Discrete-Ordinates Methods for Radiative Transfer in the Non-Relativistic Stellar Regime

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Overview

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The Equations of Radiative Transfer

The Basic Equations

A transport equation for the angular intensity, $I(t, \overrightarrow{r}, \overrightarrow{\Omega}, E)$:

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

and an equation for the material temperature, $T(t, \overrightarrow{r})$:

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

where c is the speed of light, σ_t is the total macroscopic cross section, σ_s is the Thompson macroscopic scattering cross section, ϕ is angular intensity integrated over all directions, C_v is the material heat capacity, and $B(E,T)$ is the Planck function:

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

The Equations of Radiative Transfer

Other Processes and Equations

- Compton Scattering
- Conduction
- Hydrodynamics

Operator Splitting

- All of these additional process and equations are treated via operator splitting.
- The hydrodynamics equations require material-motion corrections to the transport equation.

The Non-Linear Solution Strategy

- The basic equations are non-linear because of the temperature dependence of the material properties and the Planck function.
- The basic technique for solving these equations is a modified Newton's method.
- The Newton's method is modified in the sense that the contributions to the Jacobian from the material properties are neglected.
- This results in a type of hybrid Newton/Picard iteration.

The Linearized Equations

- The first step in the linearization process is to difference the transport and material temperature equations in time. For simplicity, we use backward-Euler differencing here, but Crank-Nicholson differencing or a second-order Gear method can also be used.
- The time-differenced equations are

$$\frac{1}{c\Delta t}(I^{n+1} - I^n) + \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I^{n+1} + \sigma_t^{n+1} I^{n+1} =$$

$$\frac{1}{4\pi}\left[\sigma_s^{n+1}\phi^{n+1} + \sigma_a^{n+1} B(T^{n+1})\right] \quad , \tag{4}$$

and

$$\frac{C_v^{n+1}}{\Delta t}(T^{n+1} - T^n) = \int_0^\infty \sigma_a^{n+1}[\ \phi^{n+1} - B(T^{n+1})\ ]\, dE \quad , \tag{5}$$

where n is the time index.

The Linearized Equations

- Let T^* denote the latest Newton iterate for the temperature.
- The linearized equations for the next Newton iteration are obtained by evaluating the material properties at T^* and linearly expanding the Planck function temperature dependence about T^*:

$$B^{n+1} = B^* + \frac{\partial B^*}{\partial T}\left(T^{n+1} - T^*\right) \quad , \tag{6}$$

  where a superscript "*" denotes a quantity evaluated at T^*.
- With the above expansion, the material temperature can be eliminated from the transport equation.
- Suppressing the temporal superscript "$n+1$", the linearized temporally-differenced transport equation can be expressed as follows.

The Linearized Equations

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I + \sigma_\tau^* I = \frac{1}{4\pi}\left[\sigma_s^* \phi + \nu\chi \int_0^\infty \sigma_a^*(E')\phi(E')\, dE'\right] + \xi \ , \quad (7)$$

$$\sigma_\tau = \sigma_t + \frac{1}{c\Delta t} \ , \quad (8a)$$

$$\nu = \frac{\int_0^\infty \sigma_a^*(E) 4\pi \frac{\partial B^*(E)}{\partial T}\, dE}{\frac{C_v^*}{\Delta t} + \int_0^\infty \sigma_a^*(E) 4\pi \frac{\partial B^*(E)}{\partial T}\, dE} \ , \quad (8b)$$

$$\chi(E) = \frac{\sigma_a^*(E)\frac{\partial B^*(E)}{\partial T}}{\int_0^\infty \sigma_a^*(E')\frac{\partial B^*(E')}{\partial T}\, dE'} \ , \quad (8c)$$

$$\xi = \sigma_a^* B^* + \frac{1}{c\Delta t} I^n - \frac{1}{4\pi}\nu\chi\left[\int_0^\infty \sigma_a^*(E') 4\pi B^*(E')\, dE' + \frac{C_v^*}{\Delta t}(T^n - T^*)\right] \ , \quad (8d)$$

The Linearized Equations

- The material temperature is calculated after the transport equation has been solved:

$$T^{n+1} = T^{*} + \frac{\int_0^\infty \Sigma_a^*(E)\left[\phi(E) - 4\pi B^*(E)\right]\, dE + \frac{C_v^*}{\Delta t}\left(T^n - T^*\right)}{\frac{C_v^*}{\Delta t} + \int_0^\infty \Sigma_a^*(E) 4\pi \frac{\partial B^*(E)}{\partial T}\, dE} \quad . \qquad (9)$$

- Note that the linearized transport equation takes the form of a steady-state neutron transport equation with within-group scattering only and fission.
- "σ_a" plays the role of the fission cross section.
- "ν", which is always less than one, plays the role of the number of neutrons per fission.
- "χ", plays the role of the fission spectrum.

Discretization of the Linearized Equations

Energy Discretization

- The multigroup method is used to discretize the equation in energy.

Angular Discretization

- The S_n method is used to discretize the equation in angle.

Discretization of the Linearized Equations

Spatial Discretization

- The requirements for spatial discretization are extremely challanging.
  - Resistance to negativities and strong damping of oscillations.
  - Asymptotic preserving with respect to the equilibrium-diffusion limit.
  - Good (if not accurate) behavior with unresolved boundary layers.
- Discontinuous methods are generally required to obtain the desired properties.
- Flux limiters can interact poorly with the solution process, so small negativities are tolerated.
- This requires special definitions for the material properties and the Planck function at negative temperatures to prevent the Newton method from breaking down.

Discretization of the Linearized Equations

Spatial Discretization

- Preservation of the equilibrium-diffusion limit is essential.
  - A formal asymptotic expansion for the analytic transport and temperature equations yields the equilbrium-diffusion approximation to leading order.
  - When such an expansion is applied to the discretized transport and temperature equations, one may or may not obtain a valid and robust discretization of the equilibrium-diffusion equation.
  - If so, the discretization is asymptotic-preserving and one can accurately zone in asymptotic regions in accordance with the spatial variation of the solution.
  - If not, the discretization is not asymptotic-preserving and one can obtain accurate results only if zone widths are small relative to a mean-free-path. Such zoning is generally prohibitively expensive.

Solution of the Linearized Transport Equation

Source Iteration

- The classic solution technique for the S_n equations is source iteration, which in its simplest form, can be expressed as follows:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I^{\ell+1} + \sigma_\tau^* I^{\ell+1} =$$

$$\frac{1}{4\pi}\left[\sigma_s^* \phi^\ell + \nu\chi \int_0^\infty \sigma_a^*(E')\phi^\ell(E')\, dE'\right] + \xi \quad , \tag{10}$$

$$\phi^{\ell+1} = \int_{4\pi} I^{\ell+1}(\overrightarrow{\Omega})\, d\Omega \quad , \tag{11}$$

  where ℓ is the iteration index.

- We have simplified the description here to avoid notational difficulties. The iteration on the scattering sources is actually nested within the iteration on the emission (fission) source.

Solution of the Linearized Transport Equation

Sweeps

- Note that all of the coupling between directions and energies occurs on the right side of Eq. (10). Thus the operator on the left side of Eq. (10) represents an independent operator for each direction and energy.
- After discretization of Eq. (10), the intensities for each direction and group usually can be ordered to achieve a block lower-triangular coefficient matrix with each block representing the unknowns associated with a single cell.
- Such systems are easily solved on a serial machine via a back-substitution process that begins where radiation enters the mesh, proceeds across the mesh in the direction of radiation flow, and ends where the radiation leaves the mesh.
- Thus the process of inverting the operator on the left side of Eq. (10) is referred to as a “sweep”.

Solution of the Linearized Transport Equation

Sweeps

- A block lower-triangular structure is not always achievable on meshes with curved cell faces. It is also possible for this to occur on any 3-D non-orthogonal mesh, but it is extremely rare if the cell faces are flat, e.g., tetrahedral meshes.
- Loss of the block lower-triangular structure greatly complicates matters, and efficiently dealing with this occurence remains an active research topic.
- Highly efficient and mature parallel sweep algorithms exist for rectangular meshes, but efficient parallel algorithms for unstructured meshes are just beginning to emerge. Unstructured-mesh sweep algorithms remains an active research topic.

Solution of the Linearized Transport Equation

Inner Source Iteration

- The inner source iteration can be expressed for group g as follows:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell_i+\frac{1}{2}} + \sigma^*_{\tau,g} I_g^{\ell_i+\frac{1}{2}} = \frac{1}{4\pi} \sigma^*_{s,g} \phi_g^{\ell_i} + Q_g \ , \tag{12}$$

$$\phi_g^{\ell_i+1} = \int_{4\pi} I_g^{\ell_i+\frac{1}{2}} \, d\Omega \ , \tag{13}$$

  where ℓ_i is the inner iteration index, and Q_g denotes the sum of the emission source and the effective fixed source for group g.

- Note that the emission source is fixed during the inner iterations.
- Note that the inner iterations are performed and converged for each group in sequence.

Solution of the Linearized Transport Equation

Outer Source Iteration

- The outer source iteration can be expressed with multigroup discretization as follows:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell_o+1} + \sigma_{\tau,g}^* I_g^{\ell_o+1} - \frac{1}{4\pi}\sigma_{s,g}^* \phi_g^{\ell_o+1} =$$

$$\frac{1}{4\pi}\nu\chi_g f^{\ell_o} + \xi \quad , g = 1, G, \tag{14}$$

$$f^{\ell_o+1} = \sum_{g=1}^{G} \sigma_{a,g}^* \phi_g^{\ell_o+1} \quad . \tag{15}$$

where ℓ_o is the outer iteration index, g is the multigroup index, G is the total number of groups, and f is the total radiation energy absorption rate.

- Note that the scattering sources carry an iteration index of $\ell_o + 1$, and thus have been converged via the inner iteration process.

Solution of the Linearized Transport Equation

Effectiveness of Source Iteration

- The spectral radius for the scattering source iterations is given by the scattering ratio, σ_s / σ_τ.
- The spectral radius for the emision source iterations is roughly given by ν.
- The scattering source iterations converge quite rapidly in typical calculations.
- With strong radiation-material coupling (large absorption cross section and small heat capacity), the emission source iterations can be prohibitively slow to converge.

Solution of the Linearized Transport Equation

Acceleration of Source Iterations

- There are two very effective techniques for accelerating the source iterations.
- The first is called diffusion-synthetic acceleration, and it is applied to the scattering source iterations.
- The second is called the linear multifrequency-grey method, and it is applied to the emission source iterations.
- Both methods are based upon the use of a diffusion approximation to accelerate the iterative convergence of the transport solution.
- Both methods are unconditionally effective and efficient in 1-D calculations, but in multidimensional calculations, their effectiveness can be degraded by severe spatial discontinuities in the cross sections.

Solution of the Linearized Transport Equation

Acceleration of Source Iterations

- The linear multifrequency-grey method takes the following form:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell_o+\frac{1}{2}} + \sigma_{\tau,g}^* I_g^{\ell_o+\frac{1}{2}} - \frac{1}{4\pi}\sigma_{s,g}^* \phi_g^{\ell_o \frac{1}{2}} = \frac{1}{4\pi}\nu\chi_g f^{\ell_o} + \xi \quad , g = 1, G, \tag{16}$$

$$-\overrightarrow{\nabla}\cdot\langle D\rangle \overrightarrow{\nabla}\mathcal{E}^{\ell_o+\frac{1}{2}} + \left[\frac{1}{c\Delta t} + \langle\sigma_a\rangle(1-\nu)\right]\mathcal{E}^{\ell_o+\frac{1}{2}} = \nu\left(f^{\ell_o+\frac{1}{2}} - f^{\ell}\right) \quad , \tag{17}$$

$$f^{\ell_o+1} = f^{\ell_o+\frac{1}{2}} + \langle\sigma_a\rangle\mathcal{E}^{\ell_o+\frac{1}{2}} \quad , \tag{18}$$

where "$\langle\cdot\rangle$" denotes a quantity that is energy-averaged with a specific weight function, and $\mathcal{E}$ is an estimate of the additive iterative error associated with the angle/energy-integrated intensity at the completion of step $\ell_o + \frac{1}{2}$.

Solution of the Linearized Transport Equation

Acceleration of Source Iterations

- Diffusion-synthetic acceleration takes the following form for group g:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell+\frac{1}{2}} + \sigma_{\tau,g}^* I_g^{\ell+\frac{1}{2}} = \frac{1}{4\pi}\sigma_{s,g}^* \phi_g^{\ell} + Q_g \quad , \tag{19}$$

$$-\overrightarrow{\nabla}\cdot D_g \overrightarrow{\nabla} \epsilon_g^{\ell+\frac{1}{2}} + (\sigma_{\tau_g}^* - \sigma_{s,g}^*)\epsilon_g^{\ell+\frac{1}{2}} = \sigma_{s,g}^*(\phi_g^{\ell+\frac{1}{2}} - \phi_g^{\ell}) \quad , \tag{20}$$

$$\phi_g^{\ell+1} = \phi_g^{\ell+\frac{1}{2}} + \epsilon_g^{\ell+\frac{1}{2}} \quad , \tag{21}$$

where ℓ denotes the scattering iteration index for group g, Q_g, denotes the emission and effective fixed source, and $\epsilon_g^{\ell+\frac{1}{2}}$ denotes an estimate for the additive intensity error associated with $\phi_g^{\ell+\frac{1}{2}}$.

Solution of the Linearized Transport Equation

Krylov Methods

- Krylov methods are iterative methods for solving a standard linear system of the following form:

$$\mathbf{A}\,\overrightarrow{x} = \overrightarrow{b} \quad , \tag{22}$$

  where $\mathbf{A}$ is an matrix, $\overrightarrow{x}$ is the solution vector, and $\overrightarrow{b}$ is the source vector.

- In general, the computational work required per iteration for a Krylov method is dominated by one or two matrix-vector multiplications carried out with the matrix, $\mathbf{A}$.

- Krylov methods are currently having an enormous impact upon our abilty to solve the S_n equations.

Solution of the Linearized Transport Equation

Krylov Methods

- One powerful advantage of Krylov methods is that the performance degradation that can occur in multidimensional calculations with the diffusion-synthetic and linear multifrequency-grey methods disappears when these acceleration schemes are recast as preconditioners.
- The implementation of preconditioned Krylov methods in existing S_n codes is surprisingly easy because the actual sequence of operations is nearly identical for both accelerated source iteration and a preconditioned Krylov method.
- Furthermore, new preconditioners that are simpler because they do not require the solution of a diffusion equation are now being developed that, when used in conjunction with a Krylov solver, result in a solution technique that is as robust as source iteration, but significantly more efficient.

Solution of the Linearized Transport Equation

Krylov Methods

- The optimal application of Krylov methods to transport is not necessarily obvious.
- For instance, let us consider the following simplified steady-state monoenergetic equation with isotropic scattering only:

$$\left(\mathbf{L} - \frac{\sigma_s}{4\pi}\mathbf{P}\right) I = Q \quad , \tag{23}$$

where $\mathbf{L}$ is the sweep operator:

$$\mathbf{L}I = \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I + \sigma_t I \quad , \tag{24}$$

and $\mathbf{P}$ is the angular integration operator:

$$\mathbf{P}I = \int_{4\pi} I \; d\Omega; \quad . \tag{25}$$

Solution of the Linearized Transport Equation

Krylov Methods

- Although one can use a Krylov method to solve Eq. (23), it is far more efficient to use a Krylov method to solve the following equation:

$$\left(\mathbf{I} - \mathbf{P}\mathbf{L}^{-1}\frac{\sigma_s}{4\pi}\right)\phi = \mathbf{P}\mathbf{L}^{-1}Q \quad . \tag{26}$$

- Note that Eq. (26) is obtained by applying $\mathbf{P}\mathbf{L}^{-1}$ to Eq. (23).
- Note that the unknowns for Eq. (26) are the angle-integrated intensities, while the unknowns for Eq. (23) are the angular intensities.
- Furthermore, the eigenvalues associated with Eq. (26) lie in a much smaller area of the complex than those associated with Eq. (26).
- Thus it is much more efficient to solve Eq. (26) with a Krylov method than Eq. (23).

Solution of the Linearized Transport Equation

Krylov Methods

- The preconditioner for Eq. (26) that is analogous to diffusion-synthetic acceleration is the operator , $\mathbf{H}$, where

$$\mathbf{H} = \left(\mathbf{I} + \mathbf{D}^{-1}\sigma_s\mathbf{I}\right) \quad , \tag{27}$$

and

$$\mathbf{D} \equiv -\overrightarrow{\nabla}\cdot\frac{1}{3\sigma_t}\overrightarrow{\nabla} + \sigma_a \quad . \tag{28}$$

Simplified Non-Relativistic Material-Motion Corrections

- For applications such as inertial-confinement fusion, material speeds remain significantly below the speed of light, e.g., $v/c < .01$.
- Although v/c is very small, failure to make any correction can result in a significant lack of energy conservation because the change in material kinetic energy due to radiation momentum deposition is not subtracted from the radiation energy field.
- Full corrections in both the Eulerian and co-moving frames significantly complicate the transport equation.
- We have defined a simple Eulerian-frame correction model that
  - conserves total (radiation plus material) energy,
  - preserves total momentum,
  - preserves the equilibrium-diffusion limit to O(v/c),
  - preserves equilibrium solutions for the angle-energy-integrated intensity and flux.

Simplified Non-Relativistic Material-Motion Corrections

- This approximation is only intended to be accurate in an angle-energy integrated sense. Differential spectral effects are not properly treated.
- The correction takes the form of a P_1-type source, in particular, the source for group g is

$$C_g(\overrightarrow{\Omega}) = \frac{1}{4\pi} C_g + \frac{3}{4\pi} \overrightarrow{C}_g \cdot \overrightarrow{\Omega} \quad , \tag{29}$$

where

$$C_g = -\frac{\sigma_{t,g}}{c} \overrightarrow{F}_{0,g} \cdot \overrightarrow{v} \quad , \tag{30}$$

$$\overrightarrow{C}_g = \frac{4}{3} \sigma_{t,g} \phi_g \frac{\overrightarrow{v}}{c} \quad . \tag{31}$$

and $\overrightarrow{F}_{0,g}$ is an approximation to the co-moving frame radiation flux:

$$\overrightarrow{F}_{0,g} = \overrightarrow{F}_g - \frac{4}{3} \phi_g \frac{\overrightarrow{v}}{c} \quad . \tag{32}$$

Simplified Non-Relativistic Material-Motion Corrections

- The radiation energy source for the material internal energy equation is

$$\mathcal{S}_e = \sum_{g=1}^{G} \left(\sigma_{a,g} \phi_g - B_g \right) \quad . \tag{33}$$

- The radiation momentum source for the material momentum equation is

$$\mathcal{S}_f = \sum_{g=1}^{G} \frac{\sigma_{t,g}}{c} \overrightarrow{F}_0 \quad . \tag{34}$$

- All material-motion correction terms are treated explicitly in time.