A Preconditioned Krylov Method for Thermal Radiation Transport Calculations

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Background

- Texas A&M University is developing a new multidisciplinary computational curriculum involving the Nuclear Engineering Department, the Computer Science Department, the Mathematics Department, and the Statistics Department.
- This curriculum will include numerical methods for multiphysics/multiscale computation, advanced programming techniques for massively parallel computation, uncertainty and error analysis for code verification and validation, and processes for large-scale multiphysics code development.
- Multiphysics coupling and multiphysics solution techniques are topics of great current interest.
- While we consider a Krylov method for thermal radiation transport today, our ultimate computational target is radiation-hydrodynamics, which combines fluid flow with thermal radiation transport, and is of fundamental importance in many high energy density physics applications.

Technical Motivation

- Thermal radiation transport is a critical component of multiphysics simulations for high energy density physics applications, and is extremely challenging from a numerical point of view.
- Cross sections strongly vary with material temperature and photon frequency.
- Problems often contain optically-thin, strongly absorbing, and highly diffusive regions.
- Diffusion-synthetic acceleration (DSA), and linear multifrequency-grey acceleration (LMFGA) are often used in thermal radiation transport calculations.
- It has recently been found that neither of these schemes is unconditionally effective.
- The deficiencies in these schemes can be essentially eliminated by recasting them as preconditioned Krylov methods.

Overview

- Krylov Solvers
- The Equations of Thermal Radiation Transport
- The Source Iteration Technique
- Diffusion-Synthetic Acceleration (DSA)
- Linear Multifrequency-Grey Acceleration (LMFGA)
- A Nested Preconditioned Krylov Method
- Final Comments

Krylov Solvers

- We consider Krylov solvers only from a blackbox point of view.
- To solve $\mathbf{A}\overrightarrow{x} = \overrightarrow{q}$, the solver is given the initial solution vector guess and the source vector.
- At each iteration step, the solver passes to the user some vector $\overrightarrow{z}$, and requires the user to pass back the vector $\overrightarrow{y} = \mathbf{A}\overrightarrow{x}$.
- It is important to recognize that $\mathbf{A}$ need never be formed. Only its action is needed.
- Convergence can be complicated to predict, but in general, a small condition number of the matrix (the ratio of the largest to smallest singular values) is desirable, and eigenvalues clustered in the complex plane are desirable .

The Equations of Thermal Radiation Transport

A Transport Equation for $I(\underline{r}, \underline{\Omega}, E, t)$:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \underline{\Omega} \cdot \underline{\nabla} I + \sigma_t I = \frac{1}{4\pi}\sigma_s \phi + \sigma_a B(T) \quad , \tag{1}$$

An equation for the *material temperature* $T(\underline{r}, t)$:

$$C_v \frac{\partial T}{\partial t} = \int_0^\infty \sigma_a [\, \phi - 4\pi B(T) \,] \, dE \quad , \tag{2}$$

where

- c is the speed of light,
- $\underline{\Omega}$ is the photon direction vector,
- $\sigma_t(\underline{r}, E, T)$ is the total macroscopic cross section,
- $\sigma_s(\underline{r}, E, T)$ is the macroscopic Thompson scattering cross section,

The Equations of Thermal Radiation Transport

- $\sigma_a(\underline{r}, E, T)$ is the macroscopic absorption cross section,
- $\phi(\underline{r}, E, t)$ is angular intensity integrated over all directions,
- $C_v(\underline{r}, T)$ is the *material heat capacity*,
- $B(E, T)$ is the *Planck function*:

$$B(E,T) = \frac{2E^3}{h^3c^2}\left[\exp\left(\frac{E}{kT}\right) - 1\right]^{-1} \quad , \tag{3}$$

- h is *Planck's constant*,
- k is *Boltzmann's constant*.

The Equations of Thermal Radiation Transport

- These equations are generally solved via Newton's method.
- After linearization, temporal discretization, and energy discretization, we obtain a temperature-independent transport equation:

$$\underline{\Omega} \cdot \underline{\nabla} I_g + \sigma^*_{\tau,g} I = \frac{1}{4\pi} \sigma^*_{s,g} \phi_g + \frac{1}{4\pi} \nu \chi_g \sum_{k=1}^{G} \sigma^*_{a,k} \phi_k \ + \xi_g \ , \quad g = 1, G, \tag{4}$$

- and an intensity-dependent temperature equation:

$$T = T^* + \frac{\sum_{g=1}^{G} \sigma^*_{a,g} \left[\phi_g - 4\pi B^*_g \right] + \frac{C^*_v}{\Delta t^k} \left(T^{k-\frac{1}{2}} - T^* \right)}{\frac{C^*_v}{\Delta t^k} + \sum_{g=1}^{G} \sigma^*_{a,g} 4\pi \frac{\partial B^*_g}{\partial T}} \ . \tag{5}$$

The Equations of Thermal Radiation Transport

- where

$$\sigma_\tau = \sigma_t + \tau \quad , \tag{6a}$$

$$\tau = \frac{1}{c\Delta t^k} \quad , \tag{6b}$$

$$\nu = \frac{\sum_{g=1}^{G} \sigma_{a,g}^* 4\pi \frac{\partial B_g^*}{\partial T}}{\frac{C_v^*}{\Delta t^k} + \sum_{g=1}^{G} \sigma_{a,g}^* 4\pi \frac{\partial B_g^*}{\partial T}} \quad , \tag{6c}$$

$$\chi_g = \frac{\sigma_{a,g}^* \frac{\partial B_g^*}{\partial T}}{\sum_{k=1}^{G} \sigma_{a,k}^* \frac{\partial B_k^*}{\partial T}} \quad , \tag{6d}$$

$$\xi_g = \sigma_{a,g}^* B_g^* + \tau \psi_g^{k-\frac{1}{2}} - \frac{1}{4\pi} \nu \chi_g \left[\sum_{k=1}^{G} \sigma_{a,k}^* 4\pi B_k^* + \frac{C_v^*}{\Delta t^k} \left(T^{k-\frac{1}{2}} - T^* \right) \right] \quad . \tag{6e}$$

Source Iteration

- The traditional method for solving the transport equation is a nested source iteration.
- Denoting the iteration index by ℓ, the inner iteration can be represented as follows:

$$\underline{\Omega} \cdot \underline{\nabla} I_g^{\ell+1} + \sigma_{\tau,g}^* I_g^{\ell+1} = \frac{1}{4\pi} \sigma_{s,g}^* \phi_g^{\ell} + \frac{1}{4\pi} \nu \chi_g \sum_{k=1}^{G} \sigma_{a,k}^* \phi_k \ + \xi_g \ , \quad (7)$$

- and the outer iteration can be represented as follows:

$$\underline{\Omega} \cdot \underline{\nabla} I_g^{\ell+1} + \sigma_{\tau,g}^* I_g^{\ell+1} - \frac{1}{4\pi} \sigma_{s,g}^* \phi_g^{\ell+1} = \frac{1}{4\pi} \nu \chi_g \sum_{k=1}^{G} \sigma_{a,k}^* \phi_k^{\ell} \ + \xi_g \ , \quad (8)$$

Source Iteration

- The operator $\underline{\Omega} \cdot \underline{\nabla} + \sigma^*_{\tau,g}$ involves no angular or energy coupling.
- When spatially discretized it takes on a block lower-triangular form with a block corresponding to the intensities within a single spatial cell for a single direction and energy.
- This operator is easily inverted using a “wavefront” or “sweep” algorithm.
- The attenuation of errors in ϕ_g determines the convergence rate of the inner iteration process.
- The attenuation of errors in $f = \sum_{g=1}^{G} \sigma^*_{a,g}\phi_g$ determines the convergence rate of the outer iteration process.

Source Iteration

- The inner iteration process can become arbitrarily slow to converge as $\sigma_{s,g}^{*} \rightarrow \sigma_{\tau,g}^{*}$.
- The outer iteration can become arbitrarily slow to converge as $\nu \rightarrow 1$ and $\tau \rightarrow 0$.
- For the case of an infinite homogeneous medium, Fourier analysis can be used to demonstrate that the most slowly converging error modes for both iterations are those that slowly vary in space.
- Thus performing a sweep is a form of relaxation: high-frequency errors are strongly attenuated, while low-frequency errors are poorly attenuated.

Diffusion-Synthetic Acceleration

- Inner source iteration with DSA takes the following form:

$$\underline{\Omega} \cdot \underline{\nabla} I_g^{\ell+\frac{1}{2}} + \sigma_{\tau,g}^* I_g^{\ell+\frac{1}{2}} = \frac{1}{4\pi}\sigma_{s,g}^* \phi_g^\ell + \frac{1}{4\pi}\nu\chi_g \sum_{k=1}^{G} \sigma_{a,k}^* \phi_k \; + \xi_g \quad , \tag{9a}$$

$$-\underline{\nabla} \cdot \frac{1}{3\sigma_{\tau,g}^*} \underline{\nabla} \delta\phi_g + \left(\sigma_{\tau,g}^* - \sigma_{s,g}^*\right) \delta\phi_g = \sigma_{s,g}^* \left(\phi_g^{\ell+\frac{1}{2}} - \phi_g^\ell\right) \quad , \tag{9b}$$

$$\phi_g^{\ell+1} = \phi_g^{\ell+\frac{1}{2}} + \delta\phi_g \quad . \tag{9c}$$

Diffusion-Synthetic Acceleration

- For the case of an infinite homogeneous medium, Fourier analysis can be used to demonstrate that this scheme completely attenuates the low-frequency error modes and grossly underestimates the high-frequency error modes.
- This is the best one can hope for in an approximate inverse.
- The scheme is unconditionally effective in 1-D and only becomes ineffective in strongly heterogeneous multidimensional problems.

Linear Multifrequency-Grey Acceleration

- Outer source iteration with LMFGA takes the following form:

$$\underline{\Omega} \cdot \underline{\nabla} I_g^{\ell+\frac{1}{2}} + \sigma_{\tau,g}^* I_g^{\ell+\frac{1}{2}} - \frac{1}{4\pi}\sigma_{s,g}^* \phi_g^{\ell+\frac{1}{2}} = \frac{1}{4\pi}\nu\chi_g f^{\ell} + \xi_g \ , \qquad \text{(10a)}$$

$$-\underline{\nabla} \cdot \langle D \rangle \underline{\nabla} \delta\Phi + \left[\langle \sigma_a \rangle (1-\nu) + \tau\right] \delta\Phi = f^{\ell+\frac{1}{2}} - f^{\ell} \ , \qquad \text{(10b)}$$

$$f^{\ell+1} = f^{\ell+\frac{1}{2}} + \langle \sigma_a \rangle \delta\Phi \qquad \text{(10c)}$$

Linear Multifrequency-Grey Acceleration

- where

$$\langle D \rangle = \sum_{g=1}^{G} \frac{\varsigma_g}{3\sigma^*_{\tau,g}} , \tag{11}$$

$$\langle \sigma_a \rangle = \sum_{g=1}^{G} \sigma^*_{a,g} \varsigma_g , \tag{12}$$

$$\varsigma_g = \frac{\frac{\chi_g}{\sigma^*_{\tau,g}}}{\sum_{k=1}^{G} \frac{\chi_k}{\sigma^*_{\tau,k}}} . \tag{13}$$

Linear Multifrequency-Grey Acceleration

- For the case of an infinite homogeneous medium, Fourier analysis can be used to demonstrate that this scheme completely attenuates the low-frequency error modes and grossly underestimates the high-frequency error modes.
- This is the best one can hope for in an approximate inverse.
- The scheme appears to be unconditionally effective in 1-D but can apparently become unstable in strongly heterogeneous multidimensional problems.

A Nested Preconditioned Krylov Method

- Our aim is to derive an equation for the absorption rate, f, from the equation for the intensity, I.
- For reasons explained shortly, the Krylov method will be used to solve a preconditioned variant of the equation for f.
- Once f is obtained, I can be obtained by solving G independent monoenergetic transport equations.
- We begin by expressing the transport equation in operator form:

$$\mathbf{A}_g I_g = \left[\frac{1}{4\pi} \nu \chi_g f + \xi_g \right] , \quad g = 1, G. \tag{14}$$

$$\mathbf{A}_g \equiv \underline{\Omega} \cdot \underline{\nabla} + \sigma^*_{\tau,g} - \frac{1}{4\pi} \sigma_{s,g} \mathbf{P} \ , \tag{15a}$$

$$\mathbf{P}\langle \cdot \rangle = \int_{4\pi} \langle \cdot \rangle \, d\Omega \tag{15b}$$

A Nested Preconditioned Krylov Method

- Solving the transport equation for I_g, we obtain

$$I_g = \mathbf{A}_g^{-1}\left[\frac{1}{4\pi}\nu\chi_g f + \mathbf{A}_g^{-1}\xi_g\right] \quad . \tag{16}$$

- Given f, this equation is solved via a preconditioned Krylov method to obtain I_g.
- Integrating the above equation over all directions, multiplying on the left by $\sigma_{a,g}^*$, and summing over all groups yields the desired equation for f:

$$\mathbf{B}f = \sum_{g=1}^{G}\sigma_{a,g}^*\mathbf{P}\mathbf{A}_g^{-1}\xi_g\,, \tag{17}$$

$$\mathbf{B} = \left[\mathbf{I} - \sum_{g=1}^{G}\sigma_{a,g}^*\mathbf{P}\mathbf{A}_g^{-1}\nu\chi_g\right]\,, \tag{18}$$

A Nested Preconditioned Krylov Method

- The action of $\mathbf{B}$ requires the solution of G independent one-group transport equations.
- These equations can be efficiently solved via a DSA-preconditioned Krylov method, yielding an overall Krylov method that is nested.
- However, it is not necessary use a preconditioned Krylov method to solve the one-group equations unless source iteration is inefficient.
- There are two advantages to solving the equation for f:
  - The rank of the f-equation is far less than that of the original transport equation - number of space points versus number of space points times number of energies times number of directions.
  - The transport operator is unbounded but $\mathbf{B}$ is compact with real eigenvalues between 0 and 1.

A Nested Preconditioned Krylov Method

- We left precondition the f equation with the operator $\mathbf{C}$:

$$\mathbf{CB}f = \mathbf{C}\sum_{g=1}^{G}\sigma_{a,g}^{*}\mathbf{PA}_{g}^{-1}\xi_{g}\,, \tag{19}$$

$$\mathbf{C} \equiv \left(\mathbf{I} + \langle\sigma_a\rangle\mathbf{H}^{-1}\nu\right)\,, \tag{20}$$

$$\mathbf{H} \equiv -\overrightarrow{\nabla}\cdot\langle D\rangle\overrightarrow{\nabla} + \left[\langle\sigma_a\rangle(1-\nu)+\tau\right]\,. \tag{21}$$

- Note that $\mathbf{H}$ is the diffusion operator from the LMFGA method.
- $\mathbf{C}$ is a very effective preconditioner.
- An infinite-medium Fourier analysis shows that $\mathbf{C}$ becomes the exact inverse of $\mathbf{B}$ when operating on eigenfunctions of $\mathbf{B}$ in the limit as the eigenvalue approaches zero.

A Nested Preconditioned Krylov Method

- We use an analogous strategy for developing a preconditioned Krylov method to solve the one-group equations:
  - We first derive an equation for ϕ_g that has a lower rank than the original monoenergetic transport equation.
  - The operator associated with this reduced-rank equation is compact with real eigenvalues between 0 and 1.
  - We use a Krylov method to solve a preconditioned variant of this equation.
  - The preconditioner contains the inverse of the diffusion operator associated with the DSA method, and is very effective because it moves the eigenvalues nearest zero to essentially one.
  - Once ϕ_g has been obtained, I_g can be obtained via a sweep for each direction and group.

A Nested Preconditioned Krylov Method

- The dominant effort required to apply the action of the overall preconditioned operator for f consists of:
  - The performance of a sweep for each direction and energy group, and the solution of a DSA diffusion equation for each energy group during each inner Krylov iteration.
  - A solution of the LMFGA diffusion equation.
- The diffusion equations themselves are solved via a precondioned Krylov method leading to a triple-nested Krylov method.
- If the diffusion solution technique is efficient, the transport solution technique will be efficient.

An Alternative Preconditioned Krylov Method

- The nested Krylov scheme we have derived is analogous to a nested source iteration with the inner iterations converged during each LMFG accelerated outer iteration.
- An alternative scheme can be developed that is analogous to a nested source iteration with one inner DSA iteration per group per LMFGA outer iteration.
- This scheme requires an equation for the multigroup scalar fluxes rather than the absorption rate and is thus of higher rank.
- However, the action of the preconditioned operator requires only a sweep for each direction and group, followed by DSA preconditioning, followed by LMFGA preconditioning.

An Alternative Preconditioned Krylov Method

- In particular, the preconditioned equation can be expressed as follows:

$$\left(\mathbf{I}+\mathbf{V}\mathbf{H}^{-1}\nu\mathbf{F}\right)\left(\mathbf{I}+\mathbf{D}^{-1}\mathbf{S}\right)\left[\mathbf{I}-\mathbf{P}\mathbf{L}^{-1}\left(\mathbf{S}+\nu\mathbf{X}\mathbf{F}\right)\right]\overrightarrow{\phi}=$$

$$\left(\mathbf{I}+\mathbf{V}\mathbf{H}^{-1}\nu\mathbf{F}\right)\left(\mathbf{I}+\mathbf{D}^{-1}\mathbf{S}\right)\mathbf{P}\mathbf{L}^{-1}\overrightarrow{\xi}\,.$$

- Fourier analysis can be used to show that these preconditioners move the eigenvalues of the basic operator that are closest to zero to essentially one.
- Thus it should be an effective scheme, but its efficiency relative to the nested scheme is not clear.
- Theory strongly suggests that the use of DSA-precontioning is critical to the effectiveness of this scheme.

Final Comments

- The nested preconditioned Krylov method has not yet been tested, but a multigroup diffusion variant has been tested and found to be highly effective.
- The strategy of obtaining a reduced-rank equation cannot be applied unless the interaction operators are low-rank.
- If the interaction operators are full rank, effective preconditioners may or may not be constructed from low-rank approximate inverses, depending upon the spectral properties of the interaction operators.
- For the case of thermal neutron transport with upscatter, an analog of the LMFGA method works very well because of the eigenvalue distribution of the thermal upscatter operator.
- Full-rank interaction terms sometimes require true multigrid preconditioners.
- This field of research is wide open and very rich.