Accelerated Radiative Diffusion Problems

Original article: Synthetic Acceleration for Radiative Diffusion Calculations [1]

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1. Problem

The equations for radiative diffusion are

$$\frac{1}{c}\frac{\partial I}{\partial t} - \nabla \cdot D(\nu)\nabla I(\nu) + \rho\kappa(E)I(E) = \rho\kappa(\nu)\beta(\nu, T) \tag{1a}$$

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot K\nabla T - \nabla \mathbb{P} u + \rho \int_0^\infty \kappa(E') \left[I(E') - \beta(E', T)\right] dE' + Q, \tag{1b}$$

where Equation 1a is the radiative diffusion equation, where c is the speed of light, I is scalar intensity $I_\nu(x) = \int_{4\pi} I_\nu(x, \Omega) d\Omega = cE$, D is the radiative diffusion constant $(3\rho\kappa)^{-1}$, κ is specific opacity [cm^2/g], and β is the angle-integrated Planck function, $\beta_\nu(T) = \int_{4\pi} B_\nu(T) d\Omega$.

Equation 1b is the heat diffusion equation with radiation and hydrodynamic effects, where ρ is material density, C_v is material heat capacity, K is thermal conductivity, $\mathbb{P}$ is the fluid pressure tensor, u is fluid velocity, and Q is heat generation per unit mass.

The energy domain can be discretized using N_g energy groups $G_i = [\nu_i, \nu_{i+1}]$ such that $\nu_0 = 0$ and $\nu_{N_g+1} = \infty$. Using this discretization, and using $\varkappa = \rho\kappa$, the diffusion equations become

$$\frac{1}{c}\frac{\partial I_k}{\partial t} - \nabla \cdot D_k \nabla I_k + \varkappa_k I_k = \varkappa_k \beta_k(T) \tag{2a}$$

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot K\nabla T - \nabla \mathbb{P} u + \sum_{g=1}^{N_g} \varkappa_g \left[I_g - \beta_g(T)\right]' + Q, \tag{2b}$$

where

$$I_k = \int_{G_k} I(\nu) d\nu \tag{3a}$$

$$\beta_k = \int_{G_k} \beta(\nu, T) d\nu \tag{3b}$$

$$D_k \nabla I_k = \int_{G_k} D(\nu) \nabla I(\nu) d\nu \tag{3c}$$

$$\varkappa_k = \frac{\int_{G_k} [\beta(\nu) - I(\nu)] \varkappa(\nu) d\nu}{\int_{G_k} [\beta(\nu) - I(\nu)] d\nu}. \tag{3d}$$

Discretizing in time using Backward Euler (time index n), with lagged coefficients, Equation 1 becomes:

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t^n} - \nabla \cdot D_k^n \nabla I_k^{n+1} + \varkappa_k^n I_k^{n+1} = \varkappa_k^n \beta_k \left(T^{n+1} \right); \qquad k = 1 \ldots N_g \tag{4a}$$

$$\rho C_v^n \frac{T^{n+1} - T^n}{\Delta t^n} = \nabla \cdot K^n \nabla T^{n+1} - \nabla \mathbb{P} u + \sum_{g=1}^{N_g} \varkappa_g^n \left[I_g^{n+1} - \beta_g (T^{n+1}) \right] + Q^{n+1}. \tag{4b}$$

The time-advanced Planck function β is approximated using the first-order Taylor expansion $\beta(T^{n+1}) \approx \beta(T^n) + \frac{\partial \beta}{\partial T}(T^{n+1} - T^n)$, which leads to the system for T^{n+1} and I^{n+1},

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t^n} - \nabla \cdot D_k^n \nabla I_k^{n+1} + \varkappa_k^n I_k^{n+1} = \varkappa_k^n \left(\beta(T^n) + \frac{\partial \beta}{\partial T} \Delta T^{n+1} \right); \qquad k = 1 \ldots N_g \tag{5a}$$

$$\rho C_v^n \frac{\Delta T^{n+1}}{\Delta t^n} = \nabla \cdot K^n \nabla T^{n+1} - \nabla \mathbb{P} u + \sum_{g=1}^{N_g} \varkappa_g^n \left[I_g^{n+1} - \beta(T^n) - \frac{\partial \beta}{\partial T} \Delta T^{n+1} \right] + Q^{n+1}. \tag{5b}$$

Finally, the temperature operator is split into the hydrodynamic and radiative contributions,

$$\rho C_v^n \frac{\Delta T^{n+1}}{\Delta t^n} = \nabla \cdot K^n \nabla T^{n+1} - \nabla \mathbb{P} u + Q^{n+1} \tag{6a}$$

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t^n} - \nabla \cdot D_k^n \nabla I_k^{n+1} + \varkappa_k^n I_k^{n+1} = \varkappa_k^n \left(\beta(T^n) + \frac{\partial \beta}{\partial T} \Delta T^{n+1} \right); \qquad k = 1 \ldots N_g \tag{6b}$$

$$\rho C_v^n \frac{\Delta T^{n+1/2}}{\Delta t^n} = \sum_{g=1}^{N_g} \varkappa_g^n \left[I_g^{n+1} - \beta(T^n) - \frac{\partial \beta}{\partial T} \Delta T^{n+1/2} \right], \tag{6c}$$

where $T^{n+1} = T^n + \Delta T^{n+1/2} + \Delta T^{n+1}$. The indices $n+1/2$ and $n+1$ in this case refer to two separate contributions in the same time step, not temperature change at an intermediate time step.

Equation 6a can be immediately solved for temperature change,

$$\Delta T^{n+1/2} = \frac{\sum_{g=1}^{N_g} \varkappa_g \left[I_g^{n+1} - \beta_g^n \right] + Q}{\frac{\rho C_v^n}{\delta t^n} + \sum_{g=1}^{N_g} \varkappa_g \frac{\partial \beta}{\partial T}}, \tag{7}$$

which is then substituted into Equation 6b to give the radiative diffusion with implicit ΔT:

$$\frac{1}{c\Delta t^n} \left(I^{n+1} - I^n \right) - \nabla \cdot D_k^n \nabla I_k^{n+1} + \varkappa_k^n I_k^{n+1} = \eta \chi_k \sum_{g=1}^{N_g} \varkappa_g I_g^{n+1} + q_k \tag{8a}$$

where

$$\eta = \left[\sum_{g=1}^{N_g} \varkappa_g \frac{\partial \beta_g}{\partial T} \right] \cdot \left[\frac{\rho C_v}{\Delta t^n} + \sum_{g=1}^{N_g} \varkappa_g \frac{\partial \beta_g}{\partial T} \right]^{-1} \tag{8b}$$

$$\chi_k = \left[\varkappa_k \frac{\partial \beta_k}{\partial T} \right] \cdot \left[\sum_{g=1}^{N_g} \varkappa_g \frac{\partial \beta_g}{\partial T} \right]^{-1} \tag{8c}$$

$$q_k = \varkappa_k \beta_k + \eta \chi_k \left[Q - \sum_{g=1}^{N_g} \varkappa_g \frac{\partial \beta_g}{\partial T} \right]. \tag{8d}$$

Equation 8a is solved for intensity, then temperature change is recovered afterward. This can be rearranged to further resemble a steady-state neutron diffusion equation,

$$-\nabla \cdot D_k \nabla I_k^{n+1} + \left(\sigma_a + \sigma_{f,k} \right) I_k^{n+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^{n+1} + S_k \tag{9}$$

where

$$\sigma_a = \frac{1}{c\Delta t^n} \tag{10a}$$

$$\sigma_{f,k} = \varkappa_k \tag{10b}$$

$$S_k = q_k + \frac{I_k^n}{c\Delta t^n}. \tag{10c}$$

Here $\sigma_{f,k} = \varkappa_k$ acts as a fission cross section, where photons are re-emitted with the "fission" spectrum χ_k, with multiplicity η, and capture cross section σ_a. The physical interpretation is that photons may be lost to material absorption or streaming in time (from $\frac{d}{dt}$). Those photons absorbed in the material are either re-emitted in the same time step, or contribute to temperature gain in the material.

The intensity equation is solved using power iteration on the fission source. Starting from initial iterate $I_k^{(0)}$, the $l+1$ iterate for intensity at the $n+1$ time step is found by solving the linear system

$$-\nabla \cdot D_k \nabla I_k^{l+1} + (\sigma_a + \sigma_{f,k}) I_k^{l+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^l + S_k. \tag{11}$$

The full iterative algorithm is found in Algorithm 1.

Algorithm 1 Unaccelerated Iteration Algorithm

while $t^n \leq t^{end}$ **do**
  $n \leftarrow n + 1$
  Compute (lagged) temperature-dependent coefficients using $T|_{t=t^{n-1}}$
  while $\left\| I^{(l)} - I^{(l-1)} \right\| > \epsilon \left\| I^{(l-1)} \right\|$ **do**
    $l \leftarrow l + 1$
    $I_k^{(l+1/2)} \leftarrow$ Source iteration on $\eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^{n+1}$ (11)
  end while
  $I_k^n \leftarrow I_k^{(l+1)}$
  Recover $\Delta T^{n+1/2}$ from I_k^n (7)
  if $K \neq 0 \wedge u \neq 0$ **then**
    Solve thermal diffusion equation for ΔT^{n+1}
  end if
  $T^{n+1} \leftarrow T^n + \Delta T^{n+1/2} + \Delta T^{n+1}$
end while

1.1 Synthetic Acceleration Method

The equation for exact error of the lth iterate (Equation 11) is

$$-\nabla \cdot D_k \nabla \epsilon_k^l + (\sigma_a + \sigma_{f,k}) \epsilon_k^l = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} \left[\epsilon_g^l + I_g^l - I_g^{l-1} \right]. \tag{12}$$

At equilibrium, this becomes

$$(\sigma_a + \sigma_{f,k}) \epsilon_k^l = \eta \chi_k \sum_{g=1}^{N_G} \sigma_{f,g} \epsilon_g^l + \eta \chi_k \sum_{g=1}^{N_G} \sigma_{f,g} \left(I_g^l - I_g^{l-1} \right) \tag{13}$$

and the group spectrum of ϵ is

$$\frac{\epsilon_k^l}{E^l} = \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \tag{14}$$

where

$$E^l = \sum_{g=1}^{N_g} \epsilon_g^l \tag{15a}$$

$$\langle \sigma_t \rangle = \left[\sum_{g=1}^{N_g} \frac{\chi_g}{\sigma_{t,g}} \right]^{-1}. \tag{15b}$$

Then, all groups of Equation 12 are summed, using this spectrum, to get

$$-\nabla \cdot \left[\langle D \rangle \nabla E^l + \langle D' \rangle E^l \right] + E^l \left[\sigma_a + \langle \sigma_f \rangle (1 - \eta) \right] = \eta r^l \tag{16}$$

where

$$\langle D \rangle = \sum_{k=1}^{N_g} D_k \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \tag{17a}$$

$$\langle D' \rangle = \sum_{k=1}^{N_g} D_k \nabla \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \tag{17b}$$

$$\langle \sigma_f \rangle = \langle \sigma_t \rangle \sum_{g=1}^{N_g} \frac{\chi_g \sigma_{f,g}}{\sigma_{t,g}} \tag{17c}$$

$$r^{l+1/2} = \sum_{g=1}^{N_g} \sigma f, g \left(I_g^{l+1/2} - I_g^l \right). \tag{17d}$$

Then the spectrum from Equation 14 can be used to calculate the groupwise correction terms from the grey correction in Equation 16. The accelerated iterative scheme becomes

$$-\nabla \cdot D_k \nabla I_k^{l+1} + \left(\sigma_a + \sigma_{f,k} \right) I_k^{l+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^l + S_k \tag{18a}$$

$$-\nabla \cdot \left[\langle D \rangle \nabla E^{l+1/2} + \langle D' \rangle E^{l+1/2} \right] + E^{l+1/2} \left[\sigma_a + \langle \sigma_f \rangle (1 - \eta) \right] = \eta r^{l+1/2} \tag{18b}$$

$$I^{l+1} = I_k^{l+1} + E^{l+1/2} \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \tag{18c}$$

The accelerated iterative algorithm is displayed in Algorithm 2

Algorithm 2 Accelerated Iteration Algorithm

while $t^n \leq t^{end}$ **do**
  $n \leftarrow n+1$
  Compute (lagged) temperature-dependent coefficients using $T|_{t=t^{n-1}}$
  while $\left\|I^{(l)} - I^{(l-1)}\right\| > \epsilon \left\|I^{(l-1)}\right\|$ **do**
    $l \leftarrow l+1$
    $I_k^{(l+1/2)} \leftarrow$ Source iteration on $\eta\chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^{n+1}$, using (18a)
    $r^{(l+1/2)} \leftarrow \sum_{g=1}^{N_g} \sigma f, g \left(I_g^{l+1/2} - I_g^l\right)$
    $E^l \leftarrow$ Grey correction equation using (18b)
    $I_k^{(l)} \leftarrow I_k^{(l+1/2)} + E^{l+1/2} \frac{\langle\sigma_t\rangle\chi_k}{\sigma_{t,k}}$ using (18c)
  end while
  $I_k^n \leftarrow I_k^{(l+1)}$
  Recover $\Delta T^{n+1/2}$ from I_k^n
  if $K \neq 0 \wedge u \neq 0$ **then**
    Solve thermal diffusion equation for ΔT^{n+1}
  end if
  $T^{n+1} \leftarrow T^n + \Delta T^{n+1/2} + \Delta T^{n+1}$
end while

2. Numerical Implementation

2.1 LD Formulation

2.2 Unaccelerated Iteration

2.3 Accelerated Iteration

2.4 Fourier Analysis and Convergence

3. Tests

3.1 Fleck and Cummings Test

3.2 Test A1, nonzero boundary conditions

3.3 Test A2, one group

3.4 Fourier-informed tests

References

[1] J. E. Morel, E. W. Larsen, and M. Matzen, "A synthetic acceleration scheme for radiative diffusion calculations," *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 34, no. 3, pp. 243–261, 1985.