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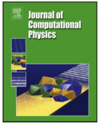

A comparison of acceleration methods for solving the neutron transport *k*-eigenvalue problem

CrossMark

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Introduction

$$\hat{\Omega}_m \cdot \nabla \psi_{g,m}\left(\vec{r}\right) + \Sigma_{t,g}\psi_{g,m}\left(\vec{r}\right) = \frac{1}{4\pi}\left[\sum_{g'=1}^{G} \Sigma_{s,g'\rightarrow g}\phi_{g'}\left(\vec{r}\right) + \frac{\chi_g}{k_{eff}}\nu\Sigma_{f,g'}\phi_{g'}\left(\vec{r}\right)\right],$$

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where

$$\phi_g = \sum_m \psi_{g,m} w_m.$$

Operator Notation

$$\mathcal{L}\Psi = \frac{1}{4\pi}\left[\mathcal{S} + \frac{1}{k_{eff}}\mathcal{F}\right]\Phi,$$

where:

$$\mathcal{L} = \hat{\Omega}\cdot\nabla + \Sigma_t$$
$$\mathcal{S} = \Sigma_s$$
$$\mathcal{F} = \chi\nu\Sigma_f$$

and

$$\Psi = \left[\psi_1, \psi_2, \dots, \psi_G\right]$$
$$\Phi = \left[\phi_1, \phi_2, \dots, \phi_G\right]$$
$$\phi = \mathcal{M}_0\psi$$

Power Iteration

Algorithm 1 Power Iteration (PI) algorithm.

Power Iteration

Input Φ^0, k^0, outer tolerance, inner tolerance, $k$max.

while $\frac{|k^{n+1}-k^n|}{k^{n+1}} >$ outer tolerance **do**

while $\|\Phi^{n+1,k+1} - \Phi^{n+1,k}\| >$ inner tolerance **and** $k < k$max **do**

Compute new flux via source iteration

$$\mathcal{L}\Psi^{n+1,k+1} = \frac{1}{4\pi}\mathcal{S}\Phi^{n+1,k} + \frac{1}{4\pi}\frac{1}{k_{eff}}\mathcal{F}\Phi^n \tag{8}$$

$$\Phi^{n+1,k+1} = \mathcal{M}_0\Psi^{n+1,k+1} \tag{9}$$

end while

Update Eigenvalue

$$k^{n+1} = \frac{W^T\mathcal{F}\Phi^{n+1}}{W^T\mathcal{F}\Phi^n}k^n \tag{10}$$

in which $W^T\vec{x}$ represents the numerical integral of $\vec{x}$ throughout the domain.

end while

Housekeeping

- JFNK: Jacobian-Free Newton-Krylov
- NKA: Nonlinear Krylov Acceleration

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- JFNK: Jacobian-Free Newton-Krylov
- NKA: Nonlinear Krylov Acceleration
- HOLO: High-Order/Low-Order Acceleration, Moment Base Acceleration
- NDA: Nonlinear Diffusion Acceleration

Motivation

H. Park, D.A, Knoll, C.K. Newman,*Nonlinear acceleration of transport criticality problems*, Nucl. Sci. Eng. 172 (2012) 53-56

- NDA to accelerate scattering source
- JFNK to accelerate the fission source in LO space

First Test

$\tau = 15$

Material properties 1-D test problems.

Property	Material 1	Material 2	Material 3
x-range (cm)	[0, 5]	$[5, \tau - 5]$	$[\tau - 5, \tau]$
Σ_t (cm^{-1})	1	1	1
Σ_s (cm^{-1})	.856	.856	.856
$\nu\Sigma_f$ (cm^{-1})	0	.144	0

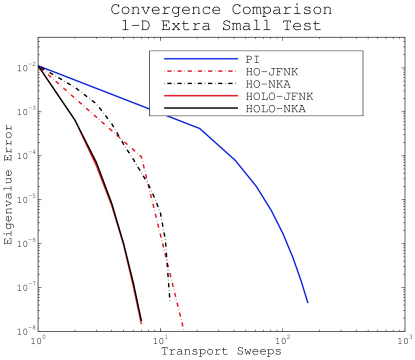

Fig. 1. Methods comparison for 1-D k-eigenvalue problem. 15 mfp domain. Dominance ratio is .3018.

First Test

$\tau = 35$ and $\tau = 210$

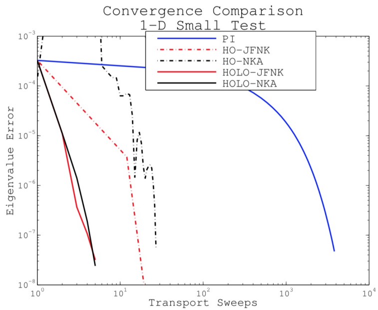

Fig. 2. Methods comparison for 1-D *k*-eigenvalue problem. 35 mfp domain. Dominance ratio is .8185.

First Test

$\tau = 35$ and $\tau = 210$

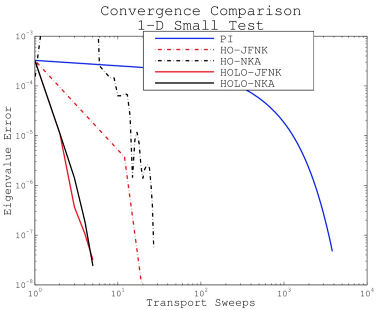

Fig. 2. Methods comparison for 1-D *k*-eigenvalue problem. 35 mfp domain. Dominance ratio is .8185.

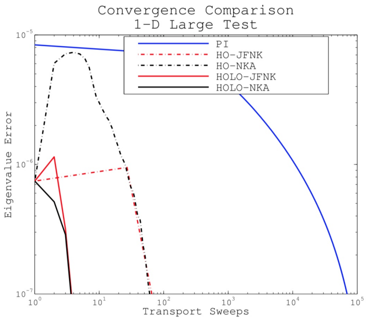

Fig. 3. Methods comparison for 1-D *k*-eigenvalue problem. 210 mfp domain. Dominance ratio is .99559.

Nonlinear Acceleration of Transport Criticality Problems

$$F\begin{pmatrix}\Phi \\ k\end{pmatrix} = \begin{pmatrix}F_{\Phi}(\Phi, k) \\ F_{k}(\Phi, k)\end{pmatrix} = 0 \tag{1}$$

Nonlinear Acceleration of Transport Criticality Problems

function aproximations

$$F_{\Phi}(\Phi, k) = \Phi - P(k)\Phi$$

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$$P_1(k) = \mathcal{M}_0 \mathcal{L}^{-1}\left[\frac{1}{4\pi}\left(\mathcal{S} + \frac{1}{k}\mathcal{F}\right)\right]$$

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$$\Phi^{n+1} = P_2(k^n)\Phi^n$$

$$P_2(k^n)\Phi^n = \mathcal{M}_0 \left(\mathcal{L} - \frac{1}{4\pi} \mathcal{S} \mathcal{M}_0 \right)^{-1} \frac{1}{4\pi k^n} \mathcal{F} \Phi^n$$

Nonlinear Acceleration of Transport Criticality Problems

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$$F_k(\Phi, k) = \left(1 - \frac{W^T \mathcal{F} P(k) \Phi}{W^T \mathcal{F} \Phi} \right) k$$

JFNK Algorithm

Algorithm 2 Jacobian-Free Newton–Krylov (JFNK) algorithm.

JFNK

Input initial iterate x_0, $\eta \in (0, 1)$.

Set $n = 0$.

while $F(x_n) >$ tolerance **do**

Compute Newton step s satisfying

$$\left\| F'(x_n)s + F(x_n) \right\| < \eta \left\| F(x_n) \right\| \tag{18}$$

by solving

$$F'(x_n)s = -F(x_n) \tag{19}$$

with GMRES.

Compute next iterate x_{n+1}

$$x_{n+1} = x_n + s. \tag{20}$$

Set $n = n + 1$.

end while

NKA Algorithm

Algorithm 3 Nonlinear Krylov Acceleration (NKA) algorithm.

NKA

Input initial iterate x_0, history length M.

Set $x_1 = x_0 - F(x_0)$

Set $n = 1$.

while $F(x_n) >$ tolerance **do**

Compute NKA Update

$$\vec{v}_{n+1} = \sum_{i=n-M+1}^{n} z_i^{(n)} \vec{v}_i + \left(F(x_n) - \sum_{i=n-M+1}^{n} z_i^{(n)} \vec{w}_i \right) \tag{21}$$

$$\vec{v}_i = x_{i-1} - x_i \tag{22}$$

$$\vec{w}_i = F(x_{i-1}) - F(x_i) \tag{23}$$

$$\vec{z}^{(n)} = \arg\min_{y \in \mathbb{R}^M} \left\| F(x_n) - \sum_{i=n-M+1}^{m} y_i \vec{w}_i \right\| \tag{24}$$

and

$$x_{n+1} = x_n + v_{n+1}. \tag{25}$$

Set $n = n + 1$.

end while

Nonlinear Elimination of the Eigenvalue

$$Ax = \lambda x$$

such that (λ^*, x^*) and (λ^*, cx^*) are pairs; with the constraint $\|x^*\| = 1$.

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$$k = \int \int \nu \Sigma_f \phi \, dV \, dE$$

$$F(\Phi) = \Phi - P\left(k\left(\Phi\right)\right)\Phi$$

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$$k\left(\Phi\right) = \int \int \nu \Sigma_f \phi dV dE$$

HOLO Methods

$$\nabla \cdot \vec{J}_g + \left(\Sigma_{t,g} - \Sigma_{s,g\rightarrow g}\right)\phi_g = \sum_{g' \neq g} \Sigma_{s,g'\rightarrow g}\phi_{g'} + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'}$$

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$$\vec{J}_g(\vec{r}) = \int_{4\pi} \vec{\Omega}\psi_g\left(\vec{\Omega},\vec{r}\right) d\vec{\Omega} = \mathcal{M}_1\psi_g$$

HOLO Methods

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$$\vec{J}_g = -\frac{1}{3\Sigma_{t,g}}\nabla\psi_g + \vec{D}_g\phi_g$$

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$$\nabla \cdot \left[-\frac{1}{3\Sigma_{t,g}}\nabla\psi_g + \vec{D}_g\phi_g\right] + \left(\Sigma_{t,g} - \Sigma_{s,g\to g}\right)\phi_g = \sum_{g'\neq g} \Sigma_{s,g'\to g}\phi_{g'} + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\phi_{g'}$$

HO Moments

Consistency term:

$$\vec{D}_g = \frac{\vec{J}_g^{HO} + \frac{1}{3\Sigma_{t,g}} \nabla \phi_g^{HO}}{\phi_g^{HO}}$$

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$$\Psi = \frac{1}{4\pi} \mathcal{L}^{-1} \left[\mathcal{S} + \frac{1}{k_{eff}} \mathcal{F} \right] \Phi$$

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$$\Phi^{HO} = \mathcal{M}_0 \Psi$$

$$\vec{J}_g = \mathcal{M}_1 \Psi$$

LO Discretization

Operator notation of NDA LO system:

$$D\Phi = \left(S_U + S_L\right)\Phi + \frac{1}{k_{eff}}\mathcal{F}\Phi.$$

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$$D\Phi = \left(S_U + S_L\right)\Phi + \frac{1}{k_{eff}}\mathcal{F}\Phi.$$

in which:

$$D_g\Phi = \nabla \cdot \left[-\frac{1}{3\Sigma_{t,g}}\nabla + \vec{D}_g\right]\phi_g + \left(\Sigma_{t,g} - \Sigma_{s,g\to g}\right)\phi_g,$$

$$\left(S_{U,g} + S_{L,g}\right)\Phi = \sum_{g'\neq g}\Sigma_{s,g'\to g}\phi_{g'}.$$

NDA Algorithm

Algorithm 4 NDA.

Nonlinear Diffusion Acceleration

Compute initial iterate $\Phi^{(0)}$, initial eigenvalue approximation k^0. Set iteration counter $m = 0$.

while $|k^m - k^{m-1}| > \tau$ **do**

Update counter, $m = m + 1$.

Execute transport sweep and compute new consistency term

$$\Psi^{(m)} = \frac{1}{4\pi}\mathcal{L}^{-1}\left(\mathcal{S} + \frac{1}{k^{m-1}}\mathcal{F}\right)\Phi^{(m-1)}, \tag{37}$$

$$\Phi^{HO} = \int \Psi^{(m)} d\hat{\Omega}, \tag{38}$$

$$\vec{J}^{HO} = \int \hat{\Omega}\Psi^{(m)} d\hat{\Omega}, \tag{39}$$

$$\hat{D}^{(m)} = \frac{\vec{J}^{HO} + \frac{1}{3\Sigma_t}\nabla\Phi^{HO}}{\Phi^{HO}}. \tag{40}$$

Solve the LO eigenvalue problem for $\Phi^{(m)}$ and k^m

$$(\mathcal{D}^{(m)} - \mathcal{S}_U - \mathcal{S}_L)\Phi^{(m)} = \frac{1}{k^{(m)}}\mathcal{F}\Phi^{(m)}. \tag{41}$$

end while

Solving LO Eigenvalue

Rewriting the LO problem:

$$F_{\Phi}\left(\Phi\right) = \left(D - S_U - S_L\right)\Phi - \frac{1}{k(\Phi)}\mathcal{F}\Phi.$$

in which:

$$k\left(\Phi\right) = \sum_{g=1}^{G}\int \nu\Sigma_{f,g}\phi_g dV.$$

Preconditioned:

$$\mathcal{M} = D - S_L - \frac{1}{k^{m-1}}\mathcal{F}.$$

Problem Set

Dominance Ratios

Dominance Ratio:

$$\rho = \frac{|k_2|}{|k_1|},$$

Dominance Ratio:

$$\rho = \frac{\left|k_2\right|}{\left|k_1\right|},$$

Scattering plus dominance Ratio:

$$\rho_{s+f} = \frac{\left|k_{PI(1)}^{n+1} - k^*\right|}{\left|k_{PI(1)}^{n} - k^*\right|}.$$

Problem Set

LRA-BWR 2g, S16, 352 × 352, $\rho = 0.97$, $\rho_{s+f} = 0.993$

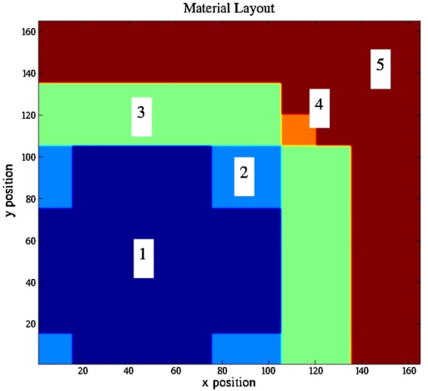

Fig. 4. LRA-BWR material layout.

Problem Set

C5G7 7g, S16, 357 × 357, $\rho = 0.77$, $\rho_{s+f} = 0.989$

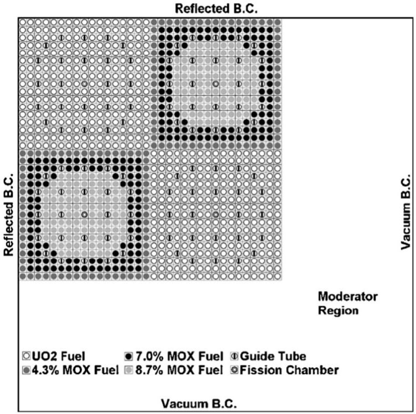

Fig. 5. C5G7MOX material layout [20].

JFNK-HO Parameter Study

HO-JFNK parameter study.

η	Max Krylovs	Sweeps	
		LRA-BWR	C5G7MOX
.001	15	1631	204
.01	15	2882	174
.1	15	2016	152
.001	30	503	179
.01	30	1030	155
.1	30	453	125
.001	150	337	165
.01	150	308	154
.1	150	314	166

JFNK-HO vs NKA-HO Study

HO-JFNK vs. HO-NKA study.

Method	Sweeps	
	LRA-BWR	C5G7MOX
HO-JFNK(.1, 15)	2016	152
HO-JFNK(.001, 30)	503	179
HO-JFNK(.1, 30)	453	125
HO-JFNK(.01, 150)	308	154
HO-JFNK(.1, 150)	314	166
HO-NKA(15)	301	121
HO-NKA(30)	262	168

Mesh Convergence Study
NDA-NCA

NDA-NCA mesh study.

Mesh size	Sweeps		k_{eff}	Error	Order
	JFNK	NKA			
0.46875	5	6	1.0014486	2.541×10^{-6}	–
0.3125	5	5	1.0014499	1.025×10^{-6}	1.97
0.234375	6	5	1.0014503	5.617×10^{-7}	2.09
0.1875	6	5	1.0014505	3.598×10^{-7}	2.00
0.15625	5	5	1.0014507	2.496×10^{-7}	2.00

Mesh Convergence Study

HO-NKA

HO-NKA(15) mesh study.

Mesh size	Sweeps	k_{eff}	Error	Order
0.937500	296	1.0014417	9.210×10^{-6}	–
0.468750	301	1.0014486	2.280×10^{-6}	2.01
0.312500	300	1.0014499	1.025×10^{-6}	1.97
0.234375	403	1.0014503	5.617×10^{-7}	2.09
0.187500	294	1.0014505	3.598×10^{-7}	2.00
0.156250	234	1.0014507	2.496×10^{-7}	2.00

HOLO vs HO Study

LRA-BWR

LRA-BWR: HO methods vs. HOLO methods.

Method	Sweeps	Time (s)	HO time (s)	LO time (s)	Factor
NDA-NCA-JFNK	5	115.04	46.04	69.00	1.00
NDA-NCA-NKA	5	140.88	46.02	94.86	1.22
NDA-PI	7	987.62	64.53	923.09	8.59
HO-JFNK(.001, 30)	503	4687.32	4687.32	–	40.75
HO-JFNK(.01, 150)	308	2893.14	2893.14	–	25.15
HO-NKA(15)	301	2768.65	2768.65	–	24.07
HO-NKA(30)	262	2410.32	2410.32	–	20.95
PI(1)	9754	89 795.33	89 795.33	–	780.56
PI(10)	12 501	115 084.21	115 084.21	–	1000.38

HOLO vs HO Study

LRA-BWR: cost breakdown

LRA-BWR: HOLO methods cost breakdown.

Method	Sweeps	LO func. evals.	Precond. const.	Precond. app.
NDA-NCA-JFNK	5	177	15	147
NDA-NCA-NKA	5	187	172	172
NDA-PI	7	1920	–	–

HOLO vs HO Study

C5G7

C5G7MOX: HO methods vs. HOLO methods.

Method	Sweeps	Time (s)	HO time (s)	LO time (s)	Factor
NDA-NCA-JFNK	6	535.48	214.92	320.56	1.00
NDA-NCA-NKA	6	635.52	214.71	420.81	1.19
NDA-PI	13	2599.61	469.37	2130.24	4.85
HO-JFNK(.001, 30)	179	6512.52	6512.52	–	12.16
HO-JFNK(.01, 150)	154	5620.18	5620.18	–	10.50
HO-NKA(15)	121	4500.79	4500.79	–	8.41
HO-NKA(30)	168	6180.89	6180.89	–	11.54
PI(1)	1454	56 387.71	56 387.71	–	105.30
PI(10)	1970	72 851.56	72 851.56	–	136.05

HOLO vs HO Study

C5G7: cost breakdown

C5G7MOX: HOLO methods cost breakdown.

Method	Sweeps	LO func. evals.	Precond. const.	Precond. app.
NDA-NCA-JFNK	6	282	16	250
NDA-NCA-NKA	6	244	228	228
NDA-PI	13	2139	–	–

Conclusion

- NKA is *generally* more efficient at solving the nonlinear HO problem.
- By moving a large portion of the problem to the LO computational space, overall work is reduced considerably.
- While JFNK and NKA applied to the HO problem can accelerate the solution when comparted to standard power iteration, they are significantly more expensive than NDA-NCA.
- NDA-NCA performance is less sensitive to mesh size and choice of parameters.
- NDA-NCA can also be preconditioned to further accelerate the solution.
- For both problems, BWR-LRA and C5G7, NDA-NCA is the most efficient by a factor of 10-40.

Thanks!
Questions?