An asymptotic preserving kinetic scheme for the M1 model of linear transport

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The UGK scheme for linear transport

Dimensionless 1D kinetic equation

$$\eta\partial_t f + v\partial_x f = \frac{\sigma}{\epsilon}(\rho - f) \tag{1}$$

Where:

- $f : (t, x, v) \mapsto f(t, x, v)$ is the particle distribution function.
- $x \in [0, 1]$ is the space variable.
- $v = \mathbf{\Omega} \cdot \mathbf{e_x} \in [-1, 1]$ is the kinetic variable.
- σ is the scattering coefficient.
- ϵ is the Knudsen number.
- η is a dimensionless number related to the transport scale.

The density is $\rho = \langle f \rangle$, where $\langle \cdot \rangle = \frac{1}{2}\int_{-1}^{1} \cdot \, \mathrm{d}v$.

Moments models

The moment hierarchy of the kinetic equation given by $\mathbf{m} = \begin{pmatrix} 1 & v \end{pmatrix}^T$ is

$$\begin{cases} \eta\partial_t \rho + \partial_x j = 0, \\ \eta\partial_t j + \partial_x q = -\dfrac{\sigma}{\epsilon} j \end{cases}, \tag{2}$$

where:

- $\rho = \langle f \rangle$ is the density.
- $j = \langle vf \rangle$ is the current density.
- $q = \langle v^2 f \rangle$ is the third moment of the distribution function.

We seek q as a function of (ρ, j). By imposing the shape of the distribution function as a function of those variables, this flux can be computed.

M1 model

Let (ρ, j) be a couple of realizable moments [1]. The distribution function $\hat{f}$ which minimizes the entropic functional $g(f) = f \ln f - f$ under the constraint $\left\langle \mathbf{m}\hat{f} \right\rangle = \begin{pmatrix} \rho & j \end{pmatrix}^T$ is

$$\hat{f}(v) = e^{\alpha + \beta v} = \rho \frac{\beta}{\sinh \beta} e^{\beta v}, \tag{3}$$

where $u = j/\rho = \coth \beta - \dfrac{1}{\beta}$. Thus, the hyperbolic $M1$ model is

$$\begin{cases} \eta \partial_t \rho + \partial_x j = 0, \\ \eta \partial_t j + \partial_x \rho \left(1 - 2\dfrac{u}{\beta}\right) = -\dfrac{\sigma}{\epsilon} j \end{cases} . \tag{4}$$

[1] There exists a **positive** distribution function which realises those moments.

Diffusion limit and **A**symptotic **P**reserving (AP) numerical scheme

At the diffusion scale ($\eta = \epsilon$), when ϵ tends to 0, the density satisfies a diffusion equation (parabolic):

$$\partial_t \rho = \partial_x \left(\frac{1}{3\sigma} \partial_x \rho \right) + \mathcal{O}(\epsilon). \tag{5}$$

A numerical scheme for the kinetic equation (1) or the M^1 moment model (4) needs to preserve the diffusion asymptotic limit. *A priori*, such a scheme doesn't ensure this property without special a special treatment of the source term.

$$\begin{tikzcd}
\boxed{\text{Moment model}} \arrow[r, "\epsilon \to 0"] \arrow[d] & \boxed{\text{Diffusion equation}} \arrow[d, dotted] \\
\boxed{\text{Numerical scheme}} \arrow[r, "\epsilon \to 0"] & \boxed{?}
\end{tikzcd}$$

A finite volume formulation

The semi-implicit finite volume formulation of the kinetic equation is

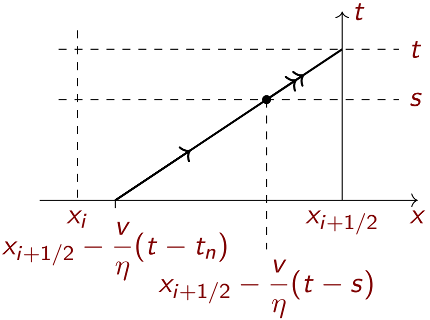
$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + \frac{1}{\Delta x}(\phi_{i+1/2} - \phi_{i-1/2}) = \nu(\rho_i^{n+1} - f_i^{n+1}) \tag{6}$$

where:

- $f_i^n = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} f(t^n, x, v)\mathrm{d}x$ is the mean value of the distribution function in cell i at time t^n.
- $\phi_{i\pm1/2} = \frac{v}{\eta \Delta t}\int_{t^n}^{t^{n+1}} f(t, x_{i\pm1/2}, v)\mathrm{d}t$ is the numerical flux between cells i and $i \pm 1$.
- $\nu = \frac{\sigma}{\eta\epsilon}$ is the collision frequency.

UGKS rests on the integral solution of the kinetic equation given by the method of characteristic:

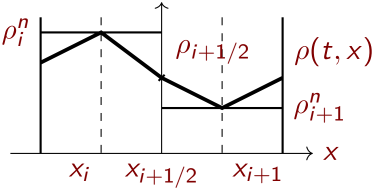
$$\begin{aligned} f(t, x_{i+1/2}, v) \approx e^{-\nu_{i+1/2}(t-t_n)} f(t^n, x_{i+1/2} - \frac{v}{\eta}(t-t_n), v) \\ + \nu_{i+1/2} \int_{t_n}^{t} e^{-\nu_{i+1/2}(t-s)} \rho(s, x_{i+1/2} - \frac{v}{\eta}(t-s)) \mathrm{d}s. \end{aligned} \tag{7}$$

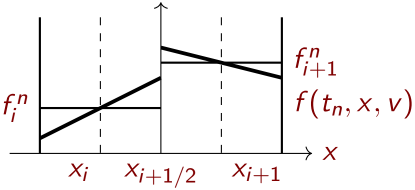


The chosen reconstructions are

$$\rho(t_n,x)=\begin{cases}\rho^n_{i+1/2}+\delta^L_x\rho^n_{i+1/2}(x-x_{i+1/2}) & x<x_{i+1/2}\\ \rho^n_{i+1/2}+\delta^R_x\rho^n_{i+1/2}(x-x_{i+1/2}) & x>x_{i+1/2}\end{cases}, \tag{8}$$

$$f(t_n,x,v)=\begin{cases}f^n_i+\delta_x f^n_i(x-x_i) & \text{si } x<x_{i+1/2}\\ f^n_{i+1}+\delta_x f^n_{i+1}(x-x_{i+1}) & \text{si } x>x_{i+1/2}\end{cases}. \tag{9}$$





The numerical flux is

$$\begin{aligned}\phi_{i+1/2}(v) =& Av\left(f_i^{n(+)}\mathbb{1}_{v>0} + f_{i+1}^{n(-)}\mathbb{1}_{v<0}\right)\\ &+Bv^2(\delta_x f_i^n \mathbb{1}_{v>0} + \delta_x f_{i+1}^n \mathbb{1}_{v<0})\\ &+Cv\rho_{i+1/2}^n\\ &+Dv^2(\delta_x^L \rho_{i+1/2}^n \mathbb{1}_{v>0} + \delta_x^R \rho_{i+1/2}^n \mathbb{1}_{v<0}),\end{aligned} \tag{10}$$

where $f_i^{n(\pm)} = f_i^n \pm \frac{\Delta x}{2}\delta_x f_i^n$ and, using the notation $w = -\sigma\Delta t/(\eta\varepsilon)$, A, B, C, D are:

$$\mathrm{A}(\Delta t, \sigma, \eta, \varepsilon) = \frac{1}{\eta w}(e^w - 1) \tag{11}$$

$$\mathrm{C}(\Delta t, \sigma, \eta, \varepsilon) = \frac{1}{\eta} - \mathrm{A}(\Delta t, \sigma, \eta, \varepsilon) \tag{12}$$

$$\mathrm{D}(\Delta t, \sigma, \eta, \varepsilon) = \frac{\varepsilon}{\sigma}(\mathrm{C}(\Delta t, \sigma, \eta, \varepsilon) - \mathrm{A}(\Delta t, \sigma, \eta, \varepsilon)) + \frac{\varepsilon}{\eta\sigma}e^w. \tag{13}$$

Asymptotic limits

Free transport limit

In the free transport limit ($\epsilon \to +\infty$), the microscopic flux tends to

$$\phi_{i+1/2} \xrightarrow[\epsilon\to\infty]{} \frac{v}{\eta}\left(f_i^{n(+)}\mathbb{1}_{v>0} + f_{i+1}^{n(-)}\mathbb{1}_{v<0}\right) - \Delta t\frac{v^2}{2\eta^2}\left(\delta_x f_i^n \mathbb{1}_{v>0} + \delta_x f_{i+1}^n \mathbb{1}_{v<0}\right), \tag{14}$$

which is the second order in space and time flux for the linear advection equation.

Diffusion limit

In the diffusion limit ($\eta = \epsilon$ and $\epsilon \to 0$), the macroscopic flux tends to

$$\left\langle \phi_{i+1/2} \right\rangle \xrightarrow[\epsilon\to 0]{} \frac{-1}{3\sigma}\frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}, \tag{15}$$

which is the two point centred scheme for the diffusion equation.

M1 closure of UGKS

Key concept: We apply the UGKS to the M^1 distribution function reconstructed from (ρ_i^n, j_i^n) at time t_n. That means the distribution function is systematically projected into the M^1 set at each time step.

$$
\begin{tikzcd}
(\rho_i^n, j_i^n) \arrow[r, "\mathscr{M}^1"] \arrow[drr, "\text{UGKS-M1}"'] & \hat{f}_i^n = e^{\alpha_i+\beta_i v} \arrow[r, "\text{UGKS}"] & f_i^{n+1} \arrow[d, "\langle \mathbf{m}\cdot \rangle"] \\
 & & (\rho_i^{n+1}, j_i^{n+1})
\end{tikzcd}
$$

Figure: UGKS-M1 scheme structure

By linearity we can exhibit two finite volume formulations for each macroscopic quantities

$$\frac{\rho_i^{n+1}-\rho_i^n}{\Delta t}+\frac{1}{\Delta x}(\Phi^\rho_{i+1/2}-\Phi^\rho_{i-1/2})=0, \tag{16a}$$

$$\frac{j_i^{n+1}-j_i^n}{\Delta t}+\frac{1}{\Delta x}(\Phi^j_{i+1/2}-\Phi^j_{i-1/2})=\frac{-\sigma}{\eta\epsilon}j_i^{n+1}, \tag{16b}$$

where:

$$\begin{aligned}\Phi^\rho_{i+1/2}&=A\left\langle v\hat{f}_i^{n+}\mathbb{1}_{v>0}+v\hat{f}_{i+1}^{n-}\mathbb{1}_{v<0}\right\rangle\\ &+B\left\langle v^2\delta_x\hat{f}_i^n\mathbb{1}_{v>0}+v^2\delta_x\hat{f}_{i+1}^n\mathbb{1}_{v<0}\right\rangle+\frac{D}{3\Delta x}(\rho_{i+1}^n-\rho_i^n)\end{aligned}, \tag{17a}$$

$$\begin{aligned}\Phi^j_{i+1/2}&=A\left\langle v^2\hat{f}_i^{n+}\mathbb{1}_{v>0}+v^2\hat{f}_{i+1}^{n-}\mathbb{1}_{v<0}\right\rangle\\ &+B\left\langle v^3\delta_x\hat{f}_i^n\mathbb{1}_{v>0}+v^3\delta_x\hat{f}_{i+1}^n\mathbb{1}_{v<0}\right\rangle+\frac{C}{3}\left\langle\hat{f}_i^n\mathbb{1}_{v>0}+\hat{f}_{i+1}^n\mathbb{1}_{v<0}\right\rangle\end{aligned}. \tag{17b}$$

Diffusion limit

In the diffusion limit ($\eta = \epsilon$ and $\epsilon \to 0$), the macroscopic flux tends to

$$\phi^{\rho}_{i+1/2} \xrightarrow[\epsilon \to 0]{} \frac{-1}{3\sigma} \frac{\rho^n_{i+1} - \rho^n_i}{\Delta x}, \tag{18}$$

which is the two point centred scheme for the diffusion equation.

Second order

The integrals $\left\langle v^k \delta_x \hat{f}_i^n \mathbb{1}_{v \lesseqgtr 0} \right\rangle$ can't be expressed in terms of (α, β) due to the non-linearity of the slope limiter.

Let $\mathbf{U} = \begin{pmatrix} \rho & j \end{pmatrix}^T$ and $\boldsymbol{\Lambda} = \begin{pmatrix} \alpha & \beta \end{pmatrix}^T$ be the vectors of conservative and entropic variables. We set

$$\mathbf{U}_i^n(x) = \begin{cases} \mathbf{U}_i^n + \delta \mathbf{U}_i^n (x - x_i) & \text{if } x < x_{i+1/2} \\ \mathbf{U}_{i+1}^n + \delta \mathbf{U}_{i+1}^n (x - x_{i+1}) & \text{if } x > x_{i+1/2} \end{cases}, \tag{19}$$

where the slope is $\delta \mathbf{U}_i^n = \frac{1}{\Delta x}(\mathbf{U}_{i+1}^n - \mathbf{U}_i^n)\phi(\mathbf{r}_i)$, $\mathbf{r}_i$ is the slope and ϕ is a TVD slope limiter. We expand $\hat{f}(\mathbf{U}_i^n(x)) = \exp\left(\boldsymbol{\Lambda}(\mathbf{U}_i^n(x)) \cdot \mathbf{m}\right)$ in Taylor series:

$$\begin{aligned} \hat{f}(\mathbf{U}_i^n(x)) &= \hat{f}(\mathbf{U}_i^n) + \frac{\mathrm{d}\widehat{\mathbf{f}}}{\mathrm{d}\mathbf{U}}(\mathbf{U}_i^n) \cdot \delta \mathbf{U}_i^n (x - x_i) \\ &= \hat{f}(\mathbf{U}_i^n) + \mathbf{J}_{\boldsymbol{\Lambda}}(\mathbf{U}_i^n)^T \mathbf{m} \hat{f}(\mathbf{U}_i^n) \cdot \delta \mathbf{U}_i^n (x - x_i), \end{aligned} \tag{20}$$

and finally we set $\delta_x \hat{f}(\mathbf{U}_i^n) = \mathbf{J}_{\boldsymbol{\Lambda}}(\mathbf{U}_i^n) \delta \mathbf{U}_i^n \cdot \mathbf{m} \hat{f}(\mathbf{U}_i^n)$.

Results

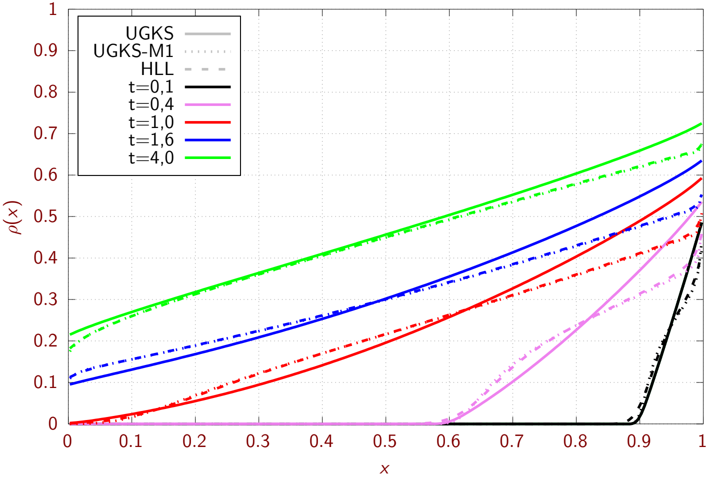


Figure: Density in the domain at time $t = 0.1, 0.4, 1.0, 1.6$ and 4.0.

Intermediate and diffusion regime

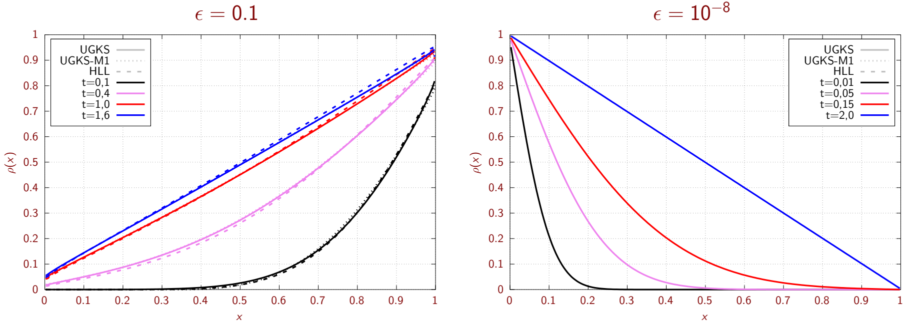


Figure: Density in the domain in the intermediate and diffusion regime

Almost null function at cell $j+1$

$$f_i^0(v) = \begin{cases} 0 & \text{if } i \neq j+1 \\ \frac{1}{|a|}\mathbb{1}_{v\in[\frac{3}{2}a,\frac{1}{2}a]} & \text{elsewhere} \end{cases}, a \in [-0.5, 0[.$$

$$\rho_j^1 = \frac{\Delta t}{\eta \Delta x}\left\langle -v^- f_{j+1}^0 \right\rangle + \mathcal{O}(\Delta t^2),$$

$$(1+\Delta t \nu) f_j^1(1) = -\frac{\Delta t^2}{\Delta x}\frac{\nu}{2\eta}\rho_{j+1/2}^0 - \frac{\Delta t^2}{\Delta x}\frac{\nu}{\eta}\left\langle v^- f_{j+1}^0 \right\rangle + \mathcal{O}(\Delta t^3),$$

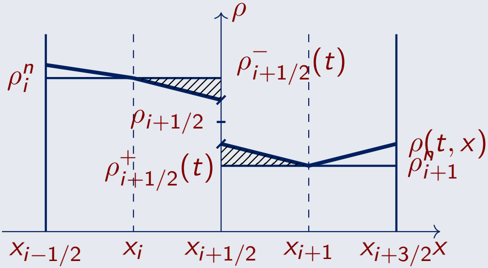
with $\rho_{j+1/2}^0 = \left\langle f_{j+1}^0 \mathbb{1}_{v<0} \right\rangle$, $\rho_{j+1/2}^0 = 1$ and $\left\langle -v^- f_{j+1}^0 \right\rangle = a$ so that

$$(1+\Delta t \nu) f_j^1(1) = \frac{\Delta t^2}{\Delta x}\frac{\nu}{\eta}\left(a - \frac{1}{2}\right) + \mathcal{O}(\Delta t^3).$$

When $a < \frac{1}{2}$ f becomes negative for Δt small enough.

Correction of the reconstruction

Time reconstruction of the interface



$$
\begin{aligned}
\rho^{n-}_{i+1/2}(t) &= \rho_i^n e^{-\nu(t-t_n)} + \rho_{i+1/2}(1-e^{-\nu(t-t_n)}),\\
\rho^{n+}_{i+1/2}(t) &= \rho_{i+1}^n e^{-\nu(t-t_n)} + \rho_{i+1/2}(1-e^{-\nu(t-t_n)}),\\
\rho(t,x) &= \begin{cases} \rho^{n-}_{i+1/2}(t) + \delta_x^L \rho^n_{i+1/2}(t)(x-x_{i+1/2}) \text{ if } x < x_{i+1/2} \\ \rho^{n+}_{i+1/2}(t) + \delta_x^R \rho^n_{i+1/2}(t)(x-x_{i+1/2}) \text{ if } x > x_{i+1/2} \end{cases},
\end{aligned}
$$

Modified UGKS

The new flux $\tilde{\phi}$ is the following:

$$\begin{aligned}
\tilde{\phi}_{i+1/2}(v) &= \phi_{i+1/2}(v) \\
&+ \frac{2F_{i+1/2}}{\Delta x} v(-\delta_x^L \rho^n_{i+1/2} \mathbb{1}_{v>0} + \delta_x^R \rho^n_{i+1/2} \mathbb{1}_{v<0}) \\
&+ G_{i+1/2} v^2(-\delta_x^L \rho^n_{i+1/2} \mathbb{1}_{v>0} + \delta_x^R \rho^n_{i+1/2} \mathbb{1}_{v<0}),
\end{aligned}$$

with

$$\begin{aligned}
F(\Delta t, \eta, \epsilon, \sigma) &= -\frac{1}{\eta}\left[e^w + \frac{1-e^w}{w}\right], \\
G(\Delta t, \eta, \epsilon, \sigma) &= -\frac{\epsilon}{2\sigma\eta}\left[we^w - 2\left(e^w + \frac{1-e^w}{w}\right)\right], \\
w &= -\frac{\sigma}{\epsilon\eta}\Delta t \in \mathbb{R}_-
\end{aligned}$$

F and G vanish in both transport and diffusion regimes.

Stability conditions

Realisibility

If σ is constant then the new scheme is stable under the condition:

$$
\begin{aligned}
\Delta t &\leq \frac{\Delta x}{A(w) + \dfrac{F(w)}{2} - \dfrac{2D(w)}{3\Delta x}} + \frac{\Delta t}{w} \frac{2F(w) + C(w) - \dfrac{4D(w)}{\Delta x}}{A(w) + \dfrac{F(w)}{2} - \dfrac{2D(w)}{3\Delta x}}, \\
0 &\leq -w \left(\min_i \mu(-|\beta_i^n|) A(w) + \frac{F(w)}{4} - \frac{D(w)}{3\Delta x} \right) + \frac{\sigma}{\epsilon} D(w).
\end{aligned}
$$

It may imply that once this inequality is satisfied the scheme may also respect a numerical second principle.

Linear-Fokker-Planck: model

Equation

$$\eta\partial_t f + v\partial_x f = \frac{\sigma}{\varepsilon}\partial_v\Big((c^2 - v^2)\partial_v f\Big), \text{ with } v \in [-c, c] \tag{21}$$

Diffusive limit

$$\partial_t\rho + \partial_x(\kappa\partial_x\rho) = 0, \text{ with } \kappa = \frac{c^2}{6\sigma} \tag{22}$$

Coefficients

The coefficients A,C,D are given by (using the notation $w = -2\sigma\Delta t/(\eta\varepsilon)$):

$$\mathrm{A}(\Delta t,\sigma,\eta,\varepsilon) = \frac{1}{\eta w}(e^{w}-1) \tag{23}$$

$$\mathrm{C}(\Delta t,\sigma,\eta,\varepsilon) = \frac{1}{\eta} - \mathrm{A}(\Delta t,\sigma,\eta,\varepsilon) \tag{24}$$

$$\mathrm{D}(\Delta t,\sigma,\eta,\varepsilon) = -\frac{\varepsilon}{2\sigma}(\mathrm{C}(\Delta t,\sigma,\eta,\varepsilon) - \mathrm{A}(\Delta t,\sigma,\eta,\varepsilon)) - \frac{\varepsilon}{2\eta\sigma}e^{w}. \tag{25}$$

Linear-Fokker-Planck: numerical tests

Result

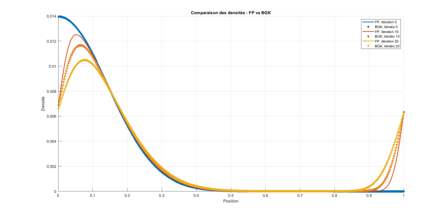


Figure: Global

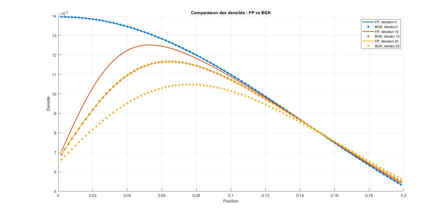


Figure: Zoom

The scheme in the electronic transport context

The electronic transport equation

$$\partial_t f + \frac{v}{\eta}\mathbf{\Omega} \cdot \nabla_{\mathbf{x}} f = \nu \left(M[f] - f \right), \tag{26}$$

Where:

- $f : (t, \mathbf{x}, v, \mathbf{\Omega}) \mapsto f(t, \mathbf{x}, v, \mathbf{\Omega})$ is the particle distribution function.
- $\mathbf{x} \in \mathrm{D}$, an open set of $\mathbb{R}^2$, is the space variable.
- $v \in \mathbb{R}_+$ is the velocity and $\mathbf{\Omega} \in \mathrm{S}^2$ is the direction.
- $\nu(\mathbf{W}) = \frac{C}{\epsilon\eta}\frac{\rho^{5/2}}{q^{3/2}}$ is the scattering coefficient.
- $M[f](v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{v^2}{2T}\right)$ is the Maxwellian ($T = \frac{2q}{3\rho}$).

The conserved variables are

$$\mathbf{W} = \begin{pmatrix} \rho & q \end{pmatrix}^T = \int_{\mathscr{S}^2} \int_0^{+\infty} \begin{pmatrix} 1 & \frac{1}{2}v^2 \end{pmatrix}^T f(t, \mathbf{x}, v, \mathbf{\Omega}) v^2 \mathrm{d}v \mathrm{d}\Omega.$$

The M1 distribution function is $\hat{f}(\boldsymbol{\Omega}) = e^{\alpha + \boldsymbol{\beta}\cdot\boldsymbol{\Omega}}$. The angular M1 moment model is

$$\begin{cases} \partial_t f_0 + \frac{v}{\eta} \nabla_{\mathbf{x}} \cdot \mathbf{f}_1 = \nu(M_0[f_0] - f_0) \\ \partial_t \mathbf{f}_1 + \frac{v}{\eta} \nabla_{\mathbf{x}} \cdot \mathbf{f}_2 = -\nu \mathbf{f}_1 \end{cases}, \tag{27}$$

where:

- $\mathbf{f}_i(t, \mathbf{x}, v) = \langle \Omega^{\otimes i} f(t, \mathbf{x}, v, \boldsymbol{\Omega}) \rangle = \int_{\mathscr{S}^2} \boldsymbol{\Omega}^{\otimes i} f(t, \mathbf{x}, v, \boldsymbol{\Omega}) \mathrm{d}\Omega$ are the angular moments,
- $\mathbf{f}_2 = \left\langle \boldsymbol{\Omega} \otimes \boldsymbol{\Omega} \hat{f} \right\rangle = f_0 \frac{u}{||\boldsymbol{\beta}||} \mathbf{I}_3 + f_0 \left(1 - 3\frac{u}{||\boldsymbol{\beta}||}\right) \frac{\boldsymbol{\beta}}{||\boldsymbol{\beta}||} \otimes \frac{\boldsymbol{\beta}}{||\boldsymbol{\beta}||}$ is the flux closed with the M1 distribution function.

Diffusion limit

In the diffusion limit ($\epsilon \to 0$), the macroscopic variables satisfies a non-linear diffusion system:

$$\begin{cases} \partial_t \rho & = \boldsymbol{\nabla}_{\mathbf{x}} \cdot \left(\dfrac{2}{3\sigma} \boldsymbol{\nabla}_{\mathbf{x}} q \right) + \mathcal{O}(\epsilon) \\ \partial_t q & = \boldsymbol{\nabla}_{\mathbf{x}} \cdot \left(\dfrac{5}{3} \dfrac{2}{3\sigma} \boldsymbol{\nabla}_{\mathbf{x}} \left(\dfrac{q^2}{\rho} \right) \right) + \mathcal{O}(\epsilon) \end{cases} . \tag{28}$$

For a uniform Cartesian grid, the finite volume formulation of the kinetic equation is

$$\frac{f_{i,j}^{n+1}-f_{i,j}^{n}}{\Delta t}+\frac{\phi_{i+1/2,j}-\phi_{i-1/2,j}}{\Delta x}+\frac{\phi_{i,j+1/2}-\phi_{i,j-1/2}}{\Delta y}= \nu(\mathbf{W}_{i,j}^{n+1})\left(M[\boldsymbol{W}_{i,j}^{n+1}]-f_{i,j}^{n+1}\right). \tag{29}$$

The integral solution of the kinetic equation

$$\begin{aligned} f(t,\mathbf{x}_{i+1/2,j},v,\boldsymbol{\Omega}) &\approx e^{-\nu^n_{i+1/2,j}(t-t_n)} f(t_n,\mathbf{x}_{i+1/2,j}-\frac{v}{\eta}(t-t_n)\boldsymbol{\Omega},v,\boldsymbol{\Omega}) \\ &+\nu^n_{i,j+1/2}\int_{t_n}^{t} e^{-\nu^n_{i+1/2,j}(t-s)} M[\mathbf{W}](s,\mathbf{x}_{i+1/2,j}-\frac{v}{\eta}(t-s)\boldsymbol{\Omega},v)\mathrm{d}s, \end{aligned} \tag{30}$$

is used to compute the microscopic fluxes using adequate reconstructions of the distribution function and of the Maxwellian.

The microscopic flux is

$$\begin{aligned}\phi_{i+1/2,j}(v,\boldsymbol{\Omega}) =& A^n_{i+1/2,j} v\Omega_x \left(f^{n(+)}_{i,j} \mathbb{1}_{\Omega_x>0} + f^{n(-)}_{i+1,j} \mathbb{1}_{\Omega_x<0} \right) \\ &+ B^n_{i+1/2,j} v^2 \Omega_x^2 (\delta_x f^n_{i,j} \mathbb{1}_{\Omega_x>0} + \delta_x f^n_{i+1,j} \mathbb{1}_{\Omega_x<0}) \\ &+ C^n_{i+1/2,j} v\Omega_x M[\mathbf{W}^n_{i+1/2,j}] \\ &+ D^n_{i+1/2,j} v^2 \Omega_x^2 \left(\delta^L_x M^n_{i+1/2,j} \mathbb{1}_{\Omega_x>0} + \delta^R_x M^n_{i+1/2,j} \mathbb{1}_{\Omega_x<0} \right),\end{aligned} \tag{31}$$

where $\delta^{LR}_x M^n_{i+1/2,j}$ are the Maxwellian slopes.

A numerical scheme for this moment model can be obtained by following the same procedure using UGKS. The finite volume formulations are

$$\frac{f_{i,j}^{0,n+1} - f_{i,j}^{0,n}}{\Delta t} + \frac{1}{\Delta x}(\chi^0_{i+1/2,j} - \chi^0_{i-1/2,j}) + \frac{1}{\Delta y}(\chi^0_{i,j+1/2} - \chi^0_{i,j-1/2}) \tag{32a}$$
$$= \nu_{i,j}^{n+1}(M_0[\mathbf{W}_{i,j}^{n+1}] - f_{i,j}^{0,n+1}),$$
$$\frac{\mathbf{f}_{i,j}^{1,n+1} - \mathbf{f}_{i,j}^{1,n}}{\Delta t} + \frac{1}{\Delta x}(\boldsymbol{\chi}^1_{i+1/2,j} - \boldsymbol{\chi}^1_{i-1/2,j}) + \frac{1}{\Delta y}(\boldsymbol{\chi}^1_{i,j+1/2} - \boldsymbol{\chi}^1_{i,j-1/2}) \tag{32b}$$
$$= -\nu_{i,j}^{n+1}\mathbf{f}_{i,j}^{1,n+1}.$$

where the fluxes are angular moments of the UGKS microscopic flux computed with $f_{i,j}^n = \hat{f}_{i,j}^n = e^{\alpha_{i,j}^n + \beta_{i,j}^n \cdot \boldsymbol{\Omega}}$.

The mesoscopic fluxes are

$$\chi^0_{i+1/2,j}(v) = A^n_{i+1/2,j} v \left\langle \Omega_x \hat{f}^n_{i,j} \mathbb{1}_{\Omega_x>0} + \Omega_x \hat{f}^n_{i+1,j} \mathbb{1}_{\Omega_x<0} \right\rangle + \frac{D^n_{i+1/2,j}}{6} v^2 M[\mathbf{W}^n_{i+1/2,j}] \left(\mathbf{\Gamma}^{nL}_{i+1/2,j} + \mathbf{\Gamma}^{nR}_{i+1/2,j} \right) \cdot \mathbf{\Psi}(v), \tag{33a}$$

$$\boldsymbol{\chi}^1_{i+1/2,j}(v) = A^n_{i+1/2,j} v \left\langle \Omega_x \boldsymbol{\Omega} \hat{f}^n_{i,j} \mathbb{1}_{\Omega_x>0} + \Omega_x \boldsymbol{\Omega} \hat{f}^n_{i+1,j} \mathbb{1}_{\Omega_x<0} \right\rangle + \frac{C^n_{i+1/2,j}}{3} v M[\mathbf{W}^n_{i+1/2,j}] \mathbf{e}_x + \frac{D^n_{i+1/2,j}}{8} v^2 M[\mathbf{W}^n_{i+1/2,j}] \left(\mathbf{\Gamma}^{nL}_{i+1/2,j} - \mathbf{\Gamma}^{nR}_{i+1/2,j} \right) \cdot \mathbf{\Psi}(v) \mathbf{e}_x. \tag{33b}$$

Diffusion limit

In the diffusion regime, the limit macroscopic flux

$$\mathbf{\Phi}_{i+1/2,j} = \left\langle \begin{pmatrix} 1 \\ \frac{1}{2}v^2 \end{pmatrix} \chi^0_{i+1/2,j}(v) \right\rangle \underset{\epsilon \to 0}{\longrightarrow} \frac{-2}{3\sigma_{i+1/2,j}} \begin{pmatrix} \dfrac{q^n_{i+1,j} - q^n_{i,j}}{\Delta x} \\ \dfrac{5}{3}\dfrac{y^n_{i+1,j} - y^n_{i,j}}{\Delta x} \end{pmatrix}, \qquad (34)$$

is the second order centred flux for the diffusion system where $y = \frac{q^2}{\rho}$.

Diffusion schemes

Different diffusion schemes can be recovered depending on the set of variables used in the Maxwellian reconstructions. To recover the "natural" diffusion scheme, the variables $(\rho, \frac{q^2}{\rho})$ have to be chosen in the Maxwellian slopes.

Angular half-moments of the M1 distribution function

The integrals of the form $\int_{\mathscr{S}^2} \Omega_x^k \Omega_y^l e^{\alpha+\boldsymbol{\beta}\cdot\boldsymbol{\Omega}} \mathbb{1}_{\Omega_x \lesseqgtr 0} \mathrm{d}\Omega$ are not analytical.

To overcome this problem, we perform a Gauss-Legendre quadrature formula on a reduced form of the half-moments:

$$\left\langle \Omega_z^k \hat{f} \mathbb{1}_{\Omega_z \geq 0} \right\rangle = f_0 \frac{||\beta||}{2\sinh ||\beta||} \int_0^1 \mu^k e^{\beta_z \mu} \mathrm{I}_0(\beta_{xy}\sqrt{1-\mu^2}) \mathrm{d}\mu. \tag{35}$$

Quadrature

In practice, to reduce the computational cost, few points are used. Consistent fluxes are recovered by performing a renormalization to ensure

$$\left\langle \Omega_z \hat{f} \mathbb{1}_{\Omega_z > 0} \right\rangle_{GL} + \left\langle \Omega_z \hat{f} \mathbb{1}_{\Omega_z < 0} \right\rangle_{GL} = \left\langle \Omega_z \hat{f} \right\rangle. \tag{36}$$

Nonlocal thermal transport

This model allows to describe nonlocal thermal transport effects. The local flux is $\phi_q^L = -\frac{10}{9\sigma}\nabla_{\mathbf{x}}\frac{q^2}{\rho}$ and the nonlocal one is $\phi_q^{NL} = \frac{1}{\eta}\left\langle v^3 \mathbf{f}_1 \right\rangle$.

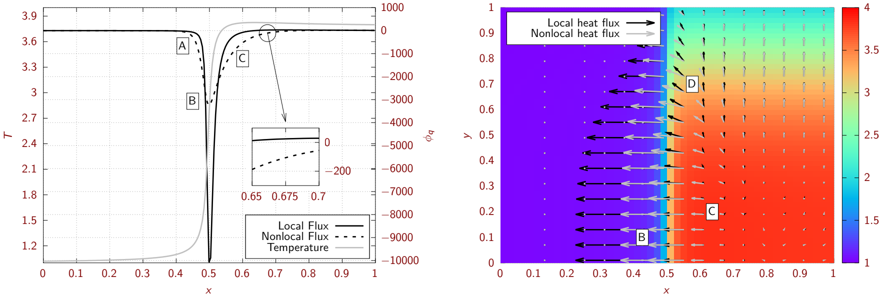


Figure: Temperature, local and nonlocal heat fluxes in the domain (**A**-preheating, **B**-flux limitation, **C**-anti-natural flux and **D**-flux rotation).

Conclusion and perspectives

- In the linear transport context, we proposed a numerical procedure to obtain numerical schemes for moment models.
  - This method is **general** and has been applied to **M1** and **M2**.
  - A **second order** extension has been proposed and the scheme has been shown to be **highly accurate**.
  - The **realizability** can be ensured under a CFL-like condition.
- This work has been extended for the M1 model of electronic transport.
  - A quadrature method has been developed to compute the **half angular moments** of the M1 distribution function.
  - **Arbitrary diffusion schemes** can be easily recovered.
  - A **second order** extension has also been proposed and the scheme has been shown to be **highly accurate**.
- This scheme is currently being adapted to unstructured meshes.
- Extension to non relaxation operators of collision

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M2 moment model

The M2 distribution function is $\hat{f}(v) = e^{\alpha+\beta v+\gamma v^2}$. For $\mathbf{m} = \begin{pmatrix} 1 & v & v^2 \end{pmatrix}^T$, the M2 moment model is

$$\begin{cases} \eta\partial_t \rho + \partial_x j &= 0, \\ \eta\partial_t j + \partial_x q &= -\dfrac{\sigma}{\epsilon} j, \\ \eta\partial_t q + \partial_x k &= \dfrac{\sigma}{\epsilon}\left(\dfrac{1}{3}\rho - q\right), \end{cases} \tag{37}$$

where $k = \left\langle v^3 \hat{f}(v) \right\rangle$.

Legendre basis

The Legendre basis $\mathbf{m} = \begin{pmatrix} 1 & v & \frac{3}{2}\left(v^2 - \frac{1}{3}\right) \end{pmatrix}^T$ can be used to recover a diagonal source term.

The FV formulation is

$$\frac{\rho_i^{n+1}-\rho_i^n}{\Delta t}+\frac{1}{\Delta x}(\Phi^{\rho}_{i+1/2}-\Phi^{\rho}_{i-1/2})=0, \tag{38a}$$

$$\frac{j_i^{n+1}-j_i^n}{\Delta t}+\frac{1}{\Delta x}(\Phi^{j}_{i+1/2}-\Phi^{j}_{i-1/2})=\frac{-\sigma}{\eta\epsilon}j_i^{n+1}, \tag{38b}$$

$$\frac{q_i^{n+1}-q_i^n}{\Delta t}+\frac{1}{\Delta x}(\Phi^{q}_{i+1/2}-\Phi^{q}_{i-1/2})=\frac{\sigma}{\eta\epsilon}\left(\frac{1}{3}\rho_i^{n+1}-q_i^{n+1}\right), \tag{38c}$$

where the first order in space UGKS-M2 fluxes are:

$$\Phi^{\rho}_{i+1/2}=A\left\langle v\hat{f}_i^n\mathbb{1}_{v>0}+v\hat{f}_{i+1}^n\mathbb{1}_{v<0}\right\rangle+\frac{D}{3\Delta x}(\rho_{i+1}^n-\rho_i^n), \tag{39a}$$

$$\Phi^{j}_{i+1/2}=A\left\langle v^2\hat{f}_i^n\mathbb{1}_{v>0}+v^2\hat{f}_{i+1}^n\mathbb{1}_{v<0}\right\rangle+\frac{C}{3}\rho_{i+1/2}^n, \tag{39b}$$

$$\Phi^{q}_{i+1/2}=A\left\langle v^3\hat{f}_i^n\mathbb{1}_{v>0}+v^3\hat{f}_{i+1}^n\mathbb{1}_{v<0}\right\rangle+\frac{D}{5\Delta x}(\rho_{i+1}^n-\rho_i^n). \tag{39c}$$

From a numerical point of view, the entropic variables are computed by solving for $\mathbf{\Lambda}$ in the non linear equation

$$\mathbf{U} = \left\langle \mathbf{m} e^{\mathbf{\Lambda}\cdot\mathbf{m}(v)} \right\rangle, \tag{40}$$

using a gradient descent algorithm. The first equation can be expressed using special functions (complementary error and Dawson functions):

$$\rho = \frac{e^{\alpha+\gamma}}{2\sqrt{|\gamma|}} \begin{cases} e^{\beta} F_+\left(\sqrt{|\gamma|} + \frac{\beta}{2\sqrt{|\gamma|}}\right) - e^{-\beta} F_+\left(-\sqrt{|\gamma|} + \frac{\beta}{2\sqrt{|\gamma|}}\right) & \gamma > 0 \\ e^{-\beta} F_-\left(-\sqrt{|\gamma|} - \frac{\beta}{2\sqrt{|\gamma|}}\right) - e^{\beta} F_-\left(\sqrt{|\gamma|} - \frac{\beta}{2\sqrt{|\gamma|}}\right) & \gamma < 0 \end{cases} \tag{41}$$

The entropic variables are then used to compute the half moments (using a similar expression) in the fluxes.

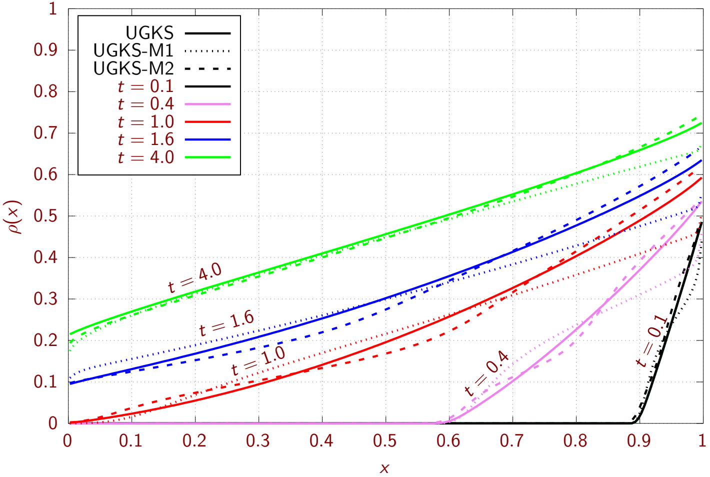


Figure: Density in the domain at time $t = 0.1, 0.4, 1.0, 1.6$ and 4.0.

Unstructured meshes

From a formal point of view, the extension to unstructured meshes is quite straightforward. The main difficulty is to obtain a good diffusion flux in the limit. Indeed, the finite volume formulation of the diffusion equation in an unstructured context is (for cell K)

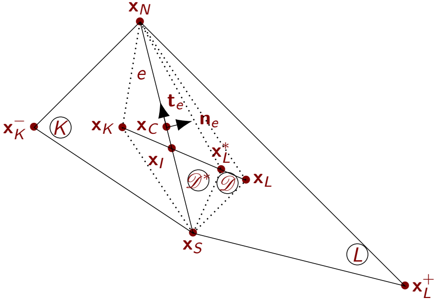
$$\frac{\mathbf{W}_K^{n+1} - \mathbf{W}_K^n}{\Delta t} = \sum_{L | e = K \cap L} \frac{|e|}{|K|} \mathbf{\Phi}_{KL/e}, \tag{42}$$

where $\mathbf{\Phi}_{KL/e} = \frac{2}{3\sigma_e} \begin{pmatrix} \nabla q \cdot \mathbf{n}_e \\ \frac{5}{3} \nabla \frac{q^2}{\rho} \cdot \mathbf{n}_e \end{pmatrix} (\mathbf{x}_e)$.

Normal gradient on general meshes

On general meshes, the approximation $(\nabla q \cdot \mathbf{n}_e)(\mathbf{x}_e) = \dfrac{q_L - q_K}{|\mathbf{x}_K - \mathbf{x}_L|}$ does not ensure the consistency of the diffusion scheme.

The main idea of the diamond scheme is to to compute the gradient on the diamond $\mathscr{D}$ using appropriate reconstructions.



$$\begin{aligned}\mathbf{P} &= \frac{1}{|\mathscr{D}|}\int_{\mathscr{D}} \nabla U \\ &= \left(\frac{U_E - U_W}{(\mathbf{x}_E - \mathbf{x}_W)\cdot \mathbf{n}_e} - \kappa \frac{U_N - U_S}{|\mathbf{e}|}\right)\mathbf{n}_e + \frac{U_N - U_S}{|\mathbf{e}|}\mathbf{t}_e\end{aligned} \tag{43}$$

Diamond Scheme in UGKS

In UGKS, the Maxwellian reconstruction determines the limit diffusion scheme. We need to define two slopes in the reconstruction:

$$\tilde{M}(t,x,y,\cdot) = M[\mathbf{W}^n_{i+1/2,j}] + \begin{cases} \delta_x^L M^n_{i+1/2,j}(x - x_{i+1/2,j}) & \text{if } x \leq x_{i+1/2,j} \\ \delta_x^R M^n_{i+1/2,j}(x - x_{i+1/2,j}) & \text{if } x \geq x_{i+1/2,j} \end{cases}. \tag{44}$$

Those slopes are computed based on the gradient of the macroscopic variables. Those gradients can be computed based on the diamond scheme. However, the Maxwellian slopes need to be defined on the half spaces, thus half gradients should be introduced.

Natural idea

The half-gradients could be computed based on the half diamond on each side of the interface.