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A fast Jacobian-Free Newton-Krylov iterative solver for eigenvalue search problems in the reactor physics

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HIGHLIGHTS

- A new nonlinear function has been developed for solving the eigenvalue problem.
- The JFNK approximation casts as an accelerated iterative approach.
- Numerical results were generated using FEMPT code.
- The results indicate that the JFNK method can converge faster than the standard procedure.

ABSTRACT

The Jacobian-Free Newton-Krylov (JFNK) method has been widely used in solving nonlinear equations arising in many applications. In this paper, the JFNK solver is examined as an alternative to the traditional power iteration method for calculation of the fundamental eigenmode in reactor analysis based on even-parity neutron transport theory. Since the Jacobian is not formed the only extra storage required is associated with the workspace of the Krylov solver used at every Newton step. A new nonlinear function is developed for the even-parity neutron transport equation utilized to solve the eigenvalue problem using the JFNK. This Newton-based method is compared with the standard iterative power method for a number of multi-groups, one and two dimensional neutron transport benchmarks. The results show that the proposed algorithm generally ends with fewer iterations and shorter run times than those of the traditional power method.

KEYWORDS

JFNK method
Even-parity neutron transport equation
Eigenvalue search
Nonlinear systems

HISTORY

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1 Introduction

The k-eigenvalue calculation in criticality problems has traditionally utilized the classical power iteration method which has slow convergence order. In practical situations, fast iterative methods applied to improve the convergence order of the power iterations. Several attempts have been made to obtain more efficient algorithms using accelerated techniques such as Chebyshev iteration (Hageman and Young, 2012) and Wielandt shift (Downar et al., 2004). Accelerated approaches to power iteration have been studied (Allen and Berry, 2002; Adams and Larsen, 2002) to improve upon the performance of power iteration methods. The Jacobian-Free Newton-Krylov (JFNK) method is a synergistic combination of Newton iterative method for nonlinear equation and Krylov subspace iterative methods for solving linear systems. In JFNK methods, the nonlinear iterative method is employed on the eigenvalue search and a linear iterative method on the system of equations (Chan and Jackson, 1984; Brown and Saad, 1990).

Subspace iterations and Krylov subspace methods, such as the Implicit Restarted Arnoldi Method (IRAM) have been successfully applied to transport (Gupta and Modak, 2004) and diffusion criticality problems (Verdú et al., 1999). These methods can also be used to find multiple eigenmodes, not only the fundamental mode. Recently, the use of JFNK methods have also been investigated in conjunction with IRAM as a tool for BWR modal analysis (Mahadevan and Ragusa, 2008). In the current work, a similar JFNK method with a new nonlinear function is explored as an alternative to the power iteration for seeking the eigenvalue of the even-parity neutron transport equation. In 2010, Martin presented the nonlinear solution scheme for implicit coupling of the convergence accelerated transport method (Martin, 2010).

In the first part of this work, a computer program has been developed based on a variational principle for

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the second order neutron transport equation. The program employs Lagrange polynomials as spatial basis functions for finite element formulation and spherical harmonics for the directional dependence of the solution. In neutronics, finite element methods developed for the first-order Boltzman transport equation and followed for its equivalent second-order forms originated by Veladimirov (Vladimirov, 1963). Synge et. al (Synge, 1957) exploited the method of hypercircle for the approximate solution of second-order and fourth-order equations in mechanics which inspired Ackroyd and Pendlebury (Ackroyd and Pendlebury, 1961) and Ackroyd (Ackroyd, 1962) to develop a hypercircle method for the first-order Boltzmann equation. A detailed review on numerical methods in neutron transport theory can be found in Lewis (1998) (Lewis and Miller, 1984). The even parity neutron transport theory has been reviewed by Ackroyd et al. (Ackroyd et al., 1987) and Ackroyd (Ackroyd, 1997).

The other sections of the paper is organized as follows: In section 2 we present the basics of Newton-Krylov method and the JFNK approximation. In section 3 the even-parity neutron transport theory is discussed, and in section 4 the application of JFNK method as an alternative fast convergence algorithm for power iteration is mentioned. We then apply the ideas developed to the multigroup even parity transport equations. Finally in sections 5 and 6 numerical results for a number of benchmarks will be presented and discussed in order to demonstrate the computational efficiency of the new approach.

2 Fundamentals of the JFNK method

Origins of the Jacobian-Free Newton-Krylov method can be traced back to publications motivated by the solution of ordinary or partial differential equations (Gear and Saad, 1983; Brown and Saad, 1990). The primary motivation in all cases appears to be the ability to perform Newton iterations without forming the Jacobian. This is a nested iteration method consisting of at least two and usually four levels. The primary levels, which give the method its name, are the loops over the Newton corrections and the loop building up the Krylov subspace out of which each Newton correction is drawn. Interior to the Krylov loop, a preconditioner is usually required, which can itself be direct or iterative.

2.1 Newton methods

The Newton iteration for arbitrary nonlinear equation $\Gamma(u) = 0$ derives from a multivariate Taylor expansion about the current point u^k:

$$\Gamma(u^{k+1}) = \Gamma(u^k)(u^{k+1} - u^k) + \text{High order terms.} \quad (1)$$

Setting the right-hand side zero and neglecting the terms of higher-order curvature yields a strict Newton method which is an iteration over a sequence of linear systems

$$\begin{aligned} &J(u^k)\delta(u^k) = -\Gamma(u^k) \\ &u^{k+1} = u^k + \delta(u^k) \quad ; \quad k = 0, 1, ... \end{aligned} \quad (2)$$

by a given initial guess u^0. Here, $\Gamma(u)$ is the vector-valued function of nonlinear residuals, $J(u)$ is its associated Jacobian matrix, u is the state vector to be found, and k is the iteration index. The Newton iteration is terminated based on a required drop in the norm of the nonlinear residual

$$\frac{\|\Gamma(u^k)\|}{\|\Gamma(u^0)\|} < \text{total residual} \quad (3)$$

For a scalar problem, discretized into n equations with n unknowns, we have

$$\Gamma(u) = \{\Gamma_1, \Gamma_2, ..., \Gamma_i, ...\Gamma_n\} \quad (4)$$

and

$$u = \{u_1, u_2, ..., u_i, ...u_n\} \quad (5)$$

In vector notation, a general element (of the i^{th} row and j^{th} column) of the Jacobian matrix is derived by

$$J_{ij} = \frac{\partial \Gamma_i(u)}{\partial u_j} \quad (6)$$

Forming each element of $J(u)$ requires taking analytic or discrete derivatives of the system of equations with respect to u which is often a cumbersome task.

2.2 Krylov subspace methods

Krylov methods are approaches for solving large linear systems introduced as direct methods in the 1950s (Hestenes and Stiefel, 1952), which their popularity took off after Reid (Reid, 1971) reintroduced them as iterative methods. There are projection or generalized projection methods (Saad, 2003) for solving $Ax = b$ using the Krylov subspace, K_j,

$$K_j = \text{span}(r_0, Ar_0, A^2r_0, ..., A^{j-1}r_0) \quad (7)$$

where $r_0 = b - Ax_0$. These methods require only matrix-vector products to carry out the iteration and not the individual elements of $\mathbf{A}$. This is a key to their use with Newton's method.

A wide variety of iterative methods such as the Generalized Minimal RESidual method (GMRES), the Bi-Conjugate Gradient STABilized (BiCGSTAB), and the Transpose-free Quasi Minimal Residual (TFQMR) fall within the Krylov taxonomy. A principal bifurcation in the family tree is applicability to non-symmetric systems.

The widely used GMRES (Saad and Schultz, 1986) is an Arnoldi-based method. In the GMRES, the Arnoldi basis vectors form the trial subspace out of which the solution is constructed. One matrix-vector product is required per iteration to create each new trial vector, and the iterations are terminated based on a by-product estimate of the residual that does not require explicit construction of intermediate residual vectors or solutions. As a result of previous studies, we tend to use GMRES almost exclusively with JFNK.

2.3 Jacobian-Free Newton-Krylov methods

In the JFNK approach, a Krylov method is used to solve the linear system of equations given by Eq. (2). An initial linear residual, r_0, is defined, given an initial guess, δu_0, for the Newton correction,

$$r_0 = -\Gamma(u) - J(u)\delta u_0 \tag{8}$$

Note that the nonlinear iteration index, k, has been dropped. This is due to the fact that the Krylov iteration is performed at a fixed k. Let j be the Krylov iteration index. Since the Krylov solution is a Newton correction, and owing that a locally optimal move was just made in the direction of the previous Newton correction, the initial guess for δu_0 in the Krylov iteration is typically zero. This is asymptotically a reasonable guess in the Newton context, as the converged value for δu should approach zero in late Newton iterations.

The action of the Jacobian in the form of matrix-vector products is approximated by

$$J(u)V = \frac{[\Gamma(u + \varepsilon V) - \Gamma(u))]}{\varepsilon} \tag{9}$$

where ε is a small perturbation and V is an arbitrary vector. The error in this approximation is proportional to ε. This matrix-free approach has many advantages which the most attractive is the Newton-like nonlinear convergence rate without costs of forming or storing the true Jacobian. In practice one forms a matrix for preconditioning purposes, so the common description of this family of methods is eschewed as fully matrix-free.

Here, we discuss various options for choosing the perturbation parameter ε in Eq. (9), which is obviously sensitive to ε for given u and V. The best value for ε to use for a scalar finite-difference of a single argument can be accurately optimized as a balance of these two quantifiable trades-offs. If ε is too large, the derivative is poorly approximated and if it is too small, the result of the finite difference is contaminated by floating-point round-off error. The ε was routinely used to set to some value larger than the square root of the machine epsilon (ε_{mach}).

When the precision is known to be limited in the evaluation of $\Gamma(u)$, then another effective formula for the evaluation of ε is (Knoll and Keyes, 2004)

$$\varepsilon = \frac{\sqrt{(1 + \|u\|)\varepsilon_{mach}}}{\|V\|} \tag{10}$$

which is used in this work.

2.4 Inexact Newton methods

Since the use of an iterative technique to solve Eq. (2) does not require the exact solution of the linear system, the resulting algorithm is categorized as an inexact Newton method. A simple inexact method results in the following convergence criteria for each linear iteration

$$\|J^k \delta u^k + \Gamma(u^k)\| < \gamma \|\Gamma(u^k)\| \tag{11}$$

where γ, the forcing factor, is a constant smaller than unity. A too large value for γ results in less work for the Krylov method but more nonlinear iterations, whereas a too small value for γ results in more Krylov iterations per Newton iteration. Several strategies for optimizing the computational work through the variable forcing term γ are given by Eisenstat and Walker (Eisenstat and Walker, 1996).

2.5 Preconditioning the JFNK method

The purpose of preconditioning the JFNK method is to reduce the number of Krylov iterations, as manifested by efficiently clustering eigenvalues of the iteration matrix. Traditionally, for linear problems, one chooses a few iterations of a simple iterative method such a classical power method as a preconditioner. A goal of the JFNK approach is to avoid forming the Jacobian matrix $J(u)$, and, as will be shown, an effective preconditioner for JFNK can typically be simpler than the strict Jacobian of the system. A linear preconditioner can be applied on the left or on the right, or on both, if suitably factored. Both strategies, left or right preconditioning, may be employed in a Jacobian-free context, and there are pros and cons to both sides of the coefficient matrix. Using right preconditioning, one solves

$$(JP^{-1})(P\delta u) = -\Gamma(u) \tag{12}$$

where P symbolically represents the preconditioning matrix. Right preconditioning is actually realized through a two-step process: First, solving

$$(JP^{-1})w = -\Gamma(u) \tag{13}$$

for w. Then solving

$$\delta u = P^{-1} w \tag{14}$$

for δu. Thus, while we may refer to the matrix P, operationally the algorithm only requires the action of P^{-1} on a vector. Note that if a distributed or segregated approach is used for preconditioning, then P^{-1} may be formed as a linear combination of approximate inverses of submatrices. This operation is done once per GMRES iteration and only the matrix elements required for the action of P^{-1} are formed.

There are various methods for choosing a preconditioning matrix like diagonal scaling, incomplete Cholesky factorization, multigrid, domain decomposition, Sparse approximate inverses, and hierarchical representations. The approach for construction of P is chosen automatically depending on the adopted Krylov subspace method. For example, in GMRES method, the diagonal scaling strategy is referred. A detailed study about preconditioning methods can be found in (Saad, 2003).

3 Even-parity neutron transport theory

Consider the one-group steady state neutron transport equation

$$\begin{aligned} &\overrightarrow{\Omega}.\nabla\Phi_0(\overrightarrow{r},\overrightarrow{\Omega}) + \Sigma_t(r)\Phi_0(\overrightarrow{r},\overrightarrow{\Omega}) = \\ &\int_{4\pi} \mathrm{d}\Omega'\, \Sigma_s(\overrightarrow{r},\overrightarrow{\Omega'},\overrightarrow{\Omega}) + \Phi_0(\overrightarrow{r},\overrightarrow{\Omega'}) + S(\overrightarrow{r},\overrightarrow{\Omega}) \end{aligned} \tag{15}$$

in volume V. Expanding the scattering kernel into series of Legendre polynomials one can write Eq. (15) in the following form

$$\begin{aligned}\overrightarrow{\Omega}.\nabla\Phi_0(\overrightarrow{r},\overrightarrow{\Omega})+\sum_{n=0}^{\infty}\frac{2n+1}{4\pi}\Sigma_{sn}(r)\times\\ \int_{4\pi}P_n(\mu_0)\Phi_0(\overrightarrow{r},\overrightarrow{\Omega'})\mathrm{d}\Omega' \;=S(\overrightarrow{r},\overrightarrow{\Omega})\end{aligned}\tag{16}$$

where $P_n(\mu_0)$ is the Legendre polynomial of order n, and $\Sigma_{sn}(r)$ is the scattering moments.

In even-parity method, the angular flux, scattering cross sections and sources are divided into even and odd parities (Ackroyd, 1978). It is well known that Eq. (16) can be cast into the pair of parity equations

$$\overrightarrow{\Omega}.\nabla\Phi_0^-(\overrightarrow{r},\overrightarrow{\Omega})+C\Phi_0^+(\overrightarrow{r},\overrightarrow{\Omega})=S^+(\overrightarrow{r},\overrightarrow{\Omega})\tag{17}$$

$$\overrightarrow{\Omega}.\nabla\Phi_0^-(\overrightarrow{r},\overrightarrow{\Omega})+G^{-1}\Phi_0^-(\overrightarrow{r},\overrightarrow{\Omega})=S^-(\overrightarrow{r},\overrightarrow{\Omega})\tag{18}$$

where C and G^{-1} denote operators for an arbitrary even function $u^+(\overrightarrow{r},\overrightarrow{\Omega})$ and odd function $u^-(\overrightarrow{r},\overrightarrow{\Omega})$ respectively defined as

$$\begin{aligned}&Cu^+(\overrightarrow{r},\overrightarrow{\Omega})=\\ &\sum_{n=0,even}^{\infty}\frac{2n+1}{4\pi}\Sigma_n\int_{4\pi}P_n(\mu_0)u^+(\overrightarrow{r},\overrightarrow{\Omega'})\mathrm{d}\Omega'\\ &G^{-1}u^-(\overrightarrow{r},\overrightarrow{\Omega})=\\ &\sum_{n=0,odd}^{\infty}\frac{2n+1}{4\pi}\Sigma_n\int_{4\pi}P_n(\mu_0)u^-(\overrightarrow{r},\overrightarrow{\Omega'})\mathrm{d}\Omega'\end{aligned}\tag{19}$$

The operators C and G^{-1} are self adjoint and positive definite.

The even and odd parity flux, source and scattering cross section are defined as

$$\begin{aligned}\Phi^{\pm}(\overrightarrow{r},\overrightarrow{\Omega})&=\frac{1}{2}[\Phi(\overrightarrow{r},\overrightarrow{\Omega})\pm\Phi(\overrightarrow{r},\overrightarrow{-\Omega})]\\ S^{\pm}(\overrightarrow{r},\overrightarrow{\Omega})&=\frac{1}{2}[S(\overrightarrow{r},\overrightarrow{\Omega})\pm S(\overrightarrow{r},\overrightarrow{-\Omega})]\\ \sigma^{\pm}(\overrightarrow{r},\overrightarrow{\Omega'},\overrightarrow{\Omega})&=\frac{1}{2}[\sigma_s(\overrightarrow{r},\overrightarrow{\Omega'},\overrightarrow{\Omega})\pm\sigma_s(\overrightarrow{r},\overrightarrow{-\Omega'},\overrightarrow{\Omega})]\end{aligned}\tag{20}$$

If the trial function Φ^+ be used instead of exact solution Φ_0^+, then volume and surface error *i.e.* $\varepsilon_V(\Phi^+)$ and $\varepsilon_{\partial V}(\Phi^+)$ would be created as the remainder of unsatisfied equations. Collecting the volume error and the surface boundary error gives (Abbassi et al., 2011)

$$\begin{aligned}\varepsilon_V(\Phi^+)+\varepsilon_{\partial V}(\Phi^+)+K^+(\Phi^+)=\\ H^{-+}(\Phi_0^-,\Phi_0^+,S^+,T)\end{aligned}\tag{21}$$

where the right hand side of Eq. (21) is a positive constant value. Total error *i.e.* sum of $\varepsilon_V(\Phi^+)$ and $\varepsilon_{\partial V}(\Phi^+)$ vanishes as Φ^+ closes the exact solution. Equation (21) suggests the following inequality for the $K^+(\Phi^+)$ functional:

$$K^+(\Phi^+)\le H^{-+}(\Phi_0^-,\Phi_0^+,S^+,T)\tag{22}$$

A good approximation for Φ_0^+ can be obtained by minimizing $\varepsilon_V(\Phi^+)+\varepsilon_{\partial V}(\Phi^+)$ with respect to the arbitrary coefficients specifying Φ^+. Minimization of $\varepsilon_V(\Phi^+)+\varepsilon_{\partial V}(\Phi^+)$ is equivalent to maximization of $K^+(\Phi^+)$, since it defines a maximum principle with trial function Φ^+:

$$\begin{aligned}K+(\Phi^+)=&\int_V\int_{4\pi}\{2(S^+\Phi^+)+2(S^-G(\overrightarrow{\Omega}.\overrightarrow{\nabla}\Phi^+))\\ &-(\overrightarrow{\Omega}.\overrightarrow{\nabla}\Phi^+G(\overrightarrow{\Omega}.\overrightarrow{\nabla}\Phi^+))-(\Phi^+C(\Phi^+))\}\mathrm{d}\Omega\,\mathrm{d}V\\ &+4\int_S\int_{\overrightarrow{\Omega}.\overrightarrow{n}<0}|\overrightarrow{\Omega}.\overrightarrow{n}|T(r,\Omega)\Phi^+\mathrm{d}\Omega\,\mathrm{d}S\\ &-2\int_S\int_{\overrightarrow{\Omega}.\overrightarrow{n}<0}|\overrightarrow{\Omega}.\overrightarrow{n}|(\Phi^+)^2\mathrm{d}\Omega\,\mathrm{d}S\end{aligned}\tag{23}$$

which expresses the spatial and angular parts of $\Phi^+(r,\Omega)$ in the equation containing S^+, S^- and T.

4 An alternative eigenvalue search method using the JFNK approximation

In order to numerically solve this eigenvalue problem the spatial domain in the multigroup equations must be discretized.

For each energy group the multi-group even-parity transport equation is

$$\begin{aligned}&-\overrightarrow{\Omega}.\overrightarrow{\nabla}G_g[\overrightarrow{\Omega}.\overrightarrow{\nabla}\Phi_g^+]+C_g[\Phi_g^+]=\\ &S_g^+-\overrightarrow{\Omega}.\overrightarrow{\nabla}G_gS_g^- \quad , \quad g=1,2,...G\end{aligned}\tag{24}$$

where the operators G_g (inverse of G^{-1}) and C_g are defined in terms of the cross-sections σ_g and σ_{sg} and in accord with the general definition (Eq. (19)). Some theoretical aspects and mathematical works (Ackroyd, 1997) leads us to multi-group functional in Eq. (25):

$$F_g^+(\Phi_g^+)=F_{sg}^+(\Phi_g^+)+F_{fg}^+(\Phi_g^+)\tag{25}$$

which $F_{sg}^+(\Phi_g^+)$ contains both up and down scattering terms and $F_{fg}^+(\Phi_g^+)$ contains fission source.

$$\begin{aligned}F_{sg}^+(\Phi_g^+)=&\sum_{g'=1}^{G}\sum_{l_{even}}\frac{2l+1}{4\pi}\sum_{sl}^{g'g}(1-\delta_{g'g})\times\\ &\int_{4\pi}P_l(\mu_0)\Phi_{g'}^+\,\mathrm{d}\Omega'\\ &+\sum_{g'=1}^{G}\sum_{l_{odd}}\frac{2l+1}{4\pi}\sum_{sl}^{g'g}(1-\delta_{g'g})\times\\ &\int_{4\pi}P_l(\mu_0)\Phi_{g'}^-\,\mathrm{d}\Omega'\end{aligned}\tag{26}$$

$$F_{fg}^+(\Phi_g^+)=\frac{\chi_g}{4\pi}\sum_{g'=1}^{G}\upsilon\sum_{fg'}\int_{4\pi}\Phi_{g'}^+(r,\Omega')\,\mathrm{d}\Omega'\tag{27}$$

where χ_g is fission spectrum. The extension of one-group even-parity neutron transport equation to multi-group approximation is straightforward

$$L_g^+=[\Phi_g^{(i+1)}]=\frac{1}{\lambda}F_{fg}^+[\Phi_g^{(i)}]\,,\quad g=1,2,...,G\tag{28}$$

where $\Phi_g^{(i)} = \int_{4\pi}[\Phi_g^+(r,\Omega)]^i \,\mathrm{d}\Omega$ is the scalar flux at i^{th} iteration and the L_g^+ is a scattering included matrix operator. In the even parity neutron transport theory, the entire L^+ operator for all groups can be written as the following matrix form

$$L^+ = \begin{bmatrix} F_1^+ & -A_{1,1}^{+2,1} & \cdots & -A_{1,n}^{+G,1} \\ \vdots & \vdots & \ddots & \vdots \\ -A_{G,1}^{+G,1} & -A_{G,n}^{+G-1,G} & \cdots & F_G^+ \end{bmatrix} \tag{29}$$

where

$$A_{g,n}^{+g,g'} = \sum_{sn}^{+g,g'} \int_V \mathrm{d}V \int_{4\pi} \mathrm{d}\Omega' P_n(\mu_0) - \sum_{sn}^{*g,g'} \int_V \mathrm{d}V \int_{4\pi} \mathrm{d}\Omega' P_n(\mu_0)[\vec{\Omega}.\vec{\nabla} G(\vec{\Omega}.\vec{\nabla})] \tag{30}$$

is the group-wise (operator) matrix element of anisotropic scattering kernel of order of n.

In traditional power method the eigenvalue λ is updated via

$$\lambda^{(i+1)} = \frac{\sum_{g'} \upsilon \sum_{fg'} \int_V \Phi_{g'}^{(i+1)} \mathrm{d}V}{\frac{1}{\lambda^{(i)}} \sum_{g'} \upsilon \sum_{fg'} \int_V \Phi_{g'}^{(i)} \mathrm{d}V} = c \sum_{g'} \upsilon \sum_{fg'} \int_V \Phi_{g'}^{(i+1)} \mathrm{d}V \tag{31}$$

where c is a constant value which is computed from previous iteration (Duderstadt et al., 1976). By initial guesses for λ and $\Phi_{g'}^{(0)}$, and solving Eq. (28) in each iteration, finally the system of $(G+1)$ equations converges.

To generalize the use of JFNK methods for coupling physical subsystems Xu and Downar (Downar, 2005) described an approach to apply the JFNK method to nested iteration schemes. These nested schemes, referred to as fixed point iterations, are defined by the function $Y(u)$ with the solution given by u, such that Eq. (28) with

$$u = \begin{bmatrix} \Phi_1^+ \\ \vdots \\ \Phi_G^+ \\ \lambda \end{bmatrix} \tag{32}$$

and the following function $\Gamma(u)$ in nonlinear system

$$\Gamma(u) = \begin{bmatrix} L_1^+[\Phi_1^+] - \frac{1}{\lambda} F_{f1}^+[\Phi_1^+] \\ \vdots \\ L_G^+[\Phi_G^+] - \frac{1}{\lambda} F_{fG}^+[\Phi_G^+] \\ \lambda - c \sum_{g'=1}^{G} \upsilon \sum_{fg'} \int_V \Phi_{g'}^+ \mathrm{d}V \end{bmatrix} \tag{33}$$

The update formula of λ (Eq. (31)) is imposed by the final equation in the nonlinear system of $G+1$ equations.

From Eq. (6), the Jacobian $(G+1, G+1)$ of the nonlinear function $\Gamma(u)$ is given by

$$J(u) = \begin{bmatrix} L_g^+ - \frac{1}{\lambda} F_{fg}^+ & \frac{1}{\lambda^2} F_{fg}^+[\Phi_g^+] \\ c \sum_{g'=1}^{G} \upsilon \sum_{fg'} \int_V \mathrm{d}V & 1 \end{bmatrix}, \quad g = 1, 2, ..., G \tag{34}$$

However, in the context of a Newton-Krylov method it is unnecessary to explicitly calculate the Jacobian in this manner, instead the construction of the Jacobian-vector product $J(u)\upsilon$ will be investigated. By using Eq. (9) the Jacobian of the nonlinear system is neither formed nor stored. Substituting $\Gamma(u)$ and $J(u)$ in Eq. (2) leads to

$$\begin{bmatrix} L_g^+ - \frac{1}{\lambda} F_{fg}^+ & \frac{1}{\lambda^2} F_{fg}^+[\Phi_g^+] \\ c \sum_{g'=1}^{G} \upsilon \sum_{fg'} \int_V \mathrm{d}V & 1 \end{bmatrix} \begin{bmatrix} \delta\Phi_g^+ \\ \delta\lambda \end{bmatrix} = - \begin{bmatrix} L_g^+[\Phi_g^+] - \frac{1}{\lambda} F_{fg}^+[\Phi_g^+] \\ \lambda - c \sum_{g'=1}^{G} \upsilon \sum_{fg'} \int_V \Phi_{g'}^+ \mathrm{d}V \end{bmatrix} \tag{35}$$

which can again be evaluated on a group-wise basis.

This is a nonsymmetrical coupled system that can be solved iteratively with Krylov subspace methods.

As is clear from Eq. (34), the goal is $\begin{bmatrix} \delta\Phi_g^+ \\ \delta\lambda \end{bmatrix} \to 0$ which means the convergence of the equations system. Because of using Jacobian free strategy, there is no need to form the left hand side of the Eq. (35). The algorithm of fast iterative JFNK method for solving eigenvalue problems presented in Fig. 1.

Aside from avoiding the inner iterations, this method has the added benefit of treating both upscatterings and downscattering equally. There are no additional iterations required over energy groups with non-negligible upscattering. Looping through energy groups in a given sequence is an artifact way to store data. In this case the coupling of energy groups is treated at the level of Newton iteration.

5 Numerical results

Numerical results were generated for a number of sample problems using a computer code named FEMPT (Abbassi et al., 2011), based on even-parity spherical harmonics and finite element method in $X-Y$ geometry, which implements the JFNK method developed for the generalized eigenvalue problem. The FEMPT is also capable of performing standard power iterations in anisotropic scattering model with no restriction on the angular approximation. This code will be used to examine the performance of the JFNK method compared to that of the classical power method and the forcing factor involved in the Newton-based approach will be studied to determine their influence on performance. To utilize the matrix-free method, the assembling approach was changed from the element based to the node based method.

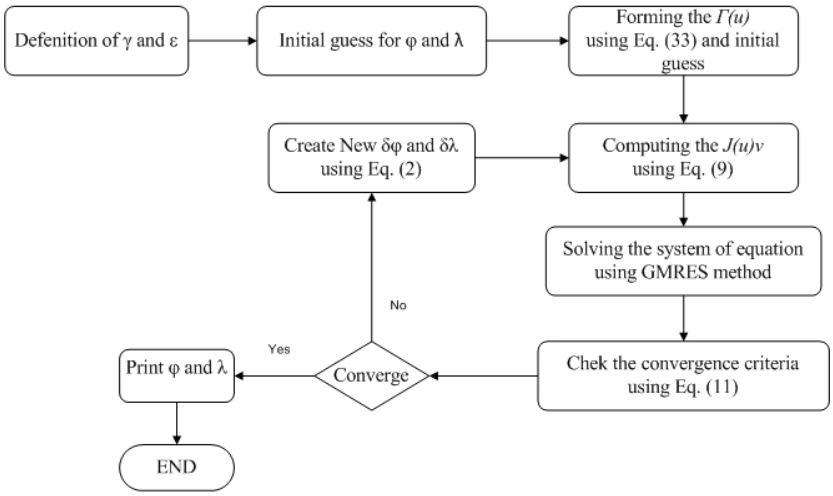

Figure 1: The algorithm of fast iterative JFNK method.

The module associated with the JFNK method was designed to interact with the FEMPT code primarily through function calls. Sparse storage is utilized for the storage of the L_g^{+j} matrices and the Preconditioned Conjugate Gradient algorithm was used to solve the within-group problem during the power iteration process. The GMRES method was used to solve the linear Newton step in all of the JFNK processes.

Two reactor benchmarks were used to evaluate the performance of the JFNK method via FEMPT:

1. *Swimming Pool Reactor*: The benchmark is a 2-D rector with five regions defined for the IAEA research program on transport theory and advanced reactor calculations (Rose, 1983). The one-group system shown in Fig. 2 is bare, the scattering is isotropic, and regions 1 and 3 contain fissile materials. Table 1 gives the nuclear data. The reference eigenvalue, is calculated by Wood and Williams (Wood and Williams, 1984) for P_3 angular approximation.

2. *Irregular 2-D Geometry Problem*: This problem is model of a hexagonal PWR assembly in which a natural uranium pin at the center is surrounded by 12 identical enriched fuel pins, as shown in Fig. 3. Thanks to the symmetry, only $\frac{1}{12}$ of assembly is simulated. This problem was also modeled by TPTRI code (Hongchun et al., 2007). The up-scattering included two-group cross-sections of each material is presented in Table 2.

Table 1: Cross-sections of swimming pool rector problem.

Region	Cross-sections (cm^{-1})		
	σ_t	$\overline{\sigma_s}$	$\upsilon\sigma_f$
1	0.60	0.53	0.079
2	0.48	0.20	0.0
3	0.70	0.66	0.043
4	0.65	0.50	0.0
5	0.90	0.89	0.0

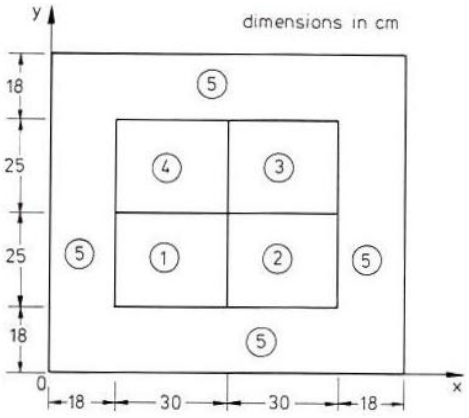

Figure 2: Geometry of swimming pool reactor (Dimensions are in cm).

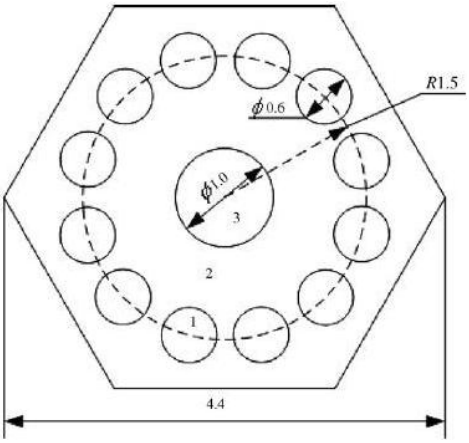

Figure 3: Geometry of PWR assembly (Dimensions are in cm).

The P_3 approximation has been used for all benchmarks. The forcing factor is set to 10^{-1} and the perturbation parameter is chosen according to Eq. (10). Comparisons made with power iteration using the tight convergence criteria set and non-preconditioned inner iterations are given in Table 3.

Table 2: Cross-sections of the hexagonal PWR assembly (cm^{-1}).

Energy group	Material zone	σ_t	σ_a	σ_s		$\upsilon\sigma_f$
				σ_{g-1}	σ_{g-2}	
1	Fuel	0.196647	0.008627	0.178	0.01002	0.006203
	Moderator	0.222064	0.000684	0.1995	0.02188	0.0
	Natural uranium	0.196647	0.008627	0.178	0.01002	0.006203
2	Fuel	0.596159	0.06957	0.001089	0.5255	0.1101
	Moderator	0.887874	0.008016	0.001558	0.8783	0.0
	Natural uranium	0.596159	0.06957	0.001089	0.5255	0.1101

From Table 3, it can be seen that for these input parameters JFNK offers an improvement in convergence of the standard power iteration and in all cases the total iteration count and the execution time is reduced.

To examine the convergence rate of the JFNK approach against the power method, the global fission source error for both benchmarks is plotted vs. the iterations in Figs. 4 and 5.

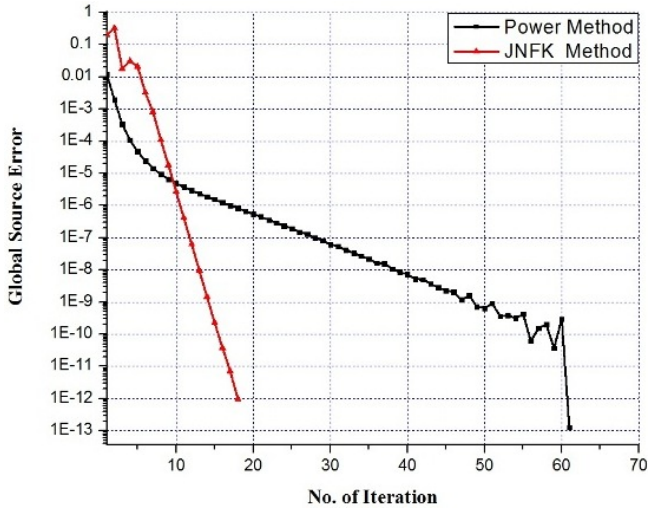

Figure 4: Convergence order of JFNK method for swimming pool reactor.

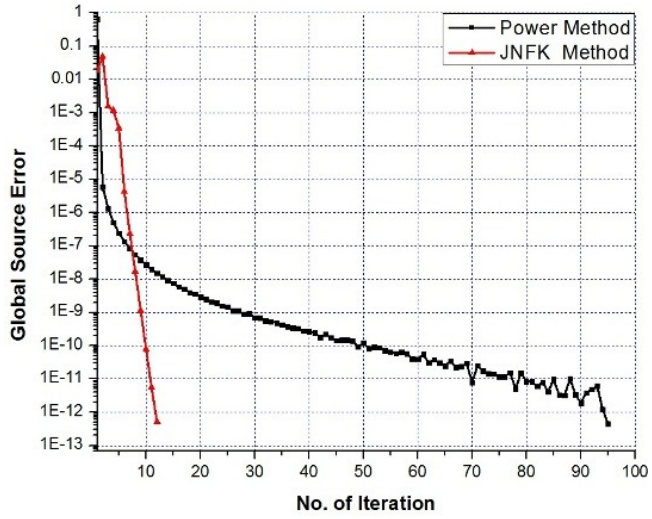

Figure 5: Convergence order of JFNK method for irregular 2-D geometry.

These plots confirm that the JFNK approach is capable of achieving impressive convergence rate. The JFNK method is theoretically sensitive to the initial guess. The proximity of the initial guess to the solution is extremely important as convergence of the Newton's method is a local and not a global quantity. For this reason the JFNK approach has been tested by using a variety of initial guesses. These are generated by first performing some number of standard power iterations, which themselves were initiated with a flat flux. The sequence of numbers of initial power iterations used was set to $\{1, 2, 3, 4, 5, 10, 15 \text{ and } 20\}$.

The number of Newton iterations and calculated eigenvalues for both benchmarks are given in Table 4. Figure 6 shows the effect of increasing the number of initial power iteration on the programs run time.

According to the Table 4, although the number of Newtons iteration have been reduced by increasing the number of initial power iterations, Fig. 5 emphasized that increasing the number of initial power iterations makes some additional computational cost. However only a few number of initial power iterations is quite enough to achieve the optimum condition.

The choice of the forcing factor sequence, γ, is an important criterion which is a constant smaller than unity. Constant values of 10^{-1}, 10^{-2}, and 10^{-3} were used and the results of these numerical experiments for JFNK are given in Figs. 7 and 8 for benchmarks 1 and 2, respectively.

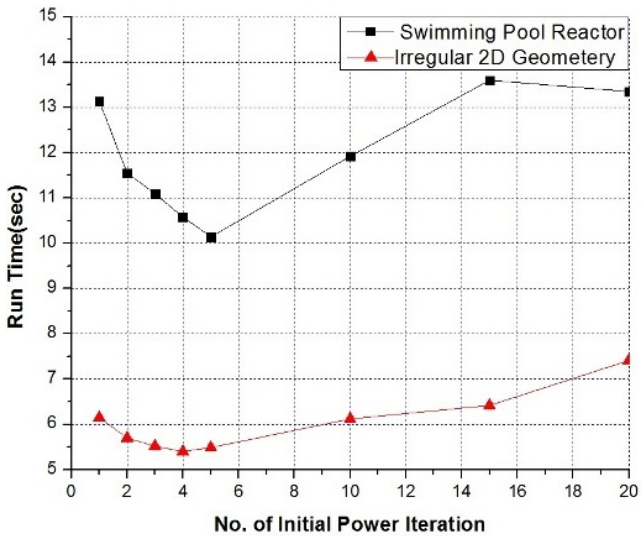

Figure 6: Effect of initial power iteration on execution time.

Table 3: Comparison between JNFK and power method results.

Benchmark	Method	K_{eff}	Newton(Krylov) iteration	Outer(Inner) iteration	Run time (sec)	Reference eigenvalue
Swimming pool reactor	Power	1.00712	-	61(1794)	33.70	1.0069 (Wood and Williams, 1984)
	JNFK	1.00767	18(173)	-	19.80	
Irregular 2-D geometry	Power	1.08532	-	95(3116)	20.60	1.085775 (Hongchun et al., 2007)
	JNFK	1.08598	12(146)	-	8.90	

Table 4: Number of Newton iterations and calculated eigenvalues according to number of initial power iteration.

No. of initial power iteration	No. of Newton's iteration		Calculated eigenvalue	
	Swimming pool reactor	Irregular 2-D geometry	Swimming pool reactor	Irregular 2-D geometry
0	18	12	1.007671	1.085983
1	11	8	1.007671	1.085981
2	9	7	1.007671	1.085973
3	8	7	1.007673	1.085975
4	7	6	1.007672	1.085982
5	6	6	1.007673	1.085980
10	5	5	1.007672	1.085976
15	4	4	1.007672	1.085979
20	3	4	1.007672	1.085979

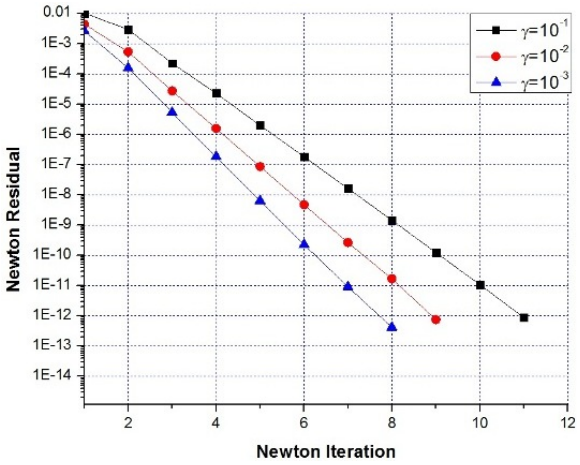

Figure 7: Convergence of JFNK method for swimming pool reactor benchmark as a function of γ.

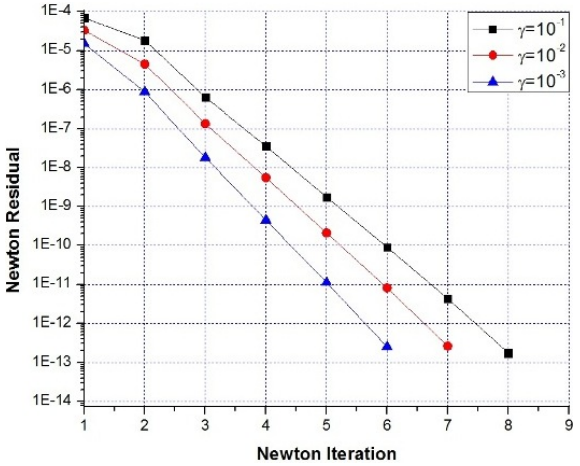

Figure 8: Convergence of JFNK method for irregular 2-D geometry benchmark as a function of γ.

Interestingly, in this case it can be seen that JFNK now performs much better and by changing the value of forcing factor the requiring number of Newton and GMRES iterations is reduced.

6 Conclusion

In this work a new nonlinear function has been developed which is capable of solving the eigenvalue problem associated with the multi-group even parity transport equations. Recognizing that the traditional power iteration can be written as a nonlinear system of equations it is possible to cast an inexact Newton method employing the Jacobian-Free approximation as an accelerated iterative approach. This method also has the benefit of not requiring any special treatment of upscattering because of within-group iterations is given equal treatment. The JFNK approach developed for the eigenvalue problems is not power iteration dependent, instead these methods rely entirely on matrix vector products in the evaluation of the nonlinear function.

Numerical results were generated using FEMPT code which solved even-parity neutron transport equation and implements the JFNK method and the traditional power method. The computational results indicate that the JFNK method can converge as fast as several times than the standard procedure.

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