PART 2: NUMERICAL APPROXIMATIONS OF KINETIC EQUATIONS

4. VELOCITY DISCRETIZATION AND D.V.M

PROBLEM: $\partial_t f + v \cdot \nabla_x f = Q(f)$

TIME VELOCITY SPACE

$$v \in \mathbb{R}^3 \xrightarrow{\text{DISCRETIZATION}} (v_1, v_2, \dots, v_N)$$

4.1 TRUNCATION OF THE VELOCITY SPACE

- SIMPLIFICATION: ASSUME THAT $v \in \mathbb{R}$ (1D CASE)
- ASSUME THAT THE "MAIN PART" OF f IS LOCATED IN A BOUNDED VELOCITY DOMAIN $[v_{min}, v_{max}]$ FOR EVERY TIME $t \leq$ SIMULATION TIME, POSITION $x \in$ SIMULATION DOMAIN

REASONABLE ASSUMPTION

REASONABLE ASSUMPTION BECAUSE

- PHYSICALLY : $\|v\| \leq$ SPEED OF LIGHT

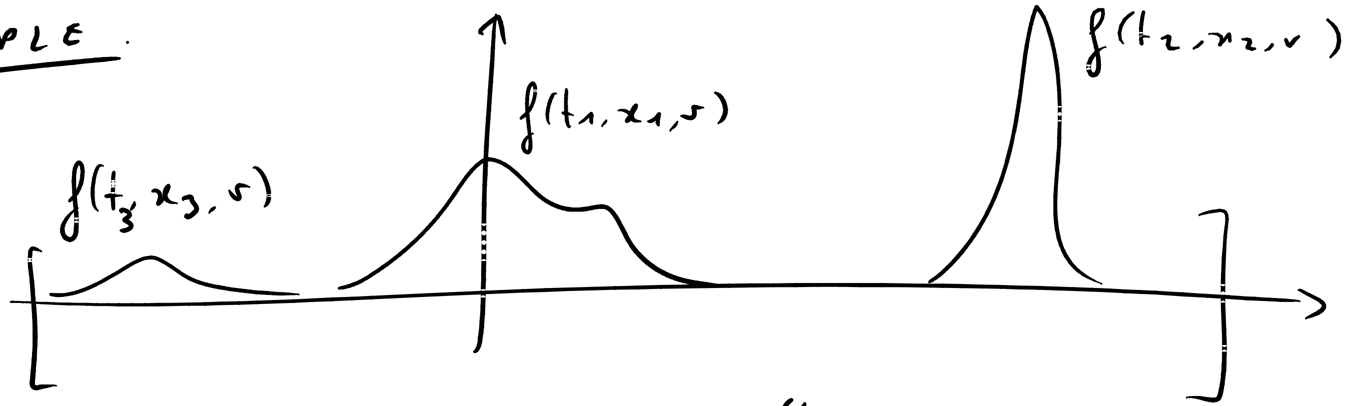
- MATHEMATICALLY :

  f is INTEGRABLE W.R.T v
  AGAINST $1, v, \frac{1}{2}\|v\|^2$

  $\Rightarrow$ f is "FASTLY DECREASING"

  $\Rightarrow$ "CONCENTRATED" SUPPORT

EXAMPLE.



v_{min} $\qquad$ v_{max}

EVERY f ARE "LOCATED" INSIDE $[v_{min}, v_{max}]$

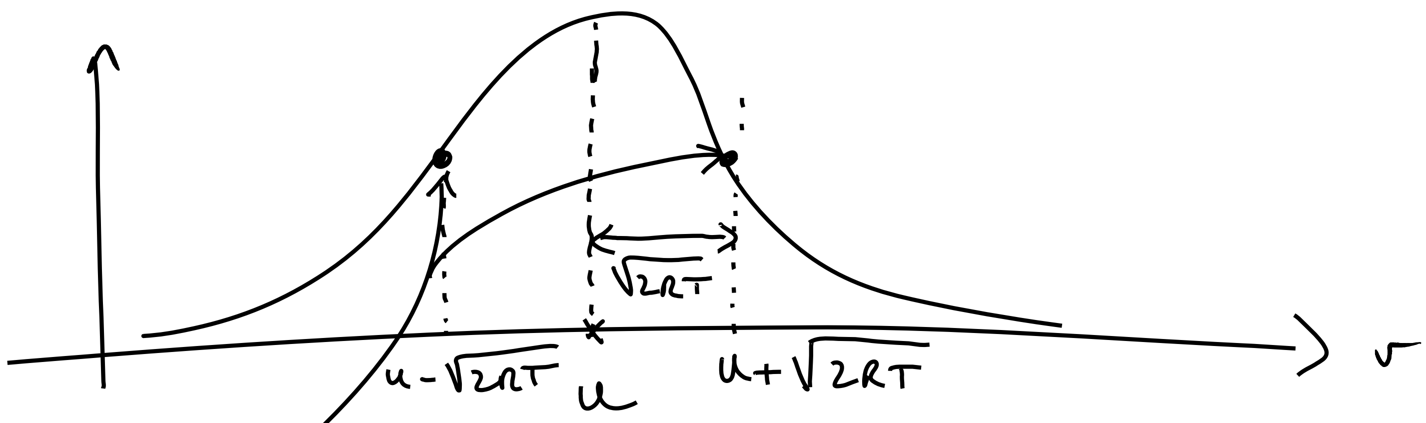
PROBLEM: HOW TO ESTIMATE THIS BOUNDS?

↳ DIFFERENT STEPS

(a) ASSUME f IS "NOT TOO FAR" FROM ITS CORRESPONDING MAXWELLIAN $M[\rho, u, T]$ FOR EVERY t, x, IN THE SENSE THAT THEIR "SUPPORT" ARE CLOSE.

↳ THE "SUPPORT" OF $M[\rho, u, T]$ CAN BE COMPUTED ANALYTICALLY

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



INFLECTION POINTS ($M''(v) = 0$)

THE ESSENTIAL PART OF $M[\rho, u, T]$ IS LOCATED INSIDE : $\left[u - 4\sqrt{2RT}\ ,\ u + 4\sqrt{2RT}\right]$

<u>EXERCISE:</u> PROVE THAT

$$v \notin \left[u - 4\sqrt{2RT}\ ,\ u + 4\sqrt{2RT}\right]$$

$$\Downarrow$$

$M[\rho, u, T](v) \leq 0{,}002\,\%$ OF THE MAXIMUM VALUE OF $M[\rho, u, T](v)$

THEN THE "SUPPORT" OF f IS CONTAINED IN THE LARGEST INTERVAL.

$$\left[u(t,x) - 4\sqrt{2RT(t,x)}\ ,\ u(t,x) + 4\sqrt{2RT(t,x)}\right]$$

TAKE:

$$v_{max} = \max_{t,x} \left(u(t,x) + 4\sqrt{2RT(t,x)} \right)$$

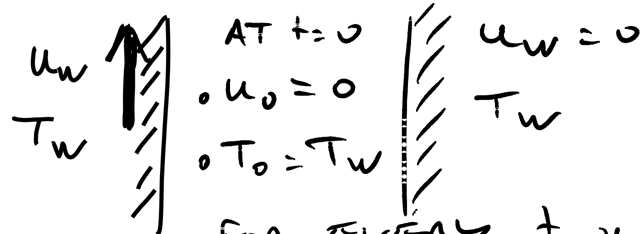
$$v_{min} = \min_{t,x} \left(u(t,x) - 4\sqrt{2RT(t,x)} \right)$$

(b) HOW TO ESTIMATE THESE VALUES ?

↳ 2 CASES

b.1: THEY CAN BE ESTIMATED BY USING THE INITIAL AND BOUNDARY DATA

EXAMPLE: COUETTE FLOW



THEN : • $0 \leq u(t,x) \leq u_w$ FOR EVERY t,x

• $T(t,x) \leq T_w$

CONSEQUENTLY :

$$\boxed{\begin{aligned} v_{max} &:= u_w + 4\sqrt{2RT_w} \\ v_{min} &:= -4\sqrt{2RT_w} \end{aligned}}$$

b.2 : THEY CANNOT BE ESTIMATED LIKE THAT

EXAMPLE : AERODYNAMICS. (EXTERNAL SUPERSONIC FLOW)

T CAN BE MUCH LARGER THAN T_∞ AND T_w

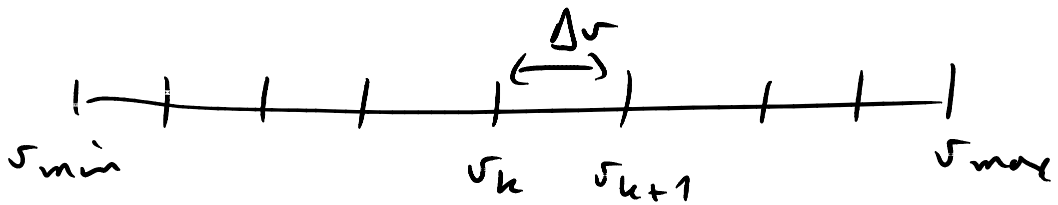
ONE SOLUTION : MAKE A FLUID SIMULATION AND THEN ESTIMATE v_{max} AND v_{min} WITH THE FLUID VALUES (NAVIER-STOKES SIMULATION)

4.2 DISCRETIZATION OF THE TRUNCATED VELOCITY SET $[v_{min}, v_{max}]$.

THE SIMPLEST : UNIFORM DISCRETIZATION (REGULAR GRID)

$$v_k = v_{min} + k\,\Delta v \qquad k = 0 \text{ TO } N$$

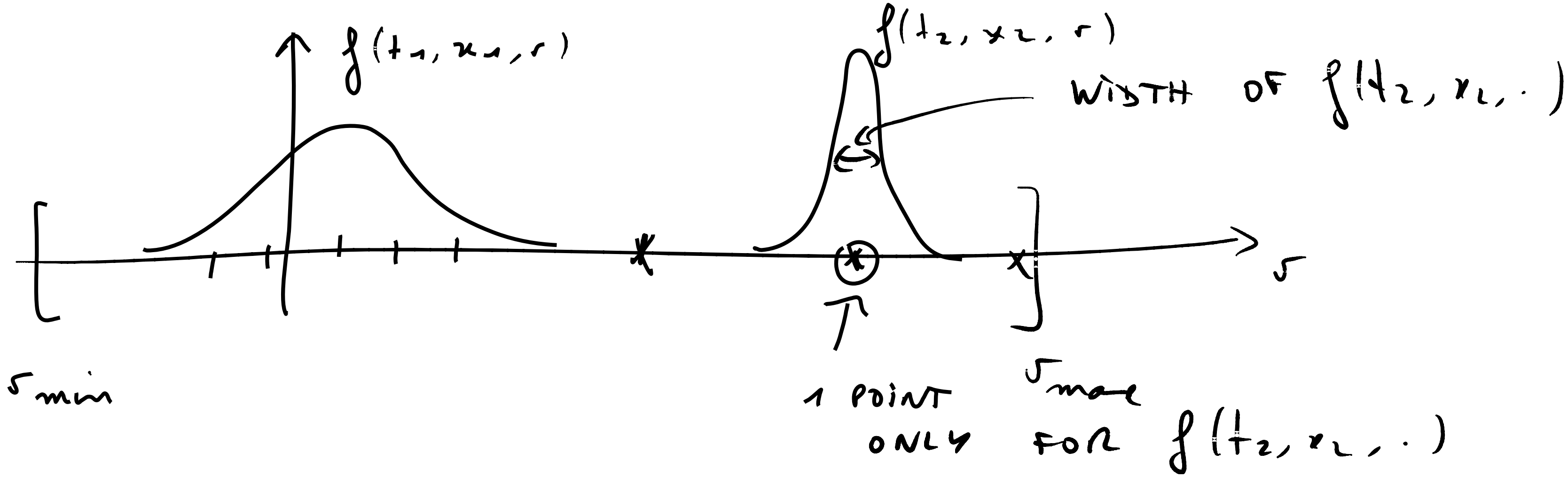
N AND Δv : $v_N = v_{min} + N\,\Delta v = v_{max}$



QUESTION: HOW TO CHOOSE Δv (OR N) ?

↳ IDEA SIMILAR TO STEP 1 FOR THE TRUNCATION

ALL THE f SHOULD BE WELL REPRESENTED ON THE GRID.



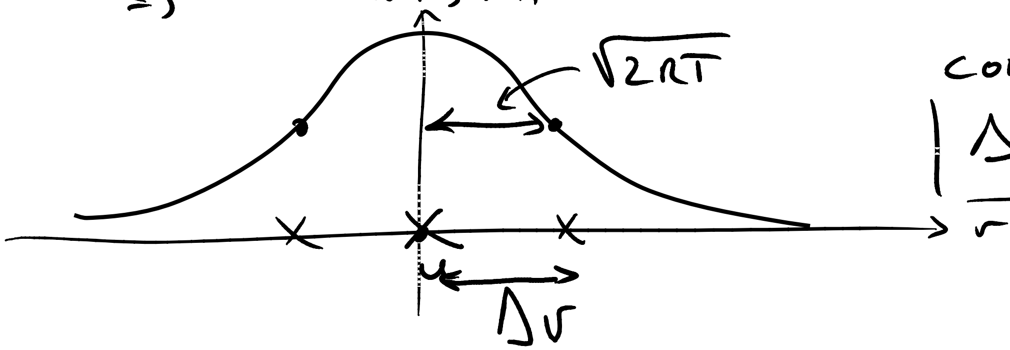
WE WANT ENOUGH POINTS TO REPRESENT f

↳ Δv MUST BE SMALL ENOUGH

WE WANT TO ESTIMATE THE "WIDTH" OF f

↳ ASSUME THAT f IS CLOSE TO $M[\rho, u, T]$

$\Rightarrow$ "WIDTH" $= 2\sqrt{2RT}$



CONSEQUENTLY:

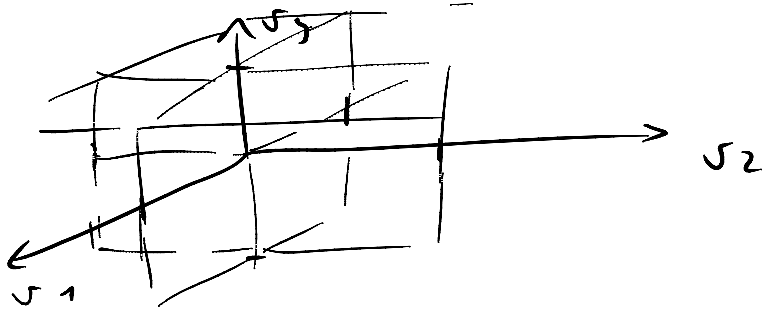
$$\boxed{\Delta v \leq \min_{t,x} \sqrt{2RT(t,x)}}$$

AGAIN, WE HAVE TO ESTIMATE A MINIMUM VALUE THAT DEPENDS ON THE MACROSCOPIC QUANTITIES

$$\boxed{\Delta v \leq \min_{t,x} \sqrt{2RT(t,x)}}$$

(USE INITIAL AND BOUNDARY DATA OR A FLUID SIMULATION)

EXERCISE: DO A SIMILAR ANALYSIS TO DEFINE SUITABLE BOUNDS AND STEPS TO REPLACE THE 3D - VELOCITY SPACE $\mathbb{R}^3$ BY A REGULAR CARTESIAN GRID



4.3 APPROXIMATION OF THE KINETIC EQUATION ON THE VELOCITY GRID

GRID $\mathbb{V} = \{ v_1, v_2, \dots, v_N \}$

↳ HOW TO APPROXIMATE

$$\underbrace{\partial_t \underbrace{f}_{(a)} + v \cdot \nabla_x f}_{(b)} = \underbrace{Q(f)}_{(c)} \quad \text{ON } \mathbb{V} \text{ ?}$$

(a) DISTRIBUTION FUNCTION :

EVERY FUNCTION φ OF v IS APPROXIMATED BY N VALUES

$$\phi = (\phi_1, \phi_2, \dots \phi_N)$$

WHERE $\phi_k \simeq \varphi(v_k)$

FOR f WE HAVE :

$$F(t,x) = \left(F_1(t,x), F_2(t,x), \dots, F_N(t,x)\right)$$

DISCRETE VELOCITY DISTRIBUTION FUNCTION

WHERE $F_k(t,x) \simeq f(t,x,v_k)$ $k = 1$ TO N

(b) TRANSPORT OPERATOR :

SIMPLE : $\left(\partial_t f + v \cdot \nabla_x f\right)(t,x,v)$

$\leadsto$ N VALUES :

$$\left(\partial_t F_k + v_k \cdot \nabla_x F_k\right)(t,x)$$

FOR $k = 1$ TO N

(c) COLLISION OPERATOR

$\hookrightarrow$ DIFFICULT : $Q(f)(t,x,v) \leadsto \left(Q_k(F)(t,x)\right)_{k=1}^{N}$

SEE NEXT SECTION

(d) MACROSCOPIC QUANTITIES

↳ HOW TO APPROXIMATE MOMENTS OF THE FORM

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} f(t,x,v)\, dv$$

ON THE GRID ?

↳ PROBLEM OF NUMERICAL INTEGRATION

↳ CHOOSE A QUADRATURE FORMULA TO APPROXIMATE INTEGRALS $\int_{\mathbb{R}^3} \varphi(v)\, dv$ ON THE GRID $\mathbb{V}$

$$\int_{\mathbb{R}} \varphi(v)\, dv \simeq \sum_{k=1}^{N} \varphi(v_k)\, \omega_k$$

WEIGHTS OF THE FORMULA.

THEN:

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} f(t,x,v)\, dv$$

$$\boxed{\simeq \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} F_k(t,x)\, \omega_k \quad \text{DENOTED BY} \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}}$$

EXERCISE: PROVE THAT WE STILL HAVE

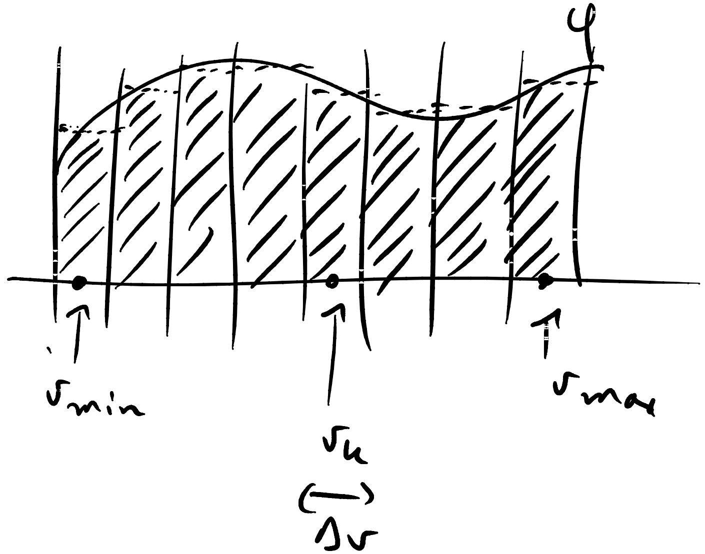
$$E = \frac{1}{2}\rho\|u\|^2 + \frac{3}{2}\rho R T$$

WHERE $\frac{3}{2}\rho R T = \sum_{k=1}^{N} \frac{1}{2}\|v_k - u\|^2 F_k\, \omega_k$

EXAMPLE: (1D CASE)

$$\mathbb{V} = \{ v_k = v_{min} + (k-1)\Delta v \quad k = 1 \text{ TO } N \}$$

USE THE MIDDLE POINT FORMULA:



$$\omega_k = \Delta v$$

$$\int_{\mathbb{R}} \varphi(v)\,dv \simeq \sum_{k=1}^{N} \varphi(v_k)\,\Delta v$$

FINALLY: DISCRETE-VELOCITY KINETIC EQUATION

$$\boxed{\partial_t F_k + v_k \cdot \nabla_x F_k = Q_k(F) \qquad k = 1 : N}$$

4.4 APPROXIMATION OF THE COLLISION OPERATOR (BGK)

WE WANT TO PRESERVE THE PROPERTIES

- $$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} Q(f)\, dv = 0 \qquad \text{(CONSERVATION)}$$

- $$\int_{\mathbb{R}^3} Q(f) \log f \, dv \leq 0 \qquad \text{(ENTROPY)}$$

THESE PROPERTY ARE VERY IMPORTANT TO DESIGN STABLE, ECONOMIC, ROBUST NUMERICAL METHODS.

EXAMPLE OF A NON-CONSERVATIVE APPROXIMATION

(1D CASE) $\mathbb{V} = \{ v_1, v_2, \ldots v_N \}$ (MIDDLE POINT FORMULA)

$$Q(f) = \frac{1}{2}\left(M[\rho, u, T] - f \right)$$

⚠

$$\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} = \int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ \frac{1}{2} v^2 \end{pmatrix} f \, dv \qquad E = \frac{1}{2}\rho u^2 + \frac{1}{2}\rho R T$$

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

CONS. PROPERTIES $\Leftrightarrow$ $\displaystyle\int \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} M[\rho, u, T] \, dv = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$

DEFINE: $\displaystyle Q_k(F_k) = \frac{1}{2}\left(M[\rho, u, T](v_k) - F_k \right)$

WHERE $\displaystyle \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} := \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2} v_k^2 \end{pmatrix} F_k \, \Delta v$

M IS APPROXIMATED BY ITS DISCRETE VALUES ON $\mathbb{V}$

THE DRAWBACK IS THAT

$$\underbrace{\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2} v_k^2 \end{pmatrix} Q_k(F)\, \Delta v}_{} \neq 0 \qquad \text{NO CONSERVATION}$$

BECAUSE

$$= \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2} v_k^2 \end{pmatrix} \frac{1}{2} \left(M[\rho,u,T](v_k) - F_k \right) \Delta v$$

$$= \frac{1}{2} \left(\sum_{k=1}^{N} \begin{pmatrix} \\ \\ \end{pmatrix} M[\rho,u,T](v_k)\, \Delta v - \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} \right)$$

$$= \frac{1}{2} \underbrace{\left(\sum_{k=1}^{N} \begin{pmatrix} \\ \\ \end{pmatrix} M[\rho,u,T](v_k)\, \Delta v - \int_{\mathbb{R}^3_v} \begin{pmatrix} 1 \\ v \\ \frac{1}{2} v^2 \end{pmatrix} M[\rho,u,T](v)\, dv \right)}_{\neq 0}$$

WE HAVE AN ERROR THAT DEPENDS ON

Δv AND ON v_{min}, v_{max}