Los Alamos NATIONAL LABORATORY

Decoupled Diffusion Synthetic Acceleration for Deterministic Neutral Particle Transport

J. M. Coale & J. S. Warsa

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Neutral Particle Transport

- Neutral particle transport processes
  - Nuclear reactors $\rightarrow$ neutron transport
  - High temperature phenomena & astrophysics $\rightarrow$ photon transport
- Numerical simulation typically involves the discrete Boltzmann transport equation
  - High dimensional, hyperbolic, integro-differential equation
  - Models particle streaming & interaction with matter
- Iterative methods are used to solve the Boltzmann transport equation

Iterative Solutions of the Boltzmann Transport Equation

- The physical regime of a problem can significantly affect iterative convergence
- In thick-diffusive regimes, iterative methods can become arbitrarily slow
  - Here scattering interactions between particles and matter dominate over particle streaming, absorption, and leakage
- The *synthetic acceleration* approach was developed in the 60's to solve this issue
  - Applies a correction to the iterative solution at each iterate
  - Correction is the solution to an *approximate* error equation
  - Improved convergence rate with extra cost per iteration
- The synthetic approach works when
  - the error equation can be solved *cheaply enough*,
  - the iterative convergence rate *improves enough*,
  - the net time-to-solution is *faster*

New Synthetic Acceleration

- Typically *diffusion synthetic acceleration* (DSA) is used to accelerate iterative solution of the transport equations
  - The diffusion approximation well approximates the error equation
  - This is because the most slowly-converging iterative error modes are linear in angle
  - Results in a very much improved iterative convergence rate
  - Scattering couples the energy-dependent diffusion equations $\rightarrow$ expensive to solve
- Previously, a method was developed to decouple the DSA equations in energy
  - Approach is to diagonalize the scattering operator in energy
  - Results in a set of “decoupled” diffusion equations that are cheaper to solve
  - The theoretical spectral radius/convergence rate of DSA iterations is **NOT** preserved
- A new decoupled DSA method improves upon the old formulation
  - Change-of-variables introduced to make diagonalization procedure “nicer”
  - The theoretical spectral radius of DSA iterations is preserved

The Boltzmann Transport Equation

- The Boltzmann Transport Equation is

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\psi + \sigma_t \psi = \frac{1}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' [\sigma_s(E' \to E)\psi(E', \boldsymbol{\Omega}')] + \frac{1}{4\pi} q$$

$$\boldsymbol{r} \in \Gamma, \quad 0 \leq E < \infty, \quad \boldsymbol{\Omega} \in \mathcal{S}, \quad \psi(\boldsymbol{r}, \boldsymbol{\Omega}) = f(\boldsymbol{\Omega}) \quad \text{for} \quad \boldsymbol{r} \in \partial\Gamma, \boldsymbol{n}_\Gamma \cdot \boldsymbol{\Omega} < 0$$

- Angular flux of particles $\psi(\boldsymbol{r}, E, \boldsymbol{\Omega})$ at position $\boldsymbol{r}$, direction $\boldsymbol{\Omega}$, and energy E
- Total and Scattering cross sections $\sigma_t(\boldsymbol{r}, E)$, $\sigma_s(\boldsymbol{r}, E' \to E)$
- Isotropic extraneous source $q(\boldsymbol{r}, E)$
- Unit sphere $\mathcal{S}$

Multigroup Approximation

- Define an energy grid: $\{E_g\}_{g=0}^{G}, \quad 0 = E_0 < \cdots < E_G < \infty$
- Apply the operator $\mathcal{P}_g^E \cdot \triangleq \int_{E_{g-1}}^{E_g} \cdot dE$

$$\mathbf{\Omega} \cdot \boldsymbol{\nabla} \mathcal{P}_g^E \psi + \mathcal{P}_g^E (\sigma_t \psi) = \frac{1}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \mathcal{P}_g^E [\sigma_s(E' \to E) \psi(E', \mathbf{\Omega}')] + \frac{1}{4\pi} \mathcal{P}_g^E q$$

- Multigroup transport equation is, for $g = 1, \ldots, G$,

$$\mathbf{\Omega} \cdot \boldsymbol{\nabla} \psi_g + \sigma_{t,g} \psi_g = \frac{1}{4\pi} \sum_{g'=1}^{G} \sigma_{s,g' \to g} \int_{4\pi} d\Omega' \psi_{g'} + \frac{1}{4\pi} q_g$$

- $\psi_g = \int_{E_{g-1}}^{E_g} \psi dE, \quad q_g = \int_{E_{g-1}}^{E_g} q dE$
- $\sigma_{t,g}$, $\sigma_{s,g' \to g}$ calculated by some weighted energy-averaging procedures

Operator Notation

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi_g + \sigma_{t,g} \psi_g = \frac{1}{4\pi} \sum_{g'=1}^{G} \sigma_{s,g' \to g} \int_{4\pi} d\Omega' \psi_{g'} + \frac{1}{4\pi} q_g$$

- Transport equation in operator notation

$$(\mathbf{L} + \mathbf{T})\psi = \frac{1}{4\pi} \mathbf{S} \mathbf{P}_0 \psi + \frac{1}{4\pi} \boldsymbol{q}$$

- Operators:

$$\mathbf{L} = \bigoplus_{g=1}^{G} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}, \quad \mathbf{T} = \bigoplus_{g=1}^{G} \sigma_{t,g}, \quad \mathbf{P}_0 = \bigoplus_{g=1}^{G} \int_{4\pi} \cdot d\Omega$$

$$\mathbf{S} = \begin{bmatrix} \sigma_{s,1\to1} & \cdots & \sigma_{s,G\to1} \\ \vdots & \ddots & \vdots \\ \sigma_{s,1\to G} & \cdots & \sigma_{s,G\to G} \end{bmatrix}$$

$$\bigoplus_{g=1}^{G} x_g \triangleq \mathrm{diag}(x_1, \ldots, x_G)$$

Source Iteration

$$\boxed{(\mathbf{L}+\mathbf{T})\psi = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\psi + \frac{1}{4\pi}\boldsymbol{q}}$$

- Solve for $\psi^{(\ell+1)}$ at iteration $\ell+1$

$$\psi^{(\ell+1)} = (\mathbf{L}+\mathbf{T})^{-1}\left[\frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\psi^{(\ell)} + \frac{1}{4\pi}\boldsymbol{q}\right]$$

- Solve for $\phi \triangleq \mathbf{P}_0\psi$, applying $\mathbf{P}_0$ on the left

$$\phi^{(\ell+1)} = \mathbf{P}_0(\mathbf{L}+\mathbf{T})^{-1}\left[\frac{1}{4\pi}\mathbf{S}\phi^{(\ell)} + \frac{1}{4\pi}\boldsymbol{q}\right]$$

The Iterative Error Equation

- Let ψ to be the exact solution to the transport equation
- Define the iterative error $\boldsymbol{e}^{(\ell+1)} = \psi - \psi^{(\ell+1)}$
- Subtract equations for ψ and $\psi^{(\ell+1)}$

$$(\mathbf{L}+\mathbf{T})\psi = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\psi + \frac{1}{4\pi}\boldsymbol{q}$$
$$(\mathbf{L}+\mathbf{T})\psi^{(\ell+1)} = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\psi^{(\ell)} + \frac{1}{4\pi}\boldsymbol{q}$$

The Iterative Error Equation

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$$(\mathbf{L} + \mathbf{T})(\psi - \psi^{(\ell+1)}) = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0(\psi - \psi^{(\ell)}) + \frac{1}{4\pi}(\boldsymbol{q} - \boldsymbol{q})$$

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$$(\mathbf{L} + \mathbf{T})\boldsymbol{e}^{(\ell+1)} = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\boldsymbol{e}^{(\ell)}$$

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- Next subtract $\frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\boldsymbol{e}^{(\ell+1)}$ from both sides

$$(\mathbf{L} + \mathbf{T} - \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0)\boldsymbol{e}^{(\ell+1)} = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0(\boldsymbol{e}^{(\ell)} - \boldsymbol{e}^{(\ell+1)})$$

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- Let ψ to be the exact solution to the transport equation
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$$(\mathbf{L} + \mathbf{T} - \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0)\boldsymbol{e}^{(\ell+1)} = \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0((\psi - \psi^{(\ell)}) - (\psi - \psi^{(\ell+1)}))$$

The Iterative Error Equation

- Let ψ to be the exact solution to the transport equation
- Define the iterative error $\boldsymbol{e}^{(\ell+1)} = \psi - \psi^{(\ell+1)}$
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The Iterative Error Equation

- Let ψ to be the exact solution to the transport equation
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- Next subtract $\frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\boldsymbol{e}^{(\ell+1)}$ from both sides

$$(\mathbf{L} + \mathbf{T} - \frac{1}{4\pi}\mathbf{S}\mathbf{P}_0)\boldsymbol{e}^{(\ell+1)} = \frac{1}{4\pi}\boldsymbol{r}^{(\ell+1)}$$

- Iterative residual $\boldsymbol{r}^{(\ell+1)} = \mathbf{S}(\boldsymbol{\phi}^{(\ell+1)} - \boldsymbol{\phi}^{(\ell)})$

Diffusion Synthetic Acceleration Equations

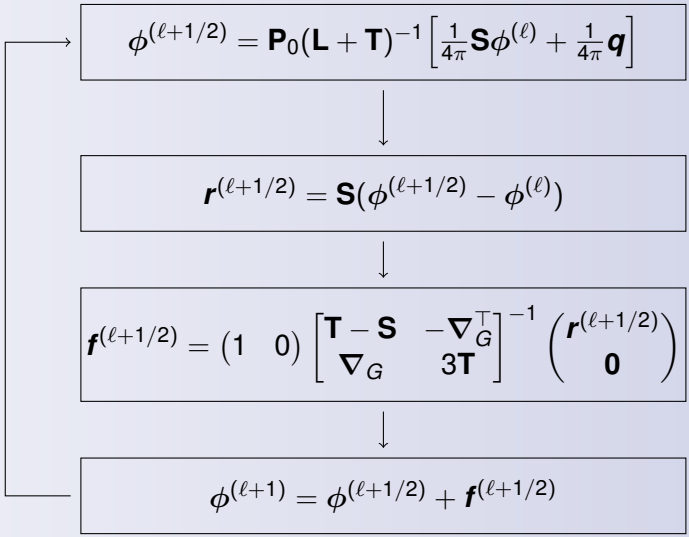
- The P_1 approximation is applied to the error equation, by taking its first two angular moments
- Zeroth & first moment operators $\mathbf{P}_0 = \bigoplus_{g=1}^{G} \int_{4\pi} \cdot d\Omega, \quad \mathbf{P}_1 = \bigoplus_{g=1}^{G} \int_{4\pi} \mathbf{\Omega} \cdot d\Omega$
- The P_1 error equations:

$$\begin{bmatrix} \mathbf{T} - \mathbf{S} & -\boldsymbol{\nabla}_G^{\top} \\ \boldsymbol{\nabla}_G & 3\mathbf{T} \end{bmatrix} \begin{pmatrix} \boldsymbol{f}^{(\ell+1)} \\ \boldsymbol{h}^{(\ell+1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{r}^{(\ell+1)} \\ \mathbf{0} \end{pmatrix}$$

- Approximate iterative errors $\boldsymbol{f}^{(\ell+1)} \approx \mathbf{P}_0 \boldsymbol{e}^{(\ell+1)}$ and $\boldsymbol{h}^{(\ell+1)} \approx \mathbf{P}_1 \boldsymbol{e}^{(\ell+1)}$
- New operators $\boldsymbol{\nabla}_G = \bigoplus_{g=1}^{G} \boldsymbol{\nabla} \cdot$,
- Boundary conditions

$$\left(\mathbf{n} \boldsymbol{h}^{(\ell+1)} + \frac{1}{2} \boldsymbol{f}^{(\ell+1)} \right) \Big|_{\boldsymbol{r} \in \partial\Gamma} = 0, \quad \mathbf{n} = \bigoplus_{g=1}^{G} \boldsymbol{n}_{\Gamma} \cdot$$

Diffusion Synthetic Acceleration Iterations



Decoupling the Diffusion Error Equation in Groups (1)

- A change of variables is introduced $\check{\boldsymbol{f}} = \mathbf{T}^{-1}\boldsymbol{f}$

$$\begin{bmatrix} \mathbf{T}-\mathbf{S} & -\boldsymbol{\nabla}_G^{\top} \\ \boldsymbol{\nabla}_G & 3\mathbf{T} \end{bmatrix} \begin{bmatrix} \mathbf{T} & 0 \\ 0 & \mathbb{I}_G \end{bmatrix} \begin{pmatrix} \check{\boldsymbol{f}}^{(\ell+1/2)} \\ \boldsymbol{h}^{(\ell+1/2)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{r}^{(\ell+1/2)} \\ \mathbf{0} \end{pmatrix}$$

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- Left apply $\mathrm{diag}(\mathbb{I}_G, \mathbf{T}^{-1})$

$$\begin{bmatrix} \mathbb{I}_G & 0 \\ 0 & \mathbf{T}^{-1} \end{bmatrix} \begin{bmatrix} (\mathbf{T}-\mathbf{S})\mathbf{T} & -\boldsymbol{\nabla}_G^\top \\ \boldsymbol{\nabla}_G\mathbf{T} & 3\mathbf{T} \end{bmatrix} \begin{pmatrix} \check{\boldsymbol{f}}^{(\ell+1/2)} \\ \boldsymbol{h}^{(\ell+1/2)} \end{pmatrix} = \begin{bmatrix} \mathbb{I}_G & 0 \\ 0 & \mathbf{T}^{-1} \end{bmatrix} \begin{pmatrix} \boldsymbol{r}^{(\ell+1/2)} \\ \mathbf{0}, \end{pmatrix}$$

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- Left apply $\mathrm{diag}(\mathbb{I}_G, \mathbf{T}^{-1})$ (assuming $\mathbf{T}^{-1}\boldsymbol{\nabla}_G\mathbf{T} = \boldsymbol{\nabla}_G$, i.e. $\frac{1}{\sigma_{t,g}}\boldsymbol{\nabla}\sigma_{t,g} = \boldsymbol{\nabla}$)

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$$\begin{bmatrix} (\mathbf{T}-\mathbf{S})\mathbf{T} & -\boldsymbol{\nabla}_G^\top \\ \boldsymbol{\nabla}_G & 3\mathbb{I}_G \end{bmatrix} \begin{pmatrix} \breve{\boldsymbol{f}}^{(\ell+1/2)} \\ \boldsymbol{h}^{(\ell+1/2)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{r}^{(\ell+1/2)} \\ \mathbf{0} \end{pmatrix}$$

- Diagonalize the group-to-group coupling term $(\mathbf{T}-\mathbf{S})\mathbf{T} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1}$

$$\begin{bmatrix} \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1} & -\boldsymbol{\nabla}_G^\top \\ \boldsymbol{\nabla}_G & 3\mathbb{I}_G \end{bmatrix} \begin{pmatrix} \breve{\boldsymbol{f}}^{(\ell+1/2)} \\ \boldsymbol{h}^{(\ell+1/2)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{r}^{(\ell+1/2)} \\ \mathbf{0} \end{pmatrix}$$

Decoupling the Diffusion Error Equation in Groups (2)

- A second change of variables is introduced

$$\hat{\boldsymbol{f}} = \mathbf{Q}^{-1}\check{\boldsymbol{f}}, \quad \hat{\boldsymbol{h}} = \mathbf{Q}^{-1}\boldsymbol{h}, \quad \hat{\boldsymbol{r}} = \mathbf{Q}^{-1}\boldsymbol{r}$$

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- Substituted into the error equation:

$$\begin{bmatrix} \mathbf{Q}^{-1} & 0 \\ 0 & \mathbf{Q}^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1} & -\boldsymbol{\nabla}_G^{\top} \\ \boldsymbol{\nabla}_G & 3\mathbb{I}_G \end{bmatrix} \begin{bmatrix} \mathbf{Q} & 0 \\ 0 & \mathbf{Q} \end{bmatrix} \begin{pmatrix} \hat{\boldsymbol{f}}^{(\ell+1/2)} \\ \hat{\boldsymbol{h}}^{(\ell+1/2)} \end{pmatrix} = \begin{pmatrix} \hat{\boldsymbol{r}}^{(\ell+1/2)} \\ \mathbf{0} \end{pmatrix}$$

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- Substituted into the error equation:

$$\begin{bmatrix} \boldsymbol{\Lambda} & \mathbf{Q}^{-1}(-\boldsymbol{\nabla}_G^{\top})\mathbf{Q} \\ \mathbf{Q}^{-1}\boldsymbol{\nabla}_G\mathbf{Q} & 3\mathbb{I}_G \end{bmatrix} \begin{pmatrix} \hat{\boldsymbol{f}}^{(\ell+1/2)} \\ \hat{\boldsymbol{h}}^{(\ell+1/2)} \end{pmatrix} = \begin{pmatrix} \hat{\boldsymbol{r}}^{(\ell+1/2)} \\ \mathbf{0} \end{pmatrix}$$

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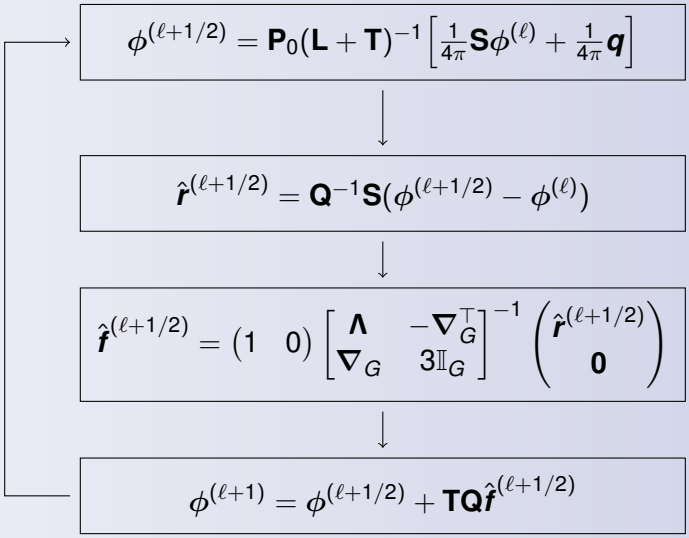
- Assuming $\mathbf{Q}^{-1}(-\boldsymbol{\nabla}_G^\top)\mathbf{Q} = -\boldsymbol{\nabla}_G^\top$ and $\mathbf{Q}^{-1}\boldsymbol{\nabla}_G\mathbf{Q} = \boldsymbol{\nabla}_G$:

$$\boxed{\begin{bmatrix} \boldsymbol{\Lambda} & -\boldsymbol{\nabla}_G^\top \\ \boldsymbol{\nabla}_G & 3\mathbb{I}_G \end{bmatrix} \begin{pmatrix} \hat{\boldsymbol{f}}^{(\ell+1/2)} \\ \hat{\boldsymbol{h}}^{(\ell+1/2)} \end{pmatrix} = \begin{pmatrix} \hat{\boldsymbol{r}}^{(\ell+1/2)} \\ \mathbf{0} \end{pmatrix}}$$

- This equation is block-diagonal in energy groups

Decoupled Diffusion Synthetic Acceleration Iterations



Decoupled Boundary Conditions

- Boundary conditions are derived by substituting the change of variables

$$\hat{\boldsymbol{f}} = \mathbf{Q}^{-1}\mathbf{T}^{-1}\boldsymbol{f}, \quad \hat{\boldsymbol{h}} = \mathbf{Q}^{-1}\boldsymbol{h}$$

  into the boundary conditions for $\boldsymbol{f}$
- After some algebra, we find:

$$\left(\mathbf{n}\hat{\boldsymbol{h}}^{(\ell+1/2)} + \frac{1}{2}\mathbf{B}\hat{\boldsymbol{f}}^{(\ell+1/2)}\right)\Big|_{\boldsymbol{r}\in\partial\Gamma} = 0, \quad \mathbf{B} = \mathbf{Q}^{-1}\mathbf{T}\mathbf{Q}$$

- Approximate, decoupled-in-energy boundary conditions:

$$\left(\mathbf{n}\hat{\boldsymbol{h}}^{(\ell+1/2)} + \frac{1}{2}\mathbf{B}^{\text{in}}\hat{\boldsymbol{f}}^{(\ell+1/2)}\right)\Big|_{\boldsymbol{r}\in\partial\Gamma} = 0, \quad \mathbf{B}^{\text{in}} = \text{diag}(\mathbf{B})$$

- Two methods are thus derived:
  - D-DSA(1) which uses the fully coupled in energy boundary conditions
  - D-DSA(2) which uses the approximate, decoupled in energy boundary conditions

Other Considerations

- Deriving discrete formulations of the decoupled equations takes special care
- For instance: Discontinuous-Galerkin finite element spatial discretization
  - involves interface conditions between mesh cells
  - interface conditions must be transformed like the boundary conditions
  - this introduces group-to-group coupling terms in the domain interior
- A decoupled-in-energy formulation is constructed by ignoring “re-coupling” terms
- Numerical tests hint that this does **not** significantly degrade convergence rate
  - use of the approximate, decoupled boundary conditions
  - ignoring “re-coupling terms” in interface conditions

1D Numerical Test Problems

- Two cross section sets:
  - C5G7 benchmark moderator (7-group water)
  - LANL 30-group uranium, excluding fission
- Fourier analysis to predict the theoretical spectral radius (1D infinite slab)
  - Details to be provided in upcoming publication
  - Fourier analysis does not take boundary conditions into account
  - Results for D-DSA(1) and D-DSA(2) are equivalent
- Numerically tested on the following problem:
  - 1D slab geometry, 50 cm long
  - 1000 spatial cells
  - Boltzmann equation discretized with step differencing
  - Double S_4 Gauss-Legendre quadrature
  - Diffusion error equations discretized with central (finite-volume) differencing

1D Numerical Results

- Fourier analysis obtained spectral radius: $\bar{\rho}^F$
- Numerically estimated spectral radius: $\bar{\rho}^N = \frac{\|\phi^{(\ell)} - \phi^{(\ell-1)}\|}{\|\phi^{(\ell+1)} - \phi^{(\ell)}\|}$
- Notation: SI $\rightarrow$ source iterations, FC-DSA $\rightarrow$ fully coupled DSA

Method	$\bar{\rho}^F$	$\bar{\rho}^N$	Iterations
SI	0.986	0.986	1600
FC-DSA	0.215	0.219	15
D-DSA(1)	0.215	0.219	15
D-DSA(2)	0.215	0.218	16

Table: C5G7 moderator cross sections

Method	$\bar{\rho}^F$	$\bar{\rho}^N$	Iterations
SI	0.822	0.821	132
FC-DSA	0.172	0.169	14
D-DSA(1)	0.172	0.169	14
D-DSA(2)	0.172	0.170	17

Table: LANL 30 uranium cross sections

2D Numerical Results

- 2D Cartesian geometry, 500 $\times$ 500 cm, 30-group water cross sections
- Linear discontinuous-Galerkin spatial discretization for transport
- Linear continuous-Galerkin spatial discretization for diffusion
- Using DSA as a *preconditioner* to GMRES
- 4×10^6 triangles on 960 MPI ranks distributed over 15 compute nodes
  - $\sim$ 4200 mesh cells per rank

Preconditioner	Iterations	Wall Time (s)
None	4734	15480.98
FC-DSA	16	2244.76
D-DSA(2)	31	262.21

Conclusion

- A decoupled-in-energy variation of the DSA method, D-DSA, was developed, analyzed and tested
- If boundary conditions remain coupled-in-energy, the approach has the same convergence rate as full DSA
- Making an approximation that decouples the boundary conditions in energy does not significantly affect convergence rate
- Some spatial discretizations can “re-couple” the equations in energy – keeping them decoupled is another approximation that also doesn’t significantly impact convergence rate

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Questions?