The lattice-Boltzmann Method

Introduction

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Part 1: LBM Theorie

- Introduction
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  - lattice BGK method
Part 2: LBM in practice

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- Boundary Conditions
- Implementation

Part 3: LBM - modeling of complex fluids

Prof. Manfred Krafczyk, TU Braunschweig

Tuesday, 22.5.07
Part 4: LBM - Parallel and HPC issues

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

Wednesday, 23.5.07

partial differential equations
e.g. Navier-Stokes

top-down
- discretisation
- truncation error
- conservation

algebraic equation

bottom-up
multi-scale analysis

discrete model
LGA or LBM

top-down vs. bottom-up
The Boltzmann equation:
\[ \frac{\partial}{\partial t} f + c \frac{\partial}{\partial x} f + K \frac{\partial}{\partial \varepsilon} f = Q(f) \]

Balance of:
- Mass
- Momentum
- Energy

\[ \partial_t \rho + \partial_x (\rho u_j) = 0 \]
\[ \partial_t (\rho u_j) + \partial_x (\rho u_j^2 + \Pi_{ij}) = 0 \]
\[ \partial_t \rho e + \partial_x (\rho u_j E_j) = 0 \]

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

Classical mechanics
- Hamilton's equation
- Liouville equation

Molecular Dynamics methods
Direct Simulation Monte Carlo

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

Neumann

Moore

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)

(a) expansion

(b) after reversing time step

cellular automata: HPP

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

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

1. Step: Propagation Fluid-Particle

2. Step: Collision Partikel / Particle
   Particle / Wall

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

\[ f_\alpha = \langle n_\alpha \rangle = \begin{cases} \text{Density:} & \rho = \sum_\alpha f_\alpha \\ \text{Massflux:} & \rho \mathbf{u} = \sum_\alpha \mathbf{c}_\alpha f_\alpha \end{cases} \]

cellular automata: LGA FHP
- Relation to macroscopic magnitudes

\[
\frac{\partial \rho}{\partial t} + \nabla(\rho u) = 0
\]

\[
\frac{\partial u}{\partial t} + (u \nabla) u = -\frac{1}{\rho} \nabla p + \nu \Delta u
\]

\[
p = c_s^2 \rho
\]

\[g(\rho) \quad \text{Nonlinear scaling term}\]

cellular automata: LGA FHP

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**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

 opendir-Boltzmann method (McNamara and Zanetti)
From lattice-Gas to lattice-Boltzmann

<table>
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LGA and LBA

Boltzmann equation

\[
\partial_t f + c \partial_x f + K \partial_c f = Q(f)
\]

\[
f = f(t, x, c)
\]
- **Boltzmann equation**

\[
\partial_t f + c \partial_x f + K \partial_c f = Q(f) \quad f = f(t, x, c)
\]

- **Invariants**

\[
\psi_k = (m, mc, \frac{1}{2} mc^2)
\]

- **Moments of distribution functions**

\[
\int f \ dx \ m \ dc = \rho(t, x) \\
\int f \ dx \ m \ dc = \rho u(t, x) \\
\int f \ dx \ mc^2 \ dc = \rho e(t, x)
\]

From Boltzmann to NS equation

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- **Boltzmann equation**

\[
\partial_t f + c \partial_x f + K \partial_c f = Q(f) \quad f = f(t, x, c)
\]

- **Invariants of collision term**

\[
\int f Q(f) \psi_k (c) \ dc = 0, \quad \psi_k = (m, mc, \frac{1}{2} mc^2)
\]

From Boltzmann to NS equation
Integration of Boltzmann equation

\[ \int c \psi_k (\partial_t f + c \partial_x f) dc = 0 \]

\[ \psi_0 = m : \quad \partial_t \rho + \partial_x \rho u = 0 \quad \partial_t \rho + \partial_x \rho u_j = 0 \]

\[ \psi_{1..3} = mc : \quad \partial_t \rho u + \partial_x \Pi = 0 \quad \partial_t \rho u_i + \partial_x \Pi_{ij} = 0 \]

\[ \psi_4 = \frac{1}{2} mc^2 : \quad \partial_t \rho e + \partial_x E = 0 \quad \partial_t \rho e + \partial_x E_j = 0 \]

\[ \Pi_{ij}(x,t) = m \int c_i c_j f dc \quad E_i(x,t) = \frac{1}{2} m \int c_i c^2 f dc \]

From Boltzmann to NS equation

- Decomposition of the velocity \( c_i = u_i + w_i \)

\[ \Pi_{ij}(x,t) = \rho u_i u_j + \rho \int_c w_i w_j f dc \]

\[ \sigma_{ij} = p \delta_{ij} + \tau_{ij} \]

- Maxwell distribution (equilibrium)

\[ f_e^{eq} = \frac{\rho}{(2\pi c_s^2)^{\frac{3}{2}}} \cdot \exp \left( -\frac{(c - u)^2}{2c_s^2} \right) \quad c_s^2 = RT \]

- "Macroscopic" momentum equation of inviscid flow

\[ \partial_t \rho u_i + \partial_x (\rho u_i u_j) = -\partial_x \left( c_s^2 \rho \delta_{ij} \right) \quad p = c_s^2 \rho \]

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

\[ \frac{\partial f}{\partial t} + c \frac{\partial f}{\partial x} = \frac{1}{\tau} (f^{eq} - f) \]

Chapman-Enskog Expansion

\[ f = f^{eq} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \ldots \]

\[ \tau_{ij}(x,t) = -\tau \rho RT (\partial_{x_i} u_j + \partial_{x_j} u_i - \frac{2}{3} \partial_{x_k} u_k \delta_{ij}) \]

\[ \nu \sim \tau \varepsilon^2 \]

From Boltzmann to Lattice Boltzmann

Energy flux

\[ E_i(x,t) = \frac{1}{2} \rho u_i^2 + \frac{1}{2} \rho u_i \int c \, w^2 \, f \, dc + \rho u_i \int_c \, w_i w_j f \, dc + \frac{1}{2} \rho \int_c \, w^2 w_j f \, dc \]

“Macrosopic” energy equation

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

\[ q_j(x,t) = -\frac{\varepsilon}{2} \frac{k}{m} \tau \rho RT \partial_{x_j} T \]

From Boltzmann to NS equation
Representation in discrete velocities

\[ f(t, x, c) \Rightarrow \tilde{f}(t, x, e_\alpha) = f_\alpha(t, x) \]

**Velocity-discrete Boltzmann Equation**

\[ \partial_t f_\alpha + e_\alpha \partial_x f_\alpha = \frac{1}{\tau} (f_\alpha^{eq} - f_\alpha) \quad \text{(STR Approximation)} \]

**Lattice Boltzmann Equation**

\[ f_\alpha(t + \Delta t, x) - f_\alpha(t, x) + e_\alpha \frac{\Delta t}{\Delta x} [f_\alpha(t + \Delta t, x + e_\alpha \Delta t) - f_\alpha(t + \Delta t, x)] = R.S. \]

\[ f_\alpha(t + \Delta t, x + e_\alpha \Delta t) - f_\alpha(t, x) = \frac{\Delta t}{\tau} (f_\alpha^{eq} - f_\alpha) \]

From Boltzmann to Lattice Boltzmann

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**Equilibrium velocity distribution for lattice Boltzmann Equation**

- no direct transfer of Maxwell distribution

\[ f_\alpha^{eq} = f^{eq} \]

**Moments of equilibrium velocity distribution shall satisfy**

\[ \int_{c=-\infty}^{\infty} f^{eq} \psi(c) dc = \sum_{e_\alpha} W_\alpha f_\alpha^{eq} \psi(e_\alpha) \]

up to 2th order!

**After linearisation**

\[ f_\alpha^{eq} = \rho \left[ 1 + \frac{e_\alpha u}{c_s^2} + uu \left( \frac{e_\alpha c_s^2}{c_s^2} - \delta_\alpha \right) \right] \]

From Boltzmann to Lattice Boltzmann
Relation to macroscopic properties

- from moments of distribution function
  - density \( \rho = \sum_{\alpha} m f_{\alpha} \)
  - mass flux \( \rho u_i = m \sum_{\alpha} e_{\alpha,i} f_{\alpha} \)
  - 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 \( \nu = c_s^2 (\tau - \frac{1}{2}) \Delta t \)

From Boltzmann to Lattice Boltzmann

Summary:

- Boltzmann equation
  \[ \partial_t f + c \partial_x f + \mathcal{Q}_c f = Q(f) \]

- BG Krook equation (STR)
  \[ \partial_t f + c \partial_x f = \frac{1}{\tau} (f_{eq} - f) \]

- Velocity discrete BGK (1. order DGL in diagonalform)
  \[ \partial_t f_{\alpha} + e_{\alpha} \partial_x f_{\alpha} = \frac{1}{\tau} (f_{\alpha}^{eq} - f_{\alpha}) \]

- Finite difference approximation
  \[ f_{\alpha}(t + \Delta t, x + e_{\alpha}\Delta t) - f_{\alpha}(t, x) = \frac{\Delta t}{\tau} (f_{\alpha}^{eq} - f_{\alpha}) \]
**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 contrast 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