Relationship Between Relaxation and Partial Convergence of Nonlinear Diffusion Acceleration for Problems with Feedback

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Outline

Multigroup Neutron Transport Equation (NTE) with Feedback

$$\begin{aligned}\hat{\mathbf{\Omega}} \cdot \nabla\psi_g(\boldsymbol{r}, \hat{\mathbf{\Omega}}) + \Sigma_{t,g}(\boldsymbol{r}, T)\psi_g(\boldsymbol{r}, \hat{\mathbf{\Omega}}) = \lambda\frac{\chi_g(\boldsymbol{r})}{4\pi}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\boldsymbol{r}, T)\phi_{g'}(\boldsymbol{r}) \\ + \sum_{g'=1}^{G}\int_{4\pi}\Sigma_{s,g'\to g}(\boldsymbol{r}, \hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}}, T)\psi_{g'}(\boldsymbol{r}, \hat{\mathbf{\Omega}}')d\Omega\end{aligned} \tag{1}$$

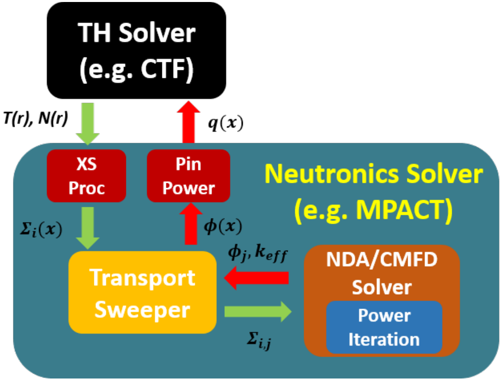
$$\int dV\sum_{g=1}^{G}\int_{4\pi}\Sigma_f\kappa\psi_g d\Omega = P \tag{2}$$

$$\boldsymbol{L}(T)T(\boldsymbol{r}) = \sum_{g=1}^{G}\Sigma_{f,g}(\boldsymbol{r}, T)\kappa\Phi_g(\boldsymbol{r}) \tag{3}$$

- The smallest $\lambda \equiv \frac{1}{k}$ eigenvalue, its corresponding eigenvector ψ, and the associated temperature distribution T are desired from this set of coupled equations.
- A normalization condition must be imposed to ensure a unique solution to the transport eigenvalue problem.

Overall Iteration Schemes

- Iteration Scheme:
  - **Picard**
  - Each Physics is solved separately
  - Easy to implement
- Transport iteration Scheme:
  - Source Iteration
  - Iterates on eigenvalue, and scattering and fission sources
  - Converges very slow
- Acceleration Scheme:
  - **Nonlinear Diffusion Acceleration (NDA)**
  - Reduce the total outer iteration number by orders of magnitude
- Eigenvalue Solver:
  - Wielandt Shifted Power Iteration



Nonlinear Diffusion Acceleration, Coarse Mesh Finite Difference

- Nonlinear Diffusion Acceleration (NDA) is a common acceleration method employed by the nuclear reactor community:
  - Low-order, transport-corrected diffusion equation
  - Nonlinear correction term $\hat{D}$ obtained from a high-order transport sweep
  - Scalar flux and eigenvalue solution used as an improved estimate for the scattering and fission source terms in a subsequent transport sweep

$$\begin{aligned}\left[-\nabla \cdot D_g(\boldsymbol{r}, T)\nabla + \Sigma_{t,g}(\boldsymbol{r}, T) + \hat{D}_g(\boldsymbol{r}, T)\right] \phi_g(\boldsymbol{r}) = \\ \sum_{g'=1}^{G} \Sigma_{s0,g' \to g}(\boldsymbol{r}, T)\phi_{g'}(\boldsymbol{r}) + \lambda\chi_g(\boldsymbol{r}) \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(\boldsymbol{r}, T)\phi_{g'}(\boldsymbol{r})\end{aligned} \tag{4}$$

- Coarse Mesh Finite Difference (CMFD) : a generalization of NDA which allows for a coarser mesh to be used on the low-order problem

Wielandt-Shifted Power Iteration

- Martix form of Equation (4):

$$\mathbf{M}\phi = \lambda \mathbf{F}\phi \tag{5}$$

- Standard power iteration (PI):

$$\mathbf{M}\boldsymbol{\phi}^{(l+1)} = \lambda^{(l)}\mathbf{F}\boldsymbol{\phi}^{(l)} \tag{6}$$

$$\lambda^{(l+1)} = \lambda^{(l)}\|\mathbf{F}\boldsymbol{\phi}^{(l)}\|/\|\mathbf{F}\boldsymbol{\phi}^{(l+1)}\| \tag{7}$$

PI converges at a rate equal to the dominance ratio (DR): λ_1/λ_2

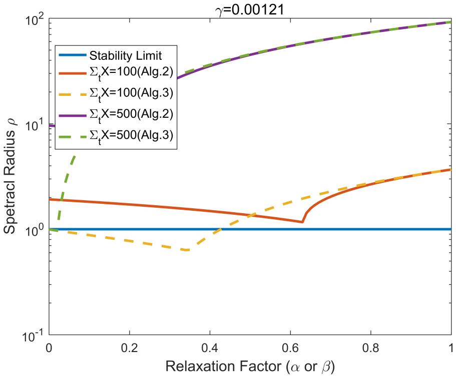
- Because the DR is close to 1 for realistic reactor problems, we can improve the spectral radius of PI using a Wielandt Shift (WS):

$$[\mathbf{M} - \lambda_s\mathbf{F}]\,\boldsymbol{\phi}^{(l+1)} = \left[\lambda^{(l)} - \lambda_s\right]\mathbf{F}\boldsymbol{\phi}^{(l)} \tag{8}$$

- In practice, this "inner" iteration procedure is not full converged, instead it is truncated at a given total number of iterations L or when some other convergence criteria is met

Picard iteration scheme is more stable than we have expected

- Drawbacks of the Picard scheme:
  - Stability is not guaranteed
  - Relaxation is always used
- Furthermore, Theoretical Analysis[1]:
  - Relaxation could not help when $\Sigma_t X > 100$
  - Hmm, the optical thickness of a 3D pincell is around 100.



- But, the multiphysics simulations have been performed for full core problems
.

[1] Brendan Kochunas/Andrew Fitzgerald/Edward Larsen: Fourier analysis of iteration schemes for k-eigenvalue transport problems with flux-dependent cross sections, in: Journal of Computational Physics 345 (2017), pp. 294–307.

More accurate CMFD solutions make iterations scheme unstable

1. Example 1–3D Pin Cell
   - Length: 380 cm, Power: 71 kW
   - L: # of power iteration, $nOuter$: # of total outer iteration

L	2	4	6	10	15	20	30	100
nOuter	33	19	15	14	14	17	21	**N/A**

2. Example 2–Vera Problem 7

Method	nOuter	Total Runtime [s]
Default	15	10230
MSED[2]	20	9749
MSED-L	12	6057

   - MSED-L: A partially converged low order MSED solve with looser convergence criteria and less aggressive Wielandt shift

[2] Ben C Yee/Brendan Kochunas/Edward W Larsen: A Multilevel in Space and Energy Solver for 3-D Multigroup Diffusion and Coarse-Mesh Finite Difference Eigenvalue Problems, in: Nuclear Science and Engineering 2019, pp. 1–24.

Goal of Research

- **Questions to be answered**:
  - Can the effect of convergence of NDA (CMFD) be theoretically investigated?
    - Previous researches on the stability of transport method always assume that NDA (CMFD) is fully converged.
  - What is the relation between partial convergence and well-known relaxation?
    - Effect of partial convergence is similar with the effect of relaxation
  - Whether the formula to determine near-optimal partial convergence can be derived?
    - An near-optimal partial convergence seems to exist
    - Reduce the computational intensity– *"why waste effort converging the low order problem with the wrong coefficients"*
    - *Stabilize the iteration scheme*
- Investigation Approach: **Fourier Analysis**

Fourier analysis is a technique that estimates the convergence properties of a method by looking at how error modes decay in a model problem*

- Procedure for Fourier analysis:
  - Define 1-D homogeneous problem with reflective boundary conditions
  - Define a "Fourier ansatz" consisting of equations of the form

$$\phi^{(l)}(x) = \phi_0 + \epsilon \sum_{\omega_j} \theta(\omega)^l e^{i\omega_j x} \,, \tag{9}$$

    where ϕ_0 is the exact solution and the second term is a "small" error of frequency ω_j
  - Substitute temporary solutions of the equations which define your method by Fourier ansatz , drop terms of $O(\epsilon^2)$ or smaller, and perform some algebra to obtain an eigenvalue problem for the decay rate $\theta(\omega)$
  - The spectral radius of the method is then given by $\rho = \max_{\omega_j} |\theta|$, $\rho < 1$ – the scheme is stable.

1. Introduction and Motivation
   - Problem of Interest
   - Motivation
2. Fourier Analysis
   - Analysis Overview
   - Model Problem
3. Analysis Results
   - Final Expression and Validation
   - Relationship between Partial Convergence and Relaxation
   - Near-Optimal Partial Convergence
4. Conclusions
5. Acknowledgement

Model Specification

- Cross section is assumed to be linearly dependent with the localized flux[3]:

$$\Sigma_i^{(n)}(x) = \Sigma_{i,0} + \Sigma_{i,1}\left(\phi^{(n)}(x) - \Phi_0\right) \tag{10}$$

  - In general the relation between cross section and the flux is not this simple. However, when the solution is close to the true solution, this approximation is reasonable.
  - Former research[4] shows this assumption can make Fourier analysis tractable and reveal the stability of the Picard scheme in neutron transport calculation with feedback.
  - A proxy multiphysics application which maintains some representative behavior while allowing for a spatially flat solution

[3] WILLIAM E KASTENBERG: Stability analysis of nonlinear space dependent reactor kinetics, in: Advances in nuclear science and technology, 1969, pp. 51–93.

[4] Brendan Kochunas/Andrew Fitzgerald/Edward Larsen: Fourier analysis of iteration schemes for k-eigenvalue transport problems with flux-dependent cross sections, in: Journal of Computational Physics 345 (2017), pp. 294–307.

Model Iteration Scheme

Algorithm 1 Model Iteration Scheme

Initialize $\phi(x)$ and $J(x)$

for $n = 0$ to N **do**

  Update the Cross Section by Equation (10)

  Calculate the CMFD coefficients and nonlinear coupling term $\hat{D}$

  Use the CMFD coefficients to form M and F

  for $l = 0$ to L **do**

    Solve $[M - \lambda_s F]\boldsymbol{\phi}^{(l+1)} = \left[\lambda^{(l)} - \lambda_s\right] F\boldsymbol{\phi}^{(l)}$

  end for

  Update the source of transport equation with coarse mesh solutions

  Perform transport sweep

end for

Important Parameters Revealed by Fourier Analysis

- Definition and Range

Symbol	c	γ	r	$\Sigma_t X$
Definition	Scattering Ratio	Feedback intensity	Wielandt shift ratio	Problem Size (mfp)
Range	< 0.96	$0 - 0.00121$	$0.66 - 0.99$	< 500

- Mathematical Expression:

$$c = \frac{\Sigma_{s,0}}{\Sigma_{t,0}} \tag{11a}$$

$$\gamma_0 = \left(\frac{\Sigma_{a,1}}{\Sigma_{a,0}} - \frac{\Sigma_{f,1}}{\Sigma_{f,0}}\right)\Phi_0 \tag{11b}$$

$$\gamma = (1-c)\gamma_0 = \frac{d\lambda}{d\phi}\frac{\nu\Sigma_{f,0}}{\Sigma_{t,0}} \tag{11c}$$

$$r = \frac{\lambda_s}{\lambda} \tag{11d}$$

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Fourier Analysis Result Expression

- Final Expression:

$$\theta(\omega) = \begin{cases} \left(\Lambda^L - \gamma\right) f_{TS}(\omega) + \left(1 - \Lambda^L(\omega)\right)\left[f_{NDA}(\omega) - \frac{3\gamma}{\omega^2} f_{TS}(\omega)\right], & \text{continuous problem} \\ \max\left|eig\left(\mathbf{T}(\omega)\right)\right|, \text{discretized problem} \end{cases} \tag{12}$$

where:

$$\mathbf{T}(\omega) = \tilde{\mathbf{H}}(\omega)(1-\gamma) - \left(1 - \Lambda^L(\omega)\right)\mathbf{1}\frac{3\Sigma_t\Delta(e^{i\Sigma_t\Delta\omega} - 1)\tilde{\mathbf{G}} + \gamma 3(\Sigma_t\Delta)^2 \frac{\mathbf{1}^T}{q}\tilde{\mathbf{H}}}{2 - 2cos(\Sigma_t\Delta\omega)}, \tag{13}$$

$$\tilde{\mathbf{H}} \in \mathbb{C}^{q\times q}, \quad \tilde{\mathbf{G}} \in \mathbb{C}^{1\times q}, \quad \mathbf{1} \in \mathbb{C}^{q}. \tag{14}$$

- q: # of fine cell per coarse mesh
- $\tilde{\mathbf{H}}, \tilde{\mathbf{G}}$[5]: Error transition matrix in the transport sweep and current calculation.

[5] Ang Zhu et al.: An optimally diffusive Coarse Mesh Finite Difference method to accelerate neutron transport calculations, in: Annals of Nuclear Energy 95 (Sept. 2016), pp. 116–124.

Fourier Analysis Result Expression

$$f_{TS}(\omega) = \frac{arctan(\omega)}{\omega} \quad (15a)$$

$$f_{NDA}(\omega) = (1 + \frac{1}{g(\omega)})f_{TS}(\omega) - \frac{1}{g(\omega)} \quad (15b)$$

$$\hat{c} = 1 - (1 - r)(1 - c) \quad (15c)$$

$$\Lambda(\omega) = \frac{1 - \tilde{c}}{1 - \tilde{c} + g(\omega)} \quad (15d)$$

$$g(\omega) = \begin{cases} \frac{1}{3}\omega^2 & \text{continuous problem} \\ \frac{2-2cos\left(\Sigma_t \Delta\omega\right)}{3\left(\Sigma_t \Delta\right)^2}, & \text{discretized problem} \end{cases}$$

- f_{TS}: error decay rate for the pure transport source iteration
- f_{NDA}: error decay rate for the NDA in problem without feedback
- $\hat{c}$: effective scattering ratio
- Λ: Error reduction rate per power iteration
- $g(\omega)$: Coefficient induced by diffusion aproximation

Validation of Fourier Analysis Results–Limitiation Check

- Continuous Case:
  1. For the case $L \to \infty, \gamma = 0$, simplied as the expression for NDA:

$$\theta(\omega) = (1 + \frac{3}{\omega^2}) f_{TS}(\omega) - \frac{3}{\omega^2} \tag{16}$$

  2. For the case $L \to \infty, \gamma \neq 0$, simplified as the expression[6] :

$$\theta(\omega) = f_{NDA}(\omega) - \gamma(1 + \frac{3}{\omega^2}) f_{TS}(\omega) \tag{17}$$

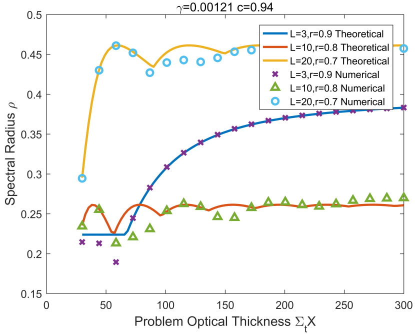
- Discretized Case, $L \to \infty, \gamma = 0$, simplied as the expression[7]:

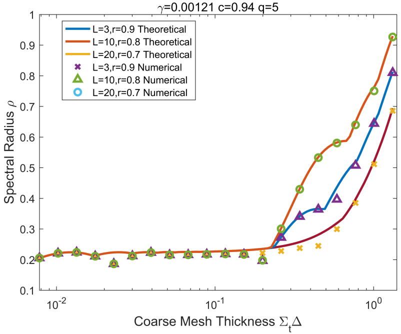
$$\mathbf{T}(\omega) = \tilde{\mathbf{H}}(\omega) - \mathbf{1}\frac{3\Sigma_t\Delta(e^{i\Sigma_t\Delta\omega} - 1)\tilde{\mathbf{G}}}{2 - 2cos(\Sigma_t\Delta\omega)}, \tag{18}$$

[6] Brendan Kochunas/Andrew Fitzgerald/Edward Larsen: Fourier analysis of iteration schemes for k-eigenvalue transport problems with flux-dependent cross sections, in: Journal of Computational Physics 345 (2017), pp. 294–307.

[7] Ang Zhu et al.: An optimally diffusive Coarse Mesh Finite Difference method to accelerate neutron transport calculations, in: Annals of Nuclear Energy 95 (Sept. 2016), pp. 116–124.

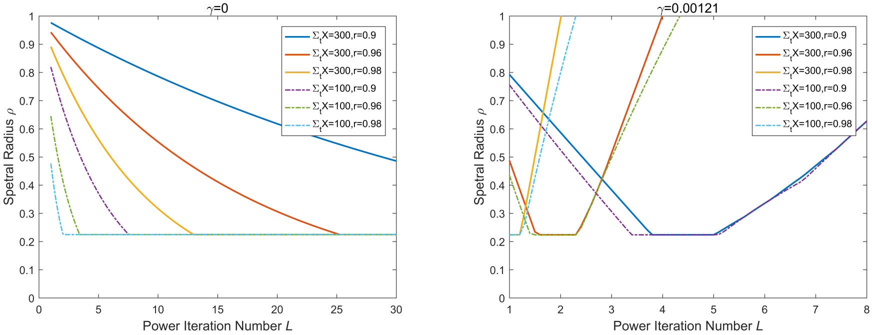
Validation of Fourier Analysis Results–Comparision with Numerical Estimation





- L, r are randomly selected to make validation convincing.
- Wave shape of spectral radius indicates that the effect of partial convergence are problem dependent.
- Fourier analysis predictions agree well with the numerical results from a test code.

Effect of Power Iteration Number



- Tightening the convergence of NDA by increasing the power iteration number or aggressiveness of Wielandt Shift will stablize the problem without feedback.
- However, it will make the Picard scheme become more stable first, then more unstable till unconverged (similiar with the relaxation).
- Near-optimal partial convergence exists but is problem-dependent.

Fourier Analysis Result of Fully Converged Nonlinear Diffusion Acceleration with Flux Relaxation

- Flux relaxation is applied when using coarse mesh flux to update the transport solution by:

$$\phi(x) = \beta\phi_j + (1-\beta)\phi(x) \tag{19}$$

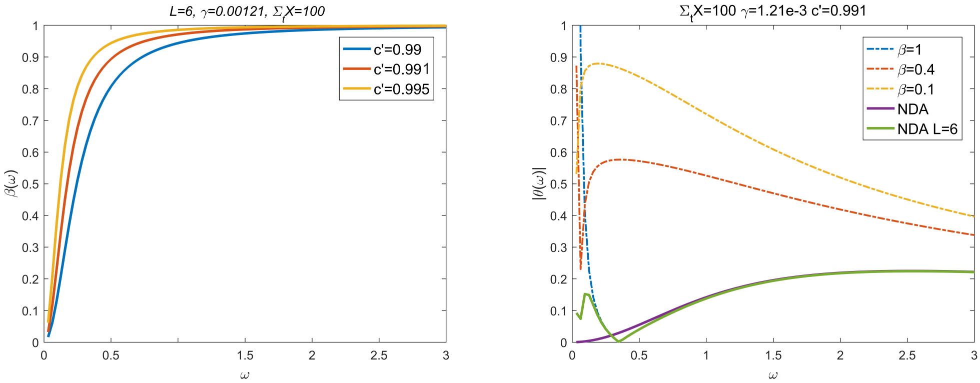
- Final Expression:

$$\theta(\omega) = \begin{cases} \left(1-\beta-\gamma\right) f_{TS}(\omega) + \beta\left[f_{NDA}(\omega) - \frac{3\gamma}{\omega^2} f_{TS}(\omega)\right], & \text{continuous problem} \\ \max\left|eig\left(\mathbf{T}(\omega)\right)\right|, \text{discretized problem} \end{cases} \tag{20}$$

where:

$$\mathbf{T}(\omega) = \tilde{\mathbf{H}}(\omega)(1-\gamma) - \beta\mathbf{1}\frac{3\Sigma_t\Delta(e^{i\Sigma_t\Delta\omega}-1)\tilde{\mathbf{G}} + \gamma 3(\Sigma_t\Delta)^2\frac{\mathbf{1}^T}{q}\tilde{\mathbf{H}}}{2-2cos(\Sigma_t\Delta\omega)} \tag{21}$$

Relation between Partial Convergence and Flux Relaxation



- Partial convergence induces the Fourier-frequency-dependent flux relaxation factor:

$$\beta(\omega) = 1 - \Lambda^{L}(\omega). \tag{22}$$

- The relaxation is mainly imposed on the relatively flat Fourier error modes.

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Derivation of the Near-Optimal Partial Convergence

- Rewrite the expression for spectral radius as for continuous case:

$$\theta(\omega) = \left(1 - \beta(\omega) - \gamma - \beta(\omega)\frac{3\gamma}{\omega^2}\right) f_{TS}(\omega) + \beta(\omega) f_{NDA} \tag{23}$$

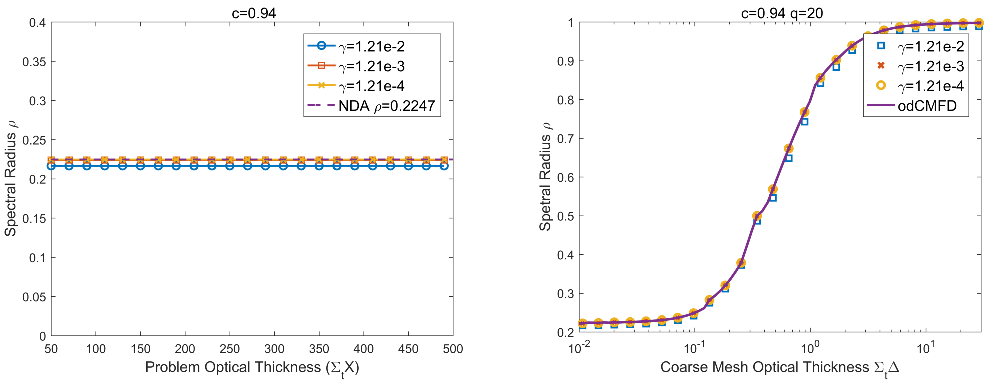
- For relatively flat fourier modes, $f_{TS}(\omega) \approx 1$
- The near optimal partial convergence should make:

$$1 - \beta(\omega) - \gamma - \beta(\omega)\frac{3\gamma}{\omega^2} \approx 0 \tag{24}$$

the near-optimal partial convergence in term of wielandt shift is:

$$r = 1 - \frac{(1 - \beta(\omega))^{\frac{1}{L}}}{1 - (1 - \beta(\omega))^{\frac{1}{L}}} \frac{\omega^2}{3(1 - c)}. \tag{25}$$

Test of Near-Optimal Partial Convergence



- $\omega = \frac{\pi}{200}$ is suggested.
- The same convergence behavior as NDA(CMFD) can be achieved theoretically.

Discussion of Near-optimal Partial Convergence

- Pros:
  - Easily to be implemented. Compatible with the CMFD and mutlilevel method such as MSED and Multilevel CMFD.
  - Stablize the scheme and reduce the computational intensity.
- Cons:
  - γ term needed to be calculated
  - Derivation is based on *NDA*, may not be optimal for CMFD.
- Conclusion: Intermediate solution to stabilize the Picard scheme with better efficiency.

Conclusions

1. The Fourier analysis of the iteration scheme accelerated by partially convergent NDA is performed.
2. The results support the observations that partial convergence can help to stabilize the multiphysics simulations, and near-optimal partial convergence exists though it is problem dependent.
3. The partial convergence is shown to be equivalent to more well understood relaxation factor, and the relaxation factor induced by partially converging the lower-order problem is mainly imposed on the flat Fourier modes.
4. The formula to determine the near-optimal partial convergence is put forward, provide people with intermediate measure to mitigate the stability issuse confronted in multiphysics simulation.

Mext Step

1. Test the prediction from the Fourier analysis in realistic problem.

2. Modify the iteration scheme in VERA-CS by using near-optimal partial convergence.

Acknowledgments

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Afterwords

1. A lot of multilevel methods are being implemented. However, be cautious about using more power iterations or more aggressive Wielandt shift in feedback problems, especially on the coarsest space/energy grid.
2. Be comfortable with a partially convergent NDA (CMFD). If it helps, just use it.
3. A batch of MC particle simulation/deterministic source iteration is a power iteration, pencil-paper results suggest that we should avoid running a lot batches/source iterations in MC/deterministic codes before applying feedback.

Numerical Result

P6 (MG)

Problem Details	
Rated Power	18 MW
k Tolerance	1e-6
ϕ Tolerance	1e-6

Reference	
n_Outer	**13**

Total Outer Iteration Number for Different Power Level

Power Level (%)	20	40	60	80	100	120	140
Default	13	13	13	13	13	13	15
PartConv	13	13	13	13	13	12	12
Difference	0	0	0	0	0	1	3

Total Run Time (min) for Different Power Level

Power Level (%)	20	40	60	80	100	120	140
Default	3.78	3.89	4.10	4.09	4.80	4.99	5.86
PartConv	3.93	3.69	3.63	3.60	3.63	3.47	3.52
Difference	-4%	5%	12%	12%	24%	31%	40%

Numerical Result

P6 (MSED)

Problem Details	
Rated Power	18 MW
k Tolerance	1e-6
ϕ Tolerance	1e-6

Reference	
n_Outer	12

Total Outer Iteration Number for Different Power Level

Power Level (%)	20	40	60	80	100	120	140
MSED	12	12	12	12	15	20	29
MSED-L	13	13	13	13	13	16	18
MSED-PC	13	13	13	13	13	13	12
Difference	0	0	0	0	2	7	17

Total Run Time (min) for Different Power Level

Power Level (%)	20	40	60	80	100	120	140
MSED	3.01	3.17	3.32	3.44	4.40	5.80	8.61
MSED-L	2.85	2.84	3.11	3.12	4.40	4.14	5.39
MSED-PC	2.92	2.91	2.90	2.92	2.92	2.97	3.03
Difference	3%	8%	13%	15%	34%	49%	65%

Numerical Result

P6 (Summary)

Problem Details	
Rated Power	18 MW
k Tolerance	1e-6
ϕ Tolerance	1e-6

Reference	
n_Outer	**13**

Total Outer Iteration Number for Different Power Level

Power Level (%)	20	40	60	80	100	120	140
Default	13	13	13	13	13	13	15
MSED-PC	13	13	13	13	13	13	12
Difference	0	0	0	0	0	0	3

Total Run Time (min) for Different Power Level

Power Level (%)	20	40	60	80	100	120	140
Default	3.78	3.89	4.10	4.09	4.80	4.99	5.86
MSED-PC	2.92	2.91	2.90	2.92	2.92	2.97	3.03
Difference	23%	25%	29%	29%	39%	41%	48%

Numerical Result

P6-MultiState

Problem Details	
Rated Power	18 MW
k Tolerance	1e-6
ϕ Tolerance	1e-6
State 1	80% Power
State 2	100% Power
State 3	120% Power
State 4	140% Power

Total Outer Iteration Number for Different Power Level

	Default	MG-PC	MSED	MSED-L	MSED-PC
Outer Number	40	38	61	53	38

Total Run Time (min) for Different Power Level

	Default	MG-PC	MSED	MSED-L	MSED-PC
Time	13.43	10.4	15.18	12.94	8.69