An asymptotic preserving unified gas kinetic scheme for the grey radiative transfer equations

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(joint work with Wenjun Sun, Kun Xu)

Introduction

- **An asymptotic limit associated with a PDE is a limit in which certain terms in the PDE are made "small" relative to other terms.**
- **This ordering in size is achieved via a scaling parameter (say ϵ) that goes to zero in the asymptotic limit.**
- **In many instances, the scale lengths associated with solutions of the limiting equation are much larger than the smallest scale lengths associated with solutions of the original PDE.**

When this is the case, asymptotic-preserving (AP) discretization schemes are necessary for near-asymptotic problems to avoid completely impractical mesh resolution requirement ($\Delta x \sim O(\epsilon),\ \epsilon \to 0$).

Aim of this talk: To present an AP scheme for the grey radiative transfer system

• Outline:

1. Governing equations
2. An AP scheme for the system
3. Asymptotic analysis, AP property
4. Numerical experiments
5. conclusions
6. Future studies

1. Governing equations

Grey radiative transfer equations:

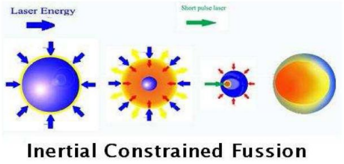
$$\frac{\epsilon^2}{c}\frac{\partial I}{\partial t} + \epsilon\vec{\Omega}\cdot\nabla I = \sigma\left(\frac{1}{4\pi}acT^4 - I\right), \qquad (1)$$

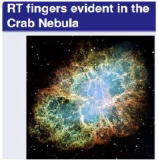
$$\epsilon^2 C_v\frac{\partial T}{\partial t} = \sigma\left(\int I d\vec{\Omega} - acT^4\right). \qquad (2)$$

$I(\vec{r},\vec{\Omega},t)$: Radiation intensity, $T(\vec{r},t)$: Material temperature,
$\sigma(\vec{r},T)$: Opacity, a: Radiation constant, c: Speed of light,
$\epsilon > 0$: Knudsen number, $C_v(\vec{r},t)$: Specific heat,
$\vec{r}$: Spatial variable, $\vec{\Omega}$: Angular variable, t: Time variable.

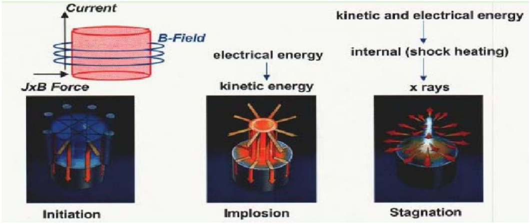
σI: absorption term; $\frac{\sigma}{4\pi}acT^4$: emission term.

Backgrounds





Z-pinch



Grey radiative transfer system finds applications in the study of ICF (inertia constrained fusion), Z-pinch, astrophysics, etc.

Numerical challenges

- **High dimensional problem**

  time: t, spatial: $\vec{r}$, direction : $\vec{\Omega}$.

- **For multi-material problems (multi-scale)**

  optically thick material: small ϵ

  optically thin material: large ϵ

- **To resolve physical scales, normally $\Delta x \sim O(\epsilon/\sigma)$**

  huge computing costs for small ϵ

- **For small ϵ, the radiation transfer behaves like diffusion**

  how to construct a scheme which can capture the diffusion behavior for small ϵ? ($\sim$ asymptotic preserving)

Formally, as $\epsilon \to 0$ (optically thick), (1)-(2) behaves like a diffusion equation.

Expand I and T in ϵ and insert the expansions into (1)-(2) $\Rightarrow$ the leading-order term satisfies (formally):
$I^{(0)} = \frac{1}{4\pi} ac(T^{(0)})^4$, and a diffusion equation

$$C_v \frac{\partial}{\partial t} T^{(0)} + a \frac{\partial}{\partial t} (T^{(0)})^4 = \nabla \cdot \frac{ac}{3\sigma} \nabla (T^{(0)})^4. \tag{3}$$

An asymptotic preserving (AP) scheme for (1)-(2) is a numerical scheme that discretizes (1)-(2) in such a way that it leads to a correct discretization of the diffusion limit (3) when ϵ/σ small.

Related results:

- AP schemes were introduced first by Larsen, Morel and Miller '87 for steady neutron transport problems
- Further developments for different non-steady problems, based on a decomposition of the distribution function between an equilibrium part and its derivation, by Klar, Jin, Pareschi, Toscani, $\cdots$ '93–'13
- A different approach by Xu & Huang '10 for rarefied gas dynamics based on a unified gas kinetic scheme (UGKS), further development by Mieussens '13 for a linear transport model.

(scalar equations are dealt with only, not coupled with other eqs.)

We want to use the idea of gas kinetic schemes to construct an AP scheme for the system (1)-(2).

2. AP scheme for the system (1)–(2)

2.1. Angular discretization

In 2D Cartesian coordinates, we can rewrite (1), (2) as

$$\begin{aligned} &\frac{\epsilon}{c}\partial_t I + \mu\partial_x I + \xi\partial_y I = \frac{\sigma}{\epsilon}\Big(\frac{1}{2\pi}\phi - I\Big), \\ &\epsilon^2 C_v \frac{\partial T}{\partial t} = \sigma\Big(\int I d\vec{\Omega} - \phi\Big), \qquad \phi = acT^4. \end{aligned} \tag{4}$$

where $\mu = \sqrt{1-\zeta^2}\cos\theta,\ \xi = \sqrt{1-\zeta^2}\sin\theta$,
$\zeta \in [0,1]$: cosine value of the angle between the propagation direction $\vec{\Omega}$ and z-axis,
$\theta \in [0, 2\pi)$: projection vector of $\vec{\Omega}$ onto the xy-plane and the x-axis.

2.1. Angular discretization

We use the usual discrete ordinate method to discretize (4) in directions.

Write the propagation direction (μ, ξ) as some discrete directions (μ_m, ξ_m), $m = 1, \cdots, M \ \ (= N(N+2)/2)$, together with the corresponding integration weights $\omega_m \Longrightarrow$ angular discretized equations:

$$
\begin{cases}
\frac{\epsilon}{c}\partial_t I_m + \mu_m \partial_x I_m + \xi_m \partial_y I_m = \frac{\sigma}{\epsilon}(\frac{1}{2\pi}\phi - I_m), \\
\epsilon^2 C_v \frac{\partial T}{\partial t} = \sigma\Big(\sum_{m=1}^{M} I_m \omega_m - \phi\Big), \qquad \phi = acT^4.
\end{cases} \tag{5}
$$

Denote $I_{i,j,m}^n$, $T_{i,j}^n$: cell average values of I_m, T at t^n in cell

$$(i,j) := \{(x,y);\ x_{i-1/2} < x < x_{i+1/2}, y_{j-1/2} < y < y_{j+1/2}\},$$

and integrate (5) $\Rightarrow$

FV discretization of (5) reads as

$$\begin{aligned} I_{i,j,m}^{n+1} &= I_{i,j,m}^n + \frac{\Delta t}{\Delta x}(F_{i-1/2,j,m} - F_{i+1/2,j,m}) \\ &+ \frac{\Delta t}{\Delta y}(H_{i,j-1/2,m} - H_{i,j+1/2,m}) + c\Delta t \frac{\sigma}{\epsilon^2}(\frac{1}{2\pi}\tilde{\phi}_{i,j} - \tilde{I}_{i,j,m}), \qquad (6) \\ C_v T_{i,j}^{n+1} &= C_v T_{i,j}^n + \Delta t \frac{\sigma}{\epsilon^2}(\sum_{m=1}^{M} \tilde{I}_{i,j,m}\omega_m - \tilde{\phi}_{i,j}), \end{aligned}$$

where $F_{i-1/2,j,m}$, $H_{i,j-1/2,m}$: numerical fluxes in the x-, y-directions, $\tilde{\phi}_{i,j}, \tilde{I}_{i,j,m}$: average of ϕ, I_m in $(t^n, t^{n+1}) \times cell(i,j)$; and

$$
\begin{aligned}
F_{i\pm1/2,j,m} &= \frac{c\mu_m}{\epsilon\Delta t}\int_{t^n}^{t^{n+1}} I_m(t, x_{i\pm1/2}, y_j, \mu_m, \xi_m)dt, \\
H_{i,j\pm1/2,m} &= \frac{c\xi_m}{\epsilon\Delta t}\int_{t^n}^{t^{n+1}} I_m(t, x_i, y_{j\pm1/2}, \mu_m, \xi_m)dt,
\end{aligned} \tag{7}
$$

and we take here approximation (implicitly in time):

$$
\tilde{I}_{i,j,m} \approx I_{i,j,m}^{n+1}, \quad \tilde{\phi}_{i,j} \approx \phi_{i,j}^{n+1}.
$$

We have to construct the numerical fluxes in (7).

2.3. Construction of the numerical fluxes

To evaluate $F_{i-1/2,j,m}$, we use the idea of gas kinetic schemes, i.e., solve (5) in the x-direction at the cell boundary $x = x_{i-1/2}$, $y = y_j$:

$$\frac{\epsilon}{c}\partial_t I_m + \mu_m \partial_x I_m = \frac{\sigma}{\epsilon}\left(\frac{1}{2\pi}\phi - I_m\right),$$
$$I_m(x, y_j, t)|_{t=t^n} = I_{m,0}(x, y_j, t^n) \tag{8}$$

to have the explicit solution

$$I_m(t, x_{i-1/2}, y_j, \mu_m, \xi_m) = e^{-\nu_{i-1/2,j}(t-t^n)} I_{m,0}\left(x_{i-1/2} - \frac{c\mu_m}{\epsilon}(t-t^n)\right)$$
$$+ \int_{t^n}^{t} e^{-\nu_{i-1/2,j}(t-s)} \frac{c\sigma_{i-1/2,j}}{2\pi\epsilon^2} \phi\left(s, x_{i-1/2} - \frac{c\mu_m}{\epsilon}(t-s)\right) ds, \tag{9}$$

where $\nu = c\sigma/\epsilon^2$, $\nu_{i-1/2,j}$: value of ν at the corresponding cell boundary. ($I_{m,0}$, ϕ to be determined)

Put (9) into (7) $\Rightarrow$

numerical flux $F_{i-1/2,j,m}$ in x,

provided the initial data $I_{m,0}(x, y_j, t^n)$ in (8), $\phi(x, y, t)$ for $t \in (t^n, t^{n+1})$ and (x, y) around $(x_{i-1/2}, y_j)$ in (9) are known.

(Flux $H_{i,j-1/2,m}$ in y can be constructed in the same manner)

- Approximate $I_{m,0}(x, y_j, t^n)$ explicitly by piecewise linear polynomials and MUSCL limiter for slopes, using known $I^n_{i,j,m}$ $\surd$

- Evaluate $\phi(x, y, t)$ implicitly by piecewise polynomials:

$$\phi(x, y_j, t) = \phi^{n+1}_{i-1/2,j} + \delta_t \phi^{n+1}_{i-1/2,j}(t - t^{n+1}) + \begin{cases} \delta_x \phi^{n+1,L}_{i-1/2,j}(x - x_{i-1/2}), & \text{if } x < x_{i-1/2}, \\ \delta_x \phi^{n+1,R}_{i-1/2,j}(x - x_{i-1/2}), & \text{if } x > x_{i-1/2}. \end{cases} \tag{10}$$

Here $\delta_t \phi^{n+1}_{i-1/2,j} = (\phi^{n+1}_{i-1/2,j} - \phi^{n}_{i-1/2,j})/\Delta t$, and

$$\delta_x \phi^{n+1,L}_{i-1/2,j} = \frac{\phi^{n+1}_{i-1/2,j} - \phi^{n+1}_{i-1,j}}{\Delta x/2}, \quad \delta_x \phi^{n+1,R}_{i-1/2,j} = \frac{\phi^{n+1}_{i,j} - \phi^{n+1}_{i-1/2,j}}{\Delta x/2}.$$

The numerical flux $F_{i-1/2,j,m}$ is obtained, provided the implicit terms $\phi^{n+1}_{i-1/2,j}, \phi^{n+1}_{i-1,j}, \phi^{n+1}_{i,j}$ are evaluated.

Remark. By (9)–(10), flux $F_{i-1/2,j,m}$ can be decomposed into

$$
\begin{aligned}
F_{i-1/2,j,m} = {} & A_{i-1/2,j}\mu_m(I^-_{i-1/2,j,m}1_{\mu_m>0} + I^+_{i-1/2,j,m}1_{\mu_m<0}) \\
& + C_{i-1/2,j}\mu_m\phi^{n+1}_{i-1/2,j} \\
& + D_{i-1/2,j}(\mu_m^2\delta_x\phi^{n+1,L}_{i-1/2,j}1_{\mu_m>0} + \mu_m^2\delta_x\phi^{n+1,R}_{i-1/2,j}1_{\mu_m<0}) \\
& + B_{i-1/2,j}(\mu_m^2\delta_x I^n_{i-1,j,m}1_{\mu_m>0} + \mu_m^2\delta_x I^n_{i,j,m}1_{\mu_m<0}) \\
& + E_{i-1/2,j}\mu_m\delta_t\phi^{n+1}_{i-1/2,j}, \qquad \text{(involved the values of } I \text{ at } t^n \text{ only)}
\end{aligned} \tag{11}
$$

where $I^-_{i-1/2,j,m}$, $I^+_{i-1/2,j,m}$ denote the boundary values:

$$
I^-_{i-1/2,j,m} = I^n_{i-1,j,m} + \frac{\Delta x}{2}\delta_x I^n_{i-1,j,m}, \quad I^+_{i-1/2,j,m} = I^n_{i,j,m} - \frac{\Delta x}{2}\delta_x I^n_{i,j,m},
$$

and $\nu = c\sigma/\epsilon^2$; the coefficients $A_{i-1/2,j} = \cdots$ are explicit functions of $\Delta t, \epsilon, \sigma, \nu$.

To evaluate $\phi^{n+1}_{\cdots}$, we take the moment of (1).

Denote $\phi = acT^4$, $\rho = \int I d\vec{\Omega}$ as before, take angular moment of (1)

$\Rightarrow$ (1), (2) can be rewritten in the macro-form:

$$\begin{cases} \frac{\epsilon^2}{c}\frac{\partial \rho}{\partial t} + \epsilon \nabla \cdot < \vec{\Omega} I > = \sigma(\phi - \rho), \qquad < \vec{\Omega} I > := \int \vec{\Omega} I d\vec{\Omega}, \\ \epsilon^2 \frac{\partial \phi}{\partial t} = \beta\sigma(\rho - \phi), \qquad \beta = \frac{4acT^3}{C_v}. \end{cases} \tag{12}$$

We discretize (12) implicitly as follows.

$$\begin{aligned} \rho^{n+1}_{i,j} &= \rho^n_{i,j} + \frac{\Delta t}{\Delta x}(\Phi^{n+1}_{i-1/2,j} - \Phi^{n+1}_{i+1/2,j}) \\ &+ \frac{\Delta t}{\Delta y}(\Psi^{n+1}_{i,j-1/2} - \Psi^{n+1}_{i,j+1/2}) + \frac{c\sigma^{n+1}_{i,j}\Delta t}{\epsilon^2}(\phi^{n+1}_{i,j} - \rho^{n+1}_{i,j}), \\ \phi^{n+1}_{i,j} &= \phi^n_{i,j} + \frac{(\beta\sigma)^{n+1}_{i,j}\Delta t}{\epsilon^2}(\rho^{n+1}_{i,j} - \phi^{n+1}_{i,j}), \end{aligned} \tag{13}$$

where

$$\Phi^{n+1}_{i\pm 1/2,j} = \frac{c}{\epsilon \Delta t} \int_{t^n}^{t^n+\Delta t} < \Omega_x I > (x_{i\pm 1/2}, y_j, t) dt,$$

$$\Psi^{n+1}_{i,j\pm 1/2} = \frac{c}{\epsilon \Delta t} \int_{t^n}^{t^n+\Delta t} < \Omega_y I > (x_i, y_{j\pm 1/2}, t) dt,$$

which can be explicitly evaluated using (9) and (11), e.g.,

$$\Phi^{n+1}_{i-1/2,j} = \sum_{m=1}^{M} \omega_m F_{i-1/2,j,m} = A_{i-1/2,j} \sum_{m=1}^{M} \omega_m \mu_m \Big(I^n_{i-1,j,m} \mathbf{1}_{\mu_m>0}$$
$$+ I^n_{i,j,m} \mathbf{1}_{\mu_m<0} \Big) + \frac{2\pi D_{i-1/2,j}}{3} \Big(\frac{\phi^{n+1}_{i,j} - \phi^{n+1}_{i-1,j}}{\Delta x} \Big)$$
$$+ B_{i-1/2,j} \sum_{m=1}^{M} \omega_m \mu_m^2 (\delta_x I^n_{i-1,j,m} \mathbf{1}_{\mu_m>0} + \delta_x I^n_{i,j,m} \mathbf{1}_{\mu_m<0}),$$

where $A_{i-1/2,j}, \cdots$ are same as before $\quad (\sigma_{i-1/2,j} = \frac{2\sigma_{i,j}\sigma_{i-1,j}}{\sigma_{i,j}+\sigma_{i-1,j}})$

($\star$ only involved the values of I at t^n)

(13) is a nonlinear system for $\phi_{i,j}^{n+1}$, $\rho_{i,j}^{n+1}$ with parameters σ, β depending on T, and is solved by a two-level iteration method,

outer iteration: a nonlinear iteration with fixed σ, β $\sim$ a linear algebraic system;

inner iteration: Gauss-Sidel iteration to solve the linear system.

After obtaining $\phi_{i,j}^{n+1}$, we take the cell boundary value $\phi_{i-1/2,j}^{n+1}$ in (10) to be

$$\phi_{i-1/2,j}^{n+1} = \frac{1}{2}(\phi_{i-1,j}^{n+1} + \phi_{i,j}^{n+1}). \tag{14}$$

With (14), the numerical fluxes (10) are determined.

The construction of our AP UGKS scheme is complete □

LOOP of the AP-UGKS: Given $I^n_{i,j,m}$ and $T^n_{i,j}$, we have $\rho^n_{i,j}$ and $\phi^n_{i,j}$. Find I^{n+1} and T^{n+1}.

1) Solve the system (13) to obtain $\phi^{n+1}_{i,j}$, $\rho^{n+1}_{i,j}$;

2) Using $\phi^{n+1}_{i,j}$ to solve the system (6) for I to get $I^{n+1}_{i,j,m}$, $T^{n+1}_{i,j}$;

3) (Corrector step) Using $I^{n+1}_{i,j,m}$ to solve $(12)_2$ (i.e. $\epsilon^2\phi_t = \beta\sigma(\rho - \phi)$) to get a new $\phi^{n+1}_{i,j}$ (explicitly given by

$$\bar{\phi}^{n+1}_{i,j} = \frac{\phi^n_{i,j} + \Delta t(\beta\sigma)^{n+1}_{i,j}\sum_{m=1}^{M}\omega_m I^{n+1}_{i,j,m}}{1 + \Delta t(\beta\sigma)^{n+1}_{i,j}} \quad).$$

And then, to give the corrected temperature by $T^{n+1}_{i,j} = (\bar{\phi}^{n+1}_{i,j}/(ac))^{1/4}$.

4) Goto 1) for the next computational step.

3. Asymptotic analysis, AP property

- **The above constructed scheme is AP**

Recalling (11), $F_{i-1/2,j,m}$ can be decomposed into

$$F_{i-1/2,j,m} = A_{i-1/2,j}\cdots + \cdots + E_{i-1/2,j}\cdots ,$$

where the coefficients satisfy $A, B \to 0$, $D \to -c/(2\pi\sigma)$ as $\epsilon \to 0$.

Thus, the corresponding macroscopic diffusion flux $(\mathrm{Diff})^{n+1}_{i-1/2,j}$:

$$(\mathrm{Diff})^{n+1}_{i-1/2,j} := \int \frac{c\mu}{2\pi\epsilon\Delta t}\int_{t^n}^{t^{n+1}} I(t, x_{i-1/2}, y_j, \mu, \xi)dtd\mu d\xi$$
$$= \frac{1}{2\pi}\sum_{m=1}^{M}\omega_m\mu_m I^m(t, x_{i-\frac{1}{2}}, y_j, \mu_m, \xi_m) \to -\frac{c}{3\sigma^{n+1}_{i-\frac{1}{2},j}}\frac{\phi^{n+1}_{i,j} - \phi^{n+1}_{i-1,j}}{\Delta x}$$

as $\epsilon \to 0$, which gives a numerical flux of the limiting diffusion equation for $\phi \rightsquigarrow$ 5 points scheme in 2D $\Rightarrow$ an AP scheme.

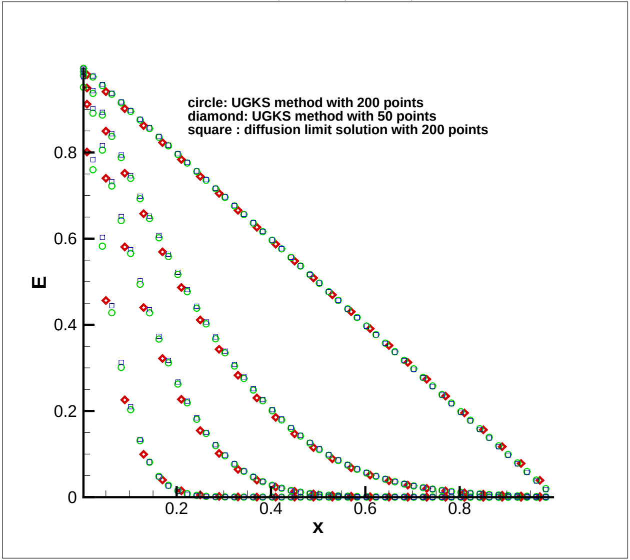
Example 1. A test for the linear kinetic equation:

$$\frac{\epsilon}{c}\partial_t I + \mu\partial_x I = \frac{\sigma}{\epsilon}\Big(\frac{1}{2\pi}\phi - I\Big),$$

where we take $\phi = \int I d\mu$, Domain: $x \in [0, 1]$, $\sigma = 1$, $\epsilon = 10^{-8}$; boundary conditions: $I_L(0, \mu) = 1$ ($\mu > 0$ and $I_R(1, \mu) = 0$ ($\mu < 0$); $\Delta x = 5 \times 10^{-3}, 2.5 \times 10^{-3} >> \epsilon$.

This problem corresponds to the equilibrium diffusion approximation.

Computed solution at $t = 0.01, 0.05, 0.15, 2.0$:



Computed solution agrees well with that of the diffusion limiting eq. $\sim$ AP property

Example 2. **(Marshak wave-2B)**

$\sigma = \frac{100}{T^3} cm^2/g$, $T = 10^{-6}$Kev, $\epsilon = 1$, specific heat=0.1$GJ/g/$Kev.

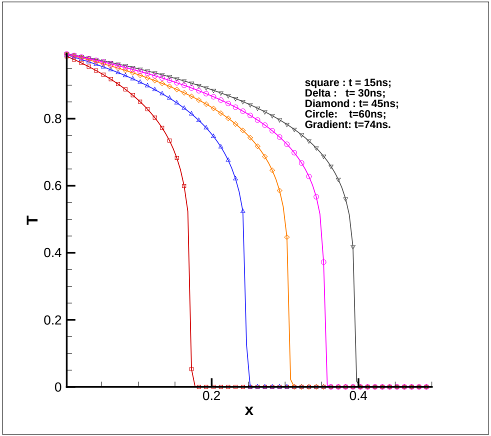
This corresponds to the equilibrium diffusion approximation.

$\Delta x = 0.005$cm (200 cells), $\Delta y = 0.01$cm (1 cell), $\Delta x, \Delta y >> \epsilon/\sigma$.

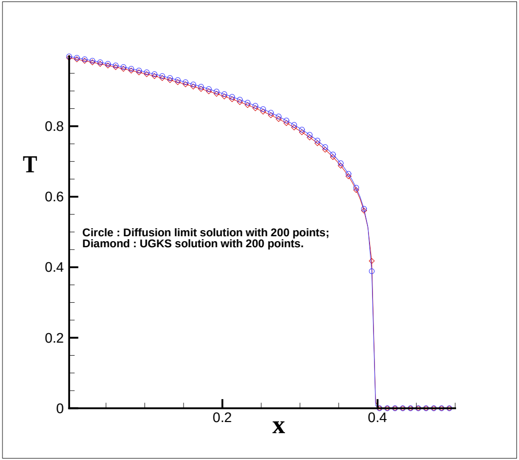
Left boundary: constant incident radiation intensity with a Planckian distribution at 1Kev;

Right boundary: outflow

Computed material temperature at $t = 15, 30, 45, 60, 74$ns



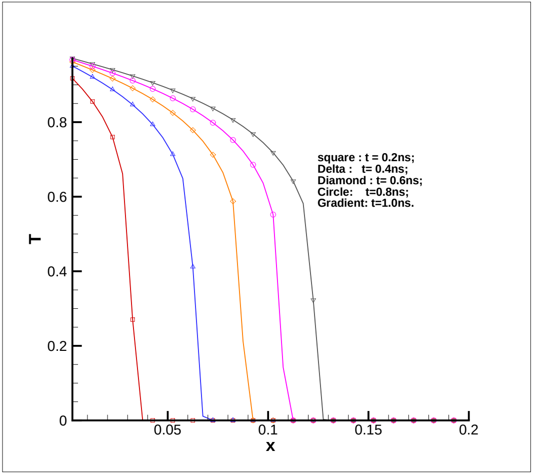
Computed material temperature for both grey radiation transfer system and diffusion limiting equation at 74ns



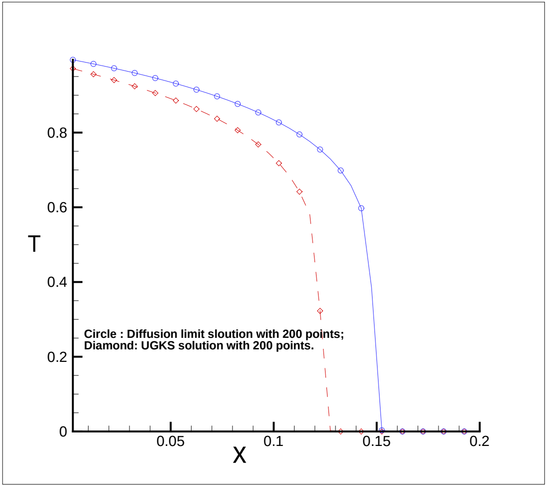
Results computed by AP UGKS agree very well with numerical solution of the diffusion limiting eq. $\sim$ AP property

Example 3. (Marshak wave-2A) the same as Example 2 except $\sigma = \frac{10}{T^3} cm^2/g$. This case violates the equilibrium diffusion approximation.

Computed radiative temperature at $t = 0.2, 0.4, 0.6, 0.8, 1.0ns$:

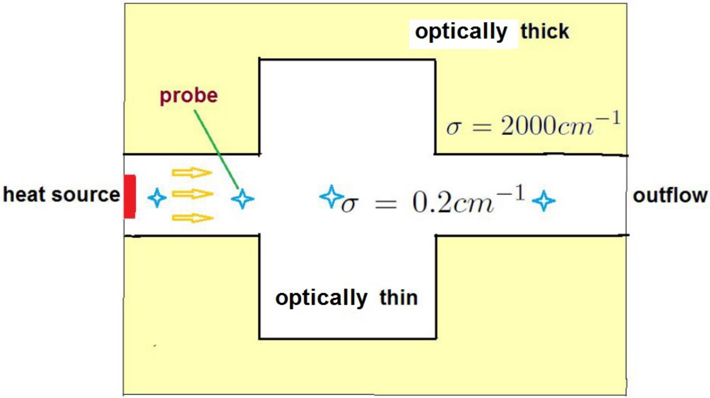


Material temperature distributions obtained by AP UGKS and the diffusion equation solution at $t = 1.0ns$: (clear difference, since not in the equilibrium diffusion approximation)



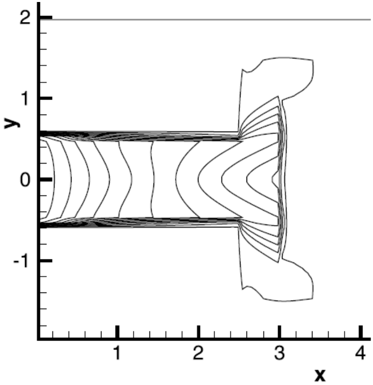
Example 4. (Tophat Test [N.A. Gentile,'01])

Domain: $[0,7]\times[-2,2]$, $\epsilon=1$; **Five probes: placed at** $(0.25,0),\cdots$ **to monitor the change of the temperature in the thin opacity material.**

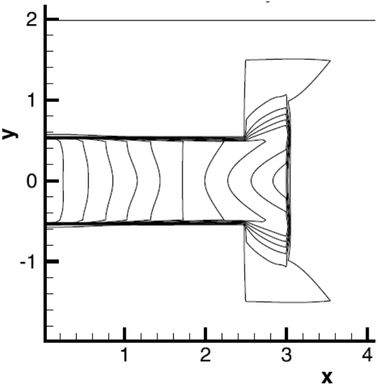


Computed material temperature at 8ns:

128 $\times$ 64 cells

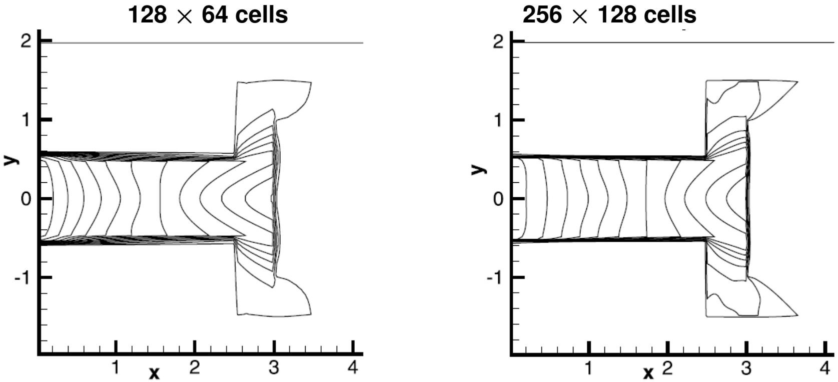


256 $\times$ 128 cells



Interface between optically thick and thin materials is captured sharply, compared with [Gentile '01 (JCP)]

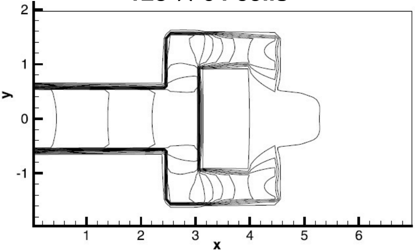
Computed radiation temperature at 8ns:



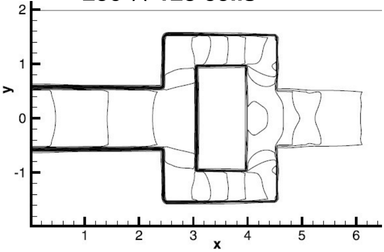
Interface between optically thick and thin materials is captured sharply.

Computed material temperature at 94ns:

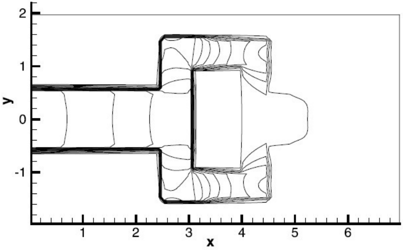
128 $\times$ 64 cells



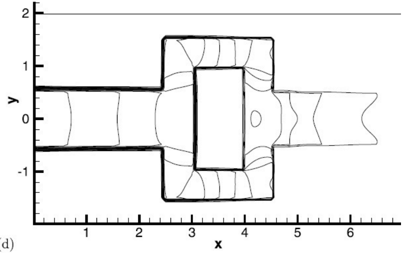
256 $\times$ 128 cells



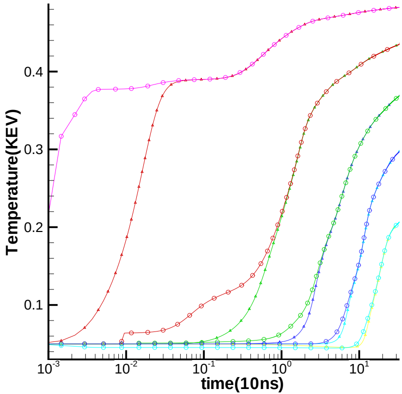
Computed radiation temperature



(d)



Time evolution of the material, radiation temperatures at 5 probes:



At the 5th probe, the temperature cools off slightly before being heated up by radiation, which is consistent with [Gentile].

But, the temperature curve here has a rapid growth initially, a slow increment, then a growth again. This is different from [Gentile], deserving further investigation.

6. Conclusions

- A unified gas scheme is constructed for the grey radiative transfer system.
- The scheme has asymptotic preserving property and works well for both optically thin and optically thick regimes.
- We believe that it should work for more general problems, say, the multi-group radiation transfer equations

7. Future studies

- Extension to the multi-group radiation transfer equations $\surd$
- Extension to the multi-material problems, quadrilateral meshes
- Extension to radiation hydrodynamics

Question: An AP scheme converges to the desired diffusion solver ?

THANK YOU !