Los Alamos NATIONAL LABORATORY

Improved Decoupled Diffusion Synthetic Acceleration Scheme for Neutral Particle Transport

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International Conference on Physics of Reactors (PHYSOR 2024)
April 24, 2024

LA-UR-24-23354

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

Multigroup Boltzmann Transport Equation

- Transport equation for the angular flux $\psi_g(\boldsymbol{r}, \boldsymbol{\Omega})$ at position $\boldsymbol{r}$, direction $\boldsymbol{\Omega}$ and energy group $g = 1, \ldots, G$

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

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

- Total and scattering cross sections $\sigma_{t,g}(\boldsymbol{r})$, $\sigma_{s,g' \to g}(\boldsymbol{r})$
- Isotropic extraneous source $q_g(\boldsymbol{r})$
- Unit sphere $\mathcal{S}$

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:

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

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

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

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
- Iterative error is $\boldsymbol{e}^{(\ell+1)} = \psi - \psi^{(\ell+1)}$
- Subtract equations for ψ and $\psi^{(\ell+1)}$

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

- Subtract $\frac{1}{4\pi}\mathbf{S}\mathbf{P}_0\boldsymbol{e}^{(\ell+1)}$ from both sides, after some manipulation:

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

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

Diffusion Synthetic Acceleration Equations

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

- The diffusion approximation is applied to the error equation:

$$\boxed{(\mathbf{L}_D+\mathbf{T}-\mathbf{S})\boldsymbol{f}^{(\ell+1)}=\boldsymbol{r}^{(\ell+1)}}$$

- Approximate iterative errors

$$\boldsymbol{f}^{(\ell+1)}\approx\mathbf{P}_0\boldsymbol{e}^{(\ell+1)}$$

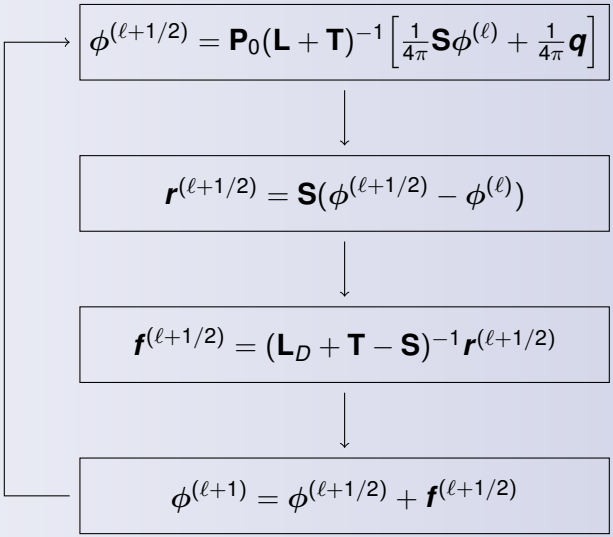
- Operators:

$$\mathbf{L}_D=\boldsymbol{\nabla}_G\mathbf{D}\boldsymbol{\nabla}_G,\quad \boldsymbol{\nabla}_G=\bigoplus_{g=1}^{G}\boldsymbol{\nabla}\cdot,\quad \mathbf{D}=\frac{1}{3}\mathbf{T}^{-1}$$

- Marshak boundary conditions

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

Diffusion Synthetic Acceleration Iterations



Decoupling the Diffusion Error Equation in Groups (1)

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

$$(\mathbf{L}_D + \mathbf{T} - \mathbf{S})\mathbf{T}\check{\boldsymbol{f}}^{(\ell+1/2)} = \boldsymbol{r}^{(\ell+1/2)}$$

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- Consider $\mathbf{L}_D\mathbf{T}$

$$\mathbf{L}_D\mathbf{T} = \boldsymbol{\nabla}_G\mathbf{D}\boldsymbol{\nabla}_G\mathbf{T}$$

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- Consider $\mathbf{L}_D\mathbf{T}$

$$\mathbf{L}_D\mathbf{T} = \frac{1}{3}\nabla_G\mathbf{T}^{-1}\nabla_G\mathbf{T}$$

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- Consider $\mathbf{L}_D\mathbf{T}$ (assuming $\mathbf{T}^{-1}\boldsymbol{\nabla}_G\mathbf{T} = \boldsymbol{\nabla}_G$, i.e. $\frac{1}{\sigma_{t,g}}\boldsymbol{\nabla}\sigma_{t,g} = \boldsymbol{\nabla}$)

$$\mathbf{L}_D\mathbf{T} = \frac{1}{3}\boldsymbol{\nabla}_G^2$$

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$$\mathbf{L}_D\mathbf{T} = \frac{1}{3}\boldsymbol{\nabla}_G^2$$

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

$$\left(\frac{1}{3}\boldsymbol{\nabla}_G^2 + \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1}\right)\check{\boldsymbol{f}}^{(\ell+1/2)} = \boldsymbol{r}^{(\ell+1/2)}$$

Decoupling the Diffusion Error Equation in Groups (2)

- A second change of variables is introduced

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

Decoupling the Diffusion Error Equation in Groups (2)

- A second change of variables is introduced

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

- Substituted into the error equation:

$$\mathbf{Q}^{-1}\left(\frac{1}{3}\nabla_G^2 + \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1}\right)\mathbf{Q}\hat{\boldsymbol{f}}^{(\ell+1/2)} = \hat{\boldsymbol{r}}^{(\ell+1/2)}$$

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$$\left(\frac{1}{3}\mathbf{Q}^{-1}\nabla_G^2\mathbf{Q} + \boldsymbol{\Lambda}\right)\hat{\boldsymbol{f}}^{(\ell+1/2)} = \hat{\boldsymbol{r}}^{(\ell+1/2)}$$

Decoupling the Diffusion Error Equation in Groups (2)

- A second change of variables is introduced

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- Substituted into the error equation:

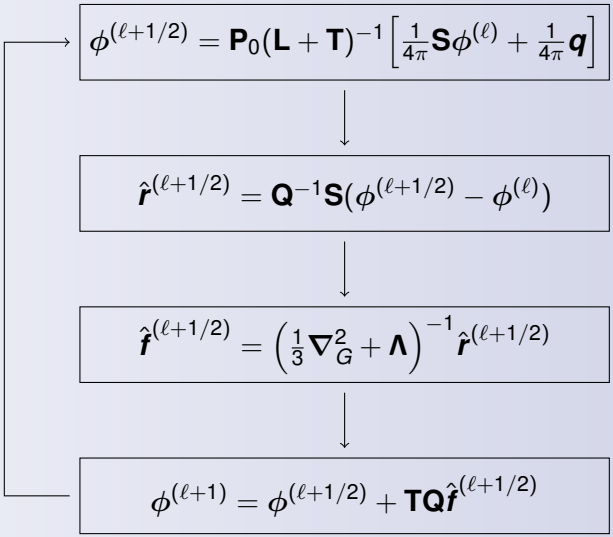
$$\left(\frac{1}{3}\mathbf{Q}^{-1}\boldsymbol{\nabla}_G^2\mathbf{Q} + \boldsymbol{\Lambda}\right)\hat{\boldsymbol{f}}^{(\ell+1/2)} = \hat{\boldsymbol{r}}^{(\ell+1/2)}$$

- Assuming $\mathbf{Q}^{-1}\boldsymbol{\nabla}_G^2\mathbf{Q} = \boldsymbol{\nabla}_G^2$:

$$\boxed{\left(\frac{1}{3}\boldsymbol{\nabla}_G^2 + \boldsymbol{\Lambda}\right)\hat{\boldsymbol{f}}^{(\ell+1/2)} = \hat{\boldsymbol{r}}^{(\ell+1/2)}}$$

- 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

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

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

$$\left(\frac{1}{3}\mathbf{n}\boldsymbol{\nabla}_G + \frac{1}{2}\mathbf{B}\right)\hat{\boldsymbol{f}}^{(\ell+1/2)}\Big|_{\boldsymbol{r}\in\partial\Gamma} = 0, \quad \mathbf{B} = \mathbf{Q}^{-1}\mathbf{T}\mathbf{Q}$$

- Approximate, decoupled-in-energy boundary conditions:

$$\left(\frac{1}{3}\mathbf{n}\boldsymbol{\nabla}_G + \frac{1}{2}\mathbf{B}^{\text{in}}\right)\hat{\boldsymbol{f}}^{(\ell+1/2)}\Big|_{\boldsymbol{r}\in\partial\Gamma} = 0, \quad \mathbf{B}^{\text{in}} = \text{diag}(\mathbf{B})$$

- 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

Numerical Test Problems

- We test the method using two cross section sets:
  - C5G7 benchmark moderator (7-group water)
  - LANL 30-group uranium, excluding fission
- We performed Fourier analysis to extract the theoretical spectral radius (1D infinite slab)
  - See paper for details
  - Fourier analysis does not take boundary conditions into account
  - Results for D-DSA(1) and D-DSA(2) are equivalent
- The method was also numerically tested on the following problem:
  - 1D slab geometry, 50 cm long
  - 1000 spatial cells
  - Boltzmann equation discretized with step difference scheme, double S_4 Gauss-Legendre quadrature
  - Diffusion error equation discretized with central difference scheme

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

Acknowledgments

This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.

Questions?