

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

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March 23, 2010

Particle Transport

Boltzmann Transport Equation:

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

Operator Form:

$$\begin{aligned} (\mathbf{L} + \mathbf{C} - \mathbf{S})\psi &= \frac{1}{k} \mathbf{F}\psi \\ \mathbf{T}\psi &= \frac{1}{k} \mathbf{F}\psi \end{aligned}$$

Define:

$$\begin{aligned} \nu &\equiv \mathbf{F}\psi \\ \mathcal{A} &\equiv \mathbf{F} \mathbf{T}^{-1} \end{aligned}$$

$$\mathcal{A}\nu = k\nu$$

Krylov Subspace Methods

- Estimate eigenpairs from Krylov subspace:

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

- Subspace constructed iteratively

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

- Krylov subspace

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

- Explicit form of \mathcal{A} not required

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:

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

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

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

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

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

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

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

- 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

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

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

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

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

Arnoldi Method Iteration

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

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

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

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

$$\mathcal{A}V_m x_i = V_m (\mu_i x_i) + v_{m+1} h_{m+1,m} e_m^T x_i$$

$$\mathcal{A}y_i = \mu_i y_i + v_{m+1} h_{m+1,m} e_m^T x_i$$

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

$$|r_i| = \|\mathcal{A}y_i - \mu_i y_i\| = |h_{m+1,m}| |e_m^T x_i|.$$

Explicitly 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

$$\int |v(x)| dx = q$$
$$p(x) = \frac{|v(x)|}{q}$$

- $p(x) dx$ is probability of picking a point in dx about x
- Neutron is given weight

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

Spatial Discretization

- Orthonormalization requires inner product between fission sources:

$$h_{jk} = \langle v_j, v_k \rangle = \int v_j(x) v_k(x) dx$$

- Discretize fission source

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

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

Inner Product of Fission Sources

- Discretization:

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

- Arnoldi vector representation:

$$v_{\Pi} = [a_1, a_2, \dots, a_B]^T$$

- Inner product of discretized fission sources:

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

Sampling from Discretized Source

- $v_{\Pi}(x)$ is a first order accurate approximation of fission source
- To sample from $v_{\Pi}(x)$, normalize

$$q = \sum_{b=1}^B |a_b|$$

$$p_b = |a_b| / q$$

- p_b is probability of sampling from bin b
- Bin b is sampled *uniformly* to determine neutron position

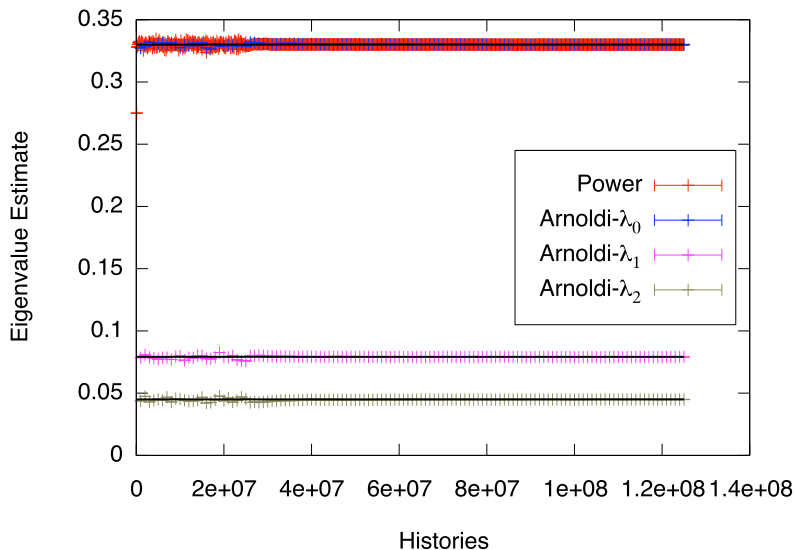
Numerical Results

- 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
- 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)

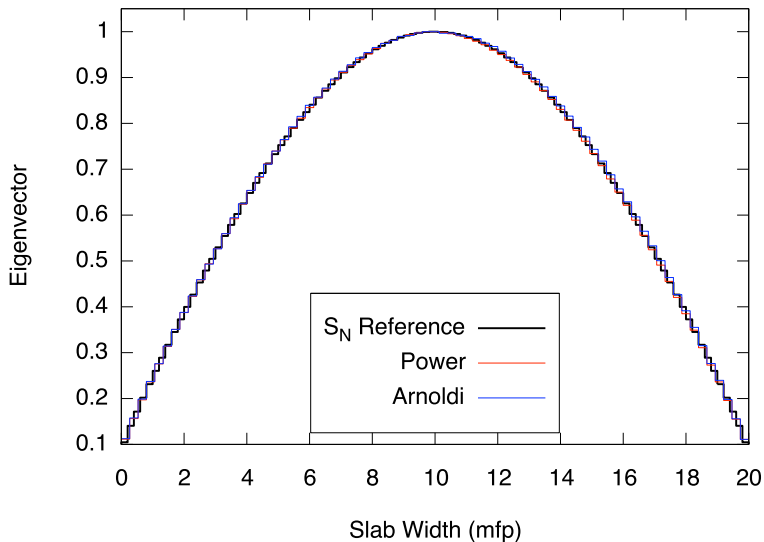
Numerical Results

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

Eigenvalue Convergence



Fundamental Eigenvector



Multiple Eigenvectors

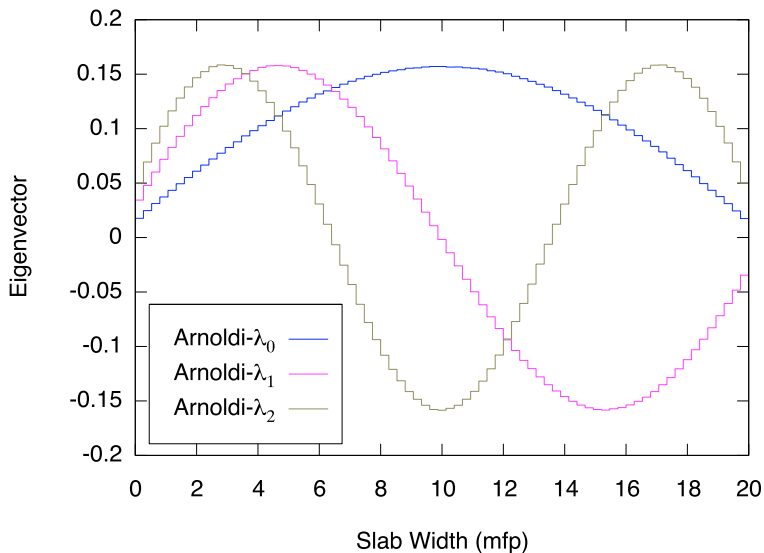


Figure of Merit

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

Figure of Merit

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

Variance

$$\sigma^2 \equiv \frac{1}{N-1} \left(\frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})^2 \right)$$

Spread

$$s \equiv \frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})^2$$

Figure of Merit

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

Variance

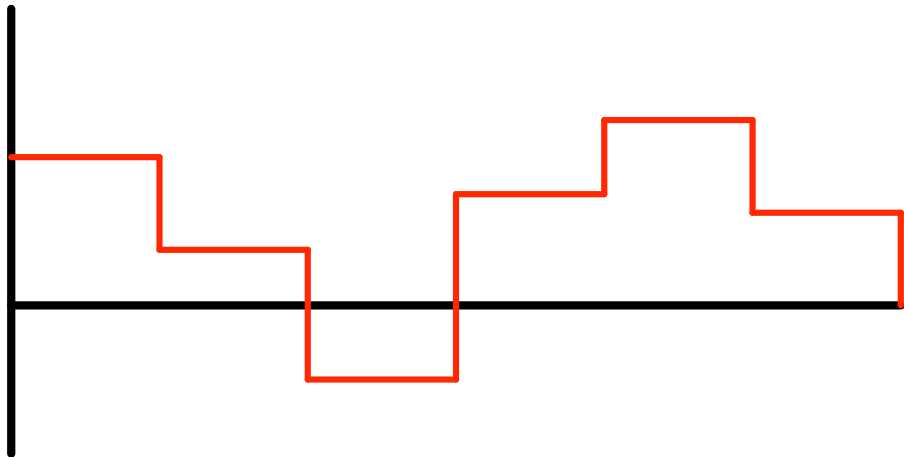
$$\sigma^2 \equiv \frac{1}{N-1} \left(\frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})^2 \right)$$

Spread

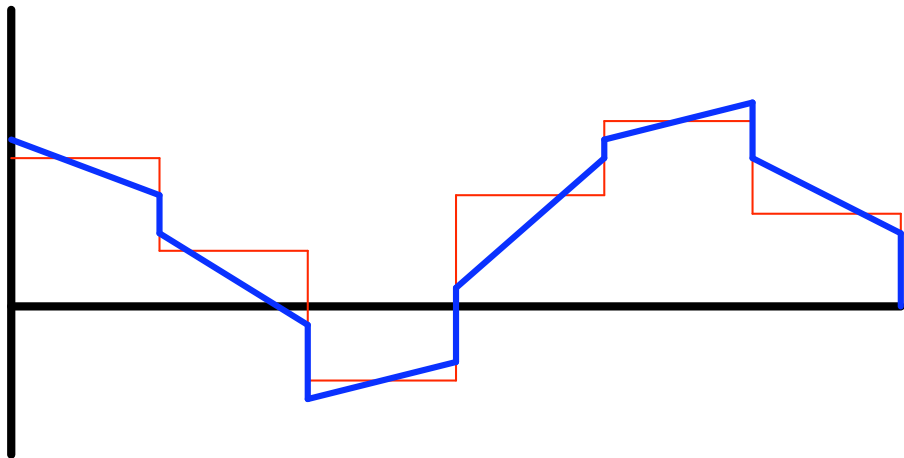
$$s \equiv \frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})^2$$

	0.2 mfp	2.0 mfp	20 mfp
Power	0.0020	0.0084	0.0201
Arnoldi	0.0018	0.0069	0.0153

Spatial Approximations



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Spatial Approximations

First Order Accurate

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

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

$$v_{\Pi} = [a_1, a_2, \dots, a_B]^T$$

Second Order Accurate

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

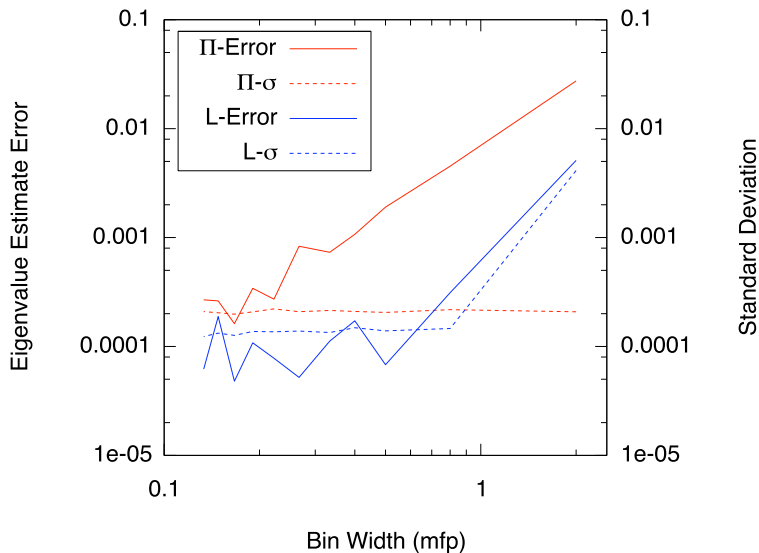
$$\mathcal{L}_b(x, \alpha_b, \beta_b) = \alpha_b + \beta_b x$$

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

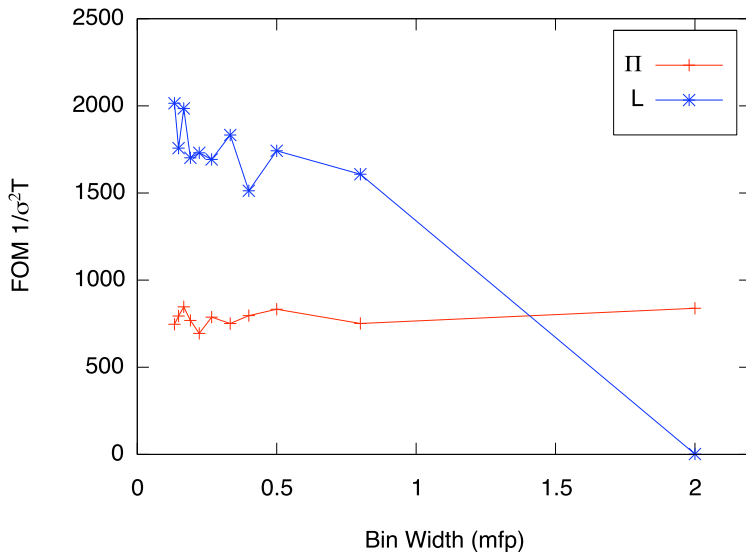
Numerical Results

- 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

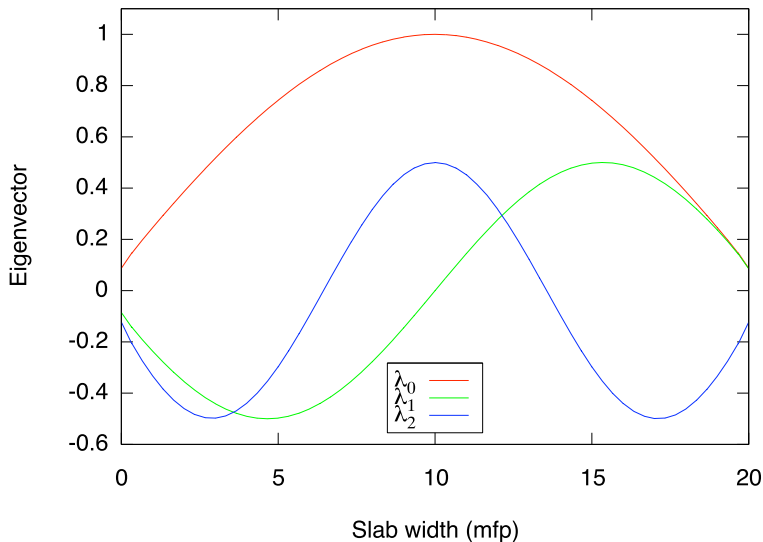
Numerical Results



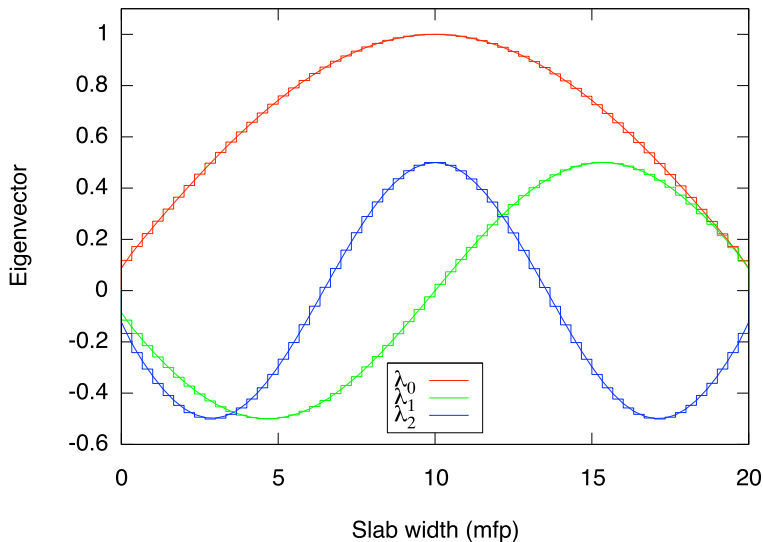
Spatial Discretization—FOM



Spatial Discretization—Eigenvectors



Spatial Discretization—Eigenvectors



Convergence in Monte Carlo Criticality Calculations

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

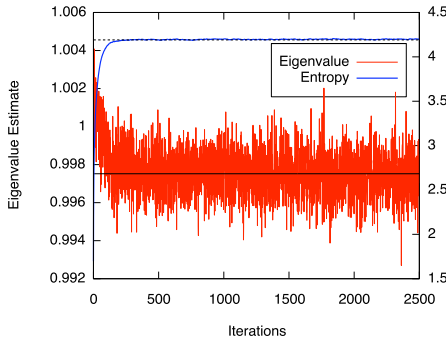
$$H(S(x)) \equiv - \sum_{b=1}^B S_b \log(S_b)$$

$$S_b = \int_{x_b}^{x_{b+1}} |v(x)| dx$$

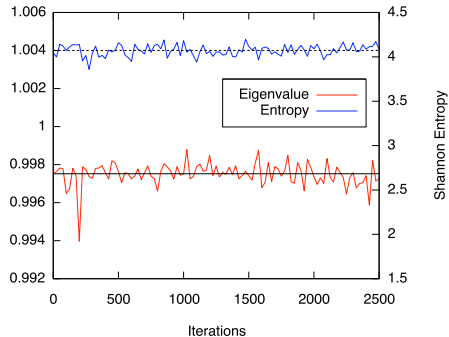
Homogeneous Geometry

- 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

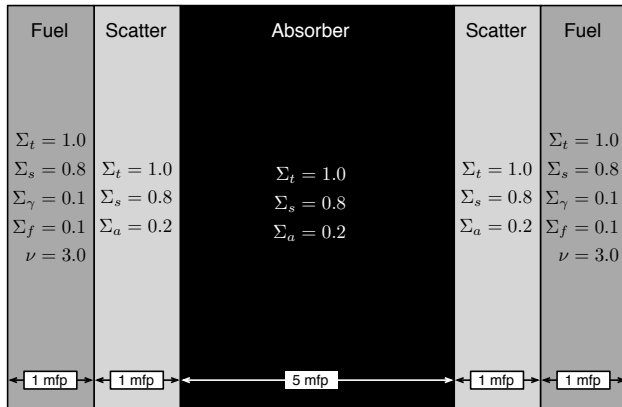


Arnoldi's Method

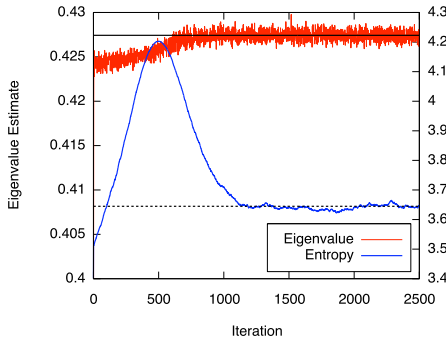
Heterogeneous Geometry

Parameters:

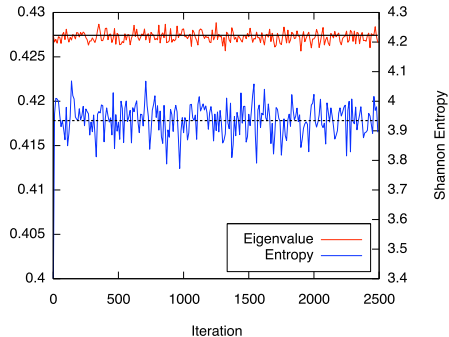
- 1×10^5 particles per iteration
- 10 iterations per Arnoldi restart
- 300 spatial bins (first order accurate)
- Source solely in left most bin
- Symmetric
- Asymmetric



Asymmetric Heterogeneous Geometry

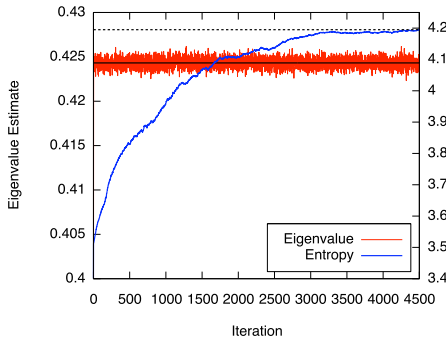


Power Method

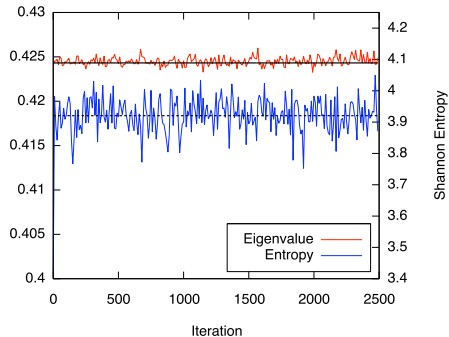


Arnoldi's Method

Symmetric Heterogeneous Geometry



Power Method



Arnoldi's Method

Conclusions

- Arnoldi's method can be used in Monte Carlo Criticality Calculations

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- Fission source is discretized
 - Discretization causes error in eigenvalue estimate
 - Second order accurate approximation reduces error and standard deviation

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- Arnoldi's method can be used in Monte Carlo Criticality Calculations
- Arnoldi's method can estimate multiple eigenvalues
- Fission source is discretized
 - Discretization causes error in eigenvalue estimate
 - Second order accurate approximation reduces error and standard deviation
- Arnoldi's method converges in just a few iterations
 - Eigenvalue estimate
 - Fission source

Questions?