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

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Outline

The Enskog equation (I)

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

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

- 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.

The Enskog equation (IV)

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

$$J_E = \sigma^2 \int \Big\{\chi\left(\boldsymbol{x} + \frac{\sigma}{2}\boldsymbol{k}\right) f(\boldsymbol{x},\boldsymbol{p}^*) f(\boldsymbol{x}+\sigma\boldsymbol{k},\boldsymbol{p}_1^*) \\ - \chi\left(\boldsymbol{x} - \frac{\sigma}{2}\boldsymbol{k}\right) f(\boldsymbol{x},\boldsymbol{p}) f(\boldsymbol{x}-\sigma\boldsymbol{k},\boldsymbol{p}_1)\Big\} (\boldsymbol{p}_r\cdot\boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p}_1 \quad (1)$$

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.
The contact value of the pair correlation function:

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

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

[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]:

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

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

The collision term $J_0(f,f)$ is the usual collision term of the Boltzmann equation for which we will employ the Shakhov collision term.

[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 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[1]:

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

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

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \nabla_{\boldsymbol{x}} f = -\frac{1}{\tau}(f - f_S) + J_1(f_{\text{MB}}, f_{\text{MB}}) \quad (6)$$

[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

Multiplying the Enskog equation with the collision invariants $1, \boldsymbol{p}$ and $\boldsymbol{p}^2/2m$ and integrating over the momentum space yields the following conservation equations for mass, momentum and energy[1]:

$$\frac{D\rho}{Dt} + \rho\nabla\boldsymbol{u} = 0 \tag{7a}$$

$$\rho\frac{D\boldsymbol{u}}{Dt} + \nabla P = -\nabla\cdot\Pi \tag{7b}$$

$$\rho\frac{De}{Dt} + P\nabla\cdot\boldsymbol{u} = -\nabla\cdot\boldsymbol{q} + \Pi : \nabla\boldsymbol{u} \tag{7c}$$

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:

$$\boldsymbol{q} = -\lambda\nabla T, \tag{8}$$

$$\Pi = -\mu_v\mathcal{I}\boldsymbol{\nabla}\cdot\boldsymbol{u} - \mu\left(\nabla u + (\nabla u)^T - \tfrac{2}{3}\mathcal{I}\boldsymbol{\nabla}\cdot\boldsymbol{u}\right) \tag{9}$$

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]:

$$\mu_v = \frac{16}{5\pi}\mu_0 b^2 \rho^2 \chi, \tag{10a}$$

$$\mu = \tau P_i = \mu_0 b\rho \left(\frac{1}{b\rho\chi} + 0.8 + \frac{4}{25}\left(1 + \frac{12}{\pi}\right) b\rho\chi\right), \tag{10b}$$

$$\lambda = \frac{5}{2}\frac{\tau P_i}{\mathrm{Pr}} = \lambda_0 b\rho \left(\frac{1}{b\rho\chi} + 1.2 + \frac{9}{25}\left(1 + \frac{32}{9\pi}\right) b\rho\chi\right), \tag{10c}$$

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

$$\mu_{\rm ref} = \frac{5}{16\sigma^2}\sqrt{\frac{m k_B T_0}{\pi}}, \qquad \lambda_{\rm ref} = \frac{75 k_B}{64 m \sigma^2}\sqrt{\frac{m k_B T_0}{\pi}}. \tag{11}$$

[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

For the dense gas the Prandtl number is:

$$\mathrm{Pr} = \frac{2}{3}\,\frac{1 + \frac{4}{5}b\rho\chi + \frac{4}{25}\left(1 + \frac{12}{\pi}\right)(b\rho\chi)^2}{1 + \frac{6}{5}b\rho\chi + \frac{9}{25}\left(1 + \frac{32}{9\pi}\right)(b\rho\chi)^2}. \tag{12}$$

The Chapman-Enskog expansion of Eq. (6) gives the relations between the relaxation time τ and the transport coefficients. It follows that the relaxation time τ is given by:

$$\tau = \frac{\mu}{P_i} \tag{13}$$

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[2], given by the ratio of the molecular diameter and the mean free path:

$$E_l = \frac{\sigma}{l} = \frac{3}{\sqrt{2}}bn\chi. \tag{14}$$

[2] 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[3]:

$$\phi(\boldsymbol{x}, p_x, t) = \int dp_y dp_z f(\boldsymbol{x}, \boldsymbol{p}, t), \tag{15}$$

$$\theta(\boldsymbol{x}, p_x, t) = \int dp_y dp_z \frac{p_y^2 + p_z^2}{m} f(\boldsymbol{x}, \boldsymbol{p}, t) \tag{16}$$

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

$$\begin{pmatrix} n \\ \rho u_x \\ \Pi_{xx} \end{pmatrix} = \int dp_x \begin{pmatrix} 1 \\ p_x \\ \frac{\xi_x^2}{m} \end{pmatrix} \phi, \tag{17}$$

$$\begin{pmatrix} \frac{3}{2} n k_B T \\ q_x \end{pmatrix} = \int dp_x \begin{pmatrix} 1 \\ \frac{\xi_x}{m} \end{pmatrix} \left(\frac{\xi_x^2}{2m} \phi + \frac{1}{2} \theta \right) \tag{18}$$

[3] 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:

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi \\ \theta\end{pmatrix} + \frac{p_x}{m}\frac{\partial}{\partial x}\begin{pmatrix}\phi \\ \theta\end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix}\phi - \phi_S \\ \theta - \theta_S\end{pmatrix} + \begin{pmatrix}J_1^{\phi} \\ J_1^{\theta}\end{pmatrix} \tag{19}$$

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

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

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

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

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

Finite difference Lattice Boltzmann

In the following, we will introduce the notation $\psi \in \{\phi, \theta\}$ to represent the reduced distributions introduced earlier.
In order to evaluate the macroscopic quantities one will replace the integrals with quadrature sums. The distribution function ψ is projected on a set of Hermite polynomials up to order N[4]:

$$\psi(x, p, t) \equiv \psi^N(x, p, t) = \omega(p_k) \sum_{\ell=0}^{N} \frac{1}{\ell!} a_\ell(x, t) H_\ell(p_k) \tag{20}$$

where the coefficients $a_\ell(x, t)$ are given by:

$$a_\ell(x, t) = \int dp \psi(x, p, t) H_\ell(p) \tag{21}$$

[4] X. Shan, X.-F. Yuan, and H. Chen, "Kinetic theory representation of hydrodynamics: a way beyond the navier–stokes equation," Journal of Fluid Mechanics 550, 413–441 (2006)

Finite difference Lattice Boltzmann

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

$$w_k = \frac{Q!}{[H_{Q+1}(r_k)]^2}. \tag{22}$$

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

$$f^k_{\text{MB}} = n g_k, \tag{23a}$$

where

$$g_k \equiv g_k\left[u, T\right] = w_k \sum_{\ell=0}^{N} H_\ell(p_k) \sum_{s=0}^{\lfloor \ell/2 \rfloor} \frac{(mT-1)^s (mu)^{\ell-2s}}{2^s s! (\ell-2s)!}, \tag{23b}$$

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:

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi_k\\ \theta_k\end{pmatrix} + \frac{p_k}{m}\frac{\partial}{\partial x}\begin{pmatrix}\phi_k\\ \theta_k\end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix}\phi_k - \phi_{S;k}\\ \theta_k - \theta_{S;k}\end{pmatrix} + \begin{pmatrix}J^{\phi}_{1;k}\\ J^{\theta}_{1;k}\end{pmatrix}. \tag{24}$$

The macroscopic quantities are evaluated as:

$$\begin{pmatrix}n\\ \rho u\\ \Pi\end{pmatrix} = \sum_{k=1}^{Q}\begin{pmatrix}1\\ p_k\\ \frac{\xi_k^2}{m}\end{pmatrix}\phi_k, \tag{25}$$

$$\begin{pmatrix}\frac{3}{2}nk_BT\\ q\end{pmatrix} = \sum_{k=1}^{Q} dp_k \begin{pmatrix}1\\ \frac{\xi_k}{m}\end{pmatrix}\left(\frac{\xi_k^2}{2m}\phi_k + \frac{1}{2}\theta_k\right) \tag{26}$$

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

Longitudinal waves

The propagation of longitudinal waves induces fluctuations in the macroscopic properties of the fluid, the amplitudes of which decay due to viscous and thermal dissipation. For simplicity we will consider small perturbations of density and pressure around the constant values ρ_0 and P_0 in a fluid homogeneous along the y and z axis, which propagates along the x axis with a small velocity $u(x,t)$:

$$\rho(x,t) = \rho_0[1 + \delta\rho(x,t)], \quad P(x,t) = P_0[1 + \delta P(x,t)] \tag{27}$$

where the perturbations $\delta\rho$ and δP are of the same order of magnitude as u. In the liniarised regime the macroscopic equations reduce to:

$$\partial_t \delta\rho + \partial_x u = 0 \tag{28a}$$

$$\partial_t u + \frac{P_0}{\rho_0}\partial_x \delta P - \frac{1}{\rho_0}\partial_x \Pi = 0 \tag{28b}$$

$$\partial_t \delta T + \frac{\partial_x q}{\rho_0 c_V T_0} + \frac{P_0}{\rho_0 c_V T_0}\partial_x u = 0 \tag{28c}$$

where the specific energy is $e = c_V T = c_V T_0(1 + \delta T)$ and $\Pi = O(u)$.

Results: Longitudinal waves

The sound speed is given by:

$$c_s^2 = \partial_\rho P + \frac{P_0}{\rho_0^2 c_V} \partial_T P \tag{29}$$

The damping coefficients:

$$\begin{aligned} \alpha_t &= \frac{\gamma \mu k^2}{\mathrm{Pr} \rho_0 c_s^2} \partial_\rho P, \quad \alpha_s = k c_s \\ \alpha_a &= \frac{k^2 \mu}{2\rho_0} \left[\frac{4}{3} + \frac{\mu_V}{\mu} + \frac{\gamma c_s^2}{\mathrm{Pr}} \left(1 - \partial_\rho P \right) \right] \end{aligned} \tag{30}$$

We will restrict our simulations to the case when the pressure perturbation vanishes at initial time $\delta P(t_0) = 0$. After some calculation one can write the full solution of the density amplitude can be written as:

$$\delta\rho(t) \approx \delta\rho_0 \left[e^{-\alpha_t t} + \left(e^{-\alpha_a t} \cos(k c_s t) - e^{-\alpha_t t} \right) \frac{1}{c_s^2} \frac{\partial P}{\partial \rho} \right] \tag{31}$$

Results: Longitudinal waves

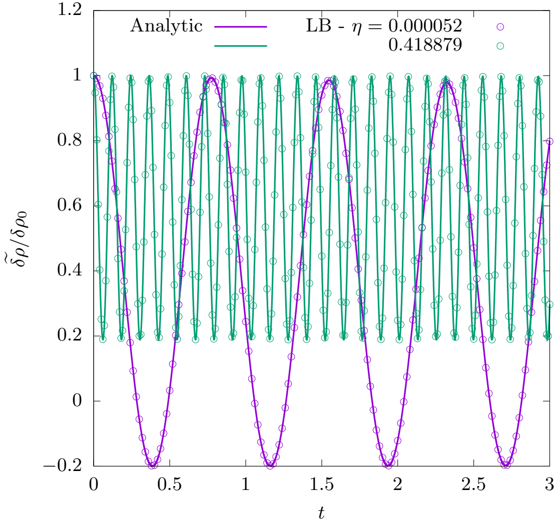


Figure: Normalized density amplitude $\delta\rho(t)/\delta\rho_0$ in comparison with the analytical prediction.

Results: Longitudinal waves

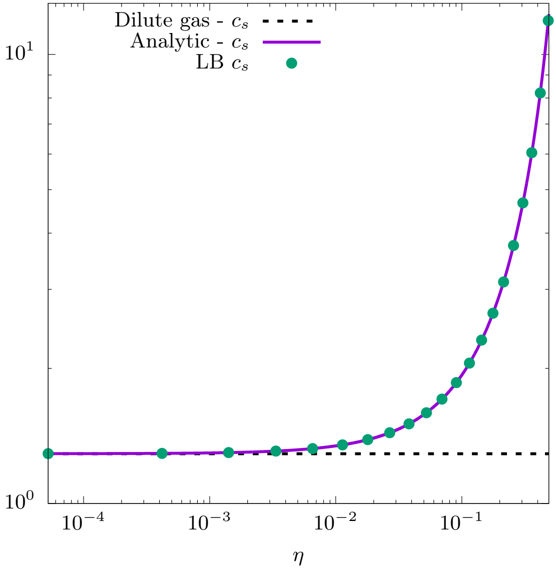


Figure: The sound speed c_s obtained from the simulation results and the analytic prediction.

Results: Longitudinal waves

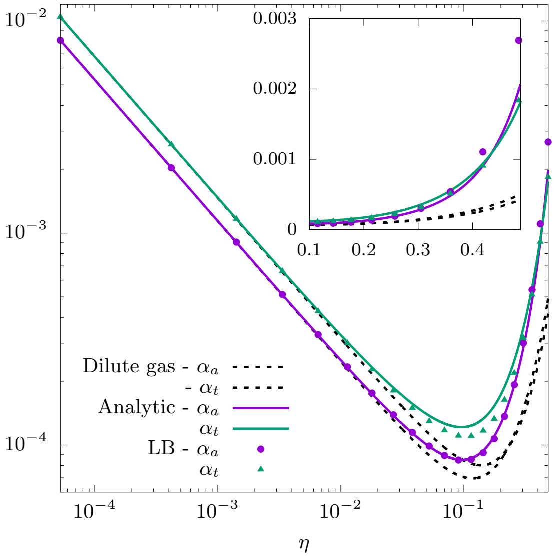
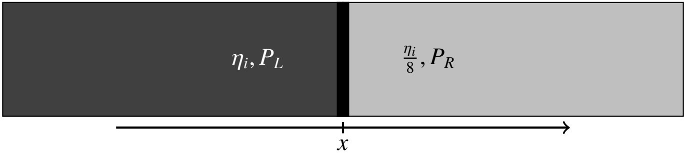


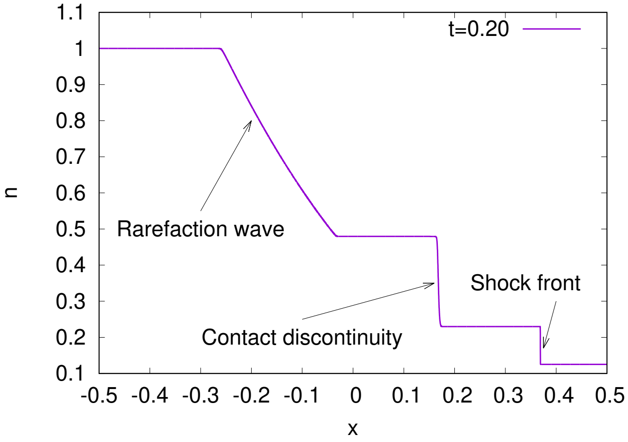
Figure: The acoustic α_a and thermal α_t mode with respect to the reduced density η.

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:

$$\frac{D\rho}{Dt} + \rho\nabla\boldsymbol{u} = 0 \tag{32a}$$

$$\rho\frac{D\boldsymbol{u}}{Dt} + \nabla P = 0 \tag{32b}$$

$$\rho\frac{De}{Dt} + P\nabla\boldsymbol{u} = 0 \tag{32c}$$

one can introduce the similarity variable:

$$\xi = \frac{x - x_0}{t}. \tag{33}$$

After some calculations, one can write 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

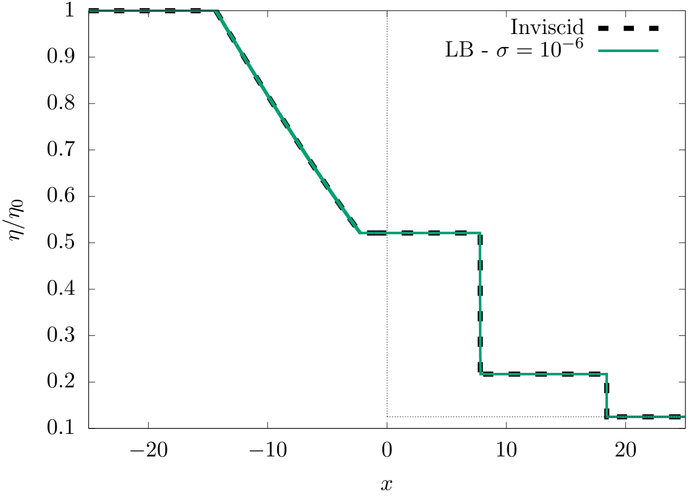


Figure: Shock wave propagation: reduced density for molecular diameter $\sigma = 10^{-6}$ at reduced density $\eta_i = 0.05$ ($E_l = 0.4825$) obtained using the LB model (solid line) and compared with the inviscid solution (dashed line).

Results: Shock wave propagation - Inviscid

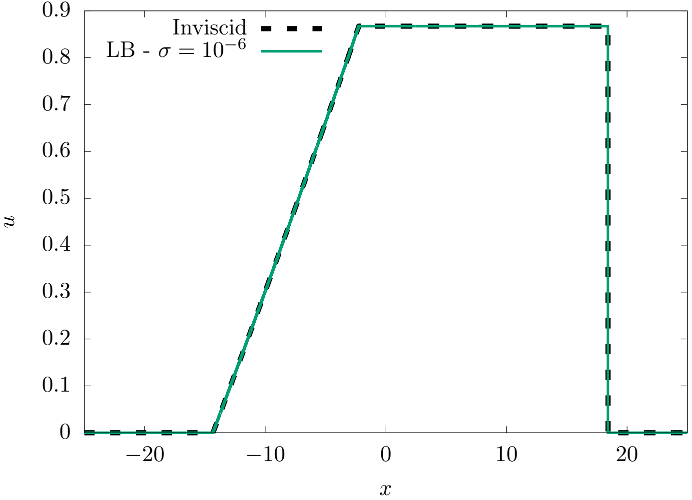
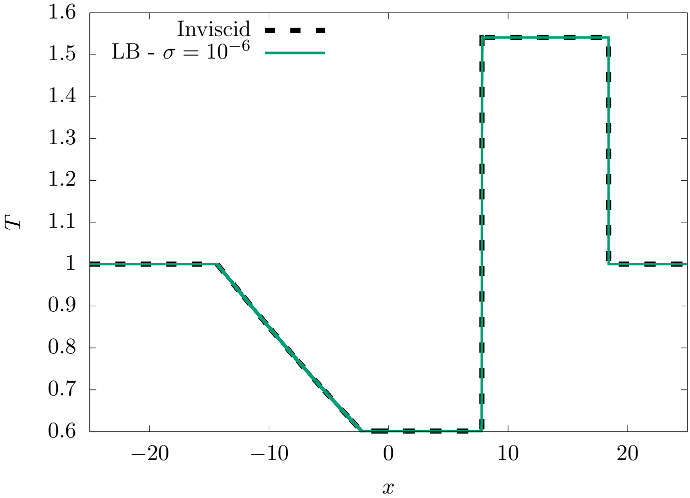


Figure: Shock wave propagation: velocity for molecular diameter $\sigma = 10^{-6}$ at reduced density $\eta_i = 0.05$ ($E_l = 0.4825$) obtained using the LB model (solid line) and compared with the inviscid solution (dashed line).

Results: Shock wave propagation - Inviscid



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Results: Shock wave propagation

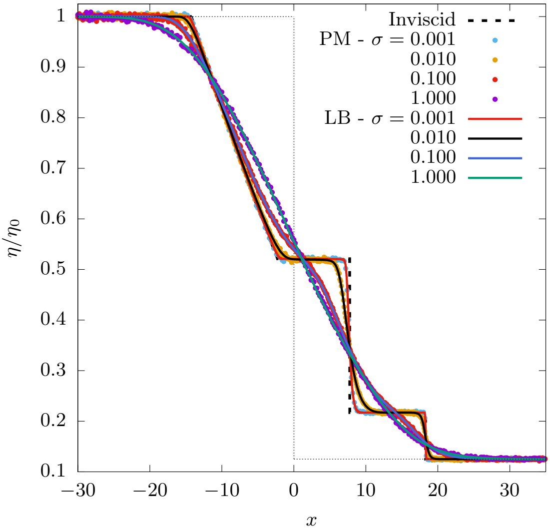


Figure: Shock wave propagation: reduced density profile for $\eta_i = 0.05$ ($E_l = 0.4825$) but with various values of the molecular diameter (implicitly various values of the relaxation time τ).

Results: Shock wave propagation

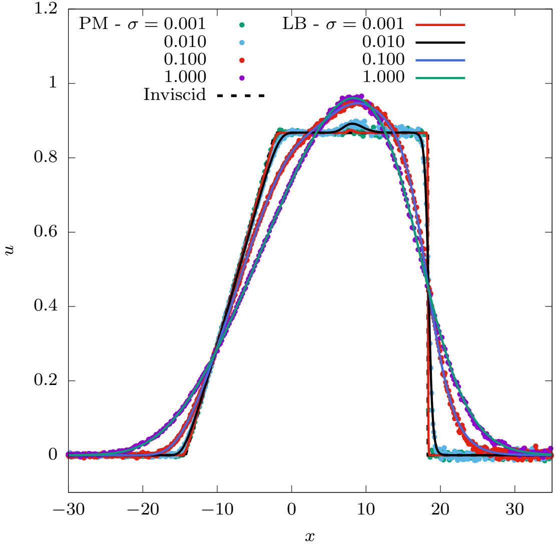


Figure: Shock wave propagation: velocity profile for $\eta_i = 0.05$ ($E_l = 0.4825$) but with various values of the molecular diameter (implicitly various values of the relaxation time τ).

Results: Shock wave propagation

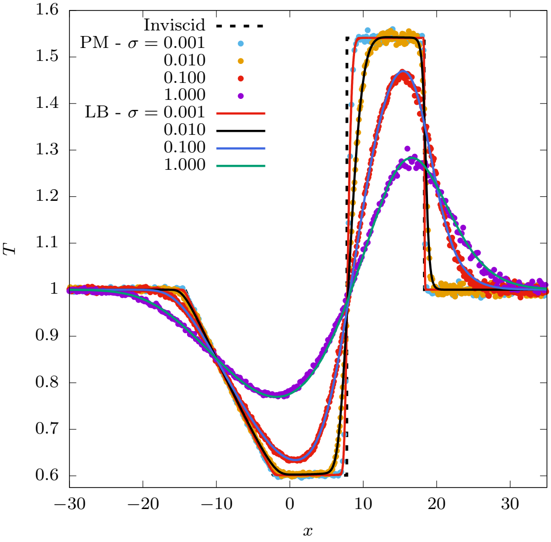


Figure: Shock wave propagation: temperature profile for $\eta_i = 0.05$ ($E_l = 0.4825$) but with various values of the molecular diameter (implicitly various values of the relaxation time τ).

Results: Shock wave propagation

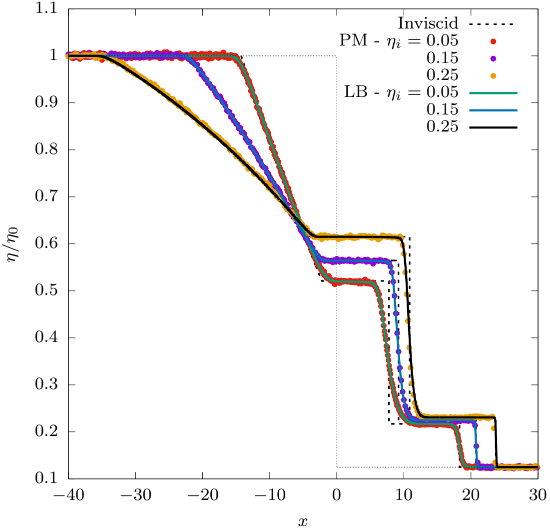
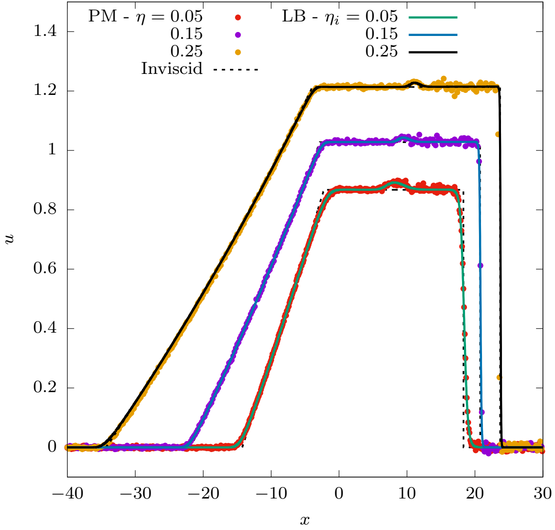


Figure: Density profiles for constant reduced density but with various values of the η at $\sigma = 0.01$ and $\eta \in \{0.05,\ 0.15,\ 0.25\}$ ($E_l \in \{0.4825,\ 1.917,\ 4.3998\}$).

Results: Shock wave propagation



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Results: Shock wave propagation

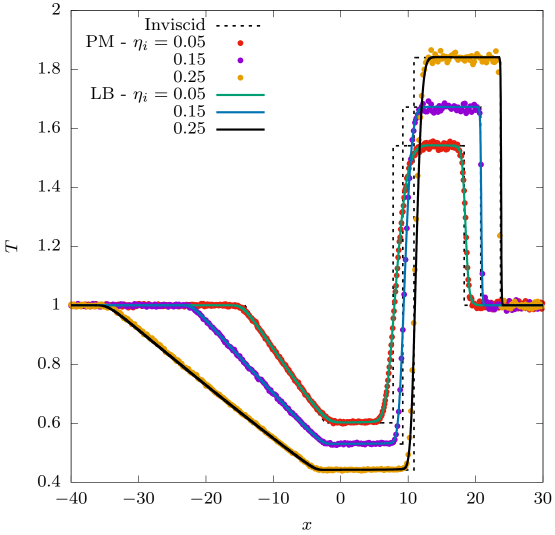

Figure: Temperature profiles for constant reduced density but with various values of the η at $\sigma = 0.01$ and $\eta \in \{0.05,\ 0.15,\ 0.25\}$ ($E_l \in \{0.4825,\ 1.917,\ 4.3998\}$).

Results: Shock wave propagation - structure at initial time

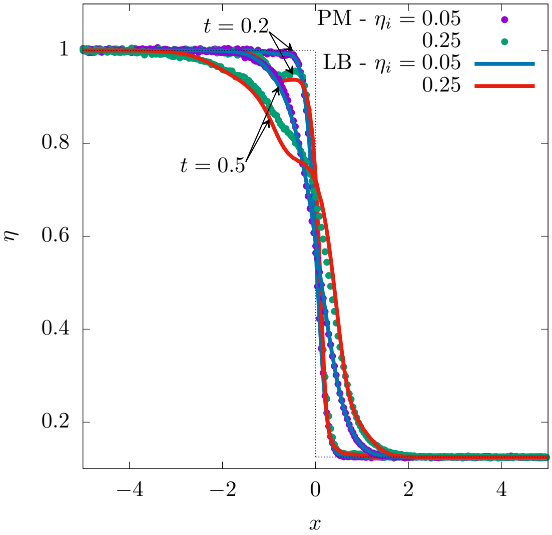

Figure: Shock wave propagation: structure at the initial time. Density profile for molecular diameter $\sigma = 1$ at reduced density $\eta_i = \{0.05, 0.25\}$ ($E_l \in \{0.4825, 4.3998\}$).

Results: Shock wave propagation

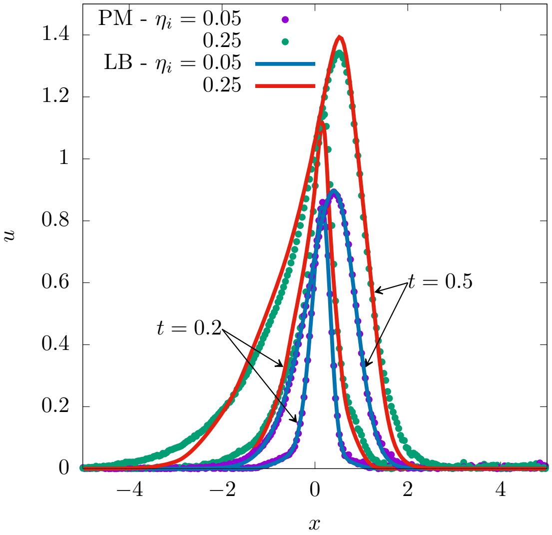

Figure: Shock wave propagation: structure at the initial time. Velocity profile for molecular diameter $\sigma = 1$ at reduced density $\eta_i = \{0.05, 0.25\}$ ($E_l \in \{0.4825, 4.3998\}$).

Results: Shock wave propagation

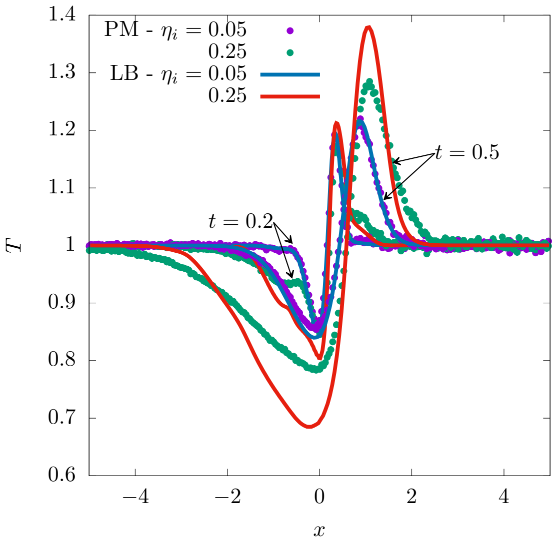

Figure: Shock wave propagation: structure at the initial time. Temperature profile for molecular diameter $\sigma = 1$ at reduced density $\eta_i = \{0.05, 0.25\}$ ($E_l \in \{0.4825, 4.3998\}$).

Conclusion

- 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).
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