Construction et analyse de schémas de Boltzmann sur réseau

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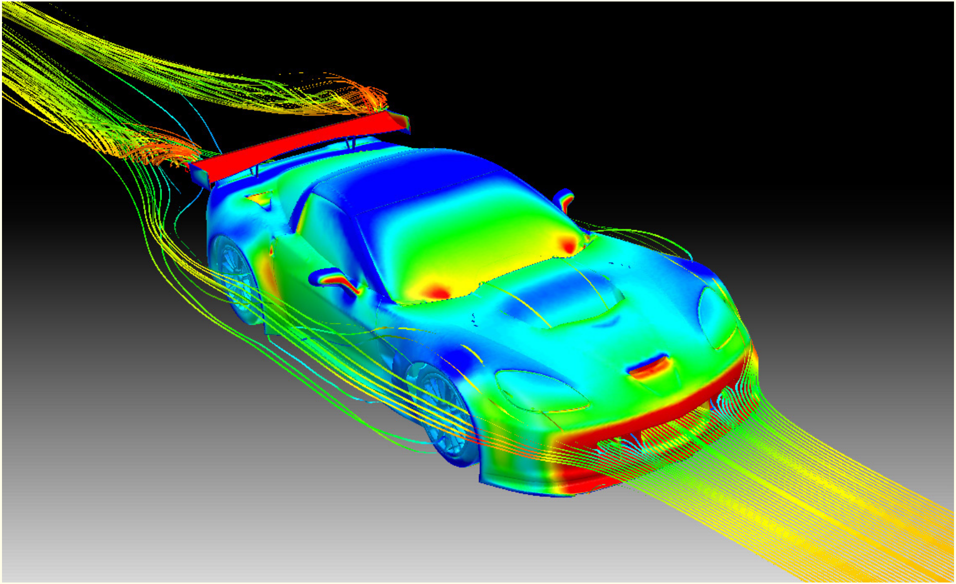
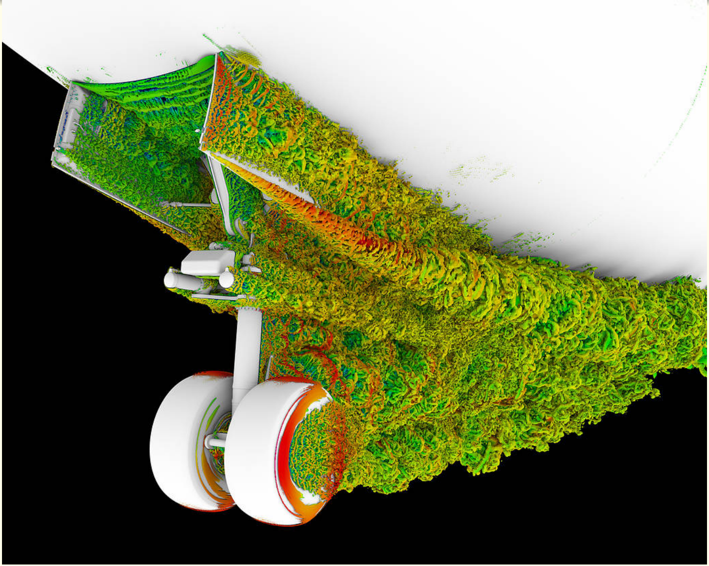
Exa's Powerflow software (2013)



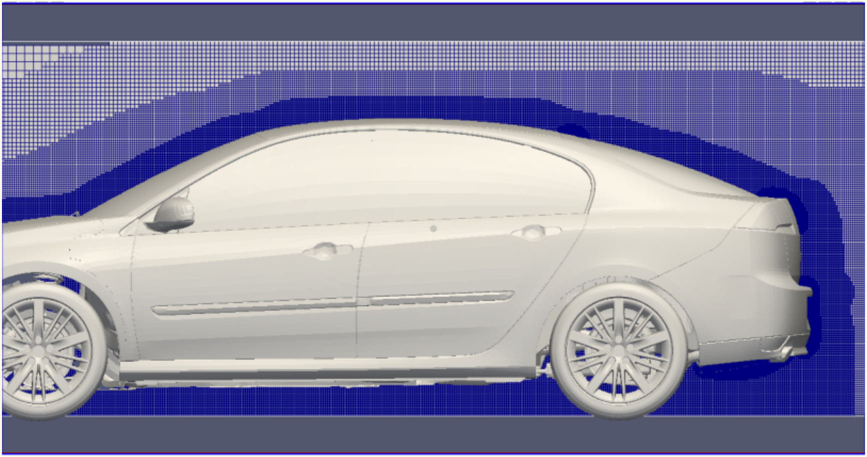
pressure field www.6speedonline.com

Exa's Powerflow software (2017)



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

LaBS-ProLB: aerodynamics software (Renault, 2013)



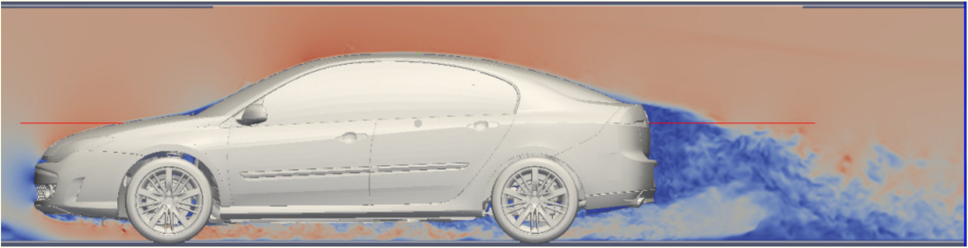
lyoncalcul.univ-lyon1.fr

186 surfaces generate 2.3 millions of triangles

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

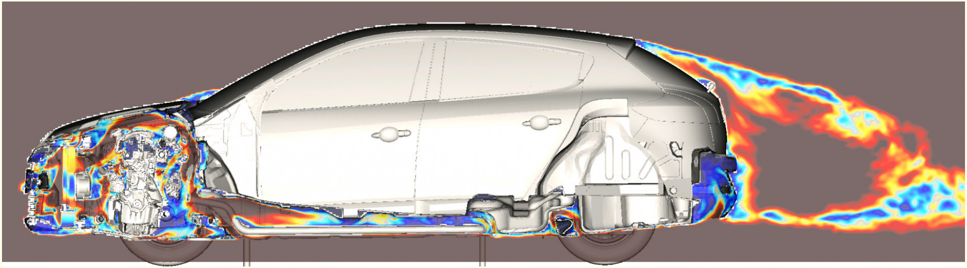
88.6 millions of meshes, 300 000 time iterations

LaBS-ProLB: aerodynamics software (Renault, 2013)



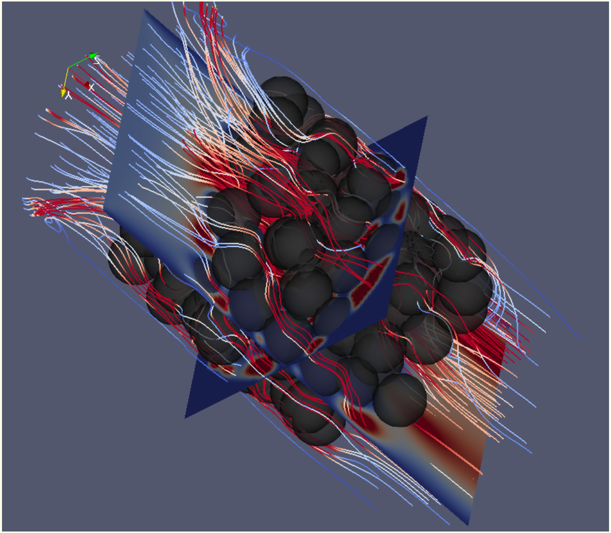
instantaneous velocity m2p2.fr

LaBS-ProLB : aérodynamique (Renault, 2013)



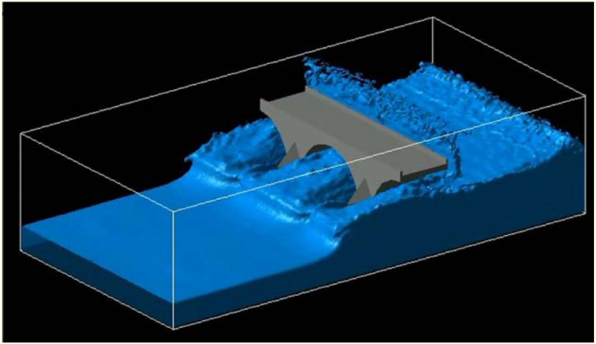
with the internal flow m2p2.fr

flows in porous media



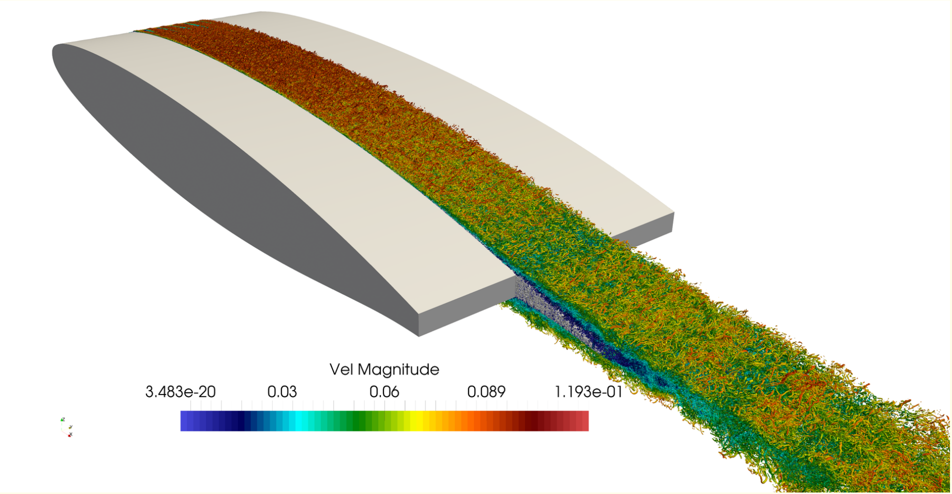
Palabos project, university of Geneva www.cfdem.com

fluid mechanics for civil engineering

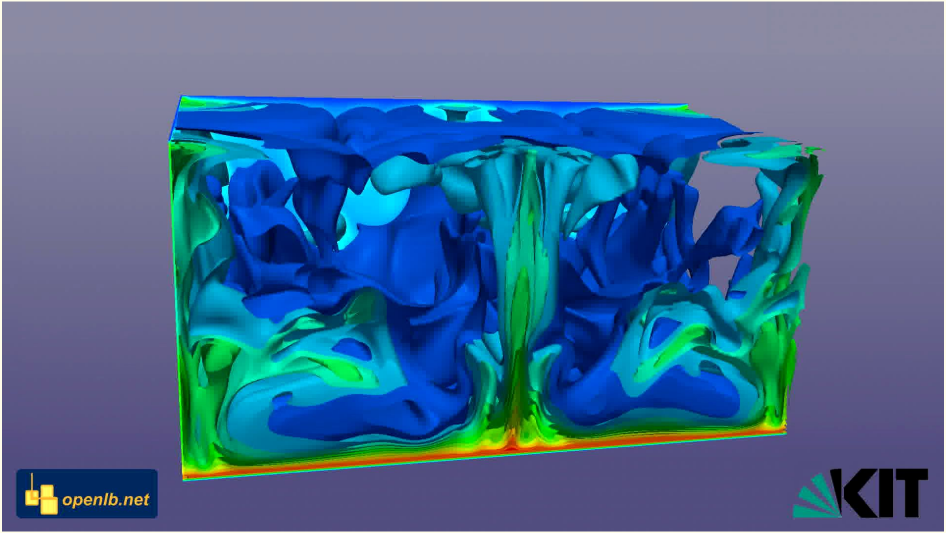


Technische Universität Braunschweig tu-braunschweig.de

virtual fluids



Open LB (Karlsruhe Institute of Technology)



Rayleigh Bénard thermal convection

www.openlb.net

Open LB (Karlsruhe Institute of Technology)

insecte

www.openlb.net

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

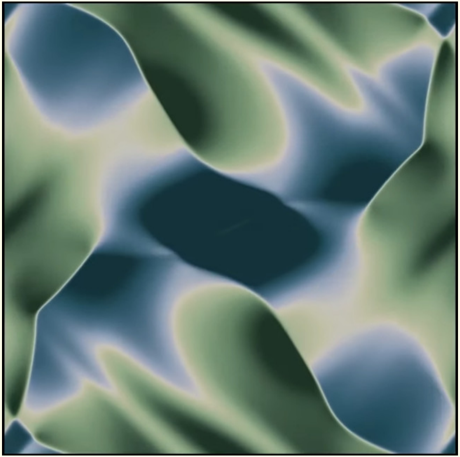
s'appuie sur le package SymPy pour décrire de manière formelle
les polynômes associés aux schémas utilisés

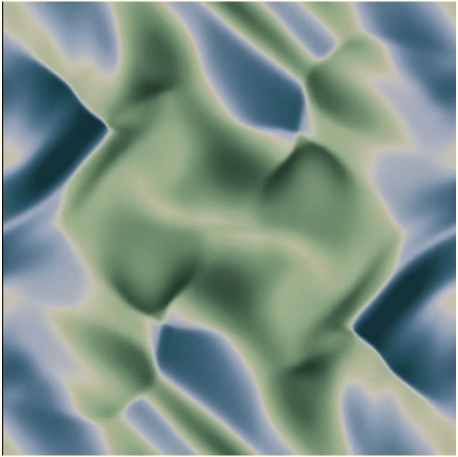
un code est ensuite généré en fonction de ces paramètres
physiques et mathématiques.

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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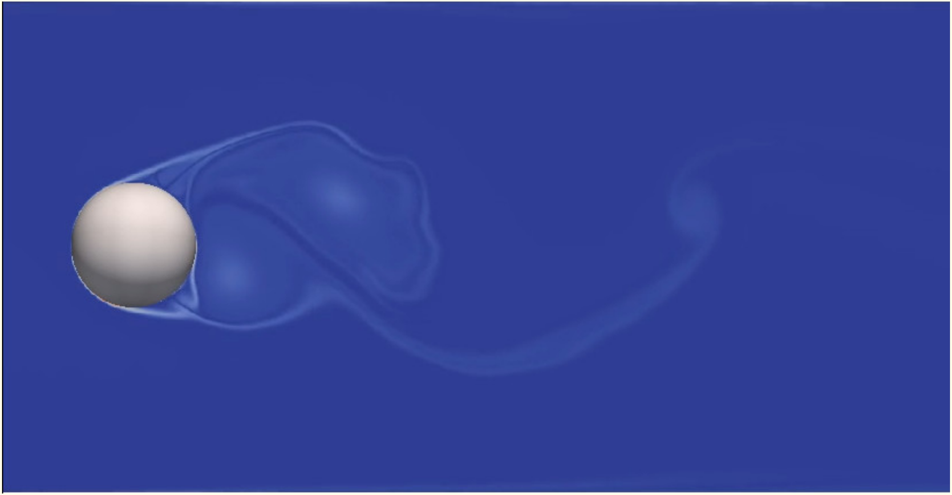
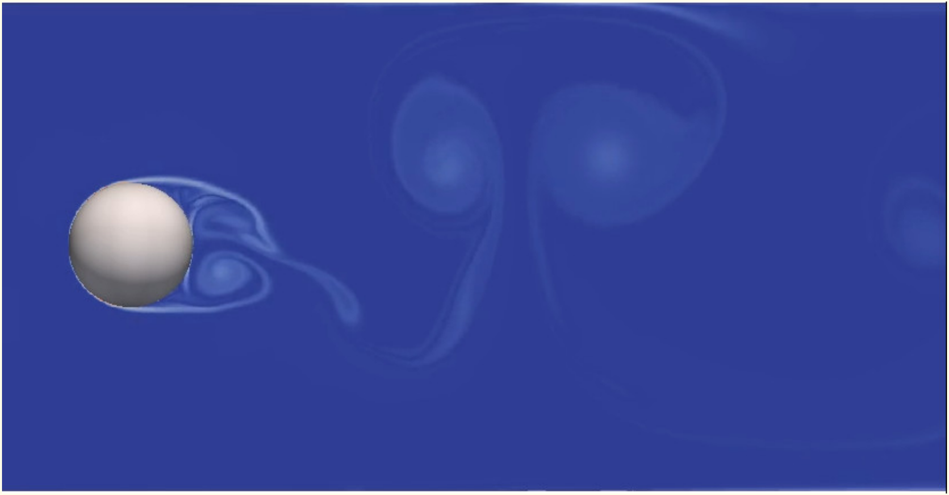
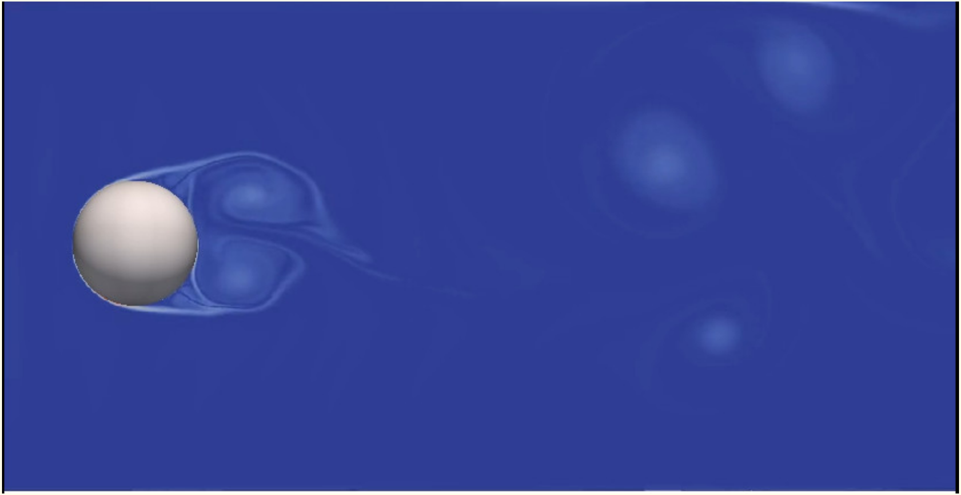


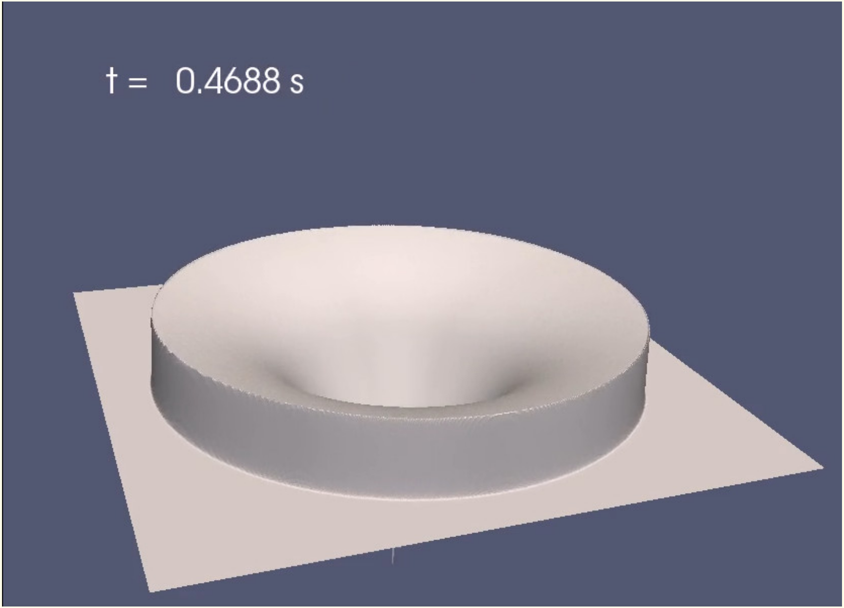
pylbm : Karman vortex street (Re = 2500)



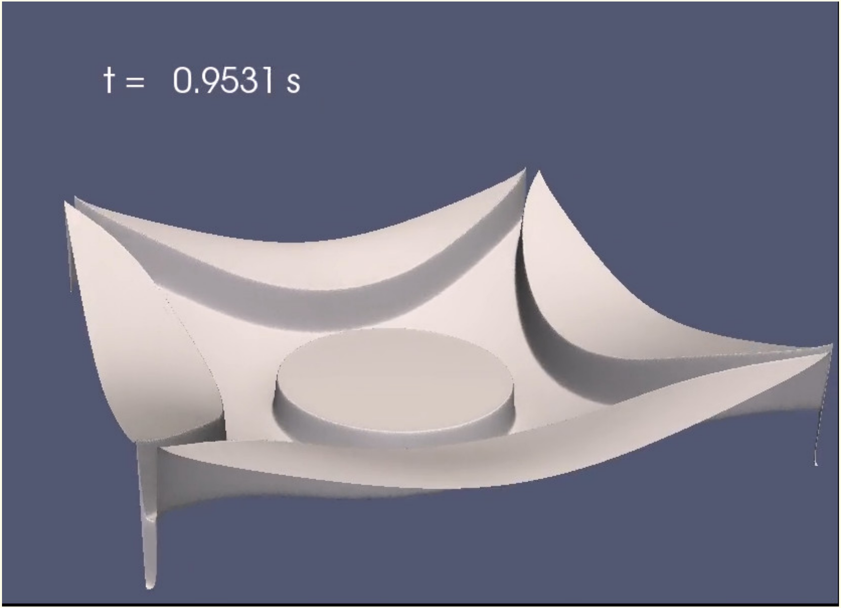
pylbm : Karman vortex street (Re = 2500)



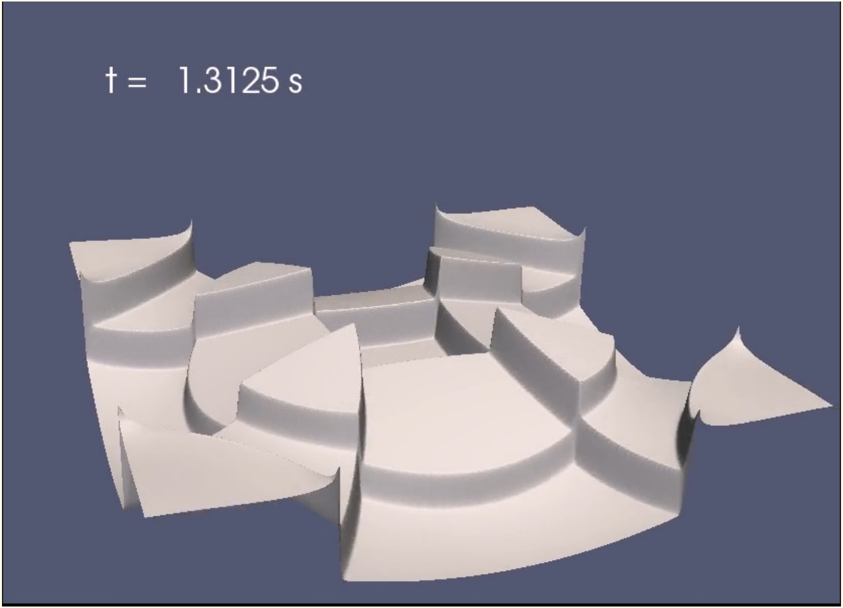
pylbm : shallow water



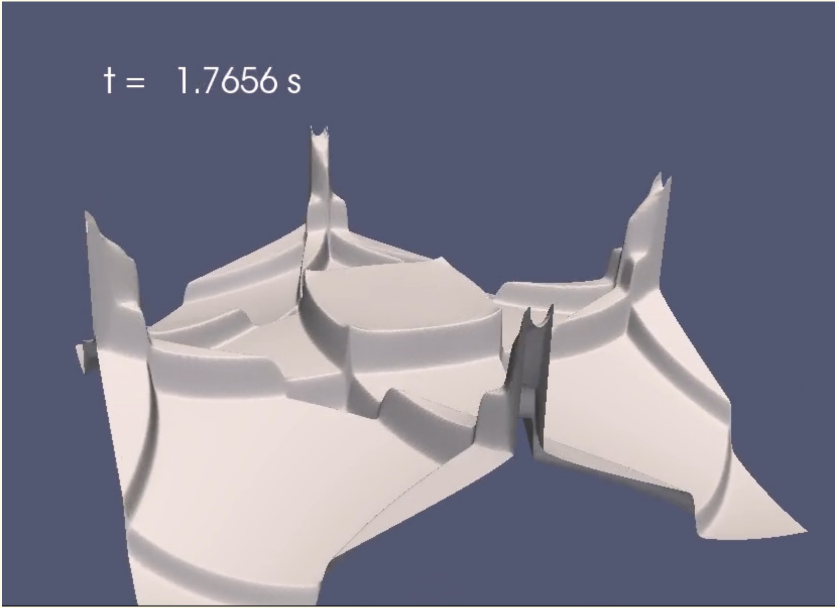
pylbm : shallow water



pylbm : shallow water

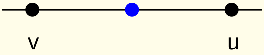


pylbm : shallow water



Discrete velocities

D1Q2 (1957)



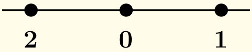
Torsten Carleman (1892-1949)

Problèmes mathématiques dans la théorie cinétique des gaz

Mittag-Leffler Institute, Stockholm

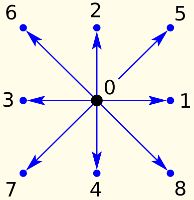
$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = v^2 - u^2, \quad \frac{\partial v}{\partial t} - \frac{\partial v}{\partial x} = u^2 - v^2$$

D1Q3 (1964)



James Broadwell (1921-2018)

D2Q9 (1969)

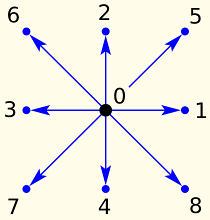


Renée Gatignol (born in 1939)

Henri Cabannes (1923 - 2016)

$$\frac{\partial f_i}{\partial t} + v_i.\nabla_x f_i = Q_i(f_0, f_1, \ldots, f_{q-1}), \; 0 \leq i < q$$

Outline



Lattice Boltzmann schemes

- equilibrium state
- alternate directions

Examples

- D1Q3 in one space dimension
- multiple relaxation times

ABCD method with Chapman Enskog for a formal analysis

- equivalent partial differential equations
- isothermal Navier Stokes
- thermal Navier Stokes with a single particle distribution

Conclusion

Equilibrium state

Boltzmann type equation $\dfrac{\partial f}{\partial t} + v\,\dfrac{\partial f}{\partial x} = Q(f)$

equilibrium state : $f(v)$ such that $\big(Q(f)\big)(v) = 0$

such an equilibrium state is parameterized
by the conserved variables W

if $Q(f) = 0$, there exists W such that $f = f_W^{\mathrm{eq}}$

the conserved variables W are appropriate moments
of the velocity distribution f

popular example : $W = (\rho,\, J)^{\mathrm{t}}$

with density $\rho = \sum_j f_j$ and momentum $J = \sum_j v_j\, f_j \equiv \rho\, u$

equilibrium state associated to a given particle distribution

$f(v) \longrightarrow W \longrightarrow f_W^{\mathrm{eq}}(v)$ with $\big(Q(f_W^{\mathrm{eq}})\big)(v) = 0$

example Maxwell-Boltzmann distribution for a gaz:
function of velocity parametrized by
the density, the mean velocity and the temperature

Alternate directions

Boltzmann equation in one space dimension

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = Q(f), \quad x \in \mathbb{R}, \ v \text{ given}$$

$$f(x, v, t) = f_0(x, v) \quad \text{initial condition}$$

two sub-problems

-1- Collision step

$$\frac{\partial f}{\partial t} = Q(f) \qquad \text{dynamical evolution}$$

$$f(x, v, t) = f_0(x, v) \qquad \text{initial condition}$$

-2- Advection step

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = 0 \qquad \text{dynamical evolution}$$

$$f(x, v, t) = f^*(x, v, t) \qquad \text{initial condition}$$

the initial condition for the advection step

is the result $f^*(x, v, t)$ of the collision step

Collision step: explicit Euler numerical scheme

collision dynamics of the Boltzmann equation: $\dfrac{\mathrm{d}f}{\mathrm{d}t} = Q(f(t))$

equilibrium state $f^{\mathrm{eq}}(t)$

constructed from $f(t)$ and such that $Q(f^{\mathrm{eq}}(t)) = 0$

$$Q(f(t)) = Q(f(t)) - Q(f^{\mathrm{eq}}(t)) \simeq \mathrm{d}Q(f^{\mathrm{eq}}(t)).\big(f(t) - f^{\mathrm{eq}}(t)\big)$$

Bhatnagar–Gross–Krook type approximation

explicit Euler scheme for $\dfrac{\mathrm{d}f}{\mathrm{d}t} = \mathrm{d}Q(f^{\mathrm{eq}}(t)).\big(f(t) - f^{\mathrm{eq}}(t)\big)$

between t and $t + \Delta t$, $\dfrac{\mathrm{d}f}{\mathrm{d}t} \simeq \dfrac{f(t+\Delta t) - f(t)}{\Delta t}$

usual notation :

$$f^*(t) = f(t+\Delta t) = f(t) + \Delta t \ \mathrm{d}Q(f^{\mathrm{eq}}(t)).\big(f(t) - f^{\mathrm{eq}}(t)\big)$$

after one time step Δt of collision, the resulting state is $f^*(x,\, v,\, t)$.

Method of characteristics for the advection

$$\frac{\partial f}{\partial t} + v\,\frac{\partial f}{\partial x} = 0 \qquad \text{dynamical evolution}$$

$$f(x,\, t) = f(x,\, 0) \qquad \text{initial condition}$$

explicit solution with the method of characteristics

$$\frac{\mathrm{d}}{\mathrm{d}t} f(y + v\,t,\, t) = \frac{\partial f}{\partial t} + v\,\frac{\partial f}{\partial x} = 0$$

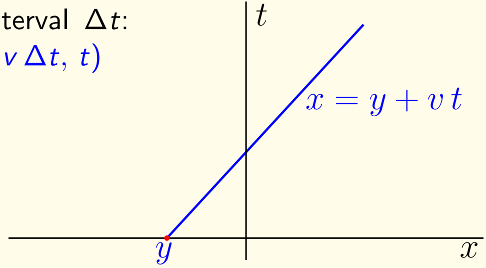
the function $t \longmapsto f(y + v\,t,\, t)$ has the same value

at time zero and at time t: $f(y + v\,t,\, t) = f(y,\, 0)$

change of variables $y = x - v\,t$: $f(x,\, t) = f(x - v\,t,\, 0)$

application with a time interval Δt:

$$f(x,\, t + \Delta t) = f(x - v\,\Delta t,\, t)$$



Finite differences for the advection

Δx space step, discrete space $x = j\,\Delta x$, j an integer

Δt time step

Δx, v and Δt chosen such that $\Delta x = |v|\,\Delta t$; $\quad \dfrac{\Delta x}{\Delta t} \equiv \lambda = |v|$

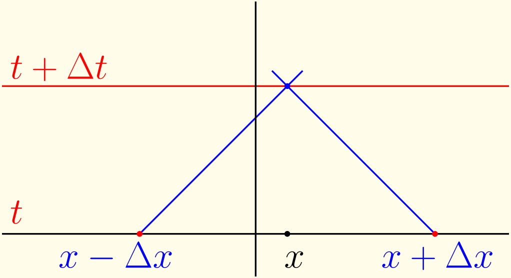
the relation $f(x,\, t + \Delta t) = f(x - v\,\Delta t,\, t)$

can be re-written as

$$f(x,\, t + \Delta t) = f(x - \Delta x,\, t) \qquad \text{if } v > 0$$

$$f(x,\, t + \Delta t) = f(x + \Delta x,\, t) \qquad \text{if } v < 0$$

Courant - Friedrichs - Lewy number always equal to 1 !



Collide - stream

One time step in one space dimension

$f(x, v, t)$ given at time t for a space location x
and for all the velocities v

How to evaluate $f(x, v, t + \Delta t)$ after one time step Δt ?

- Collision step : local in space and nonlinear

  BGK type dynamical evolution $\dfrac{\partial f}{\partial t} = \mathrm{d}Q(f^{\mathrm{eq}}(t)).\big(f(t) - f^{\mathrm{eq}}(t)\big)$

  Euler explicit scheme

  Sauro Succi *et al* (1989), Dominique d'Humières (1992), ...

  $$f^*(x, v, t) = f(x, v, t) + \Delta t \ \mathrm{d}Q(f^{\mathrm{eq}}(x, v, t)).\big(f(x, v, t) - f^{\mathrm{eq}}(x, v, t)\big)$$

- Advection step : non local in space and linear

  Dynamical evolution $\dfrac{\partial f}{\partial t} + v\,\dfrac{\partial f}{\partial x} = 0$

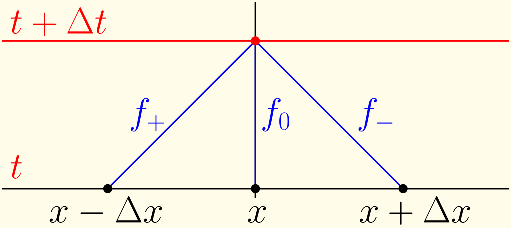
  Initial condition $f(x, v, t) = f^*(x, v, t)$

  Characteristics : $f(x, v, t + \Delta t) = f^*(x - v\,\Delta t, v, t)$

D1Q3: three discrete velocities

Lattice velocity $\lambda \equiv \dfrac{\Delta x}{\Delta t}$ fixed

three velocities $v \in \{-\lambda,\, 0,\, +\lambda\}$



discrete time evolution

$$f_-(x,\, t + \Delta t) = f_-^*(x + \Delta x,\, t)$$
$$f_0(x,\, t + \Delta t) = f_0^*(x,\, t)$$
$$f_+(x,\, t + \Delta t) = f_+^*(x - \Delta x,\, t)$$

how to construct the field $f^* = (f_-^*,\, f_0^*,\, f_+^*)$ after the collision ?

Moments

Conserved moments

density $\rho = f_- + f_0 + f_+$ $\rho^* = \rho$

momentum $J = -\lambda\, f_- + \lambda\, f_+$ $J^* = J$

Non conserved moment

energy $\varepsilon = \lambda^2\,(f_- - 2\, f_0 + f_+)$

Equilibrium value $\varepsilon^{\mathrm{eq}}$ of the non conserved moment ε

$\varepsilon^{\mathrm{eq}} =$ simple function of the conserved moments

$\varepsilon^{\mathrm{eq}} = \alpha\, \lambda^2\, \rho$, α without dimension

Relaxation (collision step)

Euler scheme

$$\varepsilon^* = \varepsilon + \frac{\Delta t}{\tau}\,(\varepsilon^{\mathrm{eq}} - \varepsilon), \qquad \varepsilon^{\mathrm{eq}} = \alpha\,\lambda^2\,\rho$$

relaxation coefficient $\quad s = \dfrac{\Delta t}{\tau}$

Relaxation of the energy during the collision step

$$\varepsilon^* = \varepsilon + s\,(\varepsilon^{\mathrm{eq}} - \varepsilon)$$

The moments $m^* = (\rho,\, J,\, \varepsilon^*)^{\mathrm{t}}$ after the collision are known

$$\left.\begin{aligned} f_-^* + f_0^* + f_+^* &= \rho \\ \lambda\,(-f_-^* + f_+^*) &= J \\ \lambda^2\,(f_-^* - 2\,f_0^* + f_+^*) &= \varepsilon^* \end{aligned}\right\} \Longleftrightarrow \left\{\begin{aligned} f_-^* &= \tfrac{1}{3}\rho - \tfrac{1}{2\,\lambda}\,J + \tfrac{1}{6\,\lambda^2}\varepsilon^* \\ f_0^* &= \tfrac{1}{3}\rho \qquad\qquad - \tfrac{1}{3\,\lambda^2}\varepsilon^* \\ f_+^* &= \tfrac{1}{3}\rho + \tfrac{1}{2\,\lambda}\,J + \tfrac{1}{6\,\lambda^2}\varepsilon^* \end{aligned}\right.$$

Moments at the new time step

as functions of moments after collision at the previous time step

$$\begin{aligned}
\rho(x,\ t+\Delta t) = \rho(x,\ t) &+ \tfrac{1}{3}\big(\rho(x+\Delta x,\ t) - 2\,\rho(x,\ t) + \rho(x-\Delta x,\ t)\big) \\
&- \tfrac{1}{2\,\lambda}\big(J(x+\Delta x,\ t) - J(x+\Delta x,\ t)\big) \\
&+ \tfrac{1}{6\,\lambda^2}\big(\varepsilon^*(x+\Delta x,\ t) - 2\,\varepsilon^*(x,\ t) + \varepsilon^*(x-\Delta x,\ t)\big)
\end{aligned}$$

$$\begin{aligned}
J(x,\ t+\Delta t) = J(x,\ t) &+ \tfrac{1}{2}\big(J(x+\Delta x,\ t) - 2\,J(x,\ t) + J(x-\Delta x,\ t)\big) \\
&- \tfrac{\lambda}{3}\big(\rho(x+\Delta x,\ t) - \rho(x+\Delta x,\ t)\big) \\
&- \tfrac{1}{6\,\lambda}\big(\varepsilon^*(x+\Delta x,\ t) - \varepsilon^*(x-\Delta x,\ t)\big)
\end{aligned}$$

$$\begin{aligned}
\varepsilon(x,\ t+\Delta t) = \varepsilon^*(x,\ t) &+ \tfrac{\lambda^2}{3}\big(\rho(x+\Delta x,\ t) - 2\,\rho(x,\ t) + \rho(x-\Delta x,\ t)\big) \\
&- \tfrac{\lambda}{2}\big(J(x+\Delta x,\ t) - J(x+\Delta x,\ t)\big) \\
&+ \tfrac{1}{6}\big(\varepsilon^*(x+\Delta x,\ t) - 2\,\varepsilon^*(x,\ t) + \varepsilon^*(x-\Delta x,\ t)\big)
\end{aligned}$$

$$\varepsilon^* = \varepsilon + s\,(\varepsilon^{\mathrm{eq}} - \varepsilon), \qquad \varepsilon^{\mathrm{eq}} = \alpha\,\rho$$

$$\varphi(x+\Delta x) - 2\,\varphi(x) + \varphi(x-\Delta x) = \Delta x^2\,\frac{\partial^2\varphi}{\partial x^2}(x) + \mathrm{O}(\Delta x^4)$$

$$\varphi(x+\Delta x) - \varphi(x-\Delta x) = 2\,\Delta x\,\frac{\partial\varphi}{\partial x}(x) + \mathrm{O}(\Delta x^3)$$

Expansion at order zero

we can remark

$$\begin{pmatrix}\rho\\ J\\ \varepsilon\end{pmatrix}(t+\Delta t) = \exp\left[-\Delta t \begin{pmatrix} 0 & \partial_x & 0 \\ \frac{2}{3}\,\lambda^2\,\partial_x & 0 & \frac{1}{3}\,\partial_x \\ 0 & \lambda^2\,\partial_x & 0 \end{pmatrix}\right]\begin{pmatrix}\rho\\ J\\ \varepsilon^*\end{pmatrix}(t)$$

[a not so simple exercice!]

$$\varepsilon(x,\ t+\Delta t) = \varepsilon^*(x,\ t) + \frac{\lambda^2}{3}\,\Delta x^2\,\frac{\partial^2\rho}{\partial x^2}(x,\ t) + \mathrm{O}(\Delta x^4)$$
$$-\lambda\,\Delta x\,\frac{\partial J}{\partial x}(x,\ t) + \mathrm{O}(\Delta x^3) + \frac{1}{6}\,\Delta x^2\,\frac{\partial^2\varepsilon^*}{\partial x^2}(x) + \mathrm{O}(\Delta x^4)$$

and $\quad \varepsilon + \mathrm{O}(\Delta t) = \varepsilon^* + \mathrm{O}(\Delta x)$

Hypotheses : $\lambda \equiv \dfrac{\Delta x}{\Delta t}$ and $0 < s \equiv \dfrac{\Delta t}{\tau} \leq 2$ are fixed

then $\quad \varepsilon^* = \varepsilon + s\,(\varepsilon^{\mathrm{eq}} - \varepsilon) = \varepsilon + \mathrm{O}(\Delta x)$

in consequence, $\varepsilon = \varepsilon^{\mathrm{eq}} + \mathrm{O}(\Delta x)$ and $\varepsilon^* = \varepsilon^{\mathrm{eq}} + \mathrm{O}(\Delta x)$

the states are close to the equilibrium

Acoustics at first order

we admit that the expansions $\varepsilon = \varepsilon^{\rm eq} + {\rm O}(\Delta x)$ and $\varepsilon^* = \varepsilon^{\rm eq} + {\rm O}(\Delta x)$ can be derived one time relative to space

then the conserved moments ρ and J satisfy the first order

acoustic model $\quad \dfrac{\partial \rho}{\partial t} + \dfrac{\partial J}{\partial x} = {\rm O}(\Delta x), \qquad \dfrac{\partial J}{\partial t} + \dfrac{\partial p}{\partial x} = {\rm O}(\Delta x)$

with $p = c_0^2 \, \rho, \; c_0 = \sqrt{\frac{\alpha+2}{3}} \, \lambda$

the sound velocity c_0 is a real number ; then $\alpha + 2 \geq 0$.

Stability: velocity of physical waves $\leq$ velocity of numerical waves

implies $\quad c_0 \leq \lambda$ and $-2 \leq \alpha \leq 1$.

Energy at first order [the devil is in the details!]

with the previous hypotheses, we have the expansions

$$\varepsilon = \alpha \, \lambda^2 \, \rho - \frac{1}{s} \, \lambda \, \Delta x \, (1 - \alpha) \, \frac{\partial J}{\partial x} + {\rm O}(\Delta x^2)$$

$$\varepsilon^* = \alpha \, \lambda^2 \, \rho + \Big(1 - \frac{1}{s}\Big) \, \lambda \, \Delta x \, (1 - \alpha) \, \frac{\partial J}{\partial x} + {\rm O}(\Delta x^2)$$

Dissipative acoustics at second order

With the hypotheses done previously,
the conserved variables ρ and J satisfy
the second order dissipative acoustic model

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = \mathrm{O}(\Delta x^2)$$

$$\frac{\partial J}{\partial t} + \frac{\partial p}{\partial x} - \frac{\lambda}{3} \Delta x \,(1-\alpha) \left(\frac{1}{s} - \frac{1}{2}\right) \frac{\partial^2 J}{\partial x^2} = \mathrm{O}(\Delta x^2)$$

pressure $p = \dfrac{\alpha + 2}{3} \lambda^2$

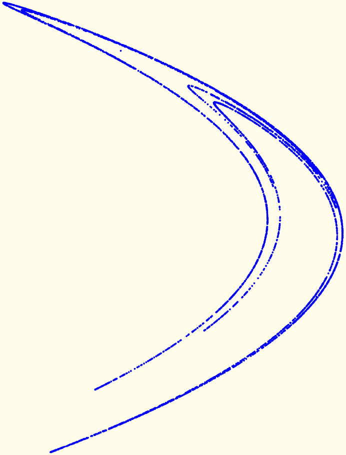
the coefficient $\sigma \equiv \dfrac{1}{s} - \dfrac{1}{2}$ is due to Michel Hénon (1987)

the dissipation coefficient satisfy $\mu = \dfrac{\lambda}{3} \Delta x \,(1-\alpha)\, \sigma$

Michel Hénon (1931 - 2013)

Hénon's relation (1987)

$$\sigma = \frac{1}{s} - \frac{1}{2}$$



Hénon's attractor (1976)

$$x_{k+1} = 1 + y_k - a\, x_k^2 \,, \;\; y_{k+1} = b\, y_k$$

$$a = 1.4 \,, \;\; b = 0.3 \,, \;\; x_0 = 1 \,, \;\; y_0 = 1$$

Synthesis for D1Q3 with two conserved moments

algorithm

moments $W = \begin{pmatrix} \rho \\ J \end{pmatrix}$, $Y = (\varepsilon)$, $m = \begin{pmatrix} W \\ Y \end{pmatrix}$

equilibrium $\varepsilon^{\mathrm{eq}} = \alpha \, \lambda \, \rho$, relaxation $W^* = W$, $\varepsilon^* = (1 - s) \, \varepsilon + s \, \varepsilon^{\mathrm{eq}}$

particles $\begin{pmatrix} f_-^* \\ f_0^* \\ f_+^* \end{pmatrix} = M^{-1} \begin{pmatrix} W \\ \varepsilon^* \end{pmatrix}$, $M = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2 & -2\,\lambda^2 & \lambda^2 \end{pmatrix}$

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

$v_- = -\lambda$, $v_0 = 0$, $v_+ = \lambda$

partial differential equations

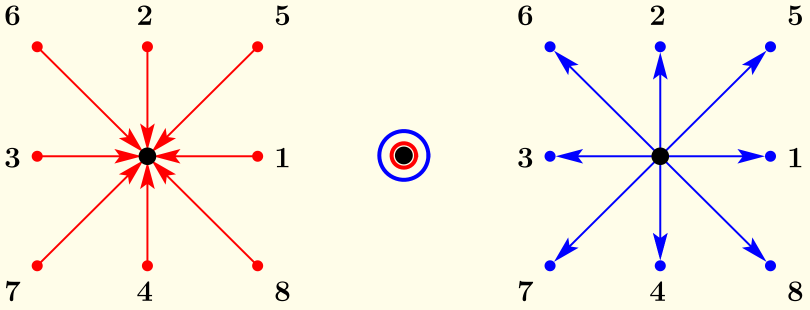
$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = \mathrm{O}(\Delta x^2) \, , \quad \frac{\partial J}{\partial t} + \frac{\partial p}{\partial x} - \mu \, \frac{\partial^2 J}{\partial x^2} = \mathrm{O}(\Delta x^2)$$

pressure $p = \dfrac{\alpha + 2}{3} \, \lambda^2$, viscosity $\mu = \dfrac{\lambda}{3} \, \Delta x \, (1 - \alpha) \, \sigma$, $\sigma = \dfrac{1}{s} - \dfrac{1}{2}$

expansion of the nonconserved moment

$$\varepsilon = \alpha \, \lambda^2 \, \rho - \frac{\lambda}{s} \, (1 - \alpha) \, \Delta x \, \frac{\partial J}{\partial x} + \mathrm{O}(\Delta x^2)$$

Lattice Boltzmann schemes



advection collision advection

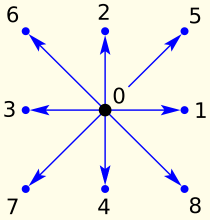
Multiple Relaxation Times lattice Boltzmann schemes

two representations :

particle and moments

$m = M\, f$

d'Humières matrix M



D2Q9

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

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

the lines of this invertible matrix are chosen orthogonal

Polynomials for generating a D2Q9 d'Humières matrix

$M_{kj} = p_k(v_{j,x},\ v_{j,y})$

orthogonality: $\sum_j M_{kj}\, M_{\ell j} = 0$ when $k \neq \ell$

c.f. Pierre Lallemand and Li-Shi Luo (2000)

k	m_k	$p_k(v_x,\ v_y)$
0	ρ	1
1	j_x	v_x
2	j_y	v_y
3	ε	$3\,(v_x^2 + v_y^2) - 4\,\lambda^2$
4	xx	$v_x^2 - v_y^2$
5	xy	$v_x\, v_y$
6	q_x	$[3\,(v_x^2 + v_y^2) - 5\,\lambda^2]\, v_x$
7	q_y	$[3\,(v_x^2 + v_y^2) - 5\,\lambda^2]\, v_y$
8	h	$[\frac{9}{2}\,(v_x^2 + v_y^2)^2 - \frac{21}{2}\,\lambda^2\,(v_x^2 + v_y^2) + 4\,\lambda^4]$

Discrete dynamics for MRT lattice Boltzmann schemes

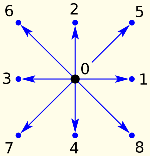
two families of moments $\quad m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}, \; m = M\, f$

conserved moments W $\qquad W \in \mathbb{R}^N$

microscopic non-conserved moments Y

equilibrium vector function

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



two steps for one time iteration

(i) nonlinear relaxation

the moment distribution m is modified locally

new moment distribution m^* after relaxation $\quad m^* \equiv \begin{pmatrix} W^* \\ Y^* \end{pmatrix}$

moments after relaxation: $W^* = W, \; Y^* = Y + S\,(Y^{\rm eq} - Y)$

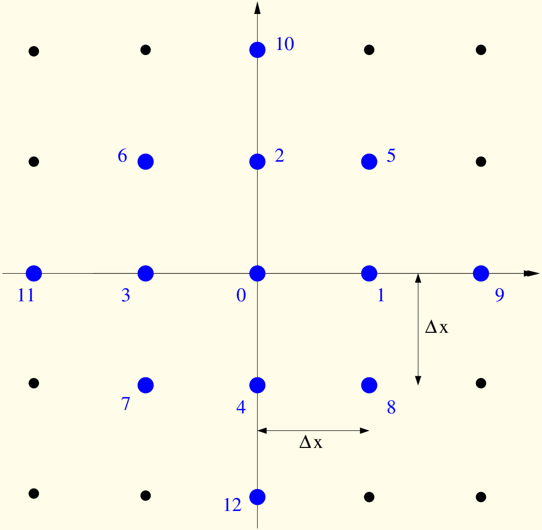
diagonal relaxation matrix S

(ii) linear advection $\quad f^* = M^{-1}\, m^*$

method of characteristics when it is exact !

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

D2Q13



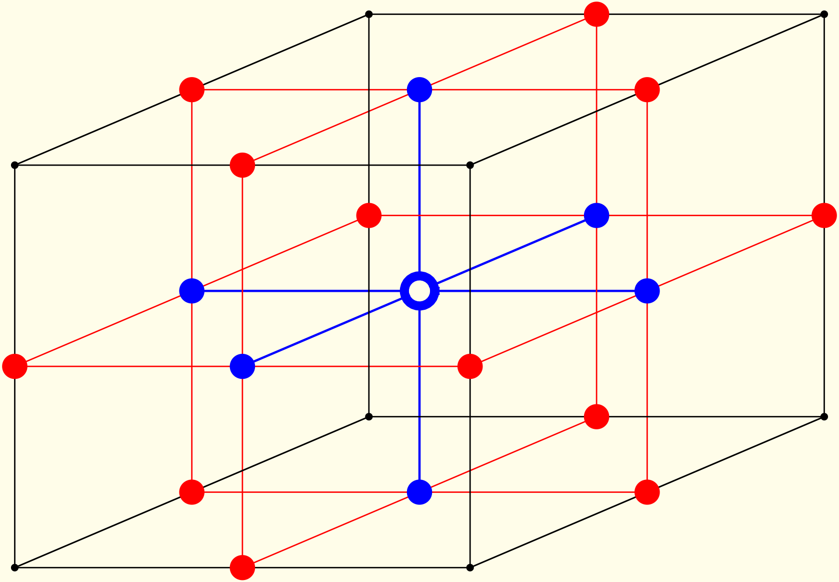
ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
h	4
x_{xe}	4
h_2	6

Polynomials for generating a D2Q13 d'Humières matrix

$M_{kj} = p_k(v_{j,x},\, v_{j,y})$

k	m_k	$p_k(v_x,\, v_y)$
0	ρ	1
1	j_x	v_x
2	j_y	v_y
3	ε	$13\,(v_x^2 + v_y^2) - 28\,\lambda^2$
4	xx	$v_x^2 - v_y^2$
5	xy	$v_x\, v_y$
6	q_x	$(v_x^2 + v_y^2 - 3\,\lambda^2)\, v_x$
7	q_y	$(v_x^2 + v_y^2 - 3\,\lambda^2)\, v_y$
8	r_x	$[\frac{35}{12}\,(v_x^2 + v_y^2)^2 - \frac{63}{4}\,\lambda^2\,(v_x^2 + v_y^2) + \frac{101}{6}\,\lambda^4]\, v_x$
9	r_y	$[\frac{35}{12}\,(v_x^2 + v_y^2)^2 - \frac{63}{4}\,\lambda^2\,(v_x^2 + v_y^2) + \frac{101}{6}\,\lambda^4]\, v_y$
10	h	$\frac{77}{2}\,(v_x^2 + v_y^2)^2 - \frac{361}{2}\,\lambda^2\,(v_x^2 + v_y^2) + 140\,\lambda^4$
11	xx_e	$[\frac{17}{12}\,(v_x^2 + v_y^2) - \frac{65}{12}\,\lambda^2]\,(v_x^2 - v_y^2)$
12	h_3	$\frac{137}{24}\,(v_x^2 + v_y^2)^3 - \frac{273}{8}\,\lambda^2\,(v_x^2 + v_y^2)^2 + \frac{581}{12}\,\lambda^4\,(v_x^2 + v_y^2) - 12\,\lambda^6$

D3Q19

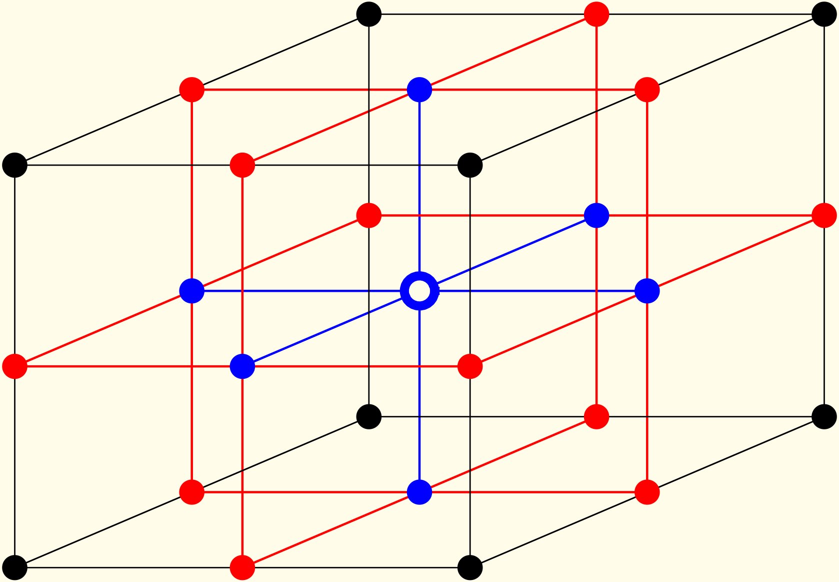


Polynomials for generating a D3Q19 d'Humières matrix

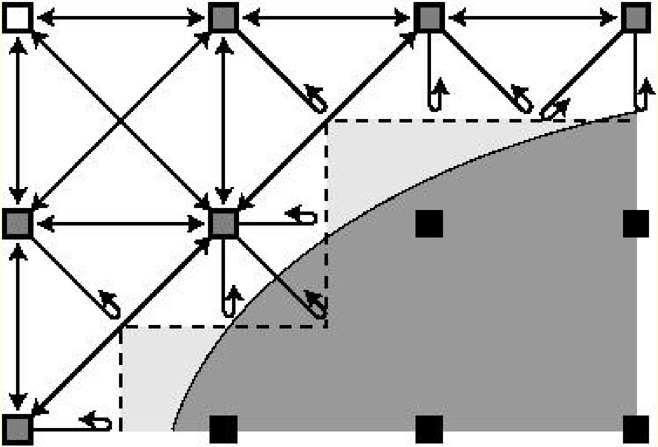
$M_{kj} = p_k(v_{j,x},\ v_{j,y},\ v_{j,z})$

k	m_k	$p_k(v_x,\ v_y,\ v_z)$
0	ρ	1
1, 2, 3	$j_x,\ j_y,\ j_z$	$v_x \quad v_y \quad v_z$
4	ε	$19\,(v_x^2+v_y^2+v_z^2)-30\,\lambda^2$
5	xx	$2\,v_x^2 - v_y^2 - v_z^2$
6	ww	$v_y^2 - v_z^2$
7, 8, 9	$xy,\ yz,\ zx$	$v_x\,v_y \quad v_y\,v_z \quad v_z\,v_x$
10	q_x	$[5\,(v_x^2+v_y^2+v_z^2)-9\,\lambda^2]\,v_x$
11	q_y	$[5\,(v_x^2+v_y^2+v_z^2)-9\,\lambda^2]\,v_y$
12	q_z	$[5\,(v_x^2+v_y^2+v_z^2)-9\,\lambda^2]\,v_z$
13, 14, 15	$x_{yz},\ y_{zx},\ z_{xy}$	$v_x\,(v_y^2 - v_z^2) \quad v_y\,(v_z^2 - v_x^2) \quad v_z\,(v_x^2 - v_y^2)$
16	h	$\frac{21}{2}\,(v_x^2+v_y^2+v_z^2)^2-\frac{53}{2}\,\lambda^2\,(v_x^2+v_y^2+v_z^2)+12\,\lambda^4$
17	xx_e	$[3\,(v_x^2+v_y^2+v_z^2)-5\,\lambda^2]\,(2\,v_x^2 - v_y^2 - v_z^2)$
18	ww_e	$[3\,(v_x^2+v_y^2+v_z^2)-5\,\lambda^2]\,(v_y^2 - v_z^2)$

D3Q27

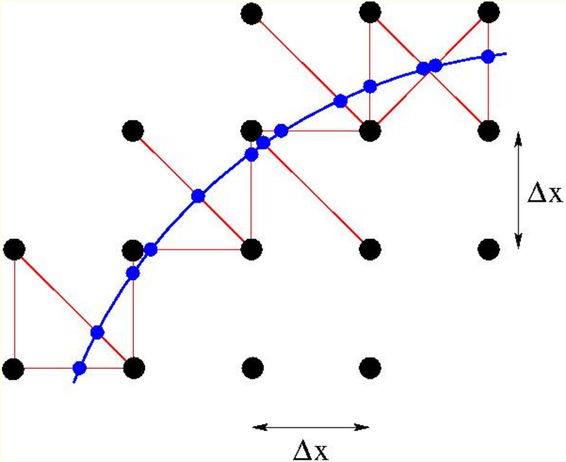


boundary conditions : staircase approximation



Ed Llewellin, Dunham university

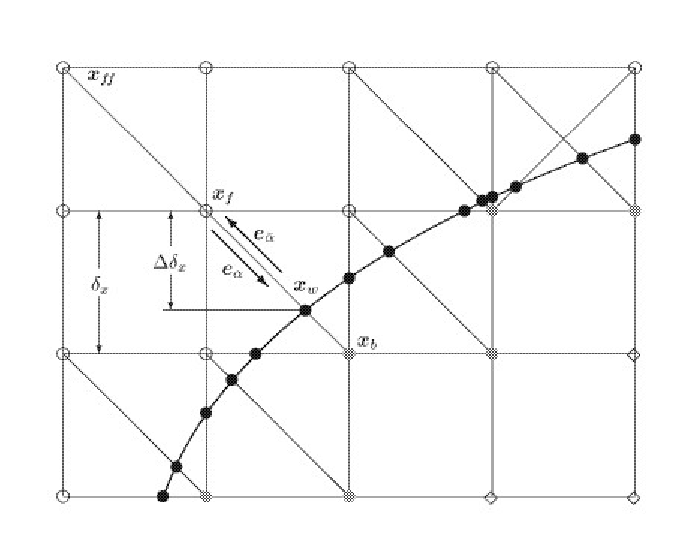
boundary conditions : precise approach



curved boundary: take into account all the red links

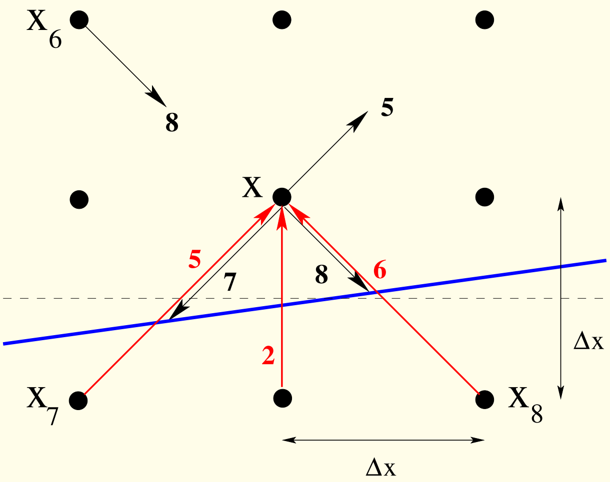
Bouzidi - Firdaouss - Lallemand boundary condition (2001)

boundary conditions : precise approach *(ii)*



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

boundary conditions : precise approach *(iii)*



"ABCD" method: exact exponential expansion

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

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

ABCD method for the analysis of a MRT scheme

two steps for one time iteration

(i) nonlinear relaxation $\quad m^* \equiv \begin{pmatrix} W^* \\ Y^* \end{pmatrix}$

$W^* = W, \; Y^* = Y + S\,(\Phi(W) - Y)$, relaxation diagonal matrix S

(ii) linear advection $\quad f^* = M^{-1}\, m^*$,

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

momentum-velocity operator matrix $\Lambda \equiv M\, \mathrm{diag}\Big(\sum_{1 \le \alpha \le d} v^\alpha\, \partial_\alpha \Big)\, M^{-1}$

advection operator in the basis of moments

exact exponential expression of the lattice Boltzmann scheme

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

$$\exp(-\Delta t\, \Lambda) = \mathrm{I} - \Delta t\, \Lambda + \frac{\Delta t^2}{2}\, \Lambda^2 + \mathrm{O}(\Delta t^2)$$

"ABCD" block decomposition $\Lambda \equiv \begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix} = \begin{pmatrix} 0 & \partial_x & 0 \\ \frac{2}{3}\lambda^2\, \partial_x & 0 & \frac{1}{3}\partial_x \\ 0 & \lambda^2 \partial_x & 0 \end{pmatrix}$

$$\Lambda^2 = \begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix} = \begin{pmatrix} \boldsymbol{A}^2 + \boldsymbol{B}\,\boldsymbol{C} & \boldsymbol{A}\,\boldsymbol{B} + \boldsymbol{B}\,\boldsymbol{D} \\ \boldsymbol{C}\,\boldsymbol{A} + \boldsymbol{D}\,\boldsymbol{C} & \boldsymbol{C}\,\boldsymbol{B} + \boldsymbol{D}^2 \end{pmatrix}$$

ABCD method for the analysis of a MRT scheme *(ii)*

analysis: Chapman Enskog expansion of lattice Boltzmann schemes
Francis J. Alexander, Shiyi Chen, James D. Sterling (1993)
Guy McNamara and Berni Alder (1993), ...

$\partial_t = \partial_{t_1} + \Delta t \, \partial_{t_2} + \mathrm{O}(\Delta t^2)$

revisited with the Taylor expansion and the "ABCD" method

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

general formal algorithm to determine

the equivalent partial differential equations of the scheme

$$\partial_{t_1} W + \Gamma_1 = 0, \quad \partial_{t_2} W + \Gamma_2 = 0$$

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

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

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

$$\Sigma \equiv S^{-1} - \tfrac{1}{2}\,\mathrm{I}, \text{ Hénon matrix } \Sigma = \mathrm{diag}\,(\sigma_e,\, \sigma_x,\, \sigma_x,\, \sigma_q,\, \sigma_q,\, \sigma_h)$$

$$\Gamma_2 = \boldsymbol{B}\ \Sigma\, \Psi_1$$

fit the parameters of the scheme $\Phi(W)$ and S

to recover Navier Stokes at second order accuracy ?

"ABCD" method: fourth order expansion

asymptotic expansion for the microscopic moments

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

partial differential equation for the conserved moments

$$\partial_t = \partial_{t_1} + \Delta t\, \partial_{t_2} + \Delta t^2\, \partial_{t_3} + \Delta t^3\, \partial_{t_4} + \mathrm{O}(\Delta t^4)$$

$$\partial_{t_1} W + \Gamma_1 = 0, \quad \partial_{t_2} W + \Gamma_2 = 0, \; \partial_{t_3} W + \Gamma_3 = 0, \quad \partial_{t_4} W + \Gamma_4 = 0$$

third order terms

$$\begin{aligned} \Psi_2(W) &= \Sigma\, \mathrm{d}\Psi_1(W).\Gamma_1(W) + \mathrm{d}\Phi(W).\Gamma_2(W) - D\,\Sigma\,\Psi_1(W) \\ \Gamma_3(W) &= B\,\Sigma\,\Psi_2(W) + \tfrac{1}{12} B_2\,\Psi_1(W) - \tfrac{1}{6}\, B\, \mathrm{d}\Psi_1(W).\Gamma_1(W) \end{aligned}$$

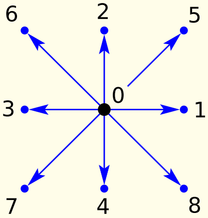
fourth order terms

$$\begin{aligned} \Psi_3(W) &= \Sigma\, \mathrm{d}\Psi_1(W).\Gamma_2(W) + \mathrm{d}\Phi(W).\Gamma_3(W) - D\,\Sigma\,\Psi_2(W) \\ &\quad + \Sigma\, \mathrm{d}\Psi_2(W).\Gamma_1(W) + \tfrac{1}{6}\, D\, \mathrm{d}\Psi_1(W).\Gamma_1(W) \\ &\quad - \tfrac{1}{12}\, D_2\,\Psi_1(W) - \tfrac{1}{12}\, \mathrm{d}\big(\mathrm{d}\Psi_1(W).\Gamma_1\big).\Gamma_1(W) \\ \Gamma_4(W) &= B\,\Sigma\,\Psi_3(W) + \tfrac{1}{4}\, B_2\,\Psi_2(W) + \tfrac{1}{6}\, B\, D_2\,\Sigma\,\Psi_1(W) \\ &\quad - \tfrac{1}{6}\, A\, B\, \Psi_2(W) - \tfrac{1}{6}\, B \Big(\mathrm{d}\big(\mathrm{d}\Phi.\Gamma_1\big).\Gamma_2(W) \\ &\quad + \mathrm{d}\big(\mathrm{d}\Phi.\Gamma_2\big).\Gamma_1(W) \Big) - \tfrac{1}{6}\, B\,\Sigma\, \mathrm{d}\big(\mathrm{d}\Psi_1(W).\Gamma_1\big).\Gamma_1(W) \end{aligned}$$

D2Q9 for isothermal Navier Stokes ?

$$\partial_t \rho + \partial_x(\rho\, u) + \partial_y(\rho\, v) = 0$$
$$\partial_t(\rho\, u) + \partial_x(\rho\, u^2 + p) + \partial_y(\rho\, u\, v) = \partial_x \tau_{xx} + \partial_y \tau_{xy}$$
$$\partial_t(\rho\, v) + \partial_x(\rho\, u\, v) + \partial_y(\rho\, v^2 + p) = \partial_x \tau_{xy} + \partial_y \tau_{yy}$$

$$p = c_s^2\, \rho$$
$$\tau_{xx} = 2\, \mu\, \partial_x u + (\zeta - \mu)\, (\partial_x u + \partial_y v)$$
$$\tau_{xy} = \mu\, (\partial_x v + \partial_y u)$$
$$\tau_{xx} = (\zeta - \mu)(\partial_x u + \partial_y v) + 2\, \mu\, \partial_y v$$



fit the parameters of the scheme !?

moments, equilibrium vector function, relaxation matrix

D2Q9 for isothermal Navier Stokes ? *(ii)*

$$M = \begin{array}{c} \left[\begin{array}{ccccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{array} \right] \end{array} \begin{array}{c} \rho \\ J_x \\ J_y \\ \varepsilon \\ xx \\ xy \\ q_x \\ q_y \\ h \end{array}$$

two families of moments $\quad m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}, \;\; m = M\, f$

conserved moments $\quad W \equiv (\rho,\, J_x = \rho\, u,\, J_y = \rho\, v)^{\mathrm{t}} \in \mathbb{R}^N$

microscopic non-conserved moments

$$Y \equiv (\varepsilon,\, xx,\, xy,\, q_x,\, q_y,\, h)^{\mathrm{t}} \in \mathbb{R}^{q-N}$$

equilibrium vector function $\quad Y^{\mathrm{eq}} = \Phi(W)$

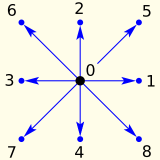
$$\mathbb{R}^N \ni W \longmapsto \Phi(W) \in \mathbb{R}^{q-N} \qquad \Phi = ??$$

ABCD method for the analysis of the D2Q9 scheme

momentum-velocity operator matrix

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

for the isothermal D2Q9 scheme



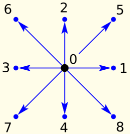
$$\begin{array}{c} \begin{array}{ccccccccc} \rho & J_x & J_y & \varepsilon & xx & xy & q_x & q_y & h \end{array} \\ \left[\begin{array}{ccc|cccccc} 0 & \partial_x & \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2\lambda^2}{3}\,\partial_x & 0 & 0 & \frac{1}{6}\,\partial_x & \frac{1}{2}\,\partial_x & \partial_y & 0 & 0 & 0 \\ \frac{2\lambda^2}{3}\,\partial_y & 0 & 0 & \frac{1}{6}\,\partial_y & -\frac{1}{2}\,\partial_y & \partial_x & 0 & 0 & 0 \\ \hline 0 & \lambda^2\,\partial_x & \lambda^2\,\partial_y & 0 & 0 & 0 & \partial_x & \partial_y & 0 \\ 0 & \frac{\lambda^2}{3}\,\partial_x & -\frac{\lambda^2}{3}\,\partial_y & 0 & 0 & 0 & -\frac{1}{3}\,\partial_x & \frac{1}{3}\,\partial_y & 0 \\ 0 & \frac{2\,\lambda^2}{3}\,\partial_y & \frac{2\,\lambda^2}{3}\,\partial_x & 0 & 0 & 0 & \frac{1}{3}\,\partial_y & \frac{1}{3}\,\partial_x & 0 \\ 0 & 0 & 0 & \frac{\lambda^2}{3}\,\partial_x & -\lambda^2\,\partial_x & \lambda^2\,\partial_y & 0 & 0 & \frac{1}{3}\,\partial_x \\ 0 & 0 & 0 & \frac{\lambda^2}{3}\,\partial_y & \lambda^2\,\partial_y & \lambda^2\,\partial_x & 0 & 0 & \frac{1}{3}\,\partial_y \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda^2\,\partial_x & \lambda^2\,\partial_y & 0 \end{array}\right] \begin{array}{c} \rho \\ J_x \\ J_y \\ \varepsilon \\ xx \\ xy \\ q_x \\ q_y \\ h \end{array} \end{array}$$

D2Q9 cannot accurately simulate Navier Stokes

Φ : vector of moments at equilibrium

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

linear system for the partial derivatives in $\nabla_W \Phi$



the best we can do

sound velocity without dimension $c_s = \frac{1}{\sqrt{3}}$: $p(\rho) = \frac{\lambda^2}{3}\,\rho$

$\Phi_\varepsilon = -2\,\lambda^2\,\rho + 3\,\rho\,(u^2 + v^2)$

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

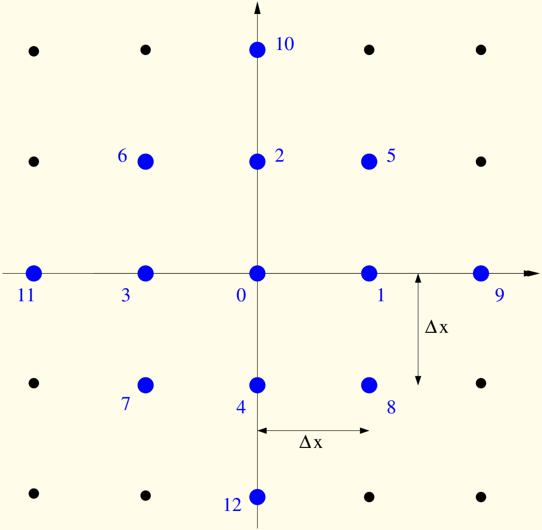
$\Phi_{qx} = -\rho\,\lambda^2\,u + 3\,\rho\,(u^2 + v^2)\,u$, $\quad \Phi_{qy} = -\rho\,\lambda^2\,v + 3\,\rho\,(u^2 + v^2)\,v$

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

lattice Boltzmann = Navier Stokes + discrepancy

$$\Delta t\,(\Gamma_2)_J = -\begin{pmatrix} \partial_x \tau_{xx} + \partial_y \tau_{xy} \\ \partial_x \tau_{xy} + \partial_y \tau_{yy} \end{pmatrix}$$
$$+\sigma_x\,\Delta t\,\partial_x \begin{pmatrix} u^3\,\partial_x \rho - v^3\,\partial_y \rho + 3\,\rho\,(u^2\,\partial_x u - v^2\,\partial_y v) \\ -v^3\,\partial_x \rho - u^3\,\partial_y \rho - 3\,\rho\,(u^2\,\partial_y u + v^2\,\partial_x v) \end{pmatrix}$$
$$+\sigma_x\,\Delta t\,\partial_y \begin{pmatrix} -v^3\,\partial_x \rho - u^3\,\partial_y \rho - 3\,\rho\,(u^2\,\partial_y u + v^2\,\partial_x v) \\ -u^3\,\partial_x \rho + v^3\,\partial_y \rho + 3\,\rho\,(-u^2\,\partial_x u + v^2\,\partial_y v) \end{pmatrix}$$

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: momentum-velocity operator matrix Λ

$$\Lambda = \begin{array}{c} \begin{matrix} \rho & J_x & J_y & \varepsilon & xx & xy & q_x & q_y & r_x & r_y & h & x_{xe} & h_2 \end{matrix} \\ \begin{bmatrix} 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ *\partial_x & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ *\partial_y & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 \\ 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\ 0 & *\partial_y & *\partial_x & 0 & 0 & 0 & *\partial_y & *\partial_x & *\partial_y & *\partial_x & 0 & 0 & 0 \\ 0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & 0 \\ 0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & 0 \\ 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_x \\ 0 & 0 & 0 & 0 & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_y \\ 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 \end{bmatrix} \end{array}$$

D2Q13 for isothermal Navier Stokes

equilibrium vector function

$$\Phi = \big(\Phi_\varepsilon,\ \Phi_{xx},\ \Phi_{xy},\ \Phi_{qx}\ ,\Phi_{qy}\ ,\ \Phi_{rx},\ \Phi_{ry},\ \Phi_{h},\ \Phi_{xxe}\ ,\ \Phi_{h_2}\big)^{\rm t}$$

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

$$\Phi_{xy} = \rho\, u\, v$$

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

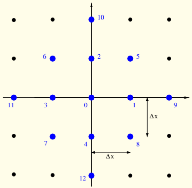
the sound velocity c_s is not constrained: $\quad p = \lambda^2\, c_s^2\, \rho$

$$\Phi_{qx} = \rho\,\big(|\mathbf{u}|^2 + 4\,\lambda^2\,c_s^2 - 3\,\lambda^2\big)\,u$$

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

$$\Phi_{rx} = \rho\,\Big(-\tfrac{7}{6}\,\lambda^2\,u^2 - 7\,\lambda^2\,v^2 - \tfrac{21}{2}\,\lambda^4\,c_s^2 + \tfrac{31}{6}\,\lambda^4\Big)\,u$$

$$\Phi_{ry} = \rho\,\Big(-7\,\lambda^2\,u^2 - \tfrac{7}{6}\,\lambda^2\,v^2 - \tfrac{21}{2}\,\lambda^4\,c_s^2 + \tfrac{31}{6}\,\lambda^4\Big)\,v$$

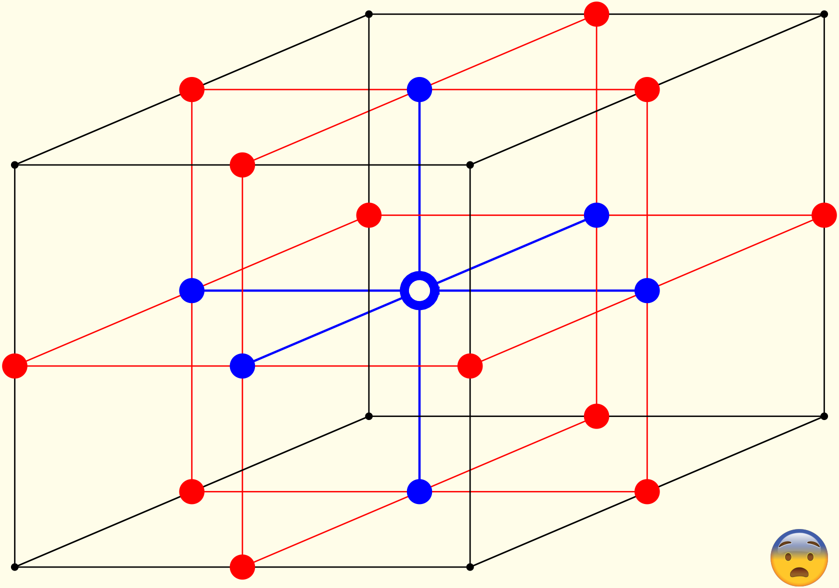


$$\mu = \rho\,\sigma_x\,\lambda\,c_s^2\,\Delta x,\quad \zeta = \rho\,\sigma_e\,\lambda\,c_s^2\,\Delta x$$

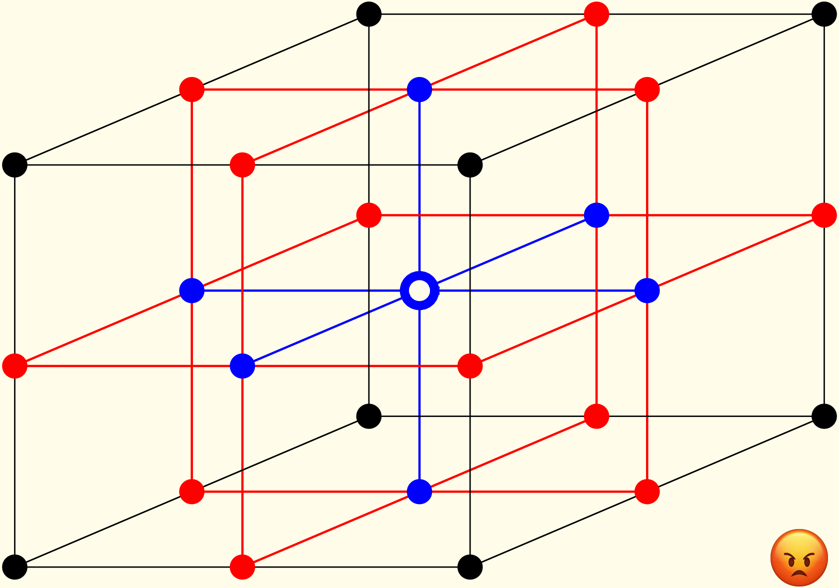
lattice Boltzmann = Navier Stokes

$$\Delta t\,\big(\Gamma_2\big)_J = -\begin{pmatrix}\partial_x\tau_{xx} + \partial_y\tau_{xy}\\ \partial_x\tau_{xy} + \partial_y\tau_{yy}\end{pmatrix}$$

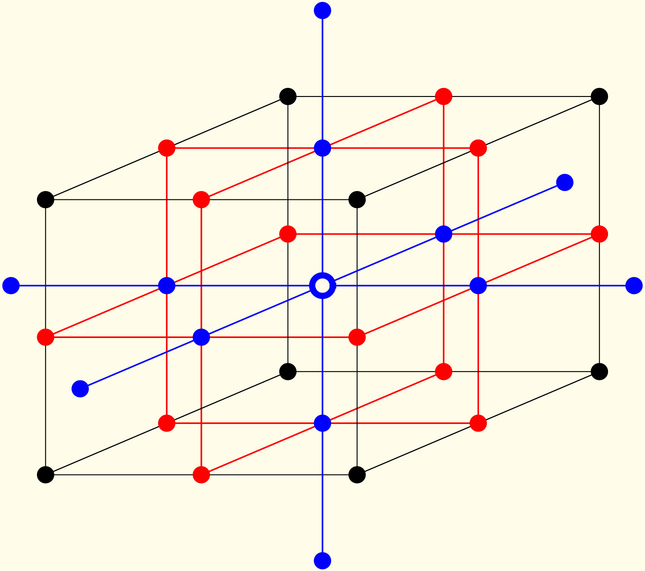
D3Q19



D3Q27



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

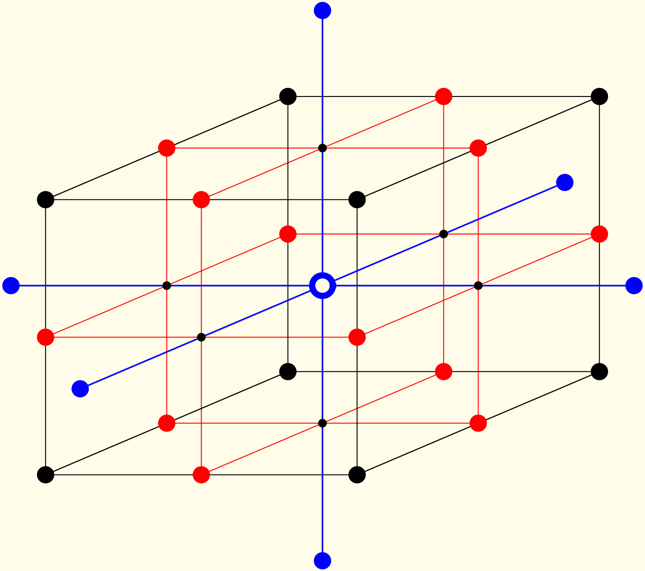
$xx_e\,,\ ww_e$

$xx_h\,,\ ww_h$

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

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

D3Q27-2 of Lallemand, d'Humières, Luo and Rubinstein



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

$xx_e\,,\ ww_e$

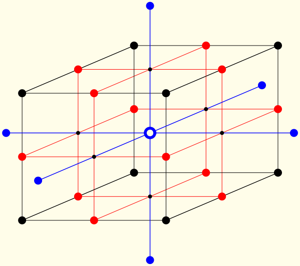
$xy_e\,,\ yz_e\,,\ zx_e$

$h2$

D3Q27-2 allows to recover isothermal Navier Stokes!

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

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



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

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

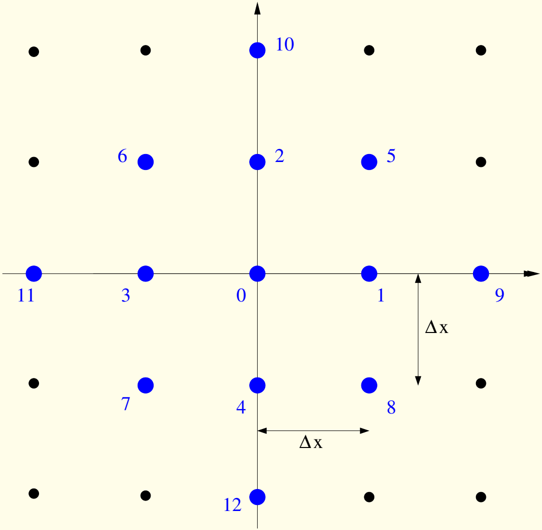
energy conservation

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

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

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

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

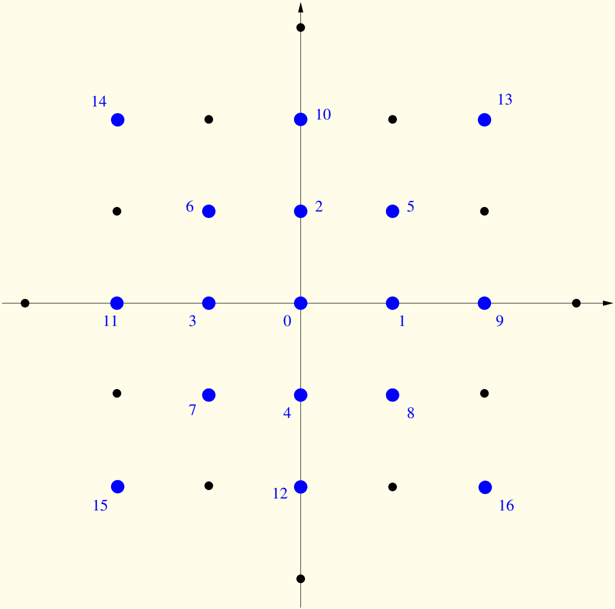
D2Q13: previous operator matrix Λ for isothermal

$$
\Lambda = \begin{array}{c}
\begin{array}{ccccccccccccc} \rho & J_x & J_y & \varepsilon & xx & xy & q_x & q_y & r_x & r_y & h & x_{xe} & h_2 \end{array} \\
\begin{bmatrix}
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_x & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_y & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & *\partial_y & *\partial_x & 0 & 0 & 0 & *\partial_y & *\partial_x & *\partial_y & *\partial_x & 0 & 0 & 0 \\
0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & 0 \\
0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & 0 \\
0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_x \\
0 & 0 & 0 & 0 & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_y \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0
\end{bmatrix}
\end{array}
$$

D2Q13: momentum-velocity operator matrix Λ

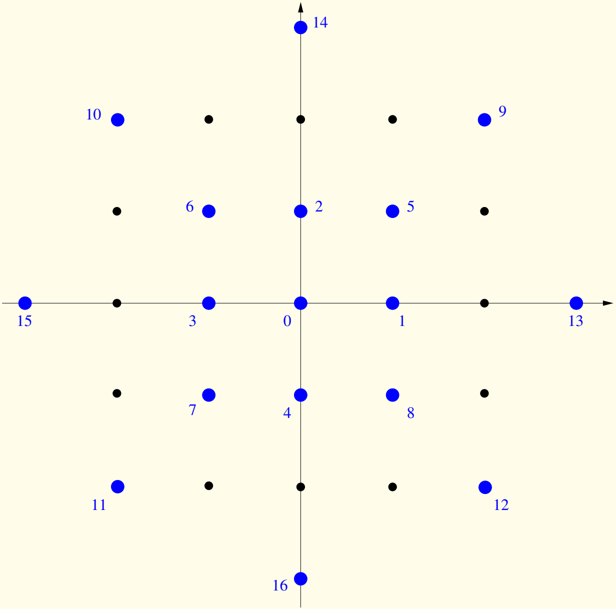
$$\Lambda = \begin{array}{c}
\begin{array}{ccccccccccccc}
\rho & J_x & J_y & \varepsilon & xx & xy & q_x & q_y & r_x & r_y & h & x_{xe} & h_2
\end{array} \\
\begin{bmatrix}
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_x & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
*\partial_y & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & 0 \\
0 & *\partial_x & *\partial_y & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & *\partial_y & *\partial_x & 0 & 0 & 0 & *\partial_y & *\partial_x & *\partial_y & *\partial_x & 0 & 0 & 0 \\
0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & 0 \\
0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & 0 \\
0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0 & 0 & *\partial_x & *\partial_x & *\partial_x \\
0 & 0 & 0 & 0 & *\partial_y & *\partial_x & 0 & 0 & 0 & 0 & *\partial_y & *\partial_y & *\partial_y \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & *\partial_x & *\partial_y & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & *\partial_x & *\partial_y & 0 & 0 & 0
\end{bmatrix}
\end{array}$$

D2Q17



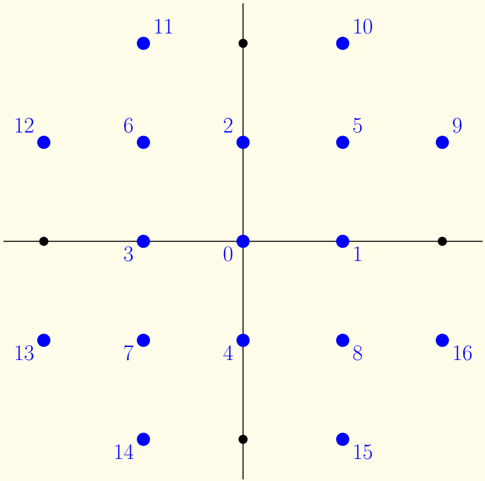
ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
s_x	7
s_y	7
h	4
x_{xe}	4
x_{ye}	4
h_3	6
h_4	8

D2V17 of Paulo Philippi and Luiz Hegele



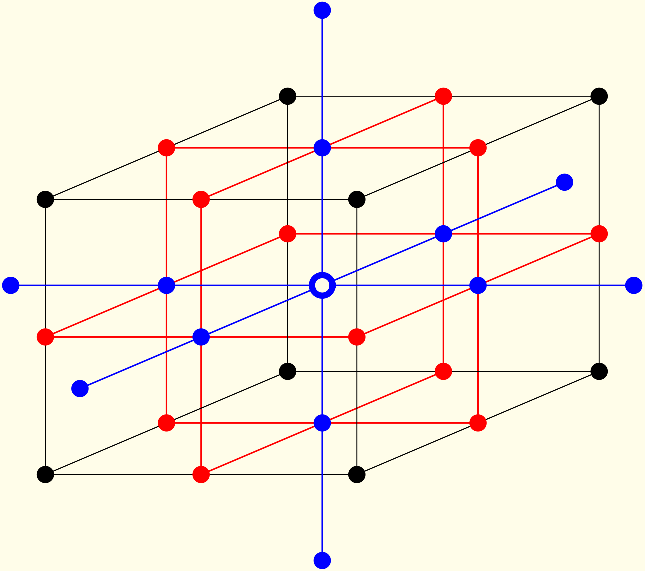
ρ	0
J_x	1
J_y	1
ε	2
xx	2
xy	2
q_x	3
q_y	3
r_x	5
r_y	5
s_x	7
s_y	7
h	4
x_{xe}	4
x_{ye}	4
h_2	6
h_3	8

D2W17 of Pierre Lallemand



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

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

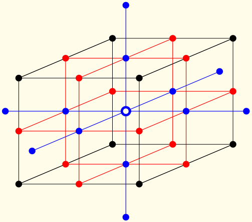
$r_x\,,\ r_y\,,\ r_z$

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

$xx_e\,,\ ww_e$

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

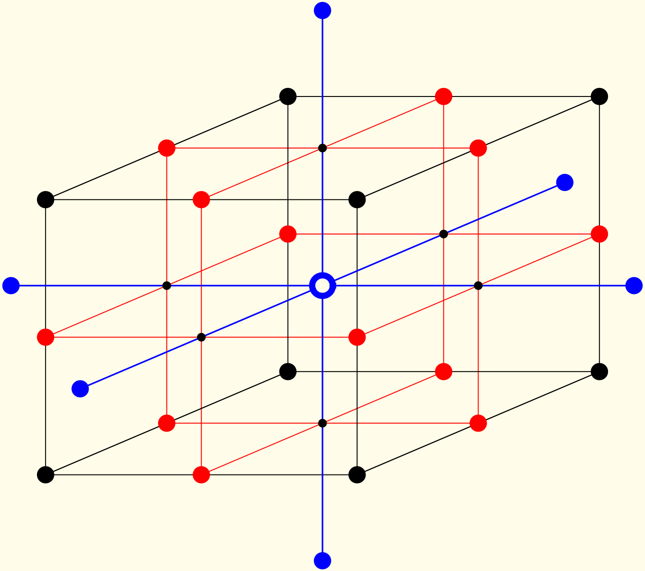
hh



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

$h3\,,\ h4$

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: equilibrium vector function

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

$\Phi_{xx} = \rho\,(2\,u^2 - v^2 - w^2)\,,\;\; \Phi_{ww} = \rho\,(v^2 - w^2)$

$\Phi_{xy} = \rho\, u\, v\,,\;\; \Phi_{yz} = \rho\, v\, w\,,\;\; \Phi_{zx} = \rho\, w\, u$

$\Phi_{qx} = \rho\, u\, \xi_q,\;\; \Phi_{qy} = \rho\, v\, \xi_q,\;\; \Phi_{qz} = \rho\, w\, \xi_q,\;\; \xi_q = |\mathbf{u}|^2 + \frac{10}{3}\, e - 3\,\lambda^2$

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

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

$\Phi_{rx} = \rho\, u\, \lambda^2\,\big(-(u^2 + 3\,v^2 + 3\,w^2) - 6\,e + 5\,\lambda^2\big)$

$\Phi_{ry} = \rho\, v\, \lambda^2\,\big(-(3\,u^2 + v^2 + 3\,w^2) - 6\,e + 5\,\lambda^2\big)$

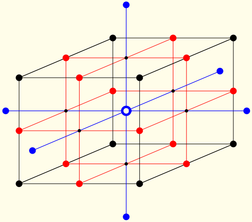
$\Phi_{rz} = \rho\, w\, \lambda^2\,\big(-(3\,u^2 + 3\,v^2 + w^2) - 6\,e + 5\,\lambda^2\big)$

$\Phi_{xxe} = \rho\,(2\,u^2 - v^2 - w^2)\,\big(\frac{9}{8}\,|\mathbf{u}|^2 + \frac{21}{4}\, e - \frac{17}{4}\,\lambda^2\big)$

$\Phi_{wwe} = \rho\,(v^2 - w^2)\,\big(\frac{9}{8}\,|\mathbf{u}|^2 + \frac{21}{4}\, e - \frac{17}{4}\,\lambda^2\big)$

$\Phi_{hh} = \rho\,\big(\frac{3}{2}\,|\mathbf{u}|^4 + 10\,(|\mathbf{u}|^2 + e)\, e - 15\,\lambda^2\,(\frac{1}{2}\,|\mathbf{u}|^2 + e) + 8\,\lambda^4\big)$

$\Phi_{xye} = \rho\, u\, v\, \beta_e,\;\; \Phi_{yze} = \rho\, v\, w\, \beta_e,\;\; \Phi_{zxe} = \rho\, w\, u\, \beta_e,\;\; \beta_e = 3\,|\mathbf{u}|^2 + 14\, e - 8\,\lambda^2$



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

$\sigma_x = \sigma_q$, then Prandtl number: $Pr = 1$

Conclusion

analysis of Multiple Relaxation Times lattice Boltzmann schemes
with the Taylor expansion method and the ABCD approach:
generalization of the Chapman Enskog methodology

inverse problem for Navier Stokes $\Phi(W) = ?, \;\; S = ?$

isothermal Navier Stokes

D3Q27 has a discrepancy for isothermal Navier Stokes

D3Q27-2 available for isothermal Navier Stokes

thermal Navier Stokes

we must impose $\gamma \equiv \frac{c_p}{c_v} = 2$ (2d), $\gamma = \frac{5}{3}$ (3d)
and a Prandtl number satisfying $Pr = 1$

D3Q27-2 available for thermal Navier Stokes

stability has not been studied in this contribution

numerical experiments are welcomed!

Formal calculus with SageMath

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

www.sagemath.org

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Merci de votre attention !