A Synthetic Acceleration Scheme for Raidative Diffusion Calculations [1]

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Outline

Radiative Diffusion Problem

Radiative Diffusion Equation:

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

$$\frac{1}{c}\frac{\partial I}{\partial t} - \nabla \cdot D(\nu) \nabla I(\nu) + \rho\kappa(E) I(E) = \rho\kappa(\nu)\beta(\nu, T), \tag{2}$$

$$I(E) = \int_{4\pi} I(E, \Omega) d\Omega = cE \tag{3}$$

$$\kappa(E) = \frac{\varkappa(E)}{\rho} \tag{4}$$

$$\beta(\nu, T) = \int_{4\pi} B_\nu(T) = \frac{8\pi h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \tag{5}$$

Standard iterative form derivation

Backward Euler, lagged coefficients:

$$\rho C_v^n \frac{T^{n+1} - T^n}{\Delta t^n} = \nabla \cdot K^n \nabla T^{n+1} - \nabla \mathbb{P} u + \rho \sum_{g=1}^{N_g} \kappa_g^n \left[I_g^{n+1} - \beta_g^{n+1}(T) \right] + Q^{n+1} \tag{6}$$

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t^n} - \nabla \cdot D_k^n \nabla I_k^{n+1} + \rho \kappa_k^n I_k^{n+1} = \rho \kappa_k^n \beta_k(T(t)); \qquad k = 1 \dots N_g. \tag{7}$$

Approximate using a first-order Taylor expansion, $\beta_k^{n+1} \approx \beta_k^n + \frac{\partial \beta_k^n}{\partial T} \Delta T^{n+1}$, and apply operator splitting:

$$\rho C_v^n \frac{\Delta T^{n+1/2}}{\Delta t^n} = \rho \sum_{g=1}^{N_g} \kappa_g^n \left[I_g^{n+1} - \left(\beta_k^n + \frac{\partial \beta_k^n}{\partial T} \Delta T^{n+1} \right) \right] + Q^{n+1} \tag{8}$$

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t^n} - \nabla \cdot D_k^n \nabla I_k^{n+1} + \rho \kappa_k^n I_k^{n+1} = \rho \kappa_k^n \left(\beta_k^n + \frac{\partial \beta_k^n}{\partial T} \Delta T^{n+1} \right); \qquad k = 1 \dots N_g \tag{9}$$

$$\rho C_v^n \frac{\Delta T^{n+1}}{\Delta t^n} = \nabla \cdot K^n \nabla T^{n+1} - \nabla \cdot \mathbb{P} u \tag{10}$$

Standard iterative form

Solving for $DeltaT^{n+1/2}$,

$$\Delta T^{n+1/2} = \left[\sum_{g=1}^{N_g} \kappa_g^n \left(I_g^{n+1} - \beta_k^n\right) + \frac{Q^{n+1}}{\rho}\right] \cdot \left[\frac{C_v^n}{\Delta t^n} + \sum_{g=1}^{N_g} \kappa_g^n \frac{\partial \beta_g^n}{\partial T}\right]^{-1} \tag{11}$$

Standard iterative form derivation

Radiative diffusion with expanded ΔT^{n+1} becomes:

$$\frac{1}{c\Delta t^n}\left(I^{n+1} - I^n\right) - \nabla\cdot D_k^n \nabla I_k^{n+1} + \rho\kappa_k^n I_k^{n+1} = \eta\chi_k \sum_{g=1}^{N_g} \rho\kappa_g I_g^{n+1} + q_k \qquad (12)$$

where

$$\eta = \left[\sum_{g=1}^{N_g} \kappa_g \frac{\partial\beta_g}{\partial T}\right] \cdot \left[\frac{C_v}{\Delta t^n} + \sum_{g=1}^{N_g} \kappa_g \frac{\partial\beta_g}{\partial T}\right]^{-1} \qquad \text{(re-emitted within time step)}$$

$$\chi_k = \left[\kappa_k \frac{\partial\beta_k}{\partial T}\right] \cdot \left[\sum_{g=1}^{N_g} \kappa_g \frac{\partial\beta_g}{\partial T}\right]^{-1} \qquad \text{(re-emission spectrum)}$$

$$q_k = \rho\kappa_k\beta_k + \eta\chi_k \left[Q - \sum_{g=1}^{N_g} \rho\kappa_g \frac{\partial\beta_g}{\partial T}\right] \qquad \text{(local source)}$$

Standard iterative form derivation, compact form

Rewrite Eq. 13 using neutron transport terms

$$-\nabla \cdot D_k \nabla I_k^{n+1} + \left(\sigma_a + \sigma_{f,k}\right) I_k^{n+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^{n+1} + S_k \tag{14a}$$

$$\Delta T^{n+1/2} = \left[\sum_{g=1}^{N_g} \kappa_g^n \left(I_g^{n+1} - \beta_k^n\right) + \frac{Q^{n+1}}{\rho}\right] \cdot \left[\frac{C_v^n}{\Delta t^n} + \sum_{g=1}^{N_g} \kappa_g^n \frac{\partial \beta_g^n}{\partial T}\right]^{-1} \tag{14b}$$

where

$$\sigma_a = \frac{1}{c\Delta t^n} \tag{15a}$$

$$\sigma_{f,k} = \rho \kappa_k \tag{15b}$$

$$S_k = q_k + \frac{I_k^n}{c\Delta t^n} \tag{15c}$$

Algorithm

while $t^j \leq t^{end}$ **do**

$j \leftarrow j + 1$

Compute (lagged) temperature-dependent coefficients using $T|_{t=t^{j-1}}$

while $\left\| I^{(s)} - I^{(s-1)} \right\| > \epsilon \left\| I^{(s-1)} \right\|$ **do**

$s \leftarrow s + 1$

Solve multigroup neutron-like diffusion equation for $I_k^{(s+1/2)}$, using $\eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^{n+1}$ for the reemission source

end while

$I_k^j \leftarrow I_k^{(s+1)}$

Recover $\Delta T^{j+1/2}$ from I_k^j

if $K \neq 0 \wedge u \neq 0$ **then**

Solve thermal diffusion equation for ΔT^{j+1}

end if

$T^{j+1} \leftarrow T^j + \Delta T^{j+1/2} + \Delta T^{j+1}$

end while

Standard iteration is slow

S_k and σ_a are both small compared to $\sigma_{f,k}$

Achievements of study

- Scheme is Linear
- Characterized well by Fourier Analysis (similar to nonlinear method which had not been characterized, at a similar computational cost)
    - Multifrequency Grey Method: frequency spectra of each iterate is used to form a one-group LO equation
- Reduced Fourier mode spectral radius from ~ 1 to ~ 0.6
- Low computational cost per iteration

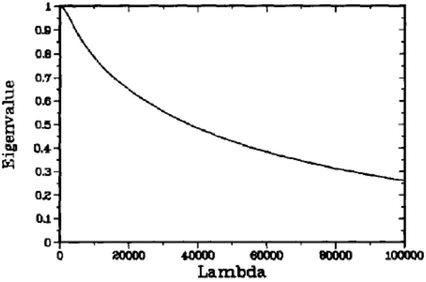


Fig. 1. Plot of unaccelerated eigenvalues for an infinite time-step.

Fourier Analysis of Unaccelerated Scheme

Using $I_k(x) = I_k e^{i\lambda x}$,

$$I_k^{l+1}\left[D_k\lambda^2 + \sigma_a + \sigma_{f,k}\right] = \eta\chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^l + S_k \tag{16}$$

which leads to

$$\omega(\lambda) = \eta \sum_{k=1}^{N_g} \frac{\sigma_{f,k}\chi_k}{\lambda^2 D_k + \sigma_a + \sigma_{f,k}} \qquad \text{spr} = \omega(0) = \eta \sum_{k=1}^{N_g} \frac{\sigma_{f,k}\chi_k}{\sigma_a + \sigma_{f,k}}. \tag{17}$$

Notably, $\lambda = 0$ (the slowest-converging eigenvalue) corresponds with the equilibrium solution, $\nabla D \nabla I = 0$

Correction term at equilibrium

Exact equation for error, $I_k = I_k^l + \epsilon_k^l$

$$\left(\sigma_a + \sigma_{f,k}\right)\epsilon_k^l = \eta\chi_k \sum_{g=1}^{N_G} \sigma_{f,g}\epsilon_g^l + \eta\chi_k \sum_{g=1}^{N_G} \sigma_{f,g}\left(I_g^l - I_g^{l-1}\right) \tag{18}$$

Summing over all groups for $E = \sum_k \epsilon$ yields

$$\frac{\epsilon_k^l}{E^l} = \frac{\langle\sigma_t\rangle\chi_k}{\sigma_{t,k}} \tag{19}$$

Spectrum of ϵ

This is the spectrum of ϵ_k^l, not I_k^l – that approximation is used for the multifrequency grey approximation

One-group equation

Equation for iterative error

$$-\nabla \cdot D_k \nabla \epsilon_k^l + (\sigma_a + \sigma_{f,k})\, \epsilon_k^l = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} \left[\epsilon_g^l + I_g^l - I_g^{l-1}\right] \tag{20}$$

plug in equilibrium spectrum, sum over all groups to get

$$-\nabla \cdot D_k \nabla E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} + (\sigma_a + \sigma_{f,k})\, E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \eta \chi_k r^l + \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \tag{21}$$

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

where

$$\langle D' \rangle = \sum_{k=1}^{N_g} D_k \nabla \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}}. \tag{22}$$

Accelerated Algorithm

The accelerated algorithm is:

while $t^j \le t^{end}$ **do**
  $j \leftarrow j+1$
  Compute temperature-dependent coefficients using $T|_{t=t^{j-1}}$
  while $\left\| I^{(s)} - I^{(s-1)} \right\| > \epsilon \left\| I^{(s-1)} \right\|$ **do**
    $s \leftarrow s+1$
    Solve multigroup diffusion equation for $I_k^{(s+1/2)}$, using $I_k^{(s)}$ for the reemission source
    Compute $r^{(s+1/2)}$
    Solve one-group error diffusion equation for $E^{(s+1/2)}$
    Compute $I_k^{(s+1)} = I_k^{(s+1/2)} + E^{(s+1/2)} \langle \sigma_t \rangle \chi_k / \sigma_{t,k}$
  end while
  $I_k^j \leftarrow I_k^{(s+1)}$
  Compute $\Delta T^{j+1/2}$ from I_k^j
  $T^{j+1} \leftarrow T^j + \Delta T^{j+1/2} + \Delta T^{j+1}$
end while

Results

Fourier eigenvalues:

$$\omega_u(\lambda) = \eta \sum_{k=1}^{N_g} \frac{\sigma_{f,k}\chi_k}{\lambda^2 D_k + \sigma_a + \sigma_{f,k}} \tag{23}$$

$$\omega_a(\lambda) = \omega_u(\lambda) + \langle\sigma_f\rangle \frac{\omega_u(\lambda) - 1}{\langle D\rangle\lambda^2 + \sigma_a + (1-\eta)\langle\sigma_f\rangle} \tag{24}$$

- ω_a is strictly $< \omega_u$
- $\omega_a(0) = 0$
- Spectral radius of the accelerated algorithm is always < 1

Numerical Results from [1]

Test problem:

- 200 μm iron slab with uniform heat generation source
- 1eV initial temperature, 140 eV equilibrium temperature
- Finite differencing scheme (Fourier Analysis was performed)

Table 3. A computational comparison of the unaccelerated and accelerated algorithms.

Iteration Method	Number of Cells	Total Iterations
Unaccelerated	10	4357
Accelerated	10	361
Unaccelerated	100	4368
Accelerated	100	560

Numerical Results from [1]

Continuous equations, finite time-step and heat capacity

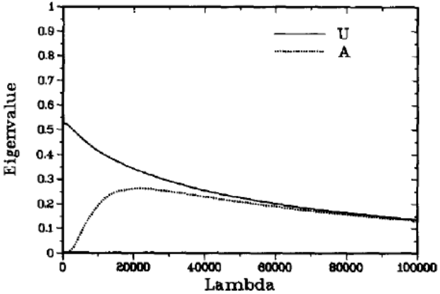


Fig. 3. Comparison of unaccelerated and accelerated eigenvalues for a finite time-step and a non-zero heat capacity.

Numerical Results

Discretized equations, infinite time-step and optically-thick cells (one-half period)

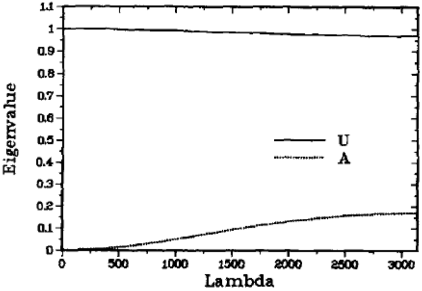
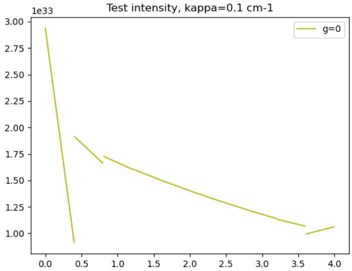


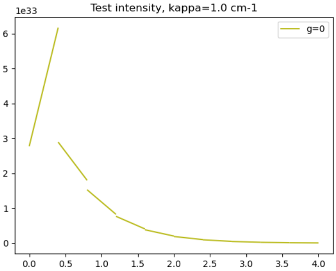
Fig. 5. Comparison of unaccelerated and accelerated eigenvalues for an infinite time-step and optically-thick cells (discrete spatial treatment).

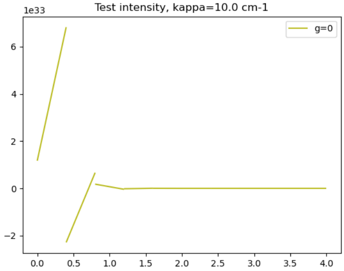
Status of LD-FEM implementation

- Test cases (using manufactured opacities, etc) demonstrate that interior cell behavior is likely correct
- Boundary cells seem to be the issue– reverse derivative, blowing up values
- At large opacity, solutions blow up nonphysically
- Temperature updates are good but oscillatory– possibly expected

Sample of results







References I

[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.