

Synthetic Acceleration for Radiative Diffusion Calculations

Notes on Morel, Larsen, Matzen 1985 [1]

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Section 1 Radiative Diffusion Equations

The radiative diffusion equations are:

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

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

where t is time, \vec{r} is position, $E = h\nu$ is photon energy, C_v is material specific heat, K is thermal conductivity, \mathbb{P} is the pressure tensor (from both material and radiation pressure), u is material velocity, κ is specific absorption opacity in units of [area/mass], ρ is material density, D is the photon diffusion coefficient, T is material temperature, $I(\vec{r}, E) = \int d\Omega I(x, \Omega, E)$ is photon intensity in units of [energy/area · time], and Q is material energy source.

Integrating Equation 1 and Equation 2 over N_g energy groups yields the multigroup radiative diffusion equations:

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot K \nabla T - \nabla \mathbb{P} u + \rho \sum_{g=1}^{N_g} \kappa_g [I_g - \beta_g(T)] + Q \quad (3)$$

$$\frac{1}{c} \frac{\partial I_k}{\partial t} - \nabla \cdot D_k \nabla I_k + \rho \kappa_k I_k = \rho \kappa_k \beta_k(T); \quad k = 1 \dots N_g \quad (4)$$

where

$$\int_k \cdot dE = \int_{E_k}^{E_{k+1}} \cdot dE \quad (5a)$$

$$I_k = \int_k I(E) dE \quad (5b)$$

$$\beta_k(T) = \int_k \beta(E, T) dE \quad (5c)$$

$$D_k \nabla I_k = \int_k D(E) \nabla I(E) dE \quad (5d)$$

$$\kappa_k = \frac{\int_g \kappa(E) [\beta(E) - I(E)] dE}{\int_g [\beta(E) - I(E)] dE} \quad (5e)$$

where the multigroup equations are only exact if the E -spectrum is known exactly within each energy group, though the approximation is close to exact when the number of energy groups is high. Rosseland- or Planck-weighted group constants are used to approximate the spectrum. Pressure \mathbb{P} , material velocity \vec{u} , thermal conductivity K , and density ρ are taken to be known exactly, since they come from hydrodynamic equations.

Discretizing in time with Backward Euler and using lagged opacity, thermal conductivity, diffusion coefficient, and heat capacity:

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

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

Then, the time advancement of β can be approximated 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 the temperature operator is split into two parts— radiative/inhomogenous source and thermal conductivity/pressure. The linearized, time-discretized equations are:

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

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

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

Where $\Delta T^{n+1/2}$ is an intermediate value for the temperature at t^{n+1} , not at an intermediate time step, and $T^{n+1/2} = T^n + \Delta T^{n+1/2}$ and $T^{n+1} = T^{n+1/2} + \Delta T^{n+1}$. $\Delta T^{n+1/2}$ can be easily evaluated algebraically from Equation 8:

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

Evaluating Equation 9 using Equation 11 yields

$$\frac{1}{c\Delta t^n} (I^{n+1} - I^n) - \nabla \cdot D_k^n \nabla I_k^{n+1} + \rho \kappa_k^n I_k^{n+1} = \dots \text{TODO} \quad (12)$$

which reduces to the final form of the multigroup diffusion equation,

$$\frac{1}{c\Delta t^n} (I^{n+1} - I^n) - \nabla \cdot D_k^n \nabla I_k^{n+1} + \rho \kappa_k^n I_k^{n+1} = \eta \chi_k \rho \sum_{g=1}^{N_g} \kappa_g I_g^{n+1} + q_k \quad (13)$$

where

$$\eta = \left[\sum_{g=1}^{N_g} \kappa_g \frac{\partial \beta_g}{\partial T} \right] \cdot \left[\frac{C_v}{\Delta t^n} + \sum_{g=1}^{N_g} \kappa_g \frac{\partial \beta_g}{\partial T} \right]^{-1} \quad (14a)$$

$$\chi_k = \left[\kappa_k \frac{\partial \beta_k}{\partial T} \right] \cdot \left[\sum_{g=1}^{N_g} \kappa_g \frac{\partial \beta_g}{\partial T} \right]^{-1} \quad (14b)$$

$$q_k = \rho \kappa_k \beta_k + \eta \chi_k \left[Q - \rho \sum_{g=1}^{N_g} \kappa_g \frac{\partial \beta_g}{\partial T} \right] \quad (14c)$$

Equation 13 resembles the steady-state neutron diffusion equation, which can be made clear by further rearranging the terms:

$$-\nabla \cdot D_k \nabla I_k^{n+1} + (\sigma_a + \sigma_{f,k}) I_k^{n+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^{n+1} + S_k \quad (15)$$

where

$$\sigma_a = \frac{1}{c\Delta t^n} \quad (16a)$$

$$\sigma_{f,k} = \rho \kappa_k \quad (16b)$$

$$S_k = q_k + \frac{I_k^n}{c\Delta t^n} \quad (16c)$$

with “fission” and “absorption” cross sections, and fission emission spectrum χ_k . The fission term will be known as the reemission term.

1(a) Iterative solution Equation 15 can be solved by source iteration, starting from some initial guess $I_k^{(0)}$ and using to compute the next iterate $I^{(1)}$, or using each iterate I_k^l to compute I_k^{l+1} . Suppressing the $n + 1$ index, the iterative equation is

$$-\nabla \cdot D_k \nabla I_k^{l+1} + (\sigma_a + \sigma_{f,k}) I_k^{l+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^l + S_k \quad (17)$$

Section 2 Acceleration Scheme

The iterative method described in subsection 1(a) can be written in operator notation as the solution to the linear system

$$\mathcal{M}x = y, \quad (18)$$

where the exact solution is denoted as x^* . The solution is solved iteratively by splitting the operator $\mathcal{M} = \mathcal{A} - \mathcal{B}$, and \mathcal{A} is easily inverted. The iterative method is then

$$\mathcal{A}x^{l+1} = \mathcal{B}x^l + y \quad (19)$$

$$x^{l+1} = \mathcal{A}^{-1} \mathcal{B}x^l + \mathcal{A}^{-1}y. \quad (20)$$

For the radiative diffusion equation (Equation 15), \mathcal{A} is the streaming and absorption operator, and \mathcal{B} is the reemission (“fission”) source. The error of the $(l + 1)$ th iterate is

$$\epsilon^{l+1} = x^* - x^{l+1} \quad (21)$$

Then the exact solution can be found from the $(l + 1)$ th iterate using

$$\mathcal{B}x^l + y = \mathcal{A}x^{l+1} \quad (22a)$$

$$y = \mathcal{A}x^{l+1} - \mathcal{B}x^l \quad (22b)$$

$$\mathcal{M}x^* = \mathcal{A}x^{l+1} - \mathcal{B}x^l \quad (22c)$$

$$x^* = \mathcal{M}^{-1} (\mathcal{A}x^{l+1} - \mathcal{B}x^l) \quad (22d)$$

$$= \mathcal{M}^{-1} (\mathcal{A}x^{l+1} - \mathcal{B}x^{l+1} + \mathcal{B}x^{l+1} - \mathcal{B}x^l) \quad (22e)$$

$$= \mathcal{M}^{-1} (\mathcal{M}x^{l+1} + \mathcal{B}(x^{l+1} - x^l)) \quad (22f)$$

$$x^* = x^{l+1} + \mathcal{M}^{-1} \mathcal{B}(x^{l+1} - x^l) = x^{l+1} + \epsilon^{l+1} \quad (22g)$$

The iteration can be accelerated by evaluating Equation 22g using an approximation $\mathcal{W} \approx \mathcal{M}$, which can be more easily inverted. Here \mathcal{M} is called the high-order operator, and \mathcal{W} is the low-order operator.

The accelerated iteration scheme is

$$x^{l+1/2} = \mathcal{A}^{-1} \mathcal{B} x^l + \mathcal{A}^{-1} y \quad (23)$$

$$x^{l+1} = x^{l+1/2} + \mathcal{W}^{-1} \mathcal{B} (x^{l+1/2} - x^l) \quad (24)$$

when solving the radiative diffusion equation, the high-order operator \mathcal{M} is the system of multigroup diffusion equations. The accelerated scheme presented in [1] uses a one-group diffusion operator as the low-order operator \mathcal{W} .

Fourier analysis of the high-order equation shows that the slowest-converging mode is $\omega(\lambda = 0)$, or

$$\omega_{\max} = \omega(0) = \eta \sum_{g=1}^{N_g} \frac{\chi_g \sigma_{f,g}}{\sigma_a + \sigma_{f,g}} \quad (25)$$

Where ω_{\max} approaches 1 as the Δt^n is increased. For small time steps, $\omega_{\max} \approx \eta$, which approaches unity for strongly coupled problems, where C_v is small or κ is large.

The most effective acceleration schemes should approximate the high-order equations accurately about $\lambda = 0$. This solution corresponds with an equilibrium solution, which will be the focus of the low-order equation. section 3 details the derivation of this result.

The multigroup equation for the error of the l th iterate of Equation 17 is

$$-\nabla \cdot D_k \nabla \epsilon_k^l + (\sigma_a + \sigma_{f,k}) \epsilon_k^l = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} [\epsilon_g^l + I_g^l - I_g^{l-1}] ; k = 1, 2, \dots, N_g \quad (26)$$

In the equilibrium limit, where the gradient term becomes zero, this equation becomes

$$(\sigma_a + \sigma_{f,k}) \epsilon_k^l = \eta \chi_k \sum_{g=1}^{N_G} \sigma_{f,g} \epsilon_g^l + \eta \chi_k \sum_{g=1}^{N_G} \sigma_{f,g} (I_g^l - I_g^{l-1}) \quad (27)$$

$$\sigma_{t,k} \epsilon_k^l = \eta \chi_k (\xi^l + r^l) \quad (28)$$

$$\epsilon_k^l = \frac{\eta \chi_k}{\sigma_{t,k}} (\xi^l + r^l) \quad (29)$$

where

$$\sigma_{t,k} = \sigma_a + \sigma_{f,k} \quad (30)$$

$$r^l = \sum_{g=1}^{N_G} \sigma_{f,g} (I_g^l - I_g^{l-1}) \quad (31)$$

$$\xi^l = \sum_{g=1}^{N_G} \sigma_{f,g} \epsilon_g^l \quad (32)$$

then, to solve for ξ^i , Equation 29 is multiplied by $\sigma_{f,k}$ and summed over all k :

$$\sum_{k=1}^{N_g} \sigma_{f,k} \epsilon_k^l = \sum_{k=1}^{N_g} \sigma_{f,k} \frac{\eta \chi_k}{\sigma_{t,k}} (\xi^l + r^l) \quad (33)$$

$$\xi^l = \eta (\xi^l + r^l) \sum_{k=1}^{N_g} \frac{\chi_k \sigma_{f,k}}{\sigma_{t,k}} \quad (34)$$

$$\xi^l = \eta (\xi^l + r^l) \frac{\langle \sigma_f \rangle}{\langle \sigma_t \rangle} \quad (35)$$

where

$$\langle \sigma_f \rangle = \langle \sigma_t \rangle \sum_{g=1}^{N_g} \frac{\chi_g \sigma_{f,g}}{\sigma_{t,g}} \quad (36)$$

$$\langle \sigma_t \rangle = \left[\sum_{g=1}^{N_g} \frac{\chi_g}{\sigma_{t,g}} \right]^{-1} \quad (37)$$

then Equation 35 can be solved for ξ^l ,

$$\xi^l = \eta (\xi^l + r^l) \frac{\langle \sigma_f \rangle}{\langle \sigma_t \rangle} \quad (38a)$$

$$\frac{\xi^l \langle \sigma_t \rangle}{\eta \langle \sigma_f \rangle} = (\xi^l + r^l) \quad (38b)$$

$$\xi^l = \frac{r^l}{\frac{\langle \sigma_t \rangle}{\eta \langle \sigma_f \rangle} - 1} \quad (38c)$$

$$\xi^l = \frac{\eta \langle \sigma_f \rangle r^l}{\langle \sigma_t \rangle - \eta \langle \sigma_f \rangle} \quad (38d)$$

yielding the final equilibrium solution of the l th iterate error,

$$\epsilon_k^l = \frac{\eta \chi_k}{\sigma_{t,k}} (\xi^l + r^l) \quad (39a)$$

$$\sigma_{t,k} = \sigma_a + \sigma_{f,k} \quad (39b)$$

$$r^l = \sum_{g=1}^{N_G} \sigma_{f,g} (I_g^l - I_g^{l-1}) \quad (39c)$$

$$\xi^l = \frac{\eta \langle \sigma_f \rangle r^l}{\langle \sigma_t \rangle - \eta \langle \sigma_f \rangle} \quad (39d)$$

$$\langle \sigma_f \rangle = \langle \sigma_t \rangle \sum_{g=1}^{N_g} \frac{\chi_g \sigma_{f,g}}{\sigma_{t,g}} \quad (39e)$$

$$\langle \sigma_t \rangle = \left[\sum_{g=1}^{N_g} \frac{\chi_g}{\sigma_{t,g}} \right]^{-1} \quad (39f)$$

Then the spectral shape (normalized) of this solution, where $E^l = \sum_{g=1}^{N_g} \epsilon_k^l$, is

$$\frac{\epsilon_k^l}{E^l} = \frac{\frac{\eta \chi_k}{\sigma_{t,k}} (\xi^l + r^l)}{\sum_{g=1}^{N_g} \frac{\eta \chi_g}{\sigma_{t,g}} (\xi^l + r^l)} \quad (40a)$$

$$= \frac{\cancel{\eta (\xi^l + r^l)} \frac{\chi_k}{\sigma_{t,k}}}{\cancel{\eta (\xi^l + r^l)} \sum_{g=1}^{N_g} \frac{\chi_g}{\sigma_{t,g}}} \quad (40b)$$

$$= \frac{\frac{\chi_k}{\sigma_{t,k}}}{\sum_{g=1}^{N_g} \frac{\chi_g}{\sigma_{t,g}}} \quad (40c)$$

$$\frac{\epsilon_k^l}{E^l} = \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}}. \quad (40d)$$

Which is exact as the time step Δt approaches infinity (in the equilibrium limit), and is equivalent to the spectral shape used to evaluate Rosseland group opacities. Then, evaluating Equation 26 using the assumed spectral shape,

$$-\nabla \cdot D_k \nabla E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} + (\sigma_a + \sigma_{f,k}) E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \eta \chi_k r^l + \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}}. \quad (41)$$

Expanding the diffusion term using the product rule,

$$\begin{aligned}
& -\nabla \cdot \left[D_k \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \nabla E^l + D_k E^l \nabla \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \right] + (\sigma_a + \sigma_{f,k}) E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \\
& \eta \chi_k r^l + \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}}. \quad (42)
\end{aligned}$$

Summing over all groups,

$$\begin{aligned}
& -\nabla \cdot \left[\left(\sum_{k=1}^{N_g} D_k \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \right) \nabla E^l + E^l \left(\sum_{k=1}^{N_g} D_k \nabla \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \right) \right] + E^l \sum_{k=1}^{N_g} (\sigma_a + \sigma_{f,k}) \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \\
& \eta r^l + \sum_{k=1}^{N_g} \eta E^l \chi_k \langle \sigma_t \rangle \sum_{g=1}^{N_g} \sigma_{f,g} \frac{\chi_g}{\sigma_{t,g}} \quad (43)
\end{aligned}$$

$$\begin{aligned}
& -\nabla \cdot \left[\left(\sum_{k=1}^{N_g} D_k \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \right) \nabla E^l + E^l \left(\sum_{k=1}^{N_g} D_k \nabla \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \right) \right] + E^l \sum_{k=1}^{N_g} (\sigma_a + \sigma_{f,k}) \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \\
& \eta r^l + \eta E^l \langle \sigma_f \rangle, \quad (44)
\end{aligned}$$

which can be written as

$$-\nabla \cdot [\langle D \rangle \nabla E^l + \langle D' \rangle E^l] + E^l \sum_{k=1}^{N_g} (\sigma_a + \sigma_{f,k}) \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \eta r^l + \eta E^l \langle \sigma_f \rangle, \quad (45)$$

where

$$\langle D \rangle = \sum_{k=1}^{N_g} D_k \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \quad (46a)$$

$$\langle D' \rangle = \sum_{k=1}^{N_g} D_k \nabla \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}}. \quad (46b)$$

Expanding the removal term,

$$E^l \sum_{k=1}^{N_g} (\sigma_a + \sigma_{f,k}) \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} = \sigma_a \sum_{k=1}^{N_g} E^l \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} + \sum_{k=1}^{N_g} E^l \frac{\langle \sigma_t \rangle \chi_k \sigma_{f,k}}{\sigma_{t,k}} \quad (47a)$$

$$= \sigma_a E^l + \langle \sigma_f \rangle E^l, \quad (47b)$$

so the one-group error diffusion equation becomes

$$-\nabla \cdot [\langle D \rangle \nabla E^l + \langle D' \rangle E^l] + E^l (\sigma_a + \langle \sigma_f \rangle) = \eta r^l + \eta E^l \langle \sigma_f \rangle \quad (48)$$

$$-\nabla \cdot [\langle D \rangle \nabla E^l + \langle D' \rangle E^l] + E^l [\sigma_a + \langle \sigma_f \rangle (1 - \eta)] = \eta r^l. \quad (49)$$

This provides an equation for the one-group iterative error of a diffusion iteration, which can be used to calculate group errors using Equation 40d. Then the set of equations for the accelerated radiative diffusion equation becomes:

$$-\nabla \cdot D_k \nabla I_k^{l+1} + (\sigma_a + \sigma_{f,k}) I_k^{l+1} = \eta \chi_k \sum_{g=1}^{N_g} \sigma_{f,g} I_g^l + S_k \quad (50)$$

$$-\nabla \cdot [\langle D \rangle \nabla E^{l+1/2} + \langle D' \rangle E^{l+1/2}] + E^{l+1/2} [\sigma_a + \langle \sigma_f \rangle (1 - \eta)] = \eta r^{l+1/2} \quad (51)$$

$$I^{l+1} = I_k^{l+1} + E^{l+1/2} \frac{\langle \sigma_t \rangle \chi_k}{\sigma_{t,k}} \quad (52)$$

where

$$r^{l+1/2} = \sum_{g=1}^{N_g} \sigma_{f,g} (I_g^{l+1/2} - I_g^l). \quad (53)$$

The full algorithm for the time-dependent problem then becomes:

Section 3 Fourier Analysis

[2]

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.
- [2] J. A. Fleck Jr and J. Cummings Jr, “An implicit monte carlo scheme for calculating time and frequency dependent nonlinear radiation transport,” *Journal of Computational Physics*, vol. 8, no. 3, pp. 313–342, 1971.

Algorithm 1 Morel, Larsen, Matzen Diffusion Acceleration Scheme [1]

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while  $t^j \leq t^{end}$  do
   $j \leftarrow j + 1$ 
  Compute temperature-dependent coefficients using  $T|_{t=t^{j-1}}$ 
  while  $\|I^{(s)} - I^{(s-1)}\| > \epsilon \|I^{(s-1)}\|$  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  $I_k^j$ 
  if  $K \neq 0 \wedge u \neq 0$  then
    Solve thermal diffusion equation for  $\Delta T^{j+1}$ 
  end if
   $T^{j+1} \leftarrow T^j + \Delta T^{j+1/2} + \Delta T^{j+1}$ 
end while

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