Variations on Diffusion-Based Synthetic Acceleration for Multigroup S_N Transport

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Multigroup S_N Transport Iterations

- Iterative solution of the transport equation can converge slowly for optically-thick problems and problems with effective scattering ratios near 1.0
- Computational efficiency can be improved with synthetic acceleration of the transport iterations
- Energy groups are coupled to one another by the scattering operators of the problem
  - Thermal neutron energy groups in reactor applications
  - Boltzmann-Compton scattering in photon transport applications
- Iterative acceleration in multigroup applications complicates the application of synthetic acceleration methods
- Synthetic acceleration can formulated to be applied as a preconditioner for more advanced iterative methods

Synthetic Acceleration

- An equation for the error in the iterative solution is found by subtracting the iterative equation from the exact equation
- The error equation is identical to the original equation with the iterative residual as a source term
- A synthetic acceleration method uses some low-order approximation to the error equation that can be solved “more easily” than the original equation
- As long as the approximate error equation is “close enough” in some sense to the original error equation, convergence will improve
- The goal is to find a low-order equation that can be solved efficiently enough and whose improvement in convergence is good enough that the overall time-to-solution is faster than it would be otherwise

Diffusion-based Synthetic Acceleration

- The diffusion equation is a linear-in-angle (Galerkin) approximation to the transport equation
- The most slowly converging error modes of simple fixed-point (source) iteration are also linear in angle
- Using the diffusion equation as the low-order approximation to the error equation therefore makes sense and will therefore also improve convergence rate
- In multigroup problems, the fully-coupled-in-energy diffusion equation must be employed as the low-order system to acheive the analytically predicted (continuous in space and angle) improvement in convergence rate (measured by the spectral radius)
- Various approximations to the fully-coupled, low-order diffusion equation will be considered that have the potential to improve overall computational efficiency
- We investigate and compare the impact that these approximations have on the analytically predicted spectral radius

Boltzmann Transport Equation

- Multigroup Boltzmann transport equation

$$\mathbf{\Omega}_m \cdot \nabla \psi_{g,m} + \sigma_{t,g} \psi_{g,m} = \frac{1}{4\pi} \sum_{g'=1}^{G} \sigma_{s,g' \to g} \phi_{g'} + q_g, \tag{1}$$

$$g = 1, \ldots, G, \quad m = 1, \ldots, M$$

- $\phi_g = \sum_{m=1}^{M} w_m \psi_{g,m}$
- Here we consider
  - Discretization in angle with the method of discrete ordinates (S_N)
  - Isotropic scattering

Operator Notation

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

- In operator notation the multigroup S_N equations become

$$\boldsymbol{L}\psi = \boldsymbol{MSD}\psi + q \qquad (2)$$

- Vectors:
  - $\psi = [\psi_1, \ldots, \psi_g, \ldots, \psi_G]^\top$
  - $\phi = [\phi_1, \ldots, \phi_g, \ldots, \phi_G]^\top$
- Operators:
  - $\boldsymbol{D}\psi = \phi$
  - $\boldsymbol{S}_{i,j} = \sigma_{s,j\to i}$
  - $\boldsymbol{M} = \frac{1}{4\pi}\boldsymbol{I}$
  - $(\boldsymbol{L}\psi)_{g,m} = \boldsymbol{\Omega}_m \cdot \nabla\psi_{g,m} + \sigma_{t,g}\psi_{g,m}$

Fixed-Point (Source) Iteration

- Given an initial guess ϕ^0, for $\ell = 0, \ldots$

$$\boldsymbol{L}\psi^{\ell+1} = \boldsymbol{MSD}\psi^{\ell} + q \tag{3}$$

- $\boldsymbol{L}$ is efficiently inverted via an S_N sweep to leverage the natural block-lower triangular structure

$$\psi^{\ell+1} = \boldsymbol{L}^{-1}\boldsymbol{MSD}\psi^{\ell} + \boldsymbol{L}^{-1}q \tag{4}$$

- Application of $\boldsymbol{D}$ on the left gives

$$\boldsymbol{D}\psi^{\ell+1} = \boldsymbol{DL}^{-1}\boldsymbol{MSD}\psi^{\ell} + \boldsymbol{DL}^{-1}q \tag{5}$$

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$$\phi^{\ell+1} = \boldsymbol{DL}^{-1}\boldsymbol{MS}\phi^{\ell} + b \tag{5}$$

$$b = \boldsymbol{DL}^{-1}q \tag{6}$$

Diffusion Synthetic Acceleration (DSA)

- Exact solution ψ

$$\boldsymbol{L}\psi = \boldsymbol{MSD}\psi + q$$

- Iterative solution $\psi^{\ell+1}$

$$\boldsymbol{L}\psi^{\ell+1} = \boldsymbol{MSD}\psi^{\ell} + q$$

- Error $e^{\ell+1} = \psi - \psi^{\ell+1}$

$$\boldsymbol{L}e^{\ell+1} = \boldsymbol{MSD}(\psi - \psi^{\ell} \pm \psi^{\ell+1}) \tag{7}$$

$$= \boldsymbol{MSD}e^{\ell+1} + r^{\ell+1} \tag{8}$$

- Iterative residual

$$r^{\ell+1} = \boldsymbol{MS}(\phi^{\ell+1} - \phi^{\ell})$$

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Diffusion Synthetic Acceleration (DSA)

- Multigroup diffusion equation for the error equation

$$-\boldsymbol{\nabla} \cdot (D_{C,g} \boldsymbol{\nabla}) f_g + \sigma_{t,g} f_g = \sum_{g'=1}^{G} \sigma_{s,g' \to g} f_{g'} + r_g \tag{9}$$

- $f = \boldsymbol{D}e$
- In operator notation

$$(\boldsymbol{L}_D + \boldsymbol{T} - \boldsymbol{S}) f = r \tag{10}$$

- Operators:
  - $(\boldsymbol{L}_D f)_g = -\boldsymbol{\nabla} \cdot (D_{C,g} \boldsymbol{\nabla}) f_g$
  - $(\boldsymbol{T} f)_g = \sigma_{t,g} f_g$

Fully-Coupled DSA (FCDSA)

$$\boxed{\phi^{\ell+1/2} = \boldsymbol{D}\boldsymbol{L}^{-1}\boldsymbol{M}\boldsymbol{S}\phi^{\ell} + b,}$$

$$\Downarrow$$

$$\boxed{r^{\ell+1/2} = \boldsymbol{S}(\phi^{\ell+1/2} - \phi^{\ell}),}$$

$$\Downarrow$$

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

$$\Downarrow$$

$$\boxed{\phi^{\ell+1} = \phi^{\ell+1/2} + f^{\ell+1/2}}$$

Decoupled DSA (DDSA)

$$\boxed{(\boldsymbol{L}_D + \boldsymbol{T} - \boldsymbol{S})f = r} \tag{11}$$

- Compute eigendecomposition

$$(\boldsymbol{T} - \boldsymbol{S}) = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1} \tag{12}$$

- Substitute with $z = \boldsymbol{Q}^{-1} f$

$$(\boldsymbol{L}_D + \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}) f^{\ell+1/2} = r^{\ell+1/2} \tag{13}$$

- Left-multiply by $\boldsymbol{Q}^{-1}$, assume commutivity with $\boldsymbol{L}_D$

(14)

- Iterative correction becomes

$$f^{\ell+1/2} = \boldsymbol{Q}(\boldsymbol{L}_D + \boldsymbol{\Lambda})^{-1}\boldsymbol{Q}^{-1} r^{\ell+1/2} \tag{15}$$

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$$(\boldsymbol{L}_D \boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{\Lambda}) z^{\ell+1/2} = r^{\ell+1/2} \tag{13}$$

- Left-multiply by $\boldsymbol{Q}^{-1}$, assume commutivity with $\boldsymbol{L}_D$

$$\boldsymbol{Q}^{-1}(\boldsymbol{L}_D \boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{\Lambda}) z^{\ell+1/2} = \boldsymbol{Q}^{-1} r^{\ell+1/2} \tag{14}$$

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Approximate & Grey DSA

- Approximate DSA (ADSA)

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

- Grey DSA (GDSA)

$$f^{\ell+1/2} = \xi(\hat{\boldsymbol{L}}_D + \hat{\sigma}_t - \hat{\sigma}_s)^{-1} \hat{r}^{\ell+1/2},$$
$$\boldsymbol{T}^{-1}\boldsymbol{S}\xi = \lambda\xi,$$
$$\hat{D}_C = \sum_{g=1}^{G} \frac{1}{3\sigma_{t,g}}\xi_g,\ \ \hat{\sigma}_t = \sum_{g=1}^{G} \sigma_{t,g}\xi_g,\ \ \hat{\sigma}_s = \sum_{g=1}^{G} (\boldsymbol{S}\xi)_g,\ \ \hat{r}^{\ell+1/2} = \sum_{g=1}^{G} r_g^{\ell+1/2}$$

Numerical Results

- We consider two 1D homogeneous test problems
  - C5G7 moderator cross sections (7-group problem)
  - Randomly generated cross sections (10-group problem)
  - 32 cm slab, S_8 Gauss-Legendre quadrature, 128 mesh cells
- Random cross section generation

$$\boldsymbol{S}_{i,j} = \sigma_{s,j\to i} = \frac{r_j c_{ij} \sigma_{t,j}}{\sum_i c_{ij}}$$

$$0.9 \le r_j \le 0.9999, \quad 0 \le c_{ij} \le 1, \quad 1.5 \le \sigma_{t,j} \le 2.5$$

Numerical Results

- C5G7 cross sections

DSA Method	Analysis	Numerical
NONE	0.98617	0.98559
FCDSA	0.21526	0.19551
ADSA	0.83849	0.83249
DDSA	0.33168	0.31738
GDSA	0.68367	0.67291

- Random 10-group cross sections

DSA Method	Analysis	Numerical
NONE	0.96258	0.96618
FCDSA	0.20976	0.18925
ADSA	0.91547	0.91455
DDSA	0.27598	0.25748
GDSA	0.54968	0.54890

Conclusion

- Spectral radii for new and existing diffusion-based synthetic acceleration methods were compared
- The new method, DDSA, uses a low-order diffusion equation that is decoupled in energy via an eigendecomposition
- It exhibits a spectral radius close to the best-case FCDSA method and smaller than GDSA and ADSA
- The DDSA low-order system is block-diagonal and can be solved one group at a time, time-to-solution could be much faster
- Especially true for large numbers of groups or if the low-order system is solved directly (especially for a parallel-decomposed mesh on large numbers of ranks)
- Future work
  - Consider computational efficiency for the methods on large-scale, MPI-parallel, highly-scattering problems with many groups
  - Compare solving the low-order all groups at once vs. solving one group (or some other number of groups) at a time
  - Consider retaining only an intermediate number of eigenmodes (even a single mode, which would closely resemble GDSA)
  - Investigate the impact of solving the low-order system iteratively vs. direct inversion (currently SuperLU)
  - Combine parallel mesh decomposition and decomposition by energy group