NE 795
Fall 2020

Computational Project

Contents

---

1 The Thermal Radiative Transfer (TRT) Problem

Create a computer code for solving the radiative transfer (RT) equation in 1D slab geometry

$$\frac{1}{c}\frac{\partial I_\nu(x,\mu,\nu,t)}{\partial t} + \mu\frac{\partial I_\nu(x,\mu,\nu,t)}{\partial x} + \varkappa_\nu(T)I_\nu(x,\mu,\nu,t) = \varkappa_\nu(T)B_\nu(T)\,, \tag{1}$$

$$0 \le x \le X\,, \quad -1 \le \mu \le 1\,, \quad 0 \le \nu < \infty\,, \quad t \ge t_0\,,$$

$$I_\nu|_{x=0} = I_\nu^{in+}\,, \quad \text{for } \mu > 0\,, \quad t \ge t_0\,, \tag{2}$$

$$I_\nu|_{x=X} = I_\nu^{in-}\,, \quad \text{for } \mu < 0\,, \quad t \ge t_0\,, \tag{3}$$

$$I_\nu|_{t=t_0} = I_\nu^0\,, \tag{4}$$

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

coupled with the material energy balance (MEB) equation

$$\frac{\partial \varepsilon}{\partial t} = \int_0^\infty \int_{-1}^1 \varkappa_\nu\Big(I_\nu - B_\nu\Big)d\mu d\nu\,, \tag{6}$$

$$\varepsilon = \varepsilon(T)\,, \tag{7}$$

$$T(x,t)|_{t=t_0} = T^0(x)\,, \quad \text{for } 0 \le x \le X\,. \tag{8}$$

2 Numerical Method for Solving the TRT Problem

- Solve this problem in multigroup approximation.
- Use the multilevel QD method and apply
  - the backward Euler temporal discretization for the RT, low-order QD and EB equations,
  - the step characteristics scheme for spatial discretization of the RT equation,
  - the finite volume scheme for discretization of the low-order QD equations.
- Detailed description of the discretization schemes for the multilevel QD method is presented in Appendix 6.2.

3 Fleck-Cummings Test

Solve a Fleck-Cummings test problem [1]. Consider the slab with $X = 4$ cm. The opacity is defined by

$$\varkappa_\nu(T) = \frac{\varkappa_0}{\nu^3}\left(1 - e^{-\frac{\nu}{T}}\right), \tag{9}$$

where $\varkappa_0 = 27$ [1]. At the left boundary there is incoming radiation with the black-body spectrum

$$I_\nu|_{x=0} = B_\nu(T_b) \quad \mu > 0\,, \tag{10}$$

where $T_b = 1$ keV. The right boundary is vacuum

$$I_\nu|_{x=X} = 0 \quad \text{for} \quad \mu < 0\,. \tag{11}$$

The initial distribution of radiation in the domain at $t = 0$ is given by

$$I_\nu|_{t=0} = B_\nu(T_0)\,, \tag{12}$$

where $T_0 = 1$ eV. The specific heat is given by

$$c_v = 0.5917 a_R (T_b)^3\,. \tag{13}$$

Use (i) uniform spatial mesh with $\Delta x = 0.4$ cm, (ii) double S_4 GL quadrature set, (iii) constant time step $\Delta t = 2 \times 10^{-3}$ sh (1 shake = 10^{-8} sec), and (iv) 17 groups ($N_g = 17$) shown in Table 1.

4 Report

In your report you need to present

1. detailed description of the computational method implemented in your code,
2. the algorithm flowchart,
3. Graphs and tables of the obtained numerical solution, namely, $T(x,t^*)$, $E(x,t^*)$, $F(x,t^*)$, $T_{rad}(x,t^*)$ for the set of moments $t^* = \{2\times10^{-3}sh, 2\times10^{-2}sh, 5\times10^{-2}sh, 1\times10^{-1}sh, 2\times10^{-1}sh, 3\times10^{-1}sh\}$ (plot each of these functions at different moments of time on the same graph to demonstrate wave-like behavior of the solution).

Table 1: The right boundaries of energy groups

g	ν_g [eV]
1	1.9047
2	3.6278
3	6.9097
4	13.161
5	25.067
6	47.744
7	90.937
8	173.21
9	329.90
10	628.35
11	1196.8
12	2279.5
13	4341.7
14	8269.5
15	15751.
16	3×10^4
17	1×10^{10}

4. Graphs and tables of energy spectrum $E_g(x,t)$ at the following moments of time $t = \{2\times 10^{-2}sh, 5\times10^{-2}sh, 3\times10^{-1}sh\}$ (plot all group energy densities at a particular moment of time as functions of space on one graph).

5. Comparison with the IMC results published in [1] (See the course website for the data based on the result shown in [1]).

6. A short instruction on how to run your code so that someone can run your code to get your results.

5 Submission

Submit online

1. an electronic copy of your report,

2. full functional version of your code with necessary input files for the test.

6 Appendix

6.1 Units and Constants

The basic units are

- distance x: $[cm]$,
- time t: $[sec]$,
- energy: $[erg]$,
- temperature T: $[^\circ K]$ $[eV]$,
- mass m: $[g]$.

Thus we have

- photon number density $n(\mathbf{x}, \mathbf{\Omega}, \nu, t)$ $\left[\frac{\#}{cm^3\ Hz\ ster}\right]$
- specific intensity $I_\nu(\mathbf{x}, \mathbf{\Omega}, \nu, t) = ch\nu n(\mathbf{x}, \mathbf{\Omega}, \nu, t)$ $\left[\frac{erg}{cm^2\ sec\ Hz\ ster}\right]$,
- monochromatic radiation energy density $E_\nu = E_\nu(\mathbf{x}, \nu, t) = \frac{1}{c}\int_{4\pi} I_\nu d\mathbf{\Omega}$ $\left[\frac{erg}{cm^3\ Hz}\right]$,
- monochromatic radiation flux $\mathbf{F}_\nu = \mathbf{F}_\nu(\mathbf{x}, \nu, t) = \int_{4\pi} \mathbf{\Omega} I_\nu d\mathbf{\Omega}$ $\left[\frac{erg}{cm^2\ sec\ Hz}\right]$,
- speed c: $\left[\frac{cm}{sec}\right]$,
- group specific intensity $I_g(\mathbf{x}, \mathbf{\Omega}, t) = \int_{\nu_g}^{\nu_{g+1}} I_\nu(\mathbf{x}, \mathbf{\Omega}, \nu, t) d\nu$ $\left[\frac{erg}{cm^2 \cdot sec \cdot ster}\right]$,
- group radiation energy density $E_g(\mathbf{x}, t) = \int_{\nu_g}^{\nu_{g+1}} E_\nu(\mathbf{x}, \nu, t) d\nu$ $\left[\frac{erg}{cm^3}\right]$,
- group radiation flux $\mathbf{F}_g(\mathbf{x}, t) = \int_{\nu_g}^{\nu_{g+1}} \mathbf{F}_\nu(\mathbf{x}, \nu, t) d\nu$ $\left[\frac{erg}{cm^3\ sec}\right]$,
- opacity $\varkappa_\nu$ $[cm^{-1}]$,
- material density ρ: $\left[\frac{g}{cm^3}\right]$.

Note that

- 1 eV = 1.6021892×10^{-19} J
- 1 erg = 6.24150934×10^{11} eV
- $k = 8.61735\times 10^{-5}\frac{eV}{^\circ K} = 1.38\times10^{-16}\ \frac{erg}{^\circ K}$
- $c = 2.99792458\times10^{10}\ \frac{cm}{s}$
- $h = 6.62613\times10^{-27}$ erg $\cdot$ s
- $\sigma_R = \frac{2\pi^5 k^4}{15c^2h^3} = 5.67\times10^{-5}\frac{erg}{cm^2\ s\ (^\circ K)^4}$

6.2 Discretization schemes

6.2.1 Temporal Discretization of the MLQD Method

We use fully implicit method applying the backward Euler scheme. The equations in this semi-continuous form at the time level $t = t^n$ are given by

- the high-order RT equations for the group intensity $I_g^n = I_g(x, \mu, t^n)$

$$\frac{1}{c\Delta t^n}\Big(I_g^n - I_g^{n-1}\Big) + \mu \frac{\partial I_g^n}{\partial x} + \varkappa_{E,g}^n I_g^n = \varkappa_{B,g}^n B_g^n \,, \tag{14a}$$

  where $\Delta t^n = t^n - t^{n-1}$, $\varkappa_{E,g}^n = \varkappa_{E,g}(T^n)$, $\varkappa_{B,g}^n = \varkappa_{B,g}(T^n)$, $B_g^n = B_g(T^n)$, $T^n = T(x, t^n)$,

- the multigroup LOQD (MLOQD) equations for the group energy densities $E_g^n = E_g(x, t^n)$ and fluxes $F_g^n = F_g(x, t^n)$

$$\frac{1}{\Delta t^n}\Big(E_g^n - E_g^{n-1}\Big) + \frac{\partial F_g^n}{\partial x} + c\varkappa_{E,g}^n E_g^n = 2\varkappa_{B,g}^n B_g^n \,, \tag{14b}$$

$$\frac{1}{c\Delta t^n}\Big(F_g^n - F_g^{n-1}\Big) + c\frac{\partial f_g^n E_g^n}{\partial x} + \tilde{\varkappa}_{R,g}^n F_g^n = 0 \,, \tag{14c}$$

  where $\tilde{\varkappa}_{R,g}^n = \tilde{\varkappa}_{R,g}(T^n)$,

$$f_g^n = \frac{\displaystyle\int_{-1}^{1} \mu^2 I_g^n d\mu}{\displaystyle\int_{-1}^{1} I_g^n d\mu} \,, \tag{14d}$$

- the grey LOQD (GLOQD) equations for the total energy density $E^n = E(x, t^n)$ and flux $F^n = F(x, t^n)$ coupled to the energy balance equation for T^n

$$\frac{1}{\Delta t^n}\Big(E^n - E^{n-1}\Big) + \frac{\partial F^n}{\partial x} + c\bar{\varkappa}_E^n E^n = c\bar{\varkappa}_B^n a_R (T^n)^4 \,, \tag{14e}$$

$$\frac{1}{c\Delta t^n}\Big(F^n - F^{n-1}\Big) + c\frac{\partial \bar{f}^n E^n}{\partial x} + \bar{\varkappa}_R^n F^n + \bar{\eta}^n E^n = 0 \,, \tag{14f}$$

$$\frac{c_v}{\Delta t^n}\Big(T^n - T^{n-1}\Big) = c\Big(\bar{\varkappa}_E^n E^n - \bar{\varkappa}_B^n a_R (T^n)^4\Big) \,, \tag{14g}$$

  where

$$\bar{f}^n = \frac{\sum_{g=1}^G f_g^n E_g^n}{\sum_{g=1}^G E_g^n} \,, \tag{14h}$$

$$\bar{\varkappa}_E^n = \frac{\sum_{g=1}^G \varkappa_{E,g}^n E_g^n}{\sum_{g=1}^G E_g^n} \,, \quad \bar{\varkappa}_B^n = \frac{\sum_{g=1}^G \varkappa_{B,g}^n B_g^n}{\sum_{g=1}^G B_g^n} \,, \tag{14i}$$

$$\bar{\varkappa}_R^n = \left(\frac{\sum_{g=1}^G \frac{1}{\tilde{\varkappa}_{R,g}^n} f_g^n E_g^n}{\sum_{g=1}^G f_g^n E_g^n} \right)^{-1} \,, \quad \bar{\eta}^n = \frac{\sum_{g=1}^G (\tilde{\varkappa}_{R,g}^n - \bar{\varkappa}_R^n) F_g^n}{\sum_{g=1}^G E_g^n} \,. \tag{14j}$$

6.2.2 Spatial Discretization of the MLQD Method

We now discretize the equations of the MLQD method in space. The spatial mesh with N_x intervals is given by

$$0 = x_{1/2} < \ldots < x_{j+1/2} < \ldots < x_{N_x+1/2} = X \,. \tag{15}$$

The multigroup RT equation for the given direction μ_m is approximated with the method of step characteristics

$$\frac{\Delta x_j}{c\Delta t^n}\Big(I^n_{g,m,j} - I^{n-1}_{g,m,j}\Big) + \mu_m\Big(I^n_{g,m,j+1/2} - I^n_{g,m,j-1/2}\Big) + \varkappa^n_{E,g,j}\Delta x_j I^n_{g,m,j} = \varkappa^n_{B,g,j}\Delta x_j B^n_{g,j}\,, \tag{16a}$$

$$I^n_{g,m,j} = \gamma^n_{g,m,j} I^n_{g,m,j-1/2} + (1-\gamma^n_{g,m,j}) I^n_{g,m,j+1/2}\,, \tag{16b}$$

$$\gamma^n_{g,m,j} = \frac{1}{\tau^n_{g,m,j}} - \frac{1}{e^{\tau^n_{g,m,j}}-1}\,, \quad \tau^n_{g,m,j} = \frac{\Delta x_j}{\mu_m}\Big(\varkappa^n_{E,g,j} + \frac{1}{c\Delta t^n}\Big)\,, \tag{16c}$$

$$\Delta x_j = x_{j+1/2} - x_{j-1/2}\,. \tag{16d}$$

$$j = 1,\ldots,N_x\,, m = 1,\ldots,M\,.$$

Here j is the index of spatial cells. Integer $\pm\frac{1}{2}$ subscripts refer to cell-edge quantities, and integer subscripts refer to cell-average quantities. The MLOQD equations are approximated by means of a finite volume method. The discretized equations have the following form:

$$\frac{\Delta x_j}{\Delta t^n}\Big(E^n_{g,j} - E^{n-1}_{g,j}\Big) + F^n_{g,j+1/2} - F^n_{g,j-1/2} + c\varkappa^n_{E,g,j}\Delta x_j E^n_{g,j} = 2\varkappa^n_{B,g,j}\Delta x_j B^n_{g,j}\,, \tag{17}$$

$$j = 1,\ldots,N_x\,,$$

$$\frac{\Delta x_{j+1/2}}{c\Delta t^n}\Big(F^n_{g,j+1/2} - F^{n-1}_{g,j+1/2}\Big) + c\Big(f^n_{g,j+1}E^n_{g,j+1} - f^n_{g,j}E^n_{g,j}\Big) + \tilde{\varkappa}^n_{R,g,j+1/2}\Delta x_{j+1/2}F^n_{g,j+1/2} = 0\,, \tag{18}$$

$$j = 0,\ldots,N_x\,,$$

$$f^n_{g,j} = \frac{\sum_{m=1}^M \mu_m^2 I^n_{g,m,j} w_m}{\sum_{m=1}^M I^n_{g,m,j} w_m}\,, \tag{19}$$

$$\tilde{\varkappa}^n_{R,g,j+1/2} = \frac{\tilde{\varkappa}^n_{R,g,j}\Delta x_j + \tilde{\varkappa}^n_{R,g,j+1}\Delta x_{j+1}}{\Delta x_j + \Delta x_{j+1}}\,. \tag{20}$$

Here, $E^n_{g,0} = E^n_g(x_{1/2})$ and $E^n_{g,N_x+1} = E^n_g(x_{N_x+1/2})$. To formulate the scheme for the GLOQD equations, we sum Eq. (17) and define the averaged opacities to derive the grey balance equation in the jth cell

$$\frac{\Delta x_j}{\Delta t^n}\Big(E^n_j - E^{n-1}_j\Big) + F^n_{j+1/2} - F^n_{j-1/2} + c\bar{\varkappa}^n_{E,j}\Delta x_j E^n_j = c\bar{\varkappa}^n_{B,j}\Delta x_j a_R\big(T^n_j\big)^4\,,\ j = 1,\ldots,N_x\,. \tag{21}$$

Then we divide Eq. (18) by $\varkappa^n_{g,j+1/2}$ and sum the resulting equations over groups. We define

$$\bar{\varkappa}^{-,n}_{R,j+1/2} = \left(\frac{\sum_{g=1}^G \frac{f^n_{g,j}E^n_{g,j}}{\tilde{\varkappa}^n_{R,g,j+1/2}+\frac{1}{c\Delta t^n}}}{\sum_{g=1}^G f^n_{g,j}E^n_{g,j}}\right)^{-1}\,, \quad \bar{\varkappa}^{+,n}_{R,j+1/2} = \left(\frac{\sum_{g=1}^G \frac{f^n_{g,j+1}E^n_{g,j+1}}{\tilde{\varkappa}^n_{R,g,j+1/2}+\frac{1}{c\Delta t^n}}}{\sum_{g=1}^G f^n_{g,j+1}E^n_{g,j+1}}\right)^{-1}\,, \tag{22}$$

$$\bar{f}_j^n = \frac{\sum_{g=1}^{G} f_{g,j}^n E_{g,j}^n}{\sum_{g=1}^{G} E_{g,j}^n}\,, \tag{23}$$

$$P_{j+1/2}^n = \sum_{g=1}^{G} \frac{F_{g,j+1/2}^{n-1}}{c\Delta t^n \bar{\varkappa}_{R,g,j+1/2}^n} \tag{24}$$

to obtain the discrete grey first-moment equation

$$c\left(\frac{\bar{f}_{j+1}^n E_{j+1}^n}{\bar{\varkappa}_{R,j+1/2}^{+,n}} - \frac{\bar{f}_j^n E_j^n}{\bar{\varkappa}_{R,j+1/2}^{-,n}}\right) + \Delta x_{j+1/2} F_{j+1/2}^n = \Delta x_{j+1/2} P_{j+1/2}^n\,,\ j = 0, \ldots, N_x\,, \tag{25}$$

where, $E_0^n = E^n(x_{1/2})$ and $E_{N_x+1}^n = E^n(x_{N_x+1/2})$. The discretized grey MEB (GMEB) equation is given by

$$\frac{c_v}{\Delta t^n}\left(T_j^n - T_j^{n-1}\right) = c\left(\bar{\varkappa}_{E,j}^n E_j^n - \bar{\varkappa}_{B,j}^n a_R (T_j^n)^4\right). \tag{26}$$

6.2.3 Iteration Algorithm

The iterations process is shown in Algorithm 1.

6.3 Auxiliary and Optional Tests

To develop your code and verify implementation of your method I recommend you to solve some auxiliary test problems.

Test A1. It is similar to the given test but there are differences in boundary and initial conditions. Incoming radiation at the left boundary

$$I_\nu|_{x=0} = B_\nu(T^*) \quad \mu > 0\,, \tag{27}$$

incoming radiation at the right boundary

$$I_\nu|_{x=4} = B_\nu(T^*) \quad \mu < 0\,, \tag{28}$$

initial conditions

$$I_\nu|_{t=0} = B_\nu(T^*)\,. \tag{29}$$

In this case the solution of the problem is the following:
$T(x,t) = T^*$, $E_g(x,t) = \frac{4\pi B_g(T^*)}{c}$, $F_g = 0$. Use $T^* = 1\ eV, 10^2\ eV, 10^3\ eV$.

Test A2. It is the given test but with just one group ($\nu_0 = 0$, $\nu_1 = \infty$). As a results you solve a one-group (grey) problem with simple analytic form of opacities and Planck source. In this problem one has

$$B_1(T) = \frac{1}{\pi}\sigma_R T^4\,, \tag{30}$$

$$\varkappa_{B,1} = \frac{\varkappa^*}{T^3}\,, \tag{31}$$

where $\varkappa^*$ is some constant that can be calculated, and hence the Planck source is given by

$$\varkappa_{B,1} B_1(T) = \frac{\varkappa^*}{\pi}\sigma_R T\,. \tag{32}$$

Algorithm 1: The iteration algorithm of the MLQD method for TRT problems

while $t^n < t^{end}$ **do**

  $s = -1$: $T^{(0)} = T^{n-1}$, $\mathfrak{f}_g^{(0)} = \mathfrak{f}_g^{n-1}$

  while $||T^{(s+1)} - T^{(s)}|| > \epsilon||T^{(s+1)}||$, $||E^{(s+1)} - E^{(s)}|| > \epsilon||E^{(s+1)}||$ **do**

    • `transport iterations (`s`-iterations)`

    $s = s + 1$

    if $s > 0$ **then**

      Update group opacities $\varkappa_{E,g}(T^{(s)})$ and $\varkappa_{B,g}(T^{(s)})$

      Solve multigroup RT eqs. for $I_g^{(s)}$

      Compute group QD factors $f_g^{(s)}$

    $l = -1$

    $T^{(\ell=0,s)} = T^{(s)}$

    while $||T^{(\ell+1,s)} - T^{(\ell,s)}|| > \tilde{\epsilon}||T^{(\ell+1,s)}||$, $||E^{(\ell+1,s)} - E^{(\ell,s)}|| > \tilde{\epsilon}||E^{(\ell+1,s)}||$ **do**

      • `low-order multigroup iterations (`ℓ`-iterations)`

      $l = l + 1$

      Update group opacities $\varkappa_{E,g}(T^{(\ell,s)})$, $\varkappa_{R,g}(T^{(\ell,s)})$, $\varkappa_{B,g}(T^{(\ell,s)})$

      Solve MLOQD eqs. for $E_g^{(\ell,s)}$ and $F_g^{(\ell,s)}$

      Compute $\bar{\varkappa}_E^{(\ell,s)}$, $\bar{\varkappa}_R^{(\ell,s)}$, $\bar{f}^{(\ell,s)}$ and $\bar{\eta}^{(\ell,s)}$

      $k = -1$

      $T^{(k=0,\ell,s)} = T^{(\ell,s)}$

      while $||T^{(k+1,\ell,s)} - T^{(k,\ell,s)}|| > \hat{\epsilon}||T^{(k+1,\ell,s)}||$,
       $||E^{(k+1,ell,s)} - E^{(k,\ell,s)}|| > \hat{\epsilon}||E^{(k+1,\ell,s)}||$ **do**

        • `grey Newton iterations (`k`-iterations)`

        $k = k + 1$

        Solve coupled GLOQD and GMEB eqs. for $E^{(k+1,\ell,s)}$, $F^{(k+1,\ell,s)}$, and $T^{(k+1,\ell,s)}$

      $T^{(\ell+1,s)} \leftarrow T^{(k,\ell,s)}$, $E^{(\ell+1,s)} \leftarrow E^{(k,\ell,s)}$

    $T^{(s+1)} \leftarrow T^{(\ell+1,s)}$, $E^{(s+1)} \leftarrow E^{(\ell+1,s)}$

  $T^n \leftarrow T^{(s+1)}$, $E^n \leftarrow E^{(s+1)}$

References

[1] J. A. Fleck & J. D. Cummings, An implicit Monte Carlo scheme for calculating time and frequency dependent nonlinear radiation transport, *Journal of Computational Physics*, **8**, 313-342 (1971).

[2] D. Y. Anistratov, Stability analysis of a multilevel quasidiffusion method for thermal radiative transfer problems, *Journal of Computational Physics*, **376**, 186-209 (2019).