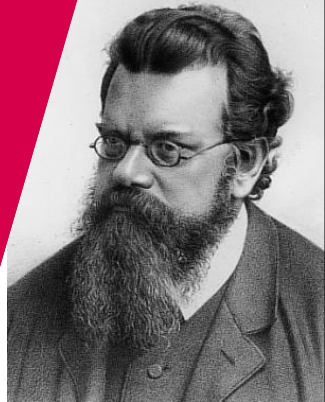


# Introduction to the Lattice Boltzmann method

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Where innovation starts

- ▶ Michael C. Sukop and Daniel T. Thorne (2006)  
*Lattice Boltzmann Modeling; an Introduction for Geoscientists and Engineers*, Springer-Verlag Berlin/Heidelberg

Practically oriented, few theoretical details, easy way to get started.

- ▶ Dieter Hänel (2004)  
*Molekulare Gasdynamik*, Springer-Verlag Berlin/Heidelberg

A quite exhaustive and yet very accessible introduction to the kinetic theory of gases. The book is available only in German.

- ▶ Sauro Succi (2001)  
*The lattice Boltzmann equation for fluid dynamics and beyond*, University Press, Oxford

Practical, numerically oriented, presents the state of the art of this method by the year 2001.

- ▶ Dieter A. Wolf-Gladrow (2000)  
*Lattice-Gas Cellular Automata and lattice Boltzmann Models*, Lecture Notes in Mathematics 1725, Springer-Verlag Berlin/Heidelberg

Focuses mainly on the lattice automata origin of the LB method, it contains a digression to the Boltzmann equation. The

discussion on symmetry properties of a lattice is a compulsory reading for LB theorists.

- ▶ U. Frisch, B. Hasslacher, Y. Pomeau, Phys. Rev. Lett., 56, 1505, 1986

First hydrodynamic Lattice Gas, many practical limitations

- ▶ G. Mc Namara, G. Zanetti, Phys. Rev. Lett., 61, 2332, 1988

Chronologically first, unviable in 3d because of collisional complexity

- ▶ F. Higuera, J. Jimenez, Europhys. Lett. 9, 662, 1989

Viable in 3d, but only at low Reynolds (high viscosity)

- ▶ F. Higuera, S. Succi, R. Benzi, Europhys. Lett. 9, 345, 1989

Viable in 3d at Reynolds as high as grid resolution allows. Inaugurates the very influential “top-down” approach

- ▶ H. Chen, S. Chen, W. Mattheus, Phys. Rev. A, 45, R5339, 1992

Galilean invariant, Single-time relaxation collisions

- ▶ Y.H. Qian, D. d’Humières, P. Lallemand, Europhys. Lett., 17, 479, 1992

Systematic theory of single-time relaxation LB

- ▶ R. Benzi, S. Succi, M. Vergassola,  
The Lattice Boltzmann Equation: Theory and Applications,  
Physics Reports, 222, 145, 1992.

Early review with many original ideas still useful today

- ▶ S. Chen, G. Doolen, Lattice Boltzmann method for fluid flows,  
Ann. Rev. Fluid Mech, 30, 329, 1998.

Very readable account of the main theory and developments up to 1998

- ▶ D. Raabe,  
Overview of the lattice Boltzmann method for nano- and microscale  
fluid dynamics in material science and engineering, Mod. Simul.  
Mater. Sci. Eng. 12, R13, 2004

Very detailed and well readable review; see handout!

- ▶ <http://www.lbmethod.org>

Offers a nice list of articles, books, etc. Home of a free implementation OpenLB/Palabos

- ▶ <http://thomas-pohl.info/work/lba.html>

Nice JAVA applet

## ► Simulation of fluids

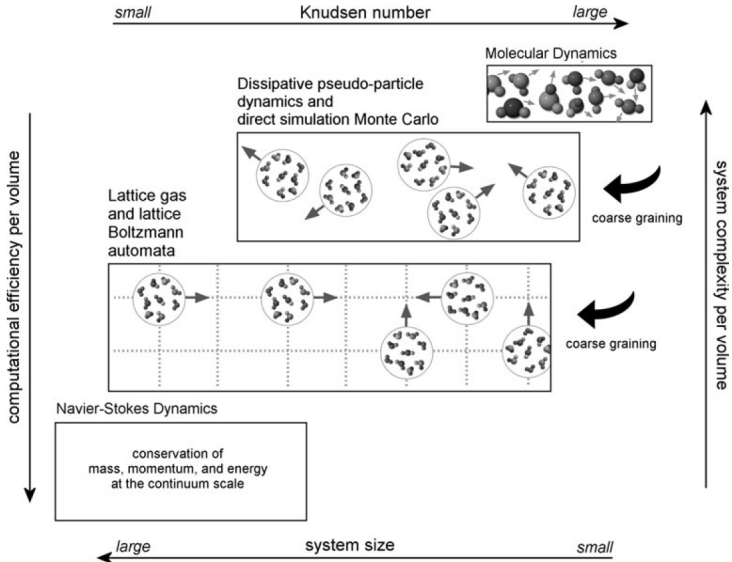
- Aiding the design of industrial products (e.g. bridges, cars, etc.)
- Allowing to analyze variables inaccessible to experiments.
- Impact of different physical phenomena can be determined easily.

## ► Simulations on different scales

- Microscale
  - Molecular dynamics simulations allow to include microscopic interactions.
  - It is computationally too expensive to reach experimental timescales.
- Macroscale
  - Although the Navier Stokes equations cannot be solved analytically numerical solutions can be found
  - Computationally efficient, huge amount of experience.
  - It cannot take into account effects arising from molecular interactions.
- Mesoscale
  - Mesoscopic simulation methods describe properties of particle ensembles
  - Typically length and timescales are on the nano to microscale.
  - Examples are DPD, SRD, LBM.

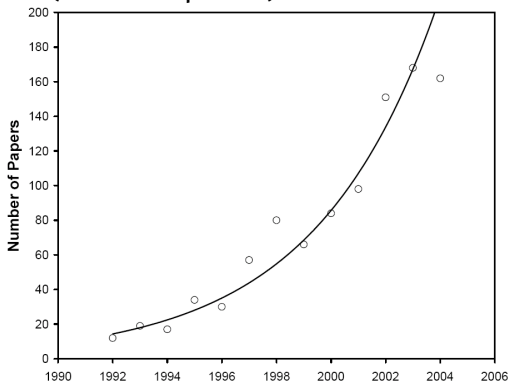
# Simulation methods in fluid dynamics

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- ▶ Alternative way to solve the Navier-Stokes equations.
- ▶ Successor of “lattice gas” models.
- ▶ Can be derived from lattice gas or by discretizing the Boltzmann equation.
- ▶ Simple, local dynamics.
- ▶ Ideal for parallel computing.
- ▶ Complex boundary conditions easy.
- ▶ Hydrodynamics: kinetic theory close to equilibrium.
- ▶ Mostly low  $Re$ , low  $Ma$ , low  $Kn$  flows.
- ▶ Extension to moderate  $Re$ ,  $Kn$  possible.
- ▶ **No noise (in contrast to lattice gas)**  $\Rightarrow \approx 100$  times faster!
- ▶ Conceptual difference to other methods: discrete velocities.

Growth in number of papers with lattice Boltzmann as a “topic” (search of article titles, abstracts, and keywords) in the Web of Science database 1992 - 2004. Solid line is fitted exponential growth curve. 2004 data may be incomplete (from Sukop et al.).



- ▶ Assumptions:
  - dilute gas
  - hard spheres
  - great velocities ( $\approx 300\text{ms}^{-1}$ )
  - only elastic collisions
- ▶  $\Rightarrow$  Exact dynamical state of system given if  $\mathbf{x}$ ,  $\mathbf{p}$  are known for every particle at some instant in time.
- ▶  $\Rightarrow$  with classical mechanics all future states are also known.
- ▶ Describe system of  $N$  particles by a distribution function (phase space!):

$$f^{(N)}(\mathbf{x}, \mathbf{p}, t) \quad (1)$$

- ▶ Time development is described by Liouville equation ( $6N$  variables).
  - real gases:  $10^{23}$  particles  $\Rightarrow 6 \cdot 10^{23}$  variables
  - solution: only use lower order distribution function ( $N = 1, 2$ )

- ▶ Let us restrict ourselves to first order (single particle) distributions.
- ▶ Then, the probability to find a particle at position  $\mathbf{x}$  and time  $t$  with momentum  $\mathbf{p}$  is given by

$$f(\mathbf{x}, \mathbf{p}, t) \quad (2)$$

- ▶ The remaining  $N - 1$  molecules are unspecified since they are indistinguishable (dilute gas).
- ▶ Probable number of molecule in range  $[\mathbf{x}, \mathbf{x} + d\mathbf{x}]$ ,  $[\mathbf{p}, \mathbf{p} + d\mathbf{p}]$ :

$$f(\mathbf{x}, \mathbf{p}, t) d\mathbf{x} d\mathbf{p} \quad (3)$$

- ▶ How does volume element  $dx dp$  evolve in time if a force  $F$  acts?

$$\mathbf{x} \rightarrow \mathbf{x} + \left(\frac{\mathbf{p}}{m}\right) dt = \mathbf{x} + \left(\frac{d\mathbf{x}}{dt}\right) dt = \mathbf{x} + d\mathbf{x} \quad (4)$$

$$\mathbf{p} \rightarrow \mathbf{p} + F dt = \mathbf{p} + \left(\frac{d\mathbf{p}}{dt}\right) dt = \mathbf{p} + d\mathbf{p} \quad (5)$$

- ▶ for  $f$ :

$$f(\mathbf{x} + d\mathbf{x}, \mathbf{p} + d\mathbf{p}, t + dt) dx dp = f(\mathbf{x}, \mathbf{p}, t) dx dp \quad (6)$$

- ▶ This is the streaming process!

- ▶ What about collisions?
- ▶ Some phase points  $(\mathbf{x}, \mathbf{p}, t)$  might not arrive at  $(\mathbf{x} + d\mathbf{x}, \mathbf{p} + d\mathbf{p}, t + dt)$ , but others might arrive there, but do not come from  $(\mathbf{x}, \mathbf{p}, t)$ ...

$\Gamma^- d\mathbf{x}d\mathbf{p}dt$  : number of molecules not arriving in  $(\mathbf{x} + d\mathbf{x}, \mathbf{p} + d\mathbf{p})$  (7)

$\Gamma^+ d\mathbf{x}d\mathbf{p}dt$  : number of molecules arriving in  $(\mathbf{x} + d\mathbf{x}, \mathbf{p} + d\mathbf{p})$  (8)

which do not come from  $(\mathbf{x}, \mathbf{p}, t)$

- ▶  $\Rightarrow$  Collisions:  $\underbrace{[\Gamma^+ - \Gamma^-]}_{\Omega} d\mathbf{x}d\mathbf{p}dt$

- ▶ But: One would have to take into account all possible molecular interactions!

- Put everything together: add collision and streaming (Eq. 6):

$$f(\mathbf{x} + d\mathbf{x}, \mathbf{p} + d\mathbf{p}, t + dt)d\mathbf{x}d\mathbf{p} = f(\mathbf{x}, \mathbf{p}, t)d\mathbf{x}d\mathbf{p} + \Omega d\mathbf{x}d\mathbf{p}dt \quad (9)$$

- By adding first order terms of a Taylor expansion of the LHS

$$f(\mathbf{x} + d\mathbf{x}, \mathbf{p} + d\mathbf{p}, t + dt) = f(\mathbf{x}, \mathbf{p}, t) + d\mathbf{x} \cdot \nabla_{\mathbf{x}} f + d\mathbf{p} \cdot \nabla_{\mathbf{p}} f + \left( \frac{\partial f}{\partial t} \right) dt + \dots \quad (10)$$

- we get the Boltzmann equation:

$$\begin{aligned} \left( f(\mathbf{x}, \mathbf{p}, t) + d\mathbf{x} \cdot \nabla_{\mathbf{x}} f + d\mathbf{p} \cdot \nabla_{\mathbf{p}} f + \left( \frac{\partial f}{\partial t} \right) dt + \dots \right) d\mathbf{x}d\mathbf{p} \\ = f(\mathbf{x}, \mathbf{p}, t)d\mathbf{x}d\mathbf{p} + \Omega d\mathbf{x}d\mathbf{p}dt \end{aligned} \quad (11)$$

- Rearranging leads to:

$$\underbrace{\mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f + \frac{\partial f}{\partial t}}_{\text{Streaming}} = \underbrace{\Omega}_{\text{Collision}} \quad (12)$$

- ▶ But we are still left with the collisions!
- ▶ 50 years later: Bhatnagar, Gross and Krook came up with an approximate solution.
- ▶ Describe collisions as a relaxation towards a Maxwell-Distribution.

$$\Omega = -\frac{1}{\tau} [f(\mathbf{x}, \mathbf{p}) - f^{\text{eq}}(\mathbf{x}, \mathbf{p})] \quad (13)$$

- ▶  $\tau$  is the rate at which the system relaxes towards a local equilibrium.
- ▶ Local equilibrium:  $f^{\text{eq}} = \rho (2\pi c_s^2)^{-D/2} \exp(-\mathbf{p}^2/2mc_s^2)$
- ▶  $c_s = \sqrt{k_B T}$ : speed of sound,  $D$ : dimension

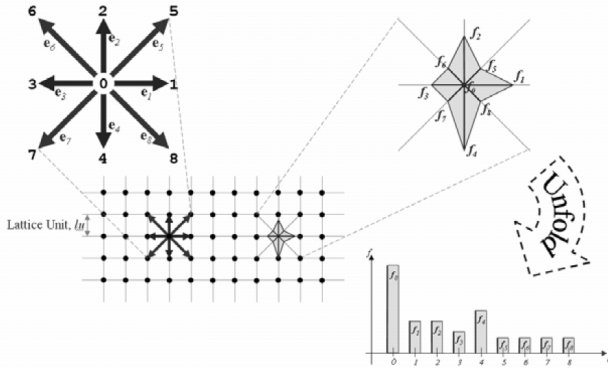
# The lattice Boltzmann equation

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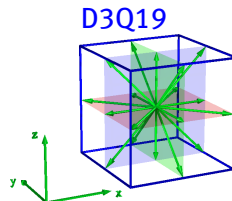
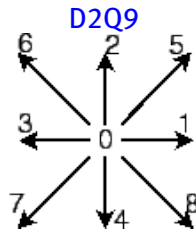
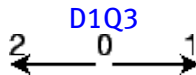
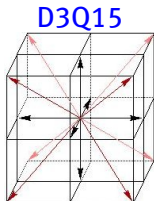
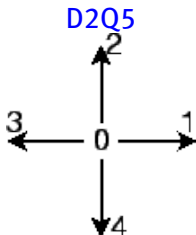
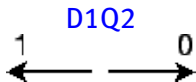
- Fluid is described as discrete particle number densities  $f_i(\mathbf{x}, t)$ .  
 $\mathbf{x}$ : lattice site     $\Delta t$ : time step     $\mathbf{e}_i$ : discrete velocities

$$\underbrace{f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t)}_{\text{Streaming/Advection}} = \underbrace{\Delta t \Omega}_{\text{Collision}}$$

- Example: D2Q9, a 2D lattice with 9 velocities



⇒ 9 distributions  
per lattice site



Physical properties of the system can be related to stochastic moments of the distribution  $f$ , e.g.

- ▶ density  $\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t)$
- ▶ momentum  $\rho \mathbf{u} = \sum_i \mathbf{e}_i f_i(\mathbf{x}, t)$
- ▶ momentum flux  
 $\rho u_k u_l + p \delta_{kl} = \sum_i e_{k,i} e_{l,i} f_i(\mathbf{x}, t)$

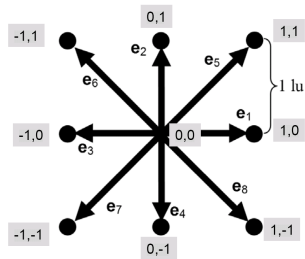


Figure : the D2Q9 lattice

# The Bhatnagar-Gross-Krook collision operator

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The popular LBGK (*Lattice Bhatnagar Gross Krook*) collision operator:

$$\Omega_i^{\text{BGK}} = \frac{1}{\tau} [f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)].$$

$$f_i^{\text{eq}} = \zeta_i \rho \left[ 1 + 3 \frac{\mathbf{e}_i \mathbf{u}}{c_s^2} + \frac{9}{2} \frac{(\mathbf{e}_i \mathbf{u})^2}{c_s^4} - \frac{3}{2} \frac{u^2}{c_s^2} \right]$$

lattice weights:  $\zeta_0 = 4/9$ ,  $\zeta_{\{1,2,3,4\}} = 1/9$ ,  $\zeta_{\{5,6,7,8\}} = 1/36$

speed of sound:  $c_s$

- ▶ The collision process is modeled as successive steps towards the local equilibrium distribution, proportional to the relaxation time  $\tau$ .
- ▶ The LBGK equation is then resolving the weakly compressible Navier-Stokes equations of a fluid with viscosity  $\nu = c_s^2 \Delta t \left( \frac{\tau}{\Delta t} - \frac{1}{2} \right)$ .
- ▶ The equation of state becomes ideal-gas like:

$$P = \sum_i f_i^{\text{eq}} c_s^2 = \rho c_s^2 = \rho k_B T.$$

- ▶ The speed of sound is known to be

$$c_s = \frac{1}{\sqrt{3}} \frac{\Delta x}{\Delta t}. \quad (14)$$

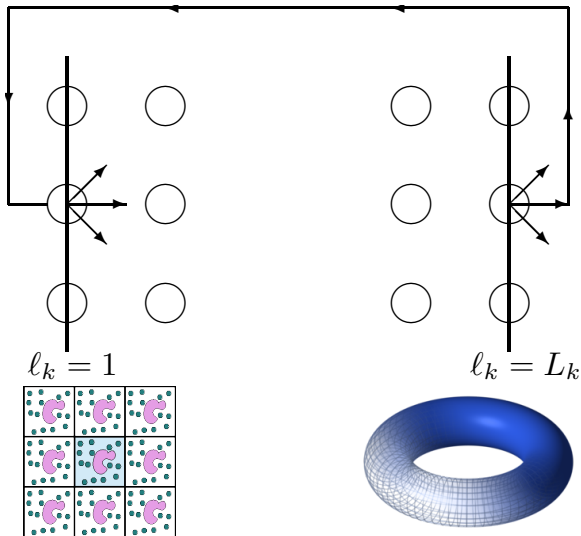
- ▶ The *kinematic* viscosity is given by

$$\nu = c_s^2 \Delta t \left( \frac{\tau}{\Delta t} - \frac{1}{2} \right). \quad (15)$$

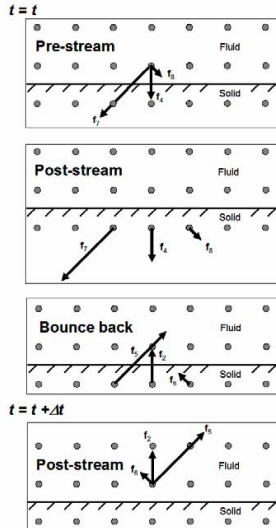
- ▶ For stability reasons  $\tau / \Delta t$  should be  $\approx 1$ .
- ▶ Assume water:  $c_s = 1480 \frac{m}{s}$ ,  $\nu \approx 10^{-6} \frac{m^2}{s}$

$$\implies \Delta t = 9.13 \cdot 10^{-13} s, \quad \Delta x = 2.34 \cdot 10^{-9} m$$

- ▶ This is small because we still have a mesoscopic method.
- ▶ But: scaling possible.



- ▶ One of the major advantages of the LBM is the easy way of implementing solid boundaries
- ▶ Just block out solid lattice sites
- ▶  $\implies$  mid-grid bounce back
- ▶ Disadvantage: slight dependence of the exact wall position on viscosity
- ▶ More complex boundary conditions solve this problem
  - solid walls
  - complex geometries
  - porous media
- ▶ Only a few lines of code needed!



- ▶ An external body force can be used to drive the flow (mimic gravity)
- ▶ Force is implemented in a velocity term:

$$\mathbf{F} = m\mathbf{a} = m \frac{d\mathbf{u}}{dt} \quad (16)$$

- density is proportional to mass
- $\tau$  is the elementary time of collisions

- ▶ Rearrange:

$$\Delta \mathbf{u} = \frac{\tau \mathbf{F}}{\rho} \quad (17)$$

- ▶ Add  $\Delta \mathbf{u}$  to the velocity used to compute  $f^{\text{eq}}$ :

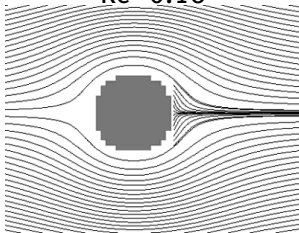
$$\mathbf{u}^{\text{eq}} = \mathbf{u} + \Delta \mathbf{u} = \mathbf{u} + \frac{\tau \mathbf{F}}{\rho} \quad (18)$$

- ▶ Other forces can be added in a similar way
- ▶ (Important to remember:  $\mathbf{u} = \mathbf{u} + \frac{1}{2} \mathbf{F}$  when writing data to disk.)

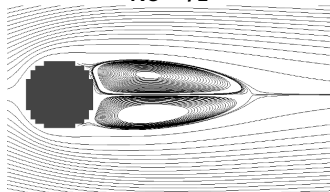
# Example: flow past a cylinder

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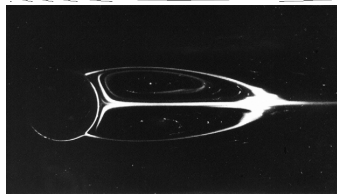
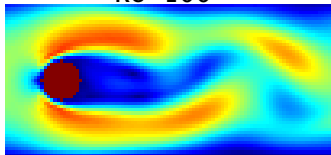
$Re=0.16$



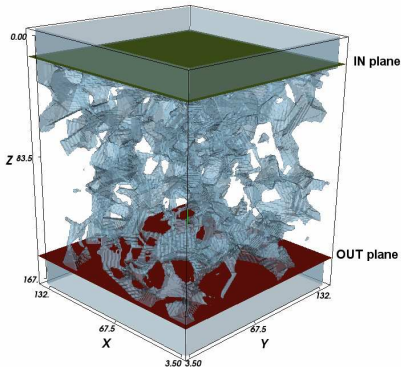
$Re=41$



$Re=100$



- ▶ The lattice Boltzmann method is very popular to study e.g. flow in porous media.
- ▶ Material properties like the permeability  $\kappa$  can be measured.



$$\kappa = -\frac{\langle u \rangle_S \rho \nu}{\langle \nabla P \rangle_S} \quad (19)$$

$\rho$ : fluid density

$\nu$ : kinematic viscosity

$\langle u \rangle_S$ : average velocity  
inside sample

$\langle \nabla P \rangle_S$ : average pressure  
gradient inside sample

## Mixtures of “simple” liquids



## Mixtures of “complex” fluids



## Particle-laden flows



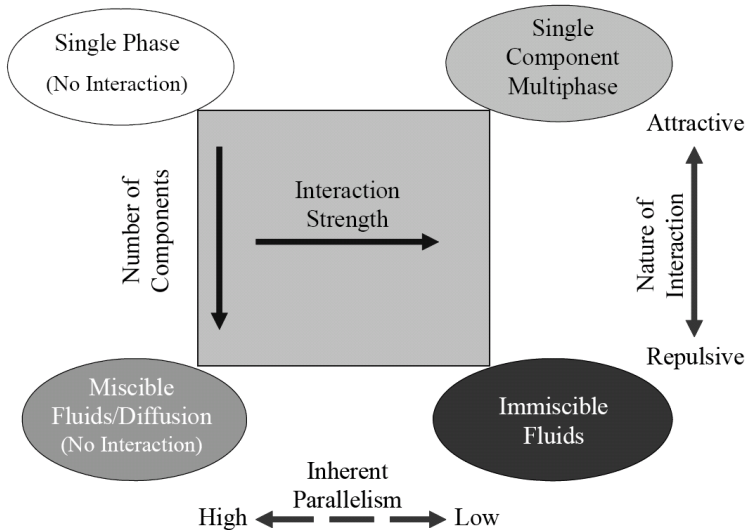
## A number of *diffuse interface* models exist:

- ▶ The colour-field model (Haliday and Care)
  - An order parameter field is introduced
  - At an interface the densities are redistributed
  - Very sharp interfaces are achieved
- ▶ The free-energy model (Oxford)
  - A free-energy term is introduced to the equation of state (EOS)
  - The free-energy has to be constructed carefully to have physical meaning
  - Physical parameters, e.g. the surface tension, can be set directly
- ▶ The pseudo-potential model (Shan and Chen)
  - Introduction of a density dependent pseudo-potential adds nonideal terms to the EOS
  - Modification of the local equilibrium function (bottom up approach)

Ref.: Dupin et al. J. Phys. A 36, 8517 (2003).

Ref.: Swift et al., Phys. Rev. E 54, 5041 (1996).

Ref.: Shan and Chen, Phys. Rev. E 47, 1815 (1993).



(from Sukop et al.)

Definition of a density-dependend pseudo-potential causing the force

$$F_{\alpha}^{SC} = \frac{dp^{\alpha}}{dt}(\mathbf{x}) = -\psi^{\alpha}(\mathbf{x}) \sum_{\alpha} g_{\alpha\bar{\alpha}} \sum_{i=0}^b \psi^{\bar{\alpha}}(\mathbf{x}') \mathbf{e}_i,$$

with the *effective mass*  $\psi^{\alpha}(\mathbf{x})$ .

This force is altering the global equilibrium velocity

$$\mathbf{u} = \frac{\sum_{\alpha} (\mathbf{u}_{\alpha} \cdot \rho_{\alpha}) / \tau_{\alpha}}{\sum_{\alpha} (\rho_{\alpha}) / \tau_{\alpha}} + \frac{\mathbf{F}^{\alpha} \cdot \tau_{\alpha}}{m_{\alpha}}.$$

**Single Component Multi Phase (SCMP):**  $F = g_{\alpha\alpha} \psi^{\alpha}(\mathbf{x}) \psi^{\alpha}(\mathbf{x}')$

**Multi Component Single Phase (MCSP):**  $F = -g_{\alpha\bar{\alpha}} \psi^{\alpha}(\mathbf{x}) \psi^{\bar{\alpha}}(\mathbf{x}')$

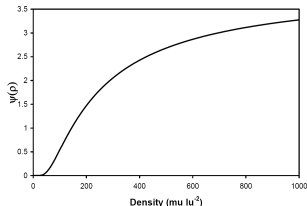
An extension of the Shan-Chen model even allows to model surfactants!

- ▶ The exact form of  $\psi(\mathbf{x})$  determines the equation of state of the model.
- ▶ The easiest:

$$\psi^\alpha(\mathbf{x}) \propto \rho \quad (20)$$

- ▶ Typical for single component multiphase:

$$\psi^\alpha(\mathbf{x}) = \psi_0 \exp(-\rho_0/\rho) \quad (21)$$

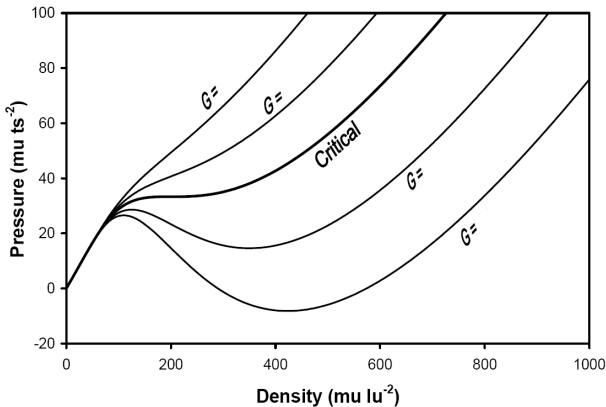


- ▶ Typical for multicomponent and multiphase:

$$\psi^\alpha(\mathbf{x}) = \psi_0 (1 - \exp(-\rho^\alpha/\rho_0)) \quad (22)$$

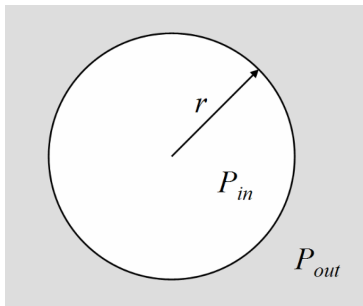
- For the single component multiphase Shan-Chen model we can write down an equation of state:

$$P = \rho k_B T + \frac{g_{\alpha\alpha} k_B T}{2} (\psi^\alpha(\mathbf{x}))^2, \quad k_B T = c_s^2 = \frac{1}{3} \quad (23)$$

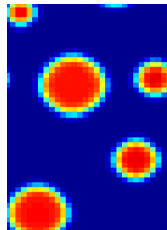


(from Sukop et al.)

- ▶ In droplets the pressure is always higher than at the outside.
- ▶ The pressure difference  $\Delta P = P_{\text{in}} - P_{\text{out}}$  depends on radius  $r$  and surface tension  $\sigma$ .



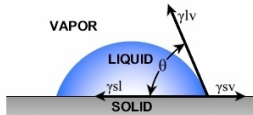
$$\Delta P = \frac{\sigma}{r} \quad (24)$$



- ▶ Study flow on (patterned) hydrophobic/hydrophilic surfaces
- ▶ Our approach: implement a repulsive “Shan-Chen like” force between surface and fluid in order to model hydrophobic surfaces:  
 $F_{wf} = \Psi^w g_{wf} \Psi^f$ ,  $\Psi^\alpha = 1 - e^{-\rho^\alpha / \rho_0}$ ,  $g_{wf}$  is an interaction parameter.
- ▶  $\Rightarrow$  variable contact angles possible

Young's Equation

$$\gamma^{sv} = \gamma^{sl} + \gamma^{lv} \cos \theta$$

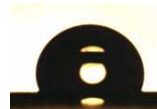


$\theta$  is the contact angle

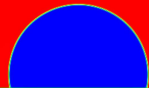
$\gamma^{sl}$  is the solid/liquid interfacial free energy

$\gamma^{sv}$  is the solid surface free energy

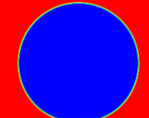
$\gamma^{lv}$  is the liquid surface free energy



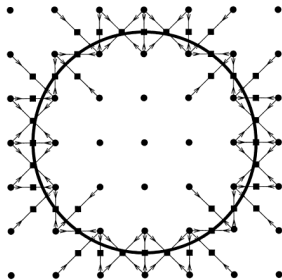
$\theta = 101^\circ$



$\theta = 160^\circ$



First proposed in 1994 by Ladd:



- ▶ Idea: particles occupy some nodes, no slip boundary conditions
- ▶ Momentum change of the fluid bouncing back is transferred to particles
- ▶ Moving wall boundary condition

$$f_i(\mathbf{x}, t) = f_i^*(\mathbf{x}, t - \Delta t) + \underbrace{2\rho\zeta_i\mathbf{e}_i\mathbf{u}_{\text{wall}}}_{\text{first order correction term}}$$

first order correction term

- ▶ Solve Newton's equations for particles (MD)

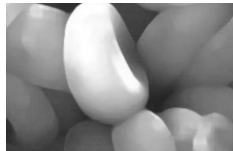
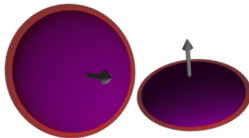
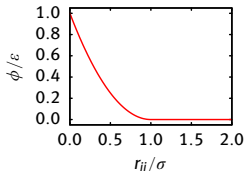
## Cell-cell interaction

repulsive Hooke potential

$$\phi(r_{ij}) = \begin{cases} \varepsilon (1 - r_{ij}/\sigma)^2 & r_{ij} < \sigma \\ 0 & r_{ij} \geq \sigma \end{cases}$$

orientation-dependent energy and  
range parameters  $\varepsilon, \sigma$

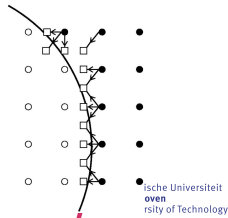
zero-energy surface approximately  
that of ellipsoids

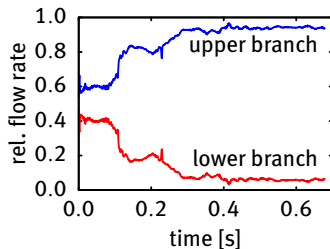
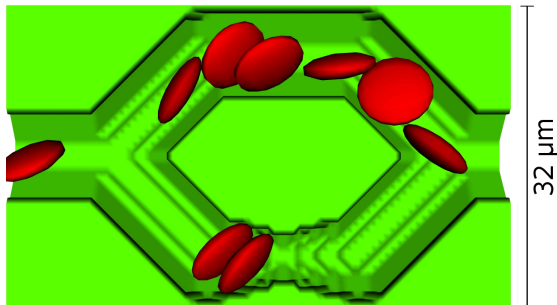


## Cell-plasma interaction

LB3D (D3Q19, BGK)

suspended rigid  
particles; ellipsoidal  
shape



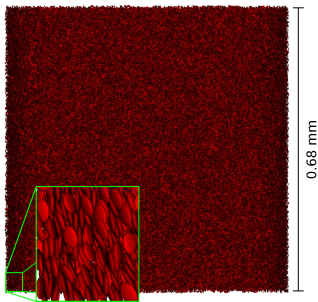


## Observations

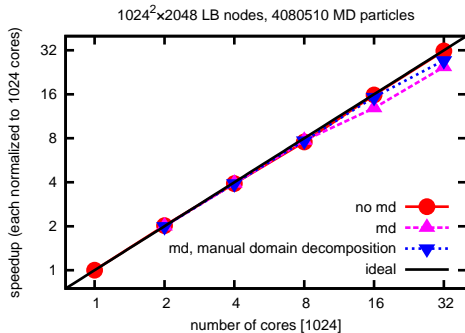
clogging visible

effect of  $\bar{\epsilon}_r$

RBCs choose faster branch as known from literature.



$1024^3$  lattice sites;  
 $2.3 \times 10^6$  particles



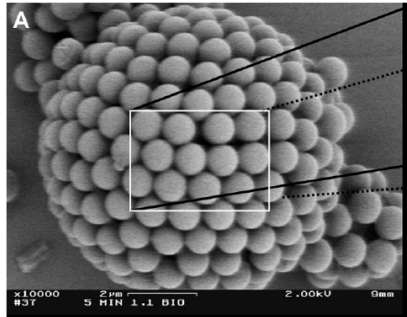
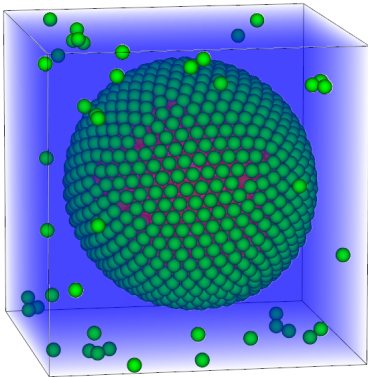
strong scaling on BlueGene/P (FZI)

Data for 32k cores

≈ 2 LB time steps per second

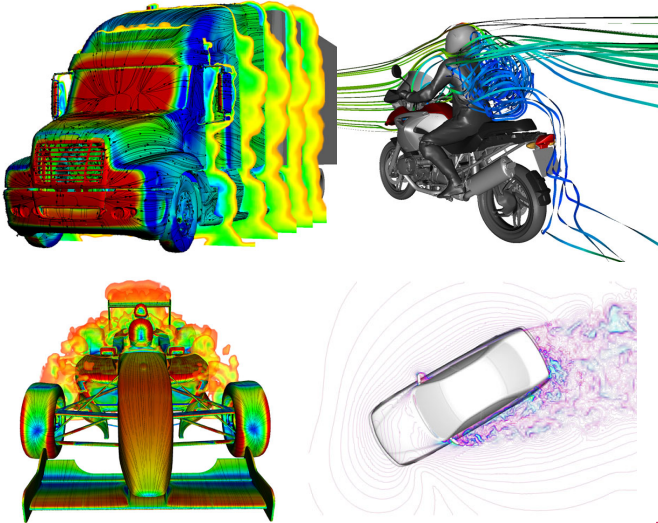
64k lattice sites per core

≈ 32 particles per core



Dinsmore et al,  
Science Vol. 298. no. 5595, pp.  
1006-1009 (2002)

## Turbulent flows (with Exa's PowerFlow)



## 1. A basic lattice Boltzmann code (15 points)

- Unpack the provided zip file and study *LBM\_SandT.m*.
- What does the code simulate?
- Identify initialization, boundary conditions, streaming, collision.

## 2. Flow around a cylinder

- Run *cylinder.m* and reproduce flow fields as on slide 23. For this, modify the maximum velocity, viscosity, cylinder diameter to achieve the required range of  $Re$ . Be careful: you might need to modify the code in order to change these values independently and to make sure to stay within the limits of stability ( $u_{max} < 0.1$ ,  $0.5 < \tau < 2$ ). (15 points)
- Change the initial condition to be able to read an arbitrary geometry from a file and study the flow to a model porous medium of your choice. (10 points)
- Compute the permeability  $\kappa$  of your porous medium (see slide 24) (15 points).

### 3. Multiphase flow

- Run *shanchen.m*. What is the code doing and what does happen if you modify the coupling parameter  $G$ ? What are the limits of phase separation and miscibility? (15 points)
- Modify the initial condition to start with a spherical droplet. (10 points)
- Compute the surface tension  $\sigma$  for different  $G$  as on slide 31. For this, let the droplet equilibrate and measure its radius as well as the pressure difference between the inside and outside. (20 points)

### 4. Play with the remaining Matlab scripts. What do they do?