SUMMARY OF LECTURE #4:

- BGK EQUATION: $\partial_t f + v \cdot \nabla_x f = Q(f)$

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

- DISCRETE VELOCITIES:

$v_k \in$ GRID $\mathbb{V}$ (N DISCRETE VELOCITIES)

- $f(t, x, v_k) \simeq F_k(t, x)$

$F(t,x) = (F_k(t,x))$ is A DISCRETE VELOCITY DISTRIBUTION FUNCTION

- $$\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} = \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} F_k(t,x)\, \omega_k$$

- DISCRETE VELOCITY APPROXIMATION OF BGK:

$$\left\| \quad \partial_t F_k + v_k \cdot \nabla_x F_k = Q_k(F) \right.$$

$$= \frac{1}{\tau}\Big(\underbrace{M[\rho, u, T]}_{\text{TO BE DEFINED}} - F_k\Big)$$

HOW TO DEFINE THE APPROXIMATION ($M_k[\rho,u,T]$) OF $M[\rho,u,T]$?

↳ CONSTRAINT: PRESERVE THE CONSERVATION PROPERTIES:

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

THAT ARE EQUIVALENT TO:

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

(WHICH IS <u>TRUE</u>)

↳ AT THE DISCRETE LEVEL, WE WANT:

$$\boxed{\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} M_k[\rho,u,T]\,\omega_k = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}}$$

("CONSERVATIVE APPROXIMATION")

BUT THE NATURAL APPROXIMATION:

$$M_k[\rho,u,T] = M[\rho,u,T](v_k) \quad \text{is } \underline{\text{NOT CONSERVATIVE}}$$

INDEED: $\displaystyle\sum_{k=1}^{N} M_k[\rho,u,T]\,\omega_k$

$$= \sum_{k=1}^{N} M[\rho,u,T](v_k)\,\omega_k$$

WHICH IS $\underline{\text{ONLY}}$ AN $\underline{\text{APPROXIMATION}}$ OF

$$\int_{\mathbb{R}^3} M[\rho,u,T](v)\,dv = \rho$$

THEREFORE: $\displaystyle\sum_{k=1}^{N} M[\rho,u,T](v_k)\,\omega_k \neq \rho$

CONSERVATIVE APPROXIMATION :

DEFINE PARAMETERS $\tilde{\rho}, \tilde{u}, \tilde{T}$ SUCH THAT

$$M_k[\rho,u,T] = M[\tilde{\rho},\tilde{u},\tilde{T}](v_k)$$

$$= \frac{\tilde{\rho}}{(2\pi\tilde{T})^{3/2}} \exp\left(-\frac{\|v_k-\tilde{u}\|^2}{2\tilde{T}}\right)$$

SATISFIES :

$$\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} M_k[\rho,u,T]\,\omega_k = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

CONSERVATION PROPERTIES
ARE ENFORCED

↳ MATHEMATICAL ANALYSIS : SEE
L. MIEUSSENS (M3AS , VOL. 8 (10) , 2000)

$$\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} M_k[\rho, u, T]\, \omega_k = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

"THERE EXISTS A DISCRETE DISTRIBUTION FUNCTION G S.T

$$\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} G_k\, \omega_k = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

AND $G_k > 0$

$$= \sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} M[\tilde{\rho}, \tilde{u}, \tilde{T}](v_k)\, \omega_k$$

THIS IS A NON-LINEAR SYSTEM OF 5 EQUATIONS AND 5 UNKNOWNS $(\tilde{\rho}, \tilde{u}, \tilde{T})$.

↳ THERE EXISTS A UNIQUE SOLUTION IF (ρ, u, T) SATISFY SOME CONSTRAINTS AND V

↳ HOW TO COMPUTE THIS SOLUTION?

⟶ NO EXPLICIT SOLUTION

⟶ NUMERICAL APPROXIMATION BY A NEWTON ALGORITHM

NON LINEAR SYSTEM: $\tilde{\rho}, \tilde{u}, \tilde{T}$ S.T

$$\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} M[\tilde{\rho}, \tilde{u}, \tilde{T}](v_k)\, \omega_k = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

LET $\vec{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$ ST. $M[\tilde{\rho}, \tilde{u}, \tilde{T}](v) = \exp(\vec{\alpha} \cdot \vec{m}(v))$

$\vec{m} = \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix}$

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

$$\Rightarrow \quad \alpha_1 = \log \frac{\tilde{\rho}}{(2\pi \tilde{T})^{3/2}} - \frac{\|u\|^2}{2T}$$

$$\left. \alpha_2 = \frac{u}{T} \qquad \alpha_3 = -\frac{1}{T} \right)$$

THE NON LINEAR SYSTEM FOR $\vec{\alpha}$ IS:

$$\sum_{k=1}^{N} \vec{m}(v_k) \exp(\vec{\alpha} \cdot \vec{m}(v_k))\, \omega_k = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

$$\Leftrightarrow \quad \boxed{\Phi(\vec{\alpha}) = 0}$$

EQUATION : $\Phi(\vec{\alpha}) = 0$

WHERE $$\Phi(\vec{\alpha}) = \sum_{k=1}^{N} \vec{m}(v_k) \exp(\vec{\alpha} \cdot \vec{m}(v_k)) \, w_k - \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}$$

NEWTON METHOD : - INITIAL GUESS $\vec{\alpha}_0$

- LINEARIZE Φ AROUND $\vec{\alpha}_0$:

$$\Phi(\vec{\alpha}) \simeq \Phi(\vec{\alpha}_0) + D\Phi(\vec{\alpha}_0) \cdot (\vec{\alpha} - \vec{\alpha}_0)$$

- $\vec{\alpha}_1$ IS SEEKED AS A ZERO OF THIS AFFINE MODEL : $\vec{\alpha}_1$ S.T

$$D\Phi(\vec{\alpha}_0) \cdot (\vec{\alpha}_1 - \vec{\alpha}_0) = - \Phi(\vec{\alpha}_0)$$ LINEAR SYSTEM 5 x 5

- ITERATE THIS : WE HAVE $\vec{\alpha}_p$, WE SOLVE

$$D\Phi(\vec{\alpha}_p) \cdot (\vec{\alpha}_{p+1} - \vec{\alpha}_p) = - \Phi(\vec{\alpha}_p)$$

UNTIL CONVERGENCE ($\| \Phi(\vec{\alpha}_p) \|$ IS SUFFICIENTLY SMALL)

INITIAL GUESS: $\vec{\alpha}_0$ TWO POSSIBILITIES

① $$\vec{\alpha}_0 = \left(\log \frac{\rho}{(2\pi T)^{3/2}} - \frac{\|u\|^2}{2T} , \frac{u}{T} , -\frac{1}{T} \right)$$

(THIS THE VALUE OF $\vec{\alpha}$ FOR A CONTINUOUS VELOCITY SPACE)

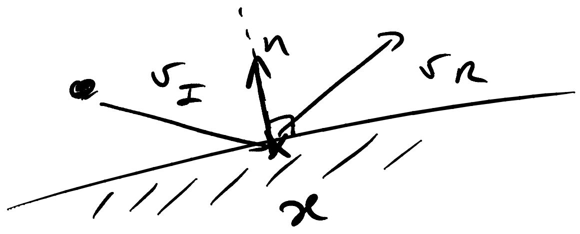
↳ WHEN WE HAVE A "NOT TOO SMALL" NUMBER OF VELOCITIES: GOOD APPROXIMATION

② $\vec{\alpha}_0 = \vec{\alpha}$ COMPUTED AT THE PREVIOUS TIME ITERATION

NEWTON ALG. CONVERGES VERY FAST

($\uparrow \leq 5$)

4.4 APPROXIMATION OF BOUNDARY COLLISIONS



v_R ST. $v_R \cdot n \geq 0$

$$f(t, x, v_R) = \mathcal{R}(f(t, x, \cdot)) \qquad (*)$$

RELATION IS S.T : ZERO MASS FLUX ACROSS THE SOLID BOUNDARY

$$\int_{\mathbb{R}^3} v \cdot n \; f(t, x, v)\, dv = 0 \qquad (**)$$

PROBLEM : HOW TO DISCRETIZE THE BOUNDARY CONDITION(*) SO AS TO PRESERVE (**) ?

4.4.1 DIFFUSE REFLECTION

$$f(t,x,v) = M[\sigma_w, u_w, T_w](v) \quad \text{FOR } v\cdot n \geq 0$$

WITH • u_w AND T_w ARE VELOCITY AND TEMPERATURE OF THE WALL

• σ_w IS DEFINED SO AS TO ENSURE (**):

$$\boxed{\sigma_w = -\frac{\left(\int_{v\cdot n\leq 0} (v\cdot n)\, f(t,x,v)\,dv\right)}{\left(\int_{v\cdot n\geq 0} (v\cdot n)\, M[1,u_w,T_w](v)\,dv\right)}}$$

AT THE DISCRETE LEVEL:

- LET M^W THE DISCRETE MAXWELLIAN S.T

$$\sum_{k=1}^{N} \begin{pmatrix} 1 \\ v_k \\ \frac{1}{2}\|v_k\|^2 \end{pmatrix} M_k^W \omega_k = \begin{pmatrix} 1 \\ u_w \\ E_w \end{pmatrix}$$

$$\left(E_w = \frac{1}{2}\|u_w\|^2 + \frac{3}{2} T_w \right)$$

(CONSERVATIVE APPROX. OF $M[1, u_w, T_w]$ ON THE GRID V)

THE DISCRETE BOUNDARY RELATION IS:

$$F_k(t,x) = \sigma_w M_k^W \quad \text{FOR } k \text{ ST } v_k \cdot n \geq 0$$

WHERE

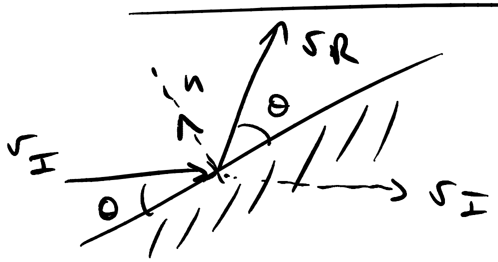
$$\sigma_w = - \frac{\sum_{k \cdot (v_k \cdot n \leq 0)} (v_k \cdot n) F_k \omega_k}{\sum_{k (v_k \cdot n \geq 0)} (v_k \cdot n) M_k^W \omega_k}$$

EXERCISE: PROVE THAT

$$\sum_{k=1}^{N} (v_k \cdot n) F_k(t,x) \omega_k = 0$$

(ZERO MASS FLUX ACROSS THE WALL IS PRESERVED)

4.4.2 SPECULAR REFECTION



SAME ANGLE FOR v_I AND v_R

$\Leftrightarrow \quad v_R = \text{Rotation}_{2\theta}(v_I)$

$\Leftrightarrow \quad v_I = \text{Rotation}_{-2\theta}(v_R)$

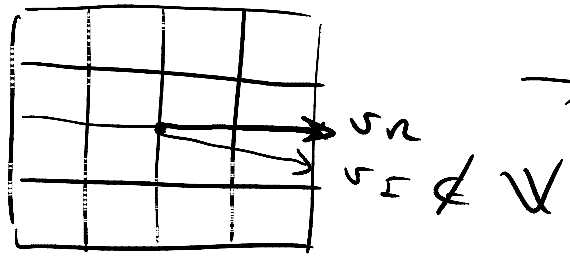
$$\boxed{f(t, x, v_R) = f(t, x, \text{Rotation}_{-2\theta}(v_R))}$$

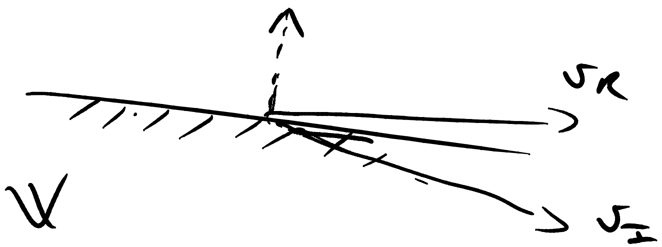
DISCRETE LEVEL: THE PROBLEM IS THAT

IF $v_R \in \mathcal{V}$ THERE IS NO REASON

FOR $v_I = \text{Rotation}_{-2\theta}(v_R) \in \mathcal{V}$

EXEMPLE (2D):

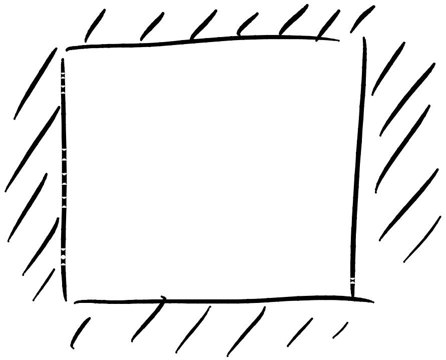




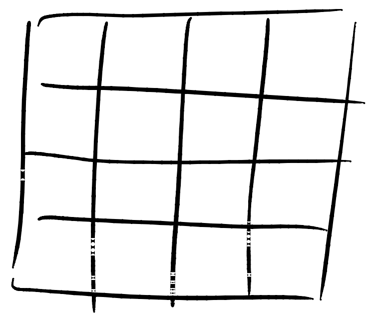
WE NEED SOME INTERPOLATION TO APPROXIMATE F AT $v_I \notin \mathbb{V}$

SO AS TO PRESERVE THE ZERO MASS FLUX CONDITION.

(EXCEPT IF THE GRID IS INVARIANT THROUGH THE ROTATION : EXAMPLE



PHYSICAL SPACE
(FOR x)



VELOCITY GRID $\mathbb{V}$

EXERCISE: PROVE THAT : FOR EVERY $v_K \in \mathbb{V}$, v_I IS NECESSARILY IN $\mathbb{V}$ TOO.)