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"

William C. Dawn

Nuclear Engineering Department
North Carolina State University
Raleigh, NC
wcdawn@ncsu.edu

May 3, 2019

NC STATE UNIVERSITY

Table of Contents

NC STATE UNIVERSITY

Outline

Why JFNK?

- Robust method for solving general nonlinear equations.
- q-quadratic convergence rate at termination [Kel95].
- Analytic form of Jacobian not required.

JFNK Challenges

- Jacobi-Free Newton-Krylov (JFNK) methods require residual form.
- Requires computationally expensive Jacobian-vector product.
- Typically, an optimized Power Iteration (PI) method is similarly efficient.

NC STATE UNIVERSITY

Outline

Multigroup Neutron Diffusion Equation

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

$\mathbf{r}$ = 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 $\left[\frac{1}{\text{cm}}\right]$,

$\Sigma_{s,g'\rightarrow g}(\mathbf{r})$ = macroscopic scatter cross section from energy group g' to energy group g $\left[\frac{1}{\text{cm}}\right]$,

G = total number of energy groups.

NEM Equations

Transverse integrated multigroup neutron diffusion equation.
Note: node indices i, j, k have been omitted.

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

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

u = coordinate direction (i.e. $u = x, y, z$),
$\overline{\Sigma_{r,g}}$ = average value of $\Sigma_{r,g}(\mathbf{r})$ in node i, j, k,
$\overline{D_g}$ = average value of diffusion coefficient in node i, j, k,
$Q_{g,u}(u)$ = transverse integrated neutron source,
$L_{g,u}(u)$ = transverse leakage.

NEM Projections

Basis functions are typically polynomials.
Zhou and Li select Legendre polynomials.

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

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

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

$a_{g,u,n}$ = expansion coefficient of $\phi_{g,u}(u)$,
$q_{g,u,n}$ = expansion coefficient of $Q_{g,u}(u)$,
$l_{g,u,n}$ = expansion coefficient of $L_{g,u}(u)$,
$f_{u,n}(u) = n^{th}$ Legendre polynomial.

Local Elimination

- Odd and even coefficients can be solved separately [Geh92].
- Zhou and Li show $a_{g,u,1}$ and $a_{g,u,3}$ can be written in terms of each other.
- $a_{g,u,1-3}$ and $a_{g,u,2-4}$ are introduced.
- Solution vector, Φ_g is length $10 \times N \times G$.

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

JFNK Theory

The m^{th} Newton step.

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

The step proceeds.

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

Inexact Newton Condition

The Newton step is solved with a Krylov solver.
GMRES and BiCGSTAB are both investigated.

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

The Krylov solver does not require an explicit Jacobian, only the Jacobian-vector product which can be approximated with finite differences.

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

Typically, $\varepsilon = \sqrt{\varepsilon_{mach}} \approx 10^{-8}$.

Choice of Physics-Based Preconditioner

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

- Preconditioner should approximate the Jacobian inverse [Kel95].
- Gill and Azmy investigate several choices of preconditioner and conclude that preconditioning with ≈ 5 PIs is ideal.
- Knoll et al. present similar results.
- Zhou and Li develop a preconditioner based on available data.
- Solved using TriDiagonal Matrix Algorithm (TDMA) and then Alternating Direction Iterative (ADI) method.
- No preconditioner comparison provided.

Convergence Rates of JFNK and PI Methods

- PI.
  - Converges linearly at a rate determined by the dominance ratio [Nak77].

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

  - Typically, $d > 0.95$ is common and the Wielandt Shift (WS) is used (to be discussed) [Geh92].

$$d' = \frac{\frac{1}{\lambda_0} - \frac{1}{\lambda'}}{\frac{1}{\lambda_1} - \frac{1}{\lambda'}}$$

- JFNK.
  - Convergence rate determined by Jacobian properties (e.g. Lipschitz constant) [Kel95].
  - Not affected by dominance ratio [Gil11].
  - Will not be affected by WS despite claim of Zhou and Li.

Outline

Verification and Validation

- No spatial convergence results.
- Single verification benchmark presented: International Atomic Energy Agency (IAEA) 3D Pressurized Water Reactor (PWR).
- Pebble bed reactor results not verified.
- λ and $\|\mathbf{R}(\mathbf{x}^m)\|$ not related so convergence of λ cannot be inferred.

Critical Boron Concentration Search

- Typically for PWRs, the critical boron concentration is desired such that $\lambda = 1.0$.
- Current algorithm is linked to the PI method.
- May be extendable to the JFNK method or may be too inefficient and undo any efficiency improvements.

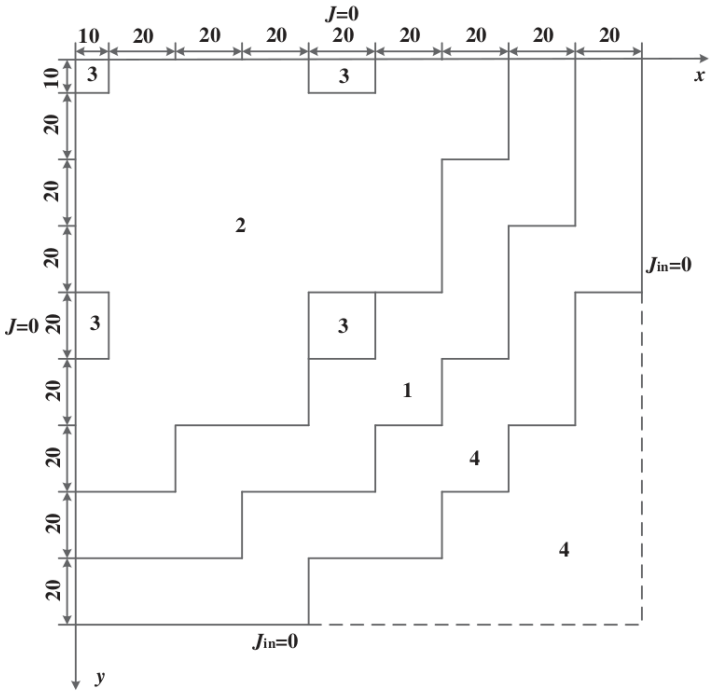
Coarse Mesh Finite Difference Formulation

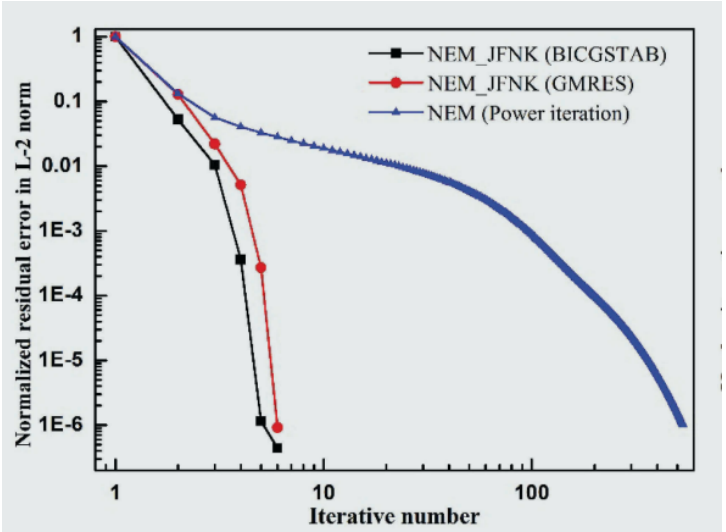
- Zhou and Li solve for Nodal Expansion Method (NEM) coefficients directly.
- Instead, a $\widetilde{D}$ can be calculated to correct the finite difference equations [Smi83; Pal97].
- Solution vector is reduced $10 \times N \times G \rightarrow N \times G$.
- Would be compatible with existing codes [Stu09b; Stu09a; Col15].
- May pose additional challenges compared to PI method.

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

Ragged Core

- After performing local elimination, 18% of solution variables in IAEA 3D PWR benchmark are unnecessary.
- This may bias results and penalize the PI method [Geh92].





Wielandt Shift

- WS can reduce PI method runtime by a factor of three or more.
- Zhou and Li do not compare the JFNK method to a PI method with the WS.
- WS could invalidate some of the results.
- JFNK may still be preferable to PI+WS [Kno11].
- WS would also be useful for a PI preconditioner.

NC STATE UNIVERSITY

Outline

Multiphysics JFNK

- Zhou and Li claim their method will be extended to include multiphysics feedback.
- Hamilton et al. present results for multiphysics JFNK.
- It was concluded that cross section processing was prohibitively inefficient.
- Required reactor-specific cross section derivatives.

Proposed Future Investigations

- Compare proposed JFNK implementation to a PI method with the WS.
- Investigate other preconditioners including PI preconditioner.
- Implement a Coarse Mesh Finite Difference (CMFD) formulation to reduce the number of solving variables.

Conclusion

When comparing algorithm efficiency, it is crucial to compare optimized computer programs.

NC STATE UNIVERSITY

Thank You!

Thank you all for coming this morning!

References I

[Col15] B. Collins et al. *MPACT Theory Manual*. Tech. rep. CASL-U-2015-0078-000. Mar. 2015.

[Daw19] W. C. Dawn. "Simulation of Fast Reactors with the Finite Element Method and Multiphysics Models." MA thesis. North Carolina State University, 2019.

[Geh92] J. C. Gehin. "A Quasi-Static Polynomial Nodal Method for Nuclear Reactor Analysis." PhD thesis. Massachusetts Institute of Technology, 1992.

[Gil11] D. F. Gill and Y. Y. Azmy. "Newton's Method for Solving k-Eigenvalue Problems in Neutron Diffusion Theory." In: *Nuclear Science and Engineering* 167.2 (Feb. 2011), pp. 141–153.

[Ham16] S. Hamilton et al. "An Assesment of Coupling Algorithms for Nuclear Reactor Core Physics Simulations." In: *Journal of Computational Physics* 311 (Feb. 2016), pp. 241–257.

[Kel95] C. T. Kelley. *Iterative Methods for Linear and Nonlinear Equations*. Society for Industrial and Applied Mathematics, 1995, p. 166.

[Kel19] C. T. Kelley. *Lecture Notes in Nonlinear Equations and Unconstrained Optimization*. Spring 2019.

[Kno11] D. A. Knoll et al. "Acceleration of k-Eigenvalue/Criticality Calculations Using the Jacobian-Free Newton-Krylov Method." In: *Nuclear Science and Engineering* 167.2 (Feb. 2011), pp. 133–140.

[Nak77] S. Nakamura. *Computational Methods in Engineering Science*. New York: Wiley, 1977.

[Pal97] S. P. Palmtag. "Advanced Nodal Methods for MOX Fuel Analysis." PhD thesis. Massachusetts Institute of Technology, 1997.

References II

[Smi83] K. S. Smith. "Nodal Method Storage Reduction by Nonlinear Iteration." In: *Transactions of the American Nuclear Society*. Vol. 44. June 1983.

[Stu09a] Studsvik. *SIMULATE-3: Advanced Three-Dimensional Two-Group Reactor Analysis Code*. Tech. rep. SSP-09/447-U. 2009.

[Stu09b] Studsvik Scandpower. *CASMO-4: A Fuel Assembly Burnup Program*. Tech. rep. SSP-09/443-U. 2009.

[Zho18] X. Zhou and F. Li. "Jacobian-Free Newton-Krylov Nodal Expansion Methods with Physics-Based Preconditioner and Local Elimination for Three-Dimensional and Multigroup k-Eigenvalue Problems." In: *Nuclear Science and Engineering* 190.3 (June 2018), pp. 238–257.

Acronyms I

ADI	Alternating Direction Iterative.
BiCGSTAB	BiConjugate Gradient STABilized.
CASL	Consortium for Advanced Simulation of LWRs.
CG	Conjugate Gradient.
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.
SPD	Symmetric Positive Definite.
TDMA	TriDiagonal Matrix Algorithm.
WS	Wielandt Shift.