Research Centre
for Gas Innovation

Lattice Boltzmann Method: An Introductory Overview

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PME-5429 | Multiscale Methods (2020)

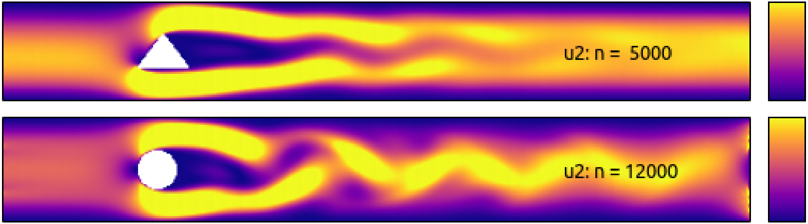
PME-5429 - Lattice Boltzmann Method

Summary of topics

- 20/10: Introduction & Kinetic Theory
- 27/10: Lattice Boltzmann & Hands-On
- 03/11: Dense Fluids & Hands-On

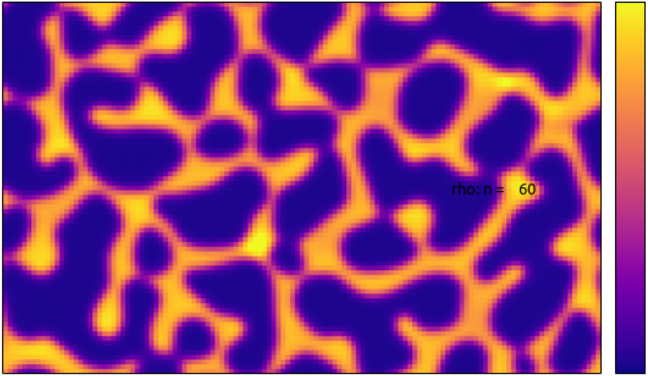
Introduction:
A quick look at the
Lattice Boltzmann method

Lattice Boltzmann Method: overview



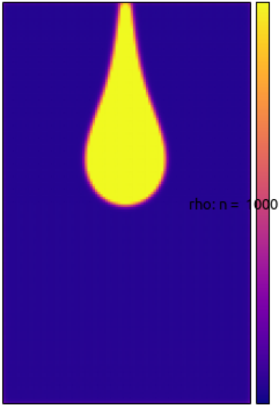
- Flow past obstacles with inlet/outlet boundary conditions

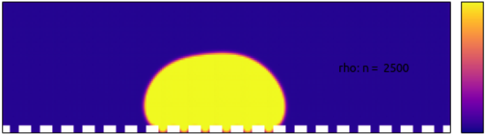
Lattice Boltzmann Method: overview



- Phase separation (periodic domain)

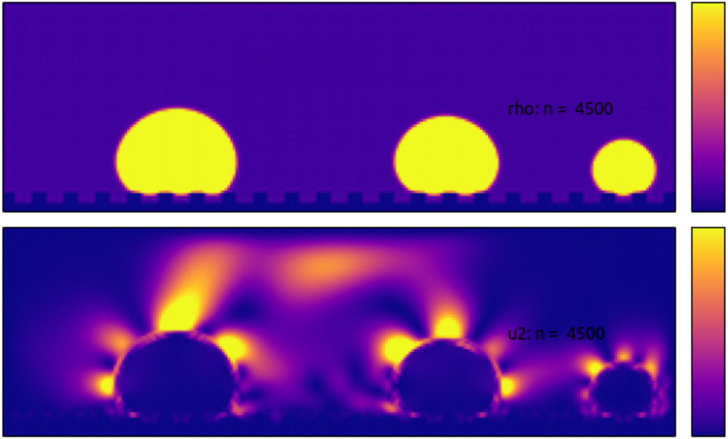
Lattice Boltzmann Method: overview





- Wetting phenomena

Lattice Boltzmann Method: overview



- Wetting phenomena

Lattice Boltzmann Method: overview

Highlights

- Intrinsically time-dependent
- Easy to implement and parallelize
- Natural description of complex flows
- Applies to both meso and macro scales
- Easy handling of irregular geometries

Limitations

- Highly-compressible flows (high Mach number)
- Substantial heat transfer
- Lattice constraints

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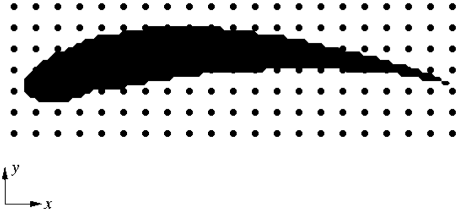
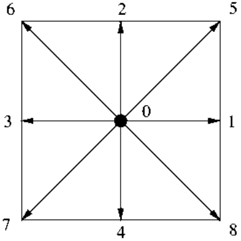
LBM algorithm in a nutshell





Simple D2Q9 scheme: at each lattice point $\mathbf{r}$:

$$\{\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4, \mathbf{e}_5, \mathbf{e}_6, \mathbf{e}_7, \mathbf{e}_8\} \qquad \text{(velocities)}$$

$$\{n_0, n_1, n_2, n_3, n_4, n_5, n_6, n_7, n_8\} \qquad \text{(`populations')}$$

where $n_\alpha = n_\alpha(\mathbf{r}, t)$

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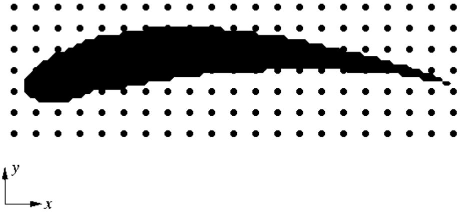
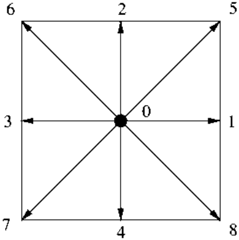




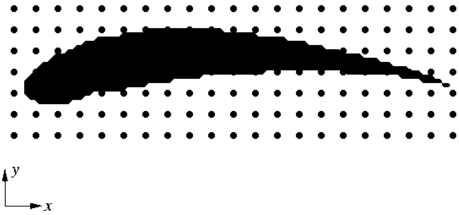
Flow fields at each lattice point $\mathbf{r}$:

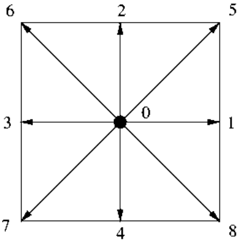
$$\rho = \sum_{\alpha=0}^{8} m\, n_\alpha \qquad \text{(mass density)}$$

$$\rho\mathbf{u} = \sum_{\alpha=0}^{8} m\mathbf{e}_\alpha\, n_\alpha \qquad \text{(momentum density)}$$

$$\tfrac{3}{2}\rho R\, T = \sum_{\alpha=0}^{8} \tfrac{1}{2}m(\mathbf{e}_\alpha - \mathbf{u})^2\, n_\alpha \qquad \text{(temperature)}$$

LBM algorithm in a nutshell





Lattice Boltzmann equation (δt = time step):

i) $n^*_\alpha(\mathbf{r}, t) = n_\alpha(\mathbf{r}, t) + \Omega_\alpha(\mathbf{r}, t)$ *collide*

ii) $n_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta t, t + \delta t) = n^*_\alpha(\mathbf{r}, t)$ *stream*

- *how is this related to fluid dynamics?*

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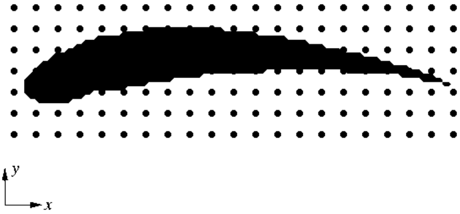

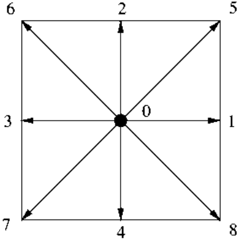

Lattice Boltzmann equation ($\delta t =$ time step):

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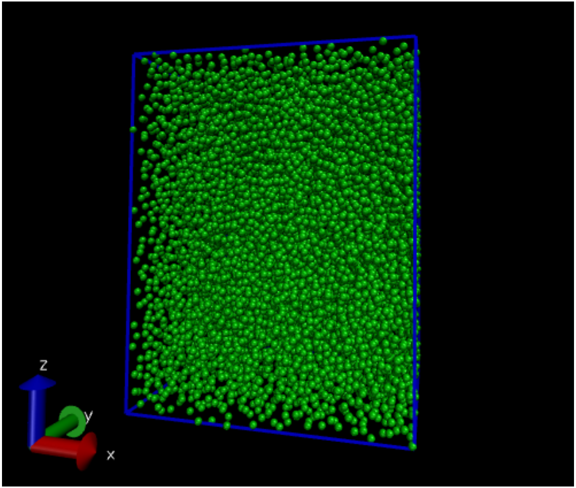
Molecular view of fluid element



- Molecular dynamics and statistics.

Part 1:
Elements of kinetic theory

1. Basic notions
2. The Boltzmann equation
3. Fluid dynamics
4. Equilibrium
5. Chapman-Enskog theory
6. Non-ideal gases: exclusion volume correction
7. The BGK collision model

Basic notions

The velocity distribution function

The probable number of molecules within $d\boldsymbol{\xi} d\mathbf{r}$ is

$$f(\mathbf{r}, \boldsymbol{\xi}, t) d\boldsymbol{\xi} d\mathbf{r}$$

where f is the *one-particle distribution function* – this is the *central object* of kinetic theory.

$n(\mathbf{r}, t) = \int f(\mathbf{r}, \boldsymbol{\xi}, t) d\boldsymbol{\xi}$ number density at $\mathbf{r}$

$N = \int n(\mathbf{r}, t)\, d\mathbf{r}$ total number of particles

(obs: sometimes other normalizations are used)

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Distribution function – macroscopic state

Number and mass densities

$$n(\mathbf{r},t) = \int f(\mathbf{r},\boldsymbol{\xi},t)d\boldsymbol{\xi} \qquad \rho(\mathbf{r},t) = m\, n(\mathbf{r},t)$$

Momentum density

$$\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) = \int m\boldsymbol{\xi}\, f(\mathbf{r},\boldsymbol{\xi},t)d\boldsymbol{\xi}$$

Kinetic energy density

$$\rho(\mathbf{r},t)e(\mathbf{r},t) = \int \tfrac{1}{2}m\xi^2\, f(\mathbf{r},\boldsymbol{\xi},t)d\boldsymbol{\xi}$$

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Hydrodynamic moments

Number and mass densities

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- $\mathbf{u}(\mathbf{r},t) =$ momentum per unit mass

$$\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) = \int m\boldsymbol{\xi}\, f(\mathbf{r},\boldsymbol{\xi},t)d\boldsymbol{\xi}$$

- $e(\mathbf{r},t) =$ kinetic energy per unit mass

$$\rho(\mathbf{r},t)e(\mathbf{r},t) = \int \tfrac{1}{2}m\xi^2\, f(\mathbf{r},\boldsymbol{\xi},t)d\boldsymbol{\xi}$$

Temperature

Thermal velocity (‘peculiar’ velocity)

$$\mathbf{C}(\mathbf{r},\boldsymbol{\xi},t) \equiv \boldsymbol{\xi} - \mathbf{u}(\mathbf{r},t) \quad \Rightarrow \quad \int \mathbf{C} f d\boldsymbol{\xi} = 0$$

$$\rho e = \int \tfrac{1}{2} m (\mathbf{u} + \mathbf{C})^2 \, f d\boldsymbol{\xi}$$

Internal (thermal) energy per unit mass

$$\rho\varepsilon(\mathbf{r},t) \equiv \int \tfrac{1}{2} m C^2 \, f d\boldsymbol{\xi}$$

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Temperature at equilibrium ($\rho = \rho_0$ and $\mathbf{u} = 0$)

$$\varepsilon = \frac{3}{2}\frac{k_B}{m}T$$

$k_B = 1.38065 \times 10^{-23}$ Joule/Kelvin $=$ Boltzmann constant

(*equipartition theorem* from statistical physics)

Temperature field

$$\varepsilon(\mathbf{r},t) = \frac{3}{2}\frac{k_B}{m}T(\mathbf{r},t)$$

- the equilibrium relation is extended to nonequilibrium
- complex molecules: center-of-mass DOFs are used

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$$\varepsilon(\mathbf{r},t) = \frac{3}{2}\frac{k_B}{m}T(\mathbf{r},t) = \frac{3}{2}R\,T(\mathbf{r},t)$$

$$R = \frac{k_B}{m} = \frac{N_A k_B}{N_A m} = \frac{\text{ideal gas constant}}{\text{molar mass}} = \text{specific gas constant}$$

The Boltzmann equation

The Boltzmann equation

Knowledge of $f(\mathbf{r}, \boldsymbol{\xi}, t)$ allows calculation of

$$
\begin{aligned}
n &= \int f \, d\boldsymbol{\xi} \\
\rho \mathbf{u} &= \int m\boldsymbol{\xi} \, f \, d\boldsymbol{\xi} && (\rho = m\,n) \\
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The Boltzmann equation governs the evolution of the distribution function

$$f(\mathbf{r}, \boldsymbol{\xi}, 0) \;\rightarrow\; f(\mathbf{r}, \boldsymbol{\xi}, t)$$

under suitable initial/boundary conditions.

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At $t = 0$, consider the cluster of molecules at $\mathbf{r}(0)$ that have velocity $\boldsymbol{\xi}(0)$. Without collisions *the number of molecules in the cluster would not change as we follow their motion*:

$$f(\mathbf{r}(t), \boldsymbol{\xi}(t), t) = f(\mathbf{r}(0), \boldsymbol{\xi}(0), t)$$

$$\text{where:} \quad \dot{\mathbf{r}}(t) = \boldsymbol{\xi}(t), \quad \dot{\boldsymbol{\xi}}(t) = \mathbf{g}(\mathbf{r}(t))$$

($m\mathbf{g}(\mathbf{r}) =$ external force field, smooth at molecular scale)

- ‘Lagrange form’ (no collisions)

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In reality, however, the number of molecules in the cluster changes, since their velocities are altered at collision events, that is

$$\frac{df(\mathbf{r}(t), \boldsymbol{\xi}(t), t)}{dt} = \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}}$$

Assumptions for rarefied gases

- only binary collisions are considered
- collisions are local
- collisions are essentially instantaneous events
- collisions are assumed to be elastic

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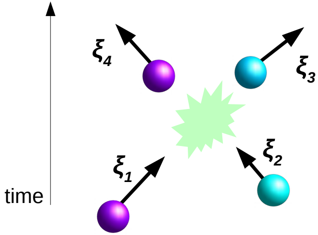
$$\left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} = \left(\frac{\partial f}{\partial t}\right)_{\text{gain}} - \left(\frac{\partial f}{\partial t}\right)_{\text{loss}}$$



$w(3,4 \leftarrow 1,2) =$
probability rate for collisions
of the type: $\underbrace{\boldsymbol{\xi}_3,\boldsymbol{\xi}_4}_{\text{after}} \leftarrow \underbrace{\boldsymbol{\xi}_1,\boldsymbol{\xi}_2}_{\text{before}}$

$$(\partial_t f(1))_{\text{loss}} = \iiint w(3,4 \leftarrow 1,2)\ f(1)f(2)\ d\boldsymbol{\xi}_2 d\boldsymbol{\xi}_3 d\boldsymbol{\xi}_4$$

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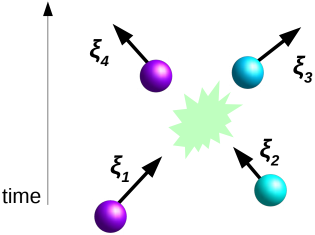

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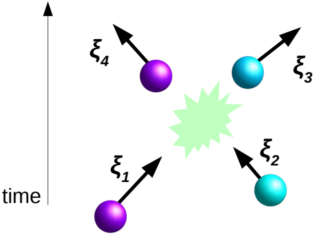

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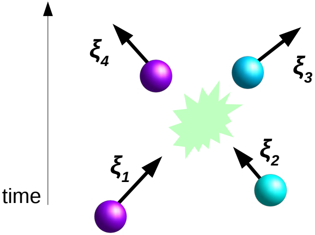

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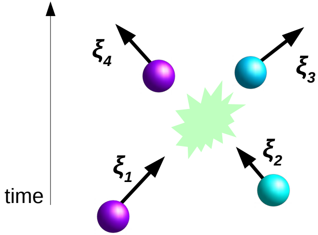

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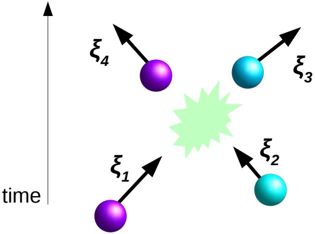
$$(\partial_t f(1))_{\text{loss}} = \int \left[\iint w(3,4 \leftarrow 1,2) d\boldsymbol{\xi}_3 d\boldsymbol{\xi}_4 \right] f(1) f(2)\, d\boldsymbol{\xi}_2$$

$$(\partial_t f(1))_{\text{gain}} = \iiint w(1,2 \leftarrow 3,4)\, f(3) f(4)\, d\boldsymbol{\xi}_2 d\boldsymbol{\xi}_3 d\boldsymbol{\xi}_4$$

The Boltzmann equation

$$\left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} = \left(\frac{\partial f}{\partial t}\right)_{\text{gain}} - \left(\frac{\partial f}{\partial t}\right)_{\text{loss}}$$



$w(3,4 \leftarrow 1,2) =$ probability rate for collisions of the type: $\underbrace{\boldsymbol{\xi}_3, \boldsymbol{\xi}_4}_{\text{after}} \leftarrow \underbrace{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2}_{\text{before}}$

$$(\partial_t f(1))_{\text{loss}} = \int \left[\iint w(1,2 \leftarrow 3,4) d\boldsymbol{\xi}_3 d\boldsymbol{\xi}_4 \right] f(1) f(2)\, d\boldsymbol{\xi}_2$$

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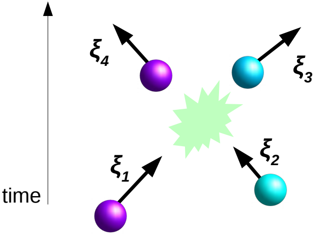

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$$(\partial_t f(1))_{\text{loss}} = \iiint w(1,2 \leftarrow 3,4)\; f(1) f(2)\; d\boldsymbol{\xi}_2 d\boldsymbol{\xi}_3 d\boldsymbol{\xi}_4$$

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The Boltzmann equation

Therefore, the dynamic equation takes the form

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{g} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = \Omega(f)$$

where

$$\Omega(f_1) = \iiint w \left(f_3 f_4 - f_1 f_2 \right) d\boldsymbol{\xi}_2 d\boldsymbol{\xi}_3 d\boldsymbol{\xi}_4$$

- $\Omega(f)$ is known as the collision integral

(obs: w is related to the scattering cross section for collisions)

The Boltzmann equation

$\Omega(f)$ has the important properties:

$$\int m\,\Omega(f)\,d\boldsymbol{\xi} = 0$$

$$\int m\boldsymbol{\xi}\,\Omega(f)\,d\boldsymbol{\xi} = 0$$

$$\int \tfrac{1}{2}m\xi^2\,\Omega(f)\,d\boldsymbol{\xi} = 0$$

Meaning: the local rate of mass, momentum, and energy changes due to collisions is zero.

- This immediately yields balance equations for mass, momentum, and kinetic energy.

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Fluid dynamics

Balance equations – mass

$$\int m\,(\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{g}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}})\,d\boldsymbol{\xi} = \int m\,\Omega(f)\,d\boldsymbol{\xi} = 0$$

- $\int m\frac{\partial f}{\partial t}d\boldsymbol{\xi} = \frac{\partial}{\partial t}\int m f d\boldsymbol{\xi} = \frac{\partial \rho}{\partial t}$
- $\int m\boldsymbol{\xi}\cdot\boldsymbol{\nabla} f d\boldsymbol{\xi} = \boldsymbol{\nabla}\cdot\int m\boldsymbol{\xi} f d\boldsymbol{\xi} = \boldsymbol{\nabla}\cdot(\rho\mathbf{u})$
- $\int m\mathbf{g}\cdot\boldsymbol{\nabla}_{\xi} f d\boldsymbol{\xi} = \mathbf{g}\cdot\int m\boldsymbol{\nabla}_{\xi} f d\boldsymbol{\xi} = \mathbf{g}\cdot\oint_{\partial\xi} m f d\mathbf{s} = 0$

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot\rho\mathbf{u} = 0$$

Balance equations – mass

$$\int m\,(\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{g}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}})\,d\boldsymbol{\xi} = \int m\,\Omega(f)\,d\boldsymbol{\xi} = 0$$

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Balance equations – mass

$$\int m\,(\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{g}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}})\,d\boldsymbol{\xi} = \int m\,\Omega(f)\,d\boldsymbol{\xi} = 0$$

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Balance equations – mass

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- $\int m \frac{\partial f}{\partial t} d\boldsymbol{\xi} = \frac{\partial}{\partial t} \int m f d\boldsymbol{\xi} = \frac{\partial \rho}{\partial t}$
- $\int m \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f d\boldsymbol{\xi} = \boldsymbol{\nabla} \cdot \int m \boldsymbol{\xi} f d\boldsymbol{\xi} = \boldsymbol{\nabla} \cdot (\rho \mathbf{u})$
- $\int m \mathbf{g} \cdot \boldsymbol{\nabla}_{\xi} f d\boldsymbol{\xi} = \mathbf{g} \cdot \int m \boldsymbol{\nabla}_{\xi} f d\boldsymbol{\xi} = \mathbf{g} \cdot \oint_{\partial \xi} m f d\mathbf{s} = 0$

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{u} = 0$$

Balance equations – mass

$$\int m\,(\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}}+\mathbf{g}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}})\,d\boldsymbol{\xi}=\int m\,\Omega(f)\,d\boldsymbol{\xi}=0$$

- $\int m\frac{\partial f}{\partial t}d\boldsymbol{\xi}=\frac{\partial}{\partial t}\int mfd\boldsymbol{\xi}=\frac{\partial\rho}{\partial t}$
- $\int m\boldsymbol{\xi}\cdot\boldsymbol{\nabla}fd\boldsymbol{\xi}=\boldsymbol{\nabla}\cdot\int m\boldsymbol{\xi}fd\boldsymbol{\xi}=\boldsymbol{\nabla}\cdot(\rho\mathbf{u})$
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$$\frac{\partial\rho}{\partial t}+\boldsymbol{\nabla}\cdot\rho\mathbf{u}=0$$

Balance equations – momentum

$$\int m\xi_i\left(\frac{\partial f}{\partial t}+\sum_j \xi_j\frac{\partial f}{\partial x_j}+\sum_j g_j\frac{\partial f}{\partial \xi_j}\right)d\boldsymbol{\xi}=\int m\xi_i\Omega(f)d\boldsymbol{\xi}=0$$

- $\int m\xi_i\frac{\partial f}{\partial t}d\boldsymbol{\xi}=\frac{\partial}{\partial t}\int m\xi_i f d\boldsymbol{\xi}=\frac{\partial(\rho u_i)}{\partial t}$
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- $\int m\xi_i\sum_j g_j\frac{\partial f}{\partial \xi_j}d\boldsymbol{\xi}=\sum_j g_j\int\left(\frac{\partial(m\xi_i f)}{\partial \xi_j}-mf\delta_{ij}\right)d\boldsymbol{\xi}=-\rho g_i$

$$\frac{\partial \rho u_i}{\partial t}+\sum_j\frac{\partial \Pi_{ij}}{\partial x_j}=\rho g_i$$

$\Pi_{ij}=$ momentum flux tensor

Balance equations – momentum

$$\int m\xi_i\Big(\frac{\partial f}{\partial t}+\sum_j \xi_j\frac{\partial f}{\partial x_j}+\sum_j g_j\frac{\partial f}{\partial \xi_j}\Big)d\boldsymbol{\xi} = \int m\xi_i\Omega(f)\,d\boldsymbol{\xi} = 0$$

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$$\frac{\partial\rho u_i}{\partial t}+\sum_j\frac{\partial \Pi_{ij}}{\partial x_j} = \rho g_i$$

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Balance equations – kinetic energy

$$\int \tfrac{1}{2}m\xi^2\left(\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}}+\mathbf{g}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}}\right)d\boldsymbol{\xi} = \int \tfrac{1}{2}m\xi^2\Omega(f)d\boldsymbol{\xi} = 0$$

- $\int \tfrac{1}{2}m\xi^2\frac{\partial f}{\partial t}d\boldsymbol{\xi} = \frac{\partial}{\partial t}\int \tfrac{1}{2}m\xi^2 f d\boldsymbol{\xi} = \frac{\partial(\rho e)}{\partial t}$
- $\int \tfrac{1}{2}m\xi^2\boldsymbol{\xi}\cdot\boldsymbol{\nabla} f d\boldsymbol{\xi} = \boldsymbol{\nabla}\cdot\int \tfrac{1}{2}m\xi^2\boldsymbol{\xi} f d\boldsymbol{\xi} = \boldsymbol{\nabla}\cdot\mathbf{Q}$
- $\int \tfrac{1}{2}m\xi^2\mathbf{g}\cdot\boldsymbol{\nabla}_{\xi} f d\boldsymbol{\xi} = \mathbf{g}\cdot\int\Big(\boldsymbol{\nabla}_{\xi}(\tfrac{1}{2}m\xi^2 f) - m\boldsymbol{\xi} f\Big)d\boldsymbol{\xi} = -\rho\mathbf{g}\cdot\mathbf{u}$

$$\frac{\partial \rho e}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{Q} = \rho\mathbf{g}\cdot\mathbf{u}$$

$\mathbf{Q} =$ kinetic energy flux vector

Balance equations – kinetic energy

$$\int \tfrac{1}{2} m\xi^2 \Big(\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}} + \mathbf{g}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}}\Big) d\boldsymbol{\xi} = \int \tfrac{1}{2} m\xi^2 \Omega(f) d\boldsymbol{\xi} = 0$$

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Balance equations – kinetic energy

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Momentum and energy fluxes

$$
\begin{aligned}
\Pi_{ij} &= \int m\xi_i\xi_j \; f \; d\boldsymbol{\xi} \\
&= \int m(u_i + C_i)(u_j + C_j) \; f \; d\boldsymbol{\xi} \\
&= \rho u_i u_j + \int mC_iC_j \; f \; d\boldsymbol{\xi}
\end{aligned}
$$

$$
\begin{aligned}
Q_j &= \int \tfrac{1}{2} m\xi^2\xi_j \; f \; d\boldsymbol{\xi} \\
&= \int \tfrac{1}{2} m(u^2 + C^2 + 2\sum_i u_iC_i)(u_j + C_j) \; f \; d\boldsymbol{\xi} \\
&= \rho e u_j + \int \tfrac{1}{2} mC^2C_j \; f \; d\boldsymbol{\xi} + \sum_k u_i \int mC_iC_j \; f \; d\boldsymbol{\xi}
\end{aligned}
$$

Momentum and energy fluxes

$$\begin{aligned}\Pi_{ij} &= \int m\xi_i\xi_j\ f\ d\boldsymbol{\xi} \\ &= \int m(u_i + C_i)(u_j + C_j)\ f\ d\boldsymbol{\xi} \\ &= \rho u_i u_j + \int mC_iC_j\ f\ d\boldsymbol{\xi}\end{aligned}$$

$$\begin{aligned}Q_j &= \int \tfrac{1}{2}m\xi^2\xi_j\ f\ d\boldsymbol{\xi} \\ &= \int \tfrac{1}{2}m(u^2 + C^2 + 2\sum_i u_iC_i)(u_j + C_j)\ f\ d\boldsymbol{\xi} \\ &= \rho e u_j + \int \tfrac{1}{2}mC^2C_j\ f\ d\boldsymbol{\xi} + \sum_k u_i \int mC_iC_j\ f\ d\boldsymbol{\xi}\end{aligned}$$

Pressure tensor and heat vector

Definitions

$$P_{ij} \equiv \int m C_i C_j \, f \, d\boldsymbol{\xi} \qquad \text{(pressure tensor)}$$

$$q_j \equiv \int \tfrac{1}{2} m C^2 C_j \, f \, d\boldsymbol{\xi} \qquad \text{(heat vector)}$$

The fluxes decompose as follows

$$\Pi_{ij} = \rho u_i u_j + P_{ij}$$

$$Q_j = \rho e u_j + q_j + \sum_i u_i P_{ij}$$

using tensor notation:

$$\mathbf{\Pi} = \rho \mathbf{u}\mathbf{u} + \mathbf{P}$$

$$\mathbf{Q} = \rho e \mathbf{u} + \mathbf{q} + \mathbf{u} \cdot \mathbf{P}$$

Note: Irving-Kirkwood expressions

The pressure tensor as implemented in LAMMPS is

$$P_{ij} = V^{-1} \sum_{a=1}^{N} \left[m(\mathbf{C}_a)_i(\mathbf{C}_a)_j + (\mathbf{r}_a)_i(\mathbf{F}_a)_j \right]$$

where sum is over all atoms inside volume V and

$$\mathbf{C}_a = \mathbf{v}_a - \mathbf{u}(\mathbf{r}_a) = \text{thermal vel. of atom `}a\text{'}$$
$$\mathbf{F}_a = \text{total force in atom `}a\text{' due to other atoms}$$

- the interatomic forces $\mathbf{F}$ are responsible for *non-ideal gas* behavior

Note: Irving-Kirkwood expressions

The pressure is the trace $P = \frac{1}{3}\sum_i P_{ii}$ or

$$P = \underbrace{\frac{Nk_BT}{V}}_{\text{kinetic}} + \sum_{a=1}^{N} \underbrace{\frac{\mathbf{r}_a \cdot \mathbf{F}_a}{3V}}_{\text{virial}}$$

- Finite-range interatomic forces are neglected in the kinetic theory of rarefied gases (collisions act merely as a thermalization mechanism)
- In order to deal with dense fluids (liquids) corrections are needed (we will return to this)

back to balance equations...

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back to balance equations...

Balance equations

The full set of balance equations

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{u} = 0 \\
&\frac{\partial \rho \mathbf{u}}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{u}\mathbf{u} = \rho \mathbf{g} - \boldsymbol{\nabla} \cdot \mathbf{P} \quad (\text{obs: } \mathbf{P}^t = \mathbf{P}) \\
&\frac{\partial \rho e}{\partial t} + \boldsymbol{\nabla} \cdot (\rho e \mathbf{u} + \mathbf{q}) = \rho \mathbf{g} \cdot \mathbf{u} - \boldsymbol{\nabla} \cdot (\mathbf{u} \cdot \mathbf{P})
\end{aligned}$$

(obs: potential energy due to $\mathbf{g}$ drops out of the equations)

Balance equations

The full set of balance equations

$$\begin{aligned}
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\frac{\partial \rho \mathbf{u}}{\partial t} + \boldsymbol{\nabla} \cdot \rho \mathbf{u}\mathbf{u} &= \rho \mathbf{g} - \boldsymbol{\nabla} \cdot \mathbf{P} \\
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\end{aligned}
$$

Meaningful only if a solution to the Boltzmann equation $f(\mathbf{r}, \boldsymbol{\xi}, t)$ is provided.

Equilibrium

Equilibrium

In equilibrium collisions do not change the velocity distribution – gains and losses cancel off so that

$$\Omega(f_0) = 0$$

and the equilibrium distribution must satisfy

$$\frac{\partial f_0}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f_0}{\partial \mathbf{r}} + \mathbf{g} \cdot \frac{\partial f_0}{\partial \boldsymbol{\xi}} = 0$$

Equilibrium

Theorem: any function with the form

$$f_0(\boldsymbol{\xi}) = c \, \exp[-b(\boldsymbol{\xi} - \mathbf{a})^2]$$

makes the collision integral vanish.

The parameters can be expressed in terms of the hydrodynamic variables $(\rho, T, \mathbf{u})$:

$$f_0(\boldsymbol{\xi}) = \frac{\rho}{m}(2\pi R\,T)^{-3/2} \exp\left[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R\,T}\right]$$

(Maxwell-Boltzmann/Maxwellian distribution)

- obs: $\Omega(f_0) = 0$ even for $\rho(\mathbf{r}, t)$, $T(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$.

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Maxwellian – properties

A few properties of the equilibrium function

$$\langle \mathbf{C} \rangle_0 = \int \mathbf{C} f_0 d\mathbf{C} = 0$$

$$\langle C \rangle_0 = \int C f_0 d\mathbf{C} = (8k_B T/m\pi)^{1/2}$$

$$\langle C^2 \rangle_0 = \int C^2 f_0 d\mathbf{C} = 3k_B T/m$$

$$\langle \psi(\mathbf{C}) \rangle_0 = \int \psi(\mathbf{C}) f_0 d\mathbf{C} = 0 \ \text{ if } \psi(\mathbf{C}) \text{ is of odd degree}$$

At standard temp/press conditions

$$\mathrm{H_2}: \quad \langle C \rangle_0 = 1644 \text{ m/s} \qquad (\rho = 0.0899 \text{ g/L})$$

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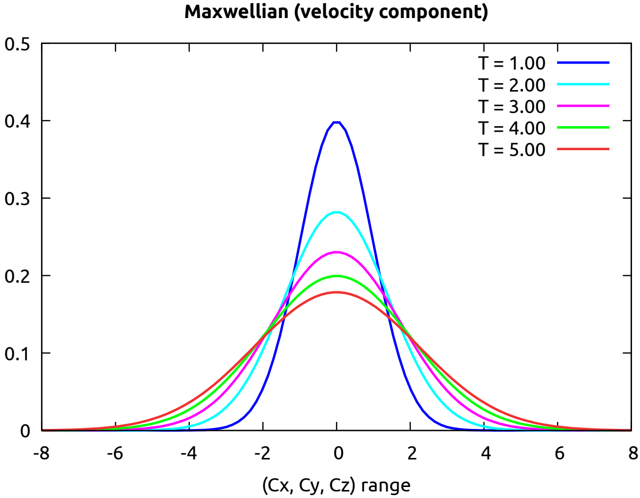

$$f(\mathbf{C}) = f(C_x)f(C_y)f(C_z), \quad f(C_x) = (\rho/m)^{1/3}(2\pi RT)^{-1/2}e^{-\frac{C_x^2}{2RT}}$$

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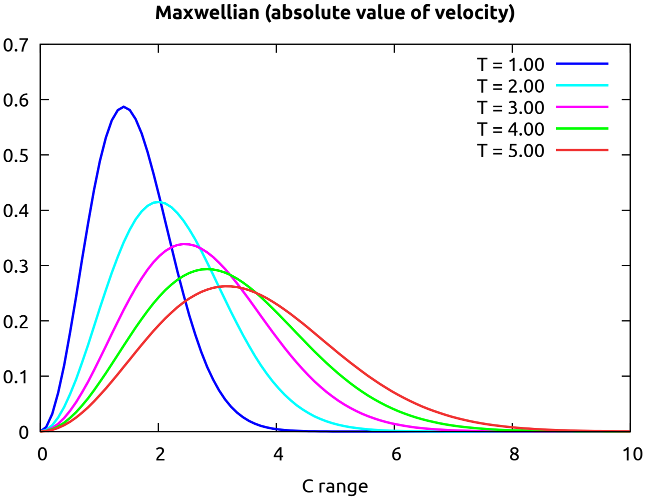

$$f(\mathbf{C})d\boldsymbol{\xi} \to 4\pi C^2 f(C)dC = 4\pi(\rho/m)(2\pi RT)^{-3/2}C^2 e^{-\frac{C^2}{2RT}}dC$$

Equilibrium – constitutive relations

Pressure tensor and heat vector at equilibrium:

$$P_{ij}(f_0) = \int mC_iC_j\, f_0\, d\boldsymbol{\xi} = \rho R\, T\, \delta_{ij} \equiv p\, \delta_{ij}$$
$$q_i(f_0) = \int \tfrac{1}{2}mC^2C_i\, f_0\, d\boldsymbol{\xi} = 0$$

where the equilibrium pressure has been identified

$$p = \rho R\, T = \tfrac{1}{3}\sum_i P_{ii}(f_0) \quad \text{(ideal gas law)}$$

These are the constitutive relations of an Euler fluid, but beware...

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Equilibrium – stationary solutions

...the function f_0 must also obey the Boltzmann equation – this imposes severe restrictions in the hydrodynamic fields.

Stationary equilibrium solutions have the form:

$$T = T_0$$

$$\mathbf{u}(\mathbf{r}) = \mathbf{u}_0 + \boldsymbol{\omega} \times \mathbf{r}$$

$$\rho(\mathbf{r}) = \rho_0 \exp\Big(-\frac{v(\mathbf{r})}{k_B T_0} - \frac{(\boldsymbol{\omega} \times \mathbf{u}_0) \cdot \mathbf{r}}{k_B T_0} - \frac{(\boldsymbol{\omega} \times \mathbf{r})^2}{2 k_B T_0} \Big)$$

where $\mathbf{g}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$; this is *hydrostatics*.

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Chapman-Enskog theory

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Task: seek for solutions of the form

$$f = f_0 + \delta f$$

Fundamental assumptions

$$\begin{aligned}
\rho &= \int m\, f\, d\boldsymbol{\xi} = \int m\, f_0\, d\boldsymbol{\xi} \\
\rho\mathbf{u} &= \int m\boldsymbol{\xi}\, f\, d\boldsymbol{\xi} = \int m\boldsymbol{\xi}\, f_0\, d\boldsymbol{\xi} \\
\tfrac{3}{2}\rho R\, T &= \int \tfrac{1}{2} m C^2\, f\, d\boldsymbol{\xi} = \int \tfrac{1}{2} m C^2\, f_0\, d\boldsymbol{\xi}
\end{aligned}$$

Deviations do not *directly* affect the local values of the basic hydrodynamic fields.

Chapman-Enskog theory

Task: seek for solutions of the form

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Fundamental assumptions

$$\begin{aligned}
\int m \left(\delta f\right) d\boldsymbol{\xi} &= 0 \\
\int m\boldsymbol{\xi} \left(\delta f\right) d\boldsymbol{\xi} &= 0 \\
\int \tfrac{1}{2} m C^2 \left(\delta f\right) d\boldsymbol{\xi} &= 0
\end{aligned}$$

Deviations do not *directly* affect the local values of the basic hydrodynamic fields.

Chapman-Enskog theory

The deviations δf, however, affect the pressure tensor and heat vector

$$P_{ij} = \rho RT\,\delta_{ij} + \int mC_iC_j\,\delta f\,d\boldsymbol{\xi}$$
$$q_i = \int \tfrac{1}{2}mC^2C_i\,\delta f\,d\boldsymbol{\xi}$$

which, *in turn*, induce changes in the hydrodynamic fields through

$$\frac{\partial\rho\mathbf{u}}{\partial t} + \boldsymbol{\nabla}\cdot\rho\mathbf{u}\mathbf{u} = \rho\mathbf{g} - \boldsymbol{\nabla}\cdot\mathbf{P}$$
$$\frac{\partial\rho T}{\partial t} + \boldsymbol{\nabla}\cdot\rho T\mathbf{u} = -\frac{2}{3R}(\boldsymbol{\nabla}\cdot\mathbf{q} + \mathbf{P}:\boldsymbol{\nabla}\mathbf{u})$$

Chapman-Enskog theory

Following this logic, deviations take the general form

$$\delta f = -f_0 \left[\mathbf{a}(\mathbf{C}) \cdot \boldsymbol{\nabla} T + \mathbf{B}(\mathbf{C}) : \boldsymbol{\nabla} \mathbf{u} \right]$$

and the task is to find vector $\mathbf{a}$ and tensor $\mathbf{B}$ by approximately solving the Boltzmann equation – once they are found we may compute

$$q_i = -\sum_j \left[\int \tfrac{1}{2} m C^2 C_i \, a_j \, f_0 \, d\boldsymbol{\xi} \right] (\boldsymbol{\nabla} T)_j$$

$$P_{ij} = \rho R T \, \delta_{ij} - \sum_{kl} \left[\int m C_i C_j \, B_{kl} \, f_0 \, d\boldsymbol{\xi} \right] (\boldsymbol{\nabla} \mathbf{u})_{kl}$$

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Chapman-Enskog theory

The result for monoatomic isotropic gases is

$$\mathbf{q} = -\lambda \boldsymbol{\nabla} T$$
$$\mathbf{P} = \rho R T\, \mathbf{I} - 2\mu \boldsymbol{\nabla} \hat{\mathbf{u}}$$

where the symmetric traceless part of $\boldsymbol{\nabla}\mathbf{u}$ is

$$(\boldsymbol{\nabla}\hat{\mathbf{u}})_{ij} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big) - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}$$

The transport coefficients for *rigid-spheres* are

$$\mu = \tfrac{5}{16}\,\sqrt{m k_B T/\pi a^4} \qquad \text{(shear viscosity)}$$
$$\lambda = \tfrac{25}{32}\,\underbrace{(3R/2)}_{c_v}\,\sqrt{m k_B T/\pi a^4} \qquad \text{(thermal conductivity)}$$

where a is the molecular diameter.

Chapman-Enskog theory

The dimensionless combination

$$\lambda / c_v \mu \approx 2.5$$

agrees well with experimental values for noble gases (Chapman-Cowling p. 249)

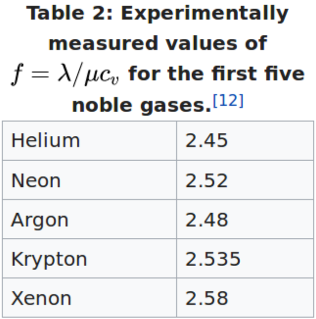

Table 2: Experimentally measured values of $f = \lambda/\mu c_v$ for the first five noble gases.[12]

Helium	2.45
Neon	2.52
Argon	2.48
Krypton	2.535
Xenon	2.58

Chapman-Enskog – Navier-Stokes

Hence the first nonequilibrium correction δf yields the constitutive relations for a viscous fluid

$$\mathbf{q} = -\lambda \boldsymbol{\nabla} T, \quad \mathbf{P} = p\mathbf{I} - 2\mu \boldsymbol{\nabla} \hat{\mathbf{u}}, \quad p = \rho R T$$

and the fluid obeys the Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}\mathbf{u}) = \rho \mathbf{g} - \boldsymbol{\nabla} p + \mu \nabla^2 \mathbf{u} + \tfrac{1}{3}\mu \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \mathbf{u})$$

$$\frac{\partial \rho c_v T}{\partial t} + \boldsymbol{\nabla} \cdot (\rho c_v T \mathbf{u}) = \lambda \nabla^2 T - p \boldsymbol{\nabla} \cdot \mathbf{u} + 2\mu(\boldsymbol{\nabla} \hat{\mathbf{u}} : \boldsymbol{\nabla} \hat{\mathbf{u}})$$

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- obs: the volume viscosity for a monoatomic gas is zero

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\end{aligned}$$

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Non-ideial gases:
(i) exclusion volume correction

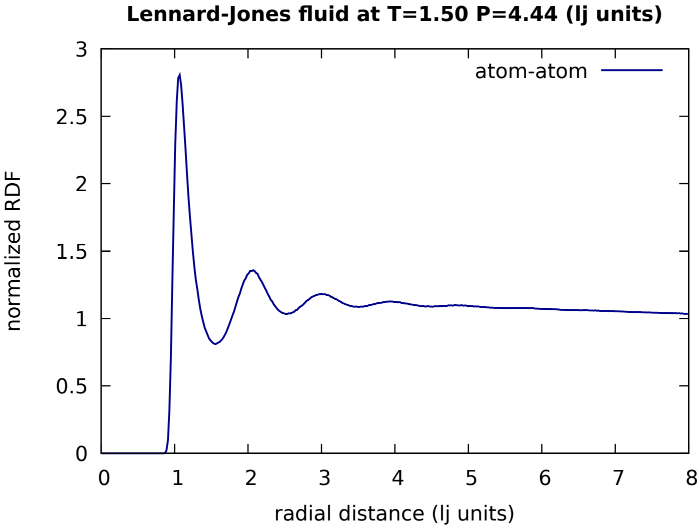
Types of corrections

At least two types of corrections are needed to describe non-ideal fluids: we must account for

- molecular exclusion volume (today)
- long-range intermolecular forces (later)

to understand look at RDFs...

Types of corrections



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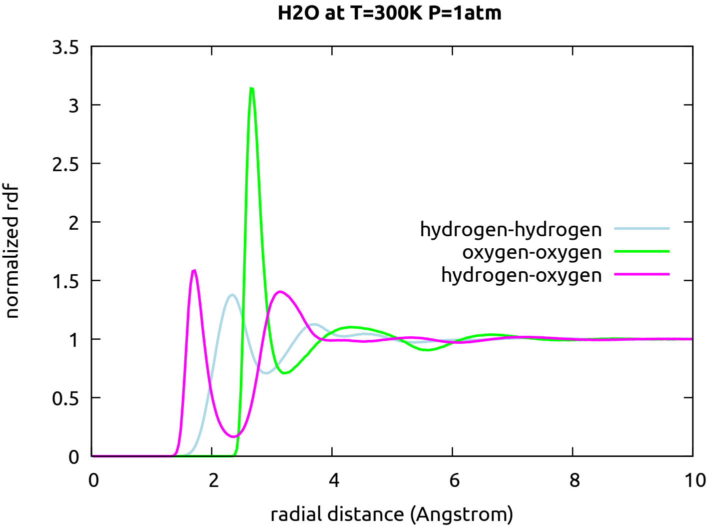

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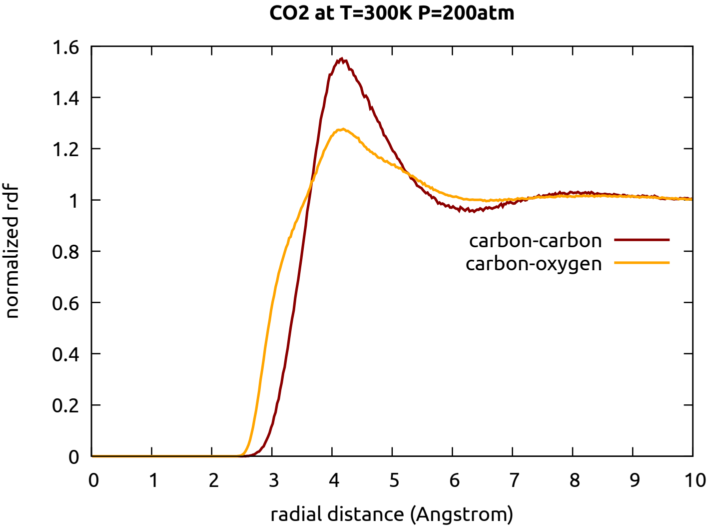

Exclusion volume

Result: if molecules have an effective diameter d

$$\left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} = \chi\big[\Omega(f) - \Theta f_0\big] \equiv \Omega_b(f)$$

i.e. the collision rate increases by the factor

$$\chi(\rho) = 1 + \tfrac{5}{8}b\rho + 0.2869(b\rho)^2 + \cdots \quad \text{where} \quad b \equiv 2\pi d^3/3m$$

while shifted by a factor '$-\Theta f_0$', where

$$\Theta(\rho, T, \mathbf{u}) = b\rho\Big\{\mathbf{C}\cdot\boldsymbol{\nabla}\log(\rho^2\chi T) + \frac{3}{5}\Big(\frac{C^2}{2RT} - \frac{5}{2}\Big)\mathbf{C}\cdot\boldsymbol{\nabla}\log T \;\cdots$$

$$+ \frac{2}{5}\Big[\frac{\mathbf{CC}}{RT} : \boldsymbol{\nabla}\mathbf{u} + \Big(\frac{C^2}{2RT} - \frac{5}{2}\Big)\boldsymbol{\nabla}\cdot\mathbf{u}\Big]\Big\}$$

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- *how does this affect the balance equations?*

Exclusion volume

New terms appear:

$$\int m\Omega_b(f)d\boldsymbol{\xi} = 0$$

$$\int m\boldsymbol{\xi}\Omega_b(f)d\boldsymbol{\xi} = -\boldsymbol{\nabla}(b\rho^2\chi R\,T) \equiv -\boldsymbol{\nabla}\cdot\boldsymbol{\Pi}_b$$

$$\int \tfrac{1}{2}m\xi^2\Omega_b(f)d\boldsymbol{\xi} = -\boldsymbol{\nabla}\cdot(b\rho^2\chi R\,T\mathbf{u}) \equiv -\boldsymbol{\nabla}\cdot(\mathbf{u}\cdot\boldsymbol{\Pi}_b)$$

These can be incorporated as a correction to the momentum flux tensor

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Exclusion volume

The balance equations are the same, except that

$$\mathbf{\Pi} = \rho\mathbf{u}\mathbf{u} + \mathbf{P} + (b\rho^2\chi R\,T)\mathbf{I}$$

$$\Pi_{ij} = \rho u_i u_j + \underbrace{(\rho R\,T + b\rho^2\chi R\,T)}_{p_b=\text{corrected equil. press.}}\delta_{ij} + \underbrace{\int mC_iC_j\,(\delta f)d\boldsymbol{\xi}}_{\text{viscous part}}$$

This effectively yields a non-ideal gas equation of state

$$p_b = \rho(1 + b\rho\chi)R\,T$$

- in practice $\chi(b\rho)$ can be adjusted to model different EOS.

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Exclusion volume

The exclusion volume corrections also affect δf and, consequently, the expressions for the viscous stress tensor and heat vector are modified:

$$\mathbf{\Pi}_{\text{viscous}} = -\eta(\boldsymbol{\nabla}\cdot\mathbf{u})\mathbf{I} - 2\mu_b\boldsymbol{\nabla}\hat{\mathbf{u}}, \quad \mathbf{Q} = -\lambda_b\boldsymbol{\nabla}T$$

where

$$\mu_b = \mu\chi^{-1}(1+\tfrac{2}{5}b\rho\chi)^2 + \tfrac{3}{5}\eta$$
$$\lambda_b = \lambda\chi^{-1}(1+\tfrac{3}{5}b\rho\chi)^2 + \tfrac{3}{2}R\eta$$

Note that a volume viscosity appears

$$\eta = 1.002\mu\chi(b\rho)^2$$

(ref: Chapman-Enskog's book, Cap. 16)

The BGK collision model

BGK collision model

The main source of difficulty in solving Boltzmann's equation is the collision integral

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{g} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = \Omega(f)$$

Simplification: adopt the *BGK collision model*

$$\Omega(f) \;\to\; \Omega_0(f) = -\frac{1}{\tau_c}(f - f_0)$$

$$f_0(\boldsymbol{\xi}; \rho, T, \mathbf{u}) = \frac{\rho}{m}(2\pi R\,T)^{-3/2} \exp\Big[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R\,T}\Big]$$

- τ_c is a model parameter known as the *relaxation time*

BGK collision model

The main source of difficulty in solving Boltzmann's equation is the collision integral

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{g} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = \Omega(f)$$

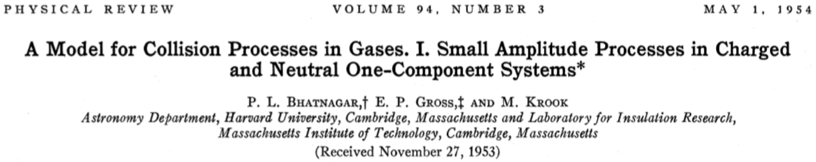
Simplification: adopt the *BGK collision model*

$$\Omega(f) \;\rightarrow\; \Omega_0(f) = -\frac{1}{\tau_c}(f - f_0)$$

$$f_0(\boldsymbol{\xi}; \rho, T, \mathbf{u}) = \frac{\rho}{m}(2\pi R\,T)^{-3/2} \exp\Big[-\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2R\,T}\Big]$$

- τ_c is a model parameter known as the *relaxation time*

BGK collision model



PHYSICAL REVIEW VOLUME 94, NUMBER 3 MAY 1, 1954

A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems*

P. L. Bhatnagar,† E. P. Gross,‡ and M. Krook
Astronomy Department, Harvard University, Cambridge, Massachusetts and Laboratory for Insulation Research, Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received November 27, 1953)

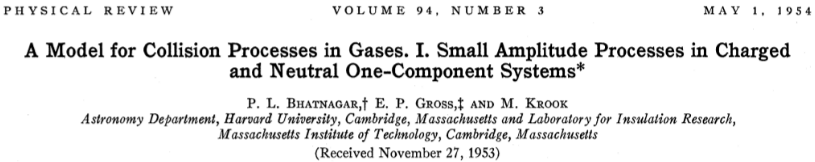
The BGK model satisfies the fundamental properties

$$\int d\boldsymbol{\xi}\, m\, \Omega_0(f) = 0$$

$$\int d\boldsymbol{\xi}\, m\boldsymbol{\xi}\, \Omega_0(f) = 0$$

$$\int d\boldsymbol{\xi}\, \tfrac{1}{2} m \xi^2\, \Omega_0(f) = 0$$

BGK collision model



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... and it is compatible with Enskog's assumptions

$$\rho = \int d\boldsymbol{\xi}\; m\; f = \int d\boldsymbol{\xi}\; m\; f_0$$

$$\mathbf{u} = \int d\boldsymbol{\xi}\; m\boldsymbol{\xi}\; f = \int d\boldsymbol{\xi}\; m\boldsymbol{\xi}\; f_0$$

$$\frac{3}{2}\rho R\, T = \int d\boldsymbol{\xi}\; \frac{1}{2} m C^2\; f = \int d\boldsymbol{\xi}\; \frac{1}{2} m C^2\; f_0$$

BGK model – transport coefficients

The Boltzmann-BGK equation reads

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{g} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}} = -\frac{1}{\tau_c}(f - f_0)$$

The Chapman-Enskog procedure yields

$$\mathbf{\Pi}_{\text{viscous}} = -2\mu \boldsymbol{\nabla} \hat{\mathbf{u}}, \quad \mathbf{q} = -\lambda \boldsymbol{\nabla} T$$

with coefficients

$$\mu = \rho R\, T\, \tau_c, \quad \lambda = \rho R\, T\, (5R/2)\, \tau_c$$

- in practice τ_c can be chosen to match the fluid's viscosity

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- $\lambda/\mu c_v = \frac{5}{3} = 1.666 \cdots \neq 2.5$

Forcing term

In order to avoid velocity gradients, we write

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c}(f - f_0) - \mathbf{g} \cdot \frac{\partial f}{\partial \boldsymbol{\xi}}$$

and approximate

$$\frac{\partial f}{\partial \boldsymbol{\xi}} \approx \frac{\partial f_0}{\partial \boldsymbol{\xi}} = -\frac{(\boldsymbol{\xi} - \mathbf{u})}{RT} f_0 = -\frac{\mathbf{C}}{RT} f_0$$

which should be valid as long as fluctuations remain small – then:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c}\left[f - f_0\left(1 + \tau_c \frac{\mathbf{C} \cdot \mathbf{g}}{RT}\right)\right]$$

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Forcing term: first implementation

Defining

$$g \equiv f_0\Big(1 + \tau_c\,(\mathbf{C}/R\,T)\cdot\mathbf{g}\Big)$$

the transport equation takes the simpler form

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c}\,(f - g)$$

‘default’ forcing style

Forcing term: first implementation

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'default' forcing style

Forcing term: second implementation

Alternatively, we may note that

$$g(\mathbf{u}, T, \rho) = f_0(\mathbf{u}, T, \rho) \times \Big(1 + \tau_c\,(\mathbf{C}/R\,T) \cdot \mathbf{g}\Big)$$
$$\approx f_0(\mathbf{u} + \Delta\mathbf{u}, T, \rho) \equiv \tilde{f}_0$$

with

$$\Delta\mathbf{u} = \tau_c\,\mathbf{g}$$

then

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c}\,(f - \tilde{f}_0)$$

'shifted velocity' forcing style

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'shifted velocity' forcing style

The basic kinetic model

The starting point for developing the Lattice Boltzmann equation will be

$$\boxed{\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{r}} = -\frac{1}{\tau_c}\left(f - g\right)}$$

To do:

- Design time-marching scheme
- Introduce discrete velocity space

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