Zhou and Li attempt to simulate both PWRs and pebble bed reactor designs. Succinctly, in reactor multiphysics

simulations, it was determined that without the calculation of cross section derivatives, the JFNK method was unacceptable as it required a burdensome amount of cross section processing time during the simulation [Ham+16].

The results of Hamilton et al. are not the end of the narrative. Applying the JFNK method to the NEM equations may be useful for certain nuclear reactor multiphysics simulations. However, insufficient data is provided by Zhou and Li to make such a conclusion. Additional attention must be paid in the application of the JFNK method to the NEM equations to determine if such an implementation would provide a benefit compared to existing methods. When drawing conclusions about improvements in computational efficiency due to a new method, it is crucial to compare optimized codes to determine if any improvement is true, or merely due to a suboptimal implementation.

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Acronyms

ADI	Alternating Direction Iterative.
BiCGSTAB	BiConjugate Gradient STABilized.
CMFD	Coarse Mesh Finite Difference.
DSA	Diffusion Synthetic Acceleration.
GMRES	Generalized Minimal Residual.
IAEA	International Atomic Energy Agency.
JFNK	Jacobi-Free Newton-Krylov.
NEM	Nodal Expansion Method.
PI	Power Iteration.
PWR	Pressurized Water Reactor.
TDMA	TriDiagonal Matrix Algorithm.
WS	Wielandt Shift.