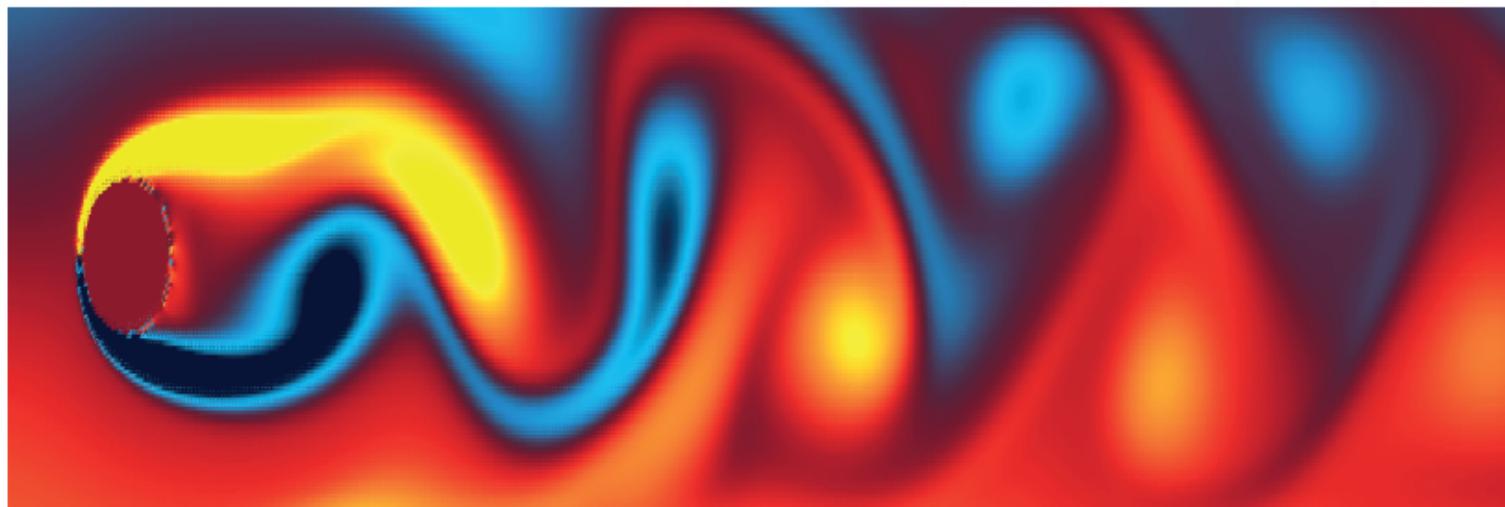


# **1er TALLER MÉTODOS DE LATTICE - BOLTZMANN**

11 al 15 de Diciembre de 2017



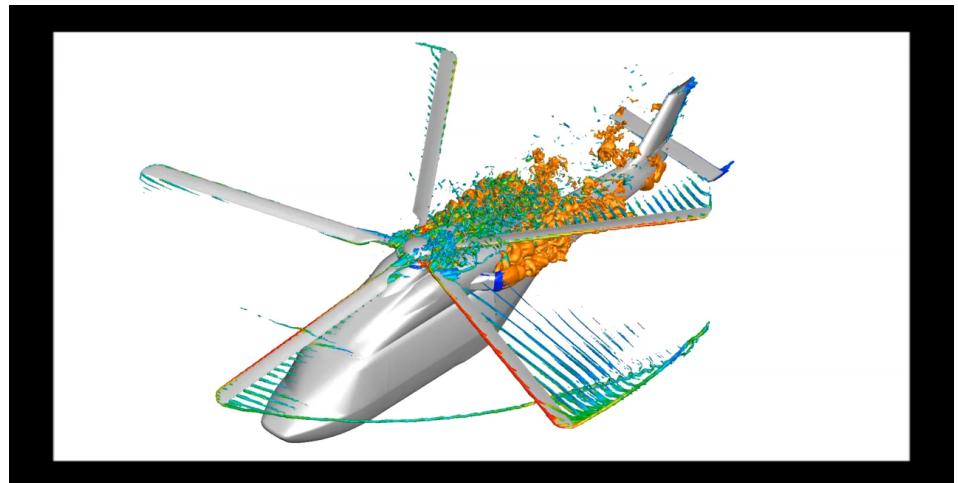
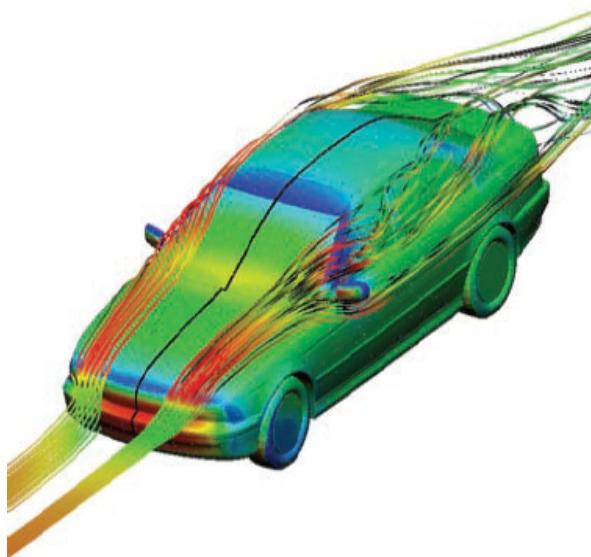
Por: Miller Mendoza Jiménez y Prof. José Daniel Muñoz Castaño

**ETH** zürich



# MOTIVACIÓN

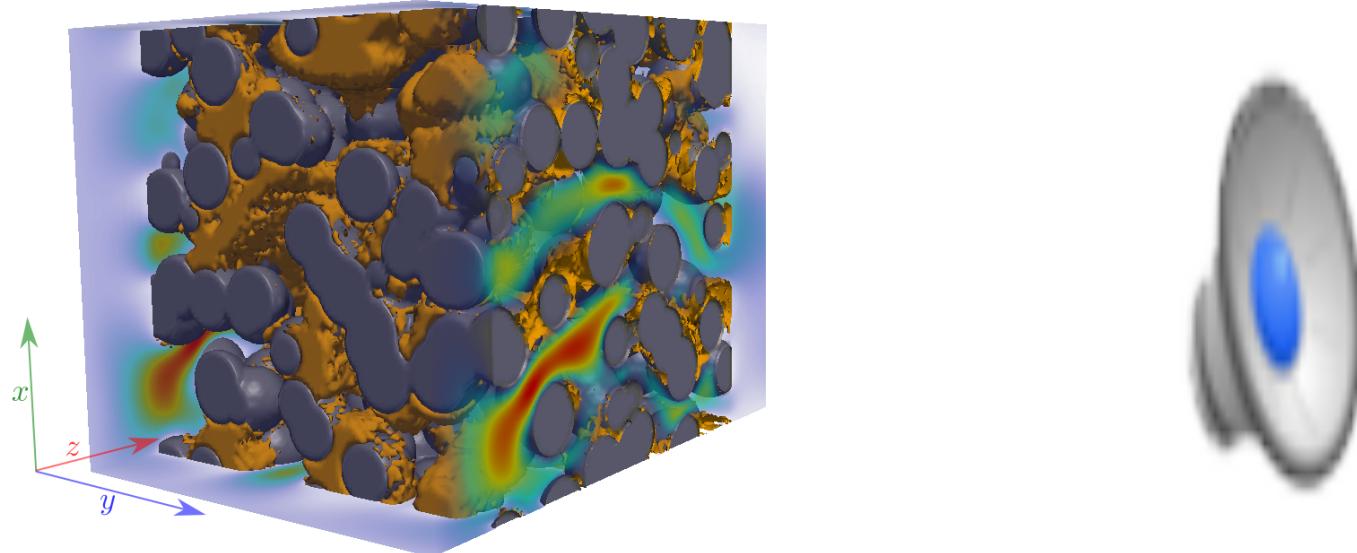
Lattice Boltzmann es un método numérico que se construyó principalmente para simular dinámica de fluidos y procesos difusivos. Sin embargo, hoy en día, las aplicaciones se han extendido a una gran variedad de sistemas físicos.



Chen, Hudong, et al. Science 301.5633 (2003): 633-636.  
<https://www.youtube.com/watch?v=8qWAdSOKIt0>

# MOTIVACIÓN

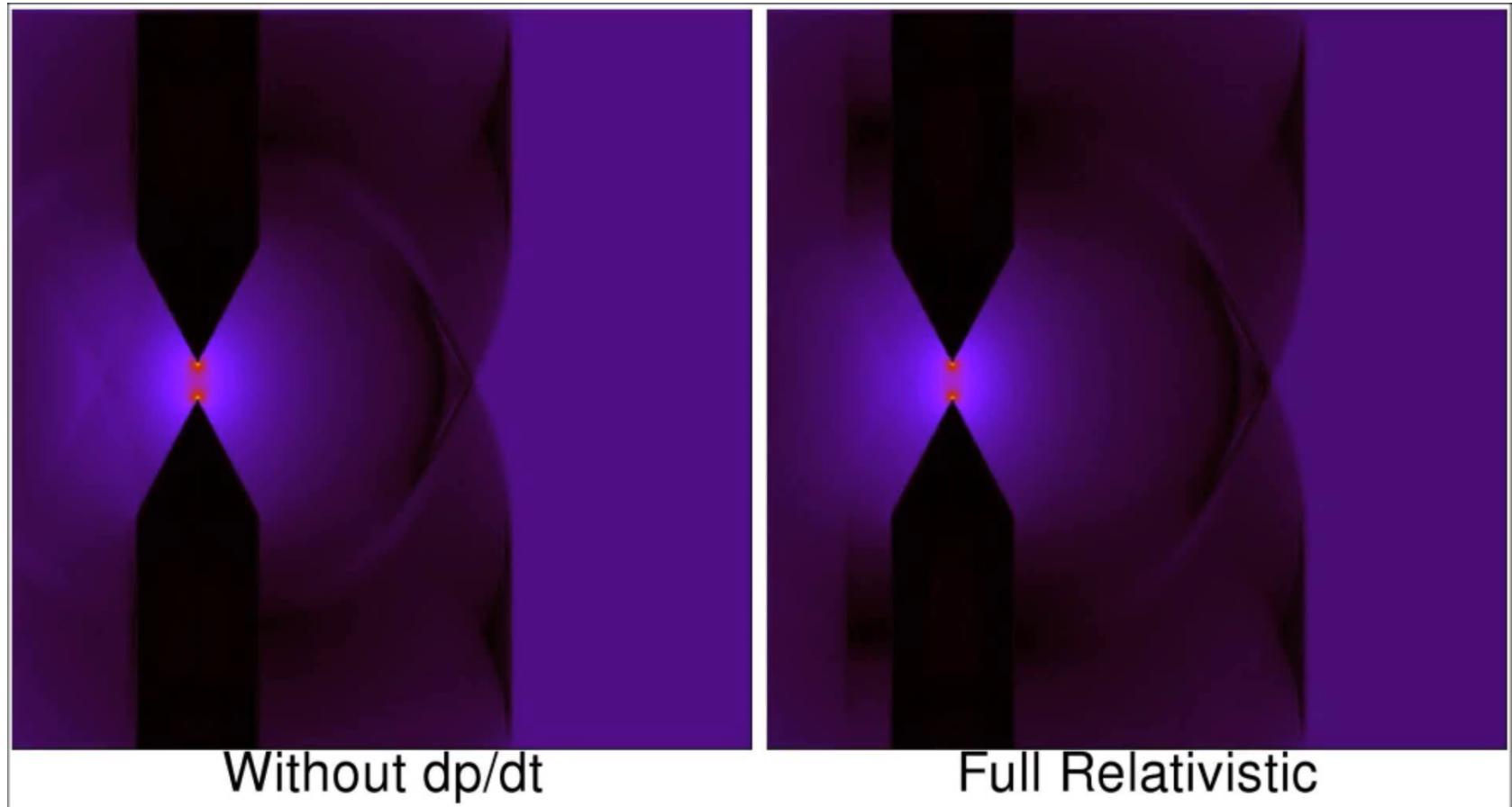
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Jäger, R. et al. Physical Review Letters 119.12 (2017): 124501.

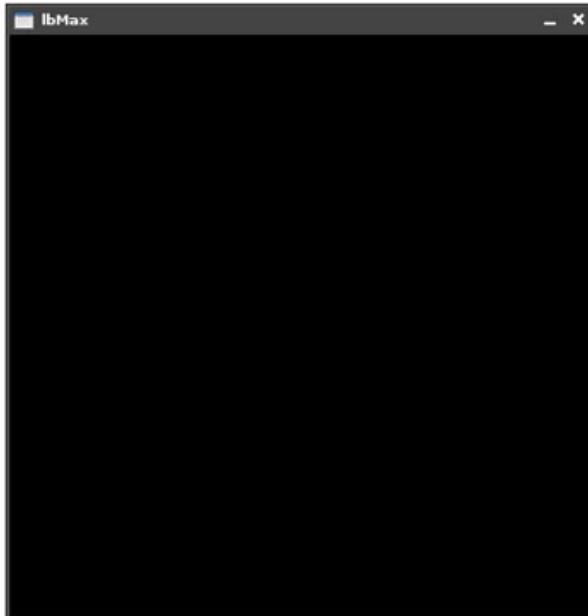
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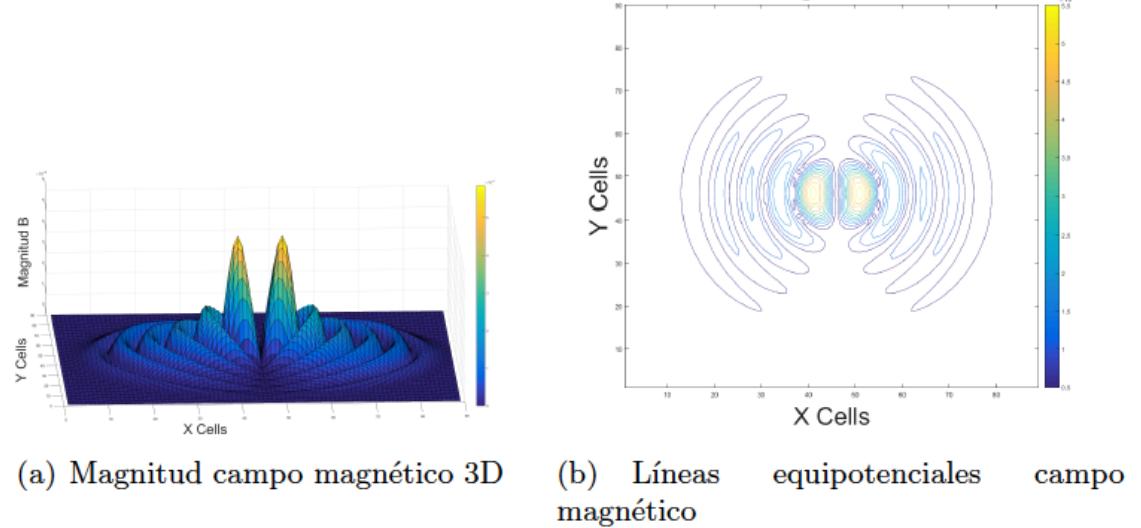


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Lattice Boltzmann es un método numérico que se construyó principalmente para simular dinámica de fluidos y procesos difusivos. Sin embargo, hoy en día, las aplicaciones se han extendido a una gran variedad de sistemas físicos.



(a) Magnitud campo magnético 3D



(b) Líneas equipotenciales campo magnético

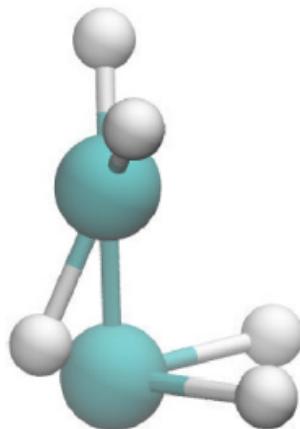
M. Mendoza, and J. D. Muñoz. Physical Review E 82.5 (2010): 056708.

Fabián Ricardo Vargas. Tesis de Maestría (2017). UNAL

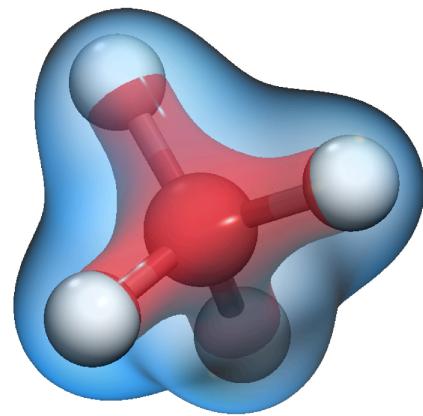
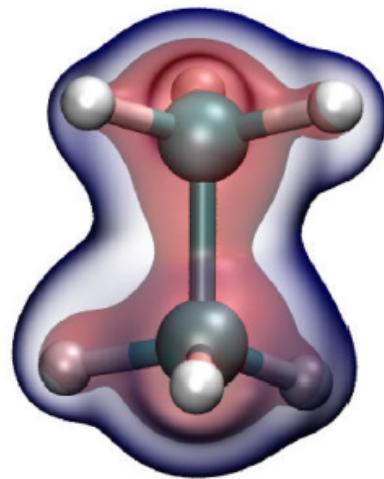
<https://www.youtube.com/watch?v=7WiHCS9jeGU>

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Molécula de etano



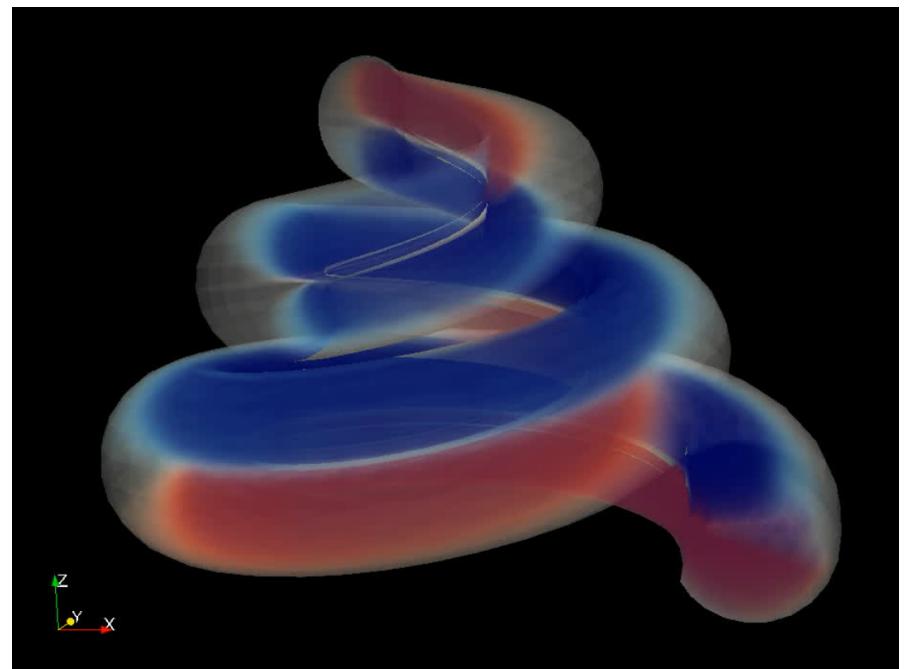
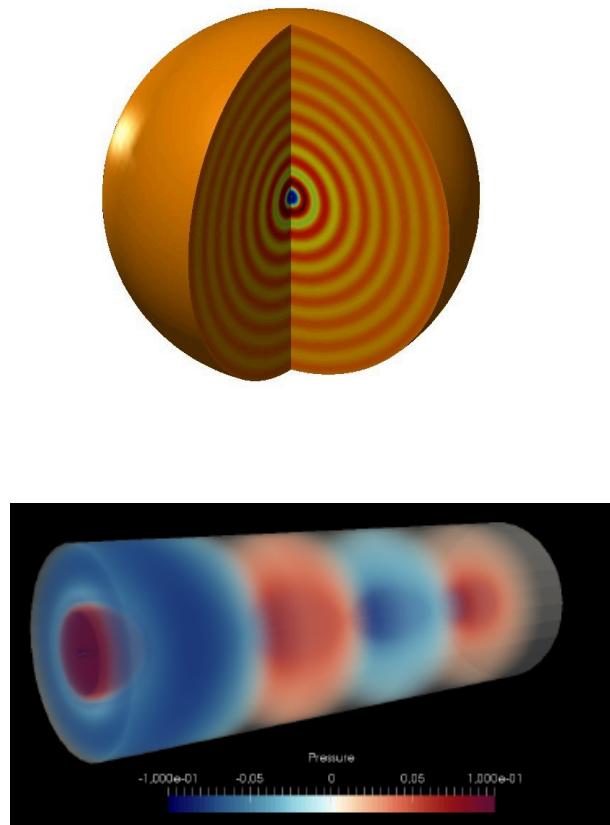
Molécula de metano

Solórzano, S. et al. Physical Review A 93.6 (2016): 062504.

Mendoza, M. et al. Physical review letters 113.9 (2014): 096402.

# MOTIVACIÓN

Lattice Boltzmann es un método numérico que se construyó principalmente para simular dinámica de fluidos y procesos difusivos. Sin embargo, hoy en día, las aplicaciones se han extendido a una gran variedad de sistemas físicos.



# POR QUÉ UTILIZAR LATTICE BOLTZMANN?

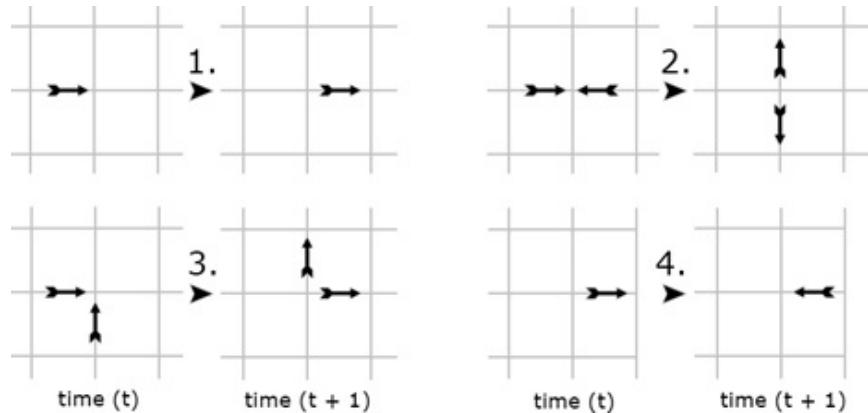
1. Se basa en teoría cinética de gases, es decir, resuelve sistemas a escala mesoscópica. Por ejemplo, en caso de fluidos, posee mas información que las ecuaciones de Navier Stokes, pero menos que dinámica molecular.
2. Ecuaciones diferenciales no-lineales pueden ser simuladas con una ecuación lineal, la ecuación de Lattice Boltzmann.
3. La propagación de la información es lineal y exacta a través del enmallado. O sea, no hay difusividad numérica.
4. Debido a que la mayoría de las operaciones son locales, es muy eficiente cuando es paralelizado en CPUs y GPUs.



**Sistemas complejos pueden ser estudiados de forma eficiente y precisa,  
sin tantos recursos computacionales.**

# HISTORIA DEL MODELO DE LATTICE BOLTZMANN

## Lattice Gas Autómata (HPP)

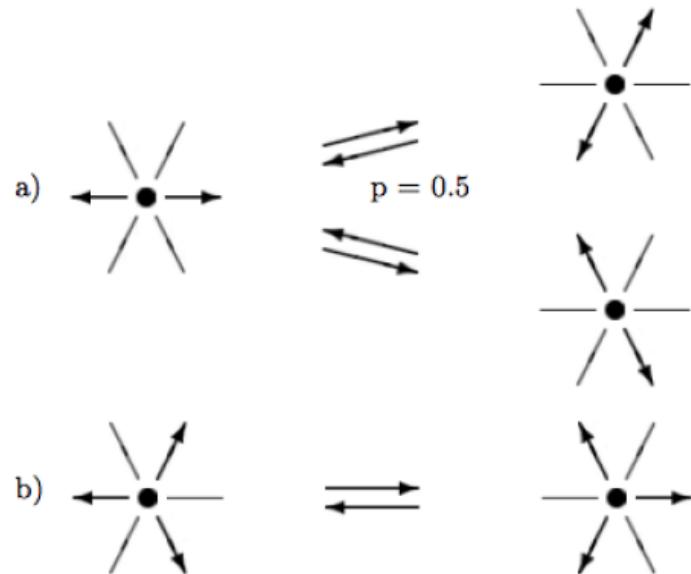


J. Hardy, Y. Pomeau, and O. de Pazzis. Molecular Dynamics of a classical lattice gas: Transport properties and time correlation functions. Phys. Rev. A, 13:1949-60, (1976).

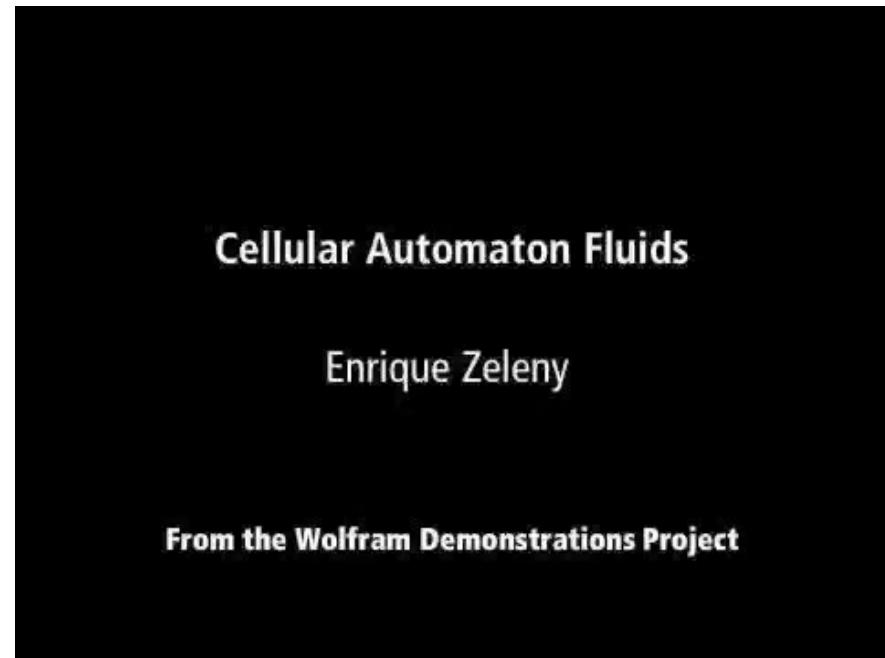
El modelo no es invariante ante rotaciones, siempre conserva el momento en cada una de las direcciones, y no cumple las ecuaciones de Navier-Stokes.

# HISTORIA DEL MODELO DE LATTICE BOLTZMANN

Lattice Gas Autómata (FHP)



U. Frisch, B. Hasslacher, and Y Pomeau. Lattice-gas automata for the Navier-Stokes equation. Phys. Rev. Lett., 56:1505 (1986).



Este modelo reproduce las ecuaciones de Navier-Stokes. Las poblaciones en cada nodo son binarias, y pueden generar ruido estadístico al calcular los campos macroscópicos. Las reglas de colisión se pueden volver más complejas al extender a 3D.

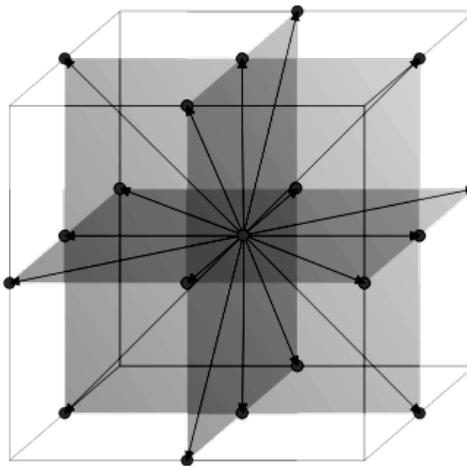
# HISTORIA DEL MODELO DE LATTICE BOLTZMANN

## Lattice Gas Autómata (FHP)

$$\begin{aligned} N_0(t + \tau, r) - N_0 = & - N_0 [((N_1 \bar{N}_2 + N_2 \bar{N}_1) \bar{N}_3 + N_3 \bar{N}_1 \bar{N}_2) \bar{N}_4 \bar{N}_5 \bar{N}_6 \\ & + \bar{N}_1 \bar{N}_2 \bar{N}_3 ((N_4 \bar{N}_5 + N_5 \bar{N}_4) \bar{N}_6 + N_6 \bar{N}_4 \bar{N}_5)] \\ & + [(N_1 N_3 \bar{N}_2 \bar{N}_4 + N_2 N_4 \bar{N}_1 \bar{N}_3) \bar{N}_5 \bar{N}_6 \\ & + (N_3 N_5 \bar{N}_4 \bar{N}_6 + N_4 N_6 \bar{N}_3 \bar{N}_5) \bar{N}_1 \bar{N}_2 \\ & + (N_1 N_5 \bar{N}_2 \bar{N}_6 + N_2 N_6 \bar{N}_1 \bar{N}_5) \bar{N}_3 \bar{N}_4] (\bar{N}_0 - N_0) \\ & + \frac{1}{2} [N_6 \bar{N}_2 (N_1 N_4 \bar{N}_3 \bar{N}_5 + N_3 N_5 \bar{N}_1 \bar{N}_4) \\ & + N_4 \bar{N}_6 (N_2 N_5 \bar{N}_1 \bar{N}_3 + N_1 N_3 \bar{N}_2 \bar{N}_5) \\ & + N_2 \bar{N}_4 (N_3 N_6 \bar{N}_1 \bar{N}_5 + N_1 N_5 \bar{N}_3 \bar{N}_6)] (\bar{N}_0 - N_0) \\ & + \frac{1}{2} [N_1 \bar{N}_5 (N_2 N_4 \bar{N}_3 \bar{N}_6 + N_3 N_6 \bar{N}_2 \bar{N}_4) \\ & + N_5 \bar{N}_3 (N_2 N_6 \bar{N}_1 \bar{N}_4 + N_1 N_4 \bar{N}_2 \bar{N}_6) \\ & + N_3 \bar{N}_1 (N_4 N_6 \bar{N}_2 \bar{N}_5 + N_2 N_5 \bar{N}_4 \bar{N}_6)] (\bar{N}_0 - N_0) \\ & + [N_4 (N_5 (N_2 N_6 \bar{N}_1 \bar{N}_3 + N_1 N_3 \bar{N}_2 \bar{N}_6) \\ & + N_2 N_3 N_6 \bar{N}_1 \bar{N}_5) + N_1 (N_2 (N_3 N_5 \bar{N}_4 \bar{N}_6 \\ & + N_4 N_6 \bar{N}_3 \bar{N}_5) + N_3 N_5 N_6 \bar{N}_2 \bar{N}_4)] (\bar{N}_0 - N_0) \end{aligned}$$

Regla de colisión para reproducir las ecuaciones de Navier-Stokes, FHP-III

# HISTORIA DEL MODELO DE LATTICE BOLTZMANN



Modelo de Lattice Boltzmann

$$N_i(\vec{x}, t) \rightarrow f_i(\vec{x}, t)$$

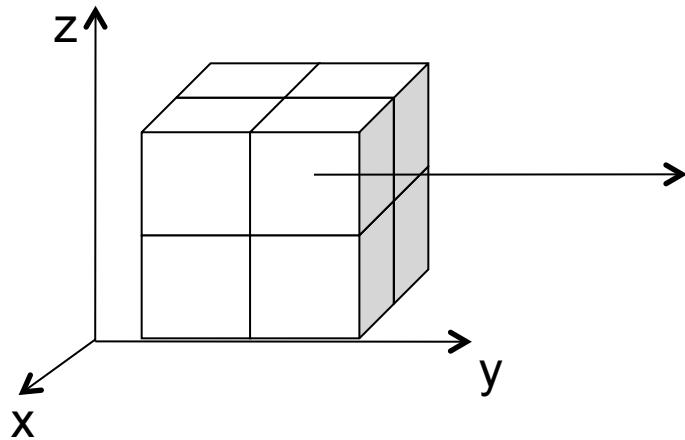
Valores = 0,1

Valores = Reales

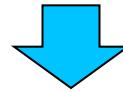
# HISTORIA DEL MODELO DE LATTICE BOLTZMANN

Modelo de Lattice Boltzmann

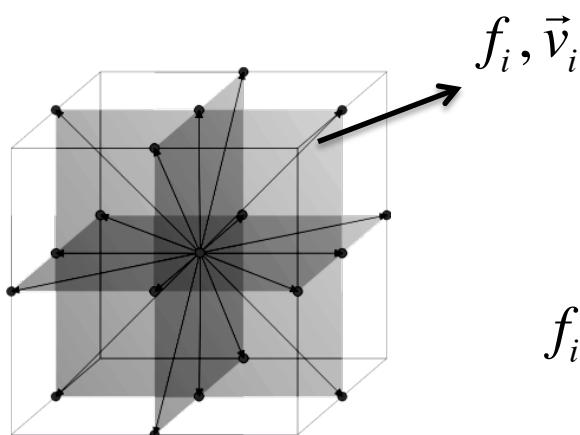
$\delta t$ : Paso de tiempo  
 $\tau$ : Tiempo de relajación



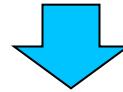
$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = \Omega_i(\vec{x}, t)$$



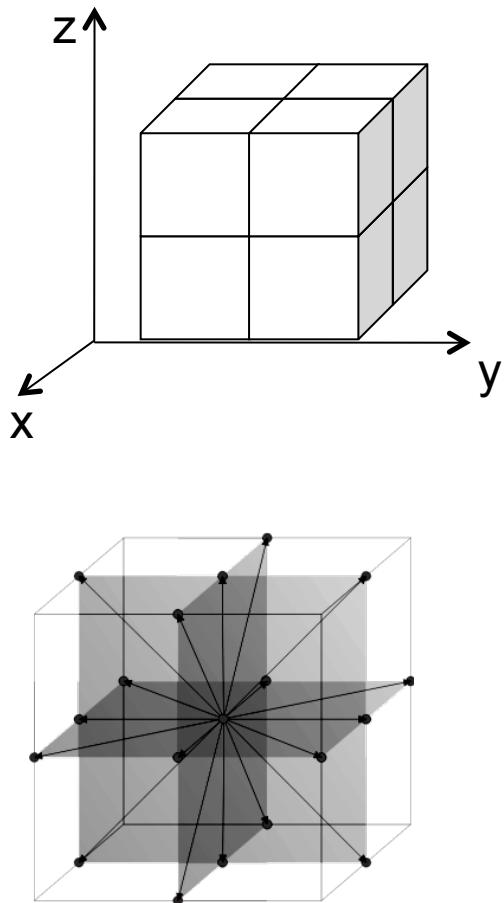
Colisión de Bhatnagar-Gross-Krook (BGK)



$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]$$



# MODELO DE LATTICE BOLTZMANN

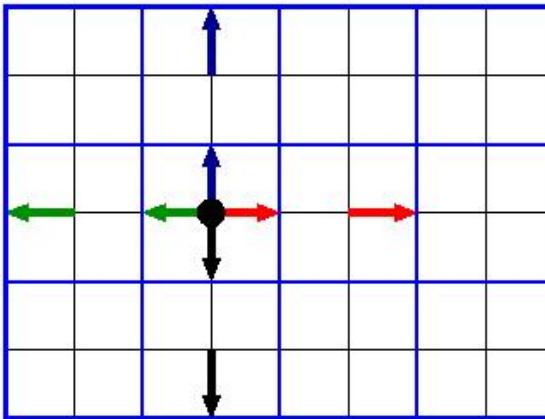


Colisión:

$$f_i^*(\vec{x}, t + \delta t) = f_i(\vec{x}, t) - \frac{1}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]$$

Transporte:

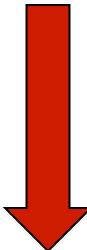
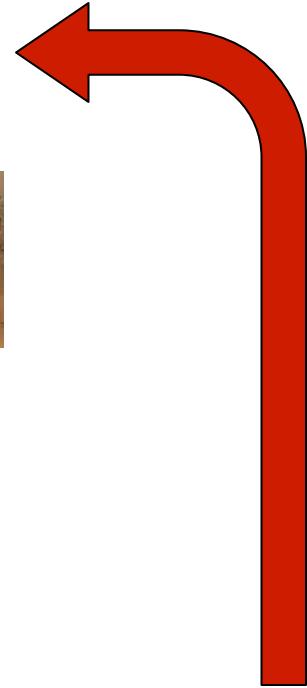
$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) = f_i^*(\vec{x}, t)$$



Operación exacta!!

# MODELO DE LATTICE BOLTZMANN

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]$$

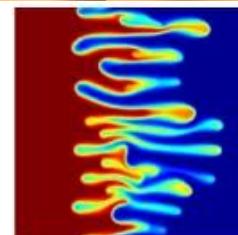


Variables macroscópicas

$$\rho = \sum_i f_i$$

$$\rho \vec{u} = \sum_i f_i \vec{v}_i$$

$$\pi_{\alpha\beta} = \sum_i f_i v_{i\alpha} v_{i\beta}$$



Distribución de equilibrio

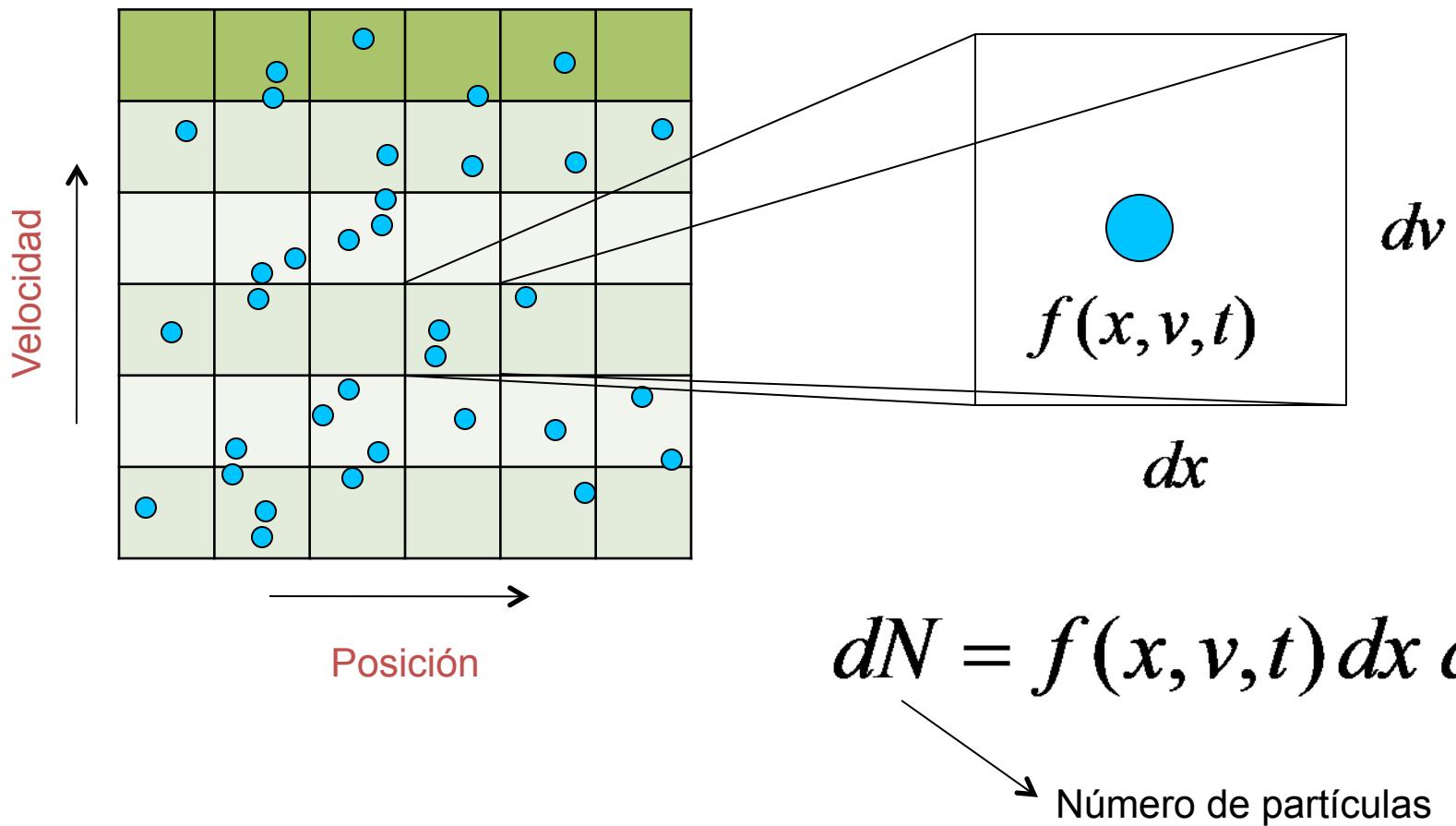
$$f_i^{eq}(x, t) = \rho \omega_i \left[ 1 + \frac{3(\vec{v}_i \cdot \vec{u})}{c_s^2} + \frac{(\vec{v}_i \cdot \vec{u})^2}{2c_s^4} - \frac{(\vec{u} \cdot \vec{u})}{2c_s^2} \right]$$

# DESARROLLO TEÓRICO

Teoría cinética de gases:

He, X., & Luo, L. S. (1997). Physical Review E, 56(6), 6811.

## Espacio de fase



# ECUACIÓN DE BOLTZMANN

Evolución de la función de distribución:

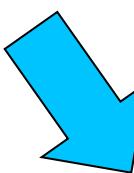
$$\frac{\partial f}{\partial t} + \vec{v}' \cdot \nabla f + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}'} f = \Omega(f)$$

Función de distribución

Velocidad microscópica

Fuerzas externas

Masa de las partículas





En equilibrio termodinámico, la solución de la ecuación de Boltzmann esta dada por la distribución de Maxwell-Boltzmann:

$$f = f^{eq}(\vec{x}, \vec{v}', t) = A e^{-\frac{m (\vec{u} - \vec{v}')^2}{kT}}$$

# ECUACIÓN DE BOLTZMANN

Las ecuaciones macroscópicas se pueden derivar de la ecuación de Boltzmann usando sus momentos:

Teoría cinética:

$$\frac{\partial f}{\partial t} + \vec{v}^! \cdot \nabla f + \frac{\vec{F}}{m} \cdot \nabla_{v^!} f = \Omega(f)$$

$$\rho = \int f d^3v$$

$$\rho \vec{u} = \int f \vec{v} d^3v$$

$$\Pi_{\alpha\beta} = \int f v_\alpha v_\beta d^3v$$

Hidrodinámica

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\frac{\partial(\rho u_i)}{\partial t} + \partial_j (\rho u_i u_j + P \delta_{ij}) = 0$$

$$\eta = \rho T \tau \quad \text{Viscosidad dinámica}$$

Momentos de la distribución

# MODELO DE LATTICE BOLTZMANN: 3 PASOS

1

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \Omega(f, f^{eq}) = -\frac{1}{\tau}(f - f^{eq})$$

Aproximación BGK

$$\rho = \int f d^3v = \int f^{eq} d^3v, \quad \rho \vec{u} = \int f \vec{v} d^3v = \int f^{eq} \vec{v} d^3v$$

2

$$f(\vec{x} + \vec{v}\delta t, \vec{v}, t + \delta t) - f(\vec{x}, \vec{v}, t) = -\frac{\delta t}{\tau}(f - f^{eq})$$

Integración en tiempo

Todavia tenemos 6+1 dimensiones

# MODELO DE LATTICE BOLTZMANN: 3 PASOS

3

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$

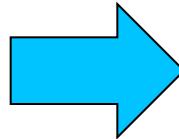
Discretización de velocidades

Tenemos que recuperar los momentos de la distribución:

$$f^{eq} = A e^{-m(\vec{u} - \vec{v})^2 / 2kT}$$

$$\rho = \int f^{eq} d^3 v \neq \sum_i f^{eq}(v_i)$$

$$\rho \vec{u} = \int f^{eq} \vec{v} d^3 v \neq \sum_i f^{eq}(v_i) \vec{v}_i$$



Al usar un pequeño  
numero de velocidades  
perdemos simetrias.

$$\Pi_{\alpha\beta} = \int f^{eq} v_\alpha v_\beta d^3 v \neq \sum_i f^{eq}(v_i) v_{i\alpha} v_{i\beta}$$

# MODELO DE LATTICE BOLTZMANN: 3 PASOS

Pero podemos usar cuadraturas:

$$f^{eq} = A e^{-m(\vec{u}-\vec{v})^2/2kT} = e^{-\vec{v}^2/2c_s^2} \sum_{n=0} \frac{1}{n!} a_n^{(n)}(\vec{x}, \vec{u}, t) H_n^{(n)}(\vec{v})$$

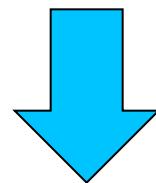
$\uparrow$

$$a_n^{(n)}(\vec{x}, \vec{u}, t) = \int f^{eq} H_n^{(n)}(\vec{v}) d^3v$$

Polinomios

---

$$a_0^{(0)}(\vec{x}, \vec{u}, t) \rightarrow \rho \quad a_1^{(1)}(\vec{x}, \vec{u}, t) \rightarrow \rho \vec{u} \quad a_2^{(2)}(\vec{x}, \vec{u}, t) \rightarrow \Pi_{\alpha\beta} \dots$$



Depende del numero de momentos a reproducir

$$\int e^{-\vec{v}^2/2c_s^2} H_m^{(m)}(\vec{v}) H_n^{(n)}(\vec{v}) d^3v = \sum_{i=0}^N \omega_i H_m^{(m)}(\vec{v}_i) H_n^{(n)}(\vec{v}_i)$$

# MODELO DE LATTICE BOLTZMANN: 3 PASOS

3

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$

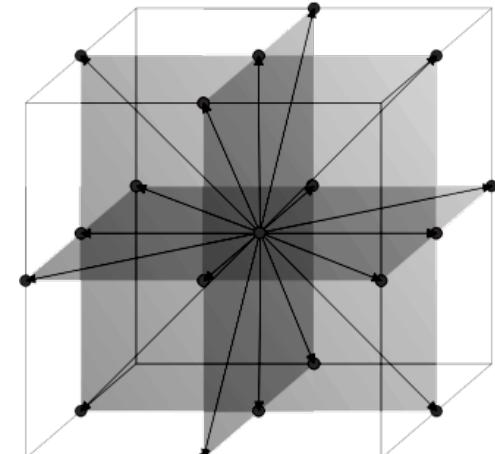
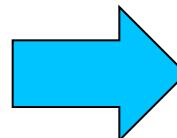
Discretización de velocidades

Ahora los momentos se recuperan de forma exacta:

$$\rho = \int f d^3v = \sum_{i=0}^N f_i$$

$$\rho \vec{u} = \int f \vec{v} d^3v = \sum_{i=0}^N f_i \vec{v}_i$$

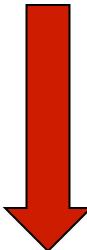
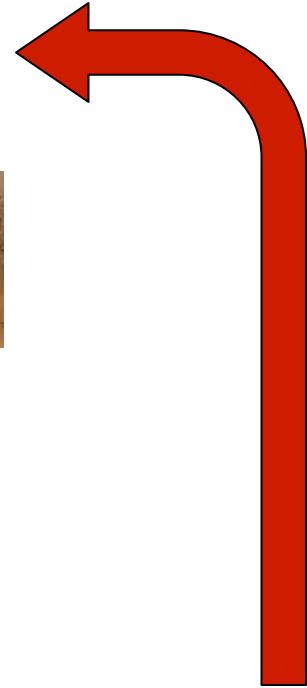
$$\Pi_{\alpha\beta} = \int f v_\alpha v_\beta d^3v = \sum_{i=0}^N f_i v_{i\alpha} v_{i\beta}$$



D3Q19

# MODELO DE LATTICE BOLTZMANN

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]$$

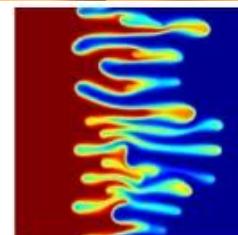


Variables macroscópicas

$$\rho = \sum_i f_i$$

$$\rho \vec{u} = \sum_i f_i \vec{v}_i$$

$$\pi_{\alpha\beta} = \sum_i f_i v_{i\alpha} v_{i\beta}$$



Distribución de equilibrio

$$f_i^{eq}(x, t) = \rho \omega_i \left[ 1 + \frac{3(\vec{v}_i \cdot \vec{u})}{c_s^2} + \frac{(\vec{v}_i \cdot \vec{u})^2}{2c_s^4} - \frac{(\vec{u} \cdot \vec{u})}{2c_s^2} \right]$$

# ALTERNATIVA A CHAPMANN-ENSKOG

Podemos derivar las ecuaciones macroscópicas por recurrencia:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \Omega(f, f^{eq}) = -\frac{1}{\tau}(f - f^{eq})$$



$$f = f^{eq} - \tau \left[ \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f \right]$$



$$\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} - \tau \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f = -\frac{1}{\tau}(f - f^{eq})$$

# ALTERNATIVA A CHAPMANN-ENSKOG

Podemos derivar las ecuaciones macroscópicas por recurrencia:

$$\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} - \tau \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f = -\frac{1}{\tau} (f - f^{eq})$$



$$f = f^{eq} - \tau \left[ \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f \right]$$



$$\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} - \tau \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f^{eq} + \tau^2 \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^3 f = -\frac{1}{\tau} (f - f^{eq})$$

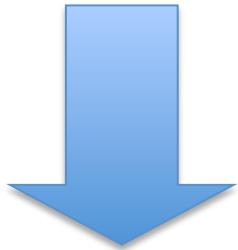
# ALTERNATIVA A CHAPMANN-ENSKOG

Conexión con el número de Knudsen y la expansión de Chapman-Enskog

$$\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} - \tau \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f^{eq} + \tau^2 \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^3 f = -\frac{1}{\tau} (f - f^{eq})$$



$$\frac{1}{t_0} \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)} f^{eq} - \frac{\tau}{t_0^2} \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2} f^{eq} + \frac{\tau^2}{t_0^3} \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^3} f = -\frac{1}{\tau} (f - f^{eq})$$



$$Kn \approx \left( \frac{\tau}{t_0} \right) \approx \left( \frac{\lambda_{mfp}}{L} \right)$$

$$\overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)} f^{eq} - \left( \frac{\tau}{t_0} \right) \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2} f^{eq} + \left( \frac{\tau}{t_0} \right)^2 \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^3} f = -\frac{t_0}{\tau} (f - f^{eq})$$

# ALTERNATIVA A CHAPMANN-ENSKOG

Conexión con el número de Knudsen y la expansión de Chapman-Enskog

$$\overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)} f^{eq} - \textcolor{red}{Kn} \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)}^2 f^{eq} + \textcolor{red}{Kn}^2 \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)}^3 f = -\frac{1}{Kn} (f - f^{eq})$$



$$\overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)} \left[ f^{eq} - \textcolor{red}{Kn} \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)} f^{eq} + \textcolor{red}{Kn}^2 \overline{\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)}^2 f^{eq} + \dots \right] = -\frac{1}{Kn} (f - f^{eq})$$

$f^{(1)}$                        $f^{(2)}$

$$Kn \approx \left( \frac{\tau}{t_0} \right) \approx \left( \frac{\lambda_{mfp}}{L} \right)$$

# ALTERNATIVA A CHAPMANN-ENSKOG

$$\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} - \tau \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f^{eq} + \tau^2 \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^3 f = -\frac{1}{\tau} (f - f^{eq})$$

Ejemplo: Ecuación de convección-difusión

$$\int -\frac{1}{\tau} (f - f^{eq}) d^3 v = 0 \quad \Rightarrow \quad \int f d^3 v = \int f^{eq} d^3 v = \Phi$$

$$\int \rightarrow \quad \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} - \tau \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f^{eq} = -\frac{1}{\tau} (f - f^{eq})$$



$$\frac{\partial \Phi}{\partial t} + \nabla \cdot (\Phi \vec{u}) - \tau \nabla \cdot (\nabla \cdot \Pi) = 0$$

$$\int f^{eq} \vec{v} d^3 v = \Phi \vec{u}$$

$$\frac{\partial \Phi}{\partial t} + \nabla \cdot (\Phi \vec{u}) - \tau c_s^2 \nabla^2 \Phi = 0$$

$$\int f^{eq} \vec{v} \vec{v} d^3 v = \Pi = c_s^2 \Phi \mathbf{1}$$

# ALTERNATIVA A CHAPMANN-ENSKOG

Caso para la ecuación de Lattice Boltzmann:

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$



$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^n f = -\frac{\delta t}{\tau} (f - f^{eq})$$



$$f = f^{eq} - \tau \sum_{n=1}^{\infty} \frac{\delta t^{n-1}}{n!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^n f$$

# ALTERNATIVA A CHAPMANN-ENSKOG

Caso para la ecuación de Lattice Boltzmann:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^n \left[ f^{eq} - \tau \sum_{m=1}^{\infty} \frac{\delta t^{m-1}}{m!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^m f \right] = -\frac{\delta t}{\tau} (f - f^{eq})$$



$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^n \left[ f^{eq} - \tau \sum_{m=1}^{\infty} \frac{\delta t^{m-1}}{m!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^m \left\{ f^{eq} - \tau \sum_{l=1}^{\infty} \frac{\delta t^{l-1}}{l!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^l f \right\} \right] = -\frac{\delta t}{\tau} (f - f^{eq})$$



$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^n f^{eq} - \tau \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{\delta t^{n+m-1}}{n!m!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^{m+n} f^{eq} = -\frac{\delta t}{\tau} (f - f^{eq})$$

# ALTERNATIVA A CHAPMANN-ENSKOG

Caso para la ecuación de Lattice Boltzmann:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^n f^{eq} - \tau \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{\delta t^{n+m-1}}{n! m!} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^{m+n} f^{eq} = -\frac{\delta t}{\tau} (f - f^{eq})$$



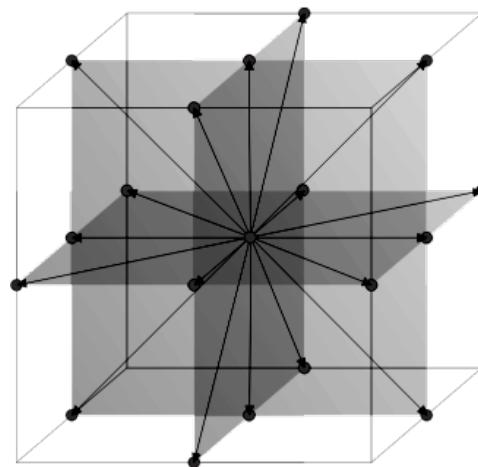
Hasta segundo orden

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f^{eq} - \tau \delta t \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} = -\frac{\delta t}{\tau} (f - f^{eq})$$



$$\left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) f^{eq} + \left( \frac{\delta t}{2} - \tau \right) \left( \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right)^2 f^{eq} = -\frac{1}{\tau} (f - f^{eq})$$

# POLINOMIOS DE HERMITE Y CUADRATURA



# MODELO DE LATTICE BOLTZMANN: 3 PASOS

1

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \Omega(f, f^{eq}) = -\frac{1}{\tau}(f - f^{eq})$$

Aproximación BGK

$$\rho = \int f d^3v = \int f^{eq} d^3v, \quad \rho \vec{u} = \int f \vec{v} d^3v = \int f^{eq} \vec{v} d^3v$$

2

$$f(\vec{x} + \vec{v}\delta t, \vec{v}, t + \delta t) - f(\vec{x}, \vec{v}, t) = -\frac{\delta t}{\tau}(f - f^{eq})$$

Integración en tiempo

Todavia tenemos 6+1 dimensiones

# MODELO DE LATTICE BOLTZMANN: 3 PASOS

3

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$

Discretización de velocidades

Tenemos que recuperar los momentos de la distribución de equilibrio:

$$\rho = \int f^{eq} d^3 v = \sum_i f^{eq}(v_i)$$

$$\rho \vec{u} = \int f^{eq} \vec{v} d^3 v = \sum_i f^{eq}(v_i) \vec{v}_i \quad \rightarrow$$

$$\Pi_{\alpha\beta} = \int f^{eq} v_\alpha v_\beta d^3 v = \sum_i f^{eq}(v_i) v_{i\alpha} v_{i\beta}$$

Al usar un pequeño  
numero de velocidades  
perdemos simetrías.

# CUADRATURA DE GAUSS

Comencemos en una dimensión. La cuadratura de Gauss se usa para aproximar el valor de una integral usando puntos de muestra:

$$\int e^{-x^2} f(x) dx \approx \sum_{i=0}^N \omega_i f(x_i)$$

Y es exacta cuando:

$$f(x) = \sum_{n=0}^N a_n H_n(x)$$

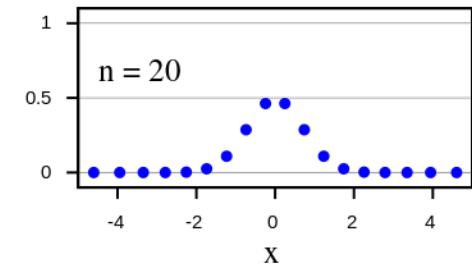
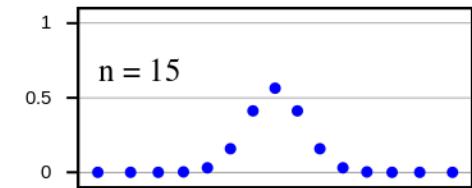
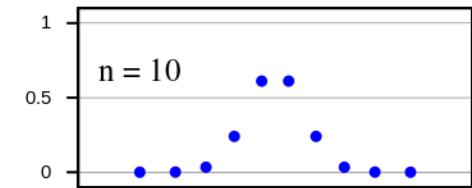
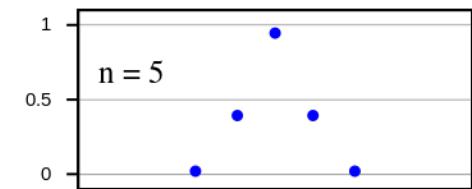
Polinomios (cualquier familia)

Existen:

$H_n(x)$ : Polinomios de Hermite  $\longrightarrow$  Gauss-Hermite

$L_n(x)$ : Polinomios de Laguerre  $\longrightarrow$  Gauss-Laguerre

...



# CUADRATURA DE GAUSS HERMITE

Por qué utilizar polinomios de Hermite?

$$\int e^{-v^2/2c_s^2} H_m(v) H_n(v) dv = \delta_{mn}$$

Forman una base ortogonal

$$\omega(\vec{v}) = e^{-\vec{v}^2/2c_s^2} = e^{-v_x^2/2c_s^2} e^{-v_y^2/2c_s^2} e^{-v_z^2/2c_s^2} = \omega(v_x) \omega(v_y) \omega(v_z)$$

Es separable: Podemos calcular la cuadratura en una dimensión y luego hacer el producto para cualquier dimensión.

Menos importante: en el caso de fluidos, la distribución de equilibrio se puede aproximar muy bien por lo que es una Gaussiana.

$$f^{eq} = A e^{-m(u-v)^2/2kT} = e^{-v^2/2c_s^2} \sum_{n=0}^{\infty} a_n(x, u, t) H_n(v)$$

Cuadratura  
Exacta!

# CUADRATURA DE GAUSS HERMITE

$$f^{eq} = Ae^{-m(u-v)^2/2kT} = e^{-v^2/2c_s^2} \sum_{n=0}^{\infty} a_n(x,u,t) H_n(v)$$

$$a_n(x,u,t) = \int f^{eq} H_n(v) dv$$

Entonces debemos resolver:

$$\boxed{\begin{aligned} H_0(v) &= 1 \\ H_1(v) &= \frac{v}{c_s} \\ H_2(v) &= \frac{1}{\sqrt{2}} \left( \frac{v^2}{c_s^2} - 1 \right) \end{aligned}}$$

$$\int e^{-v^2/2c_s^2} H_m(v) H_n(v) dv = \sum_{i=0}^N \omega_i H_m(v_i) H_n(v_i)$$

↑  
↑  
Incógnitas

Para las ecuaciones de Navier Stokes se necesita satisfacer la cuadratura para

$$m, n \in [0, 1, 2]$$

# CUADRATURA DE GAUSS HERMITE

$$f^{eq} = Ae^{-m(u-v)^2/2kT} = e^{-v^2/2c_s^2} \sum_{n=0}^{\infty} a_n(x, u, t) H_n(v)$$

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$$\int e^{-v^2/2c_s^2} H_m(v) H_n(v) dv = \sum_{i=0}^N \omega_i H_m(v_i) H_n(v_i)$$



$$v_i = -1, 0, 1$$

$$c_s = 1 / \sqrt{3}$$

$$\omega = 1/6, 2/3, 1/6$$

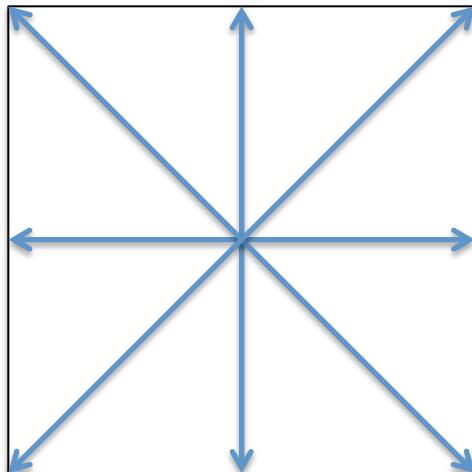
$$\xleftarrow{\hspace{1cm}} \quad v_1 = -1 \quad v_0 = 0 \quad v_2 = 1 \xrightarrow{\hspace{1cm}}$$

$$\omega_1 = 1/6 \quad \omega_0 = 2/3 \quad \omega_1 = 1/6$$

# CUADRATURA DE GAUSS HERMITE

$$\omega(\vec{v}) = e^{-\vec{v}^2/2c_s^2} = e^{-v_x^2/2c_s^2} e^{-v_y^2/2c_s^2} e^{-v_z^2/2c_s^2} = \omega(v_x)\omega(v_y)\omega(v_z)$$

En dos dimensiones:



$$\vec{v}_i = (1,1)$$

$$\omega_i = (1/6)(1/6) = 1/36$$

$$\vec{v}_i = (0,0)$$

$$\omega_i = (2/3)(2/3) = 4/9$$

D2Q9

$$c_s = 1/\sqrt{3}$$



$$v_1 = -1$$

$$v_0 = 0$$

$$v_2 = 1$$

$$\omega_1 = 1/6$$

$$\omega_0 = 2/3$$

$$\omega_1 = 1/6$$

# CUADRATURA DE GAUSS HERMITE

$$f^{eq} = A e^{-m(u-v)^2/2kT} = e^{-v^2/2c_s^2} \sum_{n=0}^2 a_n(x,u,t) H_n(v)$$



$$f_i^{eq} = \omega_i \sum_{n=0}^2 a_n(x,u,t) H_n(v_i)$$

$$a_n(x,u,t) = \sum_{i=0}^N f_i^{eq} H_n(v_i) = \int f^{eq} H_n(v) dv$$

$$\boxed{\begin{aligned} H_0(v) &= 1 \\ H_1(v) &= \frac{v}{c_s} \\ H_2(v) &= \frac{1}{\sqrt{2}} \left( \frac{v^2}{c_s^2} - 1 \right) \end{aligned}}$$

Estos coeficientes se pueden escribir en función de los momentos:

$$\boxed{a_0 = \Pi_0 \quad , \quad a_1(v) = \frac{\Pi_1}{c_s} \quad , \quad a_2(v) = \frac{1}{\sqrt{2}} \left( \frac{\Pi_2}{c_s^2} - 1 \right)}$$

# CUADRATURA DE GAUSS HERMITE

$$f^{eq} = A e^{-m(u-v)^2/2kT} = e^{-v^2/2c_s^2} \sum_{n=0}^2 a_n(x, u, t) H_n(v)$$



$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1 v_i}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2}{c_s^2} - \Pi_0 \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) \right]$$

$$\boxed{\begin{aligned} H_0(v) &= 1 \\ H_1(v) &= \frac{v}{c_s} \\ H_2(v) &= \frac{1}{\sqrt{2}} \left( \frac{v^2}{c_s^2} - 1 \right) \end{aligned}}$$



$$v_1 = -1$$

$$v_0 = 0$$

$$v_2 = 1$$

$$\omega_1 = 1/6$$

$$\omega_0 = 2/3$$

$$\omega_1 = 1/6$$

Entonces, conocidos los momentos de la distribución de equilibrio en el continuo, podemos calcular la función de equilibrio discreta. Podemos también imponer estos momentos a algo deseado, como fue hecho en el caso de ondas.

# CUADRATURA DE GAUSS HERMITE

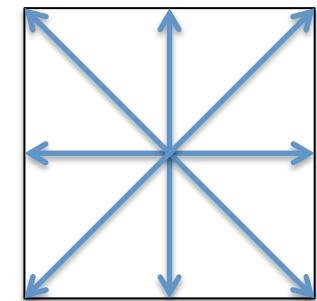
En 2D:

$$f^{eq} = A e^{-m(\vec{u}-\vec{v})^2/2kT} = e^{-\vec{v}^2/2c_s^2} \sum_{n=0}^2 a_n^{(n)}(\vec{x}, \vec{u}, t) H_n^{(n)}(\vec{v})$$



$H_0(v) = 1$
$H_1^{(1)\alpha}(v) = \frac{v^\alpha}{c_s}$
$H_2^{(2)\alpha\beta}(v) = \frac{1}{\sqrt{2}} \left( \frac{v^\alpha v^\beta}{c_s^2} - \delta^{\alpha\beta} \right)$

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$



D2Q9

$$c_s = 1/\sqrt{3}$$

Entonces, conocidos los momentos de la distribución de equilibrio en el continuo, podemos calcular la función de equilibrio discreta. Podemos también imponer estos momentos a algo deseado, como fue hecho en el caso de ondas.

# CUADRATURA DE GAUSS HERMITE

Caso fluidos 2D:

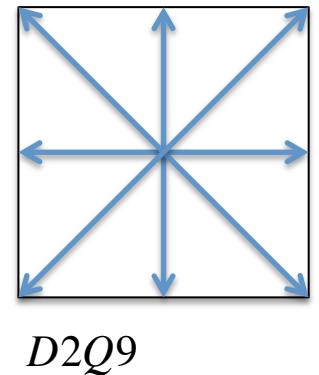
$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$\Pi_0 = \rho \quad \Pi_1^{(1)\alpha} = \rho u^\alpha \quad \Pi_2^{(2)\alpha\beta} = \rho c_s^2 + \rho u^\alpha u^\beta$$

$H_0(v) = 1$
$H_1^{(1)\alpha}(v) = \frac{v^\alpha}{c_s}$
$H_2^{(2)\alpha\beta}(v) = \frac{1}{\sqrt{2}} \left( \frac{v^\alpha v^\beta}{c_s^2} - \delta^{\alpha\beta} \right)$



$$f_i^{eq} = \omega_i \rho \left[ 1 + \frac{u^\alpha v_i^\alpha}{c_s^2} + \frac{1}{2} \frac{(v_i^\alpha u^\alpha)^2}{c_s^4} + \frac{u^\alpha u^\alpha}{2c_s^2} \right]$$



$$c_s = 1/\sqrt{3}$$

Entonces, conocidos los momentos de la distribución de equilibrio en el continuo, podemos calcular la función de equilibrio discreta. Podemos también imponer estos momentos a algo deseado, como fue hecho en el caso de ondas.

# EJEMPLO: ECUACION DE POISSON

La ecuación de Poisson:

$$\nabla^2 \Phi = \rho$$

Se puede obtener como el límite estacionario de la ecuación de difusión:

$$\frac{\partial \Phi}{\partial t} = D \nabla^2 \Phi - D \rho = 0$$

Entonces vamos a resolver la ecuación de difusión con fuente y esperamos a que la solución llegue al estado estacionario.

# EJEMPLO: ECUACION DE POISSON

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] + \delta t S_i$$



$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n f_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$



$$f_i = f_i^{eq} - \tau \sum_{n=1}^{\infty} \frac{\delta t^{n-1}}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n f_i + \tau S_i$$

# EJEMPLO: ECUACION DE POISSON

En el límite estacionario:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} (\vec{v}_i \cdot \nabla)^n f_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$

$$f_i = f_i^{eq} - \tau \sum_{n=1}^{\infty} \frac{\delta t^{n-1}}{n!} (\vec{v}_i \cdot \nabla)^n f_i + \tau S_i$$

Reemplazando por recurrencia:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} (\vec{v}_i \cdot \nabla)^n \left[ f_i^{eq} - \tau \sum_{m=1}^{\infty} \frac{\delta t^{m-1}}{m!} (\vec{v}_i \cdot \nabla)^m f_i + \tau S_i \right] = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$

# EJEMPLO: ECUACION DE POISSON

Y así sucesivamente:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} (\vec{v}_i \cdot \nabla)^n f_i^{eq} - \tau \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\delta t^{n+m-1}}{n!m!} (\vec{v}_i \cdot \nabla)^{m+n} f_i + \tau \sum_{n=1}^{\infty} \frac{\delta t^n}{n!} (\vec{v}_i \cdot \nabla)^n S_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$



$$\begin{aligned} & \sum_{n=1}^{\infty} \frac{\delta t^n}{n!} (\vec{v}_i \cdot \nabla)^n f_i^{eq} - \tau \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\delta t^{n+m-1}}{n!m!} (\vec{v}_i \cdot \nabla)^{m+n} f_i^{eq} + \tau^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \sum_{l=1}^{\infty} \frac{\delta t^{n+m+l-2}}{n!m!l!} (\vec{v}_i \cdot \nabla)^{m+n+l} f_i \\ & - \tau^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\delta t^{n+m-1}}{n!m!} (\vec{v}_i \cdot \nabla)^{m+n} S_i + \tau \sum_{n=1}^{\infty} \frac{\delta t^n}{n!} (\vec{v}_i \cdot \nabla)^n S_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i \end{aligned}$$

Si hacemos que:

$$\begin{aligned} \sum_{i=0}^N f_i^{eq} &= \Pi_0^{(0)} = \Phi \quad , \quad \sum_{i=0}^N f_i^{eq} v_i^\alpha = \Pi_1^{(1)\alpha} = 0 \quad , \quad \sum_{i=0}^N f_i^{eq} v_i^\alpha v_i^\beta = \Pi_2^{(2)\alpha\beta} = c_s^2 \Phi \delta^{\alpha\beta} \quad , \quad \sum_{i=0}^N f_i^{eq} v_i^\alpha v_i^\beta \dots = \Pi_n^{(n)\alpha\beta\dots} = 0 \\ \sum_{i=0}^N S_i &= \Pi_0^{(0)} = -D\rho \quad , \quad \sum_{i=0}^N S_i v_i^\alpha \dots = \Pi_n^{(n)\alpha\dots} = 0 \end{aligned}$$

# EJEMPLO: ECUACION DE POISSON

Así, en 1D tenemos hasta una expansión de segundo orden:

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1 v_i}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2}{c_s^2} - \Pi_0 \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) \right]$$

$$f_i^{eq} = \omega_i \left[ \Phi + \frac{1}{2} \left( \frac{\Phi c_s^2}{c_s^2} - \Phi \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) \right]$$

$$S_i = \omega_i \left[ -D\rho + \frac{1}{2} \left( \frac{0}{c_s^2} + D\rho \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) \right] \quad D = c_s^2(\tau - \delta t / 2)$$



$$c_s^2 = \frac{1}{3}$$

$$v_1 = -1 \quad \omega_1 = 1/6$$

$$v_0 = 0 \quad \omega_0 = 2/3$$

$$v_2 = 1 \quad \omega_1 = 1/6$$

# EJEMPLO: ECUACION DE POISSON

Así, en 1D tenemos hasta una expansión de cuarto orden:

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{1}{2} \left( \frac{\Pi_2}{c_s^2} - \Pi_0 \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) + \frac{1}{24} \left( \frac{\Pi_4}{c_s^4} - 6 \frac{\Pi_2}{c_s^2} + 3\Pi_0 \right) \left( \frac{v_i^4}{c_s^4} - 6 \frac{v_i^2}{c_s^2} + 3 \right) \right]$$

$$f_i^{eq} = \omega_i \left[ \Phi + \frac{1}{2} \left( \frac{\Phi c_s^2}{c_s^2} - \Phi \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) + \frac{1}{24} \left( \frac{0}{c_s^4} - 6 \frac{\Phi c_s^2}{c_s^2} + 3\Phi \right) \left( \frac{v_i^4}{c_s^4} - 6 \frac{v_i^2}{c_s^2} + 3 \right) \right]$$

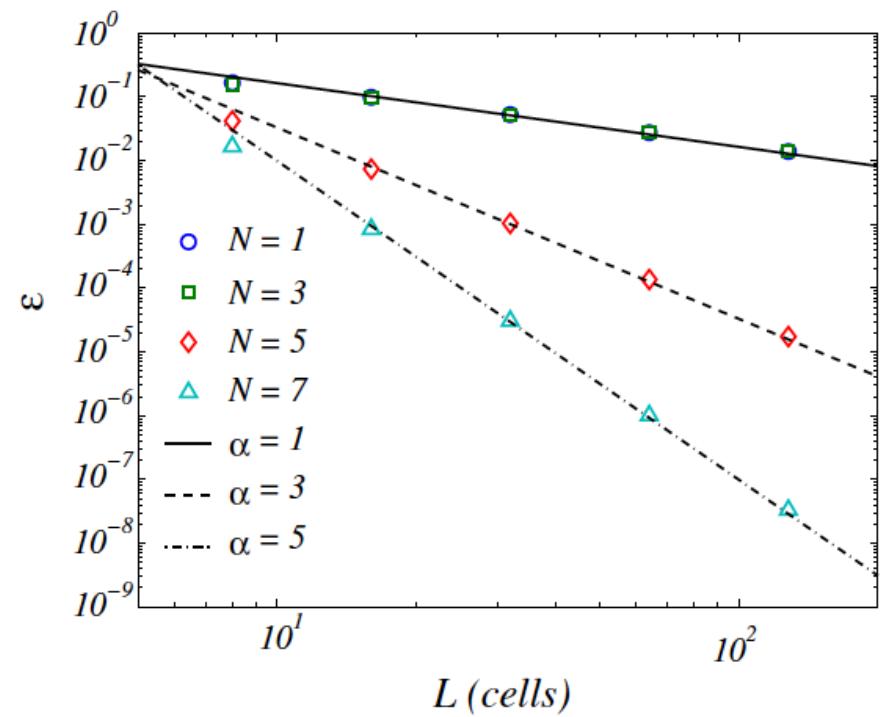
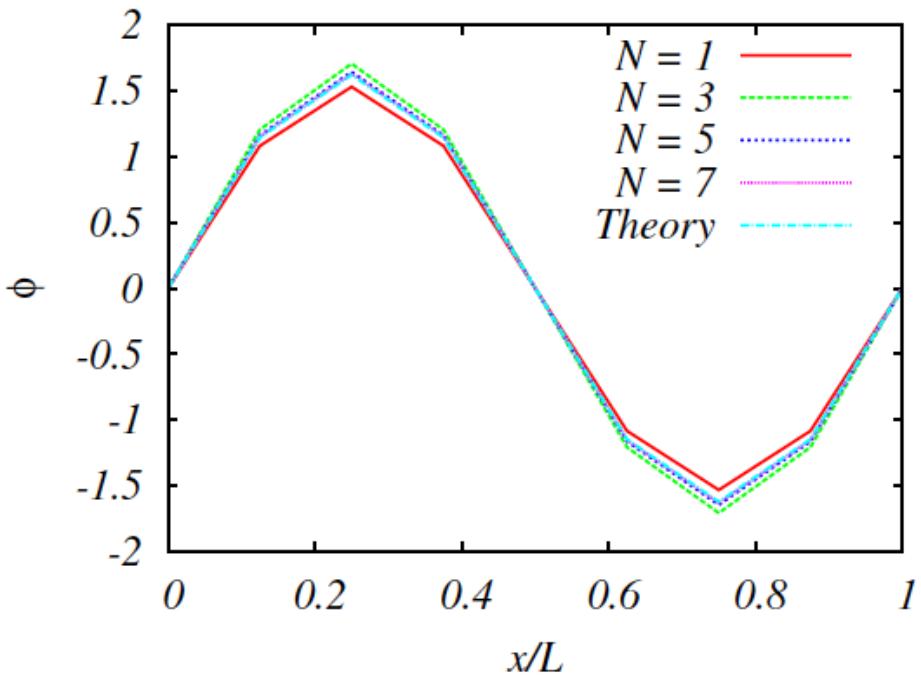
$$S_i = \omega_i \left[ -D\rho + \frac{1}{2} \left( \frac{0}{c_s^2} + D\rho \right) \left( \frac{v_i^2}{c_s^2} - 1 \right) + \frac{1}{24} \left( \frac{0}{c_s^4} - 6 \frac{0}{c_s^2} - 3D\rho \right) \left( \frac{v_i^4}{c_s^4} - 6 \frac{v_i^2}{c_s^2} + 3 \right) \right]$$

$$D = c_s^2 (\tau - \delta t / 2)$$

$$0.6979533220196831 \xrightarrow{} c_s^2$$

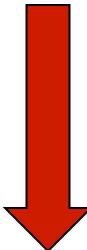
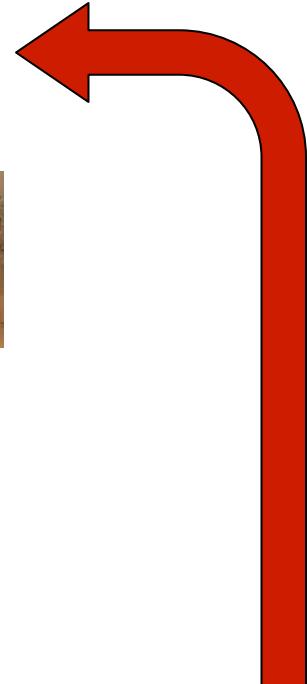
w[0] = 0.4766698865892074; v[0]=0;  
w[1] = 0.2339147378268247; v[1]=1;  
w[2] = 0.2339147378268247; v[2]=-1;  
w[3] = 0.02693818934482545; v[3]=2;  
w[4] = 0.02693818934482545; v[4]=-2;  
w[5] = 0.0008121295337461138; v[5]=3;  
w[6] = 0.0008121295337461138; v[6]=-3;

# EJEMPLO: ECUACION DE POISSON



# MODELO DE LATTICE BOLTZMANN

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]$$

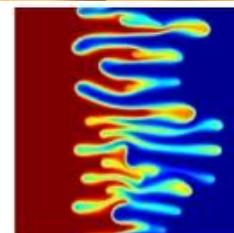
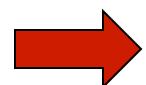


Variables macroscópicas

$$\rho = \sum_i f_i$$

$$\rho \vec{u} = \sum_i f_i \vec{v}_i$$

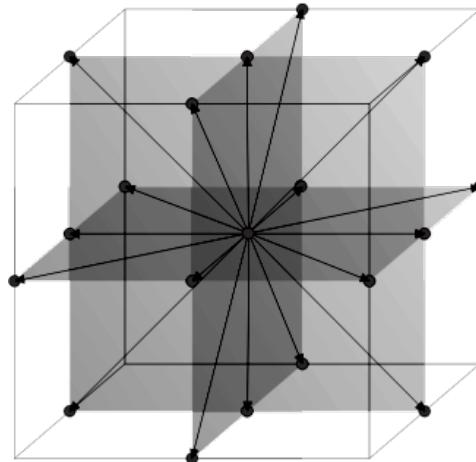
$$\pi_{\alpha\beta} = \sum_i f_i v_{i\alpha} v_{i\beta}$$



Distribución de equilibrio

$$f_i^{eq}(x, t) = \rho \omega_i \left[ 1 + \frac{3(\vec{v}_i \cdot \vec{u})}{c_s^2} + \frac{(\vec{v}_i \cdot \vec{u})^2}{2c_s^4} - \frac{(\vec{u} \cdot \vec{u})}{2c_s^2} \right]$$

# LATTICE BOLTZMANN PARA FLUIDOS



Regla de suma de Einstein: Índices repetidos se suman

$$\nabla \cdot \vec{N} = \partial_\alpha N^\alpha = \partial_0 N^0 + \partial_1 N^1 + \partial_2 N^2$$

# LATTICE BOLTZMANN PARA FLUIDOS

Caso fluidos:

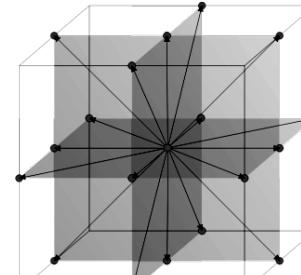
$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$\Pi_0 = \rho \quad \Pi_1^{(1)\alpha} = \rho u^\alpha \quad \Pi_2^{(2)\alpha\beta} = \rho c_s^2 + \rho u^\alpha u^\beta$$

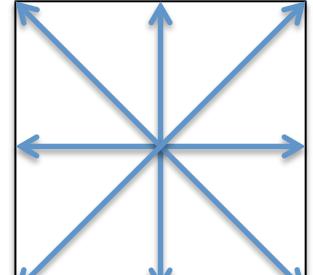
$H_0(v) = 1$
$H_1^{(1)\alpha}(v) = \frac{v^\alpha}{c_s}$
$H_2^{(2)\alpha\beta}(v) = \frac{1}{\sqrt{2}} \left( \frac{v^\alpha v^\beta}{c_s^2} - \delta^{\alpha\beta} \right)$



$$f_i^{eq} = \omega_i \rho \left[ 1 + \frac{u^\alpha v_i^\alpha}{c_s^2} + \frac{1}{2} \frac{(v_i^\alpha u^\alpha)^2}{c_s^4} + \frac{u^\alpha u^\alpha}{2c_s^2} \right]$$



D3Q19



D2Q9

$$c_s = 1/\sqrt{3}$$

# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación matriz:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n f_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$



$$f_i = f_i^{eq} - \tau \sum_{n=1}^{\infty} \frac{\delta t^{n-1}}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n f_i = f_i^{eq} + f_i^{neq}$$



$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n \left( f_i^{eq} - \tau \sum_{m=1}^{\infty} \frac{\delta t^{m-1}}{m!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^m f_i \right) = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$

# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación matriz:

$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n \left( f_i^{eq} - \tau \sum_{m=1}^{\infty} \frac{\delta t^{m-1}}{m!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^m f_i \right) = -\frac{\delta t}{\tau} (f_i - f_i^{eq})$$



Hasta  $\nabla^2$

$$\left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i^{eq} + \left( 1 - \frac{\delta t}{2\tau} \right) \left[ -\tau \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^2 f_i^{eq} \right] = -\frac{1}{\tau} (f_i - f_i^{eq})$$

$$\left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left[ f_i^{eq} + \left( 1 - \frac{\delta t}{2\tau} \right) f^{neq} \right] = -\frac{1}{\tau} (f_i - f_i^{eq})$$

# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación matriz:

$$\sum_i^N f_i^{neq} = 0 \quad , \quad \sum_i^N f_i^{neq} v_i = 0$$

$$\left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left[ f_i^{eq} + \left( 1 - \frac{\delta t}{2\tau} \right) f^{neq} \right] = -\frac{1}{\tau} (f_i - f_i^{eq})$$



$$\sum_{i=0}^N \rightarrow \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left[ f_i^{eq} + \left( 1 - \frac{\delta t}{2\tau} \right) f^{neq} \right] = -\frac{1}{\tau} (f_i - f_i^{eq})$$



$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0}$$

# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación matriz:

$$\sum_i^N f_i^{neq} = 0 \quad , \quad \sum_i^N f_i^{neq} v_i = 0$$

$$\sum_{i=0}^N v_i \rightarrow \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left[ f_i^{eq} + \left( 1 - \frac{\delta t}{2\tau} \right) f^{neq} \right] = -\frac{1}{\tau} (f_i - f_i^{eq})$$



$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \Pi_2^{(2)} + \left( 1 - \frac{\delta t}{2\tau} \right) \nabla \cdot \Pi_2^{(2), neq} = 0$$

$$\Pi_2^{(2), neq \alpha\beta} = \sum_{i=0}^N f_i^{neq} v_i^\alpha v_i^\beta \approx -\tau \sum_{i=0}^N \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i^{eq} v_i^\alpha v_i^\beta \approx -\tau \partial_\gamma \cdot \Pi_3^{(3) \alpha\beta\gamma}$$

# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación de conservación del momento:

$$\frac{\partial \rho u^\alpha}{\partial t} + \partial_\beta \Pi_2^{(2)\alpha\beta} - \left( \tau - \frac{\delta t}{2} \right) \partial_\beta \partial_\gamma \Pi_3^{(3)\alpha\beta\gamma} = 0$$

Ahora bien:

$$\Pi_2^{(2)\alpha\beta} = \rho c_s^2 \delta^{\alpha\beta} + \rho u^\alpha u^\beta, \quad \Pi_3^{(3)\alpha\beta\gamma} = \rho c_s^2 \left( \delta^{\alpha\beta} u^\gamma + \delta^{\alpha\gamma} u^\beta + \delta^{\beta\gamma} u^\alpha \right) + \rho u^\alpha u^\beta u^\gamma$$

Tenemos:

$$\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = - \partial_\alpha \left( \rho c_s^2 \right) + \left( \tau - \frac{\delta t}{2} \right) \partial_\beta \partial_\gamma \Pi_3^{(3)\alpha\beta\gamma}$$

Bajos Mach:

$$\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = - \partial_\alpha \left( \rho c_s^2 \right) + \nu \partial_\beta^2 \left( \rho u^\alpha \right) + 2\nu \partial_\alpha \partial_\beta \left( \rho u^\beta \right), \quad \nu = c_s^2 \left( \tau - \frac{\delta t}{2} \right)$$

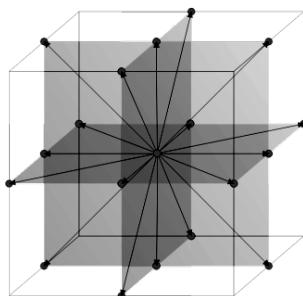
# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación de conservación del momento:

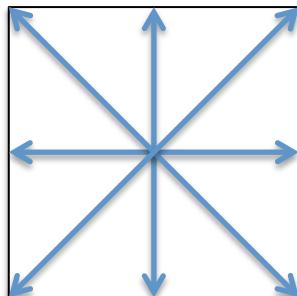
$$\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = -\partial_\alpha (\rho c_s^2) + \nu \partial_\beta^2 (\rho u^\alpha) + 2\nu \partial_\alpha \partial_\beta (\rho u^\beta), \quad \nu = c_s^2 \left( \tau - \frac{\delta t}{2} \right)$$

En el límite incompresible:

$$\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = -\partial_\alpha (\rho c_s^2) + \eta \partial_\beta^2 u^\alpha, \quad \eta = \rho c_s^2 \left( \tau - \frac{\delta t}{2} \right)$$



D3Q19



D2Q9



$$\Pi_3^{(3)\alpha\beta\gamma} = \rho c_s^2 (\delta^{\alpha\beta} u^\gamma + \delta^{\alpha\gamma} u^\beta + \delta^{\beta\gamma} u^\alpha)$$

# LATTICE BOLTZMANN PARA FLUIDOS

Ecuación de conservación del momento:

$$\frac{\partial \rho u^\alpha}{\partial t} + \partial_\beta \Pi_2^{(2)\alpha\beta} = \eta \partial_\beta^2 u^\alpha$$

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

Introducir otra ecuación de estado:

$$\Pi_2^{(2)\alpha\beta} = P \delta^{\alpha\beta} + \rho u^\alpha u^\beta, \quad P = P(\rho)$$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0}$$

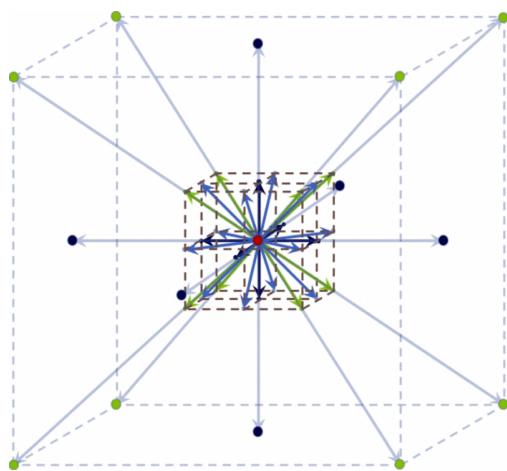
$$\boxed{\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = -\partial_\alpha P + \eta \partial_\beta^2 u^\alpha}$$

# LATTICE BOLTZMANN PARA FLUIDOS

Con una función de equilibrio:

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$
$$+ \omega_i \left[ \frac{1}{6} \left( \frac{\Pi_3^{(3)\alpha\beta\gamma}}{c_s^2} - \frac{(\delta^{\alpha\beta} \Pi_1^{(1)\gamma} + \delta^{\alpha\gamma} \Pi_1^{(1)\beta} + \delta^{\beta\gamma} \Pi_1^{(1)\alpha})}{c_s} \right) \left( \frac{v_i^\alpha v_i^\beta v_i^\gamma}{c_s^3} - \frac{(\delta^{\alpha\beta} v_i^\gamma + \delta^{\alpha\gamma} v_i^\beta + \delta^{\beta\gamma} v_i^\alpha)}{c_s} \right) \right]$$

Podemos reproducir



$$\Pi_3^{(3)\alpha\beta\gamma} = \rho c_s^2 (\delta^{\alpha\beta} u^\gamma + \delta^{\alpha\gamma} u^\beta + \delta^{\beta\gamma} u^\alpha) + \rho u^\alpha u^\beta u^\gamma$$

D3Q41

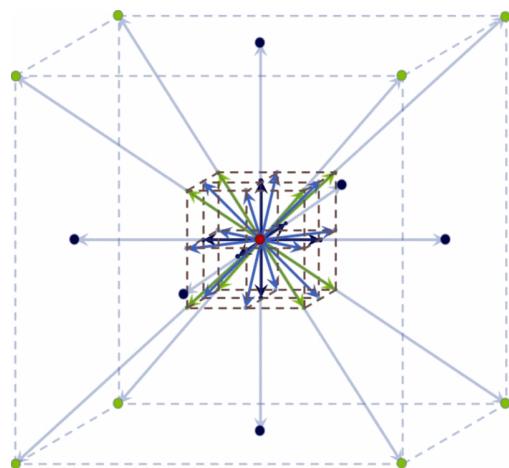
$$c_s^2 = 1 - \sqrt{\frac{2}{5}}$$

# LATTICE BOLTZMANN PARA FLUIDOS

Una función de equilibrio:

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right] \\ + \omega_i \left[ \frac{1}{6} \left( \frac{\Pi_3^{(3)\alpha\beta\gamma}}{c_s^2} - \frac{(\delta^{\alpha\beta} \Pi_1^{(1)\gamma} + \delta^{\alpha\gamma} \Pi_1^{(1)\beta} + \delta^{\beta\gamma} \Pi_1^{(1)\alpha})}{c_s} \right) \left( \frac{v_i^\alpha v_i^\beta v_i^\gamma}{c_s^3} - \frac{(\delta^{\alpha\beta} v_i^\gamma + \delta^{\alpha\gamma} v_i^\beta + \delta^{\beta\gamma} v_i^\alpha)}{c_s} \right) \right]$$

Es útil para:



$$\Pi_0 = \rho \quad \Pi_1^{(1)\alpha} = \rho u^\alpha \quad \Pi_2^{(2)\alpha\beta} = \rho T + \rho u^\alpha u^\beta$$

$$\Pi_3^{(3)\alpha\beta\gamma} = \rho T (\delta^{\alpha\beta} u^\gamma + \delta^{\alpha\gamma} u^\beta + \delta^{\beta\gamma} u^\alpha) + \rho u^\alpha u^\beta u^\gamma$$

D3Q41

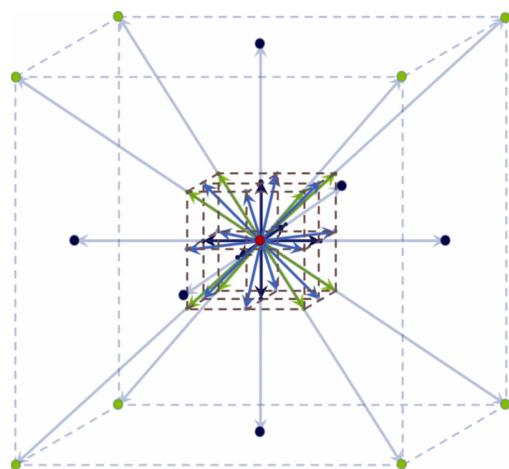
$$c_s^2 = 1 - \sqrt{\frac{2}{5}}$$

# LATTICE BOLTZMANN PARA FLUIDOS

Una función de equilibrio:

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right] \\ + \omega_i \left[ \frac{1}{6} \left( \frac{\Pi_3^{(3)\alpha\beta\gamma}}{c_s^2} - \frac{(\delta^{\alpha\beta} \Pi_1^{(1)\gamma} + \delta^{\alpha\gamma} \Pi_1^{(1)\beta} + \delta^{\beta\gamma} \Pi_1^{(1)\alpha})}{c_s} \right) \left( \frac{v_i^\alpha v_i^\beta v_i^\gamma}{c_s^3} - \frac{(\delta^{\alpha\beta} v_i^\gamma + \delta^{\alpha\gamma} v_i^\beta + \delta^{\beta\gamma} v_i^\alpha)}{c_s} \right) \right]$$

Es útil para:



$$\Pi_0 = \rho \quad \Pi_1^{(1)\alpha} = \rho u^\alpha \quad \Pi_2^{(2)\alpha\beta} = \rho T g^{\alpha\beta} + \rho u^\alpha u^\beta$$

$$\Pi_3^{(3)\alpha\beta\gamma} = \rho T (g^{\alpha\beta} u^\gamma + g^{\alpha\gamma} u^\beta + g^{\beta\gamma} u^\alpha) + \rho u^\alpha u^\beta u^\gamma$$

D3Q41

$$c_s^2 = 1 - \sqrt{\frac{2}{5}}$$

# FORZAMIENTO II

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] + \delta t S_i + \frac{\delta t}{2} [S_i(\vec{x}, t) - S_i(\vec{x} - \vec{v}_i \delta t, t - \delta t)]$$

Shi, B., Deng, B., Du, R., & Chen, X. (2008). Computers & Mathematics with Applications, 55(7), 1568-1575; J.-D. Debus, M. Mendoza, S. Succi, and H. J. Herrmann, Phys. Rev. E 93, 043316 (2016).



$$\sum_{n=1}^{\infty} \frac{\delta t^n}{n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n f_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \sum_{n=1}^{\infty} \frac{\delta t^{n+1}}{2n!} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^n S_i$$



Hasta  $\nabla^2$ ,  $\delta t^2$

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^2 f_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) S_i$$

# FORZAMIENTO II

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^2 f_i = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) S_i$$



$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i = -\frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^2 f_i - \frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) S_i$$



$$\begin{aligned} & \delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left( -\frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right)^2 f_i - \frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) S_i \right) \\ &= -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) S_i \end{aligned}$$

# FORZAMIENTO II

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left( -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \cancel{\delta t S_i} \right) = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i + \frac{\delta t^2}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) S_i$$



$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left( -\frac{\delta t}{\tau} (f_i - f_i^{eq}) \right) = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$

Considerando:  $f_i = f_i^{eq} + f_i^{neq}$

$$\sum_i^N f_i^{neq} = 0 \quad , \quad \sum_i^N f_i^{neq} v_i = 0$$

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left( -\frac{\delta t}{\tau} (f_i - f_i^{eq}) \right) = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$



$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = \Gamma_0}$$

$$\boxed{\Gamma_0 = \sum_{i=0}^N S_i}$$

# FORZAMIENTO II

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i + \frac{\delta t}{2} \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) \left( -\frac{\delta t}{\tau} (f_i - f_i^{eq}) \right) = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$

Considerando:  $f_i = f_i^{eq} + f_i^{neq}$

$$\sum_i^N f_i^{neq} = 0 \quad , \quad \sum_i^N f_i^{neq} v_i = 0$$

$$\delta t \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i^{eq} + \delta t \left( 1 - \frac{\delta t}{2\tau} \right) \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i^{neq} = -\frac{\delta t}{\tau} (f_i - f_i^{eq}) + \delta t S_i$$

Sumando:

$$\frac{\partial \rho u^\alpha}{\partial t} + \partial_\beta \Pi_2^{(2)\alpha\beta} = - \left( 1 - \frac{\delta t}{2\tau} \right) \partial_\beta \Pi_2^{(2),neq\alpha\beta} + \Gamma_1^{(1)\alpha}$$

Ahora bien:

$$f_i^{neq} \approx -\tau \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i^{eq} - \tau S_i$$

$$\Pi_2^{(2),neq\alpha\beta} \approx -\tau \partial_\gamma \Pi_3^{(3)\alpha\beta\gamma} - \tau \Gamma_2^{(2)\alpha\beta}$$

Hay opciones

# FORZAMIENTO II

$$\frac{\partial \rho u^\alpha}{\partial t} + \partial_\beta \Pi_2^{(2)\alpha\beta} = -\left(1 - \frac{\delta t}{2\tau}\right) \partial_\beta \Pi_2^{(2),neq\alpha\beta} + \Gamma_1^{(1)\alpha}$$

Ahora bien:

$$f_i^{neq} \approx -\tau \left( \frac{\partial}{\partial t} + \vec{v}_i \cdot \nabla \right) f_i^{eq} - \tau S_i$$

$$\Pi_2^{(2),neq\alpha\beta} \approx -\tau \partial_\gamma \Pi_3^{(3)\alpha\beta\gamma} - \tau \Gamma_2^{(2)\alpha\beta}$$

Hay opciones



$$\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = -\partial_\alpha (\rho c_s^2) + \eta \partial_\beta^2 u^\alpha + \Gamma_1^{(1)\alpha}, \quad \eta = \rho c_s^2 \left( \tau - \frac{\delta t}{2} \right)$$

# FORZAMIENTO II

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$S_i = \omega_i \left[ \Gamma_0 + \frac{\Gamma_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Gamma_2^{(2)\alpha\beta}}{c_s^2} - \Gamma_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

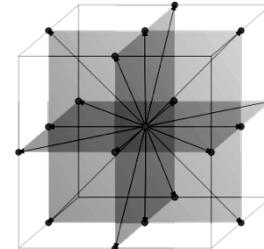
$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] + \delta t S_i + \frac{\delta t}{2} [S_i(\vec{x}, t) - S_i(\vec{x} - \vec{v}_i \delta t, t - \delta t)]$$


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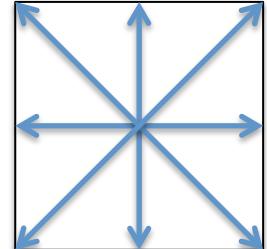
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = \Gamma_0$$

Bajo Mach y límite incompresible

$$\rho \frac{\partial u^\alpha}{\partial t} + \rho u^\beta \partial_\beta u^\alpha = -\partial_\alpha (\rho c_s^2) + \eta \partial_\beta^2 u^\alpha + \Gamma_1^{(1)\alpha}, \quad \eta = \rho c_s^2 \left( \tau - \frac{\delta t}{2} \right)$$



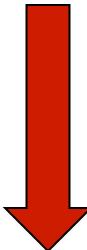
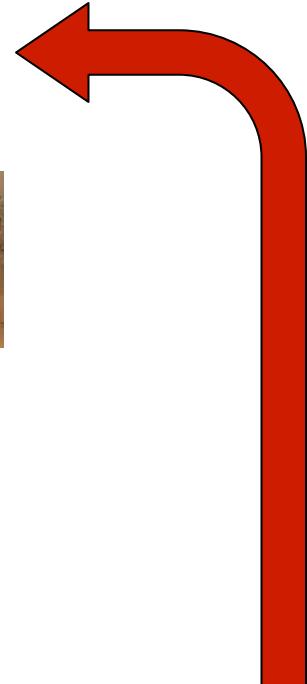
D3Q19



D2Q9

# MODELO DE LATTICE BOLTZMANN

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)]$$

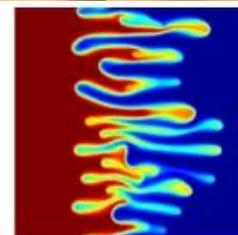


Variables macroscópicas

$$\rho = \sum_i f_i$$

$$\rho \vec{u} = \sum_i f_i \vec{v}_i$$

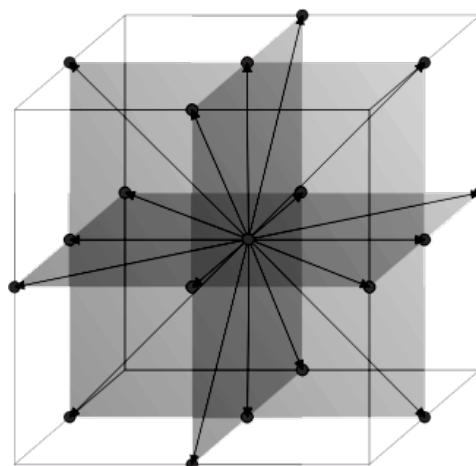
$$\pi_{\alpha\beta} = \sum_i f_i v_{i\alpha} v_{i\beta}$$



Distribución de equilibrio

$$f_i^{eq}(x, t) = \rho \omega_i \left[ 1 + \frac{3(\vec{v}_i \cdot \vec{u})}{c_s^2} + \frac{(\vec{v}_i \cdot \vec{u})^2}{2c_s^4} - \frac{(\vec{u} \cdot \vec{u})}{2c_s^2} \right]$$

# ENTROPIC LATTICE BOLTZMANN MODEL



# LATTICE BOLTZMANN MODEL

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$S_i = \omega_i \left[ \Gamma_0 + \frac{\Gamma_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Gamma_2^{(2)\alpha\beta}}{c_s^2} - \Gamma_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] + \delta t S_i + \frac{\delta t}{2} [S_i(\vec{x}, t) - S_i(\vec{x} - \vec{v}_i \delta t, t - \delta t)]$$


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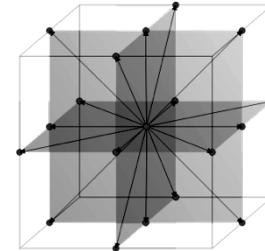
Imponiendo:

$$\Pi_0 = \sum_{i=0}^N f_i$$

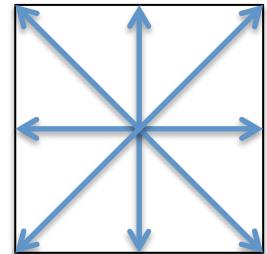
$$\Gamma_0 = \sum_{i=0}^N S_i$$

Se obtiene:

$$\boxed{\frac{\partial \Pi_0}{\partial t} + \partial_\alpha \Pi_1^{(1)\alpha} = \Gamma_0 + \left( \tau - \frac{\delta t}{2} \right) \partial_\beta \partial_\gamma \Pi_2^{(2)\beta\gamma}}$$



D3Q19



D2Q9

# LATTICE BOLTZMANN MODEL

$$f_i^{eq} = \omega_i \left[ \Pi_0 + \frac{\Pi_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Pi_2^{(2)\alpha\beta}}{c_s^2} - \Pi_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$S_i = \omega_i \left[ \Gamma_0 + \frac{\Gamma_1^{(1)\alpha} v_i^\alpha}{c_s^2} + \frac{1}{2} \left( \frac{\Gamma_2^{(2)\alpha\beta}}{c_s^2} - \Gamma_0 \delta^{\alpha\beta} \right) \left( \frac{v_i^\alpha v_i^\beta}{c_s^2} - \delta^{\alpha\beta} \right) \right]$$

$$f_i(\vec{x} + \vec{v}_i \delta t, t + \delta t) - f_i(\vec{x}, t) = -\frac{\delta t}{\tau} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] + \delta t S_i + \frac{\delta t}{2} [S_i(\vec{x}, t) - S_i(\vec{x} - \vec{v}_i \delta t, t - \delta t)]$$


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Imponiendo:

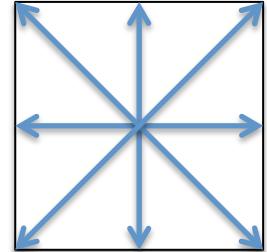
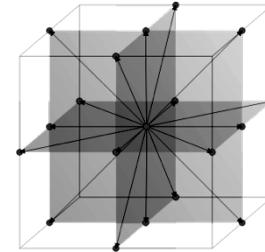
$$\Pi_0 = \sum_{i=0}^N f_i \quad \Pi_1^{(1)} = \sum_{i=0}^N f_i v_i$$

$$\Gamma_0 = \sum_{i=0}^N S_i \quad \Gamma_1^{(1)} = \sum_{i=0}^N S_i v_i$$

Se obtiene:

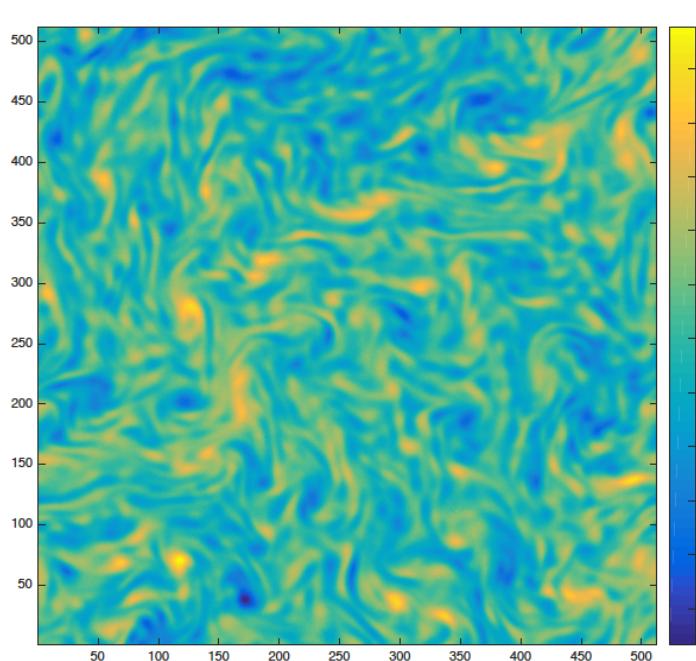
$$\frac{\partial \Pi_1^{(1)\alpha}}{\partial t} + \partial_\beta \Pi_2^{(2)\alpha} = \Gamma_1^{(1)} + \left( \tau - \frac{\delta t}{2} \right) \partial_\beta \partial_\gamma \Pi_3^{(3)\alpha\beta\gamma}$$

$$\frac{\partial \Pi_0}{\partial t} + \partial_\alpha \Pi_1^{(1)\alpha} = \Gamma_0$$



# POR QUÉ ENTROPIC LATTICE BOLTZMANN

1. La forma mas natural de eliminar inestabilidades numéricas es usar los principios de la teoría cinética de gases, es decir, asegurar que el modelo siempre maximice la entropía.
2. Al reducir las inestabilidades del modelo, se pueden modelar fluidos a números de Reynolds mucho mas altos. Es decir:



$$\nu = c_s^2(\tau - \delta t / 2), \quad \text{Re} = \frac{UL}{\nu}, \quad \tau \rightarrow \frac{\delta t}{2}$$

$$\text{Re} = 51200$$

Importante: Con este formalismo no se pueden eliminar las inestabilidades debidas a que  $f^{eq}$  toma valores negativos.

# ENTROPIA EN LA TEORIA DE BOLTZMANN

Teorema H en la teoría cinética de gases:

$$-S = H = k_B \int f \ln f d^3v \quad \frac{dH}{dt} \leq 0$$



Ludwig Boltzmann in 1872

Es una consecuencia de la ecuación de Boltzmann (en el continuo):

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \Omega(f)$$

Y se cumple:

$$\frac{dH}{dt} = 0 \iff f = f^{eq} = A e^{-m(u-v)^2/2kT}$$

# ENTROPIC LATTICE BOLTZMANN

En lattice cúbicos (D2Q9, D3Q19, ...) el teorema H es [1]:

$$H = \sum_{i=0}^N f_i \ln\left(\frac{f_i}{\omega_i}\right) \quad \frac{dH}{dt} \leq 0$$

Entonces la idea es hacer que la evolución del sistema siempre minimice la función H sin cambiar las ecuaciones macroscópicas:



Se puede utilizar un algoritmo de Newton.

Note que si la distribución toma valores negativos, H queda indefinida.

[1] I. V. Karlin, A. Ferrante, and H. C. Öttinger, *Europhys. Lett.* 47, 182 1999

# RECORDEMOS...

$$f^{eq} = A e^{-m(u-v)^2/2kT} = e^{-v^2/2c_s^2} \sum_{n=0}^2 a_n(x, u, t) H_n(v)$$



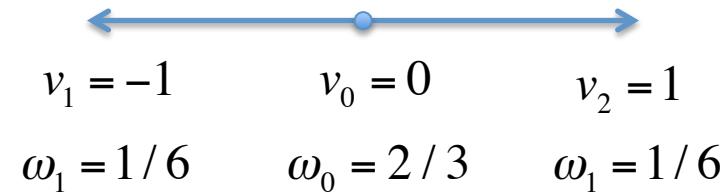
$$f_i^{eq} = \omega_i \sum_{n=0}^2 a_n(x, u, t) H_n(v_i)$$

$$a_n(x, u, t) = \sum_{i=0}^2 f_i^{eq} H_n(v_i) = \int f^{eq} H_n(v) dv$$

$H_0(v) = 1$
$H_1(v) = \frac{v}{c_s}$
$H_2(v) = \frac{1}{\sqrt{2}} \left( \frac{v^2}{c_s^2} - 1 \right)$

Estos coeficientes se pueden escribir en función de los momentos:

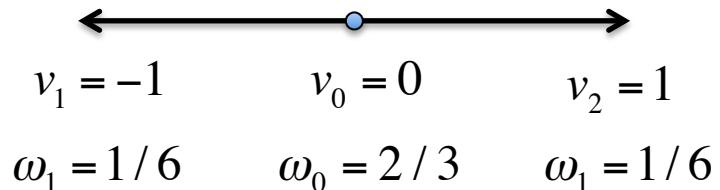
$a_0 = \Pi_0$	$, \quad a_1 = \frac{\Pi_1}{c_s}$	$, \quad a_2 = \frac{1}{\sqrt{2}} \left( \frac{\Pi_2^2}{c_s^2} - 1 \right)$
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# ENTROPIC LATTICE BOLTZMANN MODEL

Primero debemos calcular los coeficientes que el lattice esta reproduciendo:

$$a_n(x,u,t) = \sum_{i=0}^2 f_i H_n(v_i)$$



Note que no es la distribución de equilibrio, es la distribución total  $f$ . Luego reconstruimos la función que el lattice esta soportando:

$$f_i^* = \omega_i \sum_{n=0}^2 a_n(x,u,t) H_n(v_i)$$

Y el residuo:

$$f_i^{res} = f_i - f_i^*$$

$$\boxed{H_0(v) = 1, \quad H_1(v) = \frac{v}{c_s}, \quad H_2(v) = \frac{1}{\sqrt{2}} \left( \frac{v^2}{c_s^2} - 1 \right)}$$

# ENTROPIC LATTICE BOLTZMANN MODEL

Redefinimos nuestra función de distribución:

$$f_i = f_i^* + \gamma f_i^{res} \quad \gamma : \text{Parámetro para optimizar}$$

Escribimos nuestra función H:

$$H = \sum_{i=0}^N f_i \ln\left(\frac{f_i}{\omega_i}\right) \rightarrow H = \sum_{i=0}^N \left(f_i^* + \gamma f_i^{res}\right) \ln\left[\frac{f_i^* + \gamma f_i^{res}}{\omega_i}\right]$$

Para minimizar H, debemos resolver

$$H'(\gamma) = F(\gamma) = \sum_{i=0}^N f_i^{res} \left(1 + \ln\left[\frac{f_i^* + \gamma f_i^{res}}{\omega_i}\right]\right) = 0$$

Podemos utilizar el método de Newton para encontrar los ceros de F.

# ENTROPIC LATTICE BOLTZMANN MODEL

Para hallar las aproximaciones a los ceros de una función  $f(x)$  uno puede usar el método de Newton:

$$x_{l+1} = x_l - \frac{f(x_l)}{f'(x_l)}$$

Iterando hasta que  $x_l$  no cambie más. Entonces:

$$F(\gamma) = \sum_{i=0}^N f_i^{res} \left( 1 + \ln \left[ \frac{f_i^* + \gamma f_i^{res}}{\omega_i} \right] \right) , \quad F'(\gamma) = \sum_{i=0}^N \frac{(f_i^{res})^2}{f_i^* + \gamma f_i^{res}}$$

Entonces la subrutina debe iterar:

$$\gamma_{l+1} = \gamma_l - \frac{\sum_{i=0}^N f_i^{res} \left( 1 + \ln \left[ \frac{f_i^* + \gamma_l f_i^{res}}{\omega_i} \right] \right)}{\sum_{i=0}^N \frac{(f_i^{res})^2}{f_i^* + \gamma_l f_i^{res}}}$$

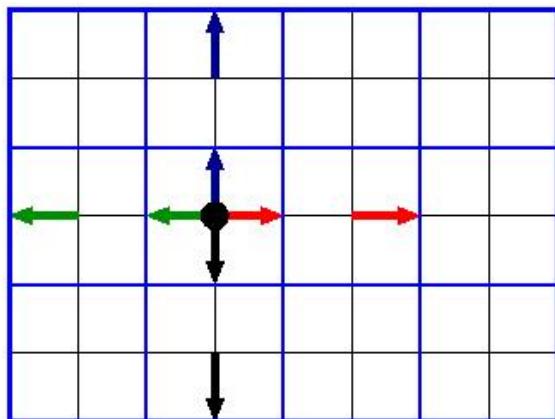
Hasta que  $\gamma_l$  no cambie.  
Como condición inicial uno  
puede escoger  $\gamma_0 = 1$ .

# ENTROPIC LATTICE BOLTZMANN MODEL

Finalmente, uno reconstruye la función de distribución con el valor final de  $\gamma$ :

$$f_i = f_i^* + \gamma f_i^{res}$$

Y continua con el paso de advección.



El modelo de lattice Boltzmann entrópico puede introducir fluctuaciones de viscosidad local. Por eso, generalmente uno usa valores efectivos de ésta para comparar con experimentos.

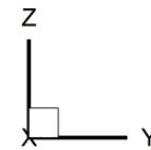
Nota: El método de Newton usualmente converge muy rápido, después de unas pocas iteraciones. Por lo tanto, el costo computacional no se incrementa demasiado.

# ENTROPIC LATTICE BOLTZMANN MODEL



Dorschner, B., Bösch, F., Chikatamarla, S. S., Boulouchos, K., & Karlin, I. V. (2016). *Journal of Fluid Mechanics*, 801, 623-651.

# ENTROPIC LATTICE BOLTZMANN MODEL



Moqaddam, A. M., Chikatamarla, S. S., & Karlin, I. V. (2017). Journal of Fluid Mechanics, 824, 866-885.