Quadrature based Lattice Boltzmann scheme for dense gases using the simplified Enskog collision operator

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24th November 2022

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Outline

1. The Enskog model
2. The simplified Enskog collision operator
3. Shock wave propagation

The Enskog equation (II)

- The dynamics of the system of particles can be described by the following *exact* kinetic equation[1]:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f = J_E =$$
$$\sigma^2 \int_{\mathbb{R}^3} d\boldsymbol{v}_* \int_{\mathcal{S}_+} d^2\hat{\boldsymbol{k}} \left\{ f_2(\boldsymbol{r}, \boldsymbol{v}', \boldsymbol{r} + \sigma\,\hat{\boldsymbol{k}}, \boldsymbol{v}'_*) - f_2(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{r} - \sigma\,\hat{\boldsymbol{k}}, \boldsymbol{v}_*) \right\} (\boldsymbol{v}_r \cdot \hat{\boldsymbol{k}}).$$

- Let us now make the following *simplifying* assumption:
  - Short-range correlations are taken into account as in Enskog theory:

$$f_2(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{r} \pm d\,\hat{\boldsymbol{k}}, \boldsymbol{v}_*, t) = \chi\left[n\left(\boldsymbol{r} \pm \frac{\sigma}{2}\hat{\boldsymbol{k}}\right)\right] f(\boldsymbol{r}, \boldsymbol{v}, t) f(\boldsymbol{r} \pm \sigma\,\hat{\boldsymbol{k}}, \boldsymbol{v}_*, t).$$

  where χ is the contact value of the pair correlation function of a hard sphere fluid.
- Non-local collision are natural when dealing with non-punctiform particles

[1] J. Karkheck and G. Stell, "Mean field kinetic theories," J. Chem. Phys. 75, 1475 (1981)

The Enskog equation (III)

- Different expression of the contact value of the pair correlation function can be used:

  - Standard Enskog Theory (SET): value of the pair correlation function in a fluid in *uniform equilibrium* with density at the contact point.

$$\chi = \chi_{\text{SET}}\left(n\left(\boldsymbol{r} \pm \frac{a}{2}\hat{\boldsymbol{k}}\right)\right) = \frac{1}{nb}\left(\frac{p^{CS}}{nk_BT} - 1\right) = \frac{1}{2}\frac{2-\eta}{(1-\eta)^3}; \; b = \frac{2\pi\sigma^3}{3}; \; \eta = \frac{\pi\sigma^3 n}{6}.$$

where p^{CS} is given by:

$$p^{CS} = nk_BT\frac{1+\eta+\eta^2-\eta^3}{(1-\eta)^3} \qquad (1)$$

The Enskog equation (III)

- Different expression of the contact value of the pair correlation function can be used:

  - Revised Enskog Theory (RET): value of the pair correlation function in a fluid in *non-uniform equilibrium* with density at the contact point.

Fischer-Methfessel approximation $\rightsquigarrow$ $\chi = \chi_{\text{RET-FM}}\left[n\left(\boldsymbol{r} \pm \frac{\sigma}{2}\hat{\boldsymbol{k}}\right)\right] = \chi_{\text{SET}}\left(\overline{n}\left(\boldsymbol{r} \pm \sigma\frac{\hat{\boldsymbol{k}}}{2}\right)\right).$

where

$$\overline{n}(\boldsymbol{r},t) = \frac{3}{4\pi\sigma^3}\int_{\mathcal{S}} n(\boldsymbol{r}_1,t)w(\boldsymbol{r},\boldsymbol{r}_1)\,d\boldsymbol{r}_1, \qquad w(\boldsymbol{r},\boldsymbol{r}_1) = \begin{cases} 1, & \|\boldsymbol{r}_1 - \boldsymbol{r}\| < \sigma \\ 0, & \|\boldsymbol{r}_1 - \boldsymbol{r}\| > \sigma \end{cases}.$$

The Enskog equation (IV)

The right-hand side is given by the Enskog collision operator J_E which reads[1]:

$$J_E = \sigma^2 \int \left\{ \chi\left(\boldsymbol{x} + \frac{\sigma}{2}\boldsymbol{k}\right) f(\boldsymbol{x}, \boldsymbol{p}^*) f(\boldsymbol{x} + \sigma\boldsymbol{k}, \boldsymbol{p}_1^*) - \chi\left(\boldsymbol{x} - \frac{\sigma}{2}\boldsymbol{k}\right) f(\boldsymbol{x}, \boldsymbol{p}) f(\boldsymbol{x} - \sigma\boldsymbol{k}, \boldsymbol{p}_1) \right\} (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} \quad (2)$$

where σ is the molecular diameter. $\boldsymbol{p_r} = \boldsymbol{p_1} - \boldsymbol{p}$ is the relative momentum and $\boldsymbol{k}$ is the unit vector giving the relative position of the two colliding particles. In the equation above, the distribution function dependence on time t was dropped for brevity. The superscript $*$ refers to the post-collision momenta.

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

By assuming that the factor χ and the distribution functions are smooth functions one can approximate these functions in the Enskog collision integral through a Taylor series near the point $\boldsymbol{x}$. The resulting terms up first order gradient are[1]:

$$J_0(f,f) = \chi \int (f^* f_1^* - f f_1) \Omega^2 (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} \tag{3}$$

$$\begin{aligned} J_1(f,f) &= \chi\sigma \int \boldsymbol{k} (f^* \boldsymbol{\nabla} f_1^* - f \boldsymbol{\nabla} f_1) \Omega^2 (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} \\ &+ \frac{\sigma}{2} \int \boldsymbol{k} \boldsymbol{\nabla} \chi (f^* f_1^* - f f_1) \Omega^2 (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} \end{aligned} \tag{4}$$

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

The collision term $J_0(f, f)$ is the usual collision term of the Boltzmann equation multiplied by χ, and is treated as such, by applying the usual relaxation time approximation. In this paper we will employ the Shakhov collision term[1], namely:

$$J_0(f, f) = -\frac{1}{\tau}(f - f^S), \tag{5}$$

where τ is the relaxation time and f_S is the equilibrium Maxwell-Boltzmann distribution times a correction factor[1]:

$$f^S = f_{\text{MB}} \left[1 + \frac{1 - \text{Pr}}{P_i k_B T}\left(\frac{\boldsymbol{\xi}^2}{5mk_B T} - 1\right)\boldsymbol{\xi} \cdot \boldsymbol{q}\right], \quad \boldsymbol{q} = \int d^3p f \frac{\boldsymbol{\xi}^2}{2m}\frac{\boldsymbol{\xi}}{m}, \tag{6}$$

where $\boldsymbol{\xi} = \boldsymbol{p} - m\boldsymbol{u}$ is the peculiar momentum, $\text{Pr} = c_P \mu / \lambda$ is the Prandtl number, $c_P = 5k_B/2m$ is the specific heat at constant pressure and $P_i = \rho RT = nk_B T$ is the ideal gas equation of state, with R being the specific gas constant. The Maxwell-Boltzmann distribution f_{MB} is given by:

$$f_{\text{MB}} = \frac{n}{(2m\pi k_B T)^{3/2}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2mk_B T}\right) \tag{7}$$

[1] E. Shakhov, "Approximate kinetic equations in rarefied gas theory," Fluid Dynamics 3, 95 – 96 (1968).

The simplified Enskog collision operator

The second term of J_E, namely $J_1(f, f)$, can be approximated by replacing the distribution functions (f^*, f_1^*, f, f_1) with the corresponding equilibrium distribution functions. By using $f^*_{\text{MB}} f^*_{\text{MB},1} = f_{\text{MB}} f_{\text{MB},1}$, and integrating over $\boldsymbol{k}$ and $\boldsymbol{p_1}$, one obtains[2]:

$$J_1(f,f) \approx J_1(f_{\text{MB}}, f_{\text{MB}}) = \\ - b\rho\chi f_{\text{MB}} \left\{ \boldsymbol{\xi} \left[\nabla \ln(\rho^2 \chi T) + \frac{3}{5}\left(\zeta^2 - \frac{5}{2}\right) \nabla \ln T \right] \right. \\ \left. + \frac{2}{5}\left[2\boldsymbol{\zeta}\boldsymbol{\zeta} : \nabla \boldsymbol{u} + \left(\zeta^2 - \frac{5}{2}\right) \nabla \cdot \boldsymbol{u} \right] \right\} \qquad (8)$$

where $\boldsymbol{\zeta} = \boldsymbol{\xi} / \sqrt{2RT}$.
With the above approximations and considering no external force, the Enskog equation becomes:

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \nabla_{\boldsymbol{x}} f = -\frac{1}{\tau}(f - f_S) + J_1(f_{\text{MB}}, f_{\text{MB}}) \qquad (9)$$

[2] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

The Chapman-Enskog expansion yields the following conservation equations for mass, momentum and energy[1]:

$$\frac{D\rho}{Dt} + \rho\nabla\boldsymbol{u} = 0 \tag{10a}$$

$$\rho\frac{D\boldsymbol{u}}{Dt} + \nabla P = -\nabla\cdot\Pi \tag{10b}$$

$$\rho\frac{De}{Dt} + P\nabla\cdot\boldsymbol{u} = -\nabla\cdot\boldsymbol{q} + \Pi : \nabla\boldsymbol{u} \tag{10c}$$

where $D/Dt = \partial_t + \boldsymbol{u}\cdot\nabla$ is the material derivative and $P = P_i(1 + b\rho\chi)$ is the equation of state of a non-ideal gas. The heat flux and the viscous part of the stress tensor $\Pi_{\alpha\beta}$ are given by:

$$\boldsymbol{q} = -\lambda\nabla T, \tag{11}$$

$$\Pi = -\mu_v\mathcal{I}\boldsymbol{\nabla}\cdot\boldsymbol{u} - \mu\left(\nabla u + (\nabla u)^T - \tfrac{2}{3}\mathcal{I}\boldsymbol{\nabla}\cdot\boldsymbol{u}\right) \tag{12}$$

where $\mathcal{I}$ is the identity matrix.

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

The bulk viscosity μ_v, shear viscosity μ and the thermal conductivity λ are given by[1]:

$$\mu_v = \frac{16}{5\pi}\mu_0 b^2\rho^2\chi, \tag{13a}$$

$$\mu = \tau P_i = \mu_0 b\rho\left(\frac{1}{b\rho\chi} + 0.8 + \frac{4}{25}\left(1 + \frac{12}{\pi}\right)b\rho\chi\right), \tag{13b}$$

$$\lambda = \frac{5}{2}\frac{\tau P_i}{\mathrm{Pr}} = \lambda_0 b\rho\left(\frac{1}{b\rho\chi} + 1.2 + \frac{9}{25}\left(1 + \frac{32}{9\pi}\right)b\rho\chi\right), \tag{13c}$$

where $\mu_0 = \mu_{\text{ref}}\sqrt{T/T_0}$ is the viscosity coefficient for hard sphere molecules, with μ_{ref} representing the viscosity coefficient for dilute gases at temperature T_0, and $\lambda_0 \equiv \lambda_{\text{ref}}$ is the reference thermal conductivity at temperature T_0. The reference values are:

$$\mu_{\text{ref}} = \frac{5}{16\sigma^2}\sqrt{\frac{mk_BT_0}{\pi}}, \qquad \lambda_{\text{ref}} = \frac{75k_B}{64m\sigma^2}\sqrt{\frac{mk_BT_0}{\pi}}. \tag{14}$$

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

From here it follows directly that the relaxation time τ is given by:

$$\tau = \frac{\mu}{P_i} \tag{15}$$

Note that the viscosity of the dense gas of a fixed reduced density η can be changed by varying the molecular diameter σ and the number density n. By using the reference mean free path $l = m/\sqrt{2}\pi\sigma^2 n\chi$, one can define the degree of denseness E_l introduced by Frezzotti and Sgarra[3], given by the ratio of the molecular diameter and the mean free path:

$$E_l = \frac{\sigma}{l} = \frac{3}{\sqrt{2}} bn\chi. \tag{16}$$

The relaxation time τ can be rewritten as the molecular diameter σ times a functional g of η:

$$\tau = \sigma g[\eta] \tag{17}$$

such that one can vary τ at constant reduced density η by changing σ.

[3] A. Frezzotti and C. Sgarra, "Numerical analysis of a shock-wave solution of the Enskog equation obtained via a Monte Carlo method," J. Stat. Phys. 73, 193–207 (1993).

Reduced distributions

The y and z degrees of freedom can be integrated out and two reduced distribution functions, ϕ and θ, can be introduced as[4]:

$$\phi(\boldsymbol{x}, p_x, t) = \int dp_y dp_z f(\boldsymbol{x}, \boldsymbol{p}, t), \tag{18}$$

$$\theta(\boldsymbol{x}, p_x, t) = \int dp_y dp_z \frac{p_y^2 + p_z^2}{m} f(\boldsymbol{x}, \boldsymbol{p}, t) \tag{19}$$

In the following, all dependencies of the reduced distribution functions will be dropped for brevity. The macroscopic moments can be evaluated as:

$$\begin{pmatrix} n \\ \rho u_x \\ \Pi_{xx} \end{pmatrix} = \int dp_x \begin{pmatrix} 1 \\ p_x \\ \frac{\xi_x^2}{m} \end{pmatrix} \phi, \tag{20}$$

$$\begin{pmatrix} \frac{3}{2} n k_B T \\ q_x \end{pmatrix} = \int dp_x \begin{pmatrix} 1 \\ \frac{\xi_x}{m} \end{pmatrix} \left(\frac{\xi_x^2}{2m} \phi + \frac{1}{2} \theta \right) \tag{21}$$

[4] V. E. Ambrus and V. Sofonea, “Quadrature-based lattice Boltzmann models, for rarefied gas flow,” in Flowing Matter, (Springer International Publishing, Cham, 2019) pp. 271–299.

Reduced distributions

The evolution equations for the reduced distribution functions are:

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi\\ \theta\end{pmatrix} + \frac{p_x}{m}\frac{\partial}{\partial x}\begin{pmatrix}\phi\\ \theta\end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix}\phi-\phi_S\\ \theta-\theta_S\end{pmatrix} + \begin{pmatrix}J_1^{\phi}\\ J_1^{\theta}\end{pmatrix} \qquad (22)$$

In the above the, ϕ_S and θ_S are given by:

$$\phi_S = f_{\text{MB}}^x\left[1+\frac{1-\text{Pr}}{5P_i m k_B T}\left(\frac{\xi_x^2}{mk_BT}-3\right)\xi_x q_x\right],$$

$$\theta_S = 2k_BT f_{\text{MB}}^x\left[1+\frac{1-\text{Pr}}{5P_i m k_B T}\left(\frac{\xi_x^2}{mk_BT}-1\right)\xi_x q_x\right]$$

$$J_1^{\phi} = -\left[\xi_x\partial_x\ln\chi + 2\xi_x\partial_x\ln\rho + \frac{3}{5}\left(\frac{\xi_x^2}{mk_BT}-1\right)\partial_x u_x + \frac{3}{10}\left(\frac{\xi_x^3}{m^2k_BT}+\frac{\xi_x}{3m}\right)\partial_x\ln T\right] f_{\text{MB}}$$

$$J_1^{\theta} = -\left[\xi_x\partial_x\ln\chi + 2\xi_x\partial_x\ln\rho + \frac{3}{5}\left(\frac{\xi_x^2}{mK_BT}-\frac{1}{3}\right)\partial_x u_x + \frac{3}{10}\left(\frac{\xi_x^3}{m^2k_BT}+\frac{7\xi_x}{3m}\right)\partial_x\ln T\right] 2mk_BT f_{\text{MB}} b\rho\chi$$

Lattice Boltzmann

When the Shakhov collision term is used in an LB model, the moments of the distribution function $\psi(x, p, t)$ $(\psi \in \{\phi, \theta\})$ up to order $N \geq 6$ are needed in order to get the evolution equations of the macroscopic fields. The momentum set $\{p_k\}$ has $Q \geq Q_{\text{min}}$ elements that belong to the set $\{r_k\}$, $1 \leq k \leq Q$, of the roots of the full-range Hermite polynomial $H_Q(p)$ and the their associated weights w_k given by

$$w_k = \frac{Q!}{[H_{Q+1}(r_k)]^2}. \tag{23}$$

The equilibrium functions $f^k_{\text{MB}} \equiv f_{\text{MB}}(x, p_k, t)$ are replaced by:

$$f^k_{\text{MB}} = n g_k, \tag{24a}$$

where

$$g_k \equiv g_k\,[u, T] = w_k \sum_{\ell=0}^{N} H_\ell(p_k) \sum_{s=0}^{\lfloor \ell/2 \rfloor} \frac{(mT-1)^s (mu)^{\ell-2s}}{2^s\, s!(\ell-2s)!}, \tag{24b}$$

and $\lfloor \ell/2 \rfloor$ is the integer part of $\ell/2$.

Lattice Boltzmann

The non-dimensionalized form of the evolution equation of the functions ϕ_k and θ_k is:

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi_k \\ \theta_k\end{pmatrix} + \frac{p_k}{m}\frac{\partial}{\partial x}\begin{pmatrix}\phi_k \\ \theta_k\end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix}\phi_k - \phi_{S;k} \\ \theta_k - \theta_{S;k}\end{pmatrix} + \begin{pmatrix}J^{\phi}_{1;k} \\ J^{\theta}_{1;k}\end{pmatrix}. \tag{25}$$

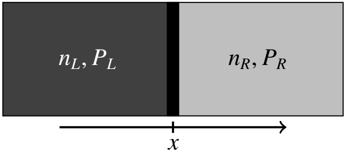
The macroscopic quantities are evaluated as:

$$\begin{pmatrix}n \\ \rho u \\ \Pi\end{pmatrix} = \sum_{k=1}^{Q}\begin{pmatrix}1 \\ p_k \\ \frac{\xi_k^2}{m}\end{pmatrix}\phi_k, \tag{26}$$

$$\begin{pmatrix}\frac{3}{2}nk_BT \\ q\end{pmatrix} = \sum_{k=1}^{Q} dp_k \begin{pmatrix}1 \\ \frac{\xi_k}{m}\end{pmatrix}\left(\frac{\xi_k^2}{2m}\phi_k + \frac{1}{2}\theta_k\right) \tag{27}$$

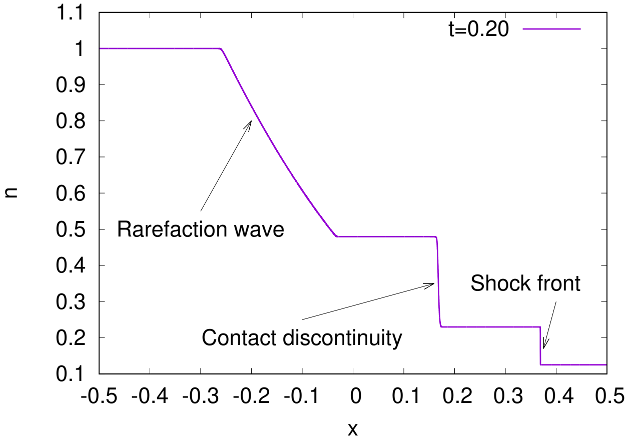
The time evolution is performed using the TVD RK-3 scheme and the advection is performed using 5^{th} order WENO numerical scheme.

1D problem: Sod shock tube



- At $t = 0$, the system consists of two semi-infinite domains separated by a thin membrane at $x = 0$.
- The system is homogeneous along y and z ($d = 1$).

1D problem: Sod shock tube - Inviscid limit



- The head of the rarefaction wave propagates at the speed of sound.
- The contact discontinuity propagates at the velocity on the plateau.
- The speed of the shock front is supersonic.

1D problem: Sod shock tube - Inviscid limit

Starting from the Euler equations:

$$\frac{D\rho}{Dt} + \rho\nabla\boldsymbol{u} = 0 \tag{28a}$$

$$\rho\frac{D\boldsymbol{u}}{Dt} + \nabla P = 0 \tag{28b}$$

$$\rho\frac{De}{Dt} + P\nabla\boldsymbol{u} = 0 \tag{28c}$$

one can introduce the similarity variable:

$$\xi = \frac{x - x_0}{t}. \tag{29}$$

In this case the Eqs. (28) reduce to:

$$\partial_\xi u - \frac{\xi - u}{\rho}\partial_\xi \rho = 0 \tag{30a}$$

$$\partial_\xi P - (\xi - u)^2 \partial_\xi \rho = 0 \tag{30b}$$

1D problem: Sod shock tube - Inviscid limit

By replacing the above equations in Eq. (28c) and assuming that $\partial_\xi \rho \neq 0$, the equations are satisfied either when $u = \xi$, corresponding to the contact discontinuity, or when:

$$u = \xi \pm c_s \tag{31}$$

The $(+)$ solution refers to the rarefaction head, travelling to the left, while the $(-)$ solution is the rarefaction tail. Since at the head of the rarefaction wave $u = u_L = 0$, the velocity of the head is constant and is given by:

$$\xi_r = -c_s \tag{32}$$

while the tail of the rarefaction wave travels with the constant value on the plateau $u = u_c$:

$$\xi_c = u_c - c_s \tag{33}$$

Replacing Eq. (31) in Eqs. (30), one obtains the system of equations for the rarefaction wave:

$$1 + \frac{1}{2c_s}\left(\partial_\rho c_s^2 \partial_\xi \rho + \partial_P c_s^2 \partial_\xi P\right) = -c_s \partial_\xi \ln \rho \tag{34a}$$

$$\partial_\xi P = c_s^2 \partial_\xi \rho \tag{34b}$$

1D problem: Sod shock tube - Inviscid limit

This system of equations can be solved numerically in conjunction with the Rankine-Hugoniot relations for the discontinuity (i.e. shock front) travelling with velocity ξ_s, given by:

$$\rho_2(u_c - \xi_s) = -\xi_s \rho_R \tag{35a}$$

$$\rho_2 u_c(u_c - \xi_s) + P_c = P_R \tag{35b}$$

$$(e_c + \frac{1}{2}\rho_2 u_c^2)(u_c - \xi_s) + u_c P_c = e_R \xi_s \tag{35c}$$

where the following notations have been introduced:

$$\rho_1 = \rho(\xi_c),\ \rho_2 = \rho(\xi_s),\ e_c = e(\rho_c, T_c),\ e_R = e(\rho_R, T_R)$$
$$P_c = P(\rho_1, T_1) = P(\rho_2, T_2),\ P_R = P(\rho_R, T_R) \tag{36}$$

where subscript 1 and 2 refer to the left and right side of the contact discontinuity. The solution is obtained using the high-precision numerical solver included in the software package Mathematica®[5].

[5] W. R. Inc., "Mathematica, Version 13.1," Champaign, IL, 2022.

Results: Shock wave propagation - Inviscid

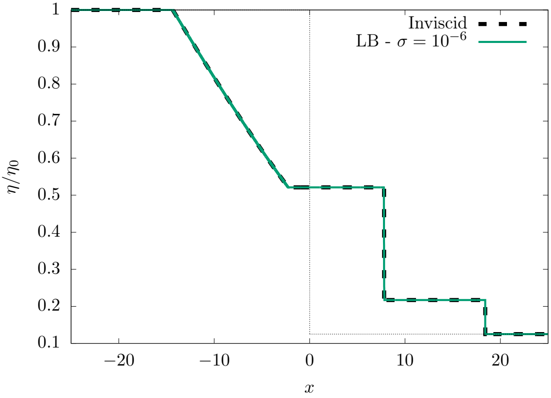


Figure: Density profiles for constant reduced density but with various values of the σ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation - Inviscid

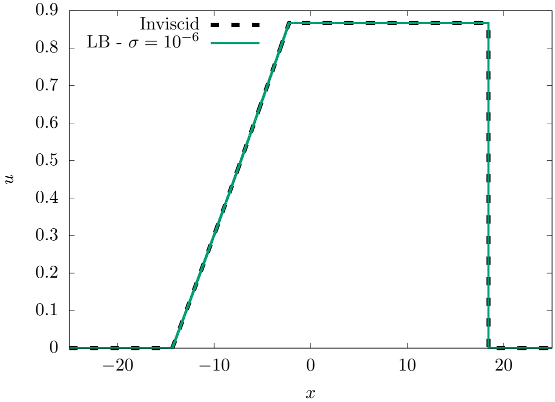


Figure: Velocity profiles for constant reduced density but with various values of the σ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation - Inviscid

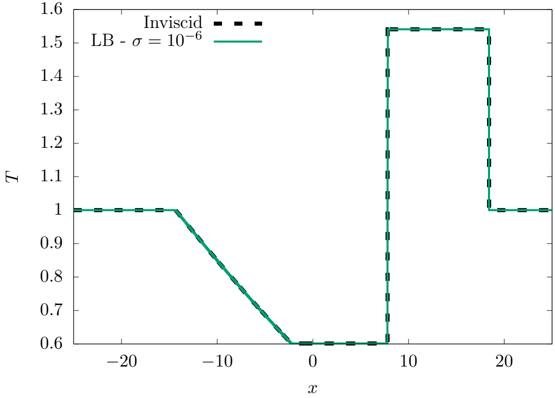


Figure: Temperature profiles for constant reduced density but with various values of the σ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation

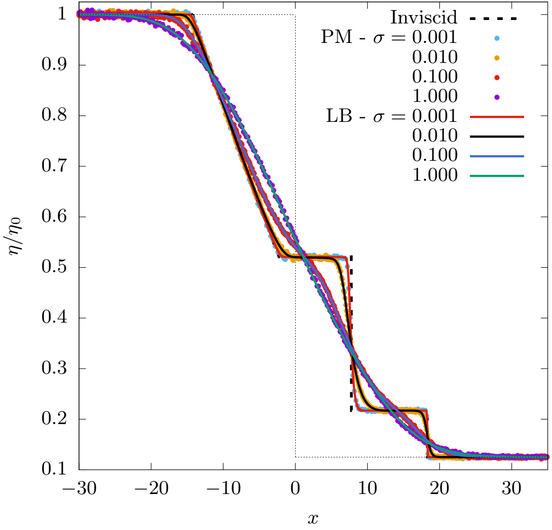


Figure: Density profiles for constant reduced density but with various values of the σ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation

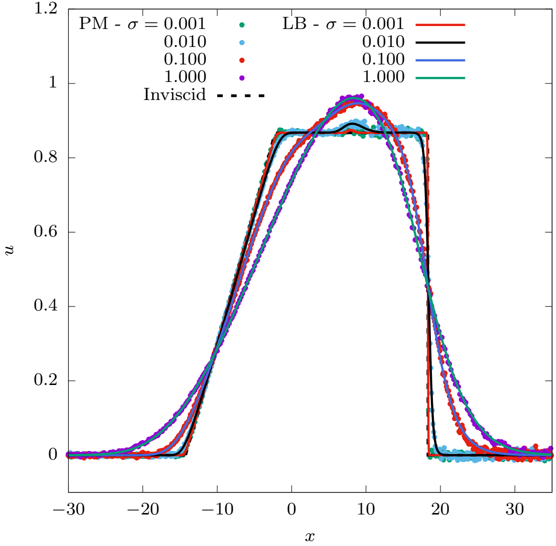
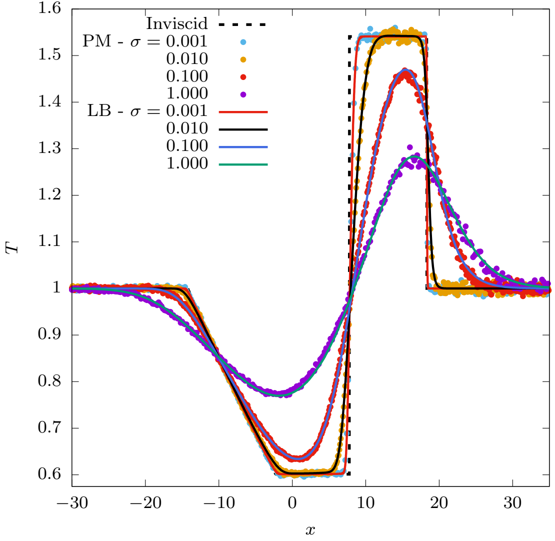


Figure: Velocity profiles for constant reduced density but with various values of the σ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation



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Results: Shock wave propagation

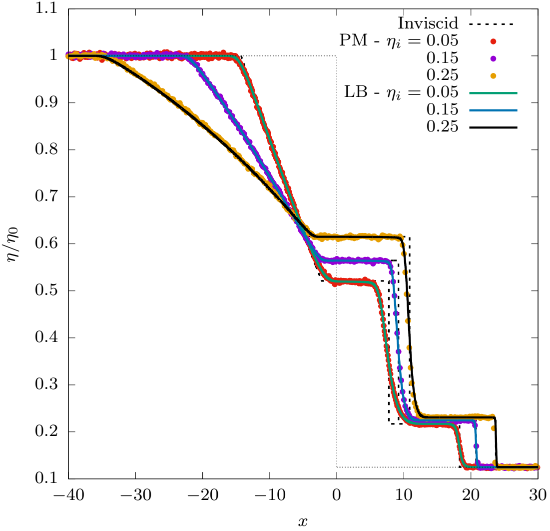

Figure: Density profiles for constant reduced density but with various values of the η at $\sigma = 0.01$ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation

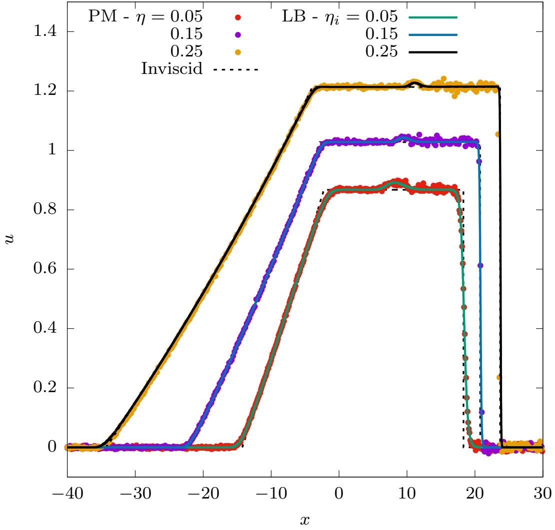

Figure: Velocity profiles for constant reduced density but with various values of the η at $\sigma = 0.01$ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation

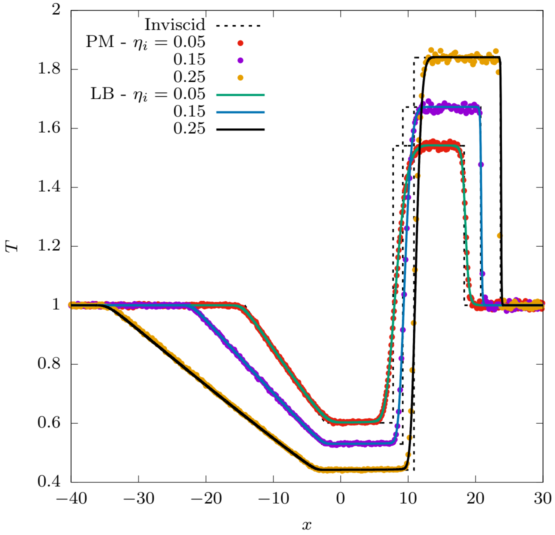

Figure: Temperature profiles for constant reduced density but with various values of the η at $\sigma = 0.01$ obtained using the LB model (solid lines) and the particle method PM (points).

Results: Shock wave propagation - structure at initial time

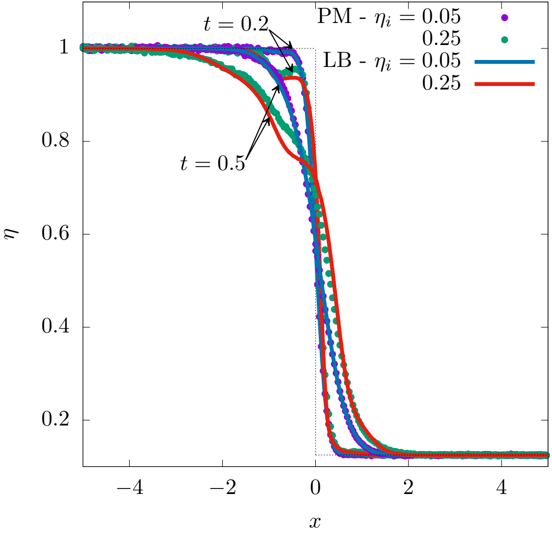

Figure: Density profiles for $\sigma = 1$ at reduced density $\eta = \{0.05, 0.25\}$ obtained using the LB model (solid lines) with $Q_x = 200$ and the PM method (points), at $t \in \{0.2, 0.5\}$.

Results: Shock wave propagation

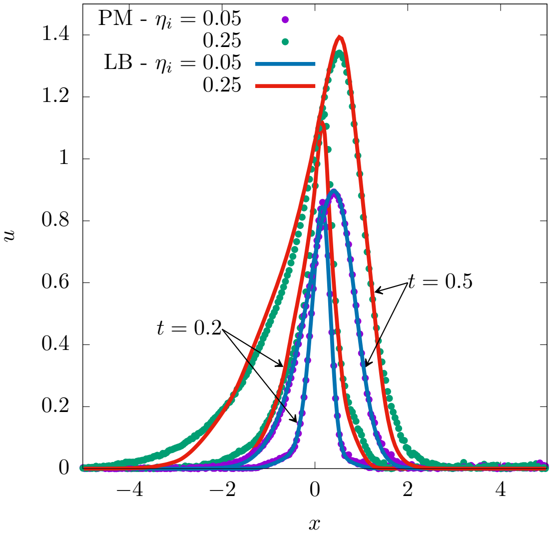

Figure: Density profiles for $\sigma = 1$ at reduced density $\eta = \{0.05, 0.25\}$ obtained using the LB model (solid lines) with $Q_x = 200$ and the PM method (points), at $t \in \{0.2, 0.5\}$.

Results: Shock wave propagation

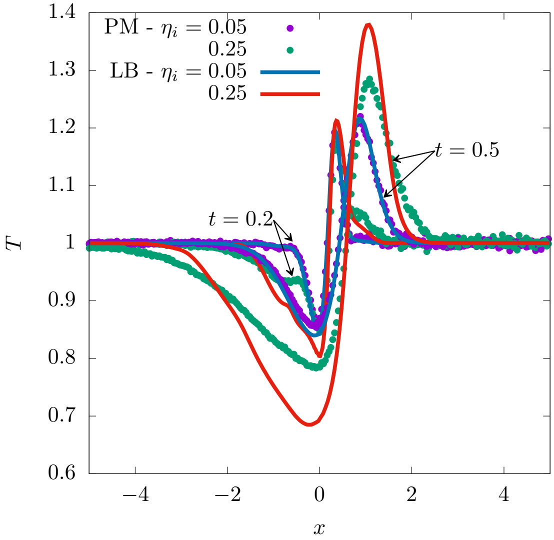

Figure: Density profiles for $\sigma = 1$ at reduced density $\eta = \{0.05, 0.25\}$ obtained using the LB model (solid lines) with $Q_x = 200$ and the PM method (points), at $t \in \{0.2, 0.5\}$.

Computational time

Method→	LB			PM	
σ	Q_x	N_x	t_{LB}	t_{PM}	$t_{\text{PM}}/t_{\text{LB}}$
0.001	8	1600	62s	186h	$\approx 1.1 \times 10^4$
0.01	8	800	32s	23h	$\approx 2.5 \times 10^3$
0.1	20	640	71s	7.25h	≈ 370
1	200	160	176s	5.8h	≈ 120

Table: Computational time comparison. As expected, the ratio $t_{\text{PM}}/t_{\text{LB}}$ increases for smaller relaxation time τ, since at constant reduced density η the relaxation time is proportional to the molecular diameter σ.

Conclusions

- The simplified Enskog collision integral can be successfully employed when dealing with moderately dense gases.
- The FDLB model successfully reproduces Particle Method results with much smaller computational time.
- Deviations of the FDLB results from the PM counterpart can be observed at the molecular scale when the denseness factor is larger than 1 (molecular diameter comparable with the mean free path).
- This work was supported through a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2021-0216, within PNCDI III PNCDI III.