Lecture 5: Kinetic theory of fluids

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Lecture 5: Kinetic Theory

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1 Goal

2 From atoms to probabilities

Fluid dynamics describes fluids as continuum media (fields); however under conditions of strong inhomogeneities (shocks, boundary layers), the continuum picture breaks down and the granular nature of matter is exposed. However, describing strongly inhomogenous fluids in terms of atoms or molecules is simply unviable. It is then very convenient to take an intermediate point of view, a
probabilistic one. What is the probability of finding a molecule at position \( \vec{r} \) in space at time \( t \) with velocity \( \vec{v} \)? This is precisely the Boltzmann probability distribution function (pdf):

\[
\Delta N = f(\vec{r}, \vec{v}; t) \Delta \vec{r} \Delta \vec{v}
\]

where \( \Delta N \) is the number of particles (atoms/molecules) in a volume \( \Delta \vec{r} \Delta \vec{v} \) of phase-space.

3 The Boltzmann equation

The BE is a continuity equation in phase space:

\[
\frac{df}{dt} = \partial_t f + \vec{v}_i \partial_{x_i} f + a_i \partial_{v_i} f = C \equiv G - L
\]

The lhs (Streaming) is a mirror of Newtonian mechanics, the rhs describes the interparticle collisions (Collide). The Stream-Collide paradigm leads to Advection-Diffusion in the macroscopic limit, but it is more general.

4 Global and local equilibria

The local equilibrium is defined by the condition

\[
C = 0
\]

namely a dynamic balance between gain and loss terms, \( G = L \). Inspection of the Boltzmann collision operator shows, after making the molecular chaos assumption

\[
f(1, 2) = f(1) f(2)
\]

shows that the logarithm of the product \( f(1)f(2) \) is conserved in the collision process. This means that it must be depend on the five collision invariants only

\[
f^{eq} = A + B_i v_i + C v^2
\]

By imposing the conservation of density, momentum and energy, one readily derives the local maxwellian distribution

\[
M(v, r; t) = A n(r; t) e^{-\xi^2(r; t)/2}
\]

where

\[
\xi_i(r; t) = (v_i - u(r; t))/v_{th(r; t)}
\]

is the peculiar speed in units of the thermal speed, and \( A = (2\pi v_{th}^3) \) is a normalization constant.

To be noted that the space-time dependence of the local equilibrium comes exclusively through the macroscopic fields.
This dependence is arbitrary, except that it must be slow in the scale of the mean free path.

Global equilibria (thermodynamics) are attained when $u = 0$ (no flow) and $v_{th} = \text{const.}$

The transient dynamics from local to global equilibria defines transport phenomena, which are key to practical applications.

## 5 From Boltzmann to Navier-Stokes

Kinetic moments: they describe the statistic in velocity space

Number density $n(r; t) = \int f(r, v; t)dv$  

Mass density $\rho(r; t) = m \int f(r, v; t)dv = nm$  

Mass current density: $J_i(r; t) = m \int f(r, v; t)v_i dv \equiv \rho u_i$  

Energy density: $e(r; t) = m \int f(r, v; t)v^2/2dv$  

Temperature $nk_BT(r; t) = m \int f(r, v; t)(v-u)^2/2 dv$  

Momentum flux: $P_{ij} = m \int f(r, v; t)v_i v_j dv$  

Energy flux: $Q_i = m \int f(r, v; t)(v^2/2)v_idv$  

Note that these quantities are statistical probes of velocity space. It happens that close enough to local equilibrium (low Knudsen) a few fields, density, velocity and temperature, capture the full story (hydrodynamics).

Project upon zeroth order basis (integrate over $\int ...dv$):

$\partial_t \rho + \partial_i J_i = 0$  

$\partial_t J_i + \partial_j P_{ij} = 0$
\[ \partial_t P_{ij} + \partial_k Q_{ijk} = \omega_P (P_{ij} - P_{ij}^{eq}) \]  
(11)

where \( Q_{ijk} = \int f v_i v_j v_k dv \).

Enslaving assumption: neglect the time derivative and replace the triple tensors with its equilibrium expressions. This delivers:

\[ P_{ij} \sim P_{ij}^{eq} + \tau P \partial_k Q_{ijk}^{eq} \]  
(12)

By computing the equilibrium tensors

\[ P_{ij}^{eq} = \rho v^2 \delta_{ij} + \rho u_i u_j \]

and

\[ Q_{ijk}^{eq} = J_i v^2 \delta_{jk} + \text{Perm} \]

6 Chapman-Enskog and higher order expansions

Formal solution of model Boltzmann equation (BGK):

\[ \partial f = \frac{1}{\tau} (f^{eq} - f) \]  
(13)

\[ f = (1 + \tau \partial)^{-1} f^{eq} \]

Formal series expansion in

\[ k \equiv \tau \partial = \tau \partial_t + v \tau \partial_x \]

(Knudsen number operator)

- Order 0 (Euler): \( f = f^{eq} \)
- Order 1 (Navier-Stokes): \( f = f^{eq} - k f^{eq} \)
- Order 2 (Burnett): \( f = f^{eq} - k f^{eq} + k^2 f^{eq} \)
- Order 3 (Super-Burnett): \( f = f^{eq} - k f^{eq} + k^2 f^{eq} + k^3 f^{eq} \)
- Order \( \infty \) (Boltzmann): .

This expansion does not converge term by term: it is the series \( 1/(1 + z) \): each term is a growing power, alternating sign, all terms must be included to obtain a finite result. Mathematically: the small parameter upfronts the space derivatives, if \( k << 1 \) all is well, otherwise no convergence.

Physically: boundary layers where \( k \) require all terms of the summation!

Going beyond the first order expansion (Navier-Stokes) typically leads to ill-posed equations. That is why transport phenomena far from equilibrium are hard to handle.
Plan

➢ Why a kinetic theory of fluids?

Flows with strong inhomogeneities expose the granular nature of matter. The atomistic/molecular description is too expensive, computationally unviable.

➢ Boltzmann equation

Intermediate: probability of finding a particle at a given position of space and time, with a given velocity.

Homogeneity is local in phase-space

➢ A modeling framework for complex flowing systems

➢ Applications

Rarefied gases, but now much more!
The Q-BBGKY hierarchy (0.1nm -> mm)

**Continuum Fields**
\[ \partial_t u + (u \cdot \nabla) u = -\frac{\nabla P}{\rho} + \nu \Delta u \]

**Probability d.f.**
\[ \partial_t f + (v \cdot \nabla) f = \frac{1}{r}(f - f^{eq}) \]

**Particles**
\[ \frac{d^2 r_i}{dt^2} = -\sum_{j>i} \nabla V_{ij} \]

**Fields again**
\[ i\hbar \partial_t \psi = H\psi \]

**Strongly heterogeneous fluids**

\[ Kn = \frac{\lambda \nabla \rho}{\rho} \approx 1 \]

**Density/Velocity/Temperature are not enough: more fields!**
I am conscious of being only an individual struggling against the stream of time. But it still remains in my power to contribute in such a way that, when the theory of gases is again revived, not too much will have to be rediscovered.

**Length Scales**

*Molecular size = range of interaction; \( S \)*

**Cross section (area):**

\[ \sigma \propto \pi S^2 / 4 \]

**Mean free path (length):**

\[ \lambda = 1 / n\sigma \]

**Mean intermolecular distance (length):**

\[ d = (1/n)^{1/3} \]

**De Broglie wavelength (quantum):**

\[ \lambda_B = \hbar / mv \]
Dilute vs Dense gases

Diluteness parameter:

$$\tilde{n} \equiv (s/d)^3$$

$$\tilde{n} \ll 1 \quad \text{Dilute gas}$$

$$\tilde{n} \approx 1 \quad \text{Dense gas} \sim \text{Liquid}$$

Formally, Boltzmann applies to Dilute Gases only. Modern KT much more general

Lengthscales hierarchy

Dilute gas \ (\text{Kin} >> \text{Pot}):\n
$$\lambda_B < s < d < \lambda < L_{\text{min}} < L_{\text{max}}$$

Dense gas \sim \text{Liquid} \ (\text{Kin} \sim \text{Pot}):\n
$$\hat{\lambda}_B < s \approx d \approx \hat{\lambda} < L_{\text{min}} < L_{\text{max}}$$

Formally, Boltzmann applies to Dilute Gases only. Modern KT much more general
The Boltzmann equation

Boltzmann: probability distribution function

\[ \Delta N(r, v; t) = f(r, v; t) \Delta r \Delta v \]

\( f \) lives in a 6-dimensional world (phase-space)
The Boltzmann kinetic equation: stream and collide

\[
\frac{df}{dt} = \frac{\partial f(1)}{\partial t} + v \frac{\partial f(1)}{\partial r} + \frac{F}{m} \frac{\partial f(1)}{\partial v} = C[f(1,2)]
\]

Free streaming: \( F = ma \)
Collisions = Dissipation

Boltzmann collision operator

\[
C[f(1,2)] = \int_{\text{Vel}} [f(1',2') - f(1,2)] g\sigma(g, \hat{\Omega}) d_2 \hat{\Omega} d_3 v_2
\]

Relative speed: \( g = |\vec{v}_2 - \vec{v}_1| \)
\( \hat{\Omega} = g\hat{\Omega} \)

Collision frequency: \( \gamma = ng\sigma \)

\( \tau_{mfp} \)
From atomistic potentials to cross section

\[ V(r) \quad \rightarrow \quad \sigma \propto \frac{\pi s^2}{4} \]

Compute cross section: binary collisions

\[
\begin{align*}
  m_1^* + m_2^* &= m_1 + m_2 = M \\
  \vec{p}_1^* + \vec{p}_2^* &= \vec{p}_1 + \vec{p}_2 = M\vec{v} \\
  \vec{p} &= m\vec{v} \\
  k_1^* + k_2^* &= k_1 + k_2 \\
  k &= \frac{mv^2}{2} \\
  \bar{g}' &= g(\sin\chi \cos\varepsilon, \sin\chi \sin\varepsilon, \cos\chi) \\
  \frac{MV^2}{2} + \frac{\mu g^2}{2} + \frac{L^2}{2\mu v^2} + V(r) &= E \\
  L &= \mu gb \\
  \mu &= \frac{m_1 m_2}{(m_1 + m_2)}
\end{align*}
\]
Atomistic details: 2-body problem

\[ \vec{v}'_1 = \vec{v}_1 - \mu_1(\vec{g}' - \vec{g}) \quad \mu_1 = m_1(m_1 + m_2) \]

\[ \vec{v}'_2 = \vec{v}_2 + \mu_2(\vec{g}' - \vec{g}) \quad \mu_2 = m_2(m_1 + m_2) \]

\[ g' = g(\sin \chi \cos \epsilon, \sin \chi \sin \epsilon, \cos \chi) \]

\[ bdb = \alpha(g, \chi) \sin \chi \rho \chi \quad \chi = \pi - \theta \]

\[ \sigma(g) \sim \frac{\pi s^2}{4} G(g/v_{th}) \]

\[ \Theta = \int \frac{(L/r^3)}{(2\pi(E - V(r)) - L/r^3)^{1/2}} \, dr \]

\[ L = \mu gb \]

Special potentials

\[ \sigma(g) \sim \frac{\pi s^2}{4} G(g/v_{th}) \]

\[ \Theta = \int \frac{(L/r^3)}{(2\pi(E - V(r)) - L/r^3)^{1/2}} \, dr \]

\[ L = \mu gb \]

Maxwell molecules:
\[ V(r) = 1/r^4: \ g \sigma \text{ const} \]

\[ V(r) = \text{Hard spheres}: \ \sigma \text{ const} \]

\[ V(r) = 1/r: \ \sigma \rightarrow \text{infinity} \]
Local equilibrium (dynamic)

Gain = Loss

\[ f(1')f(2') = f(1)f(2) \]

\[ -\ln f = A + \vec{B} \cdot \vec{v} + Cv^2 / 2 \]

Lagrange multipliers

Exact (family of) solutions:

\[ f_{eq}(r,v,t) = n(r,t) \frac{e^{-[(v-m(r,t))^2/2v^2]}}{[2\pi \nu^2 n(r,t)]^{3/2}} \]

\[ v_{\infty} = (kT/m) \]

Local equilibrium: dynamic balance

\[ C(1,2) = 0 \]

Gain = Loss

\[ f(1')f(2') = f(1)f(2) \]

\[ \ln f \quad \text{Collision-invariant!} \]

\[ -\ln f_{eq} = A + \vec{B} \cdot \vec{v} + Cv^2 / 2 \]
Local equilibrium: MME constraints

\[
\int f^{eq} d\vec{v} = n \\
\int f^{eq} v_a d\vec{v} = n u_a \\
(v_{th}^2 = kT / m) \\
\int f^{eq} v_a v_b d\vec{v} = n u_a u_b + n v_{th}^2 \delta_{ab}
\]

Local equilibrium (dynamic)

Gain=Loss

\[ f'(1) f'(2) = f(1) f(2) \]

\[-\ln f = A + \vec{B} \cdot \vec{v} + C v^2 / 2 \]

Lagrange multipliers

Exact family of solutions:

\[ f^{eq}(r, v; t) = n(r; t) \frac{e^{-[v-m(r;t)]^2/2v_{th}^2}}{(2\pi v_{th}^2(r; t))^{3/2}} \]

\[ v_{th}^2 = (kT / m) \]
Maxwell-Boltzmann equilibria

\[ f^{eq}(r,v;t) = n(r;t) \frac{e^{-\frac{v^2(r,t)}{2}}}{\left[2\pi V^2_{th}(r,t)\right]^{3/2}} \]

\[ c(r,t) = \frac{\left|v - u(r,t)\right|}{V_{th}(r,t)} \]

- **Galilean invariance:**
  BM depends on relative speed, not the absolute one!

- **The macro-fields can vary in space and time**
  (on scales above the mean free path)
  This generates TRANSPORT phenomena

- **The BM equils support NO dissipation!**
  (Note c = -c relative velocity invariance)

Part II: from Boltzmann to Navier-Stokes
Transport phenomena: (out of equilibrium)

\[ f = f^{\text{eq}} + f^{\text{neq}} \]

- Non-equi breaks c = c parity invariance in vel space;
- Reversing velocity does not bring the system back home.
  **IRREVERSIBILITY → DISSIPATION**

**Kinetic Theory: science of time and evolution**

The macroscopic world is irreversible

\[ t \neq -t \]

Why does time flow ‘one-way’ only?

Approach to thermal equilibrium (2nd Law)

- Hot
- Cold
- Time
  **Transport Processes**
Kinetic Moments

**Mass density:**
\[ \rho(r, t) = m \int_{\text{Vol}} f(r, v; t) d_v \]

**Current density:**
\[ J_a = \rho u_a(r, t) = m \int_{\text{Vol}} v_a f(r, v; t) d_v, \ a = x, y, z \]

**Momentum Flux:**
\[ P_{ab} = m \int_{\text{Vol}} v_a v_b f(r, v; t) d_v \]
\[ Tr(P_{ab}) = m \int_{\text{Vol}} v^2 f(r, v; t) d_v = 2K \]

**Mom-Mom Flux:**
\[ Q_{abc} = m \int_{\text{Vol}} v_a v_b v_c f(r, v; t) d_v \]

**Energy Flux:**
\[ q_a = m \int_{\text{Vol}} v^2 v_a f(r, v; t) d_v \]

---

Kinetic moments: project upon velocity space

1. **Project (1, v_a, v_a^*v_b):**

\[ \partial_t \rho + \partial_a J_a = C_0 = 0 \]
\[ J_a(r, t) = m \int_{\text{Vol}} v_a f(r, v; t) d_v \]
\[ \partial_t J_a + \partial_a P_{ab} = C_a = 0 \]
\[ P_{ab}(r, t) = m \int_{\text{Vol}} v_a v_b f(r, v; t) d_v \]
\[ \partial_t P_{ab} + \partial_a Q_{abc} = C_{ab} \neq 0 \]
\[ Q_{abc}(r, t) = m \int_{\text{Vol}} v_a v_b v_c f(r, v; t) d_v \]
\[ \partial_t Q_{abc} + \partial_a R_{abcd} = C_{abc} \]
\[ R_{abcd}(r, t) = m \int_{\text{Vol}} v_a v_b v_c v_d f(r, v; t) d_v \]

.................................
2. Enslaving/Weak non-equil closure

\[
\begin{align*}
\mathcal{C}_{ab} &= -\gamma_{ab} (P_{ab} - P_{ab}^{eq}) \\
\mathcal{P}_{ab} &= P_{ab}^{eq} + \gamma_{ab}^{-1} \partial_a \partial_b Q_{abc}^{eq} \\
\end{align*}
\]

(Only c is summed upon)

\[
\partial_t J_a + \partial_j P_{ab}^{eq} = -\partial_b (\gamma_{ab}^{-1} \partial_j Q_{abc}^{eq})
\]

(Advection+ Pressure) (Dissipation)

Hydrodynamics: equilibrium constraints

If \( f^{eq} \) is a local Maxwellian:

- \( P_{ab}^{eq} = \int f^{eq} v_a v_b d\vec{v} = \rho u_a u_b + \rho v_{th}^2 \delta_{ab} \)

- \( Q_{abc}^{eq} = \int f^{eq} v_a v_b v_c d\vec{v} = \rho u_a v_{th}^2 \delta_{bc} + \rho u_a u_b u_c \)

Microscopic derivation:

\[
\begin{align*}
p &= \rho v_{th}^2 \\
\mu_{ab} &= \rho v_{th}^2 \gamma_{ab}^{-1}
\end{align*}
\]
The ever-shifting battle: stream and collide

Macro field

\[ Kn \equiv \frac{\lambda}{L} \ll 1 \]

From Boltzmann to Navier-Stokes: weak non-equilibrium

\[ f = f^{eq} + f^{neq} \quad f^{neq} \approx (\nabla f + \lambda \nabla V) f^{eq} + hot \]

Weak departure from local equilibrium (herd effect)

\[ Kn = \frac{|f^{neq}|}{|f^{eq}|} \ll 1 \]

Order params:
- \( n=n(r,t) \)
- \( u=u(r,t) \)
- \( T=T(r,t) \)
Transport phenomena: formal solution

\[ C(f, f) = -\frac{(f - f^{eq})}{\tau} \]

\[ (1 + \tau \partial) f = f^{eq} \quad f = (1 + \tau \partial)^{-1} f^{eq} \]

\[ f^{(0)} = f^{eq} \quad \text{Euler} \]
\[ f^{(1)} = (1 - \tau \partial) f^{eq} \quad \text{Navier-Stokes} \]
\[ f^{(2)} = (1 - \tau \partial + \tau^2 \partial^2) f^{eq} \quad \text{Burnett} \]
\[ f^{(3)} = (1 - \tau \partial + \tau^2 \partial^2 - \tau^3 \partial^3) f^{eq} \quad \text{SuperBurnett} \]

Kinetic moments: sampling velocity space

\[ < c^n > = \int f(\vec{r}, \vec{v}, t) c^n d\vec{v} \quad c = (v-u)/V_{th} \]

Samples
\[ v \approx u \pm \sqrt{n} V_{th} \quad c \equiv v'/V_{th} \]

\[ < v_a > = u_a \]
\[ < v_a v_b > = u_a u_b + < v'_a v'_b > \]
\[ < v_a v_b v_c > = u_a u_b u_c + u_a v_{th}^2 \delta_{bc} + < v'_a v'_b v'_c > \]

Hydrodynamics \[ < c^n > = a_n (\langle c^2 \rangle)^{n/2} \]
Kinetic theory \[ < c^n > = a_n (\langle c^2 \rangle)^{n/2} \]

Molecular freedom (no enslaving)
The jungle of kinetic tensors!

\[ \frac{\partial T_{ij}}{\partial t} = \rho_0 \left( \frac{\partial U_{ij}}{\partial \rho} + \frac{\partial U_{ij}}{\partial \rho_0} - \frac{1}{2} \frac{\partial U_{ij}}{\partial T} + \frac{\partial U_{ij}}{\partial T} - \frac{2}{3} \frac{\partial U_{ij}}{\partial \rho} \right) + \frac{\partial U_{ij}}{\partial \rho_0} + \frac{\partial U_{ij}}{\partial \rho_0} - \frac{2}{3} \frac{\partial U_{ij}}{\partial T} \]
\[ - \frac{\partial}{\partial \rho} \left( Q_{ij} \frac{\partial T}{\partial \rho} - 2 \frac{\partial T}{\partial \rho} \right) + \frac{\partial}{\partial \rho_0} \left( Q_{ij} \frac{\partial T}{\partial \rho_0} - 2 \frac{\partial T}{\partial \rho_0} \right) + \frac{\partial}{\partial \rho_0} \left( Q_{ij} \frac{\partial T}{\partial \rho_0} - 2 \frac{\partial T}{\partial \rho_0} \right) = \frac{\delta T_{ij}}{\delta t} \]

(2.13a)

\[ \frac{\partial Q_{ij}}{\partial t} = \rho_0 \left( \frac{\partial U_{ij}}{\partial \rho} + \frac{\partial U_{ij}}{\partial \rho_0} - \frac{1}{2} \frac{\partial U_{ij}}{\partial T} + \frac{\partial U_{ij}}{\partial T} - \frac{2}{3} \frac{\partial U_{ij}}{\partial \rho} \right) + \frac{\partial U_{ij}}{\partial \rho_0} + \frac{\partial U_{ij}}{\partial \rho_0} - \frac{2}{3} \frac{\partial U_{ij}}{\partial T} \]
\[ + \rho_0 \left( \frac{\partial U_{ij}}{\partial \rho} + \frac{\partial U_{ij}}{\partial \rho_0} - \frac{1}{2} \frac{\partial U_{ij}}{\partial T} + \frac{\partial U_{ij}}{\partial T} - \frac{2}{3} \frac{\partial U_{ij}}{\partial \rho} \right) + \rho_0 \left( \frac{\partial U_{ij}}{\partial \rho_0} + \frac{\partial U_{ij}}{\partial \rho_0} - \frac{2}{3} \frac{\partial U_{ij}}{\partial \rho} - \frac{2}{3} \frac{\partial U_{ij}}{\partial \rho} \right) \]
\[ - \left( \frac{\partial \rho_0}{\partial \rho} + \frac{\partial \rho_0}{\partial \rho_0} - \frac{1}{2} \frac{\partial \rho_0}{\partial T} + \frac{\partial \rho_0}{\partial T} - \frac{2}{3} \frac{\partial \rho_0}{\partial \rho} \right) \]
\[ + \left( \frac{\partial \rho_0}{\partial \rho} + \frac{\partial \rho_0}{\partial \rho_0} - \frac{1}{2} \frac{\partial \rho_0}{\partial T} + \frac{\partial \rho_0}{\partial T} - \frac{2}{3} \frac{\partial \rho_0}{\partial \rho} \right) \]
\[ \left( \frac{\partial \rho_0}{\partial \rho} + \frac{\partial \rho_0}{\partial \rho_0} - \frac{1}{2} \frac{\partial \rho_0}{\partial T} + \frac{\partial \rho_0}{\partial T} - \frac{2}{3} \frac{\partial \rho_0}{\partial \rho} \right) \]
\[ = \frac{\delta Q_{ij}}{\delta t} \]

(2.13b)

Microscopic foundations of viscosity

Collision invariants and variants

1

2

1

2'

\[ m'_1 + m'_2 = m_1 + m_2 \]
\[ m'_1 V'_1 + m'_2 V'_2 = m_1 V_1 + m_2 V_2 \]
\[ m'_1 V'^2_1 + m'_2 V'^2_2 = m_1 V^2_1 + m_2 V^2_2 \]

The magnificent 5

Less magnificent 6

\[ m'_1 V'_1 + m'_2 V'_2 V'_2 = m_1 V'_1 + m_2 V'_2 V'_2 \]
**Microscopic foundations of viscosity**

\[ xx : 1 \times 1 + (-1) \times (-1) = 2 \rightarrow 0 \times 0 + 0 \times 0 = 0 \]

\[ xy : 1 \times 0 + (-1) \times (0) = 0 \rightarrow 0 \times 1 + 0 \times (-1) = 0 \]

\[ yy : 0 \times 0 + 0 \times 0 = 0 \rightarrow 1 \times 1 + 1 \times 1 = 2 \]

---

**Viscosity = Momentum-flux diffusivity**

\[ \sigma_{xy} = \frac{F_y}{A_y} = -\nu \hat{v}_y (\rho u_x) \]

*Momentum is lost on the wall, This information propagates inside via momentum-conserving collisions. This is how the wall drives the bulk fluid. No collisions, no drag.*
Solving the BE

Lives in 3+3+1 dimensions
Collision operator: integral, quadratic

COMPUTATIONAL NIGHTMARE!

Solving the BE (aargh!)

Direct Simulation Monte Carlo

Model Equations

Discrete Velocity Models
Direct Simulation MonteCarlo

Mimics (simulates) molecular motion with simple stochastic rules.

Till recently the only method in d=3+3

Very expensive (fluctuations $1/\sqrt{\Delta t}$) convergence

Stream-Collide paradigm

$$\hat{r}_i = r_i + v_i \Delta t;$$

$$\hat{v}_i = v_i + a_i \Delta t$$

$$v_i \Delta t < \lambda$$
Collisions

Prob of i-j colli in dt:

\[ p_{ij} = n V_{ij} \sigma(V_{ij}) \Delta t \equiv \frac{\Delta t}{\tau_{ij}} \]

Perform i-j colli:

Draw \( r_{ij} \in [0,1] \);
If \( r_{ij} < p_{ij} \); Collide
Else ;

Select another \((i,j)\) and try again

Model Boltzmann: BGK

- Bhatnagar-Gross-Krook (BGK), 1954

**Single-time relaxation**

\[ C(f,q) = \frac{(f^{eq} - f)}{\tau} \]

**Multi-time relaxation**

\[ C(f,q) = \int \Omega(\tilde{v},\tilde{v}') (f^{eq} - f)(\tilde{v}',\tilde{r};t)d\tilde{v}' \]

Still STRONGLY non-linear !!!
Model Boltzmann II: discrete velocities

- Kac, Carleman, Broadwell (60’s)

**Discrete velocity models**

\[
\partial_t f_i + v_i \partial_x f_i = \sum_{jkl} \sigma_{ij}^{kl} f_k f_l - \sum_{jkl} \sigma_{ij}^{kl} f_i f_j
\]

\((i,j) \leftrightarrow (k,l)\)

**NOT targeted to hydrodynamics!**

**Special solutions of the BE**

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**Practical use of Boltzmann-like equation: beyond rarefied media!**

- **Systems far from local equilibrium**
- **Neutron transport**
- **Shock waves**
- **Gamma rays transport**
- **Shuttle re-entry**
- **Electron flows**
- **Traffic/cellular flows**
Summary

1. The Boltzmann equation lives between molecules and continuum fields: probability distribution functions.

2. In its original derivation it applies only to dilute gases.

3. It is hard to solve directly, typically via direct MonteCarlo.

4. Close to local equilibrium delivers the macroscopic equations of continuum mechanics, including the EoS and transport coefficients.

5. Far from equilibrium one must solve the full Boltzmann, very hard task. Model equations provide useful approximate solutions, both analytical and numerical.

Assignments

1. Show that in a dilute gas the mean free path is larger than the mean intermolecular distance: give actual numbers for standard air.

2. What fraction of air molecules move faster than 1000 m/s in standard conditions?

3. Same for air molecules in a car moving at 100 Km/h (in the Lab frame).

4. For the brave: Solve the time-independent BGK equation in d=1 for an isothermal fluid (T=const) at rest (u=0). Initial conditions f0 gaussian in x and v. Boundary conditions, zero at plus/minus infinity. Does a solution exist?
End of Lecture