

Kinetic Modelling of Dense Gases and Liquid-Vapor Flows via Enskog-Type Equations

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Séminaire de Physique Théorique, Tours, 10.09.2026



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Why study dense gases and liquid-vapor flows?

- **Vacuum technology & MEMS/NEMS:** gas flows in micro- and nano-devices routinely cross from the dilute (rarefied) to the dense regime as channel size shrinks and pressure increases – pumps, sensors, micro-nozzles.
- **Gas storage, transport & extraction:** high-pressure pipeline transport, natural gas and shale-gas extraction through nanoporous media, where the mean free path becomes comparable to the pore size.
- **Aerospace:** spacecraft re-entry and high-altitude flight sample a wide range of densities along the trajectory, from free-molecular to near-continuum.
- **Evaporation & phase-change processes:** droplet evaporation in spray combustion and inkjet printing, boiling and condensation in heat pipes and thermal-management systems, thin-film deposition.
- **Multiphase / interfacial phenomena:** liquid-vapor coexistence and phase separation are central to condensation, cavitation, and nucleation processes in both natural and industrial settings.
- Common challenge: continuum (Navier-Stokes-Fourier) models break down once density or confinement effects become significant – a **kinetic** description is needed.



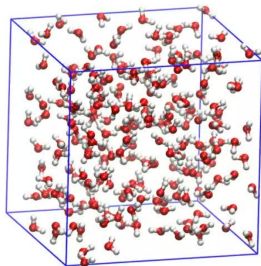
Macroscopic: $n, \mathbf{u}, T$
(Navier-Stokes-Fourier)



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$$N_A = 6.02 \times 10^{23}$$

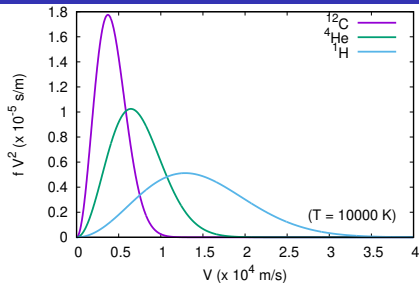


Microscopic: $(\mathbf{x}_i, \mathbf{p}_i)$
(MD)

Mesoscale approach



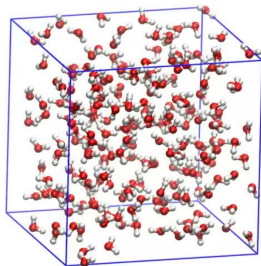
Macroscopic: $n, \mathbf{u}, T$
(Navier-Stokes-Fourier)



Mesoscopic: $f(\mathbf{x}, \mathbf{p}, t)$
(Boltzmann)

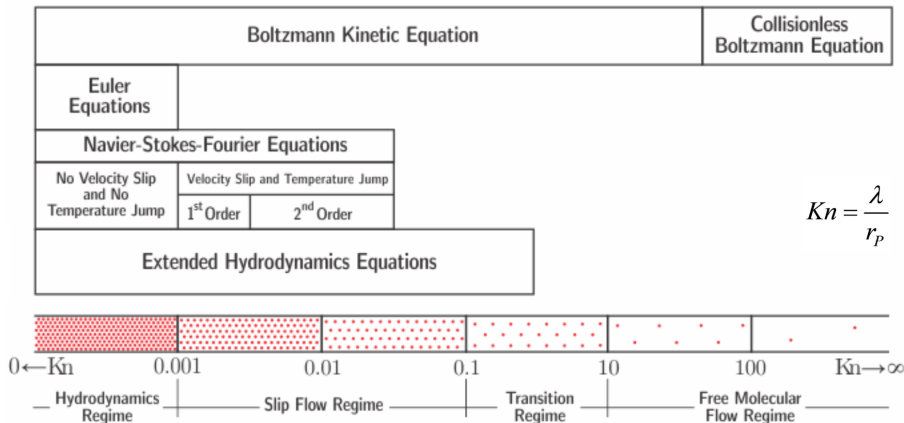


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Microscopic: $(\mathbf{x}_i, \mathbf{p}_i)$
(MD)

Flow regimes - Knudsen range



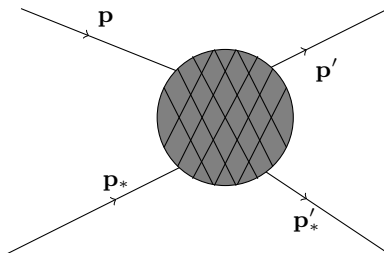
- $Kn = \lambda/r_p$ ($\lambda \equiv$ mean free path; $r_p \equiv$ characteristic channel length).
- Hydrodynamic regime (NSF): $Kn \rightarrow 0$.
- Ballistic regime (Vlasov): $Kn \rightarrow \infty$.

The Boltzmann equation.

Limits of applicability of the Navier-Stokes equations.

- The Navier-Stokes equations apply to a wide range of common problems, from laminar flows to turbulent flows.
- In the case of non-Newtonian fluids (creams, gels), the Navier-Stokes equations can be extended by allowing the transport coefficients (μ , μ_v , λ) to depend on the kinematic state of the fluid (for example, on the shear rate).
- The Navier-Stokes equations lose their applicability when the assumptions behind them are no longer reasonable:
 - The corpuscular nature of the fluid's constituents becomes important, invalidating the continuum assumption. Formally, the mean free path λ_{mfp} becomes comparable to the scale L over which the fluid properties vary, $\text{Kn} = \lambda_{\text{mfp}}/L \gtrsim 1$.
 - The dissipative fields τ_{ij} , q_i become comparable to the non-dissipative ones:
 $|\tau_{ij}|/P \gtrsim 1$, $q_i/E \gtrsim 1$.

The Boltzmann equation



- In order to manage these degrees of freedom, one defines the single-particle distribution function $f_1(\mathbf{x}, \mathbf{p}, t)$. For hard spheres of diameter a , its exact time evolution is given by the first BBGKY equation:

$$\partial_t f_1 + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{x}} f_1 + \mathbf{F} \cdot \nabla_{\mathbf{p}} f_1 = J[f_2] = a^2 \int_{\mathbb{R}^3} \int_{S_+^2} \left(\frac{|\mathbf{p} - \mathbf{p}_*|}{m} \cdot \hat{\mathbf{n}} \right) \left[\underbrace{f_2(\mathbf{x}, \mathbf{p}', \mathbf{x} + a\hat{\mathbf{n}}, \mathbf{p}_*; t)}_{\Gamma^+ \text{ (gain term)}} - \underbrace{f_2(\mathbf{x}, \mathbf{p}, \mathbf{x} - a\hat{\mathbf{n}}, \mathbf{p}_*; t)}_{\Gamma^- \text{ (loss term)}} \right] d\hat{\mathbf{n}} d\mathbf{p}_*. \quad (1)$$

where the collision term $J[f_2]$ represents the difference between the particles that, as a result of collisions, enter (Γ^+) or leave (Γ^-) the streamline.

- In formulating the equation that bears his name, Boltzmann made the following assumptions:
 - 1 Only binary collisions are taken into account;
 - 2 Collisions occur at a point;
 - 3 Collisions are instantaneous;
 - 4 The colliding particles are completely uncorrelated (*Stosszahlansatz*):
$$f_2(\mathbf{x}_1, \mathbf{x}_2, \mathbf{p}_1, \mathbf{p}_2, t) = f(\mathbf{x}_1, \mathbf{p}_1, t)f(\mathbf{x}_2, \mathbf{p}_2, t).$$
- In what follows, we will consider only perfectly elastic collisions.

- The particles leaving the streamline are particles that initially had momentum $\mathbf{p}$ and that collide with a particle of momentum $\mathbf{p}_*$:

$$\Gamma^- = \int d\mathbf{p}_* d\mathbf{p}' d\mathbf{p}'_* \delta_{\mathbf{p}} \delta_E \frac{|\mathbf{p} - \mathbf{p}_*|}{m} \frac{d\sigma}{d\Omega} f f_*, \quad (2)$$

where $\mathbf{p}'$ and $\mathbf{p}'_*$ represent the momenta of the particles after the collision, $f f_* |\mathbf{p} - \mathbf{p}_*|/m$ represents the flux of interacting particles, $d\sigma/d\Omega$ represents the differential cross section of the process, and $\delta_{\mathbf{p}}$ and δ_E ensure conservation of total momentum and energy, as follows:

$$\delta_{\mathbf{p}} \equiv \delta(\mathbf{p} + \mathbf{p}_* - \mathbf{p}' - \mathbf{p}'_*), \quad \delta_E = \delta(E + E_* - E' - E'_*). \quad (3)$$

- The particles entering the streamline are particles with some momentum $\mathbf{p}'$, which, following a collision with a particle of momentum $\mathbf{p}'_*$, will have momentum $\mathbf{p}$:

$$\Gamma^+ = \int d\mathbf{p}_* d\mathbf{p}' d\mathbf{p}'_* \delta_{\mathbf{p}} \delta_E \frac{|\mathbf{p}' - \mathbf{p}'_*|}{m} \frac{d\sigma}{d\Omega} f' f'_*. \quad (4)$$

- Let the function H be defined as follows:

$$H = \int d\mathbf{x} d\mathbf{p} f \ln f. \quad (5)$$

- Using eq. (1) one can compute the time derivative of H :

$$\begin{aligned} \frac{dH}{dt} &= \int d\mathbf{x} d\mathbf{p} J[f](1 + \ln f) \\ &= \frac{1}{4} \int d\mathbf{x} d\mathbf{p} d\mathbf{p}_* d\mathbf{p}' d\mathbf{p}'_* \delta_{\mathbf{p}} \delta_E \frac{d\sigma}{d\Omega} \frac{|\mathbf{p}' - \mathbf{p}'_*|}{m} \\ &\quad \times (f' f'_* - f f_*) (\ln f + \ln f_* - \ln f' - \ln f'_*). \end{aligned} \quad (6)$$

- The term on the last line can be written as:

$$(f' f'_* - f f_*) (\ln f + \ln f_* - \ln f' - \ln f'_*) = f' f'_* \left(1 - \frac{f f_*}{f' f'_*} \right) \ln \frac{f f_*}{f' f'_*}.$$

- Given that $(1 - x) \ln x \leq 0$ and $d\sigma/d\Omega \geq 0$, it follows that:

$$\frac{dH}{dt} \leq 0. \quad (7)$$

- Entropy stops increasing when $dH/dt = 0$, i.e., the system is in thermodynamic equilibrium:

$$\frac{dH}{dt} = \int d\mathbf{x} J[f, 1 + \ln f], \quad J[f, \psi] = \int d\mathbf{p} J[f] \psi. \quad (8)$$

- Quantities ψ for which $J[f, \psi] = 0$ are called *collision invariants*. Due to conservation of particle number, momentum, and energy:

$$J[f, 1] = 0, \quad J[f, \mathbf{p}] = 0, \quad J[f, \mathbf{p}^2/2m] = 0. \quad (9)$$

- The condition $dH/dt = 0$ implies $J[f^{(\text{eq})}, 1 + \ln f^{(\text{eq})}] = 0$, so $1 + \ln f^{(\text{eq})}$ must be a linear combination of the collision invariants (9), giving:

$$f^{(\text{eq})} = N \exp [-\alpha(\mathbf{p} - \mathbf{p}_0)^2]. \quad (10)$$

- Here N , α , and $\mathbf{p}_0$ are related to the particle density n , temperature T , and macroscopic velocity $\mathbf{u}$, respectively.

- Matching N , α , $\mathbf{p}_0$ to the physical moments $(n, \mathbf{u}, T)$ of $f^{(\text{eq})}$ gives:

$$\alpha = \frac{1}{2mK_B T}, \quad (11a)$$

$$N = \frac{n}{(2\pi m K_B T)^{3/2}}, \quad (11b)$$

$$\mathbf{p}_0 = m\mathbf{u}. \quad (11c)$$

- Substituting into eq. (10) yields the **Maxwell-Boltzmann distribution**:

$$f^{(\text{eq})}(\mathbf{x}, \mathbf{p}, t) = \frac{n}{(2\pi m K_B T)^{\frac{3}{2}}} \exp \left[-\frac{(\mathbf{p} - m\mathbf{u})^2}{2mK_B T} \right]. \quad (12)$$

- **Definition.** The absolute moment of order s of f is:

$$M_{i_1, i_2, \dots, i_s}^{(s)} = \int d\mathbf{p} f p_{i_1} p_{i_2} \dots p_{i_s}, \quad (13)$$

where i_ℓ ($\ell = 1, 2, \dots, s$) are Cartesian indices (x, y or z).

- **Definition.** The central moment of order s of f is:

$$\mu_{i_1, i_2, \dots, i_s}^{(s)} = \int d\mathbf{p} f \xi_{i_1} \xi_{i_2} \dots \xi_{i_s}. \quad (14)$$

where $\xi = \mathbf{p} - m\mathbf{u}$ represents the peculiar momentum.

- The relation between the central moments and the absolute moments is:

$$\mu_{i_1, i_2, \dots, i_s}^{(s)} = \sum_{\ell=0}^s \binom{s}{\ell} (-m)^\ell M_{(i_1 \dots i_{s-\ell}}^{(s-\ell)} u_{i_{s-\ell+1}} \dots u_{i_s}. \quad (15)$$

- **Remark:** in general, the central moments provide information about the intrinsic properties of the fluid; the absolute moments also contain information about its macroscopic state of motion.

- Particle density (absolute = central moment for $s = 0$):

$$n = M^{(0)} = \mu^{(0)} = \int d\mathbf{p} f. \quad (16)$$

- Momentum density (first-order absolute moment); note

$$\mu_i^{(1)} = M_i^{(1)} - m u_i M^{(0)} = 0:$$

$$\rho u_i = M_i^{(1)} = \int d\mathbf{p} f p_i. \quad (17)$$

- Stress tensor (second-order central moment), T_{ij} = transfer of i -th momentum component in direction j :

$$T_{ij} \equiv \frac{1}{m} \mu_{ij}^{(2)} = \int d\mathbf{p} f \frac{\xi_i \xi_j}{m}. \quad (18)$$

- Trace $\Rightarrow$ pressure and temperature; relation to absolute moment:

$$\frac{1}{2} T_{ii} = \frac{3}{2} n K_B T = \frac{3}{2} P, \quad \frac{1}{m} M_{ij}^{(2)} = T_{ij} + \rho u_i u_j.$$

- Heat flux (from the third-order moments), representing transfer of internal energy in direction i :

$$q_i = \frac{1}{2m^2} \mu_{ijj}^{(3)} = \int d\mathbf{p} f \frac{\xi^2}{2m} \frac{\xi_i}{m}. \quad (19)$$

- Relation to the third-order absolute moment:

$$\frac{1}{2m^2} M_{ijj}^{(3)} = q_i + \left(\frac{3}{2} n K_B T + \frac{1}{2} \rho \mathbf{u}^2 \right) u_i + T_{ij} u_j,$$

- where the blue term is the energy transfer by macroscopic convection, and the red term is the mechanical work per unit time done by the stress forces.

Conservation equations of the fluid medium. $(n, \mathbf{u}, T)$

- Applying the **transport theorem** to a microscopic quantity ψ produces, in general, an unclosed equation for its macroscopic flux Ψ .
- Among all choices of ψ , a privileged place is held by the **collision invariants** $\psi \in \{1, p_i, \mathbf{p}^2/2m\}$, for which $J[f, \psi] = 0$: the collision term drops out entirely.
- For $\psi = 1$, we obtain the mass conservation equation:

$$\partial_t n + \nabla \cdot (n\mathbf{u}) = 0.$$

- For $\psi = p_i$ we obtain the momentum conservation equation:

$$\partial_t(\rho u_i) + \partial_j(T_{ij} + \rho u_i u_j) = n F_i.$$

- For $\psi = \mathbf{p}^2/2m$, we obtain the energy conservation equation:

$$\partial_t \left(\frac{3}{2} n K_B T + \frac{\rho \mathbf{u}^2}{2} \right) + \partial_i \left(q_i + \frac{3}{2} n K_B T u_i + T_{ij} u_j + \frac{1}{2} \rho \mathbf{u}^2 u_i \right) = n u_i F_i. \quad (20)$$

- We have obtained three equations governing the transport of mass, momentum and energy. Note, however, that the resulting system is not closed: the evolution of n depends on $\mathbf{u}$, that of $\mathbf{u}$ depends on T_{ij} , and the evolution of the temperature depends on $\mathbf{q}$.
- In order to close the system of equations, a constitutive equation for T_{ij} and a model for $\mathbf{q}$ are required.

The relaxation-time approximation (the BGK model).

- In the case of a fluid very close to equilibrium, we can approximate f_* , f' and f'_* by the corresponding $f^{(\text{eq})}$:

$$J[f] \simeq \int d\mathbf{p}_* d\mathbf{p}' d\mathbf{p}'_* \delta_{\mathbf{p}} \delta_E \frac{|\mathbf{p} - \mathbf{p}_*|}{m} \frac{d\sigma}{d\Omega} (f^{(\text{eq})'} f'^{(\text{eq})}_* - f f^{(\text{eq})}_*).$$

In the first term in brackets, $f^{(\text{eq})'} f'^{(\text{eq})}_* = f^{(\text{eq})} f^{(\text{eq})}_*$ (by the H-theorem).
Consequently:

$$J[f] \simeq -(f - f^{(\text{eq})}) \int d\mathbf{p}_* d\mathbf{p}' d\mathbf{p}'_* \delta_{\mathbf{p}} \delta_E \frac{|\mathbf{p} - \mathbf{p}_*|}{m} \frac{d\sigma}{d\Omega} f^{(\text{eq})}_*.$$

- A term proportional to $f - f^{(\text{eq})}$ has appeared in $J[f]$.
- The integral on the right depends on the properties of $d\sigma/d\Omega$, but in general it can be interpreted as the inverse of a **relaxation time** τ .
- In this way one obtains the BGK (Bhatnagar-Gross-Krook) approximation - or the relaxation-time approximation - of the collision term:

$$J_{\text{BGK}}[f] = -\frac{1}{\tau} (f - f^{(\text{eq})}). \quad (21)$$

- A priori, the Maxwellian $f^{(\text{eq})}$ appearing in $J_{\text{BGK}}[f]$ is defined with respect to arbitrary parameters n_{eq} , $\mathbf{u}_{\text{eq}}$ and T_{eq} :

$$f^{(\text{eq})} = \frac{n_{\text{eq}}}{(2\pi m K_B T_{\text{eq}})^{3/2}} \exp \left[-\frac{(\mathbf{p} - m\mathbf{u}_{\text{eq}})^2}{2m K_B T_{\text{eq}}} \right]. \quad (22)$$

- These parameters are determined by requiring that $J_{\text{BGK}}[f]$ preserve the collision invariants:

$$J_{\text{BGK}}[f, 1] = 0, \quad J_{\text{BGK}}[f, \mathbf{p}] = 0, \quad J_{\text{BGK}} \left[f, \frac{\mathbf{p}^2}{2m} \right] = 0.$$

- One can see that the relations above require:

$$\begin{aligned} n_{\text{eq}} = n &= \int d\mathbf{p} f, \\ \mathbf{u}_{\text{eq}} = \mathbf{u} &= \frac{1}{\rho} \int d\mathbf{p} f \mathbf{p}, \\ T_{\text{eq}} = T &= \frac{2}{3n K_B} \int d\mathbf{p} f \frac{\xi^2}{2m}. \end{aligned}$$

- In addition, $dH/dt \leq 0$.

In order to construct solutions of the Boltzmann equation, Chapman and Enskog made the following assumptions:

- ① When the mean free path $\lambda \ll L$ (the channel size), f can be written as a series in powers of the Knudsen number $\text{Kn} = \lambda/L$:

$$f = f^{(0)} + f^{(1)}\text{Kn} + f^{(2)}\text{Kn}^2 + \dots \quad (23)$$

- ② In the regime $\lambda \ll L$, the evolution of f is dominated by collisions, such that $J[f] \sim \text{Kn}^{-1}$ (or $\tau = \tilde{\tau}\text{Kn}$).

- ③ f depends on $\mathbf{x}$ and on t only through n , $\mathbf{u}$ and T .

- We will use a simplified variant of the C-E method, namely:

$$f = f^{(0)} + \delta f, \quad J[f] \simeq J_{\text{BGK}}[f] = -\frac{1}{\tilde{\tau}\text{Kn}}\delta f. \quad (24)$$

- Since $J[f] \sim \text{Kn}^{-1}$ we have:

$$f^{(0)} = f^{(\text{eq})}. \quad (25)$$

- At order Kn^0 , the BGK equation gives the non-equilibrium part directly in terms of τ :

$$\delta f = -\tau \left[\partial_t f^{(\text{eq})} + \frac{\mathbf{p}}{m} \cdot \nabla f^{(\text{eq})} + \mathbf{F} \cdot \nabla_{\mathbf{p}} f^{(\text{eq})} \right]. \quad (26)$$

- Since $\psi \in \{1, \mathbf{p}, \mathbf{p}^2/2m\}$ are collision invariants, $n, \mathbf{u}, T$ are unaffected by δf and obey the **Euler equations** at zeroth order.
- Every dissipative flux is simply a **moment of δf** , and therefore **proportional to τ** :

$$\tau_{ij} = - \int d\mathbf{p} \delta f \frac{p_i p_j}{m} \quad (\text{stress}) \quad (27)$$

$$\delta q_i = \int d\mathbf{p} \delta f \frac{\xi^2}{2m} \frac{p_i}{m} \quad (\text{heat flux}) \quad (28)$$

$\Rightarrow$ The relaxation time τ is the *single* microscopic input that sets the magnitude of all transport coefficients.

The constitutive equations.

- Evaluating the stress moment gives :

$$\tau_{ij} = \tau n K_B T \left(\partial_j u_i + \partial_i u_j - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right).$$

- For the Newtonian fluid, the constitutive equation for τ_{ij} is

$$\tau_{ij} = \mu \left(\partial_j u_i + \partial_i u_j - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right) + \mu_v (\nabla \cdot \mathbf{u}) \delta_{ij}. \quad (29)$$

- In the BGK model, the **dynamic viscosity coefficient** is $\mu = \tau P = \tau n K_B T$, while the **bulk viscosity coefficient** vanishes, $\mu_v = 0$.
- for the heat flux one obtains:

$$\delta q_i = -\kappa \partial_i T, \quad \kappa = \frac{5}{2m} \tau K_B P, \quad (30)$$

where κ is the **thermal conductivity coefficient**.

- Together with the constitutive equation for T_{ij} , eq. (30) closes the system of equations for n , $\mathbf{u}$ and T .

The Enskog equation

- The dynamics of the system of particles can be described by the following *exact* kinetic equation¹:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \frac{\mathcal{F}[n]}{m} \cdot \nabla_{\mathbf{p}} f = J_E = \sigma^2 \int_{\mathbb{R}^3} d\mathbf{v}_* \int_{S_+} d^2 \hat{\mathbf{k}} \left\{ f_2(\mathbf{r}, \mathbf{v}', \mathbf{r} + \sigma \hat{\mathbf{k}}, \mathbf{v}'_*) - f_2(\mathbf{r}, \mathbf{v}, \mathbf{r} - \sigma \hat{\mathbf{k}}, \mathbf{v}_*) \right\} (\mathbf{v}_r \cdot \hat{\mathbf{k}}).$$

- Short-range correlations are taken into account as in Enskog theory:

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

- χ encodes the *static structure* of the fluid: it boosts the local collision rate above the dilute-gas value, reflecting the fact that dense hard spheres are more likely to be found in contact.
- Physically, χ plays the same role here that the equilibrium radial distribution function $g(\sigma)$ plays in equilibrium statistical mechanics — the question is only *which density* to evaluate it at, since the two colliding spheres sit at different points $\mathbf{r} \pm \sigma \hat{\mathbf{k}}/2$.

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

The Enskog equation

- Different expressions 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:

$$\chi = \chi_{\text{SET}} \left(n \left(\mathbf{r} \pm \frac{a}{2} \hat{\mathbf{k}} \right) \right) = \frac{1}{nb} \left(\frac{p^{CS}}{nk_B T} - 1 \right) = \frac{1}{2} \frac{2 - \eta}{(1 - \eta)^3}, \quad b = \frac{2\pi\sigma^3}{3},$$

where p^{CS} is given by the Carnahan-Starling equation of state:

$$p^{CS} = nk_B T \frac{1 + \eta + \eta^2 - \eta^3}{(1 - \eta)^3}, \quad \eta = \frac{\pi\sigma^3 n}{6}. \quad (31)$$

- **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):

$$\chi = \chi_{\text{RET-FM}} \left[n \left(\mathbf{r} \pm \frac{\sigma}{2} \hat{\mathbf{k}} \right) \right] = \chi_{\text{SET}} \left(\bar{n} \left(\mathbf{r} \pm \sigma \frac{\hat{\mathbf{k}}}{2} \right) \right),$$

where

$$\bar{n}(\mathbf{r}, t) = \frac{3}{4\pi\sigma^3} \int_S n(\mathbf{r}_1, t) w(\mathbf{r}, \mathbf{r}_1) d\mathbf{r}_1, \quad w(\mathbf{r}, \mathbf{r}_1) = \begin{cases} 1, & \|\mathbf{r}_1 - \mathbf{r}\| < \sigma \\ 0, & \|\mathbf{r}_1 - \mathbf{r}\| > \sigma \end{cases}.$$

The Enskog collision operator

- The right-hand side is given by the Enskog collision operator J_E^2 :

$$J_E = \sigma^2 \int \left\{ \chi \left(\mathbf{x} + \frac{\sigma}{2} \mathbf{k} \right) f(\mathbf{x}, \mathbf{p}^*) f(\mathbf{x} + \sigma \mathbf{k}, \mathbf{p}_1^*) - \right. \\ \left. \chi \left(\mathbf{x} - \frac{\sigma}{2} \mathbf{k} \right) f(\mathbf{x}, \mathbf{p}) f(\mathbf{x} - \sigma \mathbf{k}, \mathbf{p}_1) \right\} (\mathbf{p}_r \cdot \mathbf{k}) d\mathbf{k} d\mathbf{p}_1 \quad (32)$$

where σ is the molecular diameter, $\mathbf{p}_r = \mathbf{p}_1 - \mathbf{p}$ is the relative momentum, $\mathbf{k}$ is the unit vector of relative position, and $*$ denotes post-collision momenta. Used in the particle method (PM).

- Taylor-expanding χ and f near $\mathbf{x}$, the first-order gradient expansion gives:

$$J_0(f, f) = \chi \int (f^* f_1^* - f f_1) \Omega^2(\mathbf{p}_r \cdot \mathbf{k}) d\mathbf{k} d\mathbf{p}_1 \quad (33)$$

$$J_1(f, f) = \chi \sigma \int \mathbf{k} (f^* \nabla f_1^* - f \nabla f_1) \Omega^2(\mathbf{p}_r \cdot \mathbf{k}) d\mathbf{k} d\mathbf{p}_1 \\ + \frac{\sigma}{2} \int \mathbf{k} \nabla \chi (f^* f_1^* - f f_1) \Omega^2(\mathbf{p}_r \cdot \mathbf{k}) d\mathbf{k} d\mathbf{p}_1 \quad (34)$$

- $J_0(f, f)$ is the usual Boltzmann collision term multiplied by χ , treated via the relaxation time approximation:

$$J_0(f, f) = -\frac{\chi}{\tau} (f - f^{eq}). \quad (35)$$

²G. M. Kremer, *An introduction to the Boltzmann equation and transport processes in gases*

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 $f_{\text{eq}}^* f_{\text{eq},1}^* = f_{\text{eq}} f_{\text{eq},1}$ and integrating over $\mathbf{k}$ and $\mathbf{p}_1$, one obtains³:

$$J_1(f, f) \approx J_1(f_{\text{eq}}, f_{\text{eq}}) = -b\rho\chi f_{\text{eq}} \left\{ \xi \cdot \left[\nabla \ln(\rho^2 \chi T) + \frac{3}{5} \left(\zeta^2 - \frac{5}{2} \right) \nabla \ln T \right] + \frac{2}{5} \left[2\zeta\zeta : \nabla \mathbf{u} + \left(\zeta^2 - \frac{5}{2} \right) \nabla \cdot \mathbf{u} \right] \right\} \quad (36)$$

where $\zeta = \xi/\sqrt{2RT}$.

With the above approximations, the Enskog equation becomes:

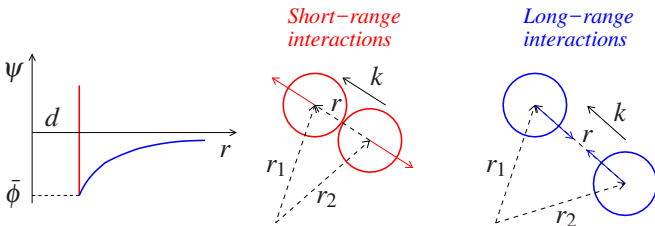
$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{x}} f + \frac{\mathcal{F}[n]}{m} \cdot \nabla_{\mathbf{p}} f = -\frac{\chi}{\tau} (f - f^S) + J_1(f_{\text{eq}}, f_{\text{eq}}) \quad (37)$$

³G. M. Kremer, *An introduction to the Boltzmann equation and transport processes in gases* (Springer-Verlag, Berlin Heidelberg, 2010).

The Enskog-Vlasov equation

- Unlike the Boltzmann equation, the Enskog-Vlasov equation has the capability of handling both the liquid and vapor phases.
- Let us consider a system of particles of mass m and diameter $d \equiv \sigma$.
- Let us assume that interactions between particles occur through the Sutherland potential:

$$\phi(\rho) = \begin{cases} +\infty, & \rho < d, \\ -\phi_a \left(\frac{\rho}{d}\right)^{-\gamma}, & \rho \geq d, \end{cases} \quad (38)$$



The Enskog-Vlasov equation

- The above simplifying assumptions lead to the following *closed* kinetic equation, which is referred to as the Enskog-Vlasov equation⁴⁵⁶⁷:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \underbrace{\frac{\mathbf{F}(\mathbf{r})}{m} \cdot \nabla_{\mathbf{v}} f}_{\text{Vlasov term}} = \underbrace{\mathbf{C}(f, f)}_{\text{Enskog term}}$$

where:

$$\begin{aligned} \mathbf{F}(\mathbf{r}) &= \int_{r > \sigma} d\mathbf{r}_* \frac{1}{r} \frac{d\phi}{dr} (\mathbf{r}_* - \mathbf{r}) n(\mathbf{r}_*), \\ \mathbf{C}(f, f) &= \sigma^2 \int_{\mathbb{R}^3} d\mathbf{v}_* \int_{\mathcal{S}_+} d^2 \hat{\mathbf{k}} \left\{ \chi_{\text{SET}}[\bar{n}(\mathbf{r} - \sigma/2\hat{\mathbf{k}})] f(\mathbf{r}, \mathbf{v}') f(\mathbf{r} + \sigma\hat{\mathbf{k}}, \mathbf{v}'_*) \right. \\ &\quad \left. - \chi_{\text{SET}}[\bar{n}(\mathbf{r} - \sigma/2\hat{\mathbf{k}})] f(\mathbf{r}, \mathbf{v}) f(\mathbf{r} - \sigma\hat{\mathbf{k}}, \mathbf{v}_*) \right\} (\mathbf{v}_r \cdot \hat{\mathbf{k}}). \end{aligned}$$

⁴L. De Sobrino, *Can. J. Phys.* 45(2), 363–385 (1967).

⁵M. Grmela, *J. Stat. Phys.* 3(3), 347–364 (1971).

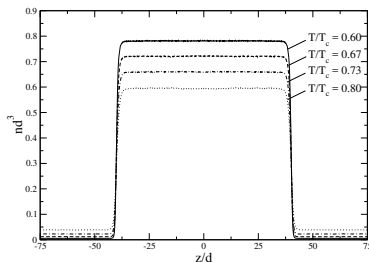
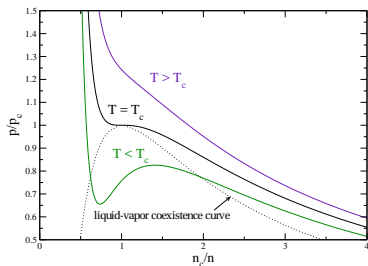
⁶J. Karkheck and G. Stell, *J. Chem. Phys.* 75(3), 1475–1487 (1981).

⁷A. Frezzotti, L. Gibelli, and S. Lorenzani, *Phys. Fluids* 17, 012012 (2005).

Liquid-vapour coexistence curve for simple liquids

- The equation of state of the fluid described by the Enskog-Vlasov equation has a generalized van der Waals form:

$$p_0(n, T) = \underbrace{nk_B T \frac{1 + \eta + \eta^2 - \eta^3}{(1 - \eta)^3}}_{\text{repulsive interactions}} - \underbrace{\frac{2\pi\sigma^3}{3} \frac{\gamma}{\gamma - 3} \phi_a n^2}_{\text{attractive interactions}}, \Rightarrow \begin{cases} T_c \simeq 0.094 \frac{4\gamma}{\gamma - 3} \frac{\phi_a}{k_B} \\ \eta_c \simeq 0.13 \end{cases}$$



- The Enskog-Vlasov equation leads to the following fluid dynamics equations⁸⁹:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + \mathbf{\Pi}) = 0,$$

$$\partial_t \left(\rho e + \frac{1}{2} \rho u^2 + \kappa |\nabla \rho|^2 \right) + \nabla \cdot \left[\mathbf{u} \left(\rho e + \frac{1}{2} \rho u^2 + \kappa |\nabla \rho|^2 \right) + \mathbf{\Pi} \cdot \mathbf{u} + \mathbf{q} \right] = 0,$$

$$\text{where } \kappa = \frac{2}{15} \frac{\gamma}{\gamma - 5} \phi_a \sigma^5.$$

- “Korteweg” contributions appear in the expressions of the stress tensor and heat flux:

$$\mathbf{\Pi} = \left(p_0 - \kappa \rho \nabla^2 \rho - \frac{\kappa}{2} |\nabla \rho|^2 \right) \mathbf{I} - \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^\top \right) - \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} + \kappa \nabla \rho \nabla \rho,$$

$$\mathbf{q} = -k \nabla T + \kappa \rho (\nabla \cdot \mathbf{u}) \nabla \rho.$$

⁸D. M. Anderson, G. B. McFadden, and A. A. Wheeler, *Annu. Rev. Fluid Mech.* 30(1), 139–165 (1998).

⁹X. He and G. D. Doolen, *J. Stat. Phys.* 107(1), 309–328 (2002).

Direct Simulation Monte Carlo (DSMC)

- Stochastic particle method for solving the Boltzmann equation, introduced by Bird¹⁰.
- Each simulated particle represents a large number of real molecules (statistical weight), keeping the particle count computationally tractable.
- Physical domain is divided into cells of size comparable to the local mean free path.
- At each time step $\Delta t \ll \tau$ (mean collision time), the motion and the collisions of particles are **decoupled**:
 - **Free flight**: particles are moved ballistically according to their velocity, $\mathbf{x} \rightarrow \mathbf{x} + \mathbf{v}\Delta t$;
 - **Collision step**: within each cell, pairs of particles are selected *stochastically* (e.g. the No-Time-Counter scheme) with a probability proportional to their relative velocity and collision cross-section;
 - post-collision velocities are sampled so as to conserve momentum and kinetic energy.
- Macroscopic quantities ($n, \mathbf{u}, T, \dots$) are recovered by sampling/averaging over the particles in each cell.
- Accuracy requires the cell size to remain smaller than λ and Δt smaller than the mean collision time τ .
- Well established for dilute (Boltzmann) gas flows; extending it to **dense** gases requires replacing the collision step with the Enskog collision mechanics $\rightarrow$ Frezzotti's scheme.

¹⁰G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford University Press (1994).

- **Non-local Nature of Enskog Collisions:** Unlike standard DSMC for the Boltzmann equation (where colliding pairs are selected locally within the same grid cell), finite molecular size σ requires non-local interaction across cell boundaries.
- **Partner Selection & Collision Mechanism:**
 - **Primary Particle:** Chosen for collision according to the collision probability modified by the local pair correlation function $\chi(\mathbf{r})$.
 - **Collision Partner:** Selected at a non-local displacement $\mathbf{r} \pm \sigma \hat{\mathbf{k}}$ by drawing a random direction unit vector $\hat{\mathbf{k}} \in \mathcal{S}_+^2$ on the contact sphere.
 - **Scattering:** An elastic hard-sphere collision is applied using post-collision momenta derived from conservation laws.
- **Key Advantages:**
 - Correctly captures excluded volume effects and collision pressure (virial contribution).
 - Naturally extends to non-uniform, dense fluids and phase-separating Enskog-Vlasov models.

- 1 **Expansion of Equilibrium:** Expand f^{eq} in a series of orthogonal polynomials (Hermite polynomials).
- 2 **Momentum Space Discretization:** Apply Gauss-Hermite quadratures to determine discrete velocity sets $\mathbf{p}_k$.
- 3 **Off-Lattice Discretization:** Numerical schemes (FD/WENO) for spatial advection and time evolution (since discrete velocities do not match grid nodes).
- 4 **Kinetic Boundary Conditions:** Implement specular, diffuse, or kinetic boundary rules.

Conservation Laws

The FDLB framework ensures exact recovery of macroscopic conservation equations for mass density n , momentum $\rho \mathbf{u}$, and energy E in thermal and non-equilibrium flows.

- **Standard Gauss-Hermite Quadrature:**

$$\int_{-\infty}^{\infty} e^{-x^2} P(x) dx \approx \sum_{i=1}^n w_i P(x_i), \quad \text{exact for polynomials up to degree } 2n - 1.$$

- **Discretization of Momentum Space¹¹:**

$$\int dp f(\mathbf{p}) P_s(p) = \sum_{k=1}^Q f_k P_s(p_k), \quad f_k = \frac{p_0 w_k}{\omega(\bar{p}_k)} f(p_k),$$

where $\bar{p}_k = p_k/p_0$ are the roots of the dimensionless weight $\omega(\bar{p}) = e^{-\bar{p}^2/2}/\sqrt{2\pi}$.

- **Polynomial Types:**

- *Full-Range Hermite* $H_Q(\bar{p})$: Q roots over $(-\infty, \infty)$ for bulk gas flows.
- *Half-Range Hermite* $h_Q(\bar{p})$: $2Q$ roots over $(-\infty, 0] \cup [0, \infty)$ tailored for half-space boundary conditions in rarefied flows.

¹¹X. W. Shan, X. F. Yuan, and H. D. Chen, *J. Fluid Mech.* **550**, 413–441 (2006).

The discrete equilibrium distribution $f_k^{\text{eq}} = n g_k$ is obtained via a truncated expansion up to polynomial order N :

- **Full-Range Hermite Expansion**¹²:

$$g_k = w_k \sum_{\ell=0}^N H_{\ell}(\bar{p}_k) \sum_{s=0}^{\lfloor \ell/2 \rfloor} \frac{1}{2^s s! (\ell - 2s)!} \left(\frac{mk_B T}{p_0^2} - 1 \right)^s \left(\frac{mu}{p_0} \right)^{\ell - 2s}.$$

- **Half-Range Hermite Expansion:** Splitting $g(p) = \theta(p)g_+(p) + \theta(-p)g_-(p)$ with Heaviside step functions $\theta(\pm p)$:

$$g_{\pm}(p) = \frac{\omega(|p|)}{p_0} \sum_{\ell=0}^{\infty} \mathcal{G}_{\ell}^{\pm} \mathfrak{h}_{\ell}(|p|),$$

where $\mathcal{G}_{\ell}^{+} = \int_0^{\infty} dp g(p) \mathfrak{h}_{\ell}(p)$ and $\mathcal{G}_{\ell}^{-} = \int_{-\infty}^0 dp g(p) \mathfrak{h}_{\ell}(-p)$.

¹²V. E. Ambruş and V. Sofonea, *J. Comput. Phys.* **316**, 1–29 (2016).

- When momentum space is separable in Cartesian coordinates (p_x, p_y) , Gauss-Hermite quadrature is evaluated along each direction:

$$\int dp_x \int dp_y f P_s(p_x) P_r(p_y) = \sum_{i=1}^{Q_x} \sum_{j=1}^{Q_y} f_{ij} P_s(p_{x,i}) P_r(p_{y,j})$$

where $H_{Q_x}(\bar{p}_{x,i}) = 0$ and $H_{Q_y}(\bar{p}_{y,j}) = 0$, with weights:

$$f_{ij} = \frac{p_{0,x} w_{x,i}}{\omega(\bar{p}_{x,i})} \frac{p_{0,y} w_{y,j}}{\omega(\bar{p}_{y,j})} f(p_{x,i}, p_{y,j})$$

- **Separability:** The discrete equilibrium PDF simplifies to $f_{ij}^{\text{eq}} = n g_{x,i} g_{y,j}$.
- Extension to 3D Cartesian grids ($Q_x \times Q_y \times Q_z$) is straightforward.

The continuum kinetic equation is discretized into a coupled set of K partial differential equations:

$$\frac{\partial f_k}{\partial t} + \frac{\mathbf{p}_k}{m} \cdot \nabla_{\mathbf{x}} f_k + \mathbf{F} \cdot (\nabla_{\mathbf{p}} f)_k = -\frac{1}{\tau} (f_k - f_k^{\text{eq}})$$

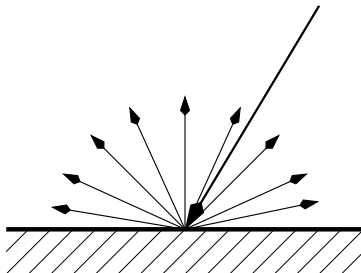
- **Off-Lattice Velocity Set:** Because $\mathbf{p}_k/m$ are roots of high-order Hermite polynomials (irrational numbers), standard stream-and-collide operations ($\mathbf{x} + \mathbf{v}_k \Delta t$) cannot be used.
- **Time Integration:**
 - 3rd-order Total Variation Diminishing Runge-Kutta (TVD-RK3)
- **Spatial Advection Schemes:**
 - 5th-order Weighted Essentially Non-Oscillatory scheme (WENO-5)

- **Specular Reflection:** Rebounds incoming momentum components along boundary normal $\hat{\mathbf{n}}$ using ghost nodes:

$$f_{k,0} = f_{\tilde{k},1}, \quad f_{k,-1} = f_{\tilde{k},2}, \quad \text{where } \mathbf{p}_{\tilde{k}} = \mathbf{p}_k - 2(\mathbf{p}_k \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}$$

- **Diffuse Reflection:** Wall density n_w is determined by enforcing zero net mass flux through the boundary:

$$\int_{\mathbf{p} \cdot \hat{\mathbf{n}} > 0} d^3p f(\mathbf{p} \cdot \hat{\mathbf{n}}) = - \int_{\mathbf{p} \cdot \hat{\mathbf{n}} < 0} d^3p f^{\text{eq}}(n_w, T_w)(\mathbf{p} \cdot \hat{\mathbf{n}})$$



Longitudinal waves

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 $u(x, t)$:

$$\rho(x, t) = \rho_0[1 + \delta\rho(x, t)], \quad P(x, t) = P_0[1 + \delta P(x, t)] \quad (39)$$

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

$$\partial_t \delta\rho + \partial_x u = 0, \quad \partial_t u + \frac{P_0}{\rho_0} \partial_x \delta P - \frac{1}{\rho_0} \partial_x \Pi = 0 \quad (40a)$$

$$\partial_t \delta T + \frac{\partial_x q}{\rho_0 c_V T_0} + \frac{P_0}{\rho_0 c_V T_0} \partial_x u = 0 \quad (40b)$$

where the specific energy is $e = c_V T = c_V T_0(1 + \delta T)$ and $\Pi = O(u)$. The sound speed is given by: $c_s^2 = \partial_\rho P + \frac{P_0}{\rho_0^2 c_V} \partial_T P$, while the damping coefficients:

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

We will restrict our simulations to the case when $\delta P(t_0) = 0$. The full solution of the density amplitude can be written as:

$$\delta\rho(t) \approx \delta\rho_0 \left[e^{-\alpha_t t} + (e^{-\alpha_a t} \cos(\alpha_s t) - e^{-\alpha_t t}) \frac{1}{c_s^2} \frac{\partial P}{\partial \rho} \right] \quad (41)$$

Results: Longitudinal waves

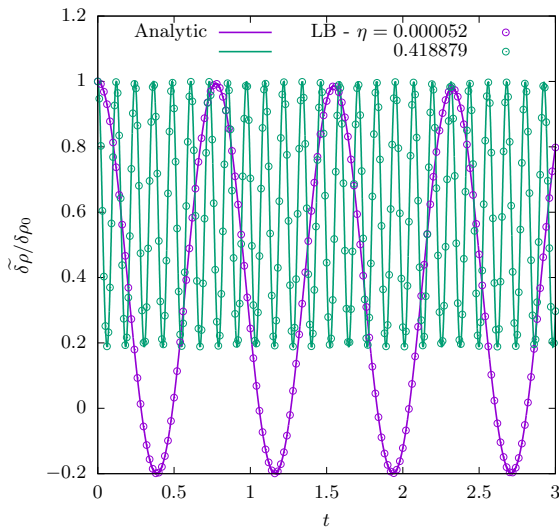


Figure: Normalized density amplitude $\delta\rho(t)/\delta\rho_0$ in comparison with the analytical prediction.

Results: Longitudinal waves

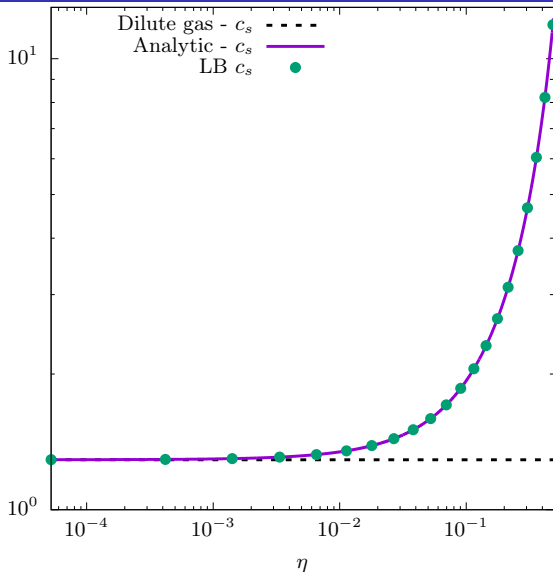


Figure: The sound speed c_s obtained from the simulation results and the analytic prediction.

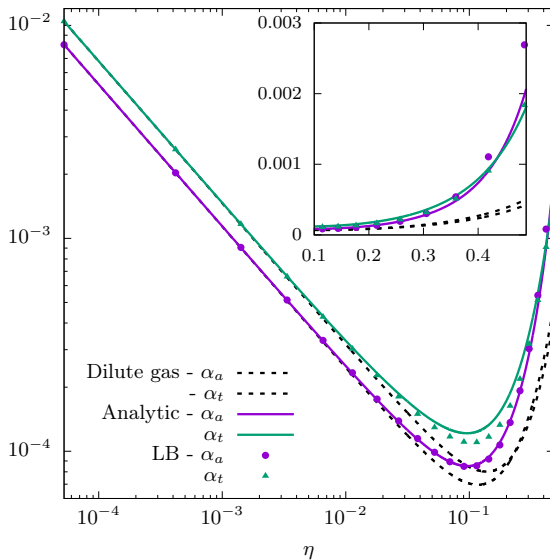
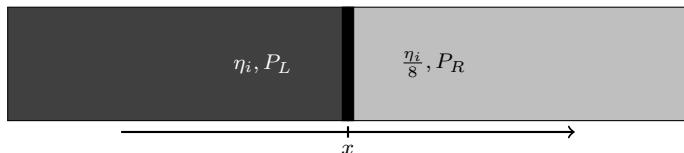


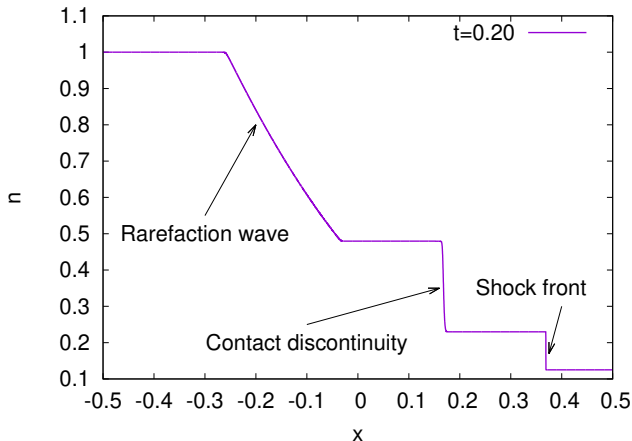
Figure: The acoustic α_a and thermal α_t mode with respect to the reduced density η .

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.

Results: Shock wave propagation

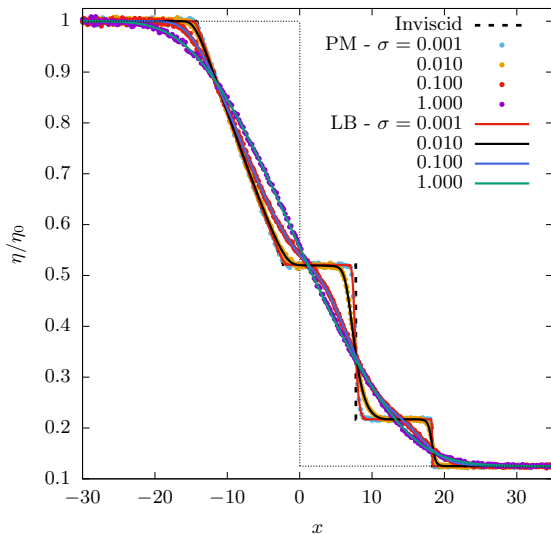
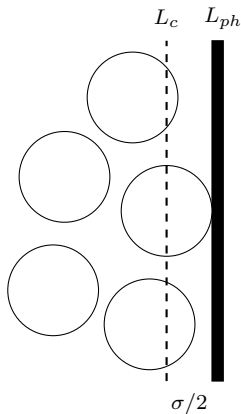
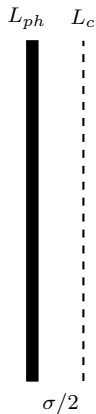
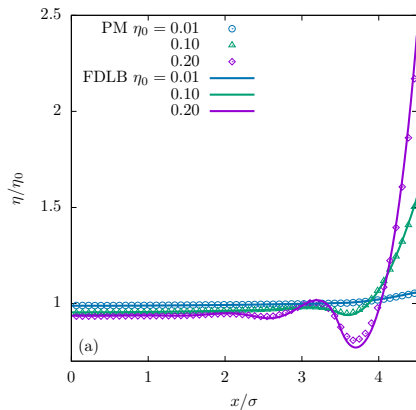


Figure: Shock wave propagation: reduced density profile for $\eta_i = 0.05$ but with various values of the molecular diameter (implicitly various values of the relaxation time τ).

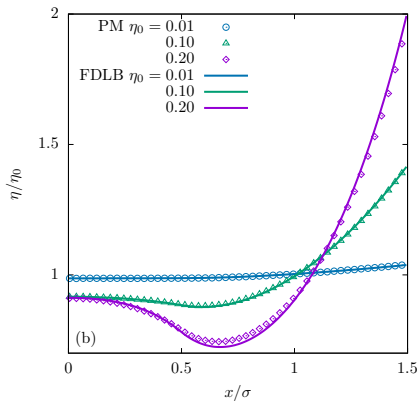
Boundary condition



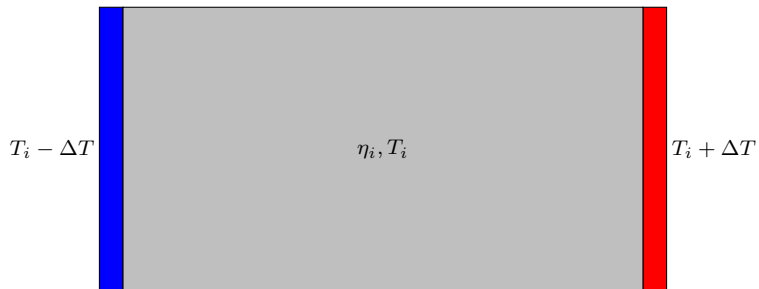
- Diffuse boundary conditions are applied at L_c . Confinement ratio defined as $R = L_{ph}/\sigma$.

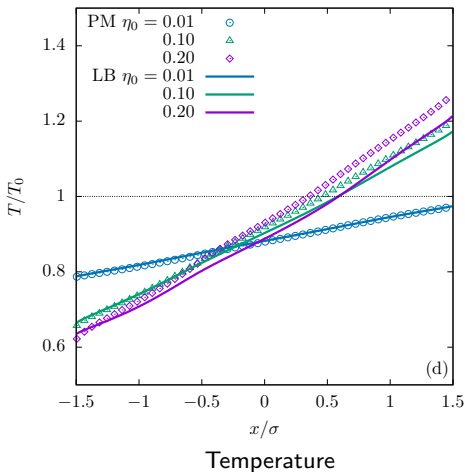
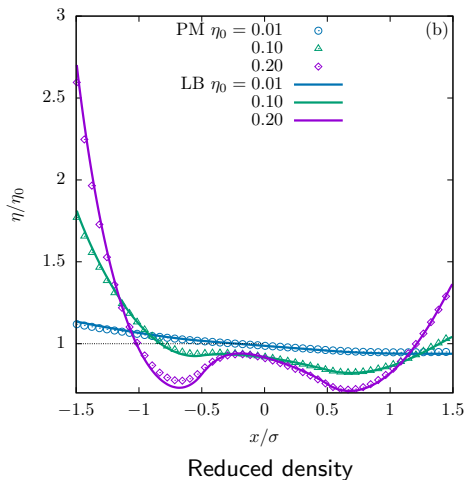


$R = 10$



$R = 4$





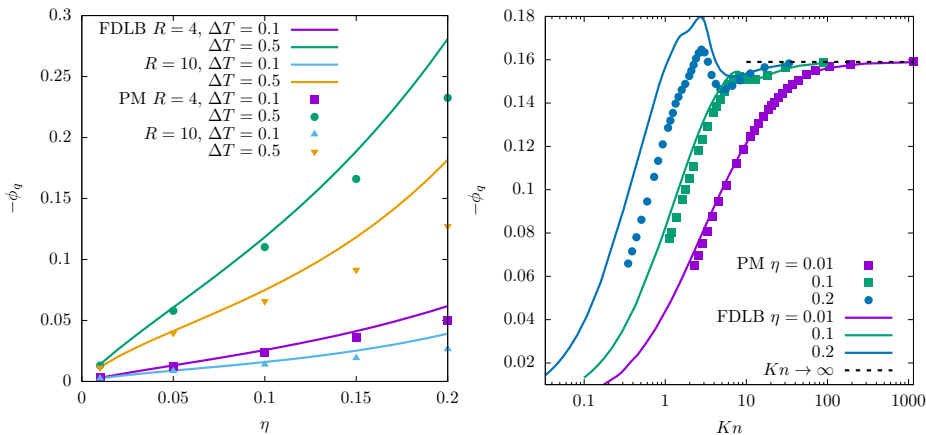
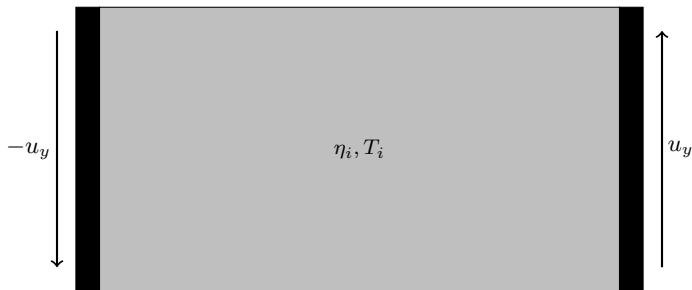
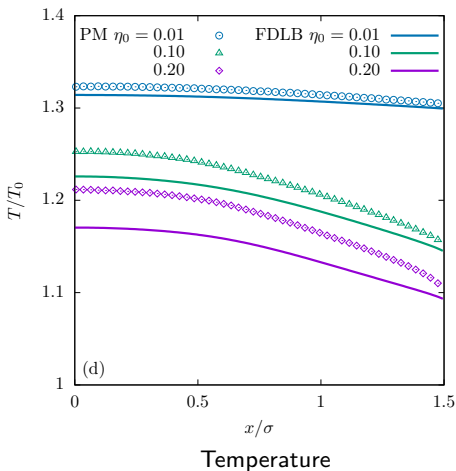
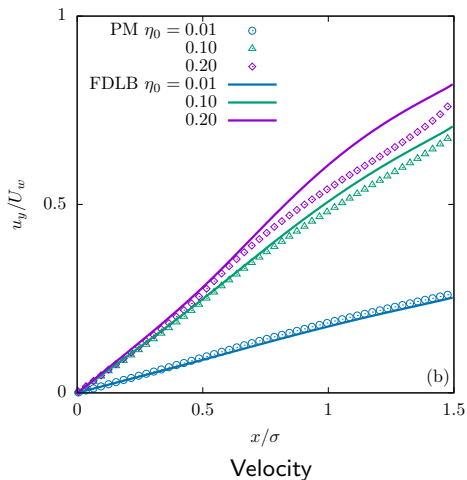
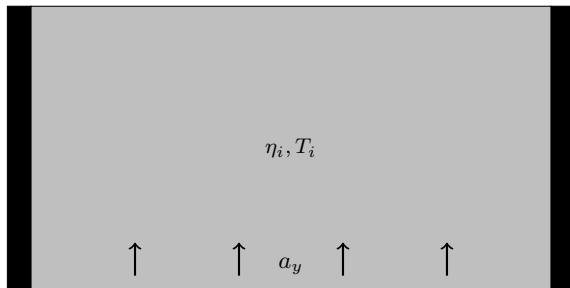


Figure: Heat transfer: (a) Heat flux ϕ_q values at temperature difference of $\Delta T = \{0.1, 0.5\}$, confinement ratios of $R = \{4, 10\}$. (b) Heat flux ϕ_q with respect to the Knudsen number Kn .

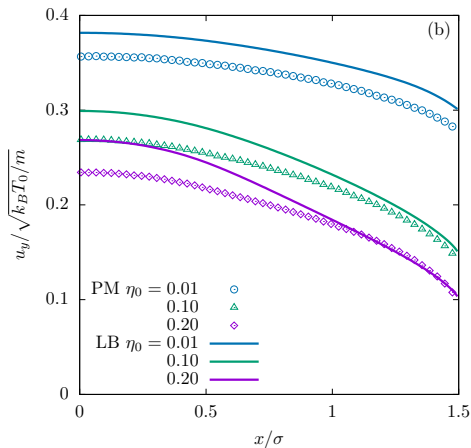


Couette flow - $U_w = 1.0$;

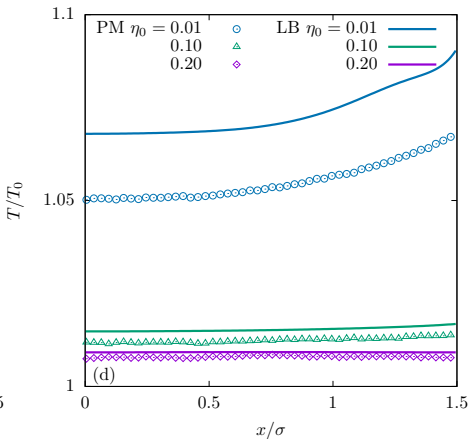




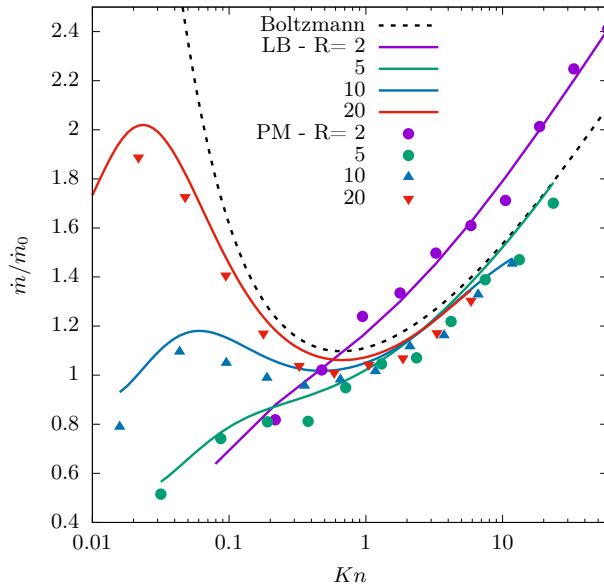
Poiseuille flow - $a_y = 0.1$



(a) Velocity



(b) Temperature



- Consider a coordinate transformation $x^i \rightarrow x^{\tilde{i}}$, which induces a metric $g_{\tilde{i}\tilde{j}}$, as follows:

$$ds^2 = \delta_{ij} dx^i dx^j = g_{\tilde{i}\tilde{j}} dx^{\tilde{i}} dx^{\tilde{j}}, \quad g_{\tilde{i}\tilde{j}} = \delta_{ij} \frac{\partial x^i}{\partial x^{\tilde{i}}} \frac{\partial x^j}{\partial x^{\tilde{j}}}.$$

- Furthermore, we note that:

$$p^{\tilde{i}} = p^i \frac{\partial x^i}{\partial x^{\tilde{i}}}, \quad F^{\tilde{i}} = F^i \frac{\partial x^i}{\partial x^{\tilde{i}}}, \quad \mathbf{p}^2 \equiv g_{\tilde{i}\tilde{j}} p^{\tilde{i}} p^{\tilde{j}}$$

- By introducing the triad vector frame and the associated one-form co-frame:

$$e_{\hat{a}} = e_{\hat{a}}^{\tilde{i}} \partial_{\tilde{i}}, \quad \omega^{\hat{a}} = \omega^{\hat{a}}_{\tilde{i}} dx^{\tilde{i}}, \quad g_{\tilde{i}\tilde{j}} dx^{\tilde{i}} dx^{\tilde{j}} = \delta_{\hat{a}\hat{b}} \omega^{\hat{a}} \omega^{\hat{b}} \quad (42)$$

the inner product $\mathbf{p}^2 \equiv \delta_{\hat{a}\hat{b}} p^{\hat{a}} p^{\hat{b}}$ is decoupled from the metric.

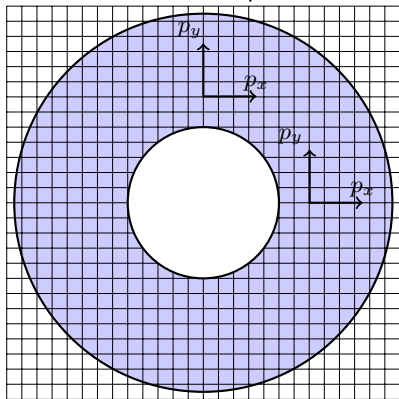
- The Enskog equation reads:

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{p^{\hat{a}}}{m} e_{\hat{a}}^{\tilde{i}} \frac{\partial f}{\partial x^{\tilde{i}}} + \left(F^{\hat{a}} - \frac{1}{m} \Gamma^{\hat{a}}_{\hat{b}\hat{c}} p^{\hat{b}} p^{\hat{c}} \right) \frac{\partial f}{\partial p^{\hat{a}}} = \\ - \frac{\chi}{\tau} (f - f^S) - b \rho \chi f^{\text{MB}} \left\{ \xi^{\hat{a}} \cdot \left[\nabla_{\hat{a}} \ln(\rho^2 \chi T) + \frac{3}{5} \left(\zeta^2 - \frac{5}{2} \right) \nabla_{\hat{a}} \ln T \right] \right. \\ \left. + \frac{2}{5} \left[2 \zeta^{\hat{a}} \zeta^{\hat{a}} : \nabla_{\hat{a}} u^{\hat{a}} + \left(\zeta^2 - \frac{5}{2} \right) \nabla_{\hat{a}} \cdot u^{\hat{a}} \right] \right\}, \quad (43) \end{aligned}$$

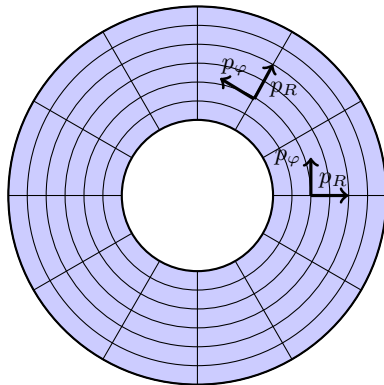
where $\zeta^{\hat{a}} = \xi^{\hat{a}} / \sqrt{2RT}$.

Spatial grid and momentum space decomposition example

Cartesian decomposition



Cylindrical decomposition



To describe the geometry of this flow, it is convenient to introduce cylindrical coordinates $\{\tilde{x}\} = \{R, \varphi, z\}$ through $x = R \cos \varphi$ and $y = R \sin \varphi$. The line element in cylindrical coordinates and the associated triad are:

$$ds^2 = dR^2 + R^2 d\varphi^2 + dz^2, \quad e_{\hat{R}} = \partial_R, \quad e_{\hat{\varphi}} = R^{-1} \partial_{\varphi}, \quad e_{\hat{z}} = \partial_z. \quad (44)$$

The Enskog equation when the flow is homogeneous with respect to φ and z reads:

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{2p^{\hat{R}}}{m} \frac{\partial(fR)}{\partial R^2} + \frac{1}{mR} \left[(p^{\hat{\varphi}})^2 \frac{\partial f}{\partial p^{\hat{R}}} - p^{\hat{R}} \frac{\partial(f p^{\hat{\varphi}})}{\partial p^{\hat{\varphi}}} \right] &= \frac{\chi}{\tau} (f - f^S) - \\ b\rho\chi f^{\text{MB}} \left\{ \xi^R \cdot \left[\partial_R \ln(\rho^2 \chi T) + \frac{3}{5} \left(\zeta^2 - \frac{5}{2} \right) \partial_R \ln T \right] \right. & \\ \left. + \frac{2}{5} \left[2\zeta^{\hat{a}} \zeta^{\hat{b}} : \nabla_{\hat{a}} u^{\hat{b}} + \left(\zeta^2 - \frac{5}{2} \right) \partial_R \cdot u^R \right] \right\}. & \quad (45) \end{aligned}$$

The advection term is implemented following Falle and Komissarov¹³.

¹³S. A. E. G. Falle and S. S. Komissarov, An upwind numerical scheme for relativistic hydrodynamics with a general equation of state, Monthly Notices of the Royal Astronomical Society 278, 586 (1996)

To describe the spherical Fourier flow we introduce spherical coordinates $\{x^{\tilde{i}}\} = \{r, \theta, \varphi\}$ through $x = r \sin \theta \cos \varphi$, $y = r \sin \theta \sin \varphi$ and $z = r \cos \theta$. The line element in spherical coordinates and its associated triad are:

$$ds^2 = dr^2 + r^2(d\theta^2 + \sin^2 \theta d\varphi^2), \quad e_{\hat{r}} = \partial_r, \quad e_{\hat{\theta}} = \frac{\partial_{\theta}}{r}, \quad e_{\hat{\varphi}} = \frac{r^{-1}}{\sin \theta} \partial_{\varphi}. \quad (46)$$

Assuming that the flow is homogeneous with respect to θ and φ , the Boltzmann equation reads:

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{3p^{\hat{r}}}{m} \frac{\partial(fr^2)}{\partial r^3} + \frac{1}{mr} \left[\left((p^{\hat{\theta}})^2 + (p^{\hat{\varphi}})^2 \right) \frac{\partial f}{\partial p^{\hat{r}}} - p^{\hat{r}} \left(\frac{\partial(f p^{\hat{\theta}})}{\partial p^{\hat{\theta}}} + \frac{\partial(f p^{\hat{\varphi}})}{\partial p^{\hat{\varphi}}} \right) \right] &= \frac{\chi}{\tau} (f - f^S) - \\ b\rho\chi f^{\text{MB}} \left\{ \xi^r \cdot \left[\partial_r \ln(\rho^2 \chi T) + \frac{3}{5} \left(\zeta^2 - \frac{5}{2} \right) \partial_r \ln T \right] \right. & \\ \left. + \frac{2}{5} \left[2\zeta^{\hat{a}} \zeta^{\hat{b}} : \nabla_{\hat{a}} u^{\hat{b}} + \left(\zeta^2 - \frac{5}{2} \right) \partial_r \cdot u^r \right] \right\}. & \quad (47) \end{aligned}$$

The advection term is implemented following Downes et al.¹⁴.

¹⁴T. P. Downes, P. Duffy, and S. S. Komissarov, Relativistic blast waves and synchrotron emission, Monthly Notices of the Royal Astronomical Society 332, 144 (2002)

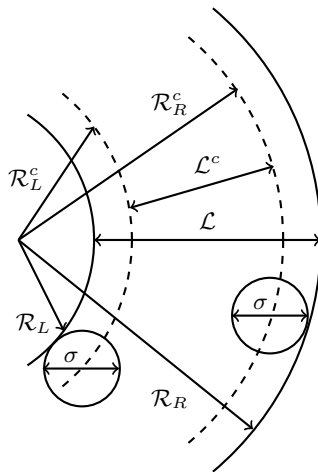


Figure: Radial coordinates used and the particle diameter σ for context. The dashed lines represent the computational domain, at a distance of $\sigma/2$ from the physical domain. the macroscopic quantities will be plotted with respect to the reduced radius $(\mathcal{R} - \mathcal{R}_L^c)/(\mathcal{R}_R^c - \mathcal{R}_L^c)$.

⁴S. Busuioc, Mesoscopic lattice Boltzmann modeling of dense gas flows in curvilinear geometries, Phys. Rev. Fluids 9, 053401 (2024).

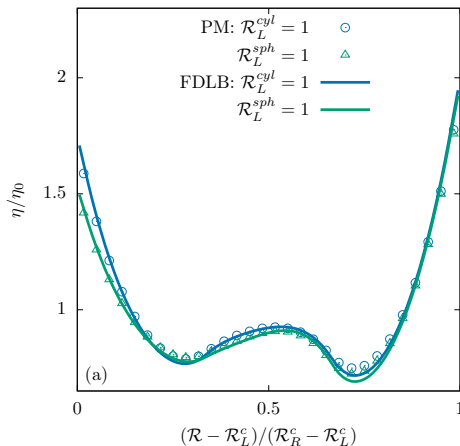


Figure: Gas at rest: Normalized reduced density η/η_0 at $\mathcal{R}_L = 1$ and variable geometry, for fixed mean reduced density $\eta_0 = 0.2$, fixed inner cylinder/sphere radius $\mathcal{R}_L = 1$ and the confinement ratio $C = 4$.

⁴S. Busuioc, Mesoscopic lattice Boltzmann modeling of dense gas flows in curvilinear geometries, Phys. Rev. Fluids 9, 053401 (2024).

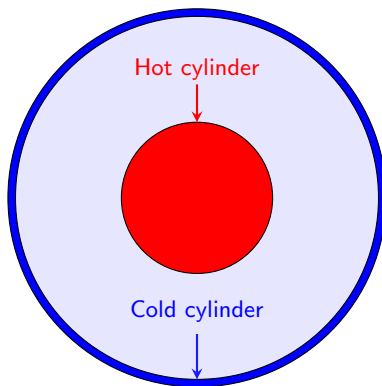


Figure: Setup of the Cylindrical Fourier flow. Temperature is given by $T_{\pm} = T_0 \pm \Delta T$.

⁴S. Busuioc, Mesoscopic lattice Boltzmann modeling of dense gas flows in curvilinear geometries, Phys. Rev. Fluids 9, 053401 (2024).

Cylindrical Fourier flow - $\Delta T = 0.1^4$

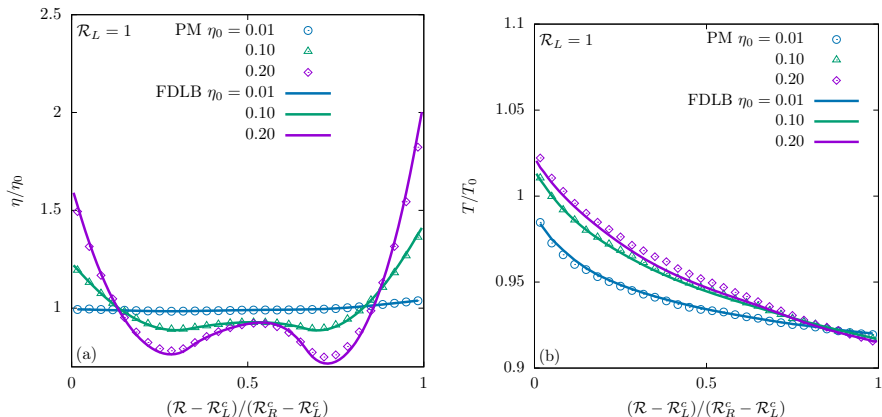


Figure: Cylindrical Fourier flow: Normalized reduced density η/η_0 and normalized temperature T/T_0 , for $\mathcal{R}_L = 1$ and the confinement ratio $C = 4$, while lines (FDLB) and points (PM) correspond to varying values of the mean reduced density $\eta_0 \in \{0.01, 0.1, 0.2\}$.

⁴S. Busuioc, Mesoscopic lattice Boltzmann modeling of dense gas flows in curvilinear geometries, Phys. Rev. Fluids 9, 053401 (2024).

Fourier flow: Geometry comparisons - $\Delta T = 0.1^4$

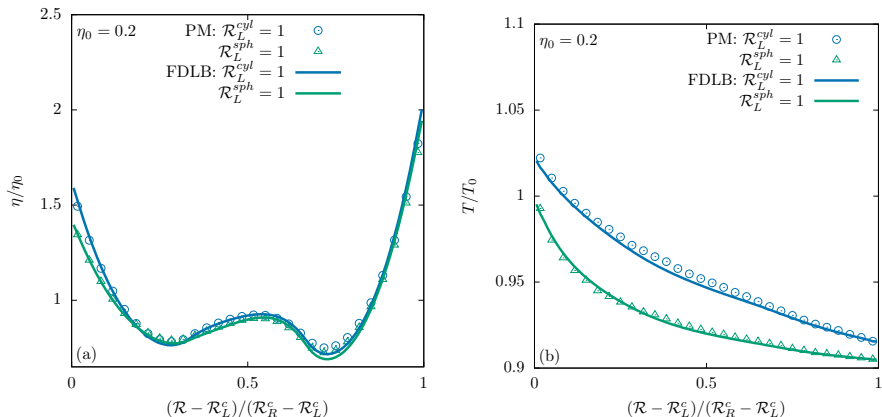


Figure: Fourier flow: Normalized reduced density η/η_0 and temperature T/T_0 for the confinement ratio $C = 4$, the inner cylinder/sphere radius $\mathcal{R}_L = 1$, three values of the mean reduced density $\eta_0 = 0.2$ and the two geometries, cylindrical and spherical.

⁴S. Busuioc, Mesoscopic lattice Boltzmann modeling of dense gas flows in curvilinear geometries, Phys. Rev. Fluids 9, 053401 (2024).

Fourier flow: Geometry comparisons⁴

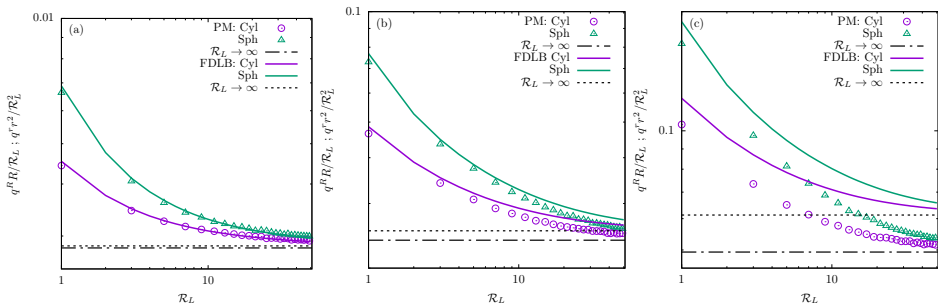


Figure: Fourier flow: The constants $q^R R / \mathcal{R}_L$, and $q^r r^2 / \mathcal{R}_L^2$ for a temperature difference of $\Delta T = 0.1$, confinement ratio of $C = 4$, mean reduced density of η_0 of (a) 0.01, (b) 0.1 and (c) 0.2, and variable inner cylinder/sphere radius $\mathcal{R}_L$. As the inner $\mathcal{R}_L$ increases, the two geometries approach a planar wall ($\mathcal{R}_L \rightarrow \infty$) and the results tend to match the results obtained in Busuioc and Sofonea⁵, which are represented as dashed lines.

⁵S. Busuioc and V. Sofonea, Bounded flows of dense gases, Phys. Rev. Fluids 9, 023401 (2024).

⁴S. Busuioc, Mesoscopic lattice Boltzmann modeling of dense gas flows in curvilinear geometries, Phys. Rev. Fluids 9, 053401 (2024).

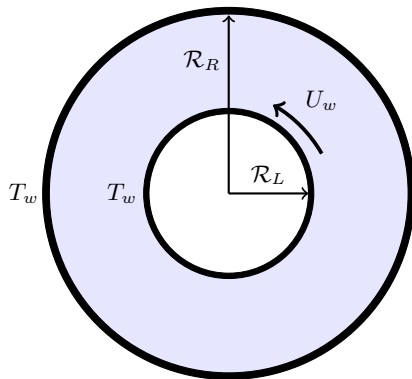
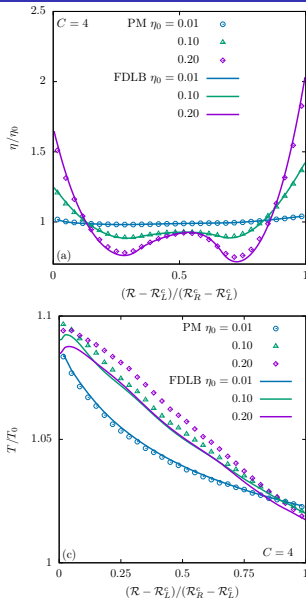


Figure: Setup of the Cylindrical Couette flow.

Cylindrical Couette flow⁴



Normalized (a) reduced density η/η_0 , (b) azimuthal velocity u_ϕ/U_w and (c) temperature T/T_0 , when the inner cylinder radius is $\mathcal{R}_L = 1$, the confinement ratio is $C = 4$, for three values of the mean reduced density $\eta_0 \in \{0.01, 0.1, 0.2\}$.

⁴S. Busuioc, Phys. Rev. Fluids 9, 053401 (2024).

The self-consistent force field is given by:

$$\mathcal{F}[n] = \int_{\varrho > \sigma} \frac{d\phi(\varrho)}{d\varrho} \frac{\mathbf{r}_1 - \mathbf{r}}{||\mathbf{r}_1 - \mathbf{r}||} n(\mathbf{r}_1) d\mathbf{r}_1 \quad (48)$$

- EV1. The direct numerical integration in (48) using the composite Simpson's 1/3 rule. As shown in Ref.¹⁵, in the one-dimensional case the following simplified expression for the x component of the self-consistent force field can be derived:

$$\mathcal{F}_1[n] = 2\pi\phi_\sigma \left[\sigma^\gamma \int_{|x-x'| > \sigma} \frac{(x' - x)n(x', t)}{|x - x'|^\gamma} dx' + \int_{|x-x'| < \sigma} (x' - x)n(x', t) dx' \right]$$

- EV2. The second one assumes that the number density n is sufficiently smooth everywhere, including the phase interface. This enables the expansion of the number density in Eq. (48) to get the following approximation of the Vlasov force :

$$\mathcal{F}_2[n] = 2a\nabla n + \kappa\nabla\Delta n = \frac{4\pi\sigma^3}{3}\phi_\sigma \frac{\gamma}{\gamma-3}\nabla n + \frac{2\pi\sigma^5}{15}\phi_\sigma \frac{\gamma}{\gamma-5}\nabla\Delta n,$$

$$\text{where } a = \frac{2\pi\sigma^3}{3}\phi_\sigma \frac{\gamma}{\gamma-3} \text{ and } \kappa = \frac{2\pi\sigma^5}{15}\phi_\sigma \frac{\gamma}{\gamma-5}.$$

¹⁵A. Frezzotti, L. Gibelli, and S. Lorenzani, Mean field kinetic theory description of evaporation of a fluid into vacuum, Phys. Fluids 17, 012102 (2005).

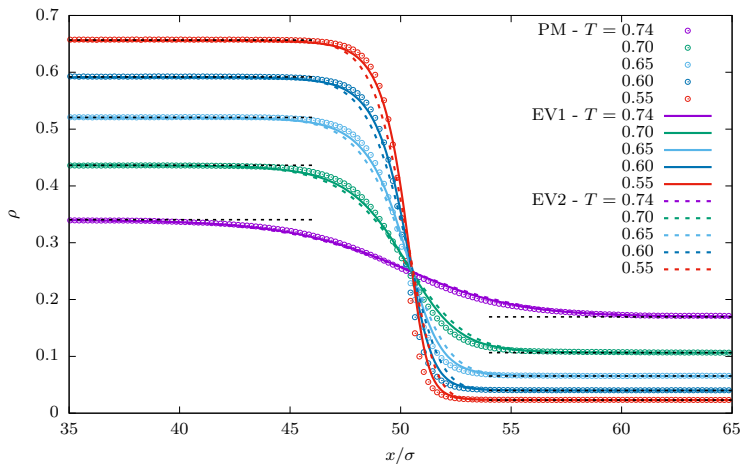


Figure: Density profiles at the liquid-vapor interface, obtained using both the PM and the FDLB methods (EV1 and EV2) at 5 constant values of the temperature T . For each T , the horizontal black-dotted lines indicate the values of both the liquid and the vapor density, as calculated according to the Maxwell construction.

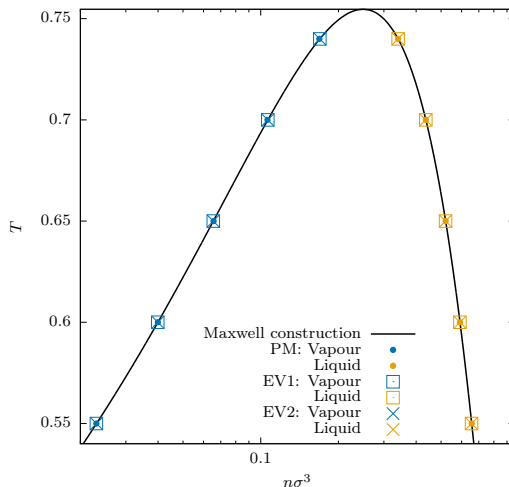


Figure: Phase diagram (fluid density $\rho = n\sigma^3$ vs temperature T) : the continuous line was traced according to the Maxwell construction for the equation of state, while the symbols denote the density values calculated numerically using the PM, as well as the EV1 and the EV2 procedures. $T_c \simeq 0.754632$.

Let us consider an Enskog-Vlasov fluid whose state is periodic along the x direction and homogeneous along the y and z directions. In the initial state ($t = 0$), the fluid density is subjected to a sinusoidal perturbation of wavelength $L = 100\sigma$ and amplitude ω :

$$\rho_i(x) \equiv \rho(x, t = 0) = A \left[1 + \omega \cos \left(\frac{2\pi x}{L} \right) \right] \quad (49)$$

The simulation is conducted in the interval $[-L/2, +L/2]$ of the x axis. For simplicity, the initial value of the fluid temperature T_i is supposed to be uniform in the whole computational domain. In Eq. (49) above, we set $A = (\rho_\ell + \rho_v)/2$, where ρ_ℓ and ρ_v are the values of the liquid and the vapor density, evaluated using the Maxwell construction at temperature T_i .

Phase separation dynamics in an Enskog-Vlasov fluid

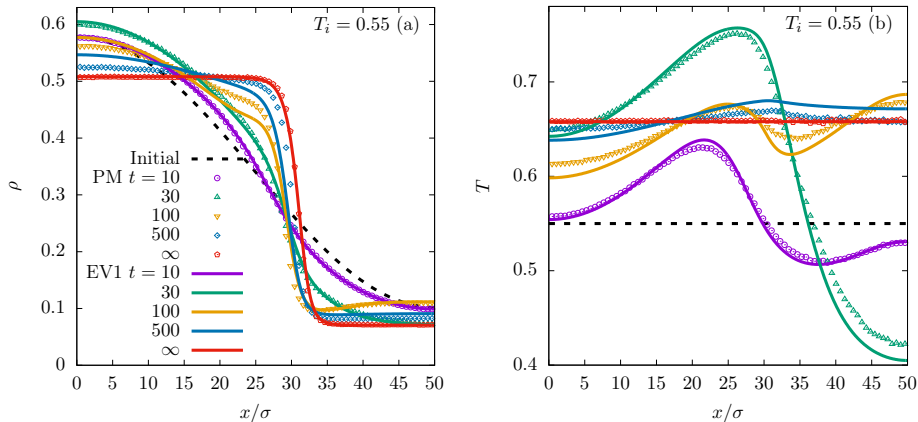


Figure: Phase separation with $(T_i, \omega) \in (0.55, 0.7)$: comparison between PM and EV1 profiles of density (a) and temperature (b) at various time instances $t \in \{0, 10, 30, 100, 500, \infty\}$. The ∞ symbol refers to the quasi-stationary state ($t = 5000$).

Phase separation dynamics in an Enskog-Vlasov fluid

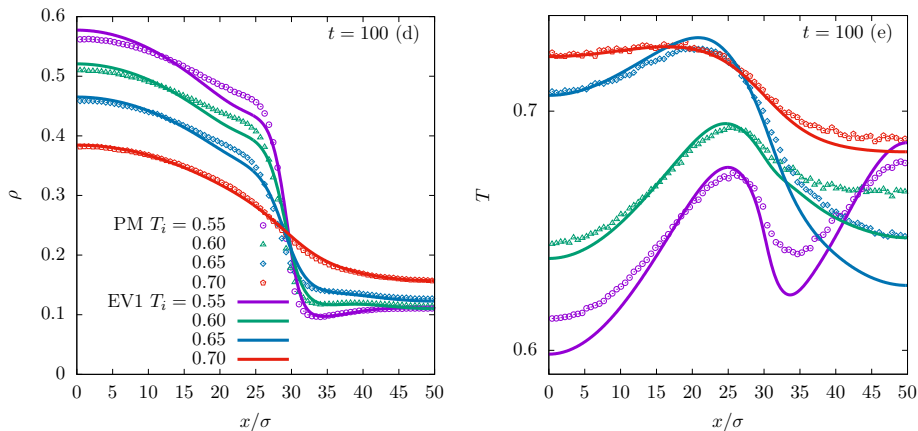


Figure: Phase separation at $t \in \{100\}$: comparison between PM and EV1 profiles of density (a) and temperature (b) for four values of the initial temperature $T_i \in \{0.55, 0.6, 0.65, 0.7\}$.

Phase separation dynamics in an Enskog-Vlasov fluid

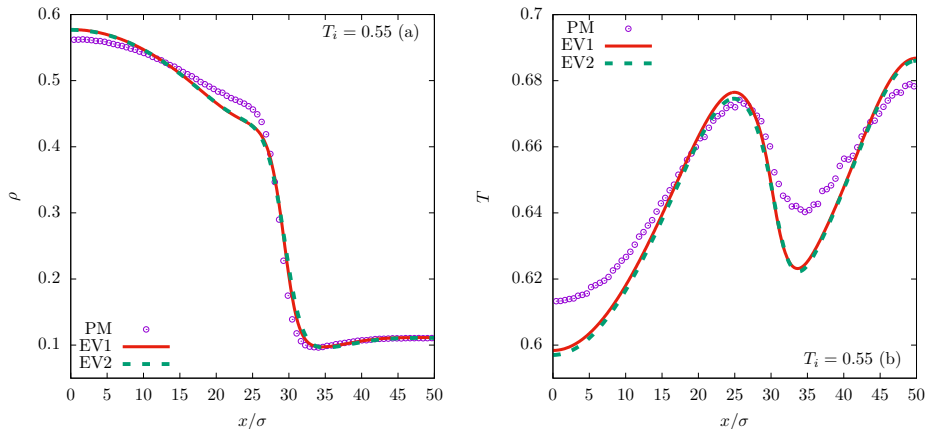


Figure: Phase separation: density and temperature profiles calculated at $t = 100$ using the PM, EV1, and EV2 methods, for $T_i = 0.55$.

Initially, a liquid slab is centered at the origin of the real axis, with symmetric smooth interfaces located at $x_0 = \pm 25\sigma$ and periodic boundary conditions. At $t = 0$, the liquid density value in the slab is set to ρ_ℓ , while the vapor density value outside the slab is set to $\rho_v/2$. At the beginning of each simulation, the left and the right liquid-vapor interface profiles are set according to:

$$\rho_i(x) = \rho_\ell + \frac{\rho_v - 2\rho_\ell}{4} \left[1 + \tanh \left(\frac{|x| - x_0}{\xi} \right) \right]; \quad (50)$$

where $\xi = \sqrt{\frac{3}{4\pi\sqrt{3}(T_c - T_i)}}$ and $x_0 = 25\sigma$.

Evaporation

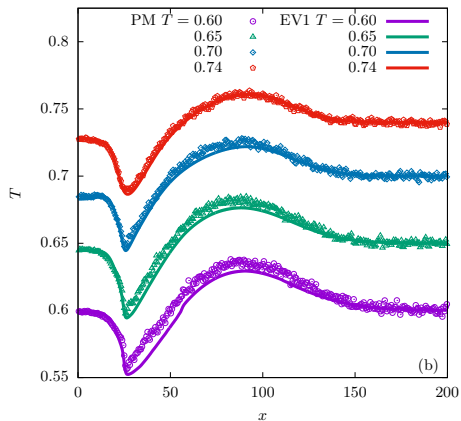
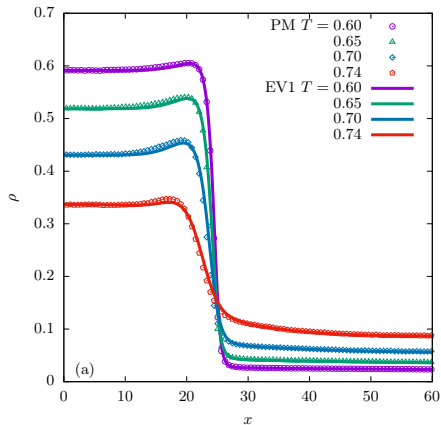


Figure: Evaporation into metastable vapor: fluid density and temperature profiles calculated at $t = 75$ for 4 values of the initial temperature T_i using the PM and the EV1 methods.

Evaporation

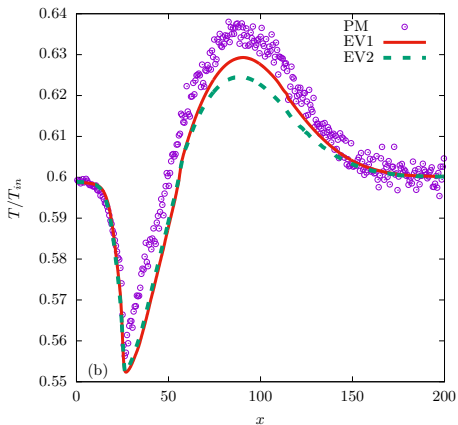
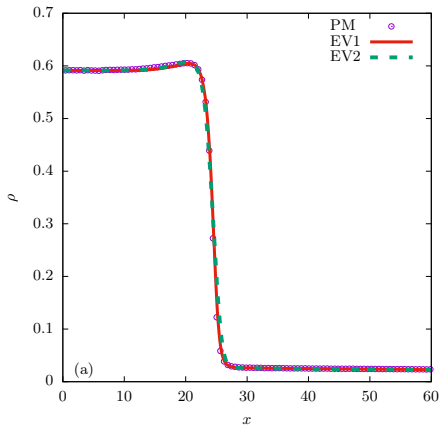


Figure: Evaporation into metastable vapor: fluid density and temperature profiles calculated at time $t = 75$ using the PM, EV1, and EV2 methods/implementations, for $T_i = 0.6$.

	Phase separation		Evaporation	
	$T = 0.55$	$T = 0.70$	$T = 0.60$	$T = 0.74$
t_{PM} (for 20 runs)	$8.2 \times 10^6 \text{s}$	$6 \times 10^6 \text{s}$	10^6s	$8.4 \times 10^5 \text{s}$
t_{EV1}	1.8×10^4	$1.8 \times 10^4 \text{s}$	$3.4 \times 10^3 \text{s}$	$3.4 \times 10^3 \text{s}$
t_{EV2}	$6 \times 10^3 \text{s}$	$6 \times 10^3 \text{s}$	$9 \times 10^2 \text{s}$	$9 \times 10^2 \text{s}$
$t_{\text{PM}}/t_{\text{EV1}}$	455	333	295	240
$t_{\text{PM}}/t_{\text{EV2}}$	1365	1000	1110	930

Table: Typical runtimes and runtime ratios.

- Starting from the Boltzmann equation, the (simplified) Enskog collision integral extends kinetic theory from dilute to moderately dense gases, while the Enskog-Vlasov equation further incorporates long-range attraction to describe liquid-vapor coexistence within a single kinetic framework.
- The Finite-Difference Lattice Boltzmann (FDLB) method, built on Gauss-Hermite quadrature and WENO/TVD-RK3 discretization, reproduces Particle-Method (DSMC) results across all test cases considered:
 - Sound and shock wave propagation;
 - Bounded flows (Couette, Fourier, Poiseuille) of dense gases;
 - Dense gas flows in curvilinear (cylindrical, spherical) geometries;
 - Phase separation and evaporation in liquid-vapor Enskog-Vlasov flows.
- Agreement with the Particle Method holds over a wide range of densities and confinement ratios, with deviations appearing only at the molecular scale.
- In all cases, the kinetic/FDLB approach achieves two to three orders of magnitude speed-up over the Particle Method, making it a practical tool for dense-gas and liquid-vapor flow simulation.
- **Outlook:** extension to fully three-dimensional liquid-vapor interfaces and curvilinear geometries.

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.