FICUS COURSE

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"Numerical methods for kinetic equations and conservation laws"

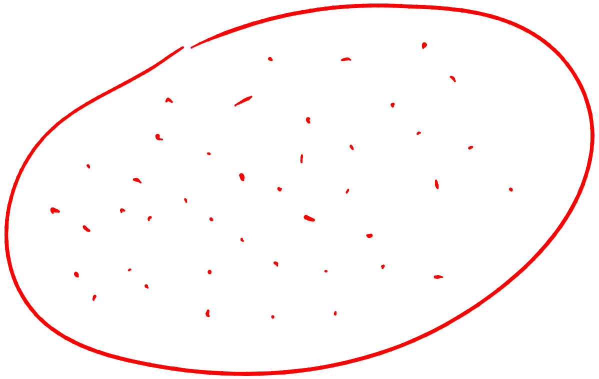
Part 1: Kinetic theory

1. Description of particle systems
2. Kinetic modelling of rarefied gases
3. From kinetic to fluid descriptions

Part 2: Numerical methods

4. Velocity discretization - DVM
5. Basic numerical approximations for time and space
6. Asymptotic Preserving (AP) numerical methods

1. Description of particle systems



particles = molecules of gas

→ 3 level of description

① microscopic description

② macroscopic description (fluid)

③ mesoscopic — (kinetic)

1.1 Microscopic description

$v(t)$ velocity $\left((v_1(t), v_2(t), v_3(t)) \right)$

$x(t)$

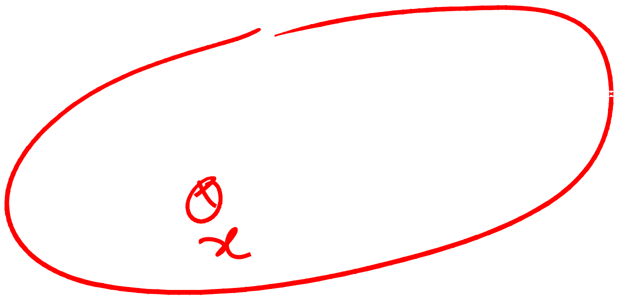
position (vector of $\mathbb{R}^3$: $(x_1(t), x_2(t), x_3(t))$)

Evolution of the system :

$$\begin{cases} \dfrac{d}{dt} x(t) = v(t) \\[2ex] m \dfrac{d}{dt} v(t) = F(t) \end{cases}$$

Newton laws

1.2 Macroscopic Description



gas: continuous fluid

$\boxed{\rho(t,x)}$ = (mass) density of the gas
(time t, position x)

= mass of gas / unit of volume
(kg / m^3)

$\boxed{u(t,x)}$ = mean velocity of the gas
(averaged
= macroscopic = bulk ...)

→ (components (u_1, u_2, u_3))

$\rho(t,x)\, u(t,x) =$ momentum (density) of the gas

$=$ momentum / unit of volume

$T(t,x) =$ temperature of the gas

$p(t,x) =$ pressure of the gas

$E(t,x) =$ total energy (density)

$=$ total energy / unit of volume

$$= \underbrace{\frac{1}{2} \rho \|u\|^2}_{\text{kinetic energy density}} + \frac{3}{2} \rho \underbrace{R}_{\text{gas constant}} T$$

evolution of the system:

↳ Euler equations of gas dynamics

$$
\begin{cases}
\partial_t \rho + \nabla\cdot(\rho u) = 0 \\
\partial_t(\rho u) + \nabla\cdot(\rho u \otimes u + p\, \mathrm{Id}) = 0 \\
\partial_t E + \nabla\cdot((E+p)u) = 0
\end{cases}
$$

1.3 Mesoscopic (Kinetic) description

- rarefied gas (not too many particles in the domain)

- distribution function :

$$f(t, x, v)$$

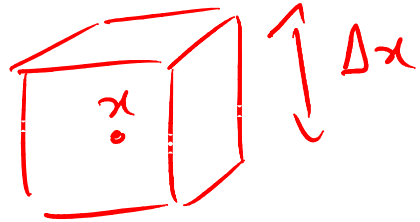
t: time, x: position, v: velocity

7 variables

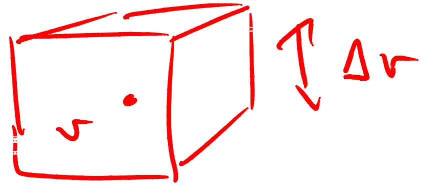
= number density of particles in the phase space

= number of particles / unit of volume in both position and velocity space

- small cube around x



small cube around v



The number of particles with position $x \pm \Delta x$ and with velocity $v \pm \Delta v$

$$= f(t, x, v) \underbrace{(\Delta x)^3}_{dx} \underbrace{(\Delta v)^3}_{dv}$$

$$dv = dv_1 dv_2 dv_3$$

$$dx = dx_1 dx_2 dx_3$$

- link with macroscopic variables :

$$\underbrace{\left(\int_{\mathbb{R}^3_v} \underbrace{f(t,x,v)\, dv \right) dx}_{\substack{\#\text{ of particles around } x \\ \text{velocity around } v}}}_{\#\text{ of particles around } x}$$

multiply by the mass of one particle (m)

$$\hookrightarrow \quad \left(\int_{\mathbb{R}^3_v} m f(t,x,v)\, dv \right) dx$$

$= \text{mass of particles around } x$

$= \underbrace{\rho(t,x)}\, dx$

$$\boxed{\rho(t,x) = \int_{\mathbb{R}^3_v} m\, f(t,x,v)\, dv}$$

notation:

$$\int_{\mathbb{R}^3_v} f(v)\, dv = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(v_1,v_2,v_3)\, dv_1\, dv_2\, dv_3$$

link between f and ρu :

$$\underbrace{\underbrace{m v \, f(t,x,v) \, dv}_{\text{\# of particles around } x \text{, velocity around } v} \, dx}_{\text{total momentum of \_\_\_\_\_\_ \_\_\_\_\_\_}}$$

$$\underbrace{\left(\int_{\mathbb{R}^3_v} m v \, f(t,x,v) \, dv \right) dx}_{\text{total momentum of particles around } x}$$

$$= \rho u(t,x) \, dx$$

$$\boxed{\rho u(t,x) = \int_{\mathbb{R}^3_v} m v f(t,x,v)\, dv}$$

$$\Rightarrow \quad \boxed{u(t,x) = \frac{1}{\rho(t,x)} \int_{\mathbb{R}^3_v} m v f(t,x,v)\, dv}$$

Exercise: prove that

① $$\boxed{E(t,x) = \int_{\mathbb{R}^3_v} \frac{1}{2} m \|v\|^2 f(t,x,v)\, dv}$$

(Notation: $\|v\|^2 = v_1^2 + v_2^2 + v_3^3$)

② $$\boxed{T(t,x) = \frac{1}{\frac{3}{2}\rho R} \int_{\mathbb{R}^3_v} \frac{1}{2} m \|v-u\|^2 f(t,x,v)\, dv}$$

hint: use ① and the relation between T and E

: write v as $(v-u)+u$

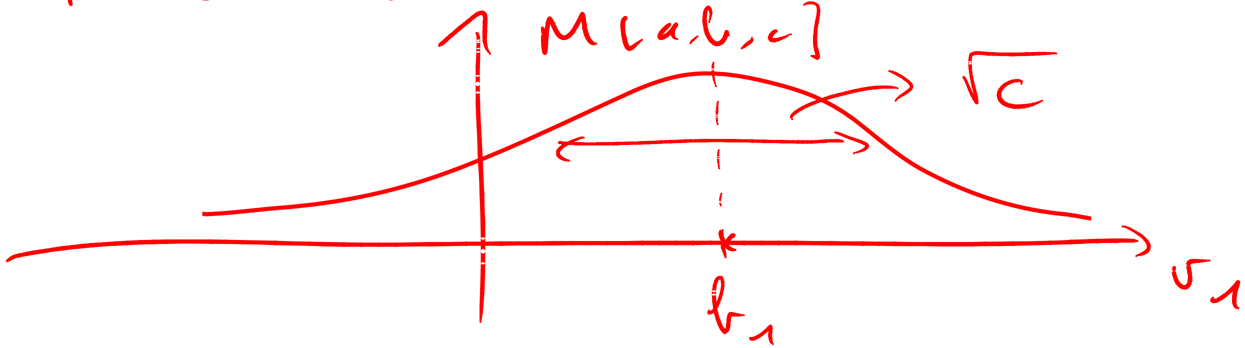
Simple (fundamental) example of distribution function:

parameters: $a \in \mathbb{R}$, $b \in \mathbb{R}^3$, $c \in \mathbb{R}$

$$\boxed{M[a,b,c](v) = \frac{m a}{(2\pi R c)^{3/2}} \exp\left(-\frac{\|v-b\|^2}{2Rc}\right)}$$

MAXWELLIAN DISTRIBUTION

(1D view v_2, v_3 fixed)



What are the macroscopic variables related to $M[a,b,c]$?

Mathematical property:

$$(*) \quad \int_0^{+\infty} e^{-x^2}\,dx = \sqrt{\pi}$$

Then:

$$\rho = \int_{\mathbb{R}^3_v} m\, M[a,b,c](v)\, dv = a$$

$$u = \frac{1}{\rho} \int_{\mathbb{R}^3_v} m v\, M[a,b,c](v)\, dv = b$$

$$T = \frac{1}{\frac{3}{2}\rho R} \int_{\mathbb{R}^3_v} \frac{1}{2} m \|v\|^2 M[a,b,c](v)\, dv = c$$

(Exercise: prove these relations)
hint: use (*) and $v \mapsto \xi = \frac{v-u}{\sqrt{2Rc}}$

Finally :

Maxwellian distribution is defined through its macroscopic quantities ρ, u, T :

$$M[\rho, u, T](v) = \frac{m\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{\|v-u\|^2}{2RT}\right)$$

$$\int_{\mathbb{R}^3_v} m \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} M[\rho, u, T](v)\, dv = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

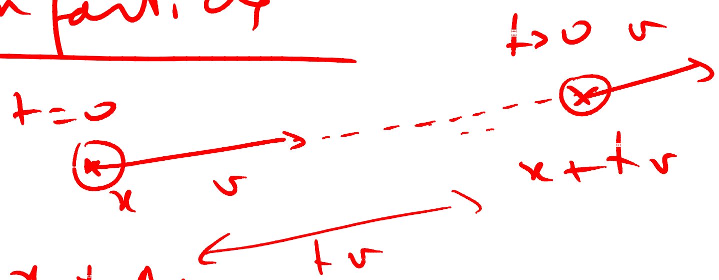
where $E = \frac{1}{2}\rho \|u\|^2 + \frac{3}{2}\rho RT$

2. Kinetic modelling of a rarefied gas

(time evolution of the system, of f)

2.1 No collision between particles

(no forces)



\# of particles at time $t=0$ at $x \pm \Delta x$,
velocity $v \pm \Delta v$

$$= f(0, x, v)\, dx\, dv$$

\# of particles at time $t>0$ at $(x+tv) \pm \Delta x$
velocity $v \pm \Delta v$

$$= f(t, x+tv, v)$$

- we have:

$$\int f(0,x,v)\,dx\,dv = \int f(t,x+tv,v)\,dx\,dv$$

- define: $\phi(t) := \int f(t,x+tv,v)\,dx\,dv$

ϕ is constant in time (see

$\Downarrow$ $\frac{d}{dt}\phi(t) = 0$

(use the chain rule)

$$\parallel$$

$$\int \Big(\underbrace{\partial_t f(t,x+tv,v) + v\cdot\nabla_x f(t,x+tv,v)}_{} \Big)\, dx\, dv$$

$= 0$ for every t, x, v

we find the following evolution equation:

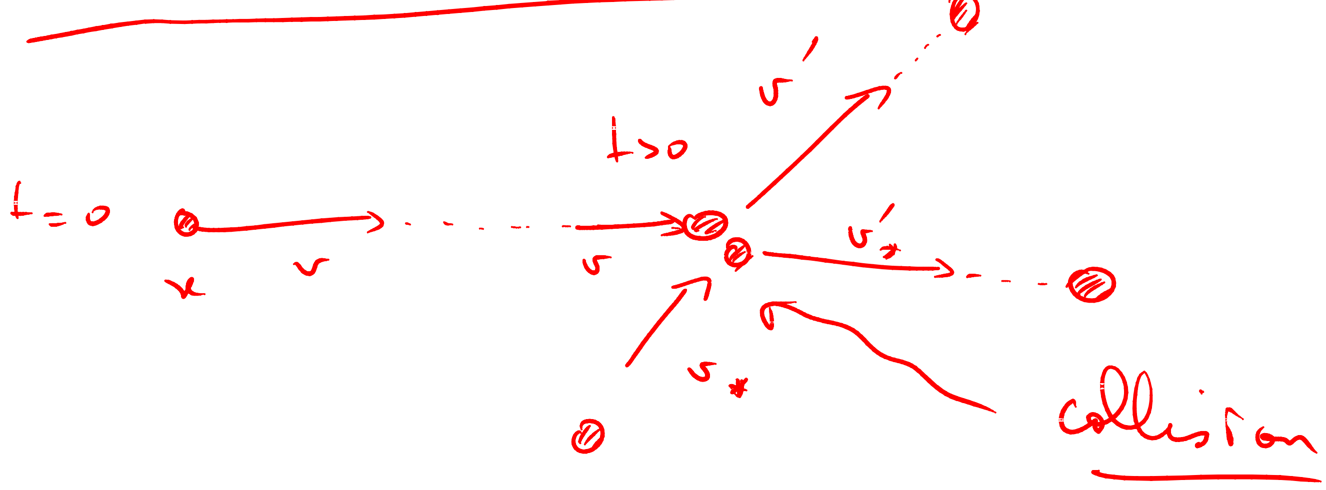
$$\boxed{\partial_t f(t,x,v) + v \cdot \nabla_x f(t,x,v) = 0}$$

transport equation

$$\left(\nabla_x f = \begin{pmatrix} \partial_{x_1} f \\ \partial_{x_2} f \\ \partial_{x_3} f \end{pmatrix} \qquad (\text{"grad } f\text{"}) \right.$$

$$\left. v \cdot \nabla_x f = v_1 \partial_{x_1} f + v_2 \partial_{x_2} f + v_3 \partial_{x_3} f \right)$$

2.2 Collisions



number of particles at $(x+tv) \pm \Delta x$, $v \pm \Delta v$
is changed by collisions

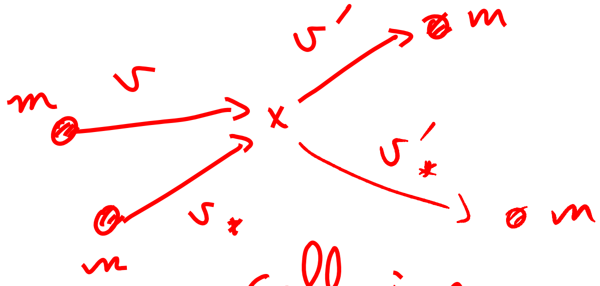
$$\boxed{\underbrace{\partial_t f + v \cdot \nabla_x f}_{\text{transport}} = \underbrace{Q(f)}_{\text{collisions}}}$$

KINETIC EQUATION

(in R.G.D.: Boltzmann equation)

2.3 Properties of the collision operator $Q(f)$

(1) Conservation properties.



collision

Assumption: in a collision

$$m + m = m + m$$

$$m v + m v_* = m v' + m v_*'$$

$$\frac{1}{2} m \|v\|^2 + \frac{1}{2} m \|v_*\|^2 = \frac{1}{2} m \|v'\|^2 + \frac{1}{2} m \|v_*'\|^2$$

before coll. after coll.

microscopic level: conservation of the mass, the momentum, the kinetic energy.

$$\boxed{\int_{\mathbb{R}^3_v} m \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} Q(f)\, dv = 0}$$

(2) entropy property:

$$\boxed{\int_{\mathbb{R}^3_v} (\log f)\, Q(f)\, dv \leq 0 \quad \text{(entropy dissipation)}}$$

(3) Equilibrium state:

$$Q(f) = 0 \iff f = M[\rho, u, T]$$

where $\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} = \int m \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} f \, dv$

eq. states are Maxwellian distributions

(4) Tends to equilibrium

homogeneous gas (no x variable)

↳ kinetic equation : $\partial_t f = Q(f)$

then:

$$f \xrightarrow[t \to +\infty]{} M[\rho, u, T]$$

" the collisions make the gas into an equilibrium state "

2.4 Conservation laws

mass conservation: $\partial_t f + v \cdot \nabla_x f = Q(f)$ (K)

we know that $\int_{\mathbb{R}^3_v} m\, Q(f)\, dv = 0$ → consequence on the kin. equation?

↳ $\int_{\mathbb{R}^3_v} m(K)\, dv$ → we find

$$\underbrace{\int_{\mathbb{R}^3} m\, \partial_t f\, dv}_{= \underbrace{\partial_t \int_{\mathbb{R}^3_v} m f\, dv}_{\rho(t,x)}} + \underbrace{\int_{\mathbb{R}^3_v} m\, v \cdot \nabla_x f\, dv}_{= \nabla_x \cdot \underbrace{\int_{\mathbb{R}^3_v} m v f\, dv}_{\rho u(t,x)}} = \cancel{\int_{\mathbb{R}} m Q(f)\, dv} = 0$$

we get : the continuity equation

$$\boxed{\partial_t \rho + \nabla_x \cdot (\rho u) = 0}$$

(remind : $v \cdot \nabla_x f = \sum_{i=1}^{3} v_i \, \partial_{x_i} f = \underbrace{\sum_{i=1}^{3} \partial_{x_i} (v_i f)}_{= \nabla \cdot (v f)}$)

where $\nabla_x \cdot V := \partial_{x_1} V_1 + \partial_{x_2} V_2 + \partial_{x_3} V_3$

" "divergence of V "

• <u>momentum conservation</u>: $\partial_t f + v \cdot \nabla_x f = Q(f)$ (K)

we know $\int m v\, Q(f)\, dv = 0$

$\downarrow \int_{\mathbb{R}^3_v} m v \,(K)\, dv \longrightarrow$ we get :

$$\underbrace{\int_{\mathbb{R}^3_v} m v\, \partial_t f \, dv}_{= \partial_t \underbrace{\int_{\mathbb{R}^3_v} m v f \, dv}_{\rho u}} + \underbrace{\int_{\mathbb{R}^3_v} m v (v \cdot \nabla_x f)\, dv}_{\nabla_x \cdot \int m v \otimes v f \, dv} = \cancel{\int m v Q(f)\, dv} = 0$$

we get:

$$\partial_t \rho u + \nabla \cdot \int m v \otimes v f \, dv = 0$$

<u>Exercise</u>: prove that:

$$\int m v \otimes v f \, dv = \rho u \otimes u + \mathbb{P}$$

where $\mathbb{P} = \int m (v-u) \otimes (v-u) f \, dv$

<u>hint</u>: write v as $(v-u)+u$

we get.

$$\boxed{\partial_t \rho u + \nabla_x \cdot (\rho u \otimes u + \mathbb{P}) = 0}$$

momentum local conservation law

parameter.

• energy conservation: $\partial_t f + v \nabla_x f = Q(f)$ (K)

we know that $\int \frac{1}{2} m \|v\|^2 Q(f)\, dv = 0$

$\int_{\mathbb{R}^3_v} \frac{1}{2} m \|v\|^2 (K)\, dv \longrightarrow$

$$\partial_t E + \nabla_x \cdot \int \frac{1}{2} m \|v\|^2 v f\, dv = 0$$

Exercise: ① Prove this ~~relation~~

② prove that:

$\int \frac{1}{2} m \|v\|^2 v f\, dv = E u + \mathbb{P} u + q$

where $q = \int \frac{1}{2} m \|v - u\|^2 (v-u) f\, dv$ heat flux vector.