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The lattice-Boltzmann Method

Introduction

Gunther Brenner

Institute of Applied Mechanics
Clausthal University

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Part 1: LBM Theorie

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- development
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- From LGA to LBA/LBM
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Part 3: LBM - modeling of complex fluids

Prof. Manfred Krafczyk, TU Braunschweig

Tuesday, 22.5.07

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Dr. Gerhard Wellein, RRZE Erlangen,
Dr. Peter Lammers, RUS Stuttgart
Thomas Zeiser, RRZE Erlangen

Wednesday, 23.5.07

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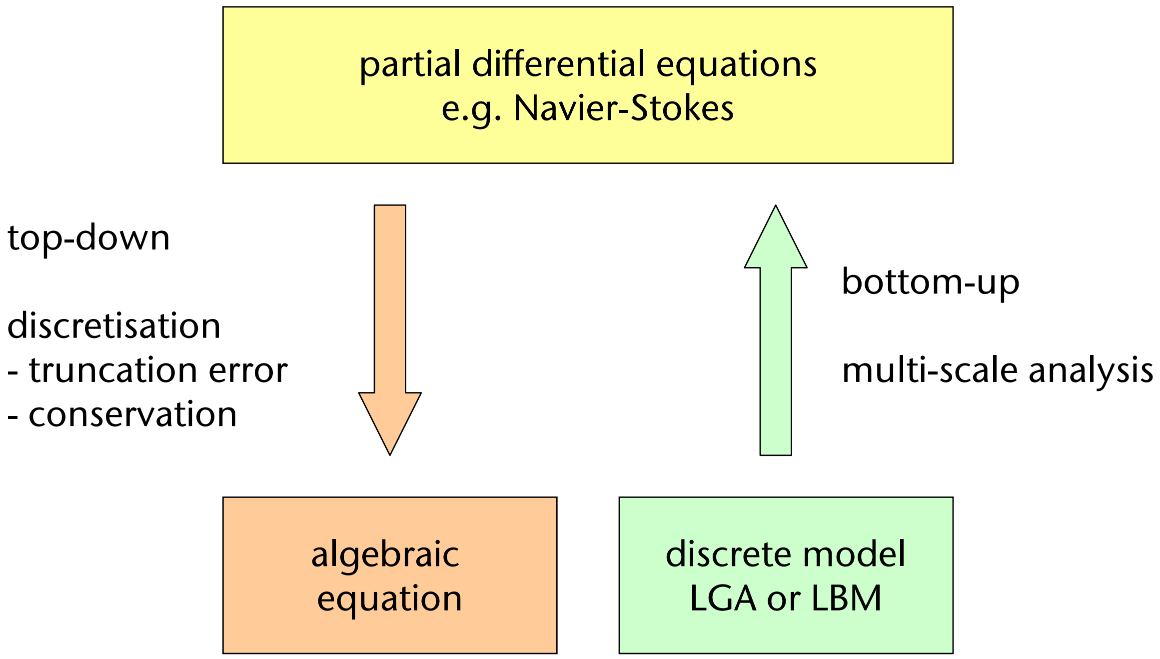


top-down vs. bottom-up

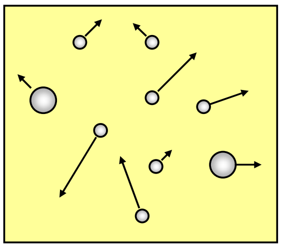
$$\partial_t \rho + \partial_{x_j} \rho u_j = 0$$
$$\partial_t \rho u_i + \partial_{x_j} \Pi_{ij} = 0$$
$$\partial_t \rho e + \partial_{x_j} E_j = 0$$

$$\Pi_{ij}(\mathbf{x},t) = \rho u_i u_j + \sigma_{ij}(\mathbf{x},t)$$
$$\sigma_{ij} \equiv -p\delta_{ij} + \tau_{ij}$$

Balance of
- Mass
- Momentum
- Energy

$$\partial_t f + \mathbf{c}\partial_{\mathbf{x}} f + \mathbf{K}\partial_{\mathbf{c}} f = Q(f)$$

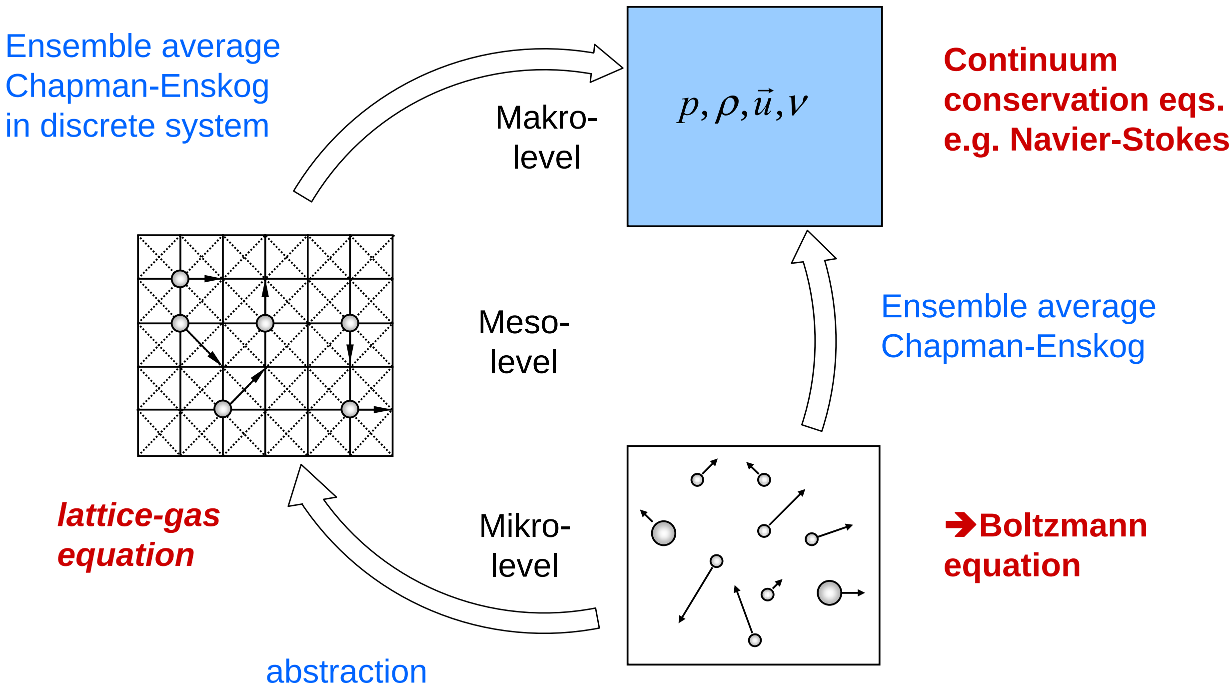
Boltzmann equation
- two particle collisions
- molecular chaos hypothesis
- external forces // collisions



Classical mechanics
- Hamiltons equation
- Liouville equation

Molecular Dynamics methods
Direct Simulation Monte Carlo

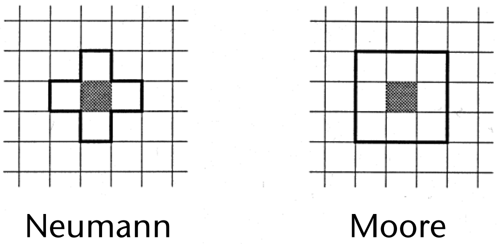
Classification



Classification

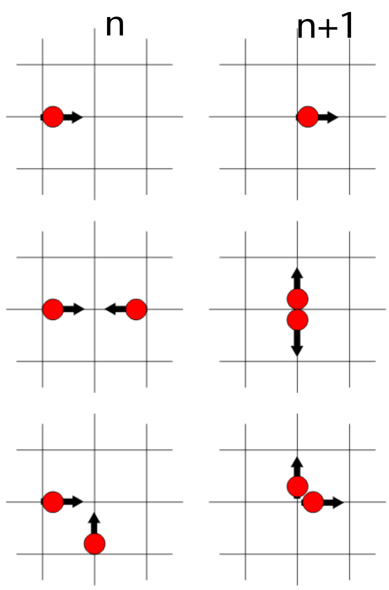
- cellular automata (CA)

  - idealized physical system
    - state defined at discrete times and locations
    - finite levels of discrete states
  - simultaneous update of state variables in discrete time steps
  - deterministic and homogeneous rules of update
  - rules depend on neighborhood states

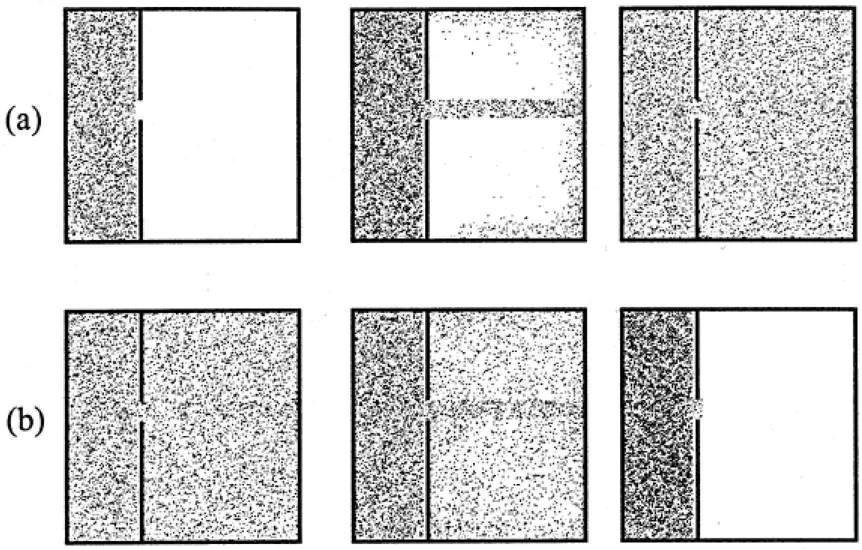


- lattice gas automata
- origin: Hardy, de Pazzi und Pomeau (1976)
  - Cartesian grid
  - propagation along grid links
    4 directions corresponding to
    4 discrete states
  - max. 1 bit each direction each node
  - simple collision rules

    „no collision“
    „head on collision“
    „transparent collision“



- example HPP LGA - Chopard (1996)



expansion

after reversing time step

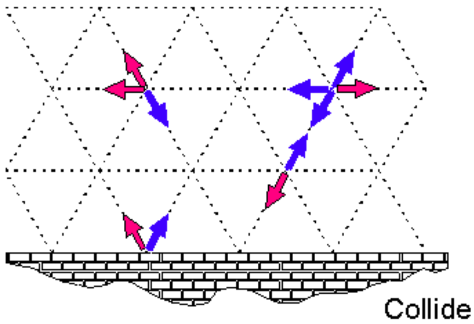
two dimensional **Lattice-Gas** Automata
FHP - Frisch, Hasslacher, Pomeau

$$n_\alpha(t+\tau, \vec{x}+\tau\vec{c}_\alpha) - n_\alpha(t,\vec{x}) = \Delta_\alpha(n_\alpha)\ , \quad \alpha = 0..6$$

1. Step: Propagation Fluid- Particle

2. Step : Collision Partikel / Particle
Particle / Wall

3. Step : Ensemble Average –
Pressure, density, fluxes, ...



$$f_\alpha = \langle n_\alpha \rangle = \begin{cases} \text{Density:} & \rho = \sum_\alpha f_\alpha \\ \text{Massflux:} & \rho\,\boldsymbol{u} = \sum_\alpha \boldsymbol{c}_\alpha f_\alpha \end{cases}$$

- Relation to macroscopic magnitudes

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

$$\frac{\partial \boldsymbol{u}}{\partial t} + g(\rho)(\boldsymbol{u}\nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu \Delta \boldsymbol{u}$$

$$p = c_s^2 \rho$$

$g(\rho)$ Nonlinear scaling term

Lattice-Gas Automata – some properties

☺ guarantees conservation principles at micro-level
☺ quite simple algorithm
☺ only Boolean operations, no truncation error, no error propagation
☺ unconditionally stable, though explicit in time

☹ solution is noisy due to averaging in finite ensemble
☹ viscosity hard to control and prescribed by collision model
☹ nonlinear scaling term in advection term is unphysical
☹ no chance for “healing”, just symptomatic treatment

⇨ lattice-Boltzmann method (McNamara and Zanetti)

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From lattice-Gas to lattice-Boltzmann

lattice Gas	lattice Boltzmann
▪ diskrete (Boolsche) states	▪ continuous distribution functions
$n_\alpha(\boldsymbol{x},t)$	$f_\alpha(\boldsymbol{x},t) = \langle n_\alpha(\boldsymbol{x},t)\rangle$
▪ collision rules	▪ relaxation term
▪ unconditionally stable	▪ conditionally stable

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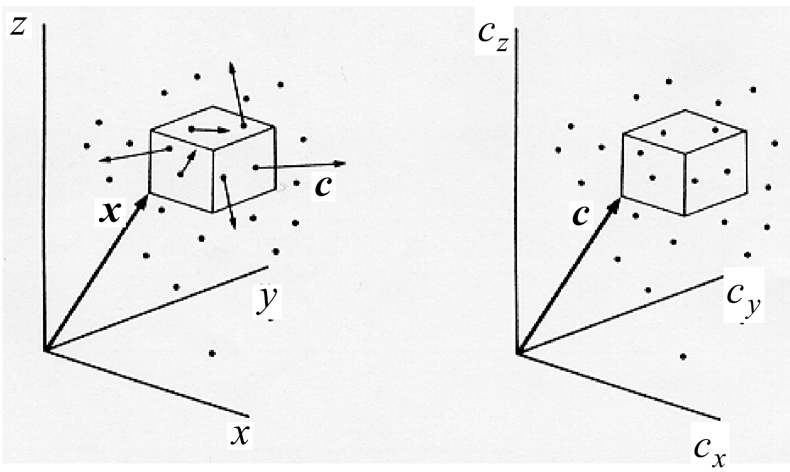
- Boltzmann equation

$$\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f + \boldsymbol{K}\partial_{\boldsymbol{c}} f = Q(f) \qquad f = f(t,\boldsymbol{x},\boldsymbol{c})$$



- Boltzmann equation

$$\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f + K\partial_c f = Q(f) \qquad f = f(t,\boldsymbol{x},\boldsymbol{c})$$

- Invariants

$$\psi_k = (m, m\boldsymbol{c}, \tfrac{1}{2}m\boldsymbol{c}^2)$$

- Moments of distribution functions

$$\begin{aligned} \int_{\boldsymbol{c}} f\, m d\boldsymbol{c} &= \rho(t,\boldsymbol{x}) \\ \int_{\boldsymbol{c}} f\, m\boldsymbol{c} d\boldsymbol{c} &= \rho\boldsymbol{u}(t,\boldsymbol{x}) \\ \int_{\boldsymbol{c}} f\, \tfrac{1}{2}m\boldsymbol{c}^2 d\boldsymbol{c} &= \rho e(t,\boldsymbol{x}) \end{aligned}$$

- Boltzmann equation

$$\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f + K\partial_c f = \boxed{Q(f)} \qquad f = f(t,\boldsymbol{x},\boldsymbol{c})$$

- Invariants of collision term

$$\int_{\boldsymbol{c}} \boxed{Q(f)}\psi_k(\boldsymbol{c})d\boldsymbol{c} = 0, \quad \psi_k = (m, m\boldsymbol{c}, \tfrac{1}{2}m\boldsymbol{c}^2)$$

- Integration of Boltzmann equation

$$\int_{\boldsymbol{c}} \psi_k (\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f) d\boldsymbol{c} = 0$$

$$\psi_0 = m: \qquad \partial_t \rho + \partial_{\boldsymbol{x}} \rho \boldsymbol{u} = 0 \qquad \partial_t \rho + \partial_{x_j} \rho u_j = 0$$

$$\psi_{1\cdots3} = m\boldsymbol{c}: \qquad \partial_t \rho \boldsymbol{u} + \partial_{\boldsymbol{x}} \boldsymbol{\Pi} = 0 \qquad \partial_t \rho u_i + \partial_{x_j} \Pi_{ij} = 0$$

$$\psi_4 = \tfrac{1}{2} m\boldsymbol{c}^2: \qquad \partial_t \rho e + \partial_{\boldsymbol{x}} \boldsymbol{E} = 0 \qquad \partial_t \rho e + \partial_{x_j} E_j = 0$$

$$\Pi_{ij}(x,t) = m\int_c c_i c_j f d\boldsymbol{c} \qquad E_i(x,t) = \tfrac{1}{2} m\int_c c_i \boldsymbol{c}^2 f d\boldsymbol{c}$$

- Decomposition of the velocity $c_i = u_i + w_i$

$$\Pi_{ij}(x,t) = \rho u_i u_j + \underbrace{\rho \int_{\boldsymbol{c}} w_i w_j f d\boldsymbol{c}}_{\sigma_{ij} = p\delta_{ij} + \tau_{ij}}$$

- Maxwell distribution (equilibrium)

$$f^{eq} = \frac{\rho}{(2\pi c_s^2)^{\frac{3}{2}}} \cdot \exp\left(-\frac{(\boldsymbol{c}-\boldsymbol{u})^2}{2c_s^2}\right) \qquad c_s^2 = RT$$

- “Macrosopic” momentum equation of inviscid flow

$$\partial_t \rho u_i + \partial_{x_j}\left(\rho u_i u_j\right) = -\partial_{x_j}\left(c_s^2 \rho \delta_{ij}\right) \qquad p = c_s^2 \rho$$

- Solution of Boltzmann equation:
  H-theorem and Maxwell distribution results in Krook equation
  (BGK Approximation)

$$\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f = \frac{1}{\tau}(f^{eq} - f)$$

- Chapman-Enskog Expansion

$$f = f^{eq} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \cdots$$

$$\tau_{ij}(\boldsymbol{x},t) = -\underbrace{\tau\,\rho RT}_{\nu \sim \tau c_s^2}(\partial_{x_i} u_j + \partial_{x_j} u_i - \tfrac{2}{3}\partial_{x_k} u_k \delta_{ij})$$

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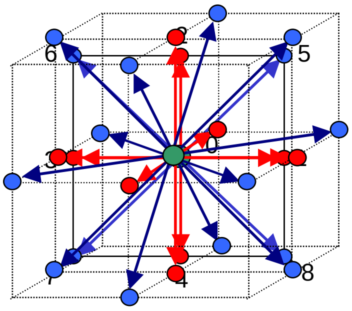
- Energy flux

$$E_i(\boldsymbol{x},t) = \underbrace{\tfrac{1}{2}\rho \boldsymbol{u}^2 u_i + \tfrac{1}{2}\rho u_i \int_{\boldsymbol{c}} \boldsymbol{w}^2 f d\boldsymbol{c}}_{convective\ transport} + \underbrace{\rho u_i \int_{\boldsymbol{c}} w_i w_j f d\boldsymbol{c}}_{work\ of\ \boldsymbol{\sigma}} + \underbrace{\tfrac{1}{2}\rho \int_{\boldsymbol{c}} \boldsymbol{w}^2 w_j f d\boldsymbol{c}}_{heatflux}$$

- “Macrosopic” energy equation

$$\partial_t \rho e + \partial_{x_j} u_j (\rho e + p) = -\partial_{x_j}(u_i \tau_{ij} + q_j)$$

$$q_j(\boldsymbol{x},t) = -\tfrac{5}{2}\tfrac{k}{m}\tau\rho RT\,\partial_{x_j} T$$



D2Q9
D3Q19

- Representation in discrete velocities

$$f(t,\boldsymbol{x},\boldsymbol{c}) \Rightarrow \tilde{f}(t,\boldsymbol{x},\boldsymbol{e}_\alpha) = f_\alpha(t,\boldsymbol{x})$$

- Velocity-discrete Boltzmann Equation

$$\partial_t f_\alpha + \boldsymbol{e}_\alpha \partial_{\boldsymbol{x}} f_\alpha = \frac{1}{\tau}(f_\alpha^{eq} - f_\alpha) \qquad \text{(STR Approximation)}$$

- Lattice Boltzmann Equation

$$\text{for} \quad \boldsymbol{e}_\alpha \Delta t = \Delta \boldsymbol{x}$$

$$f_\alpha(t+\Delta t, x) - f_\alpha(t,\boldsymbol{x}) + \boldsymbol{e}_\alpha \frac{\Delta t}{\Delta \boldsymbol{x}}\left[f_\alpha(t+\Delta t, \boldsymbol{x}+\boldsymbol{e}_\alpha \Delta t) - f_\alpha(t+\Delta t, x)\right] = R.S.$$

$$f_\alpha(t+\Delta t, \boldsymbol{x}+\boldsymbol{e}_\alpha \Delta t) - f_\alpha(t,\boldsymbol{x}) = \frac{\Delta t}{\tau}(f_\alpha^{eq} - f_\alpha)$$

- Equlibrium velocity distribution for lattice Boltzmann Equation
  - no *direct* transfer of Maxwell distribution

$$f_\alpha^{eq} = f^{eq} \quad ?$$

- Moments of equilibrium velocity distribution shall satisfy

$$\int_{c=-\infty}^{\infty} f^{eq}\, \psi(\boldsymbol{c})\, d\boldsymbol{c} \cong \sum_{\boldsymbol{e}_\alpha} W_\alpha\, f_\alpha^{eq}\, \psi(\boldsymbol{e}_\alpha)$$

up to 2th order !

- After linearisation

$$f_\alpha^{eq} = t_p \rho \left\{1 + \frac{\boldsymbol{e}_\alpha \boldsymbol{u}}{c_s^2} + \frac{\boldsymbol{u}\boldsymbol{u}}{c_s^2}\left(\frac{\boldsymbol{e}_\alpha \boldsymbol{e}_\alpha}{c_s^2} - \delta_\alpha\right)\right\}$$

Relation to macroscopic properties

- from moments of distribution function
  - density $\rho = m\sum_\alpha f_\alpha$
  - massflux $\rho u_i = m\sum_\alpha e_{\alpha,i} f_\alpha$
  - momentum flux $\tau_{ij} = m\sum_\alpha e_{\alpha,i} e_{\alpha,j} (f_\alpha^{eq} - f_\alpha)$
- from scale analysis (Chapman Enskog)
  - pressure $p = c_s^2 \rho$
    (weakly compressible)
  - viscosity $\nu = c_s^2 \left(\tau - \tfrac{1}{2}\right)\Delta t$

Summary:

- Boltzmann equation

$$\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f + K\partial_c f = Q(f)$$

- BG Krook equation (STR)

$$\partial_t f + \boldsymbol{c}\partial_{\boldsymbol{x}} f = \frac{1}{\tau}(f^{eq} - f)$$

- Velocity discrete BGK (1. order DGL in diagonalform)

$$\partial_t f_\alpha + \boldsymbol{e}_\alpha \partial_{\boldsymbol{x}} f_\alpha = \frac{1}{\tau}(f_\alpha^{eq} - f_\alpha)$$

- Finite difference approximation

$$f_\alpha(t + \Delta t, \boldsymbol{x} + \boldsymbol{e}_\alpha \Delta t) - f_\alpha(t, \boldsymbol{x}) = \frac{\Delta t}{\tau}(f_\alpha^{eq} - f_\alpha)$$

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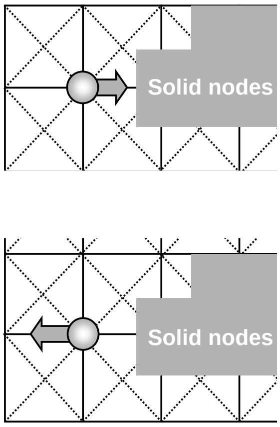
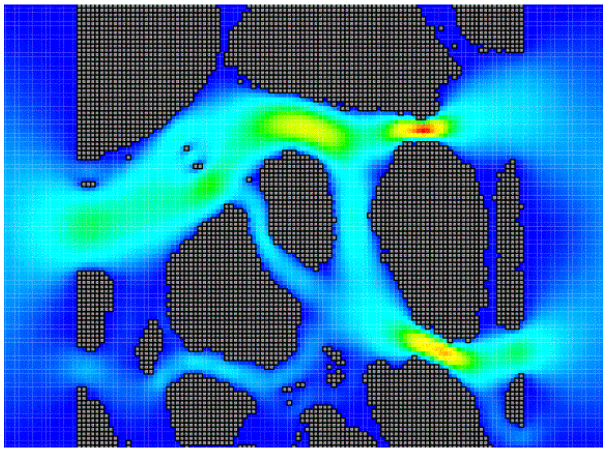
Boundary Conditions for complex geometries

- MAC approach to describe geometry
- no-slip wall boundary condition applying “bounce back”
- allows to represent arbitrarily complex structures
- allows quasi automatic generation of meshes





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Advantage of LBM

- simple, explicit Algorithms
  - low memory requirements
  - data locality
  - high Performance on many processor architectures
  - advantages regarding parallel processing

- complex geometries via immersed boundaries
  - Cartesian grids
  - Modeling of geometry from Computer Tomography or other interferometry

Summary LBM Theory

- LBM is not an attempt to duplicate exactly microscopic processes like in molecular dynamics schemes
- LBM is an abstraction of these processes
- LBM leads to a solution of the Navier-Stokes equations in certain limits such as low Mach number and weak compressibility
- simple algorithmic structure (stream – relax)
- Note: In contrats to LGA, LBM does have stability limits

Variants of LBM

- incompressible fluids
- Multi-time relaxation scheme (improvement of stability)
- Spezies transport and chemical reactions, combustion
- energy transport (often hybrid methods)
- turbulence models (ke, LES, ...)
- free surface / immiscible fluids
- multi-phase flows
- non-Newtonian fluids
- Composite grids / local grid refinement / non-Cartesian grids
- Higher order boundary conditions / curved boundaries