5. BASIC NUMERICAL METHODS FOR DISCRETE VELOCITY KINETIC EQUATIONS

5.1 ONE DIMENSION CASE

- DISCRETE VELOCITY KIN. EQ:

$$\partial_t F_k + v_k \partial_x F_k = Q_k(F) = \frac{1}{\tau}\left(M_k[\rho,u,T] - F_k\right)$$

- FINITE DIFFERENCE APPROXIMATIONS:

$x \in \mathbb{R}$: DISCRETIZED WITH NODES $x_i = i\Delta x$
(i FROM $-\infty$ TO $+\infty$)

$t \geq 0$: ——— — DISCRETE TIMES $t_n = n\Delta t$
($n \geq 0$)

- $F_k(t_n, x_i) \simeq F^n_{ki}$ $\left(\simeq f(t_n, x_i, v_k)\right)$

- $\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}(t_n, x_i) \simeq \begin{pmatrix} \rho^n_i \\ \rho^n_i u^n_i \\ E^n_i \end{pmatrix} = \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2} v_k^2 \end{pmatrix} F^n_{ki}\, \omega_k$

NUMERICAL METHOD :

- BASED ON FINITE DIFFERENCE APPROXIMATION

- $1^{\underline{ST}}$ ORDER EXPLICIT TIME DISCRETIZATION
(BACKWARD EULER EXPLICIT SCHEME)

- $1^{\underline{ST}}$ ORDER UPWIND SCHEME IN SPACE
$\left(\forall a \in \mathbb{R} : \quad a^+ = \max(a,0) \quad a^- = \min(a,0) \right)$

NUMERICAL SCHEME : $\partial_t F_k + v_k . \partial_x F_k = \frac{1}{\tau} \left(M_k[\rho, u, T] - F_k \right)$

$$\boxed{\begin{gathered} \frac{F_{ki}^{n+1} - F_{ki}^{n}}{\Delta t} + v_k^+ \frac{F_{ki}^{n} - F_{ki-1}^{n}}{\Delta x} + v_k^- \frac{F_{ki+1}^{n} - F_{ki}^{n}}{\Delta x} = \frac{1}{\tau_i^n} \left(M_k[\rho_i^n, u_i^n, T_i^n] - F_{ki}^n \right) \\ k = 1 \text{ TO } N \\ i \in \mathbb{Z} \quad , \quad n \geq 0 \end{gathered}}$$

IF $\left(F_{ki}^{n}\right)_{k,i}$ THEN $\left(F_{ki}^{n+1}\right)_{ki}$ CAN BE COMPUTED

PROPERTIES OF THE SCHEME :

① IT PRESERVES THE POSITIVITY OF (F^n_{ki})

$$\left(F^n_{ki} \geq 0 \quad \forall k,i \quad \Rightarrow \quad F^{n+1}_{ki} \geq 0 \quad \forall k i \right)$$

UNDER A CONSTRAINT ON THE TIME STEP.

② IT IS CONSERVATIVE : WE HAVE DISCRETE CONSERVATION LAWS

③ IT IS STABLE.

↳ SEE NEXT SLIDE

1 ASSUME $F^n_{ki} \geq 0 \quad \forall k, i$

THEN:

$$F^{n+1}_{ki} = \underbrace{\left(1 - \frac{\Delta t}{\Delta x}|v_k| - \frac{\Delta t}{z^n_i}\right)}_{\geq 0 \text{ IF } \Delta t \left(\frac{|v_k|}{\Delta x} + \frac{1}{z^n_i}\right) \leq 1} \overbrace{F^n_{ki}}^{\geq 0} + \overbrace{\frac{\Delta t}{\Delta x} v_k^+ F^n_{k\,i-1}}^{\geq 0} \overbrace{- \frac{\Delta t}{\Delta x} v_k^- F^n_{k\,i+1}}^{\geq 0}$$

$$+ \underbrace{\frac{\Delta t}{z^n_i} M_k[\rho^n_i, u^n_i, T^n_i]}_{\geq 0}$$

THEREFORE: $F^{n+1}_{ki} \geq 0 \quad \forall k, i$ IF

$$\boxed{\Delta t \leq \frac{1}{\frac{v_{max}}{\Delta x} + \frac{1}{\min_i z^n_i}}}$$

CFL CONDITION

FINALLY: IF $F^0_{ki} \geq 0 \quad \forall k\, i$ THEN $F^n_{ki} \geq 0 \quad \forall k\, i\, n$

(IF CFL CONDITION IS SATISFIED AT EVERY n)

NOTE : THE CFL CONDITION IS RESTRICTIVE WHEN :

- v_{max} IS LARGE (HIGH SPEED FLOWS)
- z^n_i IS SMALL (DENSE GASES = CLOSE TO CONTINUOUS REGIMES ↳ SEE CHAPTER 6).

② DISCRETE CONSERVATION LAWS : TAKE $\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2} v_k^2 \end{pmatrix} (\,-\,)\, \omega_k$

$$\hookrightarrow \frac{1}{\Delta t} \begin{pmatrix} \rho_i^{n+1} - \rho_i^n \\ \rho_i^{n+1} u_i^{n+1} - \rho_i^n u_i^n \\ E_i^{n+1} - E_i^n \end{pmatrix} + \frac{1}{\Delta x} \left(\Phi^n_{i+\frac{1}{2}} - \Phi^n_{i-\frac{1}{2}} \right) = 0$$

CONSERVATION PROP. OF THE DISCRETE COLLISION OPERATOR.

WITH : $\boxed{\Phi^n_{i+\frac{1}{2}} = \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2} v_k^2 \end{pmatrix} \left(v_k^- F^n_{k\,i+1} + v_k^+ F^n_{k\,i} \right) \omega_k}$

NUMERICAL FLUX

GLOBAL CONSERVATION PROPERTIES :

EXAMPLE : TOTAL MASS $\mathcal{M}^n = \sum_{i=-\infty}^{+\infty} \rho^n_i \, \Delta x \quad \left(\simeq \int_{\mathbb{R}} \rho \, dx \right)$

↳ TAKE $\sum_{i=-\infty}^{+\infty}$ (CONSERVATION LAW OF ρ^n_i) Δx ⟶

$$\frac{\mathcal{M}^{n+1} - \mathcal{M}^n}{\Delta t} + \underbrace{\sum_{i=-\infty}^{+\infty} \left(\Phi^{n,1}_{i+\frac{1}{2}} - \Phi^{n,1}_{i-\frac{1}{2}} \right)}_{=0} = 0$$

$= 0$ SINCE EVERY TERM VANISHES !!

THEN . $\mathcal{M}^{n+1} = \mathcal{M}^n = \dots = \mathcal{M}^0$

CONSERVATION OF THE TOTAL MASS .

3 STABILITY :

$$\|F^n\| = \sum_{k,i} |F^n_{ki}| \, w_k \, \Delta x \qquad (\text{"NORM" OF } F^n = (F^n_{ki}))$$

UNDER THE CFL CONDITION : $\|F^n\| \leq \|F^0\|$

(THE NORM OF F^n IS CONTROLLED BY THE INITIAL DATA) = STABILITY

PROOF : CFL CONDITION $\Rightarrow$ $F^n_{ki} \geq 0$ (IF $F^0_{ki} \geq 0$) $\forall k, i$ (⊕)

$$\Rightarrow \|F^n\| = \sum_{k\,i} F^n_{ki} \, w_k \, \Delta x = \mathcal{M}^n$$

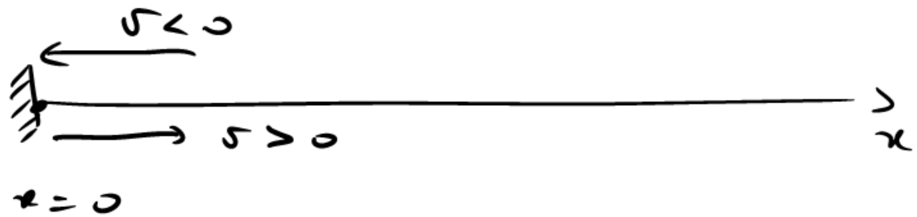
$$(C) \Rightarrow \mathcal{M}^n = \mathcal{M}^0 \left(= \|F^0\| \right)$$

THEN $\|F^n\| = \|F^0\|$.

5.2 NUMERICAL APPROXIMATION OF BOUNDARY COLLISIONS (1D)

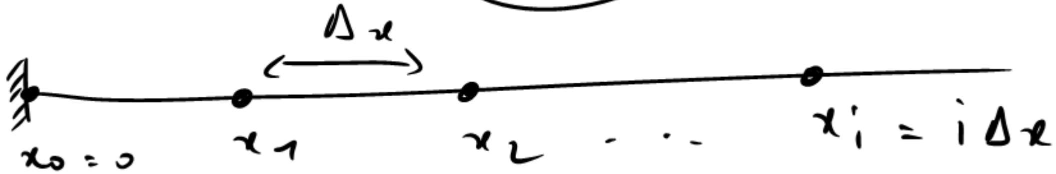
$$\partial_t f + v \partial_x f = Q(f) \rightsquigarrow \frac{F^{n+1}_{ki} - F^n_{ki}}{\Delta t} + v_k^+ \frac{F^n_{ki} - F^n_{ki-1}}{\Delta x} + v_k^- \frac{F^n_{ki+1} - F^n_{ki}}{\Delta x} = Q_k(F^n_i)$$

- ASSUME THAT WE HAVE A BOUNDARY AT $\underline{x = 0}$.
  (PROBLEM : $x \in [0, +\infty[$)
- SPECULAR REFLECTION :



$$f(t, x=0, \underset{v>0}{v}) = f(t, x=0, \underset{-v<0}{-v})$$

- NUMERICALLY :



↳ THE SCHEME IS DEFINED FOR $\underline{i \geq 0}$

IF (F^n_{ki}) IS KNOWN $\forall k = 1$ TO N, $\forall i \geq 0$ → COMPUTE (F^{n+1}_{ki}) $\forall k = 1$ TO N, $\forall i \geq 0$

PROBLEM : IF $i = 0$ → THE SCHEME

NEEDS $F^{n}_{k,-1}$ → NOT DEFINED

FOR $v_k > 0$ ONLY.

(FOR $v_k < 0$: EVERY TERM IS KNOWN ⇒ F^{n+1}_{k0} CAN BE DEFINED)

→ HOW TO COMPUTE F^{n+1}_{k0} FOR $v_k > 0$?

↳ WE CANNOT USE THE SCHEME.

↳ USE THE SPECULAR REFLECTION.

$F^{n+1}_{k0} = F^{n+1}_{k'0}$ (WHERE k' S.T $v_{k'} = -v_k$)

(FOR k S.T $v_k > 0$)

THEN : F^{n+1}_{ki} CAN BE DEFINED FOR EVERY k, i, n

EXERCISE: ① DO THE SAME ANALYSIS FOR THE DIFFUSE REFLECTION

② DO THE SAME FOR THE BOUNDARY VALUE PROBLEM $x \in [0,1]$ (TWO BOUNDARIES)

6. ASYMPTOTIC PRESERVING SCHEMES

- REMEMBER THAT WHEN $\varepsilon \to 0$ (DENSE GAS) (IN RESCALED VARIABLES) THE MACROSCOPIC QUANTITIES ARE SOLUTIONS OF THE EULER EQUATIONS (ASYMPTOTIC REGIME)

- WHAT DOES HAPPEND AT THE NUMERICAL LEVEL?

- USE RESCALED VARIABLES SUCH THAT THE SCHEME READS :

$$\left\{ \frac{F_{ki}^{n+1} - F_{ki}^{n}}{\Delta t} + v_k^{+} \frac{F_{ki}^{n} - F_{ki-1}^{n}}{\Delta x} + v_k^{-} \frac{F_{ki+1}^{n} - F_{ki}^{n}}{\Delta x} = \frac{1}{\varepsilon} \frac{1}{Z_i^n} \left(M_k(\rho_i^n, u_i^n, T_i^n) - F_{ki}^n \right) \right.$$

THE SCHEME IS STABLE IF

$$\Delta t \leq \frac{1}{\frac{v_{max}}{\Delta x} + \frac{1}{\min_i (\varepsilon Z_i^n)}} = O(\varepsilon) \text{ WHEN } \varepsilon \ll 1$$

– IN THE FLUID REGIME :

$$\varepsilon \to 0 \quad \Rightarrow \quad \Delta t \to 0$$

↳ THE SCHEME CANNOT BE USED

(TOO EXPENSIVE)

– IDEA OF ASYMPTOTIC PRESERVING SCHEMES (SHI JIN)
(A. P.)

→ SCHEME WHICH IS UNIFORMLY STABLE W.R.T. ε

(Δt SHOULD BE INDEPENDENT OF ε)

→ THE SCHEME OBTAINED AT THE LIMIT $\varepsilon = 0$ MUST BE CONSISTENT WITH THE ASYMPTOTIC LIMIT OF THE KINETIC EQUATION (EULER EQUATIONS).

↳ GENERAL IDEA : TIME IMPLICIT SCHEMES

(BECAUSE THESE SCHEMES ARE KNOWN TO BE FREE OF CFL CONDITION)

EXAMPLE 1 :

TAKE THE EXPLICIT SCHEME AND WE REPLACE

$$\frac{1}{\varepsilon z_i^n}\left(M(\rho_i^n, u_i^n, T_i^n] - F_{u\,i}^n\right)$$

BY

$$\frac{1}{\varepsilon z_i^n}\left(M(\rho_i^n, u_i^n, T_i^n) - F_{u\,i}^{n+1}\right)$$

↳ THE SCHEME READS :

$$\underbrace{\left(1 + \frac{\Delta t}{\varepsilon z_i^n}\right)}_{\geq 0} F_{u\,i}^{n+1} = \underbrace{\left(1 - \frac{\Delta t}{\Delta x}|v_u|\right)}_{\geq 0} F_{u\,i}^n + \overbrace{\frac{\Delta t}{\Delta x} v_u^+ F_{u\,i-1}^n - \frac{\Delta t}{\Delta x} v_u^- F_{u\,i+1}^n + \frac{\Delta t}{\varepsilon z_i^n} M(\rho_i^n, u_i^n, T_i^n]}^{\geq 0}$$

if $\boxed{\Delta t \leq \dfrac{1}{\frac{v_{max}}{\Delta x}}}$ CFL CONDITION DOES NOT DEPEND ON ε.

|| THE SCHEME IS UNIFORMLY STABLE W.R.T ε

BUT : THE LIMIT $\varepsilon \to 0$ IS NOT CORRECT

THE SCHEME READS :

$$F^{n+1}_{ki} = \frac{1}{1+\frac{\Delta t}{\varepsilon z^n_i}} \left(\left(1 - \frac{\Delta t}{\Delta x} |v_k|\right) F^n_{ki} + (\quad) - (\quad) \right)$$

$$\simeq O(\varepsilon) \to 0 \quad + \quad \frac{\Delta t / \varepsilon z^n_i}{1 + \Delta t / \varepsilon z^n_i} \xrightarrow[\varepsilon \to 0]{} 1 \quad M[\rho^n_i, u^n_i, T^n_i]$$

WHEN $\varepsilon \longrightarrow 0$:

$$F^{n+1}_{ki} \xrightarrow[\varepsilon \to 0]{} M[\rho^n_i, u^n_i, T^n_i]$$

FOR $\varepsilon = 0$.

$$F^{n+1} = M[\rho^n, u^n, T^n]$$

$$F^n = M[\rho^{n-1}, u^{n-1}, T^{n-1}]$$

ETC . . .

$F^n = F^0$ FOR EVERY n.

THE FLOW DOES NOT EVOLVE.

$\Rightarrow$ THIS SCHEME IS NOT A.P.

EXAMPLE 2 : EVALUATE M AT t_{n+1} :

$$\frac{1}{\varepsilon}\left(M_k[\rho,u,T] - F\right) \rightsquigarrow \frac{1}{\varepsilon^n_i}\left(M_k[\rho^{n+1}_i, u^{n+1}_i, T^{n+1}_i] - F^{n+1}_{ki}\right)$$

THEN :

(UNIFORMLY STABLE W.R.T ε)

$$\left[F^{n+1}_{ki} = \frac{1}{1+\frac{\Delta t}{\varepsilon \varepsilon^n_i}}\left(\quad\right) + \frac{\Delta t/\varepsilon\varepsilon^n_i}{1+\Delta t/\varepsilon\varepsilon^n_i} M_k[\rho^{n+1}_i, u^{n+1}_i, T^{n+1}_i] \right.$$

$$\varepsilon \to 0 \Rightarrow \boxed{F^{n+1}_{ki} = M_k[\rho^{n+1}_i, u^{n+1}_i, T^{n+1}_i]}$$

NO TIME SHIFT.

CORRECT LIMIT. (AS IN THE CONTINUS CASE)

THEN :

$$\Phi^n_{k\,i+\frac{1}{2}} \underset{(\varepsilon=0)}{=} \sum_{k=1}^{N} v_k \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}v_k^2 \end{pmatrix} M_k[\rho^n_i, u^n_i, T^n_i]$$

$$\Rightarrow \frac{1}{\Delta x}\left(\Phi^n_{k\,i+\frac{1}{2}} - \Phi^n_{k\,i-\frac{1}{2}}\right) \underset{(\varepsilon=0)}{\simeq} \int_{\mathbb{R}} v \begin{pmatrix} 1 \\ v \\ \frac{1}{2}v^2 \end{pmatrix} M[\rho,u,T]\, dv$$

EULER FLUXES

AT THE LIMIT $\varepsilon = 0$: (ρ^n_i, u^n_i, T^n_i) SATISFY

A DISCRETE APPROXIMATION OF THE EULER EQUATIONS

$\Rightarrow$ THE <u>SCHEME IS AP</u>

<u>PROBLEM</u>: NON-LINEAR IMPLICIT SCHEME

(F^{n+1} IS DIFFICULT TO BE COMPUTED

$\hookrightarrow$ EXPENSIVE)

EXAMPLE 3 : TIME SPLITTING SCHEME

(CORON - PERTHAME)

DECOMPOSE KINETIC EQ INTO TWO EQ. :

TRANSPORT STEP : SOLVE $\partial_t f + v \partial_x f = 0$
for $t \in [0, \Delta t]$

COLLISION STEP : SOLVE $\partial_t f = \frac{1}{\varepsilon^2} \left(M[\rho, u, T] - f \right)$
for $t \in [0, \Delta t]$

ρ, u, T ARE CONSTANT !!!

$\Rightarrow$ CAN BE SOLVED EXACTLY :

$$f(\Delta t, x, v) = e^{-\Delta t/\varepsilon^2} f(0, x, v) + \left(1 - e^{-\Delta t/\varepsilon^2}\right) M[\rho, u, T]$$

FINALLY THE SCHEME READS:

TRANSPORT STEP: $$\frac{f_{ki}^{n+\frac{1}{2}} - f_{ki}^{n}}{\Delta t} + v_k^{+} \frac{f_{ki}^{n} - f_{ki-1}^{n}}{\Delta x} + v_k^{-} \frac{f_{ki+1}^{n} - f_{ki}^{n}}{\Delta t} = 0$$

COLLISION STEP: $$f_{ki}^{n+1} = e^{-\frac{\Delta t}{\varepsilon z_i^n}} f_{ki}^{n+\frac{1}{2}} + \left(1 - e^{-\frac{\Delta t}{\varepsilon z_i^n}}\right) M\underbrace{\left[\rho_i^{n+1}, u_i^{n+1}, T_i^{n+1}\right]}_{=\left[\rho_i^{n+\frac{1}{2}}, u_i^{n+\frac{1}{2}}, T_i^{n+\frac{1}{2}}\right]}$$

EXERCISE: PROVE THAT THIS SCHEME IS

1. UNIFORMLY STABLE W.R.T ε
2. A.P.

HERE f_{ki}^{n+1} CAN BE COMPUTED EXPLICITELY.