From Cellular Automata to Lattice Boltzmann Models

Dieter A. Wolf-Gladrow
Alfred Wegener Institute for Polar and Marine Research,
POB 12 01 61
D-27515 Bremerhaven, Federal Republic of Germany
Dieter.Wolf-Gladrow@awi.de
Dresden

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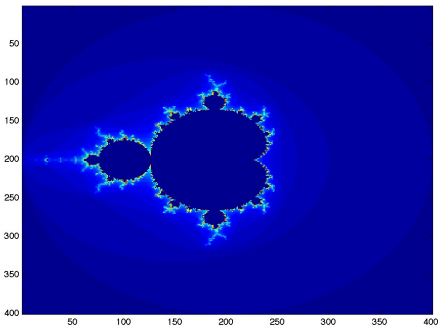
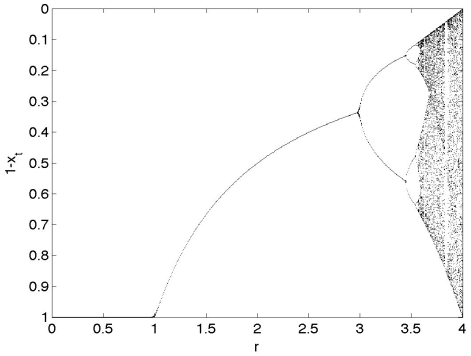
Simple models for complex phenomena

Simulation of complex phenomena in space and time with simple mathematical models

Well-known examples of simple models with complex outcome:

1. Ising model (1D: Ising, 1925; 2D: Onsager, 1944, phase transition)
2. Mandelbrot set: iteration of $z_{n+1} = z_n^2 + c$, c and $z_n \in \mathbb{C}$
3. Logistic map: $x_{n+1} = r x_n (1 - x_n)$, $x_n \in \mathbb{R}$ (May, 976)





Cellular automata: discrete in space, time, and state

Characterization of cellular automata (CA):

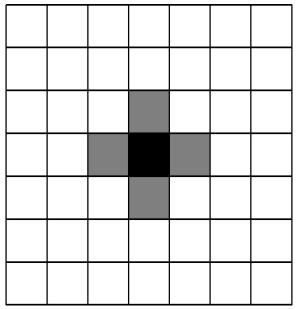
- CA are regular arrangements of single *cells* of the same kind.
- Each cell holds a finite number of discrete states.
- The states are updated simultaneously ('synchronously') at discrete time levels.
- The update rules are uniform in space and time.
- The rules for the evolution of a cell depend only on a local neighborhood of cells.

Cellular automata: history

- Norbert Wiener and Aturo Rosenblueth, The mathematical formulation of the problem of conduction of impulses in a network of connected excitable elements, specifically in cardiac muscle. Arch. Inst. Cardiol. Mexico, 16, 205-265, 1946.
- Stanislas Ulam (1952, 1962): growth processes.
- John von Neumann further developed CA in order to construct self-reproducing CA ('the robot that is able to rebuild itself').
- Konrad Zuse (Rechnender Raum 1969; English translation: Calculating Space, 1970).
- Early 1970ies Conway: 'Game of Life': it has the power of a universal Turing machine: that is, anything that can be computed algorithmically can be computed within Conway's Game of Life.
- Wolfram (1983, 1984): systematic investigation of one-dimensional CA.

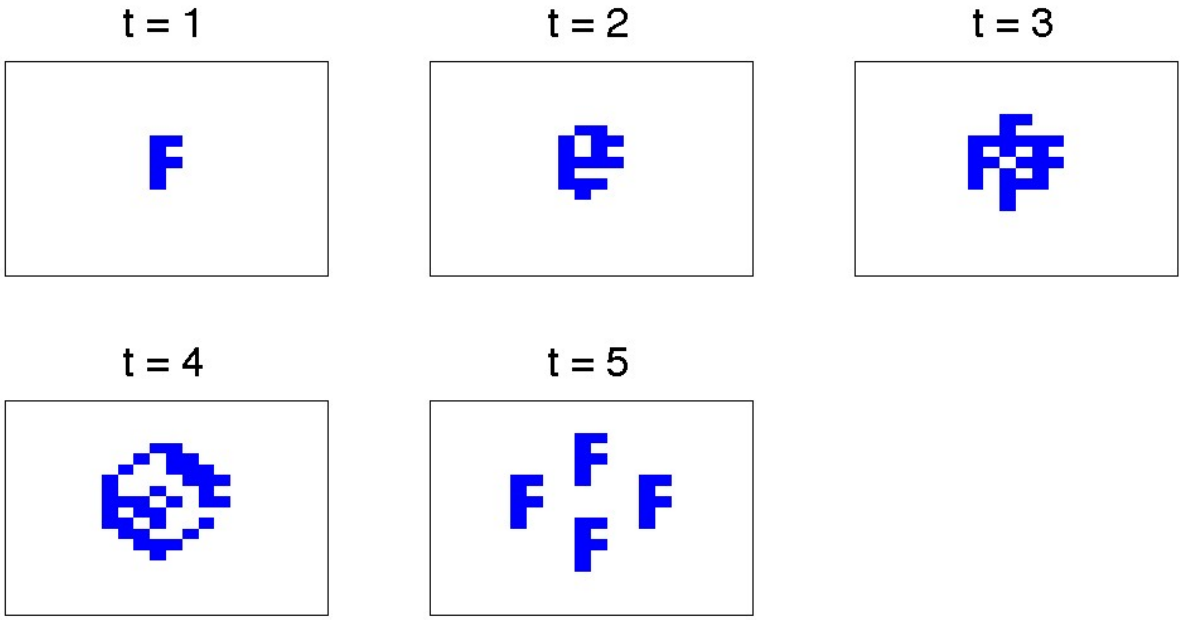
Fredkin's game

Fredkin's game is defined on the smallest von Neumann neighborhood encompassing 4 cells (grey) with two possibles states per cell: dead or alive, white or black, off or on, 0 or 1.

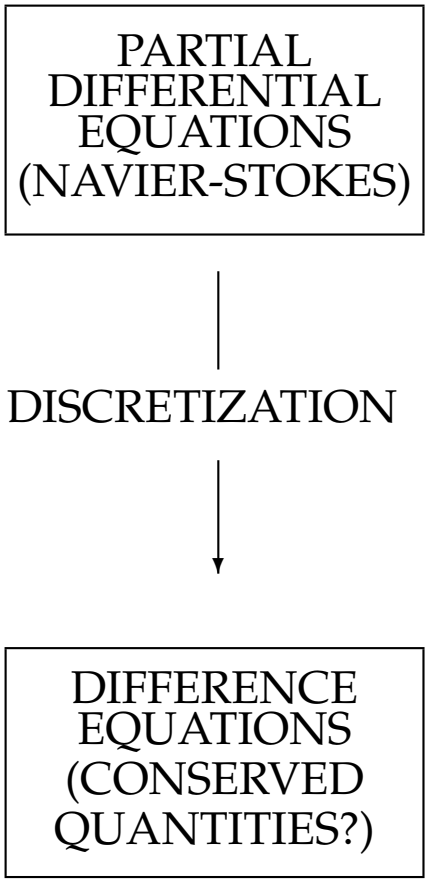


The rules of Fredkin's game are simple: for each cell

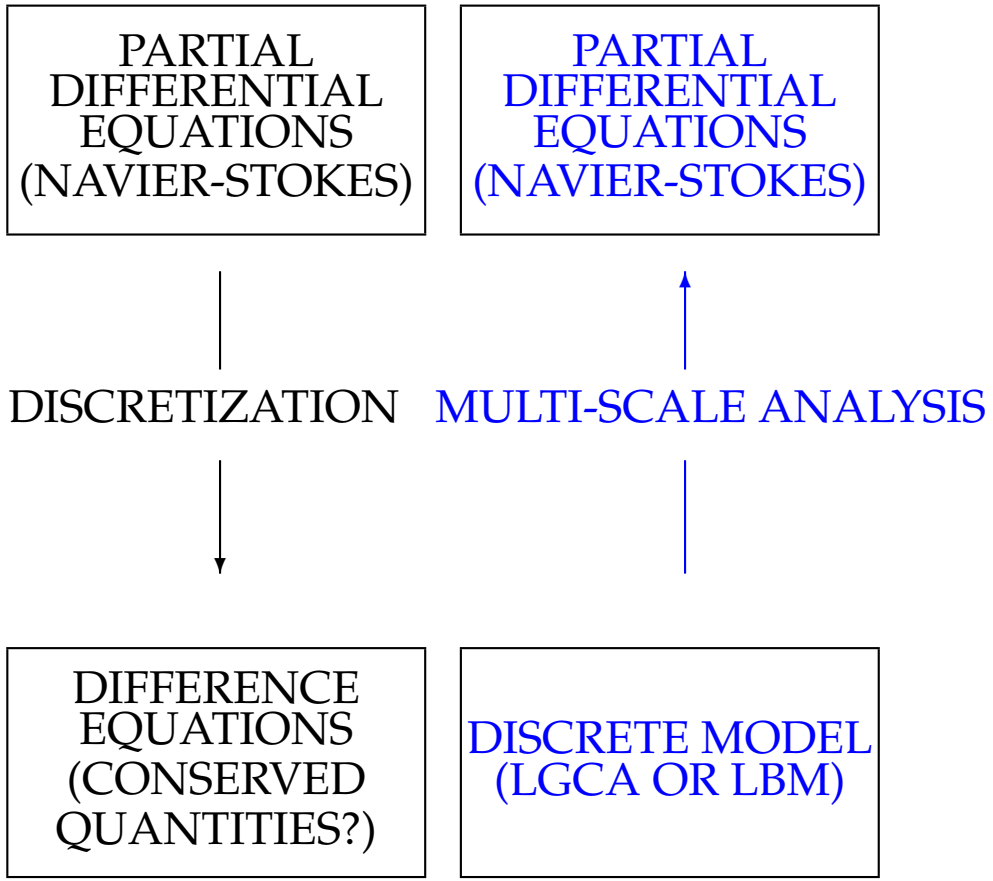
- count the number of live cells, N, of the 4 neighbors: $N = 0$,1,2,3, or 4;
- even or odd: each cell with an even number $(0, 2, 4)$ of live neighbors will be dead at the next time level and alive otherwise.


t = 1
t = 2
t = 3
t = 4
t = 5

Simulation of fluid flows: top-down



Simulation of fluid flows: top-down versus bottom up



Simulation of fluid flows with Lattice-Gas Cellular Automata (LGCA)

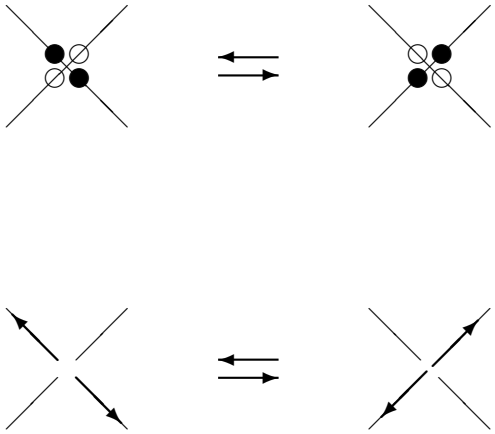
Fluid flow: continuity and Navier-Stokes equations are based on conservation of mass and momentum.

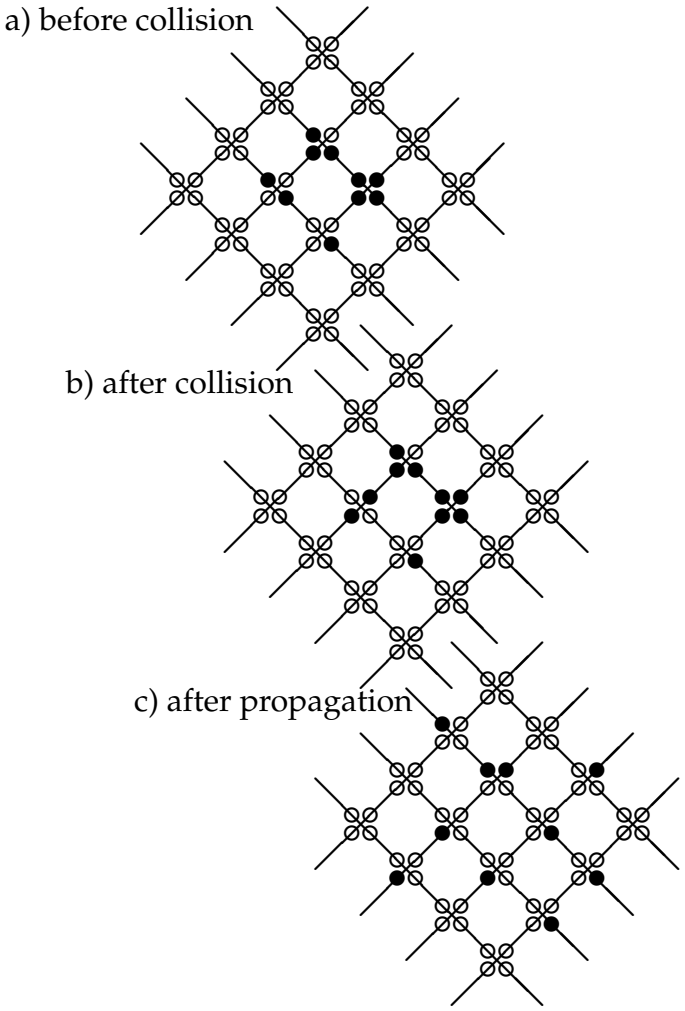
Basic idea of LGCA for fluid dynamics: create an artificial micro-world that

- is much simpler than the real world,
- possesses built-in conservation laws for mass and momentum (and nothing else), and
- leads to continuity and Navier-Stokes equations in the 'macroscopic limit' (averaging over space).

LGCA (in contrast to CA): split update rule into collision and propagation.

Hardy, Pomeau, and de Pazzis (1973, HPP)




a) before collision
b) after collision
c) after propagation

HPP

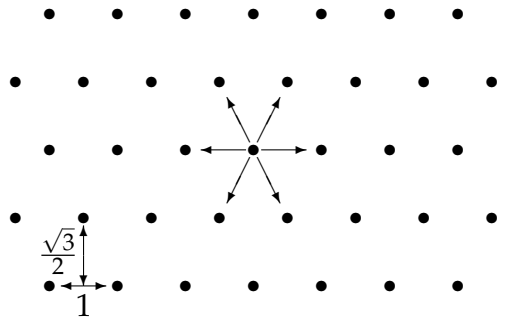
- 2D, square lattice
- 4 cells per node
- 4 lattice velocities = vectors that link neighboring lattice nodes
- identical particles with mass $m = 1$
- momentum = mass * lattice velocity
- succession of collision and propagation
- 1 type of collision only: head-on, conserves mass and momentum
- **However: HPP does not lead to Navier-Stokes**

Symmetry of the lattice

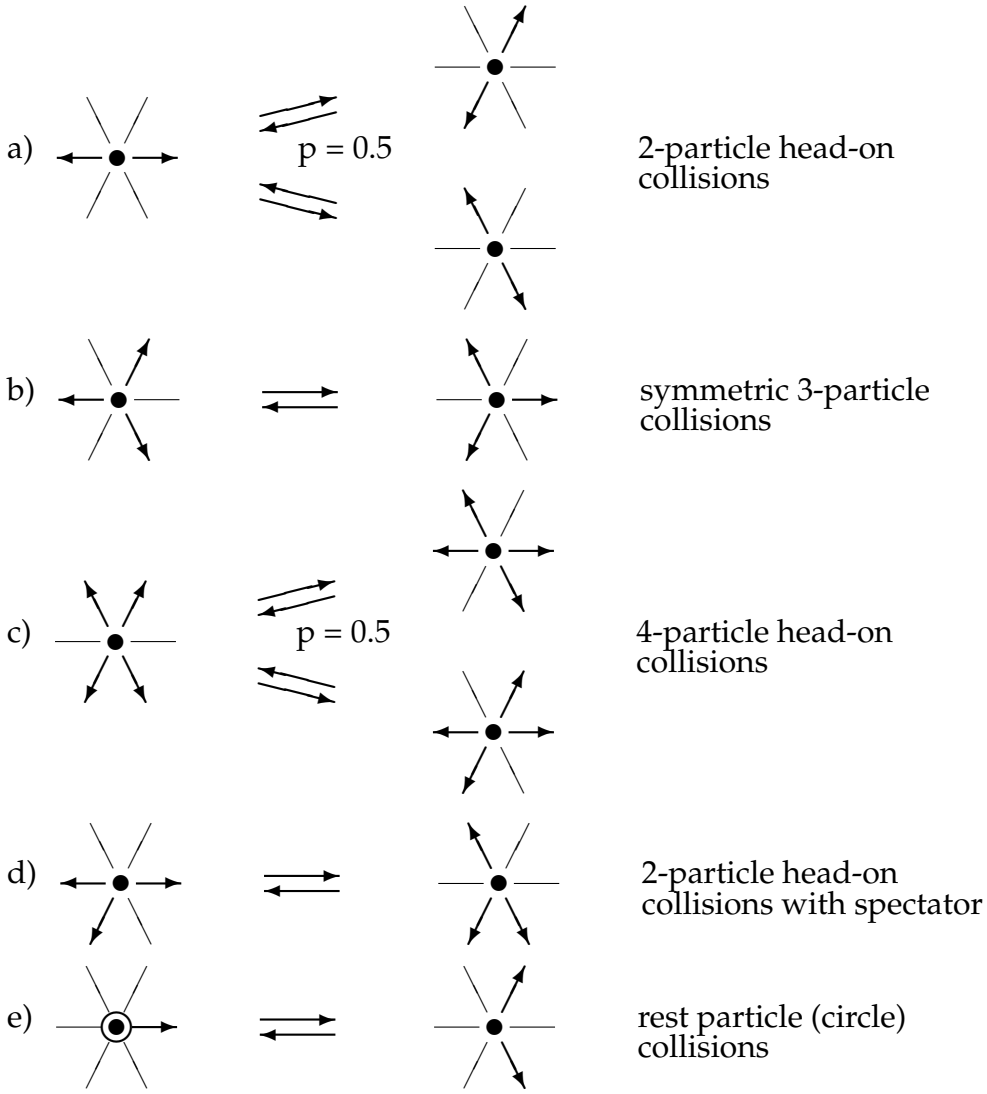
HPP fails to yield Navier-Stokes because of 'not enough symmetry' of the underlying lattice. 4-fold symmetry of the square lattice is 'too coarse a resolution with respect to angle'.

Frisch, Hasslacher, and Pomeau (1986, FHP): triangular lattice with 6-fold symmetry (in 2D) is enough to yield Navier-Stokes.

FHP: 6 (or 7) cells per node; several types of collisions.



FHP


a)
p = 0.5
2-particle head-on collisions
b)
symmetric 3-particle collisions
c)
p = 0.5
4-particle head-on collisions
d)
2-particle head-on collisions with spectator
e)
rest particle (circle) collisions

Mass and momentum density

Calculate mean occupation numbers, N_i, by averaging over a large number (32 x 32) of lattice nodes ('coarse graining'):

$$N_i(t, \boldsymbol{r}) = \langle n_i(t, \boldsymbol{r}) \rangle$$

where $n_i(t, \boldsymbol{r}) \in \{0, 1\}$ is the occupation number of cell i of the node at location $\boldsymbol{r}$ and at time t.

Mass and momentum density are defined as follows:

$$\rho(t, \boldsymbol{r}) := \sum_i N_i(t, \boldsymbol{r})$$

$$\boldsymbol{j}(t, \boldsymbol{r}) := \sum_i \boldsymbol{c}_i N_i(t, \boldsymbol{r})$$

where the $\boldsymbol{c}_i$ are the lattice velocities.

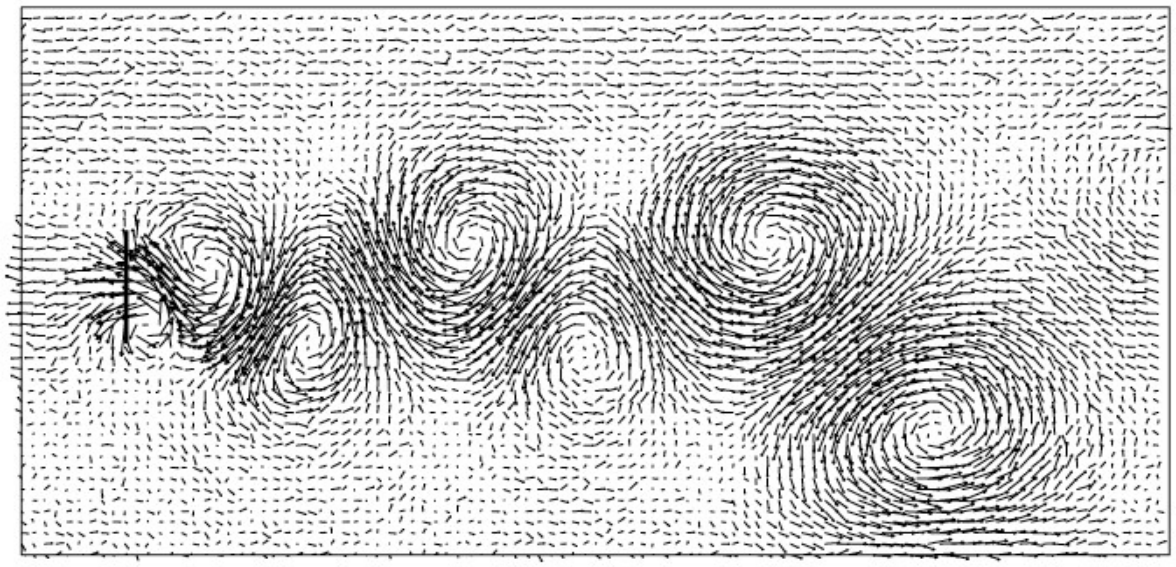


Figure 1: Simulation with PI-LGCA of a Karman vortex street in 2D at a Reynolds number of 80: flow past a plate. The figure shows the perturbation of the velocity after 80 000 time steps. The homogeneous flow field was subtracted to make the eddies clearly visible. The lattice consists of 6400 times 3200 nodes (Wolf-Gladrow et al., 1991).

Computational aspects

The state of a single cell can be described by one bit: 0 = empty, 1 = occupied.

32 (or 64) bits can be stored in a single integer variable.

Logical operators (C) or logical functions (FORTRAN) work bitwise on whole integers.

Collisions can be expressed in terms of logical operations (and, exclusive or, inclusive or, not).

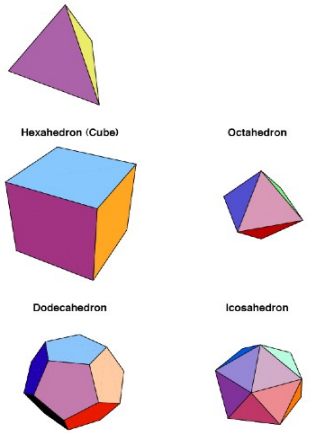
Propagation can be realized by shifts of bits.

LGCA are well adapted for massive parallel computers because collisions are local and propagation involves nearest neighbors only.

The LGCA method is numerically stable (no rounding errors).

Desperately seeking a lattice for simulations in three dimensions

2D: lattice made of plane-filling regular polygons
3D: five regular polytopes: the Platonic solids



No space-filling regular polytope in 3D with sufficient symmetry!

Solution: use face-centered hypercube (FCHC) in 4D and 'project' back to 3D.

FCHC: 24 lattice velocities $\Rightarrow$ collision rules quite complicated (use look-up tables instead of logical functions).

LGCA for fluid dynamics: diseases

disease	cause	therapy/cure	remarks
non-isotropic advection term	lattice tensor of 4th rank is non-isotropic	higher symmetry of lattice add inner degree of freedom multi-speed models	HPP $\rightarrow$ FHP HPP $\rightarrow$ PI
violation of the Galilei invariance	Fermi-Dirac distributions	rescaling (symptomatic treatment)	FHP, FCHC, PI
spurious invariants	regular lattices	as many collisions as possible	Zanetti invariants
noise	Boolean variables	averaging (coarse graining)	enormous memory demand
pressure depends explicitly on velocity		multi-speed models	Chen et al. 1989

Lattice Boltzmann Models (LBMs)

McNamara and Zanetti (1988) introduced LBM in order to get rid of the noise in LGCA.

Basic idea: Replace particles with unit mass by **packages of particles** with variable mass. Use the same lattices as for LGCA (because same symmetry constraints apply), use same collision operators as for LGCA, however, replace the discrete occupation numbers ($n_i = 0$ or 1) by the mean occupation numbers (Fermi-Dirac distributions). Keep succession of collision and propagation.

Further developments: Replace Fermi-Dirac distributions by **Boltzmann distributions** and simplify the collision operator (**BGK approximation**).

Microdynamics of LGCA ($n_i = 0$ or 1):

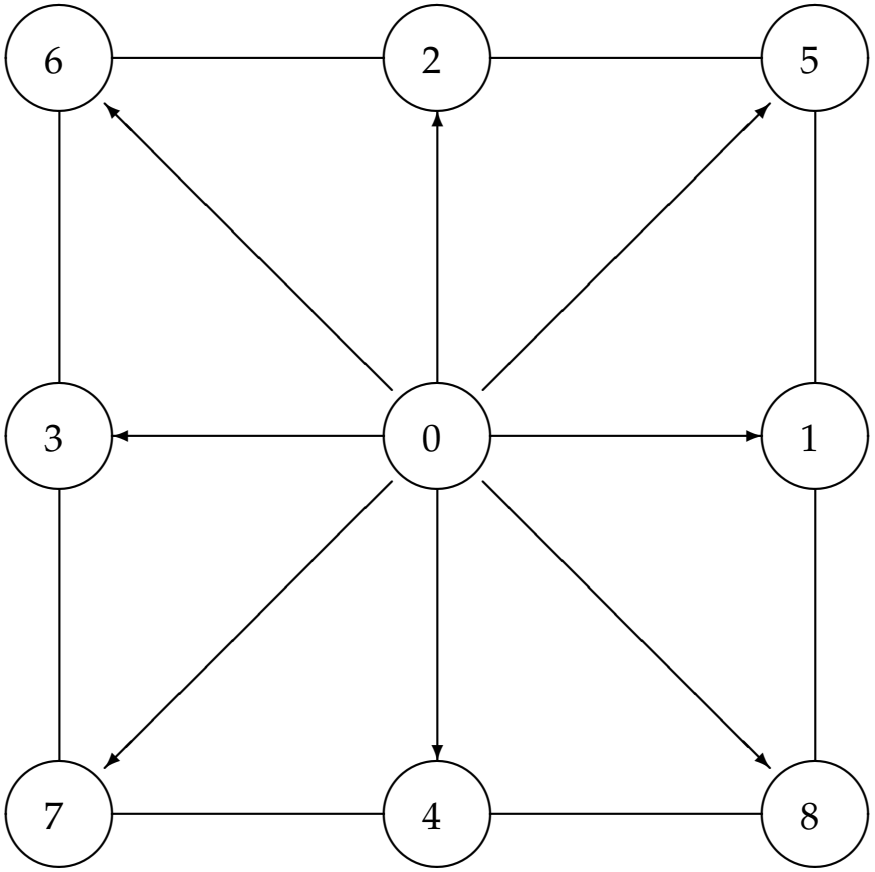
$$n_i\left(\boldsymbol{x} + \boldsymbol{c}_i\Delta t, t + \Delta t\right) - n_i\left(\boldsymbol{x}, t\right) = \underbrace{\Delta_i(n_j)}_{\text{collisions}}$$

Lattice Boltzmann equation with BGK approximation ($F_i \geq 0$, real):

$$F_i\left(\boldsymbol{x} + \boldsymbol{c}_i\Delta t, t + \Delta t\right) - F_i\left(\boldsymbol{x}, t\right) = -\frac{1}{\tau}\left(F_i - F_i^{(eq)}\right) = -\omega\left(F_i - F_i^{(eq)}\right)$$

BGK approximation (Bhatnagar, Gross, and Krook, 1953; Welander, 1954): Collisions lead to approach to equilibrium. Replace complicated collisions by simple relaxation of non-equilibrium distributions towards equilibrium distributions on a time scale τ (non-dimensional; Δt is hidden in τ).

D2Q9 = LBM in 2 dimensions with 9 lattice velocities



D2Q9

$$\rho(\boldsymbol{x},t) = \sum_i F_i(\boldsymbol{x},t) \quad \text{mass} \tag{1}$$

$$\boldsymbol{j}(\boldsymbol{x},t) = \rho(\boldsymbol{x},t)\boldsymbol{v}(\boldsymbol{x},t) = \sum_i \boldsymbol{c}_i F_i(\boldsymbol{x},t) \quad \text{momentum} \tag{2}$$

Distribution functions $F_i(\boldsymbol{x},t)$ = fluid at rest ($W_i > 0$) plus small perturbations $f_i(\boldsymbol{x},t)$

$$F_i(\boldsymbol{x},t) = W_i + f_i(\boldsymbol{x},t)$$

with $|f_i(\boldsymbol{x},t)| << W_i$.

D2Q9: derive equilibrium distributions - it's a kind of magic

1. step: Fluid at rest distributions W_i are derived from the following constraints: **moments up to order 4 over the W_i are equal to the corresponding moments over the Boltzmann distribution**

$$w_B(v) = \rho_0 \frac{m}{2\pi k_B T} \exp\left[-mv^2/2k_B T\right]$$

The odd moments vanish and the even moments read

$$\begin{aligned}
\sum_i W_i &= \int d\boldsymbol{v}\, w_B(v) = \rho_0 \\
\sum_i W_i c_{i\alpha} c_{i\beta} &= \int d\boldsymbol{v}\, w_B(v) v_\alpha v_\beta = \rho_0 \frac{k_B T}{m} \delta_{\alpha\beta} \\
\sum_i W_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} &= \int d\boldsymbol{v}\, w_B(v) v_\alpha v_\beta v_\gamma v_\delta \\
&= \rho_0 \left(\frac{k_B T}{m}\right)^2 (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}).
\end{aligned}$$

$\Rightarrow$

$$W_0 = \frac{4}{9}\rho_0, \quad W_m = \frac{1}{9}\rho_0 \quad m = 1,2,3,4, \quad W_n = \frac{1}{36}\rho_0 \quad n = 5,6,7,8$$

Maximum entropy principle

2. step: In order to derive the equilibrium distributions $F_i^{(0)}$ one applies the maximum entropy principle with the entropy relative to the fluid at rest distributions (W_i)

$$S(\rho, \boldsymbol{j}) := -\frac{k}{m} \sum_i F_i^{(0)}(\rho, \boldsymbol{j}) \ln \frac{F_i^{(0)}(\rho, \boldsymbol{j})}{W_i}.$$

and the definition of mass and momentum

$$\begin{aligned} \rho(\rho, \boldsymbol{j}) &= \sum_i F_i^{(0)}(\rho, \boldsymbol{j}) \\ \boldsymbol{j}(\rho, \boldsymbol{j}) &= \sum_i \boldsymbol{c}_i F_i^{(0)}(\rho, \boldsymbol{j}). \end{aligned}$$

as constraints.

Maximize entropy ... after some calculus and algebra ...

$$F_i^{(0)}(\rho, \boldsymbol{j}) = \frac{W_i}{\rho_0} \left\{ \rho + \frac{m}{k_B T} \boldsymbol{c}_i \cdot \boldsymbol{j} + \frac{m}{2\rho k_B T} \left[\frac{m}{k_B T} (\boldsymbol{c}_i \cdot \boldsymbol{j})^2 - \boldsymbol{j}^2 \right] \right\}. \qquad (3)$$

LBM algorithm

The algorithm proceeds as follows:

1. Initial values of $\rho(\boldsymbol{x}, t)$ and $\boldsymbol{j}(\boldsymbol{x}, t) \Rightarrow F_i^{(0)}(\rho(\boldsymbol{x}, t), \boldsymbol{j}(\boldsymbol{x}, t))$; set $F_i = F_i^{(0)}$.
2. Apply lattice Boltzmann equation

$$\boxed{F_i\left(\boldsymbol{x} + \boldsymbol{c}_i, t + \Delta t\right) = \left(1 - \omega\right) F_i\left(\boldsymbol{x}, t\right) + \omega F_i^{(0)}\left(\boldsymbol{x}, t\right)}$$

3. $F_i \Rightarrow \rho(\boldsymbol{x}, t)$ and $\boldsymbol{j}(\boldsymbol{x}, t)$
4. $\rho(\boldsymbol{x}, t)$ and $\boldsymbol{j}(\boldsymbol{x}, t) \Rightarrow F_i^{(0)}$; proceed with the second step of the algorithm.

Construction of other LBMs

In order to construct a LBM for a given partial differential equation one has to specify 3 items:

1. A kinetic equation (collision and propagation); for example: the lattice Boltzmann equation with BGK approximation.
2. A lattice with sufficient symmetry.
3. Equilibrium distributions: make an **ansatz**.

LBM for the diffusion equation

Temperature T

1. Kinetic equation: the lattice Boltzmann equation with BGK approximation reads:

$$T_m(\boldsymbol{x} + \boldsymbol{c}_m, t + \Delta t) = (1 - \omega) T_m(\boldsymbol{x}, t) + \omega T_m^{(0)}(\boldsymbol{x}, t)$$

2. Square lattice in 2D has sufficient symmetry for diffusion.

3. Linear ansatz for equilibrium distributions:

$$T_m^{(0)} = \gamma_0 + \gamma_1 T.$$

   The free parameters of the equilibrium distributions (here: γ_0 and γ_1) are constrained by the definition of T as the sum over all $T_m^{(0)}$ per node $\Rightarrow$

$$T_m^{(0)} = \frac{T}{2D}$$

4. The resulting LBM at $\omega = 1$ is identical to the standard finite difference scheme at its stability limit (Wolf-Gladrow, 1995).

5. A small modification (replace the constant ω by the temperature dependent $\omega(T)$) leads to a LBM for the non-linear diffusion model (Wolf-Gladrow, 1995).

$$\frac{\partial T}{\partial t} = \boldsymbol{\nabla}\left[\kappa(T)\boldsymbol{\nabla}T\right]$$

$$\kappa(T) = \left[\frac{1}{\omega(T)} - \frac{1}{2}\right]\frac{1}{D}.$$

For $\kappa(T) = T$ a solution reads

$$T(x,t) = \frac{1}{6t}\left(A^2t^{2/3} - x^2\right) \quad \text{for} \quad |x| < At^{1/3}$$

and $T(x,t) = 0$ otherwise.

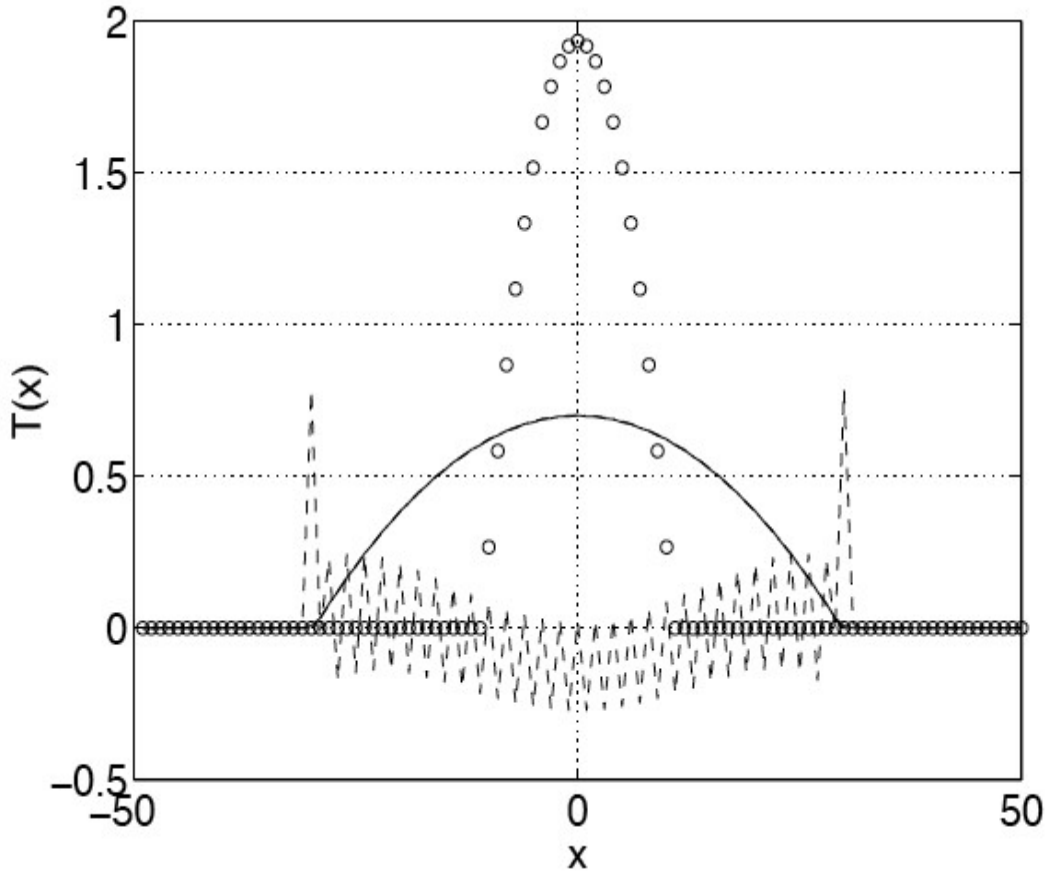


Figure 2: Integration of the nonlinear diffusion equation by the LBM. The initial distribution is marked by circles. The numerical solution at t = 210 (solid line) is indistinguishable from the analytical solution (dashed-dotted line; not visible). The broken line shows the difference between numerical and analytical solution multiplied by 100. (Wolf-Gladrow et al., 2000).

Who needs LBM?

Succi (2001)

- **Don't use**
  - Strong compressibility.
  - Substantial heat transfer effects.
- **Can use**
  - Turbulent flows in simple geometry (cubes, channels).
- **Should use**
  - Single and multiphase flows in grossly irregular geometries (porous media, oil and water, flow past cars).
- **Must use**
  - Flow with suspended particles.
  - Hydrodynamic problems with additional physics.

Applications

1. Flow past obstacles
2. Flow through porous media
3. Multi-phase flow (free surfaces, oil and water)
4. Animations, movies

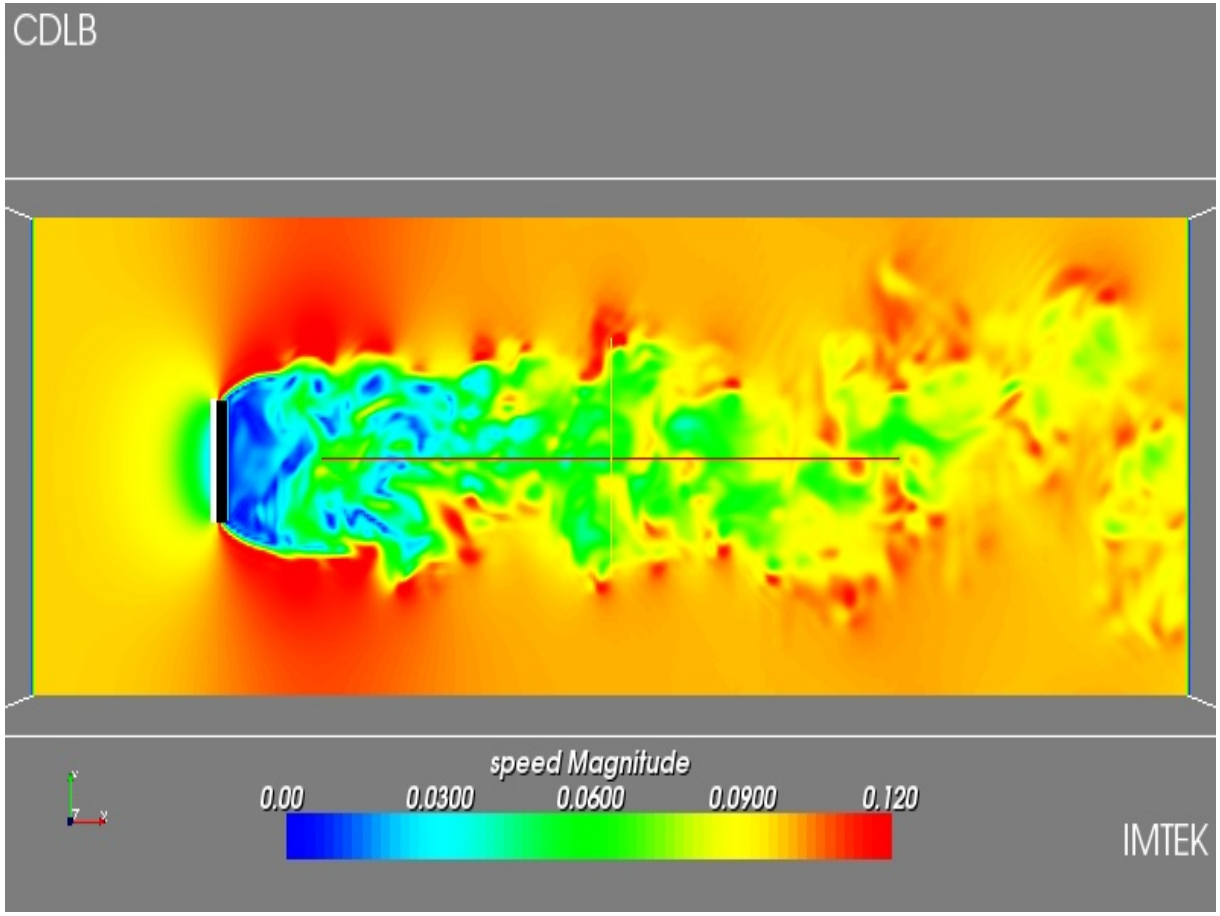


Figure 3: Flow past an obstacle. Source: www.bfg.uni-freiburg.de/Projects/dlb/re1350000slice.jpg

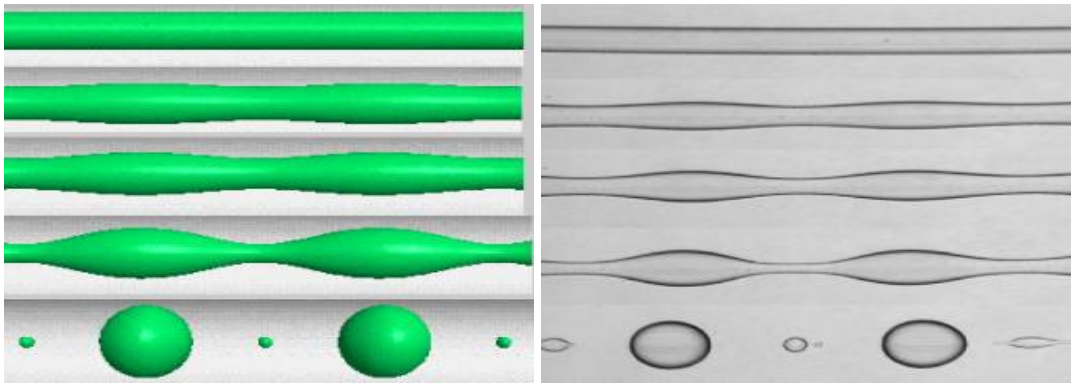


Figure 4: J. Hagedorn has performed a series of runs simulating multiple fluids through a tube. Parameters have been varied to investigate the effects of tube radius, tube length, wetting parameters, and other parameters on the stability of the fluid structure. Results [left panel] are very similar to experimental results [right panel] generated by Dr. Kalman Migler of the Polymers Division of MSEL ...

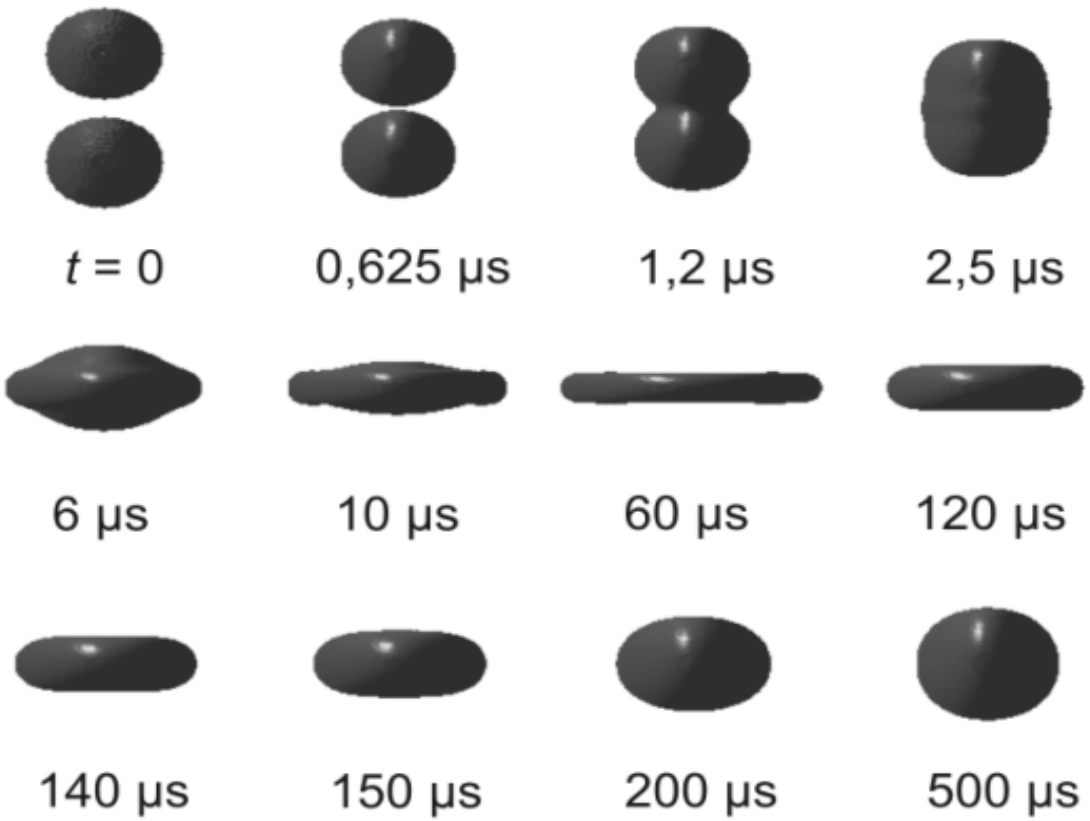


Figure 5: Muli-phase flow: central collision of two droplets (Danijel Babic, Moritz von Stosch, University of Aachen).

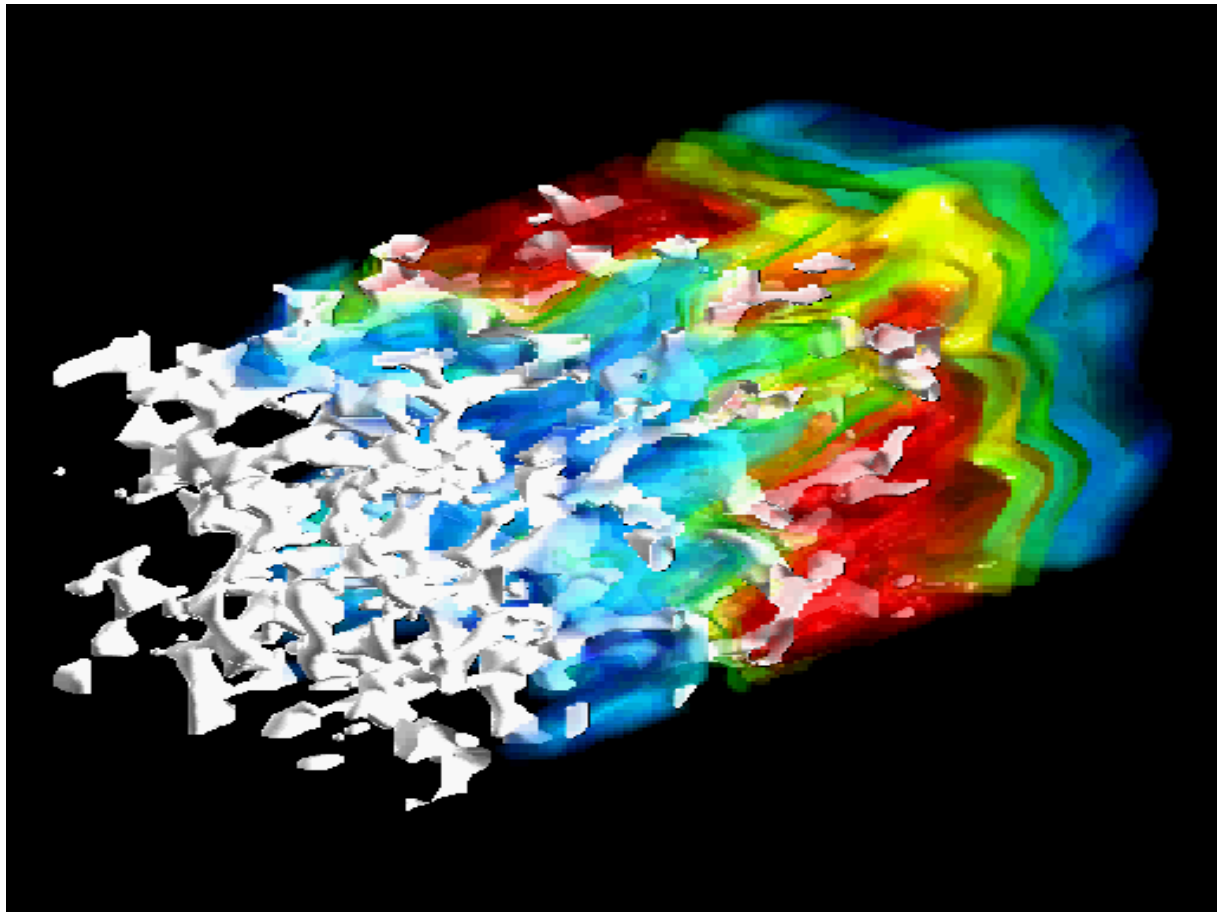


Figure 6: Study of a reactive flow through a porous structure using the Lattice Boltzmann technique. The structure is rendered by isosurfaces and the flow and species concentration (color) with volume rendering.

Figure 7: Xiaoming Wei, Ye Zhao, Zhe Fan, Wei Li, Feng Qiu, Suzanne Yoakum-Stover, and Arie Kaufman IEEE Transactions on Visualization and Computer Graphics, 10(6):719-729, 2004.

Open ends

CA: reversible computation in 3D (Miller and Fredkin, 2005)

LGCA: for fluid dynamics largely replaced by LBM; growth of tumors

LBMs:

1. high flexibility (compared to LGCA) due to choice of kinetic equation, lattice, equilibrium distributions;
2. improvement of stability by modification of the collision operator;
3. local refinements;
4. LBMs for other differential equations;
5. applications, applications, applications, ...

Thanks for your attention!

Literature

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