Cloud Computing mit mathematischen Anwendungen

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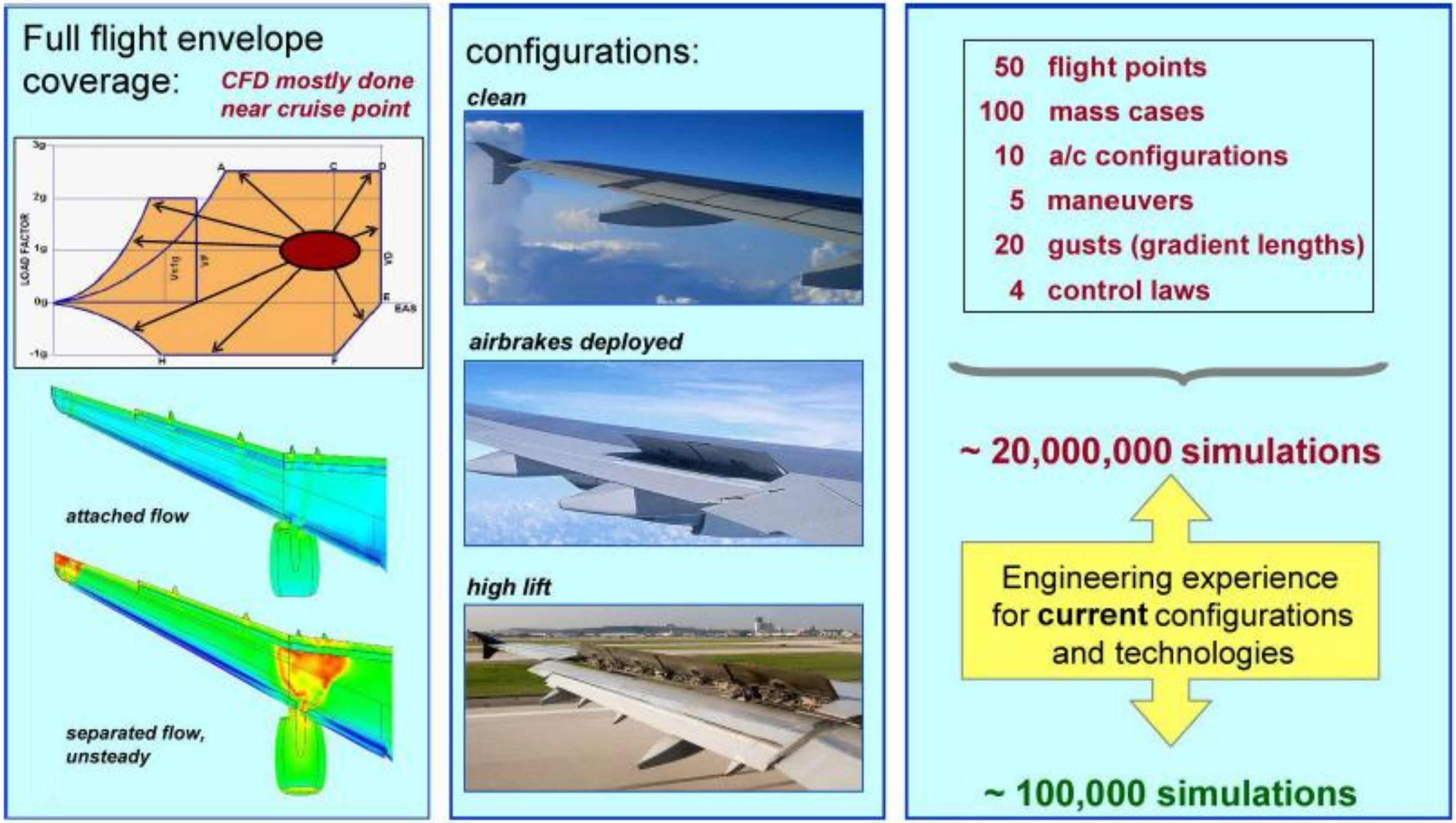
11. Numerical Simulation and Optimization

Vision: Digital Aircraft



Source: DLR

- Example: Airbus 380

How can we scale to this Dimension?

- **Extension of the Parallel Programming Model**
  - Fully asynchronous
  - Dataflow driven
  - Implicitly load balanced
  - Exclusively uses local locks instead of global barriers
  - Should work well with large multi-core CPUs

```
for(k = 0; k < KDIM; k++)
   for (j = 0; j < JDIM; j++)
      for (i = 0; i < IDIM; i++) {};
BARRIER;
for(k = 0; k < KDIM; k++) …
```

```
for(k = get_k_index(); k != -1; k = get_next_k_index(k))
   for (j = 0; j < JDIM; j++)
      for (i = 0; i < IDIM; i++) {};
 for(k = get_k_index(); k != -1; k = get_next_k_index(k)) …
```

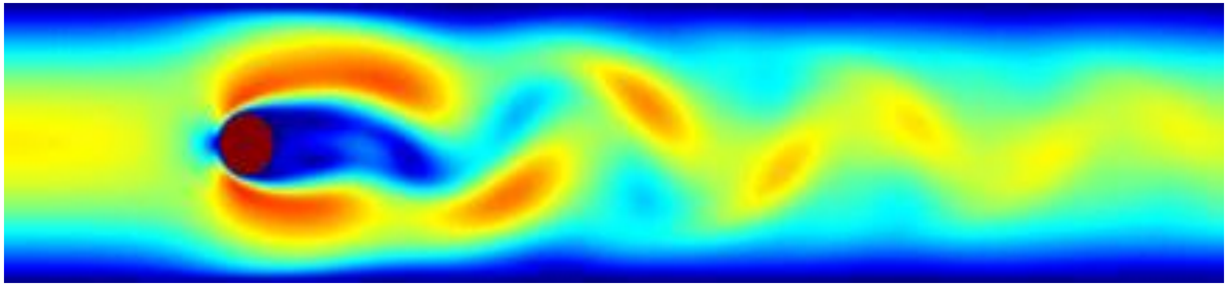
J.Jägersküpper (DLR), C.Simmendinger (T-Systems SfR). A Novel Shared-Memory Thread-Pool Implementation for Hybrid Parallel CFD Solvers, EuroPar 2011, (to appear).

Computational Fluid Dynamics (CFD)

- Predicting the behavior of fluids
- Important in e.g. aerospace-, civil-, or mechanical engineering
- Numerical simulation of fluid flows
  - Traditional method: solves the conservation equations of macroscopic properties (i. e., mass, momentum, and energy)
  - Lattice Boltzmann method (LBM): models the fluid consisting of fictitious particles, which perform consecutive propagation and collision processes over a discrete lattice
  - LBM is efficient when dealing with complex boundaries and the incorporation of microscopic interactions

What are Lattice Boltzmann Methods (LBM)?

- Lattice Boltzmann methods are numerical techniques for the simulation of fluid flows.
- Solve the incompressible, time-dependent **Navier-Stokes** equation numerically
- Represent **complex physical phenomena**, ranging from multiphase flows to chemical interactions between the fluid and the borders
- Molecular description of a fluid incorporating physical terms
- A collection of resources on the lattice Boltzmann method can be found on the website of **LBmethod**.



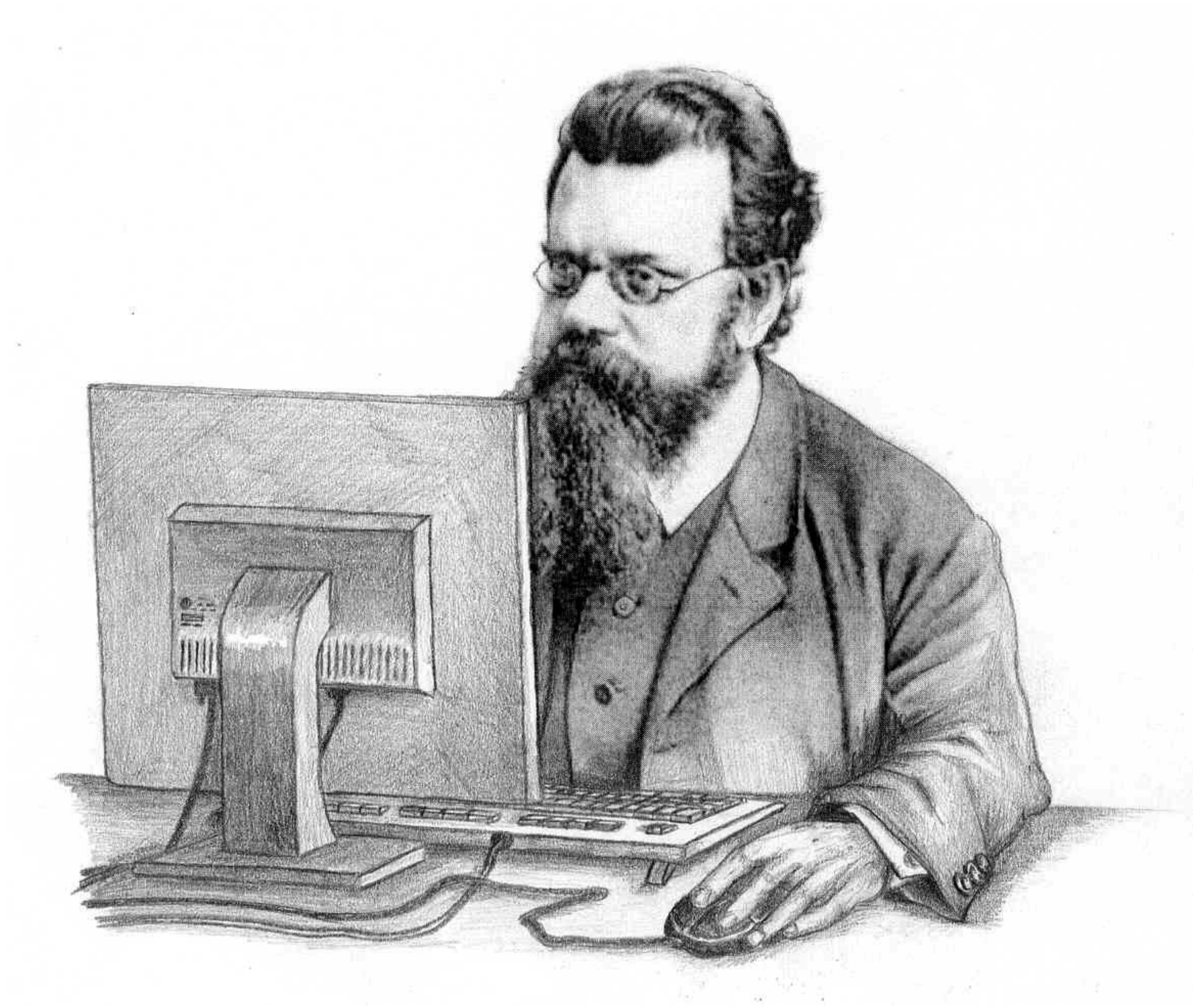
http://www.lbmethod.org/animations/karman.gif

2D flow past a cylinder
Source:
http://www.lbmethod.org

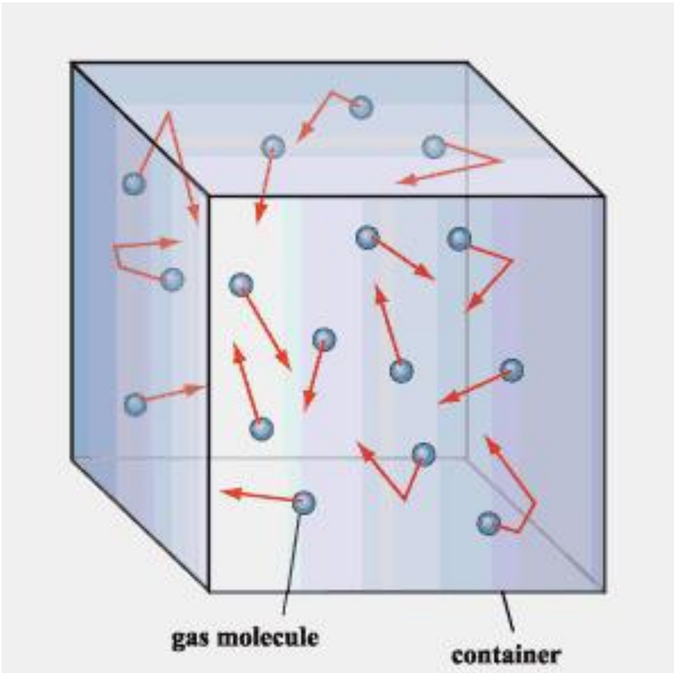
Where does LBM come from?

- Discrete representations of the Boltzmann equation (Kinetic gas theory)
- **Boltzmann equation** is the analogue of the **Navier-Stokes equation** at a molecular level, where it describes the evolution of the **probability distribution function** for a molecule to be present at a given point in the space of positions and velocities, the 6-dimensional phase space.
- The molecular model is able to capture transport phenomena such as friction, diffusion and temperature transport and derive the corresponding transport coefficients.

Ludwig Boltzmann (1844-1906)



Kinetic Gas Theory (Boltzmann Equation)



- Free elastic particles
- No external forces
- Constant velocity
- Large number (ca. 10^{20})

Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \frac{\partial f}{\partial \mathbf{x}} = \Omega(f, f')$$

Particle probability density function **Ω**

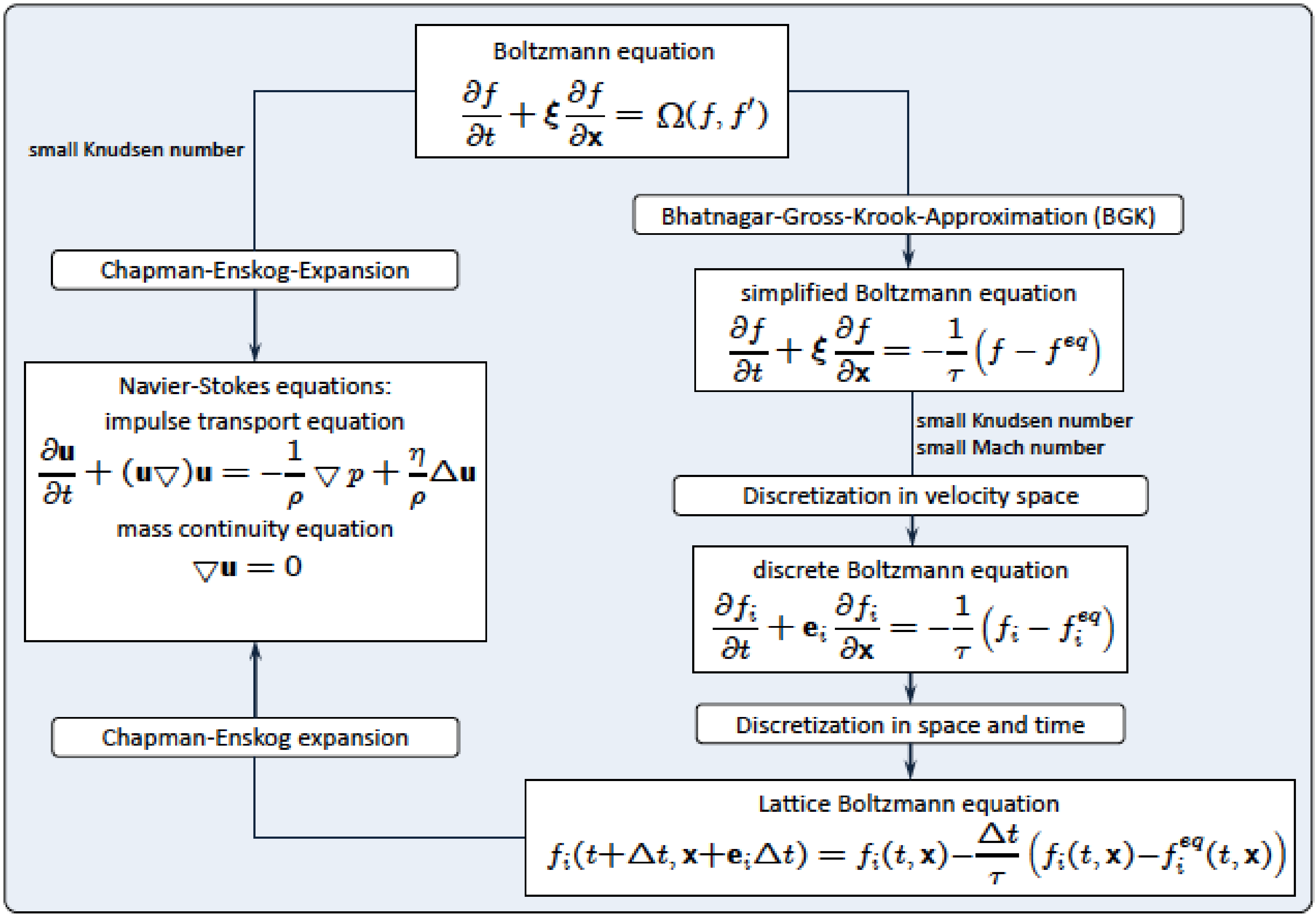
f = Mass density

$\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$: Position

$\xi = (\xi_1, \xi_2, \xi_3)$: Velocity

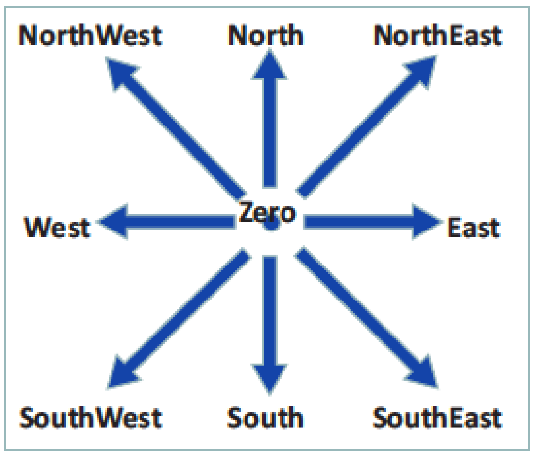
t : Time

Lattice Boltzmann Equation

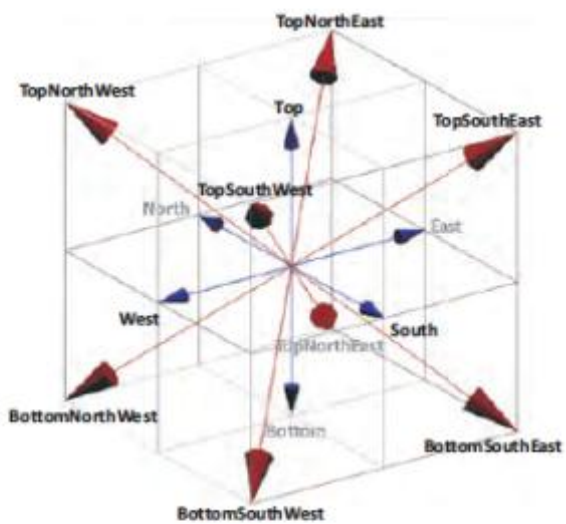


Discretization

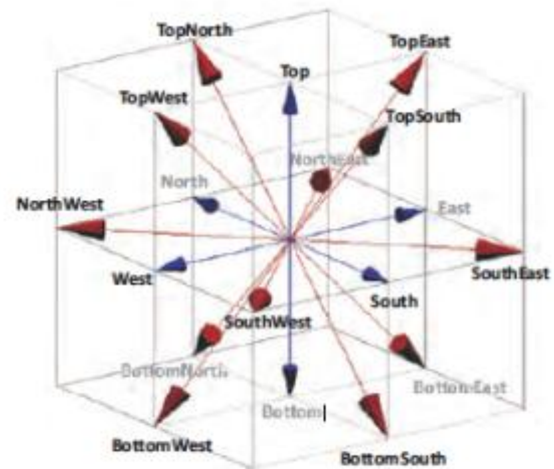
- Discretization on a lattice with stencils of dimension d and number of microscopic velocities q: DdQq



D2Q9



D3Q15



D3Q19

Lattice Boltzmann Methods (LBM)

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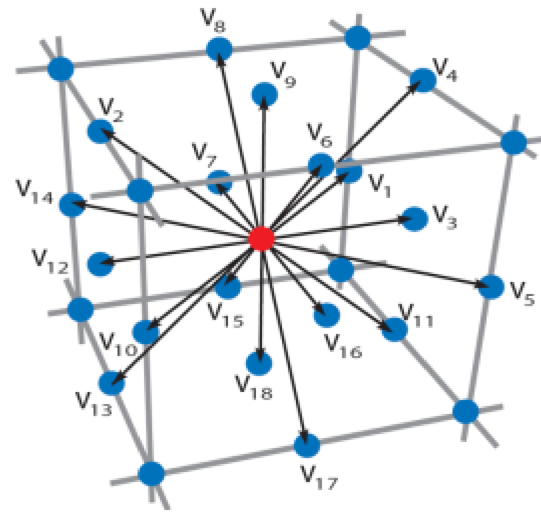
D3Q19



Idea: coupling model parameter $h \in \mathbb{R}_{>0}$ with discretisation parameter: *Lattice DdQq*

Macroscopic moments:

density $\rho = \sum_{i=0}^{q-1} f_i$, velocity $\rho \boldsymbol{u} = \sum_{i=0}^{q-1} \boldsymbol{v_i} f_i$

Time loop $t = t_0, t_0 + h^2, t_0 + 2h^2, ..., t_1$

Position space loop $\boldsymbol{r} \in \Omega_h$

(1) Collision $\tilde{f}_i(t, \boldsymbol{r}) = f_i(t, \boldsymbol{r}) - \frac{1}{3\nu + 1/2}\left(f_i(t, \boldsymbol{r}) - M_{f_i}^{eq}(t, \boldsymbol{r})\right)$

(2) Streaming $f_i(t + h^2, \boldsymbol{r} + h^2 \boldsymbol{v_i}) = \tilde{f}_i(t, \boldsymbol{r})$

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OpenLB: Overview

openlb.org

2D and 3D fluid flow simulations based on LBM

- Computational framework:
  - Open Source (GPL2)
  - C++, object oriented, template-based
- Features in latest release 0.6:
  - Multi-physics models (multiphase, thermal)
  - Hybrid parallelisation (MPI & OpenMP)
  - Automated build-in pre-processing:
    - Voxelisation from STL-files
    - Setting of boundary conditions
  - XML interface for input parameters
  - Visualization (built-in and VTK)
- Current project partners:

  EMCL/KIT (Karlsruhe), Mevis (Bremen)

2009

2007

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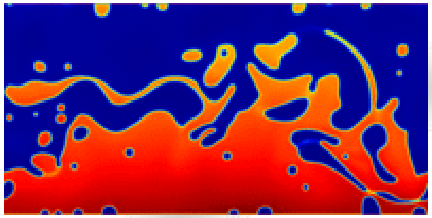
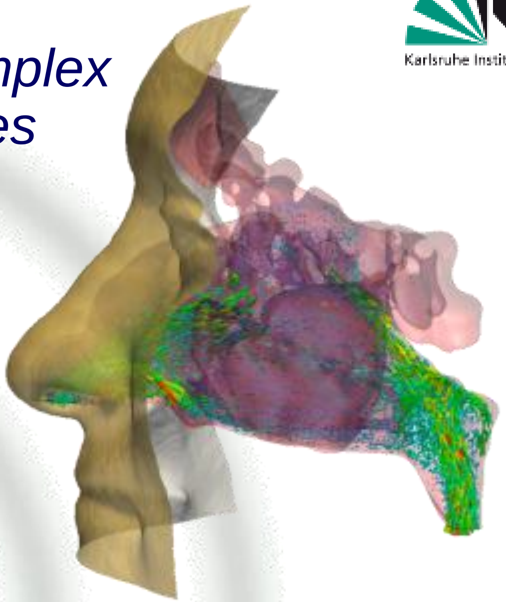
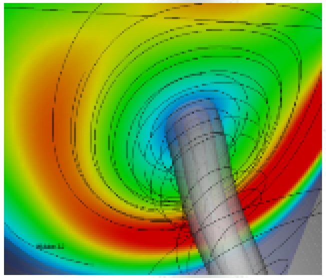
OpenLB: Applications



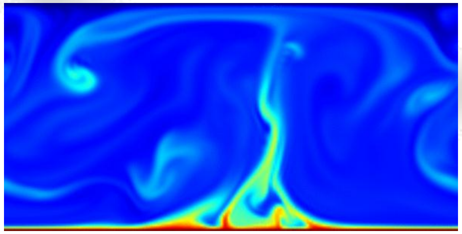
Multiphase flows



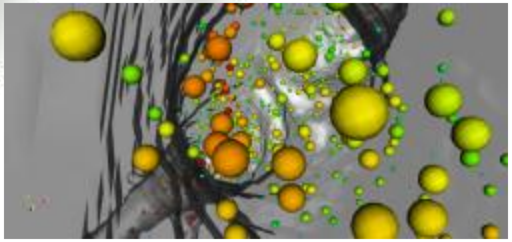
Flows in complex geometries



Turbulent flows



Thermal flows



Particle flows

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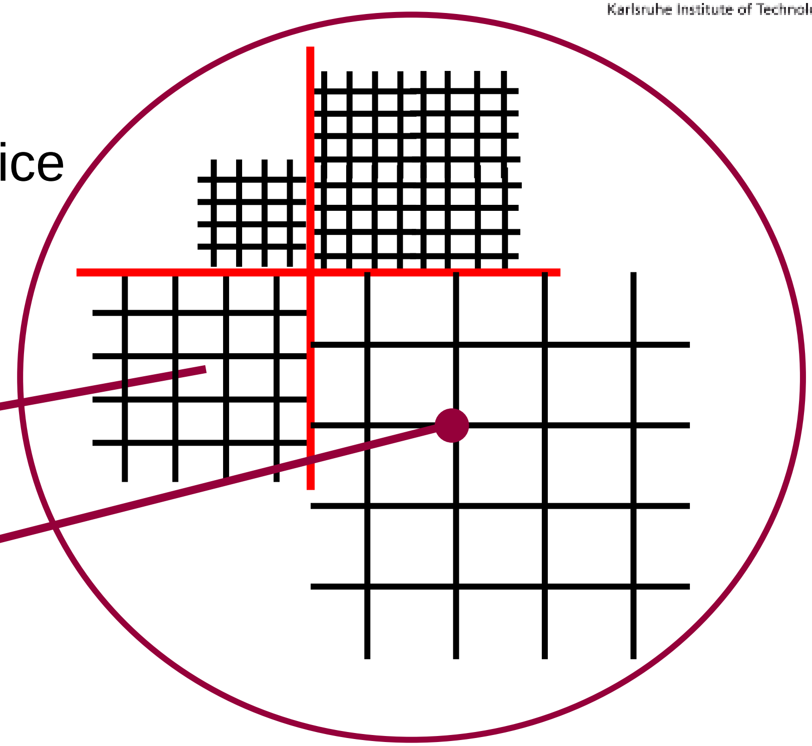
Data Structure Design

SuperLattice

Multi-block ansatz

BlockLattice

Cell



Data:

- Distribution function f_i

Methods:

- Compute density
- Compute velocity
- Compute stress tensor
- Execute collision step

Example: distinction between fluid cell and boundary cell

Example: inhomogeneous fluids

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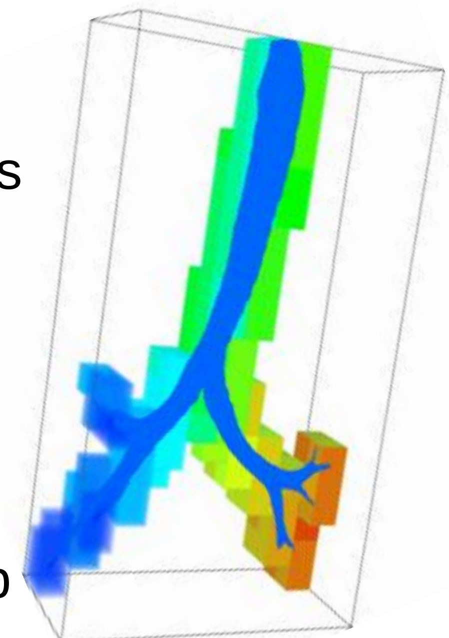
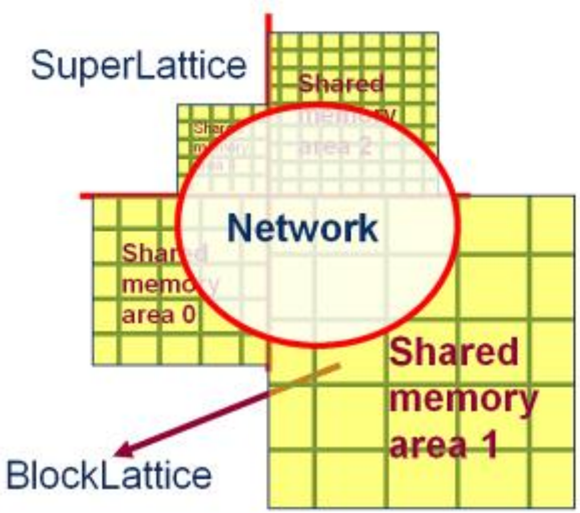
Parallelisation: Hybrid Concept

- For distributed and/or shared memory platforms
- Based on domain decomposition
- Sparse multi-block representation of geometries
- OpenMP for intra-block parallelism
- MPI for inter-block parallelism





Time loop

Collision step

> Blocking

> Communicating

> Writing to ghost cells

Streaming step

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Hausaufgabe 10: OpenLB

Installieren Sie das OpenLB-System entsprechend der Anleitung auf http://www.openlb.org/. Instanzieren Sie mit AWS zunächst ein Amazon Linux System (m1.large), basierend auf dem Image ami-8e1fece7.

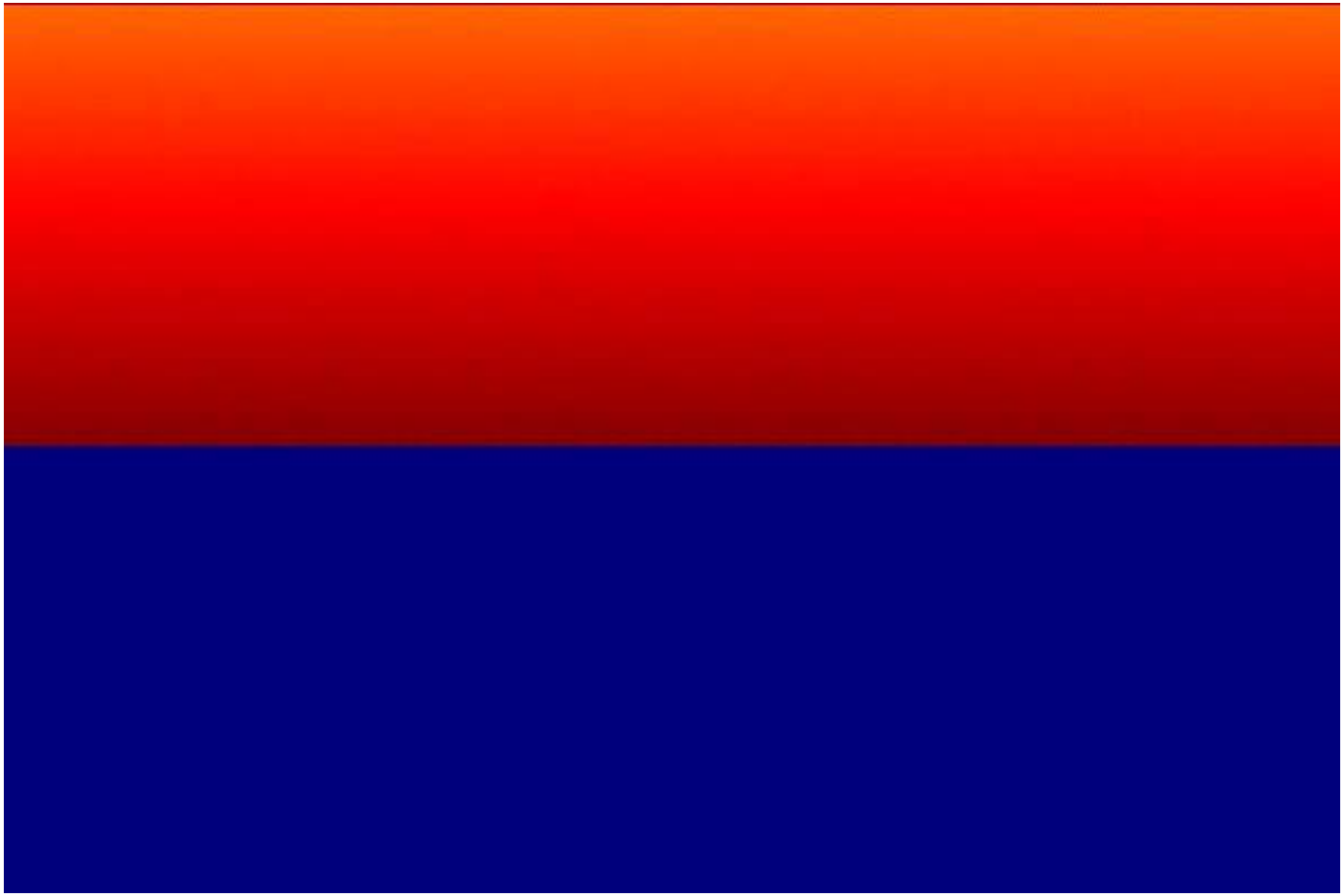
- Einloggen auf dem Server mit
  ssh –i <keyname>.pem ec2-user@<server-ip>
- Installation der Requirements
  sudo yum install mpi-devel;
  sudo yum install blas-devel;
  sudo yum install gcc-c++;
  sudo yum install make
- Laden des OpenLB-Pakets
  wget http://www.openlb.org/openlb/download.php?cat=30_Download\&file=olb-0.6r0.tgz
- Auspacken des Pakets
  tar -zxf *olb-0.6r0.tgz; cd olb-0.6r0
- In Makefile.inc die folgenden Optionen aktivieren:
  CXX := mpicc
  PARALLEL_MODE := MPI
- Übersetzen des Pakets
  export MPI_HOME=/usr/lib64/openmpi
  export PATH=$MPI_HOME/bin:$PATH
  export LD_LIBRARY_PATH=$MPI_HOME/lib:$LD_LIBRARY_PATH
  make

Hausaufgabe 10: OpenLB

Probieren Sie nun einige der Beispiele aus und stellen Sie die Ergebnisse grafisch dar.

- Installation des Grafikpakets und des Filmkonverters
  sudo yum install imageMagick
  sudo yum install ffmpeg
- Wechsel in das Beispielverzeichnis. Durchführen einer Simulation. Erzeugen eines Films aus den einzelnen gif-Bildern.
  cd examples
  cd cavity2d; make
  mpirun –np 8 cavity2d
  cd tmp
  convert –delay 5 *.gif cavity2d.mpg
- Die vti-Files können auch mit dem Programm Paraview studiert werden:http://www.paraview.org/

Example



- Rayleigh-Taylor instability in 2D, generated by a heavy fluid penetrating a light one. http://cloudvorlesung.s3.amazonaws.com/multiComponent2d.mpg

Good to know

- **All course info is on http://studium.kit.edu**
- **http://www.math.kit.edu/mitglieder/lehre/cloudcomp2011s/**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