Failure of Rayleigh Quotient Iteration for Certain Alpha-Eigenvalue Calculations

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The Alpha-Eigenvalue Equation

$$(\underbrace{\mathbf{S}}_{\text{scattering}} + \underbrace{\mathbf{F}}_{\text{fission}} - \underbrace{\mathbf{H}}_{\text{streaming}})\psi = \alpha \underbrace{\mathbf{V}^{-1}}_{\text{velocity}} \psi \tag{1}$$

$$V = \begin{bmatrix} V_1 & & & \\ & V_2 & & \\ & & \ddots & \\ & & & V_G \end{bmatrix} \quad H = \begin{bmatrix} H_1 & & & \\ & H_2 & & \\ & & \ddots & \\ & & & H_G \end{bmatrix} \tag{2}$$

$$F = \begin{bmatrix} \nu\sigma^f_{11} & \nu\sigma^f_{12} & \cdots & \nu\sigma^f_{G1} \\ \nu\sigma^f_{21} & \nu\sigma^f_{22} & & \\ \vdots & & \ddots & \\ \nu\sigma^f_{G1} & & & \nu\sigma^f_{GG} \end{bmatrix} \quad S = \begin{bmatrix} \sigma^s_{11} & \sigma^s_{12} & \cdots & \sigma^s_{G1} \\ \sigma^s_{21} & \sigma^s_{22} & & \\ \vdots & & \ddots & \\ \sigma^s_{G1} & & & \sigma^s_{GG} \end{bmatrix} \tag{3}$$

Calculating the α-Eigenvalue Using Rayleigh Quotient

For a given square matrix $\mathbf{M} \in \mathbb{C}^{n \times n}$ and nonzero vector $\mathbf{x} \in \mathbb{C}^n$, the Rayleigh quotient $R(\mathbf{M}, \mathbf{x}) \in \mathbb{R}$ is defined as:

$$R(\mathbf{M}, \mathbf{x}) := \frac{\mathbf{x}^* \mathbf{M} \mathbf{x}}{\mathbf{x}^* \mathbf{x}}. \tag{4}$$

In ARDRA, we obtain an iterate for the eigenvalue α_n using the corresponding eigenvector iteration ψ_n:

$$\alpha_n = \rho(\psi_n) \equiv \frac{\langle \psi_n, (\mathbf{S} + \mathbf{F} - \mathbf{H}) \psi_n \rangle}{\langle \psi_n, \mathbf{V}^{-1} \psi_n \rangle}. \tag{5}$$

Some care needed in how we invert our matrices since we must keep the matrices non-negative.

RQ Algorithm in ARDRA

Given $\alpha_n, \psi_n \geq 0$:

- If $\alpha_n \geq 0$, solve for ψ_{n+1} as follows:

$$\psi_{n+1} = (\mathbf{H} + \alpha_n \mathbf{V}^{-1})^{-1}(\mathbf{S} + \mathbf{F})\psi_n \tag{6}$$

$(\mathbf{H} + \alpha_n \mathbf{V}^{-1})$ is positive.

- If $\alpha_n < 0$, solve for ψ_{n+1} as follows:

$$\psi_{n+1} = \mathbf{H}^{-1}(-\alpha_n \mathbf{V}^{-1} + \mathbf{S} + \mathbf{F})\psi_n. \tag{7}$$

Method usually works except for some interesting cases...

Method usually works....(Supercritical Slab)

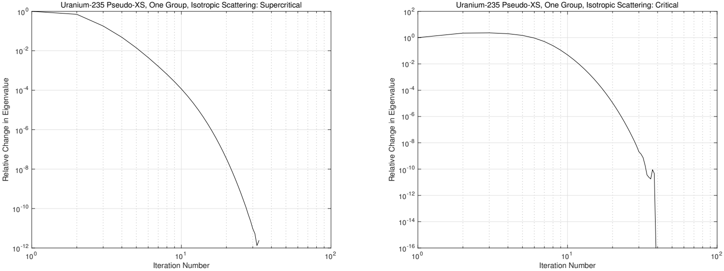

Figure: RQI Doesn't Fail

...but when it doesn't work, it's painful :(

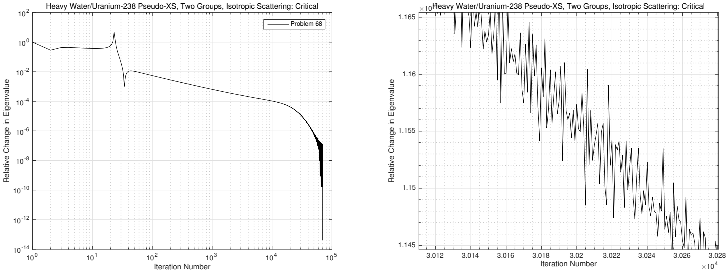

Figure: RQI Struggles...

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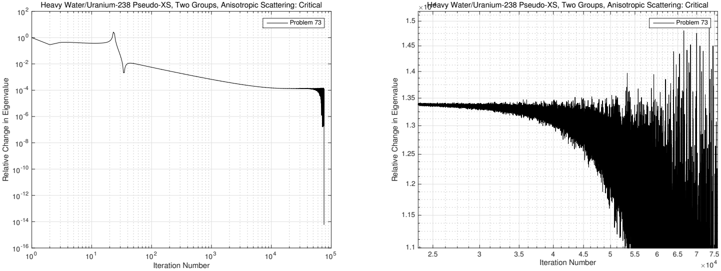

Figure: RQI Struggles...

Sood Criticality Benchmark Problem 68 (SCB-68)

- $k_{\text{eff}} = 1.00$, $\alpha = 0.00$
- Two Energy Groups
- Isotropic Scattering
- Finite Slab

Table 49: Fast Energy Group Macroscopic Cross Sections (cm^{-1}) for U-D_2O

Material	ν_2	Σ_{2f}	Σ_{2c}	Σ_{22s}	Σ_{12s}	Σ_2	χ_2
U-D_2O	2.50	0.002817	0.008708	0.31980	0.004555	0.33588	1.0

Table 50: Slow Energy Group Macroscopic Cross Sections (cm^{-1}) for U-D_2O

Material	ν_1	Σ_{1f}	Σ_{1c}	Σ_{11s}	Σ_{21s}	Σ_1	χ_1
U-D_2O	2.50	0.097	0.02518	0.42410	0.0	0.54628	0.0

Table 51: Critical Dimension, r_c, for Two-Group D_2O System

Problem	Identifier	Geometry	r_c (mfp)	r_c (cm)	Reference
68	UD2O-2-0-SL	Slab	284.367	846.632726	8,35,36

Sood Criticality Benchmark Problem 72 (SCB-72)

- $k_\infty = 1.000196$
- Two Energy Groups
- Anisotropic Scattering
- Infinite

Table 56: Fast Energy Group Cross Sections for Linearly Anisotropic Scattering (cm^{-1}) for U-D_2O

Material	ν_2	Σ_{2f}	Σ_{2c}	Σ_{22s_0}	Σ_{22s_1}	Σ_{12s_0}	Σ_{12s_1}	Σ_2	χ_2
D_2O	2.50	0.002817	0.008708	0.31980	0.06694	0.004555	-0.0003972	0.33588	1.0

Table 57: Slow Energy Group Cross Sections for Linearly Anisotropic Scattering (cm^{-1}) for U-D_2O

Material	ν_1	Σ_{1f}	Σ_{1c}	Σ_{11s_0}	Σ_{11s_1}	Σ_{21s}	Σ_1	χ_1
D_2O	2.50	0.097	0.02518	0.42410	0.05439	0.0	0.54628	0.0

Sood Criticality Benchmark Problem 73 (SCB-73)

- $k_{\text{eff}} = 1.00$, $\alpha = 0.00$
- Two Energy Groups
- Anisotropic Scattering
- Finite Slab

Table 56: Fast Energy Group Cross Sections for Linearly Anisotropic Scattering (cm^{-1}) for U-D_2O

Material	ν_2	Σ_{2f}	Σ_{2c}	Σ_{22s_0}	Σ_{22s_1}	Σ_{12s_0}	Σ_{12s_1}	Σ_2	χ_2
D_2O	2.50	0.002817	0.008708	0.31980	0.06694	0.004555	-0.0003972	0.33588	1.0

Table 57: Slow Energy Group Cross Sections for Linearly Anisotropic Scattering (cm^{-1}) for U-D_2O

Material	ν_1	Σ_{1f}	Σ_{1c}	Σ_{11s_0}	Σ_{11s_1}	Σ_{21s}	Σ_1	χ_1
D_2O	2.50	0.097	0.02518	0.42410	0.05439	0.0	0.54628	0.0

Table 58: Critical Dimension, r_c, for Two-Group Linearly Anisotropic Scattering for U-D_2O Reactor

Problem	Identifier	Geometry	r_c (mfp)	r_c (cm)	Reference
73	UD2O-2-1-SL	Slab	336.05	1000.506133	25

Infinite Medium Two-Group Problem with Self-Scattering and Fission

RQI will converge for all matrices $A \in \mathbb{R}^{2\times 2}$. Want to mimic behavior of previous failures using some sort of parameter. Only non-symmetric matrix is the fission matrix **F**. Ideas as to how to do this?

$$(\underbrace{\mathbf{S}}_{\text{scattering}} + \underbrace{\mathbf{F}}_{\text{fission}} - \underbrace{\mathbf{\Sigma}}_{\text{total XS}})\psi = \alpha \underbrace{\mathbf{V}^{-1}}_{\text{velocity}} \psi \tag{8}$$

$$V = \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix} \quad \Sigma = \begin{bmatrix} \sigma_1^t & 0 \\ 0 & \sigma_2^t \end{bmatrix} \tag{9}$$

$$F = \begin{bmatrix} \nu\sigma_{11}^f & \nu\sigma_{12}^f \\ \nu\sigma_{21}^f & \nu\sigma_{22}^f \end{bmatrix} \quad S = \begin{bmatrix} \sigma_{11}^s & 0 \\ 0 & \sigma_{22}^s \end{bmatrix} \tag{10}$$

Observations

- Heavy water, uranium-238 like systems seem prone to this behavior.
- Need to investigate eigenvalue spectrum. Requires reconstructing the matrices which is possible.
- Want to do analysis where a system approaches critical.
- Any suggestions?