Une analyse asymptotique des schémas de Boltzmann sur réseau

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atelier "Schémas numériques de type Boltzmann"

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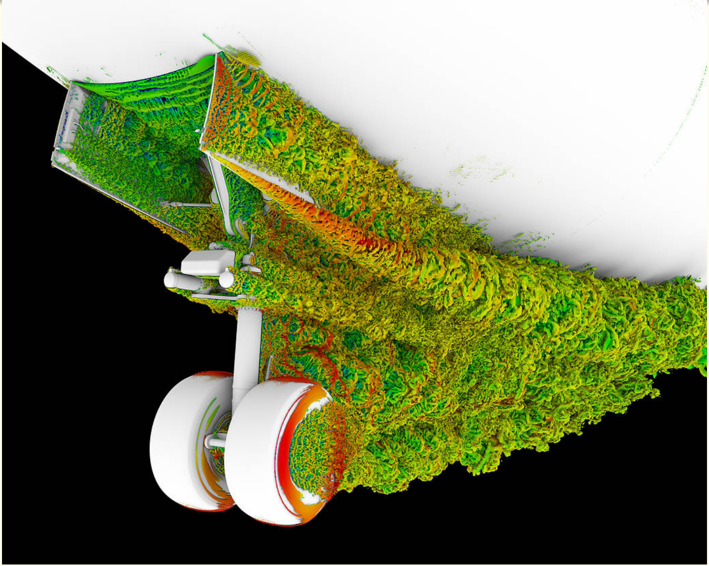
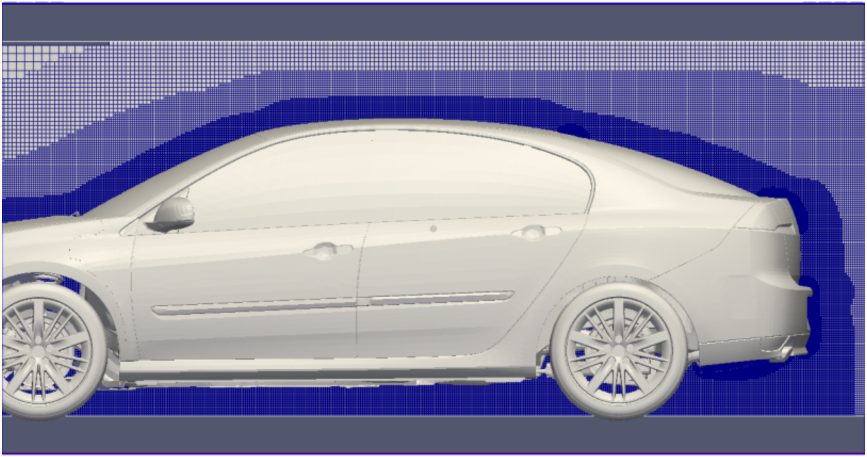
Exa's Powerflow software (2017)



complex vortex structure under the Boeing 777 www.nasa.gov

LaBS-ProLB: aerodynamics software (Renault, 2013)



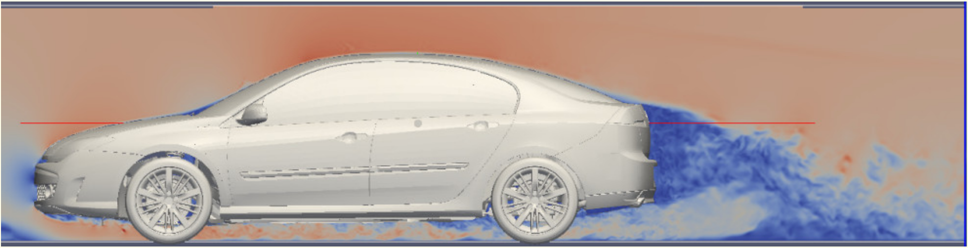
lyoncalcul.univ-lyon1.fr

186 surfaces generate 2.3 millions of triangles

10 levels of mesh refinement (octree) size of the smallest mesh: 1.25 mm

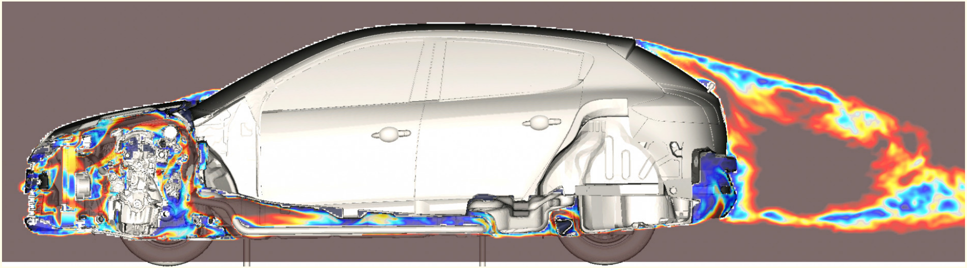
88.6 millions of meshes, 300 000 time iterations

LaBS-ProLB: aerodynamics software (Renault, 2013)



instantaneous velocity m2p2.fr

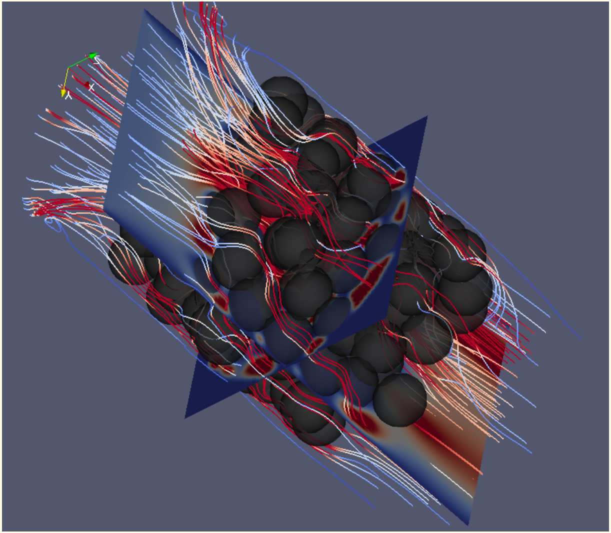
LaBS-ProLB : aérodynamique (Renault, 2013)



with the internal flow

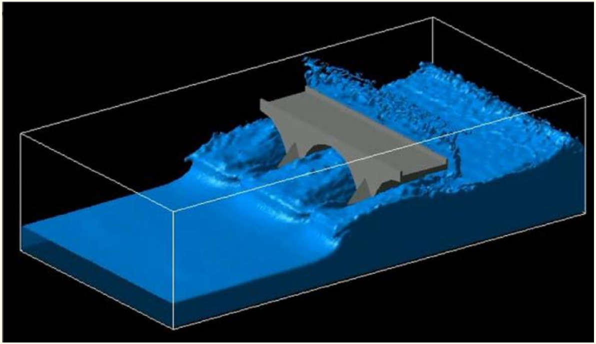
m2p2.fr

flows in porous media



Palabos project, university of Geneva www.cfdem.com

fluid mechanics for civil engineering



Technische Universität Braunschweig tu-braunschweig.de

pylbm

Loïc Gouarin (CMAP, Écolpe Polytechnique)
et Benjamin Graille (LMO Orsay)

github.com/pylbm
www.imo.universite-paris-saclay.fr/∼ benjamin.graille/pylbm.php
www.youtube.com/channel/UCEfCyEjGAZx1UsjaqRmtcVg/videos

module Python permettant d'utiliser
différentes méthodes de Boltzmann sur réseau

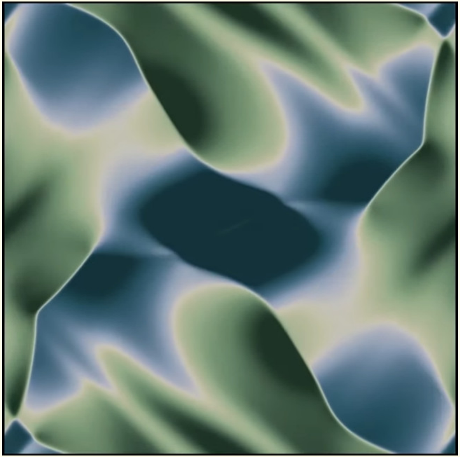
s'appuie sur le package SymPy pour décrire de manière formelle
les polynômes associés aux schémas utilisés

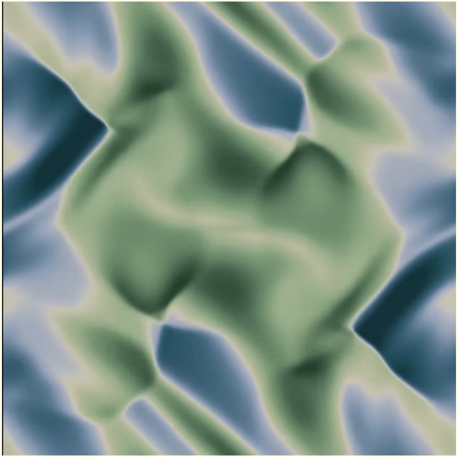
un code est ensuite généré en fonction de ces paramètres
physiques et mathématiques.

l'utilisateur peut créer des domaines complexes
s'appuyant sur l'union de formes simples

logiciel disponible à l'adresse pylbm.readthedocs.io

pylbm : Orsag-Tang vortex





pylbm : Karman vortex street (Re = 2500)

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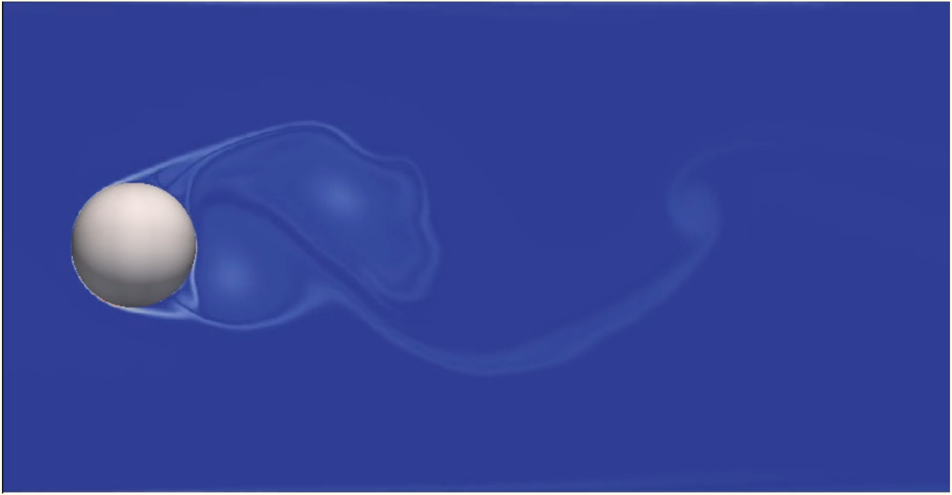
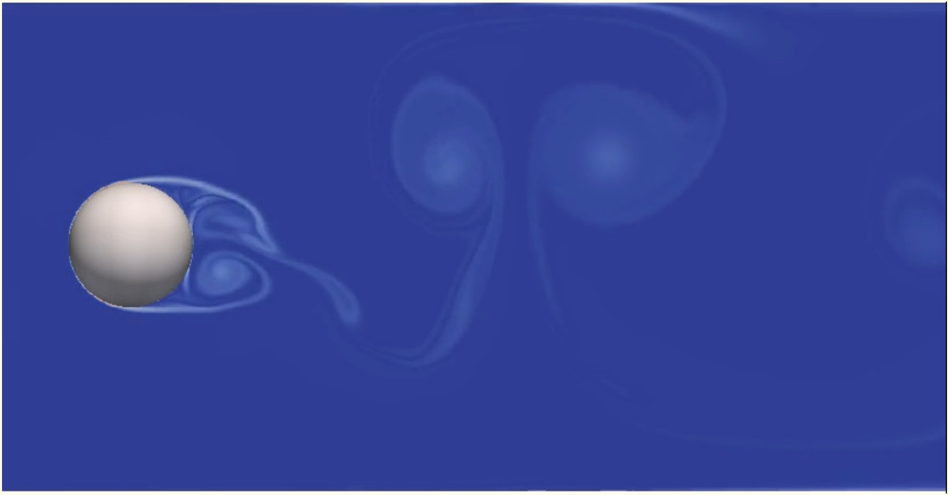
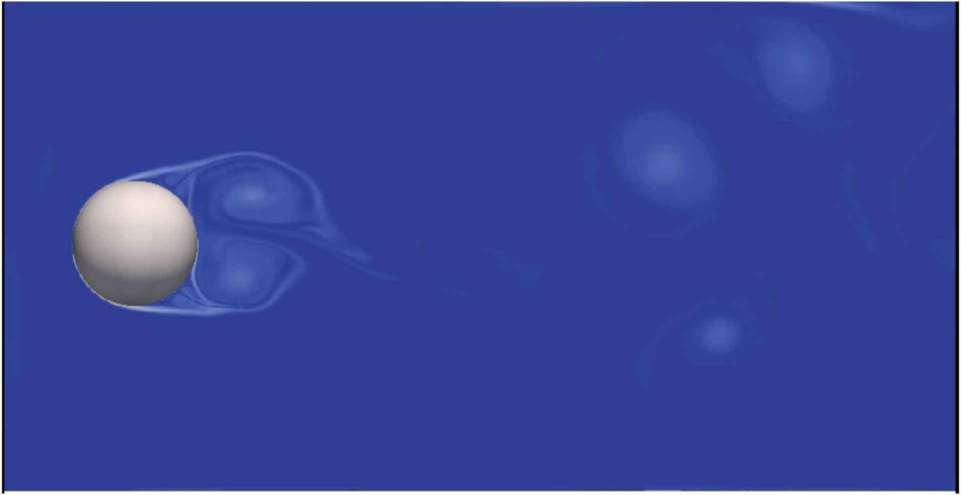


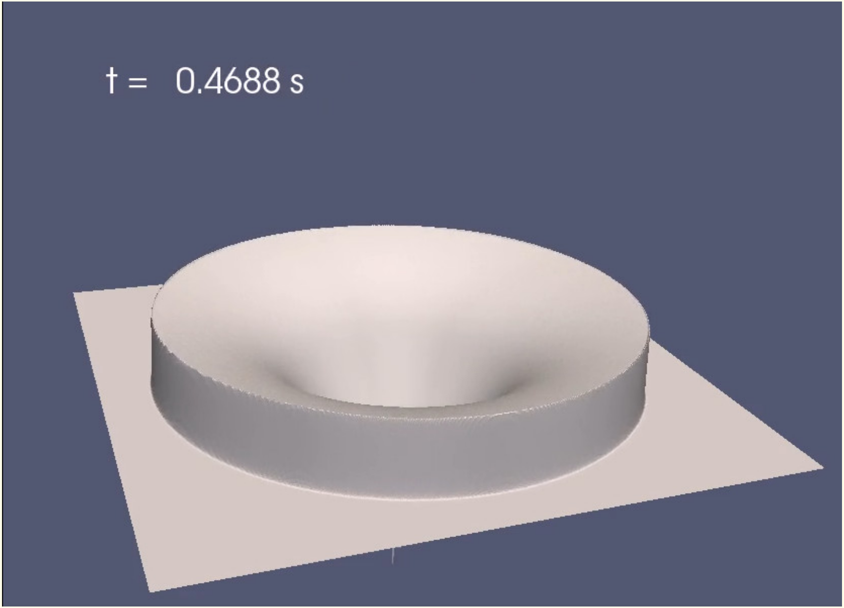
pylbm : Karman vortex street (Re $= 2500$)



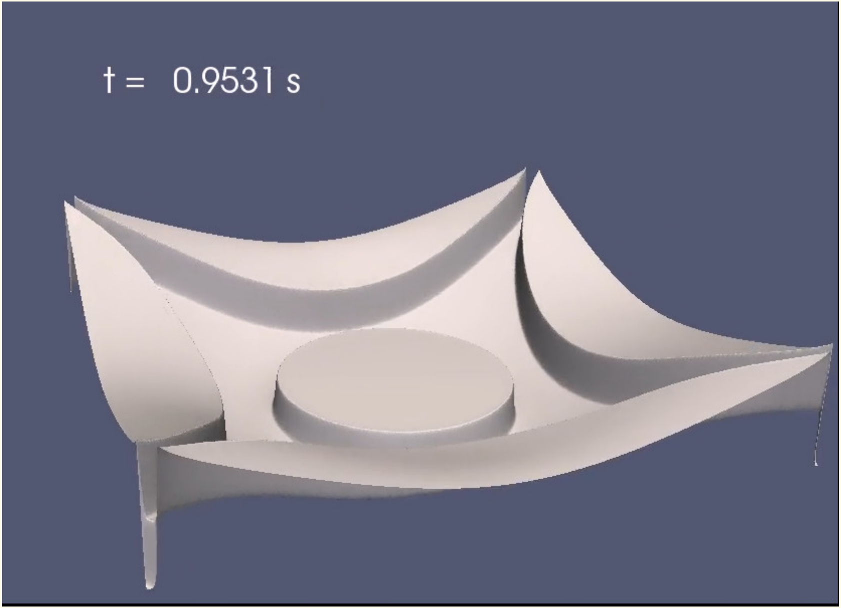
pylbm : Karman vortex street (Re = 2500)



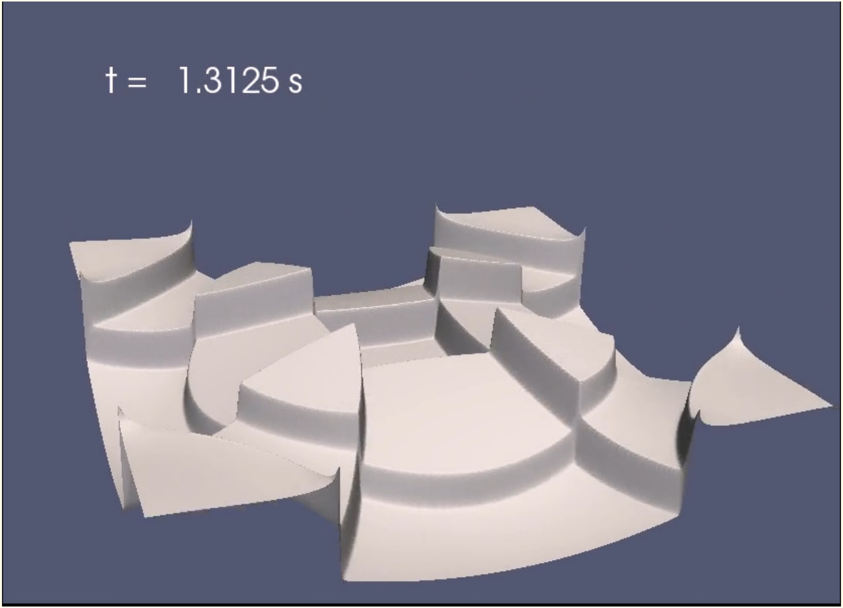
pylbm : shallow water



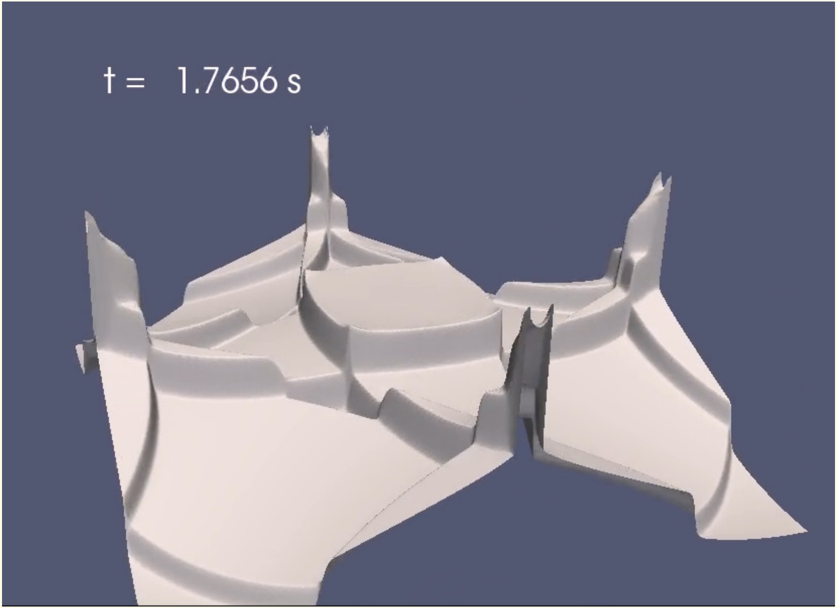
pylbm : shallow water



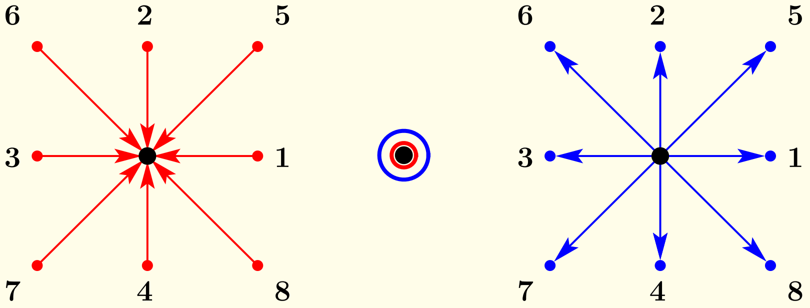
pylbm : shallow water



pylbm : shallow water



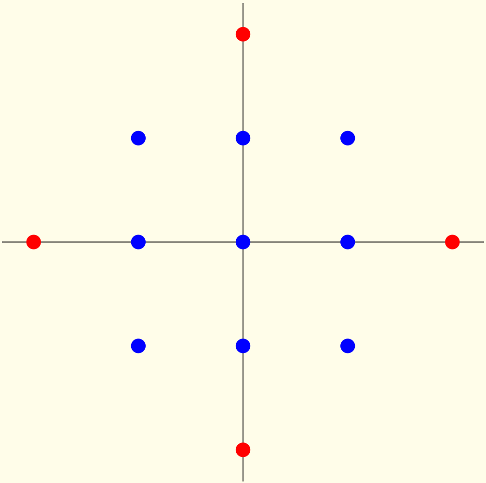
"collide-stream" for lattice Boltzmann schemes



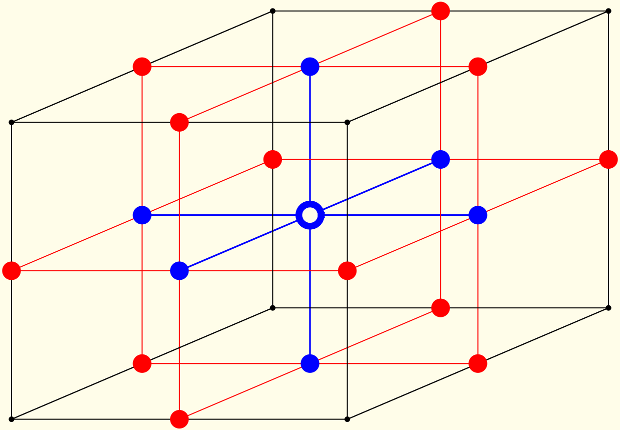
advection collision advection

D2Q9 scheme

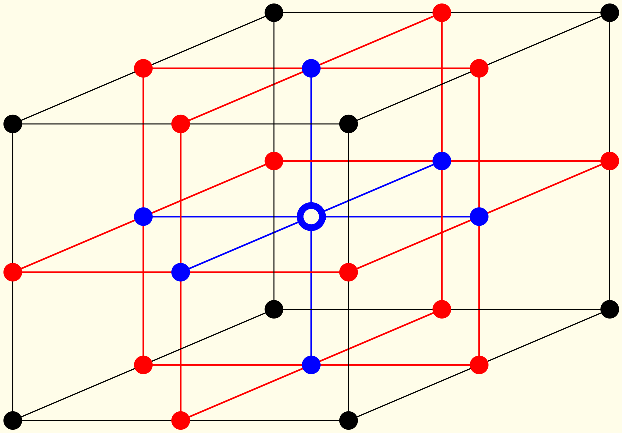
D2Q13



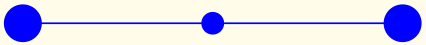
D3Q19



D3Q27



D1Q2, D1Q3



D1Q2 : Torsten Carleman (1892-1949)

D1Q3 : James Broadwell (1921-2018)

interior algorithm

Boltzmann model with a finite number of velocities

$$\frac{\partial f_i}{\partial t} + v_i . \nabla_x f_i = Q_i(f), \; 0 \leq i < q$$

$m = M\, f$: vector of moments $m \in \mathbb{R}^q$:

constant invertible matrix M ("d'Humières matrix", 1992)

$$m_k \equiv \sum_{0 \leq j < q} M_{kj} \; f_j \,, \; 0 \leq k < q$$

N conservation laws $(1 \leq N < q)$

the N first moments of the collision kernel are equal to zero:

$$\sum_{0 \leq j < q} M_{kj} \; Q_j(f) = 0 \,, \quad \forall f \in \mathbb{R}^q, \; 0 \leq k < N$$

divide the vector of moments into two families: $m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}$

N conservation laws for macroscopic variables W

$$\frac{\partial W_k}{\partial t} + \sum_{1 \leq \alpha \leq d} \sum_{0 \leq j < q} M_{kj} \; v_j^\alpha \; \frac{\partial f_j}{\partial x_\alpha} = 0 \,, \quad 0 \leq k < N$$

$q - N$ nonconserved moments or microscopic variables Y

interior algorithm *(ii)*

$$\frac{\partial f_i}{\partial t} + v_i . \nabla_x f_i = Q_i(f), \ 0 \leq i < q$$

equilibrim states $f^{\rm eq}$ defined by the conditions $Q(f^{\rm eq}) = 0$

characterized with a regular vector field $\Phi : \mathbb{R}^N \longrightarrow \mathbb{R}^{q-N}$

$$f^{\rm eq} = M^{-1} \begin{pmatrix} W \\ \Phi(W) \end{pmatrix}$$

the vector field $W \longmapsto Y^{\rm eq} \equiv \Phi(W)$ defines the equilibrium states

hypothesis : the jacobian matrix ${\rm d}Q(f^{\rm eq})$ at equilibrium

is diagonalizable with real eigenvalues and real eigenvectors

$$M \, {\rm d}Q(f^{\rm eq}) \, M^{-1} = -{\rm diag}\left(0, \ldots, 0, \frac{1}{\tau_1}, \ldots, \frac{1}{\tau_{q-N}}\right), \ \tau_\ell > 0$$

MRT hypothesis: the jacobian operator ${\rm d}Q(f^{\rm eq})$

admits the matrix M^{-1} as a matrix of eigenvectors

Bhatnagar-Gross-Krook type hypothesis

the state f is close to equilibrium $f^{\rm eq}$

collision kernel Q approximated at first order:

$$Q(f) \simeq Q(f^{\rm eq}) + {\rm d}Q(f^{\rm eq}).(f - f^{\rm eq}) \ \simeq {\rm d}Q(f^{\rm eq}).(f - f^{\rm eq})$$

interior algorithm *(iii)*

Lattice Boltzmann scheme with multiple relaxation times

(d'Humières, 1992)

f_j : discrete particle distribution with velocity v_j

moments $m = (W\,,\ Y)^{\rm t} \equiv M\, f$

$$\frac{\partial f_i}{\partial t} + v_i . \nabla_x f_i = \big({\rm d}Q(f^{\rm eq}).(f - f^{\rm eq}) \big)_i ,\ \ 0 \le i < q$$

(i) "collide": nonlinear relaxation, neglect the advection operator

$$\frac{\partial W}{\partial t} = 0\,,\ \ \frac{\partial Y}{\partial t} = -{\rm diag}\big(\frac{1}{\tau_1},\, \ldots,\, \frac{1}{\tau_{q-N}}\big)(Y - \Phi(W))$$

use a simple forward Euler scheme:

$$W^* = W\,,\ \ Y^* = Y + S\,(\Phi(W) - Y),\ \ S = {\rm diag}\ \big(\frac{\Delta t}{\tau_k}\big)$$

$$f^* = M^{-1} \begin{pmatrix} W^* \\ Y^* \end{pmatrix};\qquad s_k = \frac{\Delta t}{\tau_k} \text{ fixed numerical parameter}$$

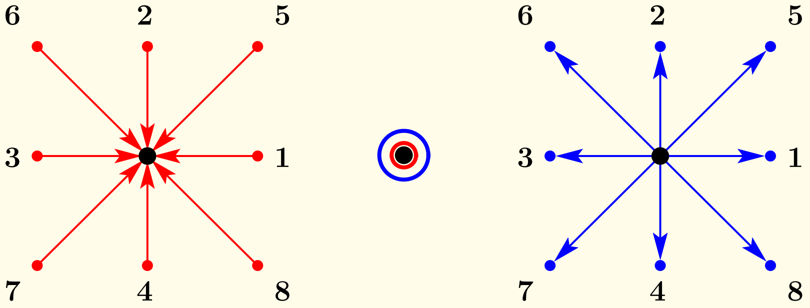
(ii) "stream": linear advection, neglect the local nonlinear collision

$$\frac{\partial f_i}{\partial t} + v_i . \nabla_x f_i = 0$$

method of characteristics when it is exact !

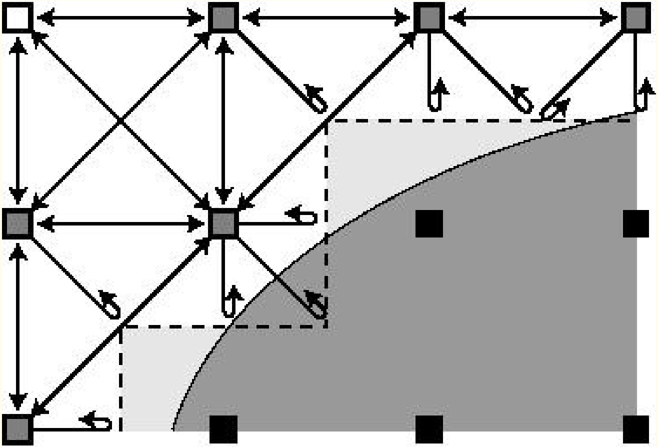
compact description: $f_j(x,\, t + \Delta t) \,=\, f_j^*(x - v_j\, \Delta t,\, t)$

interior algorithm *(iv)*



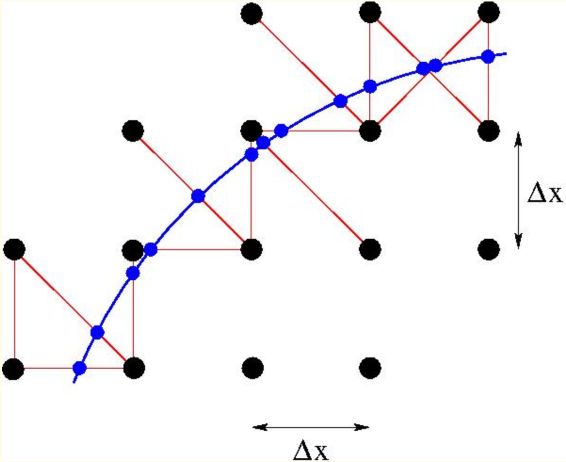
advection	collision	advection
f	$m,\ W^*,\ Y^*,\ f^*$	f

boundary conditions : staircase approximation



Ed Llewellin, Dunham university

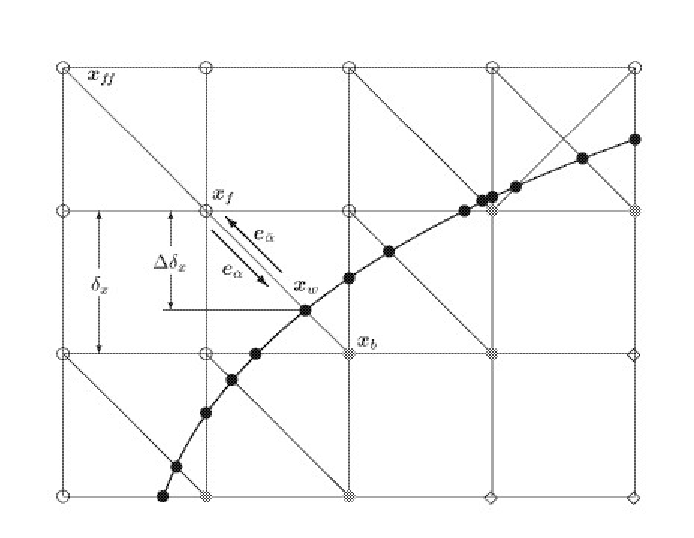
boundary conditions : precise approach



curved boundary: take into account all the red links

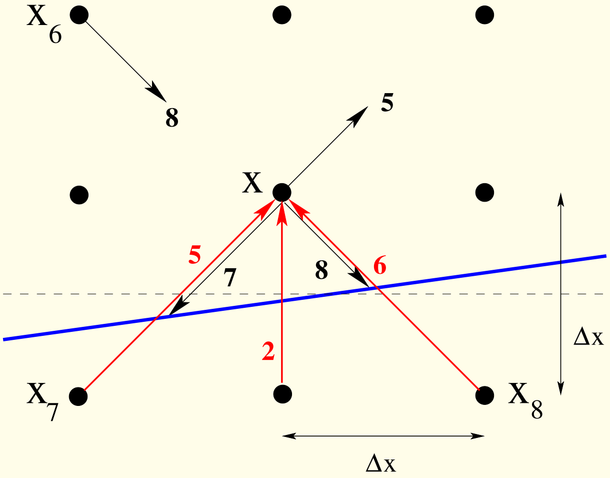
Bouzidi - Firdaouss - Lallemand boundary condition (2001)

boundary conditions : precise approach *(ii)*



Mei, Yu, Shyy, Luo, *Phys. Rev. E*, april 2002

boundary conditions : precise approach *(iii)*



"ABCD" method: exact exponential expansion

$$f_j(x,\, t+\Delta t) \,=\, f_j^*(x - v_j\,\Delta t,\, t)$$

$$\begin{aligned}
m_k(x, t+\Delta t) &= \sum_j M_{kj}\, f_j^*(x - v_j\,\Delta t,\, t) \\
&= \sum_{j\,\ell} M_{kj}\,(M^{-1})_{j\ell}\; m_\ell^*(x - v_j\,\Delta t,\, t) \\
&= \sum_{j\,\ell} M_{kj}\,(M^{-1})_{j\ell}\; \sum_{n=0}^{\infty} \frac{1}{n!}\Big(-\Delta t \sum_\alpha v_j^\alpha\,\partial_\alpha\Big)^n\, m_\ell^*(x,\, t) \\
&= \sum_\ell \sum_{n=0}^{\infty} \frac{1}{n!} \sum_j M_{kj}\,\Big(-\Delta t \sum_\alpha v_j^\alpha\,\partial_\alpha\Big)^n\,(M^{-1})_{j\ell}\; m_\ell^*(x,\, t) \\
&= \sum_\ell \Big[\, \sum_{n=0}^{\infty} \frac{1}{n!}\,\big(-\Delta t\,\Lambda\big)^n_{k\ell} \Big]\; m_\ell^*(x,\, t) \\
&= \sum_\ell \exp(-\Delta t\,\Lambda)_{k\ell}\; m_\ell^*(x,\, t) \\
&= \Big(\exp(-\Delta t\,\Lambda)\; m^*(x,\, t)\Big)_k
\end{aligned}$$

"ABCD" method: exact exponential expansion *(ii)*

$$f_j(x,\ t + \Delta t) \ = \ f_j^*(x - v_j\, \Delta t,\ t)$$

Momentum-velocity operator matrix

$$\Lambda = M \ \mathrm{diag} \Big(\textstyle\sum_{1 \leq \alpha \leq d} v^\alpha\, \partial_\alpha \Big)\ M^{-1}$$

$$m(x, t + \Delta t) = \exp(-\Delta t\, \Lambda)\ m^*(x,\ t)$$

$$\exp(-\Delta t\, \Lambda) = \mathrm{I} - \Delta t\, \Lambda + \frac{\Delta t^2}{2}\, \Lambda^2 + \ldots + (-1)^k\, \frac{\Delta t^k}{k!}\, \Lambda^k + \ldots$$

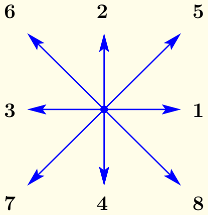
important elementary remark to obtain the final results

block decomposition $\quad \Lambda \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}$

$$\Lambda^2 = \Lambda\, \Lambda \equiv \begin{pmatrix} A_2 & B_2 \\ C_2 & D_2 \end{pmatrix} \quad \text{with} \quad \begin{pmatrix} A_2 & B_2 \\ C_2 & D_2 \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

$$A_2 = A^2 + B\, C,\ \ B_2 = A\, B + B\, D,\ \ C_2 = C\, A + D\, C,\ \ D_2 = C\, B + D^2$$

example: D2Q9 scheme



$$\lambda = \frac{\Delta x}{\Delta t}$$

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{bmatrix} \begin{matrix} \rho \\ J_x \\ J_y \\ \varepsilon \\ xx \\ xy \\ q_x \\ q_y \\ h \end{matrix}$$

the lines of this invertible matrix are chosen orthogonal

example: D2Q9 scheme *(ii)*

Momentum-velocity operator matrix $\Lambda \equiv M \,\mathrm{diag}\big(\sum_\alpha v^\alpha \, \partial_\alpha \big) \, M^{-1}$

$1 \leq \alpha \leq 2 =$ space dimension

Block decomposition $\Lambda \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}$

Operator matrix Λ for the isothermal D2Q9 scheme

ρ	J_x	J_y	ε	xx	xy	q_x	q_y	h	
0	∂_x	∂_y	0	0	0	0	0	0	ρ
$\frac{2\lambda^2}{3}\,\partial_x$	0	0	$\frac{1}{6}\,\partial_x$	$\frac{1}{2}\,\partial_x$	∂_y	0	0	0	J_x
$\frac{2\lambda^2}{3}\,\partial_y$	0	0	$\frac{1}{6}\,\partial_y$	$-\frac{1}{2}\,\partial_y$	∂_x	0	0	0	J_y
0	$\lambda^2\,\partial_x$	$\lambda^2\,\partial_y$	0	0	0	∂_x	∂_y	0	ε
0	$\frac{\lambda^2}{3}\,\partial_x$	$-\frac{\lambda^2}{3}\,\partial_y$	0	0	0	$-\frac{1}{3}\,\partial_x$	$\frac{1}{3}\,\partial_y$	0	xx
0	$\frac{2\,\lambda^2}{3}\,\partial_y$	$\frac{2\,\lambda^2}{3}\,\partial_x$	0	0	0	$\frac{1}{3}\,\partial_y$	$\frac{1}{3}\,\partial_x$	0	xy
0	0	0	$\frac{\lambda^2}{3}\,\partial_x$	$-\lambda^2\,\partial_x$	$\lambda^2\,\partial_y$	0	0	$\frac{1}{3}\,\partial_x$	q_x
0	0	0	$\frac{\lambda^2}{3}\,\partial_y$	$\lambda^2\,\partial_y$	$\lambda^2\,\partial_x$	0	0	$\frac{1}{3}\,\partial_y$	q_y
0	0	0	0	0	0	$\lambda^2\,\partial_x$	$\lambda^2\,\partial_y$	0	h

"ABCD" method: asymptotic expansion at second order

Asymptotic hypothesis: emerging partial differential equations

$$\partial_t W + \Gamma_1 + \Delta t \, \Gamma_2 = \mathrm{O}(\Delta t^2)$$

Γ_j: vector obtained after j space derivations
of the conserved moments W
and the equilibrium vector $\Phi(W)$.

Non-Conserved moments:

$$Y = \Phi(W) + \Delta t \, S^{-1} \, \Psi_1 + \mathrm{O}(\Delta t^2)$$

General nonlinear "Vilnius" algorithm at second order

$$\Gamma_1 = A \, W + B \, \Phi(W)$$

$$\Psi_1 = \mathrm{d}\Phi(W).\Gamma_1 - (C \, W + D \, \Phi(W))$$

$$\Gamma_2 = B \, \Sigma \, \Psi_1$$ with Σ the Hénon matrix: $\Sigma \equiv S^{-1} - \frac{1}{2} \, \mathrm{I}$

"ABCD" method: fourth order expansion

asymptotic expansion for the microscopic moments

$$Y = \Phi(W) + S^{-1} \left(\Delta t \, \Psi_1(W) + \Delta t^2 \, \Psi_2(W) + \Delta t^3 \, \Psi_3(W) \right) + \mathrm{O}(\Delta t^4)$$

partial differential equation for the conserved moments

$$\partial_t W + \Gamma_1(W) + \Delta t \, \Gamma_2(W) + \Delta t^2 \, \Gamma_3(W) + \Delta t^3 \, \Gamma_4(W) = \mathrm{O}(\Delta t^4)$$

third order terms

$$\Psi_2(W) = \Sigma \, \mathrm{d}\Psi_1(W).\Gamma_1(W) + \mathrm{d}\Phi(W).\Gamma_2(W) - D \, \Sigma \, \Psi_1(W)$$

$$\Gamma_3(W) = B \, \Sigma \, \Psi_2(W) + \tfrac{1}{12} B_2 \, \Psi_1(W) - \tfrac{1}{6} \, B \, \mathrm{d}\Psi_1(W).\Gamma_1(W)$$

fourth order terms

$$\begin{aligned} \Psi_3(W) = {} & \Sigma \, \mathrm{d}\Psi_1(W).\Gamma_2(W) + \mathrm{d}\Phi(W).\Gamma_3(W) - D \, \Sigma \, \Psi_2(W) \\ & + \Sigma \, \mathrm{d}\Psi_2(W).\Gamma_1(W) + \tfrac{1}{6} \, D \, \mathrm{d}\Psi_1(W).\Gamma_1(W) \\ & - \tfrac{1}{12} \, D_2 \, \Psi_1(W) - \tfrac{1}{12} \, \mathrm{d} \left(\mathrm{d}\Psi_1(W).\Gamma_1 \right).\Gamma_1(W) \end{aligned}$$

$$\begin{aligned} \Gamma_4(W) = {} & B \, \Sigma \, \Psi_3(W) + \tfrac{1}{4} \, B_2 \, \Psi_2(W) + \tfrac{1}{6} \, B \, D_2 \, \Sigma \, \Psi_1(W) \\ & - \tfrac{1}{6} \, A \, B \, \Psi_2(W) - \tfrac{1}{6} \, B \left(\mathrm{d} \left(\mathrm{d}\Phi.\Gamma_1 \right).\Gamma_2(W) \right. \\ & \left. + \, \mathrm{d} \left(\mathrm{d}\Phi.\Gamma_2 \right).\Gamma_1(W) \right) - \tfrac{1}{6} \, B \, \Sigma \, \mathrm{d} \left(\mathrm{d}\Psi_1(W).\Gamma_1 \right).\Gamma_1(W) \end{aligned}$$

FD, *Asymptotic Analysis*, 2022.

"ABCD" method: zero-order expansion

expand one iteration of the scheme:

$$m(x, t + \Delta t) = \exp(-\Delta t \, \Lambda) \; m^*(x, \, t) \,, \qquad m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}$$

$$m + \Delta t \, \partial_t m + \tfrac{1}{2} \, \Delta t^2 \, \partial_t^2 m + \mathrm{O}(\Delta t^3) = \\ = m^* - \Delta t \, \Lambda \, m^* + \tfrac{1}{2} \, \Delta t^2 \, \Lambda^2 \, m^* + \mathrm{O}(\Delta t^3)$$

replace the vector m by its two components W and Y

$$W + \Delta t \, \partial_t W + \tfrac{1}{2} \, \Delta t^2 \, \partial_t^2 W + \mathrm{O}(\Delta t^3) = \\ = W - \Delta t \, (A \, W + B \, Y^*) + \tfrac{1}{2} \, \Delta t^2 \, (A_2 \, W + B_2 \, Y^*) + \mathrm{O}(\Delta t^3)$$

$$Y + \Delta t \, \partial_t Y + \tfrac{1}{2} \, \Delta t^2 \, \partial_t^2 Y + \mathrm{O}(\Delta t^3) = \\ = Y^* - \Delta t \, (C \, W + D \, Y^*) + \tfrac{1}{2} \, \Delta t^2 \, (C_2 \, W + D_2 \, Y^*) + \mathrm{O}(\Delta t^3)$$

at zero-order: $Y - Y^* = \mathrm{O}(\Delta t)$ and $Y^* \equiv Y + S \, (\Phi(W) - Y)$

the matrix S is supposed fixed

then $Y = \Phi(W) + \mathrm{O}(\Delta t)$ and $Y^* = \Phi(W) + \mathrm{O}(\Delta t)$

"ABCD" method: first-order expansion

$$Y^* = \Phi(W) + \mathrm{O}(\Delta t)$$

second-order partial differential equations reduced at first-order:

$$\partial_t W + \mathrm{O}(\Delta t) = -\big(A\,W + B\,Y^*\big) + \mathrm{O}(\Delta t)$$

then $\quad \partial_t W + \Gamma_1 = \mathrm{O}(\Delta t) \quad$ with $\quad \Gamma_1 = A\,W + B\,\Phi(W)$

we report this result for the microscopic variables

$$\partial_t Y = \mathrm{d}\Phi(W).\partial_t W + \mathrm{O}(\Delta t) = \mathrm{d}\Phi(W).(-\Gamma_1) + \mathrm{O}(\Delta t)$$

$$\partial_t Y = -\,\mathrm{d}\Phi(W).\Gamma_1 + \mathrm{O}(\Delta t)$$

but we know that

$$Y + \Delta t\,\partial_t Y + \mathrm{O}(\Delta t^2) = Y^* - \Delta t\,(C\,W + D\,Y^*) + \tfrac{1}{2} + \mathrm{O}(\Delta t^2)$$

then $\quad Y - Y^* = -\Delta t\,\partial_t Y - \Delta t\,(C\,W + D\,Y^*) + \mathrm{O}(\Delta t^2)$

and $\quad S\,(Y - \Phi) = \Delta t\,\big(\mathrm{d}\Phi(W).\Gamma_1 - (C\,W + D\,\Phi)\big) + \mathrm{O}(\Delta t^2)$

finally

$$Y = \Phi + \Delta t\; S^{-1}\,\big(\mathrm{d}\Phi(W).\Gamma_1 - (C\,W + D\,\Phi)\big) + \mathrm{O}(\Delta t^2)$$

and $\quad \Psi_1 = \mathrm{d}\Phi(W).\Gamma_1 - (C\,W + D\,\Phi)$

"ABCD" method: non-conserved moments at first-order

$$\Psi_1 = \mathrm{d}\Phi(W).\Gamma_1 - (C\,W + D\,\Phi)$$

Hénon matrix: $\Sigma \equiv S^{-1} - \frac{1}{2}\,\mathrm{I}$

$$Y = \Phi(W) + \Delta t\ S^{-1}\ \Psi_1 + \mathrm{O}(\Delta t^2)$$

then

$$\begin{aligned} Y^* &= Y + S\,(\Phi - Y) \\ &= Y - \big(\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2)\big) \\ &= \Phi(W) + \left(\Sigma + \tfrac{1}{2}\,\mathrm{I}\right)\big(\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2)\big) - \big(\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2)\big) \\ &= \Phi(W) + \left(\Sigma - \tfrac{1}{2}\,\mathrm{I}\right)\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2) \end{aligned}$$

and

$$\begin{aligned} Y &= \Phi(W) + \left(\Sigma + \tfrac{1}{2}\,\mathrm{I}\right)\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2) \\ Y^* &= \Phi(W) + \left(\Sigma - \tfrac{1}{2}\,\mathrm{I}\right)\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2) \end{aligned}$$

"ABCD" method: second-order expansion

$$Y^* = \Phi(W) + \big(\Sigma - \tfrac{1}{2}\,\mathrm{I}\big)\,\Delta t\,\Psi_1 + \mathrm{O}(\Delta t^2)$$

$$\partial_t W + \tfrac{1}{2}\,\Delta t\,\partial_t^2 W + \mathrm{O}(\Delta t^2) =$$

$$= (A\,W + B\,Y^*) + \tfrac{1}{2}\,\Delta t\,(A_2\,W + B_2\,Y^*) + \mathrm{O}(\Delta t^2)$$

$$A_2 = A^2 + B\,C,\; B_2 = A\,B + B\,D$$

$$\partial_t W = -\Gamma_1 + \mathrm{O}(\Delta t) = -(A\,W + B\,\Phi(W)) + \mathrm{O}(\Delta t)$$

then

$$\partial_t^2 W = -\partial_t\big(\Gamma_1 + \mathrm{O}(\Delta t)\big) = -\,\mathrm{d}\Gamma_1.\partial_t W + \mathrm{O}(\Delta t)$$

$$= \mathrm{d}\Gamma_1.\Gamma_1 + \mathrm{O}(\Delta t)$$

$$= A\,\Gamma_1 + B\,\mathrm{d}\Phi.\Gamma_1 + \mathrm{O}(\Delta t)$$

$$\partial_t W = -\tfrac{1}{2}\,\Delta t\,(A\,\Gamma_1 + B\,\mathrm{d}\Phi.\Gamma_1) - \mathbf{A\,W} - B\,\big(\mathbf{\Phi} + (\Sigma - \tfrac{1}{2}\mathrm{I})\,\Delta t\,\Psi_1\big)$$

$$+\tfrac{1}{2}\,\Delta t\,\big((A^2 + B\,C)\,W + (A\,B + B\,D)\,\Phi\big) + \mathrm{O}(\Delta t^2)$$

$$= -\mathbf{A\,W} - \mathbf{B\,\Phi} - \Delta t\,\Big[\tfrac{1}{2}(A\,(A\,W + B\,\Phi)) + \tfrac{1}{2}\,B\,\mathrm{d}\Phi.\Gamma_1$$

$$+B\,\Sigma\,\Psi_1 - \tfrac{1}{2}B\,(\,\mathrm{d}\Phi.\Gamma_1 - C\,W - D\,\Phi)$$

$$-\tfrac{1}{2}\,(A^2 + B\,C)\,W - \tfrac{1}{2}\,(A\,B + B\,D)\,\Phi\Big] + \mathrm{O}(\Delta t^2)$$

$$= -\mathbf{A\,W} - \mathbf{B\,\Phi} - \Delta t\,B\,\Sigma\,\Psi_1 + \mathrm{O}(\Delta t^2)$$

$$\partial_t W = -\Gamma_1 - \Delta t\,B\,\Sigma\,\Psi_1 + \mathrm{O}(\Delta t^2) \qquad \text{and} \qquad \Gamma_2 = B\,\Sigma\,\Psi_1$$

"ABCD" Taylor expansion method

$$\Lambda = M \,\mathrm{diag}\left(\sum_{1 \leq \alpha \leq d} v^\alpha \, \partial_\alpha \right) M^{-1} \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

$$m\,(x, t + \Delta t) \equiv \begin{pmatrix} W \\ Y \end{pmatrix} (x, t + \Delta t) = \exp\left(-\Delta t \, \Lambda\right) \, m^*(x, \, t)$$

$$W^* = W \,, \quad Y^* = Y + S \left(\Phi(W) - Y \right)$$

hypotheses: $M, \ \Lambda, \ S$ and $\lambda \equiv \frac{\Delta x}{\Delta t}$ are **fixed**

asymptotic expansion of the non-conserved moments

$$Y = \Phi(W) + \Delta t \, S^{-1} \, \Psi_1 + \mathrm{O}(\Delta t^2)$$

emerging asymptotic partial differential equations

$$\partial_t W + \Gamma_1 + \Delta t \, \Gamma_2 = \mathrm{O}(\Delta t^2)$$

Γ_j: vector obtained after j space derivations
of the conserved moments W and the equilibrium $\Phi(W)$

general nonlinear ABCD algorithm at second order

$$\Gamma_1 = A \, W + B \, \Phi(W)$$

$$\Psi_1 = \mathrm{d}\Phi(W).\Gamma_1 - \left(C \, W + D \, \Phi(W) \right)$$

$$\Gamma_2 = B \, \Sigma \, \Psi_1$$ with Σ the Hénon matrix: $\Sigma \equiv S^{-1} - \frac{1}{2} \, \mathrm{I}$

possible to **recover formally the Navier-Stokes equations?**

formal calculus with SageMath

SageMath: free open-source mathematics software system
licensed under the GNU General Public License.

It builds on top of many existing open-source packages:
NumPy, SciPy, matplotlib, Sympy, Maxima, GAP, FLINT, R, ...

www.sagemath.org

what lattice Boltzmann scheme for Naver-Stokes ?

- Isothermal Navier-Stokes

  D2Q9 and D2Q13

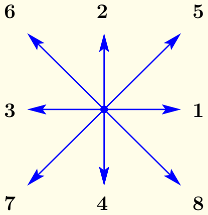
  D3Q19, D3Q27, D3Q33 and D3Q27-2

- Navier-Stokes with energy conservation

  D2Q13, D2Q17, D2V17 and D2W17

  D3Q33 and D3Q27-2

D2Q9



$$\lambda = \frac{\Delta x}{\Delta t}$$

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{bmatrix} \begin{matrix} \rho \\ J_x \\ J_y \\ \varepsilon \\ xx \\ xy \\ q_x \\ q_y \\ h \end{matrix}$$

the lines of this invertible matrix are chosen orthogonal

D2Q9 *(ii)*

Momentum-velocity operator matrix $\Lambda \equiv M \, \mathrm{diag}\big(\sum_\alpha v^\alpha \, \partial_\alpha \big) \, M^{-1}$

$1 \leq \alpha \leq 2 =$ space dimension

Block decomposition $\Lambda \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}$

Operator matrix Λ for the isothermal D2Q9 scheme

	ρ	J_x	J_y	ε	xx	xy	q_x	q_y	h
ρ	0	∂_x	∂_y	0	0	0	0	0	0
J_x	$\frac{2\lambda^2}{3}\,\partial_x$	0	0	$\frac{1}{6}\,\partial_x$	$\frac{1}{2}\,\partial_x$	∂_y	0	0	0
J_y	$\frac{2\lambda^2}{3}\,\partial_y$	0	0	$\frac{1}{6}\,\partial_y$	$-\frac{1}{2}\,\partial_y$	∂_x	0	0	0
ε	0	$\lambda^2\,\partial_x$	$\lambda^2\,\partial_y$	0	0	0	∂_x	∂_y	0
xx	0	$\frac{\lambda^2}{3}\,\partial_x$	$-\frac{\lambda^2}{3}\,\partial_y$	0	0	0	$-\frac{1}{3}\,\partial_x$	$\frac{1}{3}\,\partial_y$	0
xy	0	$\frac{2\,\lambda^2}{3}\,\partial_y$	$\frac{2\,\lambda^2}{3}\,\partial_x$	0	0	0	$\frac{1}{3}\,\partial_y$	$\frac{1}{3}\,\partial_x$	0
q_x	0	0	0	$\frac{\lambda^2}{3}\,\partial_x$	$-\lambda^2\,\partial_x$	$\lambda^2\,\partial_y$	0	0	$\frac{1}{3}\,\partial_x$
q_y	0	0	0	$\frac{\lambda^2}{3}\,\partial_y$	$\lambda^2\,\partial_y$	$\lambda^2\,\partial_x$	0	0	$\frac{1}{3}\,\partial_y$
h	0	0	0	0	0	0	$\lambda^2\,\partial_x$	$\lambda^2\,\partial_y$	0

first order partial differential equations

at first order $\Gamma_1 = A\, W + B\, \Phi(W)$

$$\Gamma_1 = \begin{cases} \partial_x J_x + \partial_y J_y \\ \frac{2}{3}\,\lambda^2\,\partial_x \rho + \frac{1}{6}\,\partial_x \Phi_\varepsilon + \frac{1}{2}\,\partial_x \Phi_{xx} + \partial_y \Phi_{xy} \\ \frac{2}{3}\,\lambda^2\,\partial_y \rho + \frac{1}{6}\,\partial_y \Phi_\varepsilon - \frac{1}{2}\,\partial_y \Phi_{xx} + \partial_x \Phi_{xy} \end{cases}$$

first order terms of the Navier-Stokes equations (Euler equations)

$$\begin{cases} \partial_t \rho + \partial_x J_x + \partial_y J_y \\ \partial_t J_x \; + \; \partial_x\big(\frac{J_x^2}{\rho} + p\big) \; + \; \partial_y\big(\frac{J_x\, J_y}{\rho}\big) \\ \partial_t J_y \; + \; \partial_x\big(\frac{J_x\, J_y}{\rho}\big) \; + \; \partial_y\big(\frac{J_y^2}{\rho} + p\big) \end{cases}$$

identify the two expressions $(J_x \equiv \rho\, u,\;\; J_y \equiv \rho\, v)$

$$\begin{cases} \Phi_\varepsilon & = & 6\, p \, - \, 4\,\lambda^2\,\rho \, + \, 3\,\rho\,(u^2 + v^2) \\ \Phi_{xx} & = & \rho\,(u^2 - v^2) \\ \Phi_{xy} & = & \rho\, u\, v \end{cases}$$

D2Q9: towards second order equations

Φ : vector of moments at equilibrium

$$\Phi = \big(\Phi_\varepsilon, \Phi_{xx}, \Phi_{xy}, \Phi_{qx}, \Phi_{qy}, \Phi_h\big)^{\rm t}$$

$$\Psi_1 = {\rm d}\Phi(W).\Gamma_1 - (C\,W + D\,\Phi(W)) \in \mathbb{R}^6$$

viscous fluxes $\quad -\Delta t\,\Gamma_2 = -\Delta t\,B\,\Sigma\,\Psi_1 =$ physical fluxes ?

$$= \begin{cases} 0 \\ \partial_j \tau_{xj} \equiv \partial_x(2\,\mu\,\partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y(\mu(\partial_x v + \partial_y u)) \\ \partial_j \tau_{yj} \equiv \partial_x(\mu(\partial_x v + \partial_y u)) + \partial_y((\zeta - \mu)(\partial_x u + \partial_y v) + 2\,\mu\,\partial_y v)) \end{cases}$$

Linear system of $2 \times 2 \times 2 \times 3 = 24$ equations,

- one equation for each of the 2 moments J_x and J_y
- one equation relative to each dimension
- one equation for each of the associated partial derivatives ∂_x and ∂_y
- one equation for each of the 3 nonconserved variables ρ, u, v
  - only $3 \times 2 = 6$ unknowns (partial derivatives of Φ_{qx} and Φ_{qy})

try to avoid unphysical terms in $\partial_x \rho$ and $\partial_y \rho$
from the second order fluxes? no solution :-(

D2Q9: towards second order equations *(ii)*

$$\Phi_\varepsilon = 3\,\rho\,(u^2+v^2) - 2\,\lambda^2\,\rho, \quad \Phi_{xx} = \rho\,(u^2-v^2), \quad \Phi_{xy} = \rho\,u\,v$$

discrepancy reduced to third order terms in velocity when

$p(\rho) = \frac{\lambda^2}{3}\,\rho$: isothermal fluid with $c_s = \frac{\lambda}{\sqrt{3}}$

$\Phi_{qx} = -\rho\,\lambda^2\,u + 3\,\rho\,(u^2+v^2)\,u, \quad \Phi_{qy} = -\rho\,\lambda^2\,v + 3\,\rho\,(u^2+v^2)\,v$

Hénon matrix $\Sigma = \mathrm{diag}\big(\sigma_e,\, \sigma_x,\, \sigma_x,\, *,\, *\,*\big)$

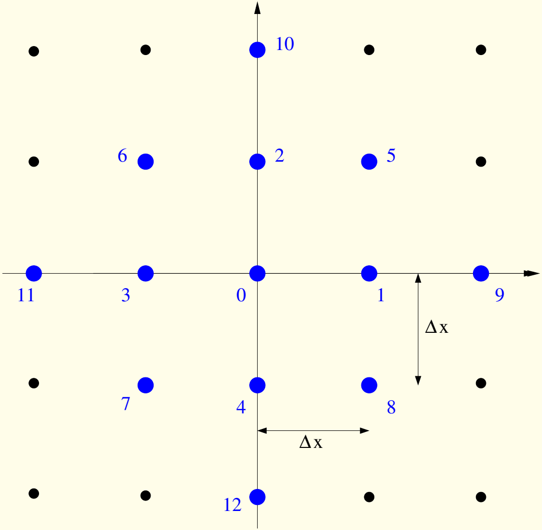
shear viscosity $\mu = \frac{\lambda}{3}\,\rho\,\sigma_x\,\Delta x$, bulk viscosity $\zeta = \frac{\lambda}{3}\,\rho\,\sigma_e\,\Delta x$

$$-\Delta t\,\Gamma_2 = \begin{pmatrix} 0 \\ \partial_j \tau_{xj} \\ \partial_j \tau_{yj} \end{pmatrix}$$

$$- \sigma_x\,\Delta t\,\partial_x \begin{pmatrix} 0 \\ u^3\,\partial_x\rho - v^3\,\partial_y\rho + 3\,\rho\,(u^2\,\partial_x u - v^2\,\partial_y v) \\ -v^3\,\partial_x\rho - u^3\,\partial_y\rho - 3\,\rho\,(u^2\,\partial_y u + v^2\,\partial_x v) \end{pmatrix}$$

$$- \sigma_x\,\Delta t\,\partial_y \begin{pmatrix} 0 \\ -v^3\,\partial_x\rho - u^3\,\partial_y\rho - 3\,\rho\,(u^2\,\partial_y u + v^2\,\partial_x v) \\ -u^3\,\partial_x\rho + v^3\,\partial_y\rho + 3\,\rho\,(-u^2\,\partial_x u + v^2\,\partial_y v) \end{pmatrix}$$

D2Q13



ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
h	4
x_{xe}	4
h_2	6

D2Q13: first order equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y = 0$$

$$\partial_t J_x + \partial_x \big(\tfrac{14}{13}\, \lambda^2\, \rho + \tfrac{1}{26} \Phi_\varepsilon + \tfrac{1}{2} \Phi_{xx} \big) + \partial_y \Phi_{xy} = 0$$

$$\partial_t J_x + \partial_x (\rho\, u^2 + p) + \partial_y (\rho\, u\, v) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y \big(\tfrac{14}{13}\, \lambda^2\, \rho + \tfrac{1}{26} \Phi_\varepsilon - \tfrac{1}{2} \Phi_{xx} \big) = 0$$

$$\partial_t J_y + \partial_x (\rho\, u\, v) + \partial_y (\rho\, v^2 + p) = 0$$

then $\quad \frac{14}{13}\, \lambda^2\, \rho + \frac{1}{26} \Phi_\varepsilon + \frac{1}{2} \Phi_{xx} = \rho\, u^2 + p,$

$\quad \frac{14}{13}\, \lambda^2\, \rho + \frac{1}{26} \Phi_\varepsilon - \frac{1}{2} \Phi_{xx} = \rho\, v^2 + p$

and $\quad \Phi_{xx} = \rho\, (u^2 - v^2),\ \Phi_{xy} = \rho\, u\, v$

$$\frac{28}{13}\, \lambda^2\, \rho + \frac{1}{13} \Phi_\varepsilon = \rho\, (u^2 + v^2) + 2\, p$$

then $\quad \Phi_\varepsilon = 13\, \rho\, |\mathbf{u}|^2 + 26\, p - 28\, \rho\, \lambda^2$

The equilibrium values of the moments of degree two are fixed with the first order Euler equations

D2Q13: second order equations

Φ : vector of moments at equilibrium

$$\Phi = \big(\Phi_\varepsilon,\, \Phi_{xx},\, \Phi_{xy},\, \Phi_{qx}\,,\Phi_{qy}\,,\, \Phi_{rx},\, \Phi_{ry},\, \Phi_h,\, \Phi_{xxe}\,,\, \Phi_{h2}\big)^{\rm t}$$

conservative first order fluxes

$$\Gamma_1 = \begin{bmatrix} \partial_x J_x + \partial_y J_y \\ \partial_x(\rho\, u^2 + p) + \partial_y(\rho\, u\, v) \\ \partial_x(\rho\, u\, v) + \partial_x(\rho\, v^2 + p) \end{bmatrix}$$

$$\Psi_1 = {\rm d}\Phi(W).\Gamma_1 - (C\, W + D\, \Phi(W)) \in \mathbb{R}^6$$

viscous fluxes $-\Delta t\, \Gamma_2 = -\Delta t\, B\, \Sigma\, \Psi_1 =$ physical fluxes ?

$$= \begin{bmatrix} 0 \\ \partial_j \tau_{xj} \equiv \partial_x(2\,\mu\,\partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y(\mu(\partial_x v + \partial_y u)) \\ \partial_j \tau_{yj} \equiv \partial_x(\mu(\partial_x v + \partial_y u)) + \partial_y((\zeta - \mu)(\partial_x u + \partial_y v) + 2\,\mu\,\partial_y v)) \end{bmatrix}$$

linear system of $2 \times 2 \times 2 \times 3 = 24$ equations

for $3 \times 4 = 12$ partial derivatives

of $\Phi_{qx}\,,\Phi_{qy}\,,\,\Phi_{rx},\,\Phi_{ry}$ relative to ρ, u and v

D2Q13: second order equations *(ii)*

after identification, we find:

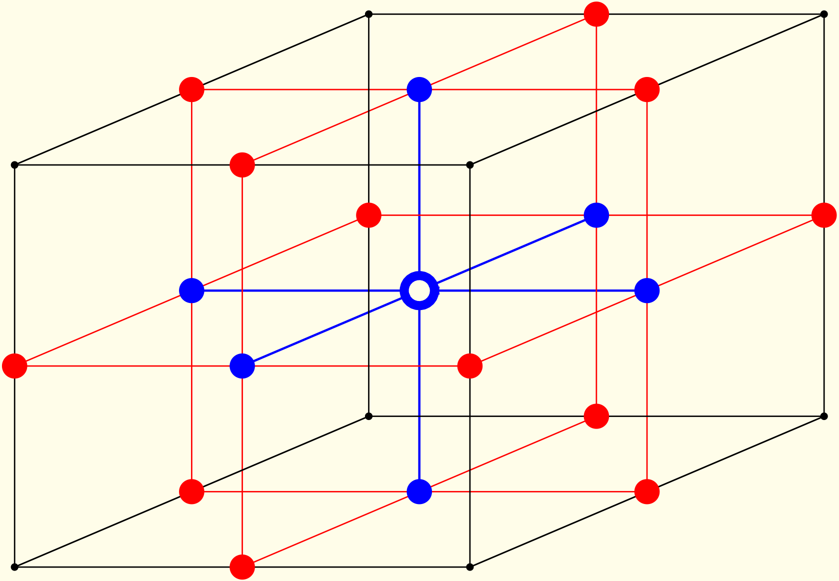
$p = \lambda^2 \, c_s^2 \, \rho$ and the parameter c_s is not constrained

$$\Phi_{qx} = \rho \left(|\mathbf{u}|^2 + 4 \, \lambda^2 \, c_s^2 - 3 \, \lambda^2 \right) u$$
$$\Phi_{qy} = \rho \left(|\mathbf{u}|^2 + 4 \, \lambda^2 \, c_s^2 - 3 \, \lambda^2 \right) v$$
$$\Phi_{rx} = \rho \left(- \tfrac{7}{6} \, \lambda^2 \, u^2 - 7 \, \lambda^2 \, v^2 - \tfrac{21}{2} \, \lambda^4 \, c_s^2 + \tfrac{31}{6} \, \lambda^4 \right) u$$
$$\Phi_{ry} = \rho \left(- 7 \, \lambda^2 \, u^2 - \tfrac{7}{6} \, \lambda^2 \, v^2 - \tfrac{21}{2} \, \lambda^4 \, c_s^2 + \tfrac{31}{6} \, \lambda^4 \right) v$$

$$\mu = \rho \, \sigma_x \, \lambda \, c_s^2 \, \Delta x$$
$$\zeta = \rho \, \sigma_e \, \lambda \, c_s^2 \, \Delta x$$

ok compared to a pure human algebraic calculus (april 2015)

D3Q19



D3Q19: moments

ρ — 4 conserved

$j_x\,,\;j_y\,,\;j_z$

ε — 6 of degree 2: fit the Euler equations

$xx\,,\;ww$

$xy\,,\;yz\,,\;zx$

$q_x\,,\;q_y\,,\;q_z$ — 6 to fit the viscous terms ?

$x\;yz$

$y\;zx$

$z\;xy$

hh — 3 without any influence

$xx_e\,,\;ww_e$

D3Q19: recovering first order isothermal equations

isothermal flow: $p \equiv c_s^2 \, \rho$

$$
\begin{aligned}
\Phi_\varepsilon &= \rho \, (19 \, |\mathbf{u}|^2 - 30 \, \lambda^2 + 57 \, c_s^2) \\
\Phi_{xx} &= \rho \, (2 \, u^2 - v^2 - w^2) \\
\Phi_{ww} &= \rho \, (v^2 - w^2) \\
\Phi_{xy} &= \rho \, u \, v \\
\Phi_{yz} &= \rho \, v \, w \\
\Phi_{zx} &= \rho \, wu
\end{aligned}
$$

Then

$$
\begin{aligned}
& \partial_t \rho + \mathrm{div}(\rho \, \mathbf{u}) = \mathrm{O}(\Delta x) \\
& \partial_t (\rho \, \mathbf{u}) + \mathrm{div} \, (\rho \, \mathbf{u} \otimes \mathbf{u}) + \nabla p = \mathrm{O}(\Delta x)
\end{aligned}
$$

the value of the sound velocity is not imposed at this step

D3Q19: recovering second order equations?

at first order relative to velocity...

the relation $c_s = \frac{\lambda}{\sqrt{3}}$ is mandatory

a total of $3 \times 3 \times 3 \times 4 = 108$ equations to solve to identify the second order terms of the Navier Stokes equations

3 equations for momentum $j_x, \ j_y, \ j_z$

3 conservation terms per equation: $\partial_x[**], \ \partial_y[**]$ and $\partial_z[**]$

3 partial derivatives $\partial_x, \ \partial_y$ and ∂_z per variable

4 nonconserved variables $\rho, \ u, \ v$ and w

$4 \times 6 = 24$ unknowns

expressions that concentrate the error to high order velocity terms

$$\Phi_{qx} = 5\,\rho\,u\,(|\mathbf{u}|^2 - \tfrac{2}{3}\,\lambda^2)$$

$$\Phi_{qy} = 5\,\rho\,v\,(|\mathbf{u}|^2 - \tfrac{2}{3}\,\lambda^2)$$

$$\Phi_{qz} = 5\,\rho\,w\,(|\mathbf{u}|^2 - \tfrac{2}{3}\,\lambda^2)$$

$$\Phi_{x\ yz} = \rho\,u\,(v^2 - w^2), \ \Phi_{x\ yz} = \rho\,u\,(v^2 - w^2), \ \Phi_{z\ xy} = \rho\,w\,(u^2 - v^2)$$

a total of 66 equations remain unsolved

D3Q19: recovering second order equations? *(ii)*

relaxation of second order moments

$$\varepsilon^* = \varepsilon + s_e \, (\Phi_\varepsilon - \varepsilon), \quad xx^* = xx + s_x \, (\Phi_{xx} - xx)$$
$$ww^* = ww + s_x \, (\Phi_{ww} - ww), \quad xy^* = xy + s_x \, (\Phi_{xy} - xy)$$
$$yz^* = yz + s_x \, (\Phi_{yz} - yz), \quad zx^* = zx + s_x \, (\Phi_{zx} - zx)$$

Hénon relations: $\sigma_x \equiv \frac{1}{s_x} - \frac{1}{2}, \qquad \sigma_e \equiv \frac{1}{s_e} - \frac{1}{2}$

shear viscosity $\mu = \frac{1}{3} \, \rho \, \sigma_x \, \Delta t \, (\lambda^2 + \mathrm{O}(|\mathbf{u}|^2))$

bulk viscosity $\zeta = \frac{2}{9} \, \rho \, \sigma_e \, \Delta t \, (\lambda^2 + \mathrm{O}(|\mathbf{u}|^2))$

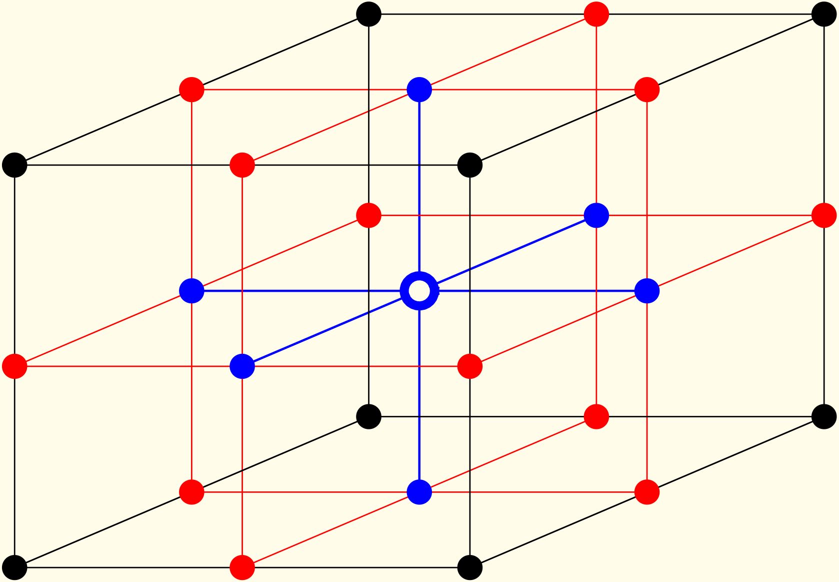
tensor of vicosities $\tau_{xx} = 2 \, \mu \, \partial_x u + \left(\zeta - \frac{2}{3} \, \mu\right) \mathrm{div} \, \mathbf{u}$

$$\tau_{yy} = 2 \, \mu \, \partial_y v + \left(\zeta - \tfrac{2}{3} \, \mu\right) \mathrm{div} \, \mathbf{u}, \quad \tau_{zz} = 2 \, \mu \, \partial_z w + \left(\zeta - \tfrac{2}{3} \, \mu\right) \mathrm{div} \, \mathbf{u}$$
$$\tau_{xy} = \mu \, (\partial_x v + \partial_y u), \quad \tau_{yz} = \mu \, (\partial_y w + \partial_z v), \quad \tau_{zx} = \mu \, (\partial_z u + \partial_x w)$$

Approximative isothermal Navier-Stokes equations at second order

$$\partial_t \rho + \mathrm{div}(\rho \, \mathbf{u}) = \mathrm{O}(\Delta x^2)$$
$$\partial_t (\rho \, \mathbf{u}) + \mathrm{div} \, (\rho \, \mathbf{u} \otimes \mathbf{u}) + \nabla p - \Delta t \; \mathrm{div} \, \tau = \Delta x \, \mathrm{O}(|\mathbf{u}|^3) + \mathrm{O}(\Delta x^2)$$

D3Q27



D3Q27: moments

ρ — 4 conserved

j_x , j_y , j_z

ε — 6 of degree 2: fit the Euler equations

xx , ww

xy , yz , zx

q_x , q_y , q_z — 7 to fit the viscous terms ?

$x\ yz$

$y\ zx$

$z\ xy$

xyz

r_x , r_y , r_z — 10 without influence

hh

xx_e , ww_e

xy_e , yz_e , zx_e

$h3$

D3Q27: recovering first order isothermal equations?

isothermal flow: $p \equiv c_s^2 \, \rho$

$$
\begin{aligned}
\Phi_\varepsilon &= \rho \, (|\mathbf{u}|^2 + 3 \, c_s^2 - 2\lambda^2) \\
\Phi_{xx} &= \rho \, (2 \, u^2 - v^2 - w^2) \\
\Phi_{ww} &= \rho \, (v^2 - w^2) \\
\Phi_{xy} &= \rho \, u \, v \\
\Phi_{yz} &= \rho \, v \, w \\
\Phi_{zx} &= \rho \, wu
\end{aligned}
$$

Then

$$
\begin{aligned}
&\partial_t \rho + \mathrm{div}(\rho \, \mathbf{u}) = \mathrm{O}(\Delta x) \\
&\partial_t (\rho \, \mathbf{u}) + \mathrm{div} \, (\rho \, \mathbf{u} \otimes \mathbf{u}) + \nabla p = \mathrm{O}(\Delta x)
\end{aligned}
$$

the value of the sound velocity is not imposed at this step

essentially analogous to the D3Q19 case...

D3Q27: recovering second order equations?

the relation $c_s = \frac{\lambda}{\sqrt{3}}$ is imposed

a total of $3 \times 3 \times 3 \times 4 = 108$ equations to solve to identify
for $4 \times 7 = 28$ unknown partial derivatives
of Φ_{qx}, Φ_{qy}, Φ_{qz}, $\Phi_{x\ yz}$, $\Phi_{y\ zx}$, $\Phi_{z\ xy}$, Φ_{xyz}
relative to ρ, u, v, and w

nonisotropic expressions for high order velocity terms errors

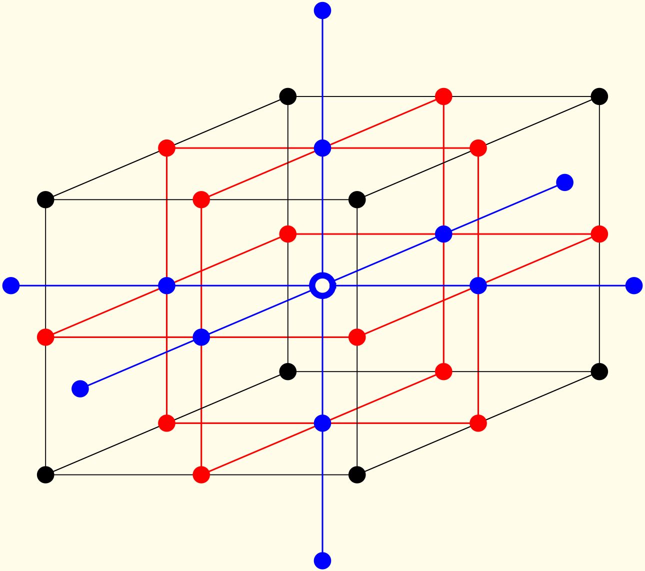
$$\Phi_{qx} = \rho\, u\, (3\,|\mathbf{u}|^2 - 2\,\lambda^2), \quad \Phi_{qy} = \rho\, v\, (3\,|\mathbf{u}|^2 - 2\,\lambda^2)$$
$$\Phi_{qz} = \rho\, w\, (3\,|\mathbf{u}|^2 - 2\,\lambda^2)$$
$$\Phi_{x\ yz} = \rho\, u\, (v^2 - w^2) - \rho\, u^3$$
$$\Phi_{y\ zx} = \rho\, v\, (w^2 - u^2) + \rho\, v^3$$
$$\Phi_{z\ xy} = \rho\, w\, (u^2 - v^2) - \rho\, w^3, \quad \Phi_{xyz} = \rho\, u\, v\, w$$

approximative isothermal Navier-Stokes equations at second order

$$\partial_t \rho + \mathrm{div}(\rho\, \mathbf{u}) = \mathrm{O}(\Delta x^2)$$
$$\partial_t(\rho\, \mathbf{u}) + \mathrm{div}\,(\rho\, \mathbf{u} \otimes \mathbf{u}) + \nabla p - \mathrm{div}\, \tau = \Delta x\, \mathrm{O}(|\mathbf{u}|^3) + \mathrm{O}(\Delta x^2)$$

a total of 56 [44] equations remain unsolved

D3Q33



D3Q33: moments

$\rho\,,\ j_x\,,\ j_y\,,\ j_z$ — 4 conserved

6 of degree 2: fit the Euler equations

ε

$xx\,,\ ww$

$xy\,,\ yz\,,\ zx$

13 to fit the viscous terms

$q_x\,,\ q_y\,,\ q_z$

$x\ yz\,,\ y\ zx\,,\ z\ xy$

xyz

$r_x\,,\ r_y\,,\ r_z$

$t_x\,,\ t_y\,,\ t_z$

10 without any influence

$xx_e\,,\ ww_e$

$xx_h\,,\ ww_h$

$xy_e\,,\ yz_e\,,\ zx_e$

$hh\,,\ h2\,,\ h4$

D3Q33: equilibrium value to recover first order

isothermal flow: $p \equiv c_s^2 \, \rho$

the sound velocity c_s is *a priori* not imposed

$$\begin{aligned} \Phi_\varepsilon &= \rho \, (11 \, |\mathbf{u}|^2 + 33 \, c_s^2 - 26 \, \lambda^2) \\ \Phi_{xx} &= \rho \, (2 \, u^2 - v^2 - w^2) \\ \Phi_{ww} &= \rho \, (v^2 - w^2) \\ \Phi_{xy} &= \rho \, u \, v \\ \Phi_{yz} &= \rho \, v \, w \\ \Phi_{zx} &= \rho \, wu \end{aligned}$$

then

$$\partial_t \rho + \mathrm{div}(\rho \, \mathbf{u}) = \mathrm{O}(\Delta x)$$

$$\partial_t (\rho \, \mathbf{u}) + \mathrm{div} \, (\rho \, \mathbf{u} \otimes \mathbf{u}) + \nabla p = \mathrm{O}(\Delta x)$$

D3Q33: second order partial differential equations

the 108 equations are completely solved

for $4 \times 13 = 52$ unknown partial derivatives

of 13 red moments relative to ρ, u, v, and w

algebraic nonlinear expressions for high order moments

$$\Phi_{qx} = \rho\, u\, (13\, |\mathbf{u}|^2 + 65\, c_s^2 - 37\, \lambda^2)$$

$$\Phi_{qy} = \rho\, v\, (13\, |\mathbf{u}|^2 + 65\, c_s^2 - 37\, \lambda^2)$$

$$\Phi_{qz} = \rho\, w\, (13\, |\mathbf{u}|^2 + 65\, c_s^2 - 37\, \lambda^2)$$

$$\Phi_{x\ yz} = \rho\, u\, (v^2 - w^2)$$

$$\Phi_{y\ zx} = \rho\, v\, (w^2 - u^2)$$

$$\Phi_{z\ xy} = \rho\, w\, (u^2 - v^2)$$

$$\Phi_{xyz} = \rho\, u\, v\, w$$

$$\Phi_{rx} + \frac{38}{13}\frac{\Phi_{tx}}{\lambda^2} = \rho\, u\, \lambda^2 \left(-\frac{161}{39}\, u^2 - \frac{345}{13}\, (v^2 + w^2) + \frac{1265}{39}\, \lambda^2 - \frac{2553}{39}\, c_s^2 \right)$$

$$\Phi_{ry} + \frac{38}{13}\frac{\Phi_{ty}}{\lambda^2} = \rho\, v\, \lambda^2 \left(-\frac{161}{39}\, v^2 - \frac{345}{13}\, (w^2 + u^2) + \frac{1265}{39}\, \lambda^2 - \frac{2553}{39}\, c_s^2 \right)$$

$$\Phi_{rz} + \frac{38}{13}\frac{\Phi_{tz}}{\lambda^2} = \rho\, w\, \lambda^2 \left(-\frac{161}{39}\, w^2 - \frac{345}{13}\, (u^2 + v^2) + \frac{1265}{39}\, \lambda^2 - \frac{2553}{39}\, c_s^2 \right)$$

D3Q33: second order partial differential equations *(ii)*

relaxation of second order moments

$$\varepsilon^* = \varepsilon + s_e\,(\Phi_\varepsilon - \varepsilon), \quad xx^* = xx + s_x\,(\Phi_{xx} - xx)$$
$$ww^* = ww + s_x\,(\Phi_{ww} - ww), \quad xy^* = xy + s_x\,(\Phi_{xy} - xy)$$
$$yz^* = yz + s_x\,(\Phi_{yz} - yz), \quad zx^* = zx + s_x\,(\Phi_{zx} - zx)$$

Hénon relations: $\sigma_x \equiv \frac{1}{s_x} - \frac{1}{2}, \qquad \sigma_e \equiv \frac{1}{s_e} - \frac{1}{2}$

shear viscosity $\mu = \rho\, c_s^2\, \lambda\, \sigma_x\, \Delta x$

bulk viscosity $\zeta = \frac{2}{3}\, \rho\, c_s^2\, \lambda\, \sigma_e\, \Delta x$

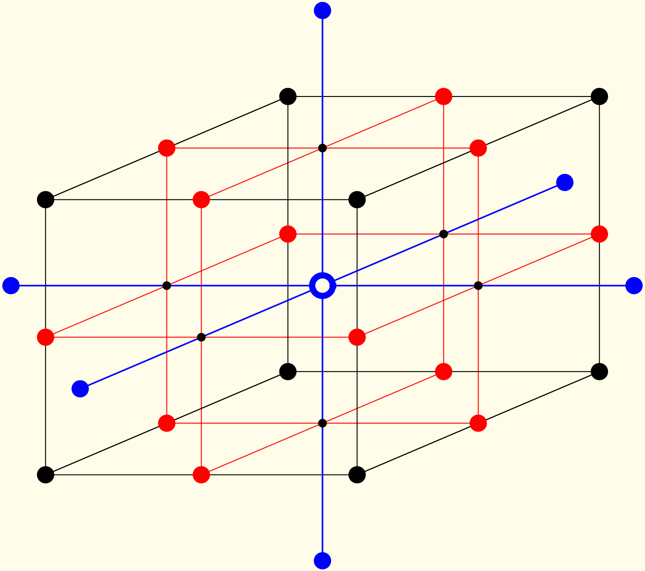
tensor of vicosities

$$\tau_{xx} = 2\,\mu\,\partial_x u + \left(\zeta - \tfrac{2}{3}\,\mu\right) \mathrm{div}\, \mathbf{u}$$
$$\tau_{yy} = 2\,\mu\,\partial_y v + \left(\zeta - \tfrac{2}{3}\,\mu\right) \mathrm{div}\, \mathbf{u}$$
$$\tau_{zz} = 2\,\mu\,\partial_z w + \left(\zeta - \tfrac{2}{3}\,\mu\right) \mathrm{div}\, \mathbf{u}$$
$$\tau_{xy} = \mu\,(\partial_x v + \partial_y u), \quad \tau_{yz} = \mu\,(\partial_y w + \partial_z v), \quad \tau_{zx} = \mu\,(\partial_z u + \partial_x w)$$

isothermal Navier-Stokes equations satisfied at second order :-)

$$\partial_t \rho + \mathrm{div}(\rho\,\mathbf{u}) = \mathrm{O}(\Delta x^2)$$
$$\partial_t(\rho\,\mathbf{u}) + \mathrm{div}\,(\rho\,\mathbf{u} \otimes \mathbf{u}) + \nabla p - \mathrm{div}\,\tau = \mathrm{O}(\Delta x^2)$$

D3Q27-2, Lallemand, d'Humières, Luo, Rubinstein (2003)



D3Q27-2: moments

$\rho\,,\ j_x\,,\ j_y\,,\ j_z$ — 4 conserved

ε — 6 of degree 2: fit the Euler equations

$xx\,,\ ww$

$xy\,,\ yz\,,\ zx$

$q_x\,,\ q_y\,,\ q_z$ — 10 to fit the viscous terms

$x\ yz\,,\ y\ zx\,,\ z\ xy$

xyz

$r_x\,,\ r_y\,,\ r_z$

hh — 7 without influence on the Navier-Stokes equations

$xx_e\,,\ ww_e$

$xy_e\,,\ yz_e\,,\ zx_e$

$h2$

D3Q27-2 allows to recover isothermal Navier Stokes !

isothermal flow: $p \equiv c_s^2 \, \rho$, c_s is *a priori* not imposed

$$
\begin{aligned}
\Phi_\varepsilon &= \rho \, (3 \, |\mathbf{u}|^2 + 9 \, c_s^2 - 8 \lambda^2) \\
\Phi_{xx} &= \rho \, (2 \, u^2 - v^2 - w^2) \\
\Phi_{ww} &= \rho \, (v^2 - w^2) \\
\Phi_{xy} &= \rho \, u \, v \,, \quad \Phi_{yz} = \rho \, v \, w \,, \quad \Phi_{zx} = \rho \, w u \\
\Phi_{qx} &= \rho \, u \, (|\mathbf{u}|^2 + 5 \, c_s^2 - 3 \, \lambda^2) \\
\Phi_{qy} &= \rho \, v \, (|\mathbf{u}|^2 + 5 \, c_s^2 - 3 \, \lambda^2) \\
\Phi_{qz} &= \rho \, w \, (|\mathbf{u}|^2 + 5 \, c_s^2 - 3 \, \lambda^2) \\
\Phi_{x \, yz} &= \rho \, u \, (v^2 - w^2) \\
\Phi_{y \, zx} &= \rho \, v \, (w^2 - u^2) \\
\Phi_{z \, xy} &= \rho \, w \, (u^2 - v^2) \\
\Phi_{xyz} &= \rho \, u \, v \, w \\
\Phi_{rx} &= \rho \, u \, \lambda^2 \left(5 \, \lambda^2 - 9 \, c_s^2 - (u^2 + 3 \, v^2 + 3 \, w^2)\right) \\
\Phi_{ry} &= \rho \, v \, \lambda^2 \left(5 \, \lambda^2 - 9 \, c_s^2 - (v^2 + 3 \, w^2 + 3 \, u^2)\right) \\
\Phi_{rz} &= \rho \, w \lambda^2 \left(5 \, \lambda^2 - 9 \, c_s^2 - (w^2 + 3 \, u^2 + 3 \, v^2)\right)
\end{aligned}
$$

vicosities $\mu = \rho \, c_s^2 \, \sigma_x \, \Delta t$, $\zeta = \frac{2}{3} \, \rho \, c_s^2 \, \sigma_e \, \Delta t$;-)

Navier - Stokes with conservation of energy

... in one space dimension

conserved variables $\rho,\ J \equiv \rho\, u,\ E = \frac{1}{2}\,\rho\, u^2 + \rho\, e$

polytropic perfect gas $p = (\gamma - 1)\,\rho\, e,\ e = c_v\, T,\ \gamma = \frac{c_p}{c_v}$

Prandtl number $Pr = \frac{\mu\, c_p}{\kappa}$

mass conservation $\partial_t \rho + \partial_x(\rho\, u) = 0$

momentum conservation

$$\partial_t(\rho\, u) + \partial_x(\rho\, u^2 + p) - \partial_x(\mu\, \partial_x u) = 0$$

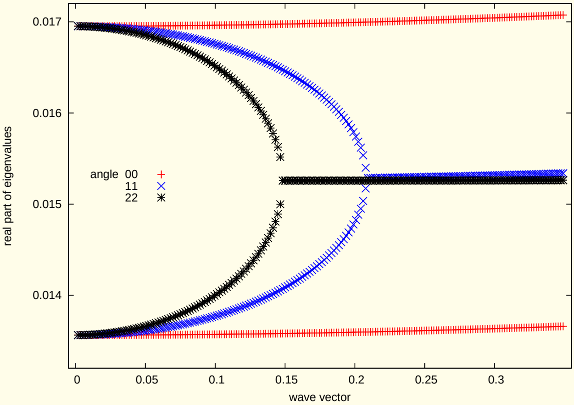
energy conservation

$$\partial_t E + \partial_x(E\, u + p\, u) - \partial_x(\mu\, u\, \partial_x u) - \frac{\gamma}{Pr}\,\partial_x(\mu\, \partial_x e) = 0$$

Fourier law of heat dissipation $-\frac{\gamma}{Pr}\,\partial_x(\mu\, \partial_x e)$

viscous work $\partial_x(\mu\, u\, \partial_x u)$

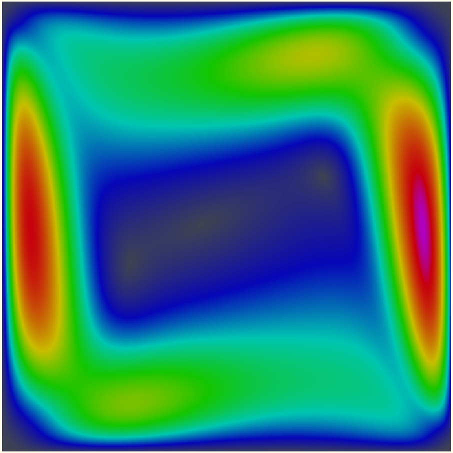
thermal Navier-Stokes with lattice Boltzmann schemes



the viscous and thermal modes merge together for a critical
wave number [P. Lallemand and L.-S. Luo, Phys. Rev. E, 2003]

linear analysis of D2Q13 lattice Boltzmann scheme
for advective acoustics and tuning the parameters of the D2Q13

De Vahl Davis thermal test case for natural convection



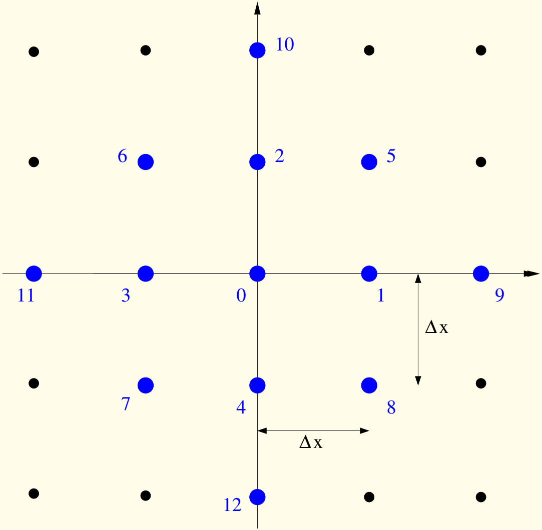
Rayleigh number $= 10^5$, Prandtl number $= 0.71$

D2Q13 lattice Boltzmann scheme with a single particle distribution

iso-velocity curves for the modulus of the fluid speed

[Pierre Lallemand and FD, CiCP, 2015]

D2Q13



ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
h	4
x_{xe}	4
h_2	6

D2Q13: isothermal operator matrix Λ

$$
\begin{array}{ccccccccccccc}
\rho & J_x & J_y & \varepsilon & xx & xy & q_x & q_y & r_x & r_y & h & x_{xe} & h_2
\end{array}
$$

$$
\Lambda = \begin{bmatrix}
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_x & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_y & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & *\partial_y & *\partial_x & 0 & 0 & 0 & *\partial_y & *\partial_x & *\partial_y & *\partial_x & 0 & 0 & 0 \\
0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & 0 \\
0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & 0 \\
0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_x \\
0 & 0 & 0 & 0 & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_y \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0
\end{bmatrix}
$$

D2Q13: momentum-velocity operator matrix Λ

$$\begin{matrix} & \rho & J_x & J_y & \varepsilon & xx & xy & q_x & q_y & r_x & r_y & h & x_{xe} & h_2 \end{matrix}$$

$$\Lambda = \begin{bmatrix}
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_x & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_y & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & *\partial_y & *\partial_x & 0 & 0 & 0 & *\partial_y & *\partial_x & *\partial_y & *\partial_x & 0 & 0 & 0 \\
0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & 0 \\
0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & 0 \\
0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_x \\
0 & 0 & 0 & 0 & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_y \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0
\end{bmatrix}$$

D2Q13: first order equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y = 0$$

$$\partial_t J_x + \partial_x \big(\tfrac{14}{13}\,\lambda^2\,\rho + \tfrac{1}{26}\varepsilon + \tfrac{1}{2}\Phi_{xx}\big) + \partial_y \Phi_{xy} = 0$$

$$\partial_t J_x + \partial_x(\rho\, u^2 + p) + \partial_y(\rho\, u\, v) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y \big(\tfrac{14}{13}\,\lambda^2\,\rho + \tfrac{1}{26}\varepsilon - \tfrac{1}{2}\Phi_{xx}\big) = 0$$

$$\partial_t J_y + \partial_x(\rho\, u\, v) + \partial_y(\rho\, v^2 + p) = 0$$

$$\partial_t \varepsilon + 11\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + 13\,(\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0$$

$$\partial_t E + \partial_x(E\, u + p\, u) + \partial_y(E\, v + p\, v) = 0$$

then $\tfrac{14}{13}\,\lambda^2\,\rho + \tfrac{1}{26}\varepsilon + \tfrac{1}{2}\Phi_{xx} = \rho\, u^2 + p,$ $\quad \Phi_{xy} = \rho\, u\, v$

$\tfrac{14}{13}\,\lambda^2\,\rho + \tfrac{1}{26}\varepsilon - \tfrac{1}{2}\Phi_{xx} = \rho\, v^2 + p$ and $\Phi_{xx} = \rho\,(u^2 - v^2)$

Lattice Boltzmann: $\tfrac{28}{13}\,\lambda^2\,\rho + \tfrac{1}{13}\varepsilon = \rho\,(u^2 + v^2) + 2\,p$ is conserved

Physics: $E \equiv \tfrac{1}{2}\,\rho\,(u^2 + v^2) + \rho\, e$ is conserved

then $p = \rho\, e\,,\ \ \gamma = 2$ and $\varepsilon = 26\, E - 28\,\lambda^2\,\rho$

$$\Phi_{qx} = \rho\, u\,(|\mathbf{u}|^2 + 4\, e - 3\,\lambda^2)\,, \quad \Phi_{qy} = \rho\, v\,(|\mathbf{u}|^2 + 4\, e - 3\,\lambda^2)$$

D2Q13: towards second order equations

Φ : vector of moments at equilibrium

$$\Phi = \big(\Phi_{xx},\, \Phi_{xy},\, \Phi_{qx}\,,\Phi_{qy}\,,\, \Phi_{rx},\, \Phi_{ry},\, \Phi_{h},\, \Phi_{xxe}\,,\, \Phi_{h2}\big)^{\mathrm{t}}$$

$$\Psi_1 = \mathrm{d}\Phi(W).\Gamma_1 - (C\,W + D\,\Phi(W)) \in \mathbb{R}^9$$

viscous fluxes $-\Delta t\, \Gamma_2 = -\Delta t\, B\, \Sigma\, \Psi_1 =$ physical fluxes ?

$$= \begin{bmatrix} 0 \\ \partial_j \sigma_{xj} \equiv \partial_x (2\,\mu\,\partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y (\mu(\partial_x v + \partial_y u)) \\ \partial_j \sigma_{yj} \equiv \partial_x (\mu(\partial_x v + \partial_y u)) + \partial_y ((\zeta - \mu)(\partial_x u + \partial_y v) + 2\,\mu\,\partial_y v)) \\ 26\,[\partial_j (u_i\,\sigma_{ij}) + \frac{\gamma}{Pr}\,(\partial_x (\mu\,\partial_x e) + \partial_y (\mu\,\partial_y e))] \end{bmatrix}$$

$3 \times 2 \times 2 \times 4 = 48$ equations to solve

- 3 equations $(j_x,\ j_y,\ E)$
- 2 conservation terms ∂_x and ∂_y per equation
- 2 partial derivatives ∂_x and ∂_y per variable
- 4 nonconserved variables $\rho,\ u,\ v,\ e$

16 unknowns

- 4 moments $\Phi_{rx},\ \Phi_{ry},\ \Phi_{h},\ \Phi_{xxe}$
- 4 partial derivatives relative to $\rho,\ u,\ v,\ e$ per moment

D2Q13: towards second order equations *(ii)*

48 equations to solve

16 unknowns

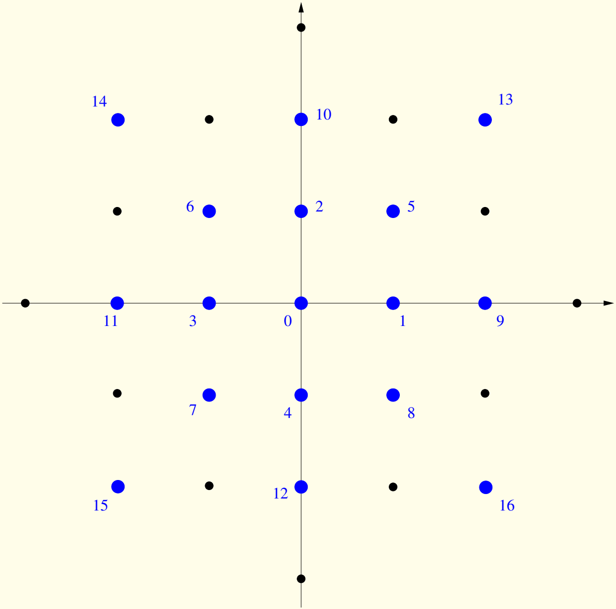
important remaining discrepancies

22 equations cannot be solved

$$\Phi_{rx} = \rho\, u\, \lambda^2 \big(\tfrac{31}{6}\, \lambda^2 - \tfrac{7}{6}\, (u^2 + 6\, v^2) - \tfrac{21}{2}\, e \big)$$
$$\Phi_{ry} = \rho\, v\, \lambda^2 \big(\tfrac{31}{6}\, \lambda^2 - \tfrac{7}{6}\, (6\, u^2 + v^2) - \tfrac{21}{2}\, e \big)$$
$$\Phi_{h} = \rho \big(\tfrac{77}{2}\, |\mathbf{u}|^4 + 308\, (|\mathbf{u}|^2 + e)\, e - 361\, \lambda^2\, (e + |\mathbf{u}|^2) + 140\, \lambda^4 \big)$$
$$\Phi_{xxe} = \rho\, (u^2 - v^2) \big(\tfrac{17}{12}\, |\mathbf{u}|^2 + \tfrac{17}{2}\, e - \tfrac{65}{12}\, \lambda^2 \big)$$

viscosities: $\mu = 2\, \rho\, e\, \sigma_x\, \Delta t\,, \quad \zeta = 0\,, \quad Pr = \frac{\sigma_x}{2\, \sigma_e}\,,$

D2Q17



ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
s_x	7
s_y	7
h	4
x_{xe}	4
x_{ye}	4
h_3	6
h_4	8

D2Q17: first order equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y = 0$$

$$\partial_t J_x + \partial_x\big(\tfrac{30}{17}\,\lambda^2\,\rho + \tfrac{1}{34}\varepsilon + \tfrac{1}{2}\Phi_{xx}\big) + \partial_y \Phi_{xy} = 0$$

$$\partial_t J_x + \partial_x(\rho\,u^2 + p) + \partial_y(\rho\,u\,v) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y\big(\tfrac{30}{17}\,\lambda^2\,\rho + \tfrac{1}{34}\varepsilon - \tfrac{1}{2}\Phi_{xx}\big) = 0$$

$$\partial_t J_y + \partial_x(\rho\,u\,v) + \partial_y(\rho\,v^2 + p) = 0$$

$$\partial_t \varepsilon + \tfrac{109}{3}\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + \tfrac{17}{3}\,(\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0$$

$$\partial_t E + \partial_x(E\,u + p\,u) + \partial_y(E\,v + p\,v) = 0$$

then $\frac{30}{17}\,\lambda^2\,\rho + \frac{1}{34}\varepsilon + \frac{1}{2}\Phi_{xx} = \rho\,u^2 + p,$ $\quad\Phi_{xy} = \rho\,u\,v$

$\frac{30}{17}\,\lambda^2\,\rho + \frac{1}{34}\varepsilon - \frac{1}{2}\Phi_{xx} = \rho\,v^2 + p$ and $\Phi_{xx} = \rho\,(u^2 - v^2)$

$\frac{60}{17}\,\lambda^2\,\rho + \frac{1}{17}\varepsilon = \rho\,(u^2 + v^2) + 2\,p$ is conserved

then $p = \rho\,e$ and $\gamma = 2$

then $\varepsilon = 34\,E - 60\,\lambda^2\,\rho$

D2Q17: first order equations *(ii)*

$$\varepsilon = 34\,E - 60\,\lambda^2\,\rho, \qquad p = \rho\,e$$

$$\partial_t\varepsilon + \tfrac{109}{3}\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + \tfrac{17}{3}\,(\partial_x q_x + \partial_y q_y) = 0$$

$$\partial_t(34\,E - 60\,\lambda^2\,\rho) + \partial_x(\varepsilon\,u + 34\,p\,u) + \partial_y(\varepsilon\,v + 34\,p\,v) = 0$$

then $\Phi_{qx} = \rho\,u\,\left(3\,|\mathbf{u}|^2 + 12\,e - 17\,\lambda^2\right)$

$\Phi_{qy} = \rho\,v\,\left(3\,|\mathbf{u}|^2 + 12\,e - 17\,\lambda^2\right)$

Φ : vector of moments at equilibrium

$$\Phi = \begin{pmatrix} \Phi_{xx},\ \Phi_{xy},\ \Phi_{qx}\,,\ \Phi_{qy} \\ \Phi_{rx},\ \Phi_{ry},\ \Phi_{sx},\ \Phi_{sy},\ \Phi_{h},\ \Phi_{xxe},\ \Phi_{xye} \\ \Phi_{h3},\ \Phi_{h4} \end{pmatrix}$$

D2Q17: second order equations

linear system of $3 \times 2 \times 2 \times 4 =$ 48 equations
for $4 \times 7 =$ 28 partial derivatives

possible reconstruction of the nonlinear functions:

$$\Phi_{rx} + \frac{2}{31}\frac{\Phi_{sx}}{\lambda^2} = \frac{1}{62}\,\rho\,u\,\lambda^2\big(221\,\lambda^2 - 101\,u^2 + 54\,v^2 - 249\,u\,e\big)$$

$$\Phi_{ry} + \frac{2}{31}\frac{\Phi_{sy}}{\lambda^2} = \frac{1}{62}\,\rho\,v\,\lambda^2\big(221\,\lambda^2 - 101\,v^2 + 54\,u^2 - 249\,u\,e\big)$$

$$\Phi_{h} = \rho\,\Big(620\,\lambda^4 + \frac{109}{2}\,|\mathbf{u}|^4 + 436\,e\,(|\mathbf{u}|^2 + e) - \frac{969}{2}\,\lambda^2\,(|\mathbf{u}|^2 + 2e)\Big)$$

$$\Phi_{xxe} = \rho\,(u^2 - v^2)\,\Big(-\frac{65}{12}\,\lambda^2 + \frac{17}{12}\,|\mathbf{u}|^2 + \frac{17}{2}\,e\Big)$$

$$\Phi_{xye} = \rho\,u\,v\,\Big(-\frac{65}{12}\,\lambda^2 + \frac{17}{24}\,|\mathbf{u}|^2 + \frac{17}{4}\,e\Big)$$

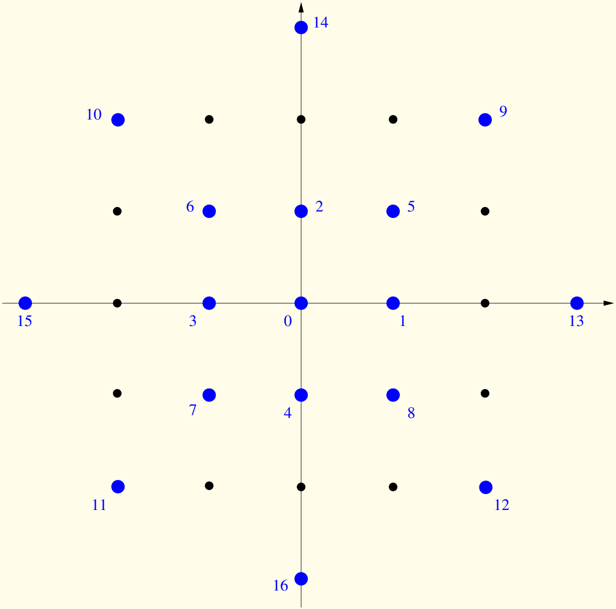
viscosities: $\mu = \rho\,e\,\sigma_x\,\Delta t$ and $\zeta = 0$

satisfy the relation $\sigma_x = \sigma_q$

Prandtl number: $Pr = 1$

and all the equations are satisfied :-)

D2V17 of Philippi and Hegele (2006)



ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
s_x	7
s_y	7
h	4
x_{xe}	4
x_{ye}	4
h_2	6
h_3	8

D2V17: non null elements of the Λ matrix

$$
\begin{bmatrix}
0 & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\ast & 0 & 0 & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\ast & 0 & 0 & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \ast & \ast & 0 & 0 & 0 & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \ast & \ast & 0 & 0 & 0 & \ast & \ast & \ast & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 \\
0 & \ast & \ast & 0 & 0 & 0 & \ast & \ast & \ast & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & 0 & 0 \\
0 & 0 & 0 & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & 0 & 0 \\
0 & 0 & 0 & 0 & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast & 0 \\
0 & 0 & 0 & 0 & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast & 0 \\
0 & 0 & 0 & 0 & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast \\
0 & 0 & 0 & 0 & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast \\
0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & \ast & \ast & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ast & \ast & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

D2V17: first order equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y = 0$$

$$\partial_t J_x + \partial_x\big(\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{40}{17}\,\rho\,\lambda^2\big) + \partial_y \Phi_{xy} = 0$$

$$\partial_t J_x + \partial_x(\rho\,u^2 + p) + \partial_y(\rho\,u\,v) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y\big(-\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{40}{17}\,\rho\,\lambda^2\big) - \tfrac{1}{2}\Phi_{xx}\big) = 0$$

$$\partial_t J_y + \partial_x(\rho\,u\,v) + \partial_y(\rho\,v^2 + p) = 0$$

$$\partial_t \varepsilon + \tfrac{95}{2}\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + \tfrac{17}{2}\,(\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0$$

$$\partial_t E + \partial_x(E\,u + p\,u) + \partial_y(E\,v + p\,v) = 0$$

Then

$$\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{40}{17}\,\rho\,\lambda^2 = \rho\,u^2 + p$$

$$-\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{40}{17}\,\rho\,\lambda^2 = \rho\,v^2 + p$$

$\Phi_{xy} = \rho\,u\,v$ and $\Phi_{xx} = \rho\,(u^2 - v^2)$

$$\tfrac{1}{34}\,\varepsilon + \tfrac{40}{17}\,\rho\,\lambda^2 = \tfrac{1}{2}\,\rho\,(u^2 + v^2) + p$$

so $\tfrac{1}{2}\,\rho\,(u^2 + v^2) + p$ must be conserved and $\gamma = 2$

in consequence, $\tfrac{1}{34}\,\varepsilon + \tfrac{40}{17}\,\rho\,\lambda^2 = E \equiv \tfrac{1}{2}\,\rho\,(u^2 + v^2) + \rho\,e$

$$\varepsilon = 34\,E - 80\,\lambda^2\,\rho$$

D2V17: first order equations *(ii)*

$$\varepsilon = 34\,E - 80\,\lambda^2\,\rho = 17\,\rho\,(u^2 + v^2) + 34\,\rho\,e - 80\,\rho\,\lambda^2$$

$$\partial_t\varepsilon + \frac{95}{2}\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + \frac{17}{2}\,(\partial_x\Phi_{qx} + \partial_y\Phi_{qy}) = 0$$

$$\partial_t E + \partial_x(E\,u + p\,u) + \partial_y(E\,v + p\,v) = 0$$

$$\partial_t\varepsilon + \partial_x(\varepsilon\,u + 34\,p\,u) + \partial_y(\varepsilon\,v + 34\,p\,v) = 0$$

then

$$\frac{95}{2}\,\lambda^2\,J_x + \frac{17}{2}\,\Phi_{qx} = \varepsilon\,u + 34\,p\,u$$

$$\frac{95}{2}\,\lambda^2\,J_y + \frac{17}{2}\,\Phi_{qy} = \varepsilon\,v + 34\,p\,v$$

and

$$\Phi_{qx} = \frac{2}{17}\,\varepsilon\,u + 4\,p\,u - \frac{95}{17}\,\lambda^2\,J_x$$

$$\Phi_{qy} = \frac{2}{17}\,\varepsilon\,v + 4\,p\,v - \frac{95}{17}\,\lambda^2\,J_y$$

$$\Phi_{qx} = (2\,|\mathbf{u}|^2 + 8\,e - 15\,\lambda^2)\,\rho\,u$$

$$\Phi_{qy} = (2\,|\mathbf{u}|^2 + 8\,e - 15\,\lambda^2)\,\rho\,v$$

D2V17: second order equations

reconstruction of the nonlinear functions:

$$\Phi_{rx} + \frac{5}{3}\,\frac{\Phi_{sx}}{\lambda^2} = \rho\, u\, \lambda^2 \left(\frac{1}{9}\, u^2 - \frac{8}{3}\, v^2 - \frac{7}{3}\, e + \frac{35}{9}\, \lambda^2 \right)$$

$$\Phi_{ry} + \frac{5}{3}\,\frac{\Phi_{sy}}{\lambda^2} = \rho\, v\, \lambda^2 \left(\frac{1}{9}\, v^2 - \frac{8}{3}\, u^2 - \frac{7}{3}\, e + \frac{35}{9}\, \lambda^2 \right)$$

$$\Phi_h = \rho \left(\frac{19}{2}\, |\mathbf{u}|^4 + 76\, e \,(|\mathbf{u}|^2 + e) - 185\, \lambda^2 \left(\frac{1}{2} |\mathbf{u}|^2 + e\right) + 100\, \lambda^4 \right)$$

$$\Phi_{xxe} = \rho\, (u^2 - v^2) \left(\frac{41}{36}\, |\mathbf{u}|^2 + \frac{41}{6}\, e - \frac{365}{36}\, \lambda^2 \right)$$

$$\Phi_{xye} = \rho\, u\, v \left(\frac{17}{24}\, |\mathbf{u}|^2 + \frac{17}{4}\, e - \frac{65}{12}\, \lambda^2 \right)$$

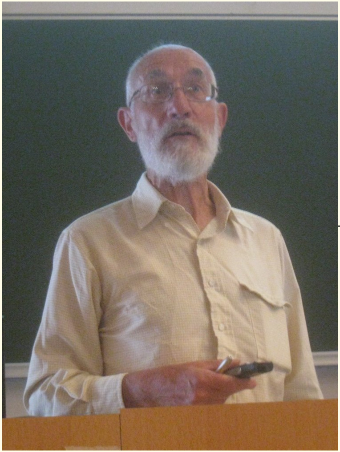
viscosities: $\mu = \rho\, e\, \sigma_x\, \Delta t$ and $\zeta = 0$

satisfy the relation $\sigma_x = \sigma_q$

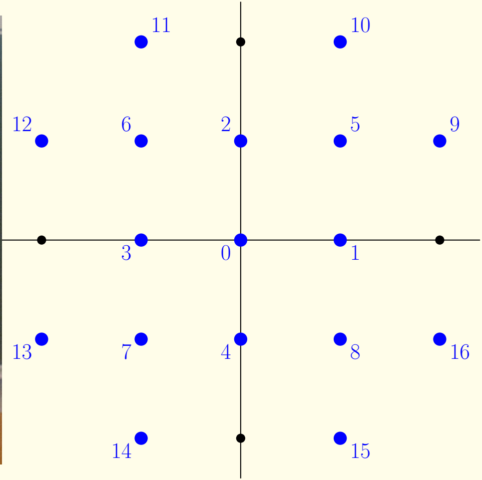
Prandtl number: $Pr = 1$

as for the D2Q17 lattice Boltzmann scheme :-)

D2W17 of Pierre Lallemand



ICMMES, Lyon, 2011



ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
x_{xe}	4
x_{ye}	4
x_{y2}	4
y_{x2}	4
h	4
x_{xxy}	4
h_3	6

D2W17: first order equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y = 0$$

$$\partial_t J_x + \partial_x\left(\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{26}{17}\,\rho\,\lambda^2\right) + \partial_y \Phi_{xy} = 0$$

$$\partial_t J_x + \partial_x(\rho\, u^2 + p) + \partial_y(\rho\, u\, v) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y\left(-\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{26}{17}\,\rho\,\lambda^2\right) - \tfrac{1}{2}\Phi_{xx}) = 0$$

$$\partial_t J_y + \partial_x(\rho\, u\, v) + \partial_y(\rho\, v^2 + p) = 0$$

$$\partial_t \varepsilon + \tfrac{259}{13}\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + \tfrac{17}{13}\,(\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0$$

$$\partial_t E + \partial_x(E\, u + p\, u) + \partial_y(E\, v + p\, v) = 0$$

then

$$\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{26}{17}\,\rho\,\lambda^2 = \rho\, u^2 + p$$

$$-\tfrac{1}{2}\,\Phi_{xx} + \tfrac{1}{34}\,\varepsilon + \tfrac{26}{17}\,\rho\,\lambda^2 = \rho\, v^2 + p$$

$\Phi_{xy} = \rho\, u\, v$ and $\Phi_{xx} = \rho\,(u^2 - v^2)$

$$\tfrac{1}{34}\,\varepsilon + \tfrac{26}{17}\,\rho\,\lambda^2 = \tfrac{1}{2}\,\rho\,(u^2 + v^2) + p$$

so $\tfrac{1}{2}\,\rho\,(u^2 + v^2) + p$ must be conserved and $\gamma = 2$

in consequence, $\tfrac{1}{34}\,\varepsilon + \tfrac{26}{17}\,\rho\,\lambda^2 = E \equiv \tfrac{1}{2}\,\rho\,(u^2 + v^2) + \rho\, e$

$$\varepsilon = 34\,E - 52\,\lambda^2\,\rho$$

D2W17: first order equations *(ii)*

$$\varepsilon = 34\,E - 52\,\lambda^2\,\rho = 17\,\rho\,(u^2 + v^2) + 34\,\rho\,e - 52\,\rho\,\lambda^2$$

$$\partial_t \varepsilon + \tfrac{259}{13}\,\lambda^2\,(\partial_x J_x + \partial_y J_y) + \tfrac{17}{13}\,(\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0$$

$$\partial_t E + \partial_x(E\,u + p\,u) + \partial_y(E\,v + p\,v) = 0$$

$$\partial_t \varepsilon + \partial_x(\varepsilon\,u + 34\,p\,u) + \partial_y(\varepsilon\,v + 34\,p\,v) = 0$$

then

$$\tfrac{259}{13}\,\lambda^2\,J_x + \tfrac{17}{13}\,\Phi_{qx} = \varepsilon\,u + 34\,p\,u$$

$$\tfrac{259}{13}\,\lambda^2\,J_y + \tfrac{17}{13}\,\Phi_{qy} = \varepsilon\,v + 34\,p\,v$$

and

$$\Phi_{qx} = \tfrac{13}{17}\,\varepsilon\,u + 26\,p\,u - \tfrac{259}{17}\,\lambda^2\,J_x$$

$$\Phi_{qy} = \tfrac{13}{17}\,\varepsilon\,v + 26\,p\,v - \tfrac{259}{17}\,\lambda^2\,J_y$$

$$\Phi_{qx} = (13\,|\mathbf{u}|^2 + 52\,e - 55\,\lambda^2)\,\rho\,u$$

$$\Phi_{qy} = (13\,|\mathbf{u}|^2 + 52\,e - 55\,\lambda^2)\,\rho\,v$$

D2W17: second order equations

reconstruction of the nonlinear functions:

$$\Phi_{rx} + \frac{171}{2}\,\Phi_{xy2} = \rho\, u\, \lambda^2 \left(\frac{85}{4}\, u^2 - 50\, v^2 + \frac{55}{4}\, e + \frac{35}{4}\, \lambda^2 \right)$$

$$\Phi_{ry} + \frac{171}{2}\,\Phi_{yx2} = \rho\, u\, \lambda^2 \left(-\, 50\, u^2 + \frac{85}{4}\, v^2 + \frac{55}{4}\, e + \frac{35}{4}\, \lambda^2 \right)$$

$$\Phi_h = \rho \left(\frac{259}{2}\, |\mathbf{u}|^4 + 1036\, (|\mathbf{u}|^2 + e)\, e - 1543\, \lambda^2 \left(\frac{1}{2}\, |\mathbf{u}|^2 + e \right) + 684\, \lambda^4 \right)$$

$$\Phi_{xxe} = \rho\, (u^2 - v^2) \left(\frac{19}{12}\, |\mathbf{u}|^2 + \frac{19}{2}\, e - \frac{91}{12}\, \lambda^2 \right)$$

$$\Phi_{xye} = \rho\, u\, v \left(\frac{3}{2}\, |\mathbf{u}|^2 + 9\, e - 7\, \lambda^2 \right)$$

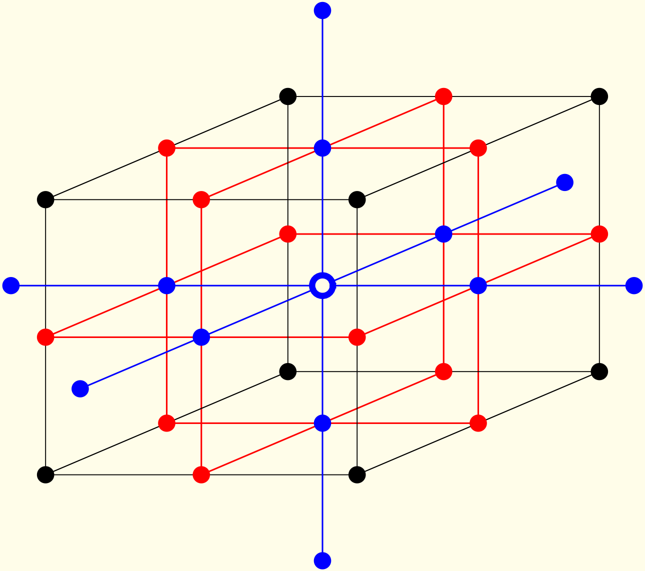
viscosities: $\mu = \rho\, e\, \sigma_x\, \Delta t$ and $\zeta = 0$

satisfy the relation $\sigma_x = \sigma_q$

Prandtl number: $Pr = 1$

as for the previous D2Q17 and D2V17 schemes :-)

D3Q33



D3Q33: moments

$\rho\,,\; j_x\,,\; j_y\,,\; j_z\,,\; \varepsilon$ — 5 conserved

$xx\,,\; ww$ — 8 to fit the Euler equations

$xy\,,\; yz\,,\; zx$

$q_x\,,\; q_y\,,\; q_z$

$x\;yz\,,\; y\;zx\,,\; z\;xy$ — 16 to fit the viscous terms

xyz

$r_x\,,\; r_y\,,\; r_z$

$t_x\,,\; t_y\,,\; t_z$

$xx_e\,,\; ww_e$

$xy_e\,,\; yz_e\,,\; zx_e$

hh

$xx_h\,,\; ww_h$ — 4 without any influence

$h3\,,\; h4$

D3Q33: first order equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y + \partial_z J_z = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y + \partial_z J_z = 0$$

$$\partial_t J_x + \partial_x\big(\tfrac{1}{3}\,\rho\,|\mathbf{u}|^2 + \tfrac{1}{3}\,\Phi_{xx} + \tfrac{2}{3}\,\rho\,e\big) + \partial_y \Phi_{xy} + \partial_z \Phi_{zx} = 0$$

$$\partial_t J_x + \partial_x(\rho\,u^2 + p) + \partial_y(\rho\,u\,v) + \partial_z(\rho\,u\,w) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y\big(\tfrac{1}{3}\,\rho\,|\mathbf{u}|^2 - \tfrac{1}{6}\,\Phi_{xx} + \tfrac{1}{2}\,\Phi_{ww} + \tfrac{2}{3}\,\rho\,e\big) + \partial_z \Phi_{yz} = 0$$

$$\partial_t J_y + \partial_x(\rho\,u\,v) + \partial_y(\rho\,v^2 + p) + \partial_z(\rho\,v\,w) = 0$$

$$\partial_t J_z + \partial_x \Phi_{zx} + \partial_y \Phi_{yz} + \partial_z\big(\tfrac{1}{3}\,\rho\,|\mathbf{u}|^2 - \tfrac{1}{6}\,\Phi_{xx} - \tfrac{1}{2}\,\Phi_{ww} + \tfrac{2}{3}\,\rho\,e\big) = 0$$

$$\partial_t J_z + \partial_x(\rho\,u\,w) + \partial_y(\rho\,v\,w) + \partial_z(\rho\,w^2 + p) = 0$$

$$\partial_t \varepsilon + \partial_x(3\,\Phi_{qx} + \rho\,u\,\lambda^2) + \partial_y(3\,\Phi_{qy} + \rho\,v\,\lambda^2) + \partial_z(3\,\Phi_{qz} + \rho\,w\,\lambda^2) = 0$$

$$\partial_t E + \partial_x(E\,u + p\,u) + \partial_y(E\,v + p\,v) + \partial_z(E\,w + p\,w) = 0$$

then
$$\left\{\begin{array}{rcl} \tfrac{1}{3}\,\rho\,|\mathbf{u}|^2 + \tfrac{1}{3}\,\Phi_{xx} + \tfrac{2}{3}\,\rho\,e &=& \rho\,u^2 + p \\ \tfrac{1}{3}\,\rho\,|\mathbf{u}|^2 - \tfrac{1}{6}\,\Phi_{xx} + \tfrac{1}{2}\,\Phi_{ww} + \tfrac{2}{3}\,\rho\,e &=& \rho\,v^2 + p \\ \tfrac{1}{3}\,\rho\,|\mathbf{u}|^2 - \tfrac{1}{6}\,\Phi_{xx} - \tfrac{1}{2}\,\Phi_{ww} + \tfrac{2}{3}\,\rho\,e &=& \rho\,w^2 + p \end{array}\right.$$

so $p = \frac{2}{3}\,\rho\,e$, $\gamma \equiv \frac{c_p}{c_v} = \frac{5}{3}$

and $\varepsilon = 22\,E - 26\,\lambda^2\,\rho$ with $E = \frac{1}{2}\,\rho\,|\mathbf{u}|^2 + \rho\,e$

$\varepsilon + 26\,\rho\,\lambda^2 = 11\,\rho\,|\mathbf{u}|^2 + 22\,\rho\,e$ and $e = \frac{1}{22\,\rho}\varepsilon - \frac{1}{2}\,|\mathbf{u}|^2 + \frac{13}{11}\,\lambda^2$

D3Q33: necessary relations for the equilibria

$$\Phi_{xx} = \rho\,(2\,u^2 - v^2 - w^2)\,,\ \Phi_{ww} = \rho\,(v^2 - w^2)$$
$$\Phi_{xy} = \rho\,u\,v\,,\ \Phi_{yz} = \rho\,v\,w\,,\ \Phi_{zx} = \rho\,w\,u$$
$$\Phi_{qx} = (13\,|\mathbf{u}|^2 + \tfrac{130}{3}\,e - 37\,\lambda^2)\,\rho\,u$$
$$\Phi_{qy} = (13\,|\mathbf{u}|^2 + \tfrac{130}{3}\,e - 37\,\lambda^2)\,\rho\,v$$
$$\Phi_{qz} = (13\,|\mathbf{u}|^2 + \tfrac{130}{3}\,e - 37\,\lambda^2)\,\rho\,w$$

[15 equations]

algebraic equations for second order partial differential equations

a total of $4 \times 3 \times 5 \times 3 = 180$ equations to solve to identify
the second order terms of the Navier Stokes equations

4 equations for momentum and energy
3 conservation terms per equation: $\partial_x[**]$, $\partial_y[**]$ and $\partial_z[**]$
5 nonconserved variables ρ, u, v, w and e
3 partial derivatives ∂_x, ∂_y and ∂_z per variable
for $5 \times 16 = 80$ partial derivatives

D3Q33: equilibria for second order equations

$$\Phi_{x\ yz} = \rho\, u\, (v^2 - w^2),\ \Phi_{y\ zx} = \rho\, v\, (w^2 - u^2),\ \Phi_{z\ xy} = \rho\, w\, (u^2 - v^2)$$

$$\Phi_{xyz} = \rho\, u\, v\, w$$

$$\Phi_{rx} + \frac{38}{13}\frac{\Phi_{tx}}{\lambda^2} = \rho\, u\, \lambda^2 \left(-\frac{161}{39}\, u^2 - \frac{345}{13}\, (v^2 + w^2) - \frac{1702}{39}\, e + \frac{1265}{39}\, \lambda^2 \right)$$

$$\Phi_{ry} + \frac{38}{13}\frac{\Phi_{ty}}{\lambda^2} = \rho\, v\, \lambda^2 \left(-\frac{161}{39}\, v^2 - \frac{345}{13}\, (w^2 + u^2) - \frac{1702}{39}\, e + \frac{1265}{39}\, \lambda^2 \right)$$

$$\Phi_{rz} + \frac{38}{13}\frac{\Phi_{tz}}{\lambda^2} = \rho\, w\, \lambda^2 \left(-\frac{161}{39}\, w^2 - \frac{345}{13}\, (u^2 + v^2) - \frac{1702}{39}\, e + \frac{1265}{39}\, \lambda^2 \right)$$

$$\Phi_{xxe} = \rho\, (2\, u^2 - v^2 - w^2)\, \left(38\, |\mathbf{u}|^2 + \frac{266}{3}\, e - 38\, \lambda^2\right)$$

$$\Phi_{wwe} = \rho\, (v^2 - w^2)\, \left(38\, |\mathbf{u}|^2 + \frac{266}{3}\, e - 38\, \lambda^2\right)$$

$$\Phi_{xye} = \rho\, u\, v\, (3\, |\mathbf{u}|^2 + 14\, e - 8\, \lambda^2)$$

$$\Phi_{yze} = \rho\, v\, w\, (3\, |\mathbf{u}|^2 + 14\, e - 8\, \lambda^2)$$

$$\Phi_{zxe} = \rho\, w\, u\, (3\, |\mathbf{u}|^2 + 14\, e - 8\, \lambda^2)$$

$$\Phi_{hh} = \rho \left(\frac{69}{2}\, |\mathbf{u}|^4 + 230\, (|\mathbf{u}|^2 + e)\, e - 325\, \lambda^2 \left(\frac{1}{2}\, |\mathbf{u}|^2 + e\right) + 152\, \lambda^4 \right)$$

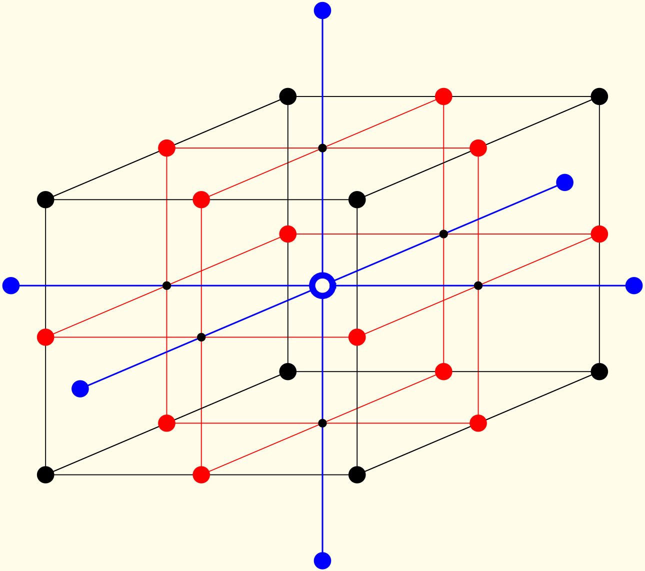
the equilibrium functions Φ_{xxh}, Φ_{wwh}, Φ_{h2}, Φ_{h4} are undetermined

satisfy the relation $\sigma_x = \sigma_q$

viscosities: $\mu = \frac{2}{3}\, \rho\, e\, \sigma_x\, \Delta t$ and $\zeta = 0$

Prandtl number: $Pr = 1$:-)

surprising D3Q27-2



D3Q27-2: moments

$\rho\,,\ j_x\,,\ j_y\,,\ j_z\,,\ \varepsilon$ — 5 conserved

$xx\,,\ ww$ — 8 to fit the Euler equations

$xy\,,\ yz\,,\ zx$

$q_x\,,\ q_y\,,\ q_z$

$x\ yz\,,\ y\ zx\,,\ z\ xy$ — 13 to fit the viscous terms

xyz

$r_x\,,\ r_y\,,\ r_z$

hh

$xx_e\,,\ ww_e$

$xy_e\,,\ yz_e\,,\ zx_e$

$h3$ — 1 without influence on the Navier-Stokes equations

D3Q27-2: Euler equations

$$\partial_t \rho + \partial_x J_x + \partial_y J_y + \partial_z J_z = 0 \qquad \partial_t \rho + \partial_x J_x + \partial_y J_y + \partial_z J_z = 0$$

$$\partial_t J_x + \partial_x\big(\tfrac{1}{3}\,\Phi_{xx} + \tfrac{1}{9}\,\varepsilon + \tfrac{8}{9}\,\rho\,\lambda^2\big) + \partial_y \Phi_{xy} + \partial_z \Phi_{zx} = 0$$

$$\partial_t J_x + \partial_x(\rho\, u^2 + p) + \partial_y(\rho\, u\, v) + \partial_z(\rho\, u\, w) = 0$$

$$\partial_t J_y + \partial_x \Phi_{xy} + \partial_y\big(-\tfrac{1}{6}\,\Phi_{xx} + \tfrac{1}{2}\,\Phi_{ww} + \tfrac{1}{9}\,\varepsilon + \tfrac{8}{9}\,\rho\,\lambda^2\big) + \partial_z \Phi_{yz} = 0$$

$$\partial_t J_y + \partial_x(\rho\, u\, v) + \partial_y(\rho\, v^2 + p) + \partial_z(\rho\, v\, w) = 0$$

$$\partial_t J_z + \partial_x \Phi_{zx} + \partial_y \Phi_{yz} + \partial_z\big(-\tfrac{1}{6}\,\Phi_{xx} - \tfrac{1}{2}\,\Phi_{ww} + \tfrac{1}{9}\,\varepsilon + \tfrac{8}{9}\,\rho\,\lambda^2\big) = 0$$

$$\partial_t J_z + \partial_x(\rho\, u\, w) + \partial_y(\rho\, v\, w) + \partial_z(\rho\, w^2 + p) = 0$$

$$\partial_t \varepsilon + \partial_x(3\,\Phi_{qx} + \rho\, u\,\lambda^2) + \partial_y(3\,\Phi_{qy} + \rho\, v\,\lambda^2) + \partial_z(3\,\Phi_{qz} + \rho\, w\,\lambda^2) = 0$$

$$\partial_t E + \partial_x(E\, u + p\, u) + \partial_y(E\, v + p\, v) + \partial_z(E\, w + p\, w) = 0$$

then
$$\left\{\begin{array}{rcl} \tfrac{1}{3}\,\Phi_{xx} + \tfrac{1}{9}\,\varepsilon + \tfrac{8}{9}\,\rho\,\lambda^2 & = & \rho\, u^2 + p \\ -\tfrac{1}{6}\,\Phi_{xx} + \tfrac{1}{2}\,\Phi_{ww} + \tfrac{1}{9}\,\varepsilon + \tfrac{8}{9}\,\rho\,\lambda^2 & = & \rho\, v^2 + p \\ -\tfrac{1}{6}\,\Phi_{xx} - \tfrac{1}{2}\,\Phi_{ww} + \tfrac{1}{9}\,\varepsilon + \tfrac{8}{9}\,\rho\,\lambda^2 & = & \rho\, w^2 + p \end{array}\right.$$

$\frac{1}{3}\,\varepsilon + \frac{8}{3}\,\rho\,\lambda^2 = \rho\,|\mathbf{u}|^2 + 3\,p$ and $e = \frac{1}{6\,\rho}\varepsilon - \frac{1}{2}\,|\mathbf{u}|^2 + \frac{4}{3}\,\lambda^2$

so $p = \frac{2}{3}\,\rho\, e$, $\gamma \equiv \frac{c_p}{c_v} = \frac{5}{3}$ and $\varepsilon = 6\,E - 8\,\lambda^2\,\rho$

D3Q27-2: necessary relations for the equilibria

$$\Phi_{xx} = \rho\,(2\,u^2 - v^2 - w^2)\,,\ \Phi_{ww} = \rho\,(v^2 - w^2)$$
$$\Phi_{xy} = \rho\,u\,v\,,\ \Phi_{yz} = \rho\,v\,w\,,\ \Phi_{zx} = \rho\,w\,u$$
$$\Phi_{qx} = \rho\,u\,(|\mathbf{u}|^2 + \tfrac{10}{3}\,e - 3\,\lambda^2)$$
$$\Phi_{qy} = \rho\,v\,(|\mathbf{u}|^2 + \tfrac{10}{3}\,e - 3\,\lambda^2)$$
$$\Phi_{qz} = \rho\,w\,(|\mathbf{u}|^2 + \tfrac{10}{3}\,e - 3\,\lambda^2)$$

[15 equations]

fit the Navier Stokes with conservation of energy at second order:

$4 \times 3 \times 3 \times 5 = 180$ equations to solve

for $5 \times 13 = 65$ partial derivatives

$$\Phi_{x\ yz} = \rho\,u\,(v^2 - w^2)$$
$$\Phi_{y\ zx} = \rho\,v\,(w^2 - u^2)$$
$$\Phi_{z\ xy} = \rho\,w\,(u^2 - v^2)$$
$$\Phi_{xyz} = \rho\,u\,v\,w$$

D3Q27-2 available for thermal Navier - Stokes !

$$
\begin{aligned}
\Phi_{rx} &= \rho\, u\, \lambda^2 \left(-(u^2 + 3\, v^2 + 3\, w^2) - 6\, e + 5\, \lambda^2 \right) \\
\Phi_{ry} &= \rho\, v\, \lambda^2 \left(-(3\, u^2 + v^2 + 3\, w^2) - 6\, e + 5\, \lambda^2 \right) \\
\Phi_{rz} &= \rho\, w\, \lambda^2 \left(-(3\, u^2 + 3\, v^2 + w^2) - 6\, e + 5\, \lambda^2 \right) \\
\Phi_{xxe} &= \rho\, (2\, u^2 - v^2 - w^2) \left(\tfrac{9}{8}\, |\mathbf{u}|^2 + \tfrac{21}{4}\, e - \tfrac{17}{4}\, \lambda^2 \right) \\
\Phi_{wwe} &= \rho\, (v^2 - w^2) \left(\tfrac{9}{8}\, |\mathbf{u}|^2 + \tfrac{21}{4}\, e - \tfrac{17}{4}\, \lambda^2 \right) \\
\Phi_{xye} &= \rho\, u\, v\, (3\, |\mathbf{u}|^2 + 14\, e - 8\, \lambda^2) \\
\Phi_{yze} &= \rho\, v\, w\, (3\, |\mathbf{u}|^2 + 14\, e - 8\, \lambda^2) \\
\Phi_{zxe} &= \rho\, w\, u\, (3\, |\mathbf{u}|^2 + 14\, e - 8\, \lambda^2) \\
\Phi_{hh} &= \rho \left(\tfrac{3}{2}\, |\mathbf{u}|^4 + 10\, (|\mathbf{u}|^2 + e)\, e - 15\, \lambda^2 \left(\tfrac{1}{2}\, |\mathbf{u}|^2 + e \right) + 8\, \lambda^4 \right)
\end{aligned}
$$

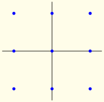
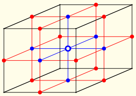
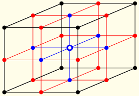
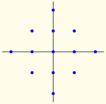
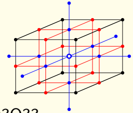
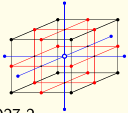
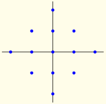
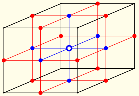
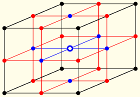
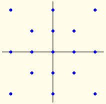
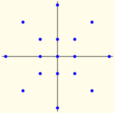
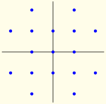
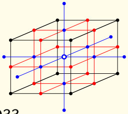
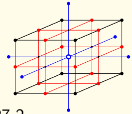
the equilibrium function is determinded for all microscopic moments

satisfy the relation $\sigma_x = \sigma_q$

viscosities: $\mu = \frac{2}{3}\, \rho\, e\, \sigma_x\, \Delta t$ and $\zeta = 0$

Prandtl number: $Pr = 1$:-)

summary for fluids with lattice Boltzmann schemes

energy	no	yes
without	 D2Q9  D3Q19  D3Q27	 D2Q13  D3Q33  D3Q27-2
with	 D2Q13  D3Q19  D3Q27	 D2Q17  D2V17  D2W17  D3Q33  D3Q27-2

conclusion

lattice Boltzmann approach without the Gauss and Hermite paradigm

less velocities than proposed in previous works

Philippi, Hegele, dos Santos, Surmas (2006): D2V37

Shan (2016): D3Q103

stability: a fundamental remaining question

extensions

changing the d'Humières matrix M:

no difficulty if M is well chosen! but to be done!

centered moments: no major difficulty? but to be done!

cumulants: a nonlinear version of the ABCD method?

coupling mass-momentum and energy with two distributions:

no major difficulty? but to be done!

vectorial schemes like $(D2Q4)^4$ or $(D3Q7)^5$:

no major difficulty? but to be done!

diffusive scaling with fixed ratio $\frac{\Delta x^2}{\Delta t}$

references

D. d'Humières. "Generalized Lattice-Boltzmann Equations", in *Rarefied Gas Dynamics*, vol. **159** of *AIAA Prog. in Astron.*, 1992.

P. Lallemand, L.S. Luo. "Theory of the Lattice Boltzmann Method: Acoustic and Thermal Properties", *Phys. Rev.E*, vol. **68**, 2003.

FD. "Equivalent partial differential equations of a lattice Boltzmann scheme", *Comput. And Mathematics with Appl.*, vol. **55**, 2008.

P. Lallemand, FD. "Comparison of Simulations of Convective Flows", *Comm. in Computational Physics*, vol. **17**, p. 1169-1184, 2015.

FD. "Nonlinear fourth order Taylor expansion of lattice Boltzmann schemes", *Asymptotic Analysis*, vol. **127**, p. 297-337, 2022.

FD, P. Lallemand. "On single distribution lattice Boltzmann schemes for the approximation of Navier Stokes equations", hal.archives-ouvertes.fr/hal-03702835, 2022.

merci de votre attention !