Explicitly Restarted Arnoldi's Method for Monte Carlo Nuclear Criticality Calculations

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Outline

- Personal Introduction
- Krylov Subspace Methods
- Power Method
- Arnoldi's Method
  - Theory
  - Monte Carlo Implementation
  - Benchmark 1D Calculations
- Eigenvalue and Fission Source Convergence
  - Power Method
  - Arnoldi's Method
- Conclusions

Krylov Subspace Methods

- Estimate eigenpairs from Krylov subspace:

$$\mathcal{K}_m(\mathcal{A}, v) \equiv \text{span}\left\{v, \mathcal{A}v, \mathcal{A}^2 v, \ldots, \mathcal{A}^{m-1} v\right\}$$

- Subspace constructed iteratively

$$v_i = \mathcal{A} v_{i-1}, \qquad \text{for } i = 1, 2, \ldots, m-1$$

- Krylov subspace

$$\mathcal{K}_m(\mathcal{A}, v) \equiv \text{span}\left\{v_0, v_1, v_2, \ldots, v_{m-1}\right\}$$

- Explicit form of $\mathcal{A}$ not required

Particle Transport

Boltzmann Transport Equation:

$$\Omega \cdot \nabla \psi(\mathbf{r}, \Omega) + \Sigma_t \psi(\mathbf{r}, \Omega) = \frac{\Sigma_s}{4\pi} \int \psi(\mathbf{r}, \Omega)\, d\Omega + \frac{1}{k} \frac{\nu \Sigma_f}{4\pi} \int \psi(\mathbf{r}, \Omega)\, d\Omega,$$

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Operator Form:

$$(\mathbf{L} + \mathbf{C} - \mathbf{S})\psi = \frac{1}{k}\mathbf{F}\psi$$

$$\mathbf{T}\psi = \frac{1}{k}\mathbf{F}\psi$$

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$$v \equiv \mathbf{F}\psi$$

$$\mathcal{A} \equiv \mathbf{F}\,\mathbf{T}^{-1}$$

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$$\mathcal{A}v = kv$$

Monte Carlo Application of Transport-Fission Operator $\mathcal{A}$

To apply $\mathcal{A}$ to v_{i-1}:

1. Sample neutron from v_{i-1}
2. Transport neutron
3. Record positions of fission neutrons
4. Repeat...

Fission Source:

$$v \equiv \mathbf{F}\psi$$

$$v_i = \mathcal{A}v_{i-1}$$

Transport-fission Operator:

$$\mathcal{A} \equiv \mathbf{F}\,\mathbf{T}^{-1}$$

$$\mathcal{A} = \mathbf{F}\left(\mathbf{L}+\mathbf{C}-\mathbf{S}\right)^{-1}$$

Krylov Subspace Method: Power Method

- Straightforward Krylov subspace method

$$v_i = \frac{1}{k_{i-1}} \mathcal{A} v_{i-1}$$

$$k_i = k_{i-1} \frac{\int \mathcal{A} v_{i-1}}{\int v_{i-1}}$$

- k_i and v_i converge to fundamental eigenpair as i becomes large
- Eigenvalue convergence proportional to dominance ratio

$$\text{DR} = \lambda_1 / \lambda_0$$

Monte Carlo Statistics

- Iterations before power method converges are discarded
  - *Inactive* iterations
- Iterations after convergence are *Active* iterations
- Calculate mean and variance of eigenvalue estimates

$$\overline{\lambda} \equiv \frac{1}{N} \sum_{n=1}^{N} \lambda_n$$

$$\sigma_{\overline{\lambda}}^2 \equiv \frac{1}{N-1} \left(\frac{1}{N} \sum_{n=1}^{N} \left(\lambda_n - \overline{\lambda} \right)^2 \right)$$

- $\sigma_{\overline{\lambda}}$ is an estimate of the statistical uncertainty of $\overline{\lambda}$

Arnoldi's Method—Alternative to Power Method

Power method has been used for more than 50 years

- Straightforward implementation
- Fundamental eigenvalue and eigenvector
- Only one Krylov basis vector is stored and used
- Slow convergence

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Arnoldi's method:

- Application of $\mathcal{A}$ same as in Power method
- Multiple eigenpairs
- All Krylov basis vectors are stored and used.
- Faster convergence

Arnoldi's Method

Krylov Subspace

$$\mathcal{K}_m(\mathcal{A}, v) \equiv \text{span}\left\{v, \mathcal{A}v, \mathcal{A}^2 v, \ldots, \mathcal{A}^{m-1} v\right\}$$

$$\mathcal{K}_m(\mathcal{A}, v) \equiv \text{span}\left\{v_0, v_1, v_2, \ldots, v_{m-1}\right\}$$

- Krylov subspace built iteratively
- Vectors are orthogonalized and normalized
- Normalized basis vectors (v_i) are called Arnoldi vectors
- All Arnoldi vectors are stored and used

Arnoldi Method Iteration

Arnoldi Iteration

$$v_1 = \frac{v}{\|v\|_2}$$

$$\tilde{v}_2 = \mathcal{A} v_1$$

$$\tilde{v}_2 = \mathcal{A} v_1 - h_{1,1} v_1$$

$$v_2 = \frac{\tilde{v}_2}{h_{2,1}}$$

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$$\tilde{v}_2 = \mathcal{A} v_1 - h_{1,1} v_1$$

$$v_2 = \frac{\tilde{v}_2}{h_{2,1}}$$

At m-th iteration

$$\tilde{v}_{m+1} = \mathcal{A} v_m - \sum_{j=1}^{m} h_{jm} v_j$$

$$v_{m+1} = \frac{\tilde{v}_{m+1}}{h_{m,m+1}}$$

$$h_{jm} = \langle \mathcal{A} v_m, v_j \rangle$$

Arnoldi Factorization

$$\mathcal{A}V_m = V_m H_m + v_{m+1} h_{m+1,m} e_m^T$$

- Columns of V_m are Arnoldi vectors
- Elements of H_m are h_{jm}
- H_m is the projection of $\mathcal{A}$ onto Krylov subspace

- $H_m \in \mathbb{R}^{m \times m}$, upper-Hessenberg matrix
- m is small, easy to calculate eigenpair of H_m, (μ_i, x_i)

Finding Ritz Pairs from Arnoldi Factorization

- (μ_i, x_i) is an eigenpair of H_m

$$\begin{aligned}
\mathcal{A}V_m &= V_m H_m &&+ v_{m+1} h_{m+1,m} e_m^T \\
\mathcal{A}V_m x_i &= V_m \left(H_m x_i\right) &&+ v_{m+1} h_{m+1,m} e_m^T x_i \\
\mathcal{A}V_m x_i &= V_m \left(\mu_i x_i\right) &&+ v_{m+1} h_{m+1,m} e_m^T x_i \\
\mathcal{A}y_i &= \mu_i y_i &&+ v_{m+1} h_{m+1,m} e_m^T x_i
\end{aligned}$$

- $y_i = V_m x_i$
- (μ_i, y_i) is a *Ritz pair* or approximated eigenpair of $\mathcal{A}$
- Residual:

$$|r_i| = \left\|\mathcal{A}y_i - \mu y_i\right\| = \left|h_{m+1,m}\right| |e_m x_i| .$$

Explicitly Restarted Arnoldi's Method

As n increases:

- Memory requirements increase
- Computational expense increases
- Effect on Ritz pair decreases

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Restarted Arnoldi's method:

- Begin with estimate of desired eigenvector
- Calculate eigenpairs of H_m after a fixed number of iterations
- Restart Arnoldi with desired eigenvectors as new starting vector
- Several iterations make up one Arnoldi *restart*

Monte Carlo Arnoldi's Method

- $\mathcal{A}$ is applied exactly as it is applied in power method
- Eigenvalues and eigenvectors estimated at end of every restart
- Mean and variance of estimates can be calculated
- Can do inactive restarts (but don't need to!)

- Orthogonalization will create negative Arnoldi vectors
  - Negative fission source
- Need to define inner product between two fission sources

Negative Sources

- To sample from negative fission source, normalize

$$\int \left|\nu(x)\right| \mathrm{d}x = q$$

$$p(x) = \frac{\left|\nu(x)\right|}{q}$$

- $p(x)\,\mathrm{d}x$ is probability of picking a point in $\mathrm{d}x$ about x
- Neutron is given weight

$$\omega = \begin{cases} 1, & \nu(x_s) > 0 \\ -1, & \nu(x_s) < 1. \end{cases}$$

Inner Product of Fission Sources

- Orthonormalization requires inner product between fission sources:

$$h_{jk} = \langle \nu_j, \nu_k \rangle = \int \nu_j(x)\nu_k(x)\,\mathrm{d}x$$

- Discretize fission source

$$\nu_\Pi(x) = \sum_{b=1}^{B} a_b \Pi_b(x)$$

$$\Pi_b(x) = \begin{cases} \left(\frac{1}{\Delta x_b}\right)^{1/2}, & x_b \leq x < x_{b+1} \\ 0, & \text{otherwise} \end{cases}$$

Spatial Discretization

- Discretization:

$$v_\Pi(x) = \sum_{b=1}^{B} a_b \Pi_b(x)$$

- Arnoldi vector representation:

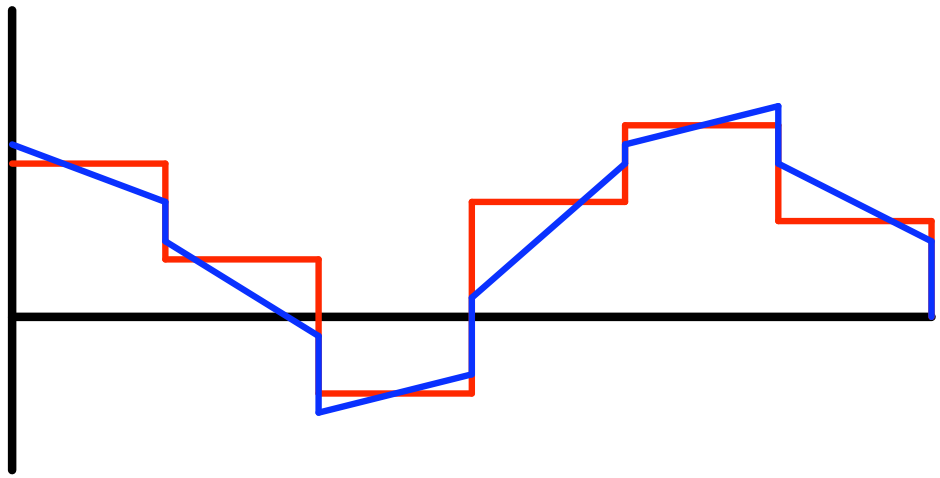
$$v_\Pi = \left[a_1, a_2, \ldots, a_B\right]^T$$

- Inner product of discretized fission sources:

$$h_{jk} = \langle v_\Pi^{(j)}, v_\Pi^{(k)} \rangle = \sum_{b=1}^{B} a_b^{(j)} a_b^{(k)}$$

Effects of Spatial Discretization

- Bias in Eigenvalue estimate
- Second order accurate approximation:
  - Reduces error
  - Reduces standard deviation
  - Increases figure of merit
  - Improves eigenvector estimate



Numerical Results

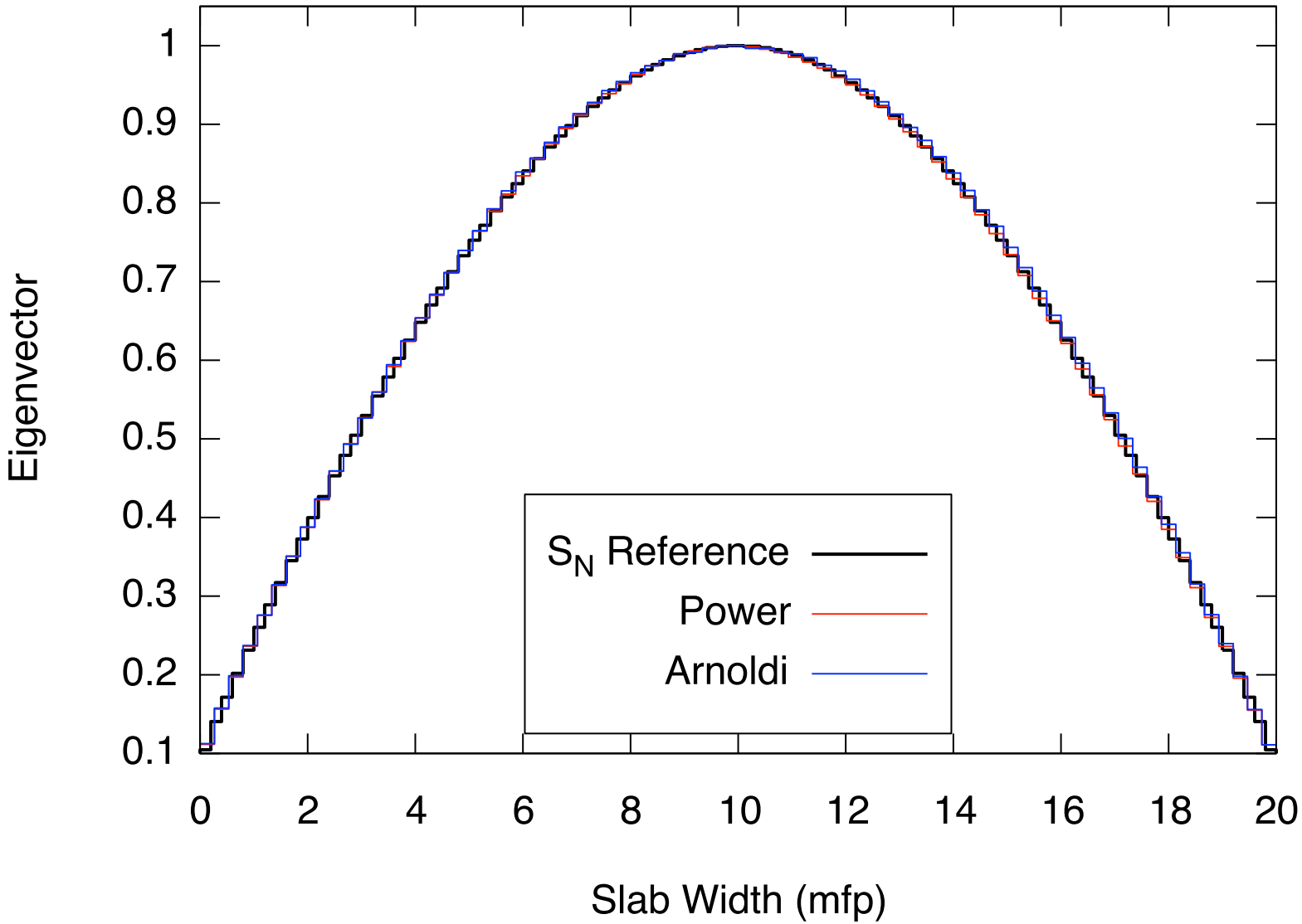
- Homogeneous slab
- $\nu\Sigma_f = 1.0$, $\Sigma_a = 0.2$, $\Sigma_s = 0.8$, $\Sigma_t = 1.0$
- 0.2, 2.0, 20 mfp thick
- Geometry and cross sections match published results

- Arnoldi's method compared with power method
- Parameters:
  - 1×10^5 particles per iteration
  - 25 inactive, 100 active Arnoldi restarts, 10 iterations per restart
  - 250 inactive, 1000 active power iterations
  - 50 spatial bins (0.2 mfp), 75 spatial bins (2.0, 20 mfp)

Numerical Results

Width (DR)	Method	Eigenvalue	Standard Deviation	Reference
0.2 (0.2400)	Power Arnoldi	0.329979 0.33008	6.3×10^{-5} 1.8×10^{-4}	0.330000
2.0 (0.4015)	Power Arnoldi	2.09593 2.09652	2.7×10^{-4} 6.9×10^{-4}	2.09599
20 (0.9079)	Power Arnoldi	4.82734 4.8290	6.3×10^{-4} 1.5×10^{-3}	4.82780

Fundamental Eigenvector



Multiple Eigenvectors

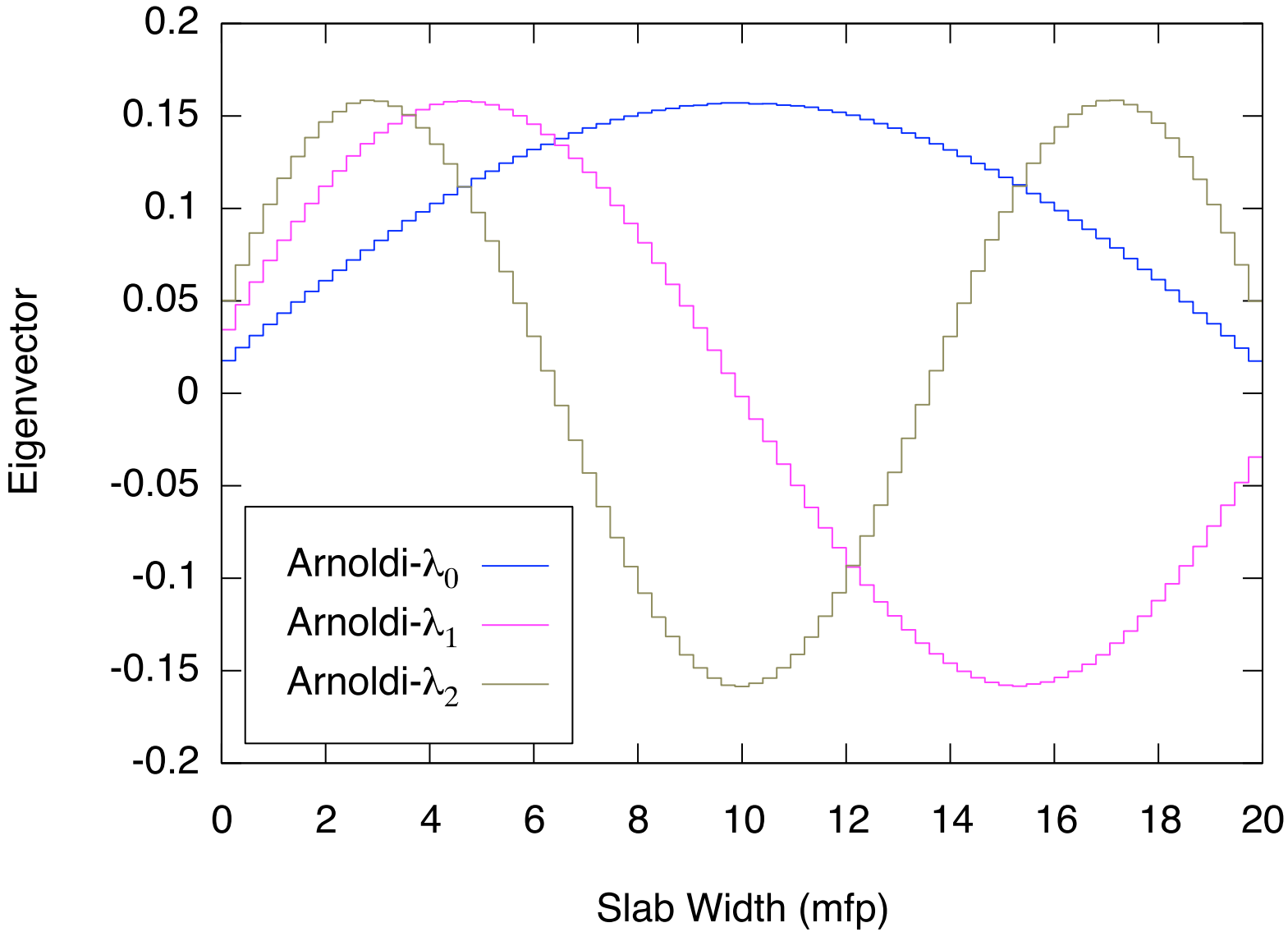


Figure of Merit

Width (mfp)	Method	Standard Deviation	FOM	Time (sec)
0.2	Power	6.3×10^{-5}	1.7×10^{6}	149.0
	Arnoldi	1.8×10^{-4}	3.3×10^{5}	95.3
2.0	Power	2.7×10^{-4}	5.5×10^{4}	258.1
	Arnoldi	6.9×10^{-4}	9.8×10^{3}	212.5
20	Power	6.3×10^{-4}	5.4×10^{3}	463.0
	Arnoldi	1.5×10^{-3}	1.1×10^{3}	378.5

Figure of Merit

$$\text{FOM} \equiv \frac{1}{\sigma^2 T}$$

Convergence in Monte Carlo Criticality Calculations

- Eigenvalue estimate converges proportional to dominance ratio λ_1/λ_0
- Fission source converges more slowly
- Shannon entropy

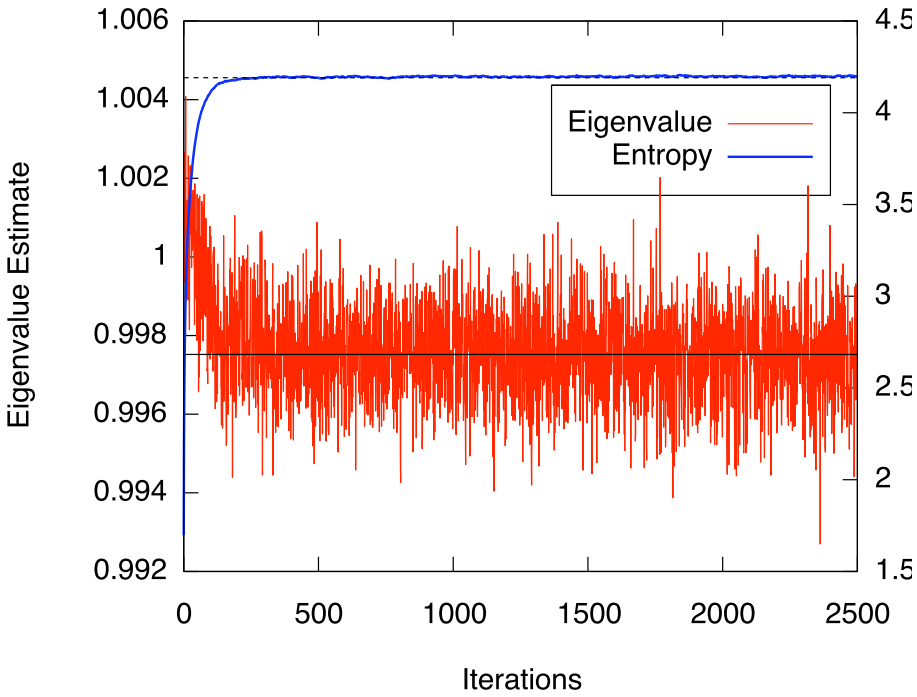
$$H\left(S(x)\right) \equiv -\sum_{b=1}^{B} S_b \log\left(S_b\right)$$

$$S_b = \int_{x_b}^{x_{b+1}} \left|v(x)\right| \mathrm{d}x$$

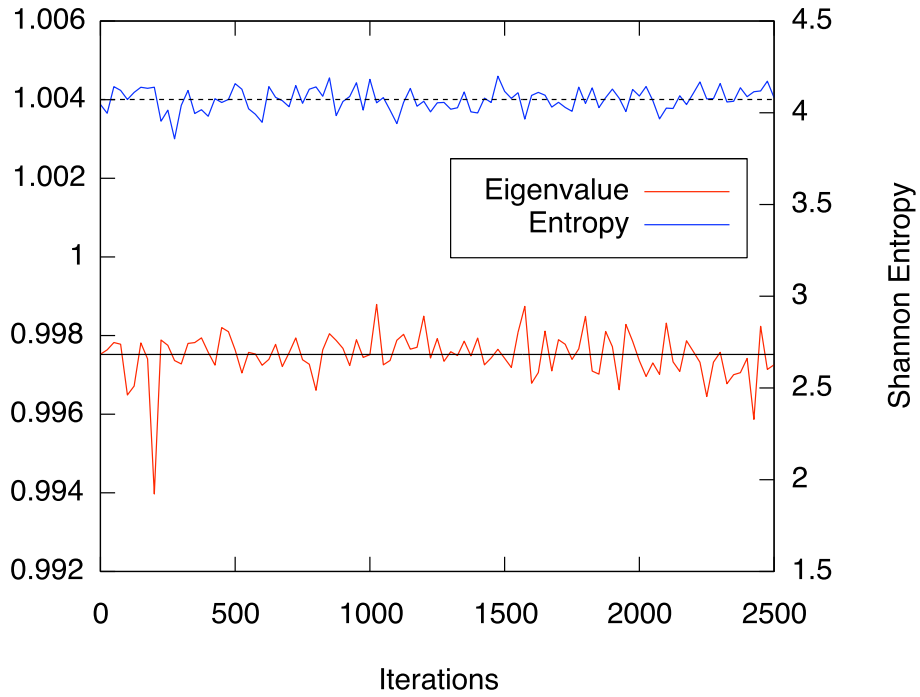
Homogeneous Geometry

- 50 mfp thick
- $\nu\Sigma_f = 1.0$, $\Sigma_a = 0.2$, $\Sigma_s = 0.8$, $\Sigma_t = 1.0$
- 5×10^5 particles per iteration
- 75 spatial bins (first order accurate)
- Source solely in left most bin

Homogeneous Geometry



Power Method

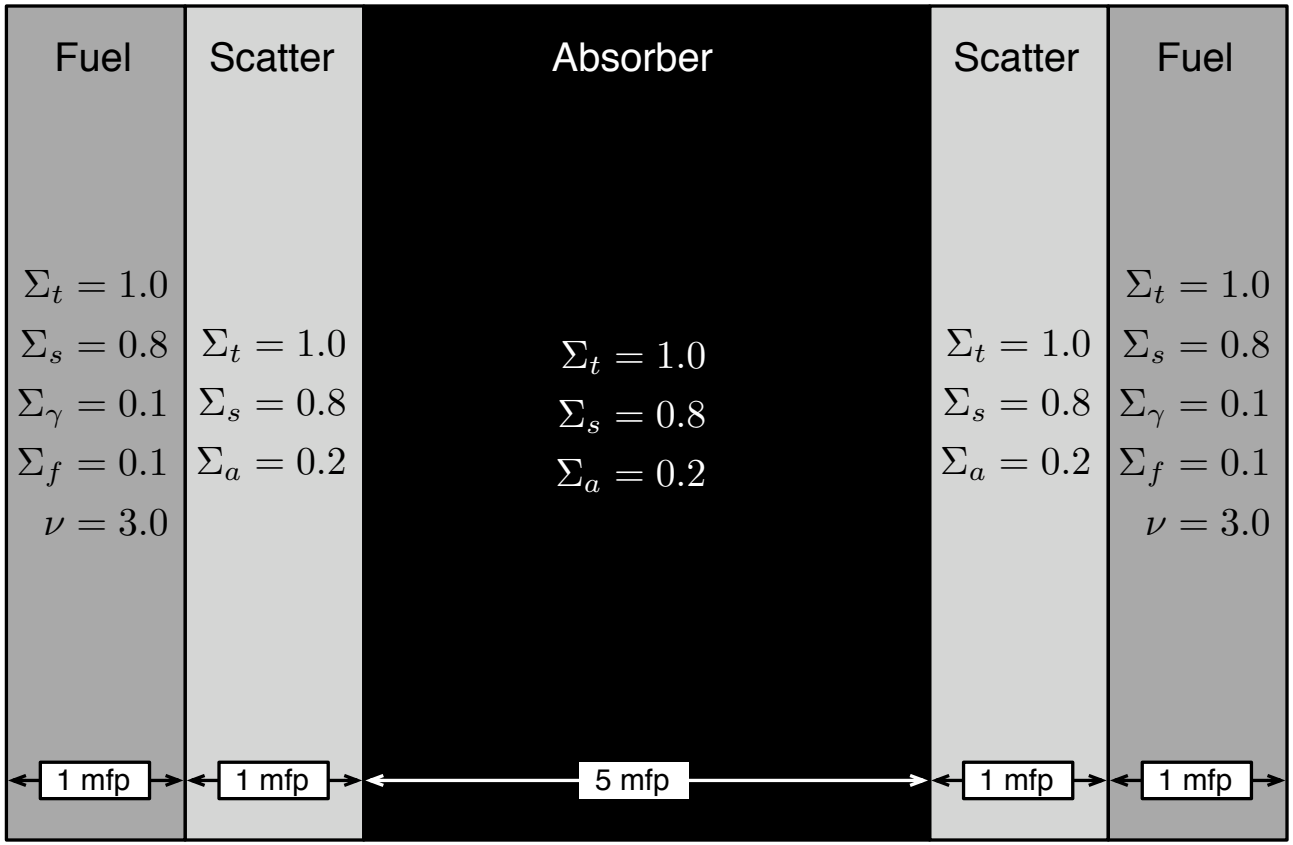


Arnoldi's Method

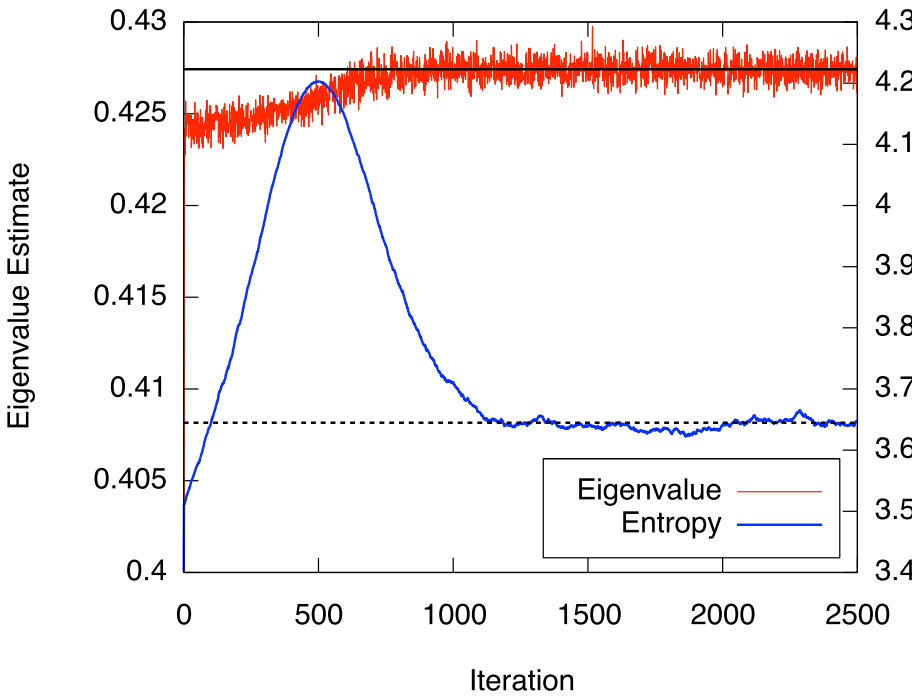
Heterogeneous Geometry

Parameters:

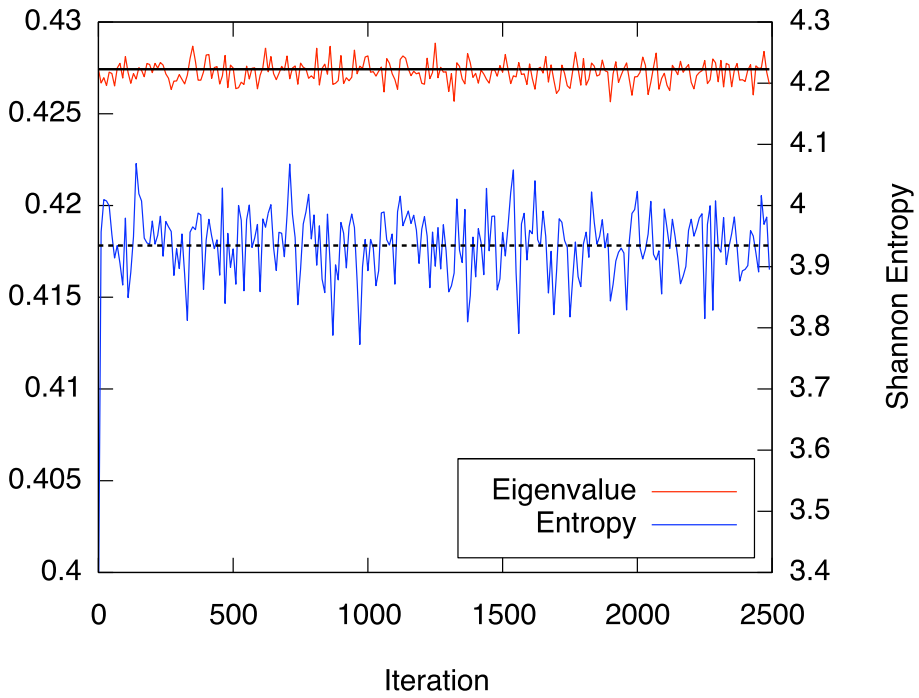
- 1×10^5 particles per iteration
- 10 iterations per Arnoldi restart
- Source solely in left most bin
- Symmetric ($DR = 0.999566$)
- Asymmetric ($DR = 0.992504$)



Asymmetric Heterogeneous Geometry

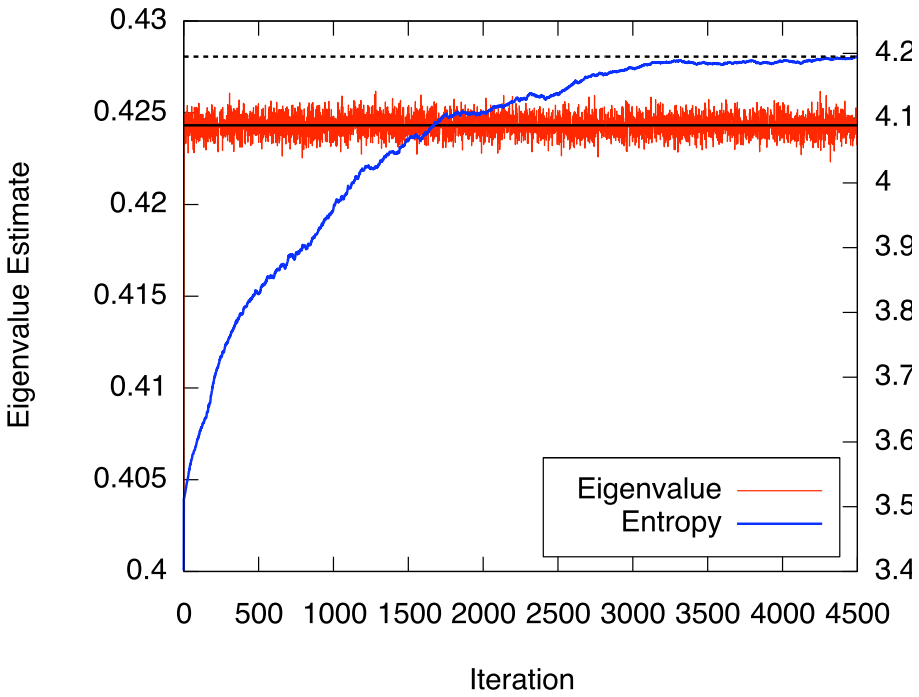


Power Method

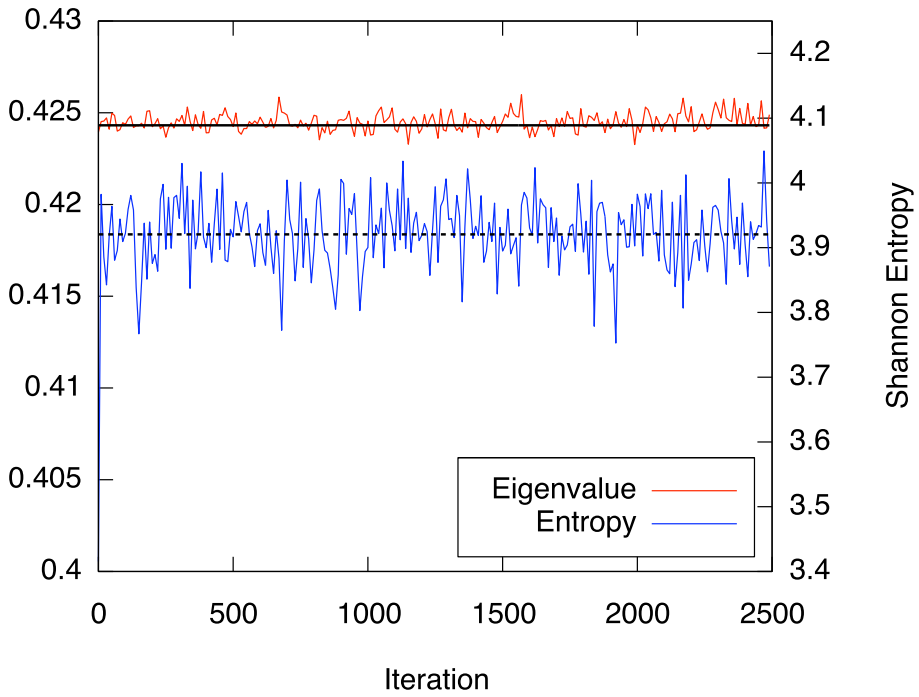


Arnoldi's Method

Symmetric Heterogeneous Geometry



Power Method



Arnoldi's Method

Conclusions

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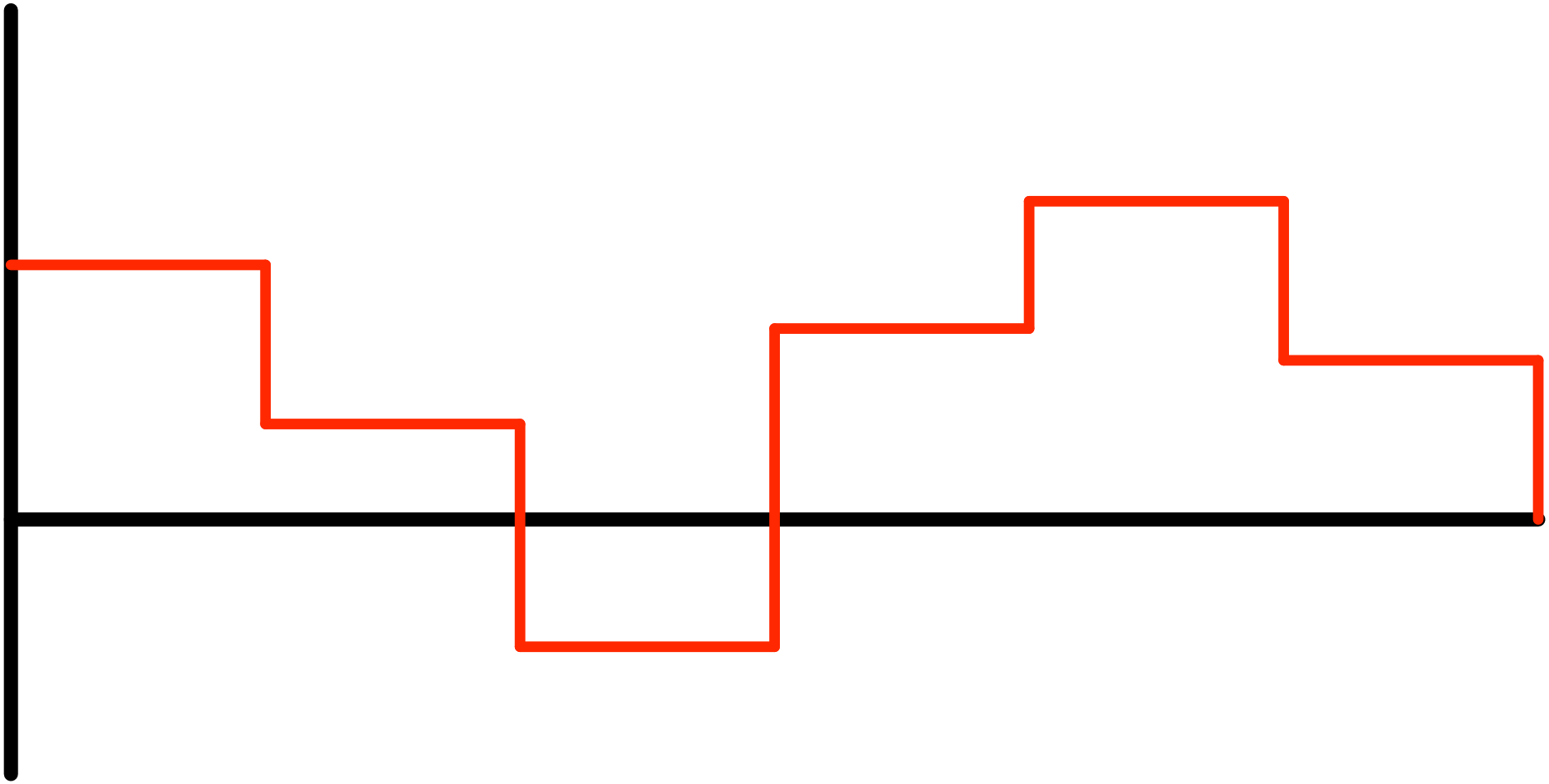
Conclusions

- Arnoldi's method can be used in Monte Carlo Criticality Calculations
- Arnoldi's method can estimate multiple eigenvalues
- Fission source is discretized
- Arnoldi's method converges in just a few iterations
  - Eigenvalue estimate
  - Fission source

Questions?

Spatial Approximations



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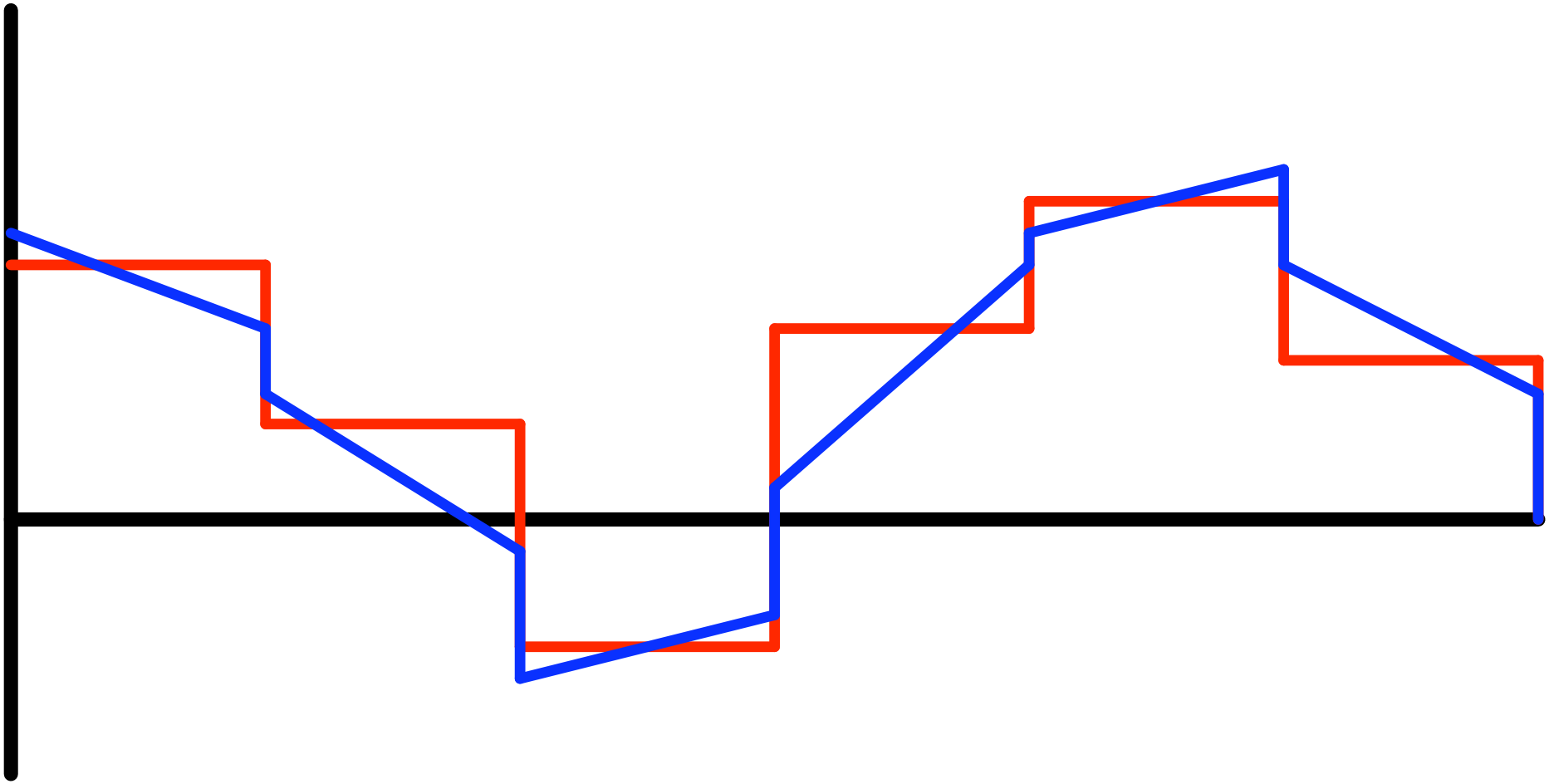


Spatial Approximations

First Order Accurate

$$v_{\Pi}(x) = \sum_{b=1}^{B} a_b \Pi_b(x)$$

$$\Pi_b(x) = \left(\frac{1}{\Delta x_b} \right)^{1/2}$$

$$v_{\Pi} = \left[a_1, a_2, \ldots, a_B \right]^T$$

Second Order Accurate

$$v_{\mathcal{L}}(x) = \sum_{b=1}^{B} \mathcal{L}_b(x, \alpha_b, \beta_b)$$

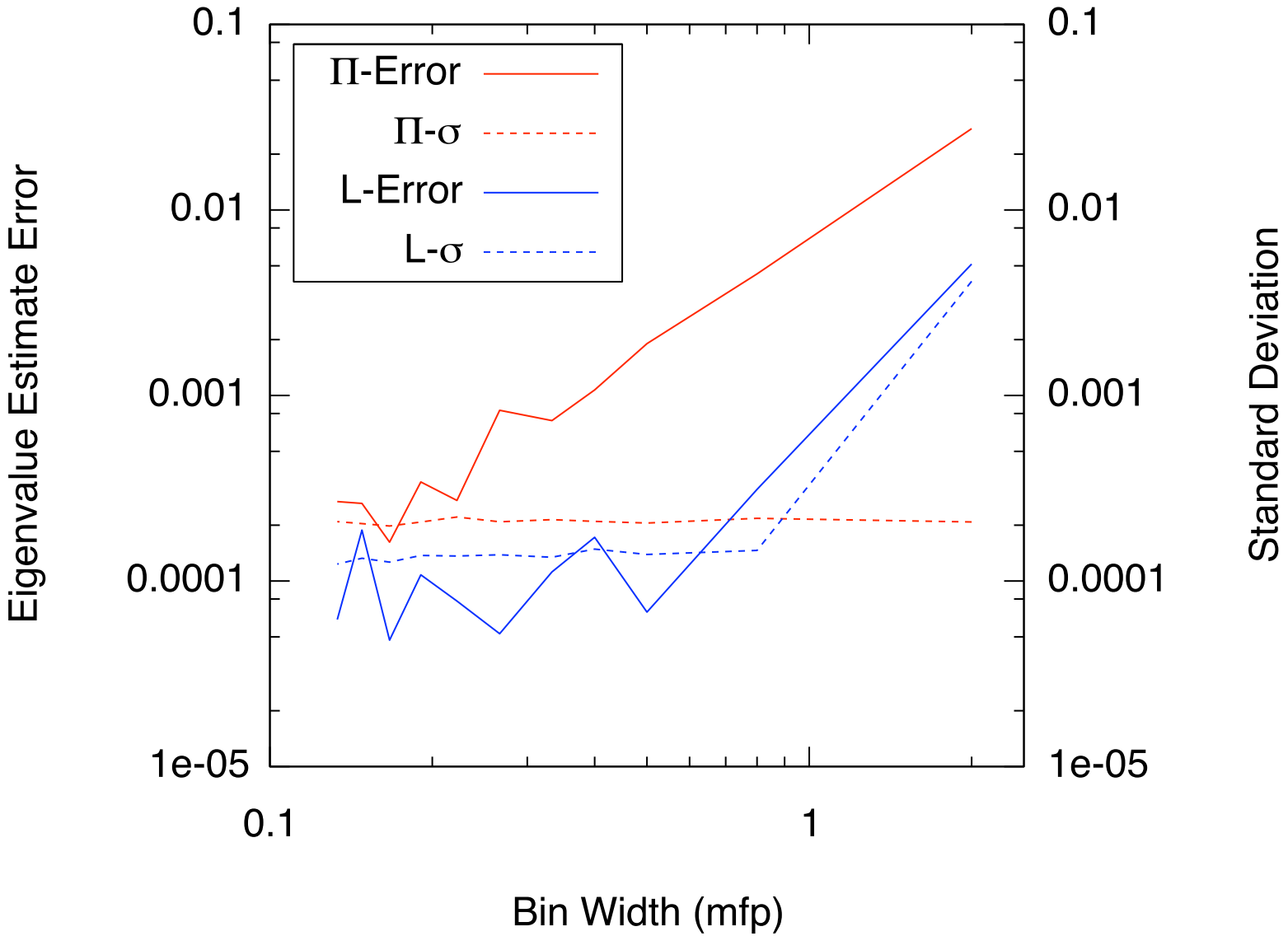
$$\mathcal{L}_b(x, \alpha_b, \beta_b) = \alpha_b + \beta_b x$$

$$v_{\mathcal{L}} = \left[\alpha_1, \beta_1, \alpha_2, \beta_2, \ldots, \alpha_n, \beta_B \right]^T$$

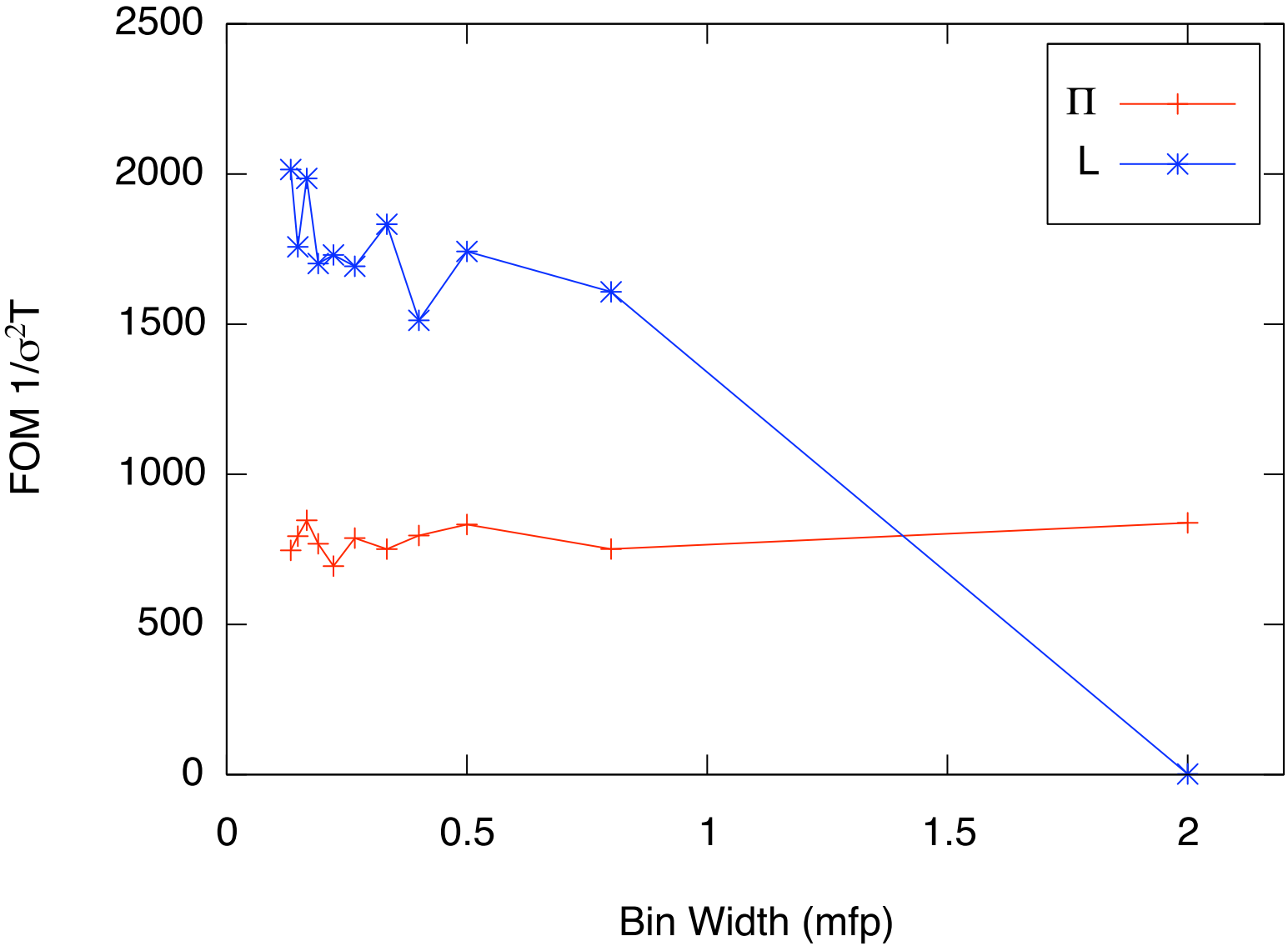
Numerical Results

- 20 mfp homogeneous thick
- $\nu\Sigma_f = 1.0$, $\Sigma_a = 0.2$, $\Sigma_s = 0.8$, $\Sigma_t = 1.0$
- 1×10^6 particles per iteration
- 50 inactive, 100 active Arnoldi restarts, 10 iterations per restart
- First and second order accurate spatial approximations
- 10–150 spatial bins

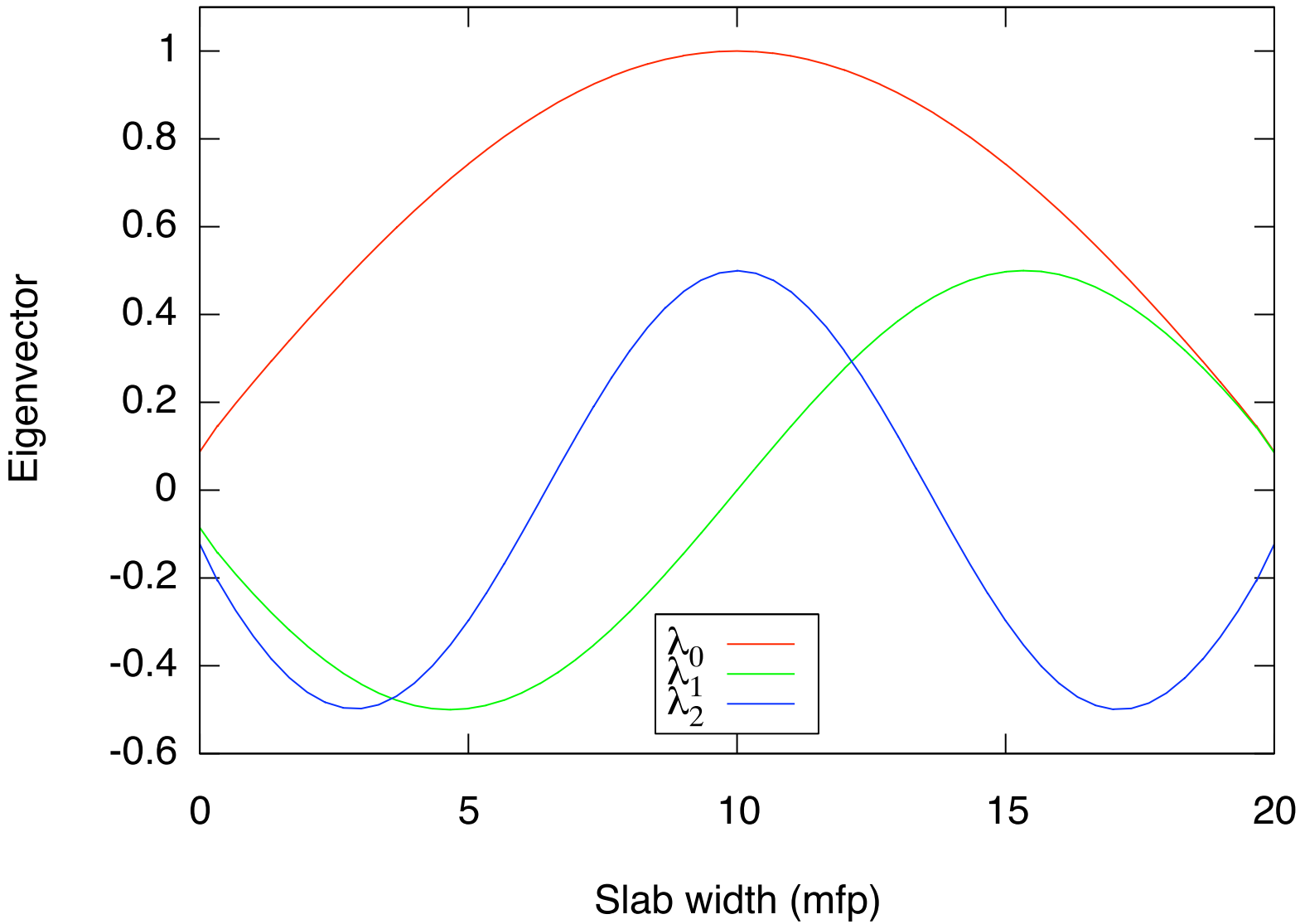
Numerical Results



Spatial Discretization—FOM



Spatial Discretization—Eigenvectors



Spatial Discretization—Eigenvectors