Massively parallel simulation of 3D transient coupled CFD problems with kinetic methods

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Outline

- The Problem: Fluid dynamics
- Kinetic Models for CFD in a nutshell
- Hierarchical data structures
- Numerical examples & parallel efficiencies on CPUs
- (Multi-)GPU-computing
- Outlook

Kinetic Models for CFD in a nutshell

Boltzmann equation (BE)

$$\frac{\partial f}{\partial t} + \vec{\xi}\,\frac{\partial f}{\partial \vec{x}} = \Omega(f)$$

Kn<<1

CE-expansion

BGK-approximation

$$\frac{\partial f}{\partial t} + \vec{\xi}\,\frac{\partial f}{\partial \vec{x}} = -\frac{1}{\tau}(f - f^{eq})$$

Navier-Stokes equation

$$\frac{\partial(\rho\vec{v})}{\partial t} + (\vec{v}\nabla)(\rho\vec{v}) = -\nabla p + \mu\Delta(\rho\vec{v})$$

continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla(\rho\vec{v}) = 0$$

Discrete BE

$$\frac{\partial f_i}{\partial t} + \vec{\xi}_i\,\frac{\partial f_i}{\partial \vec{x}} = -\frac{1}{\tau}(f_i - f_i^{eq})$$

FD-Discretization

Lattice BE

$$f_i(t+\Delta t, \vec{x} + \vec{\xi}_i \Delta t) - f(t,\vec{x}) = -\frac{1}{\tau}(f_i - f_i^{eq})$$

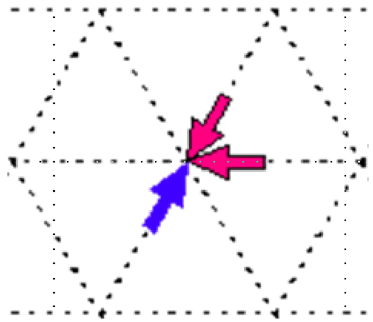
Kn, Ma <<1

Chapman-Enskog expansion

Lattice Boltzmann Equation (LBE)

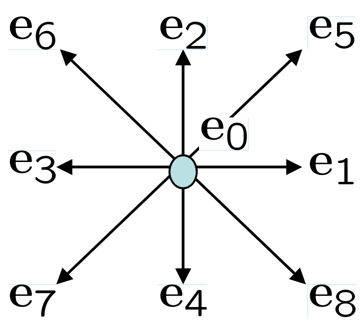
$$f_i(t+\Delta t, \mathbf{x}+\mathbf{e}_i \Delta t) = f_i(t, \mathbf{x}) + \Omega_i, \quad i = 0, \ldots, b-1$$

f	Mass fractions
e	Microscopic velocity of the particles
t	Time
x	Space



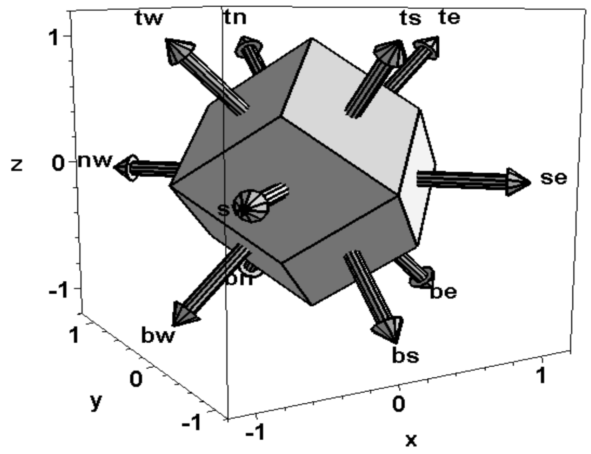
d2q6-Model

Wolfram 86, Hasslacher 86



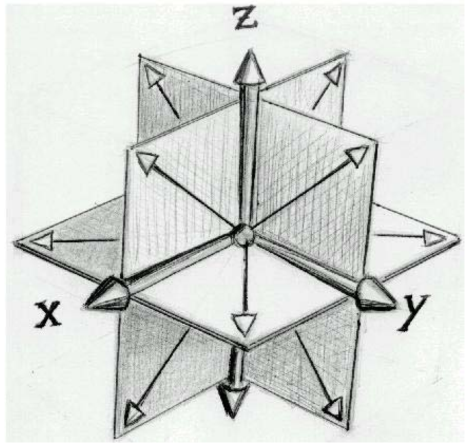
d2q9-Model

Qian 92



d3q13-Model

d'Humieres 01



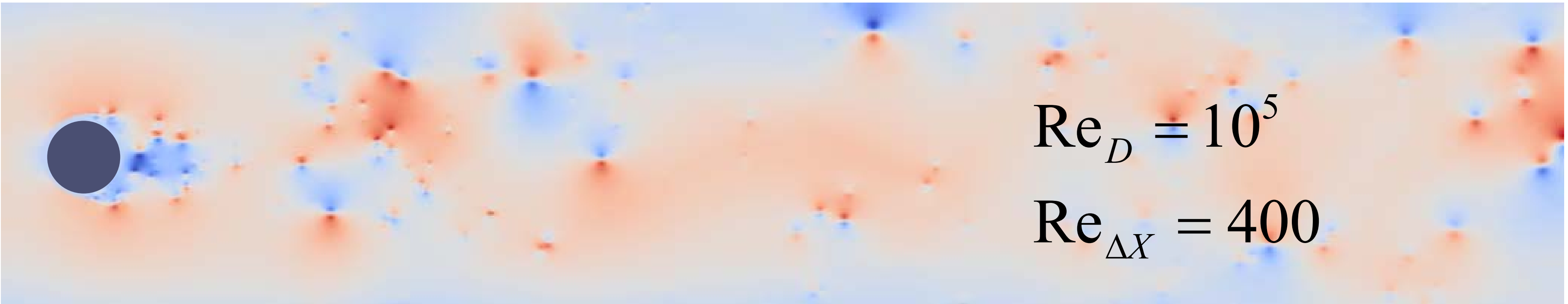
d3q19-Model

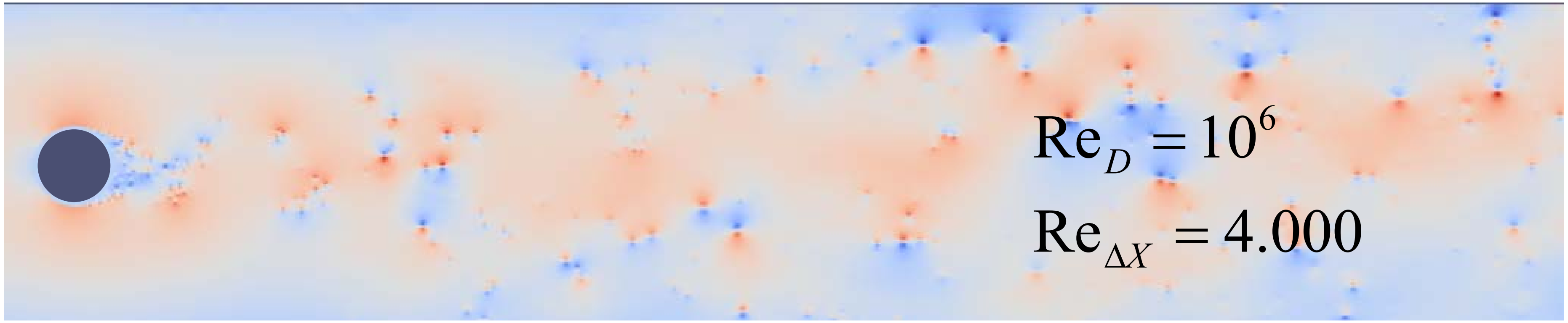
Qian 92

Cascaded LB: testing stability limits …

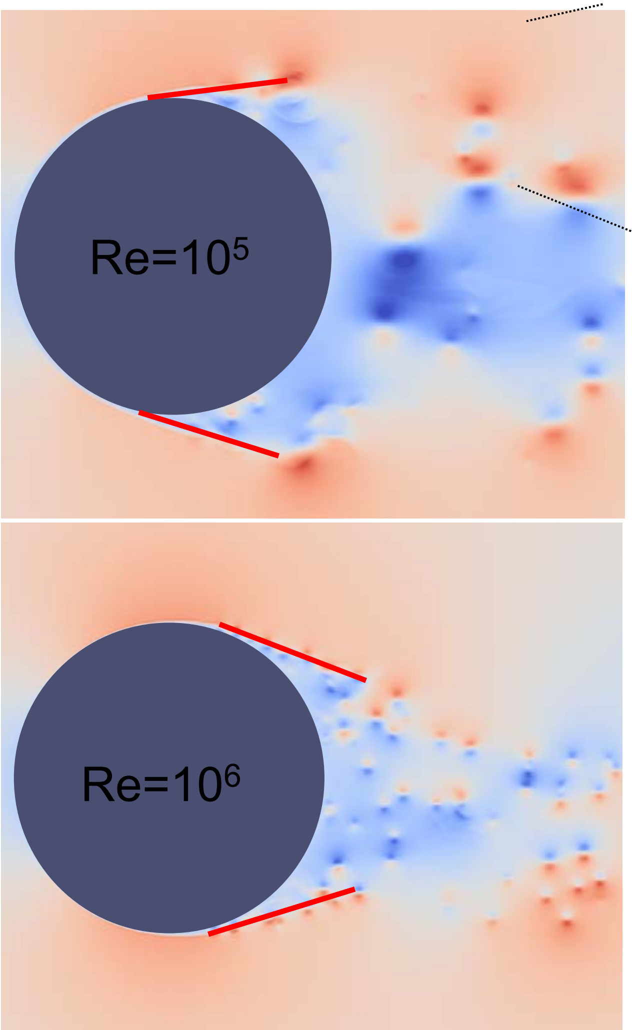
D2Q9, two grid levels, GPU (single precision)

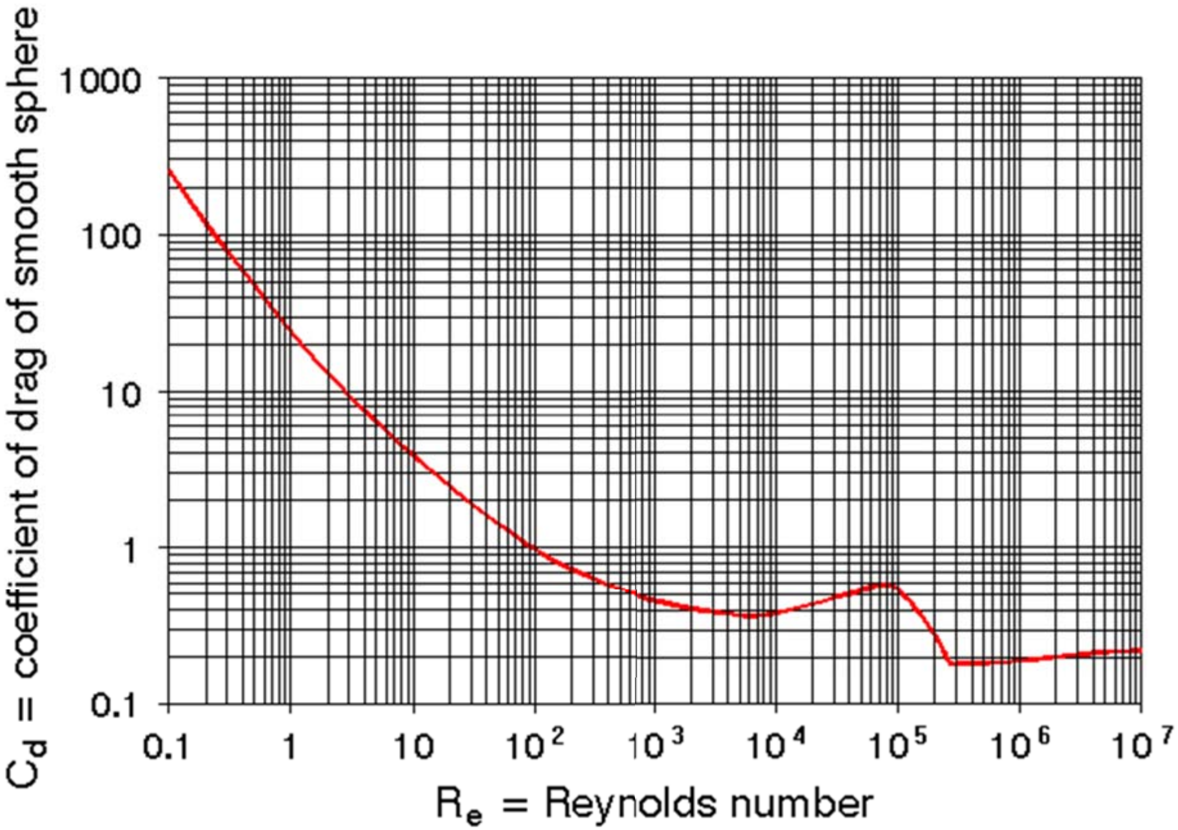
Each level holds 2.048 x 10.990 grid nodes ($2\times10^{8}\,DOF$) $\dfrac{\Delta x_{coarse}}{\Delta x_{fine}} = 2$



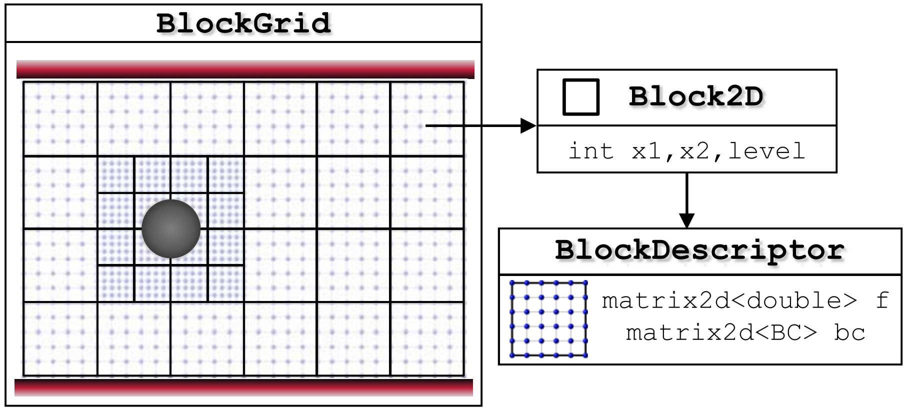


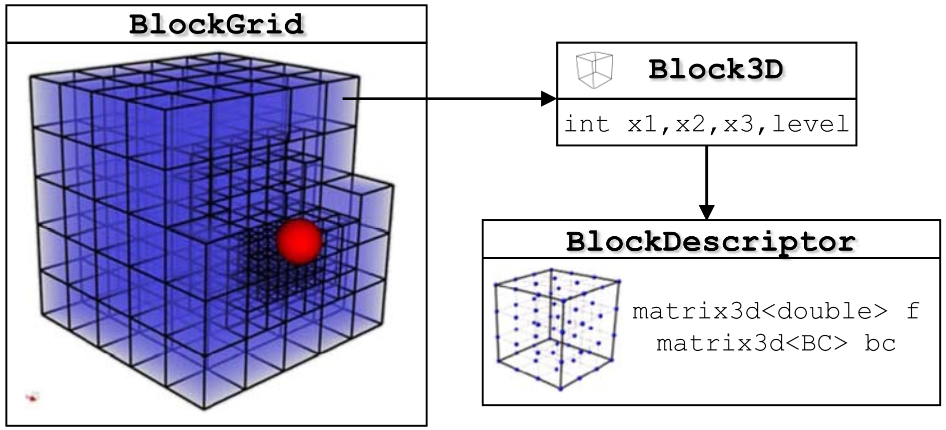
…reveals 2d „drag crisis“





Data structures: hierarchical grids



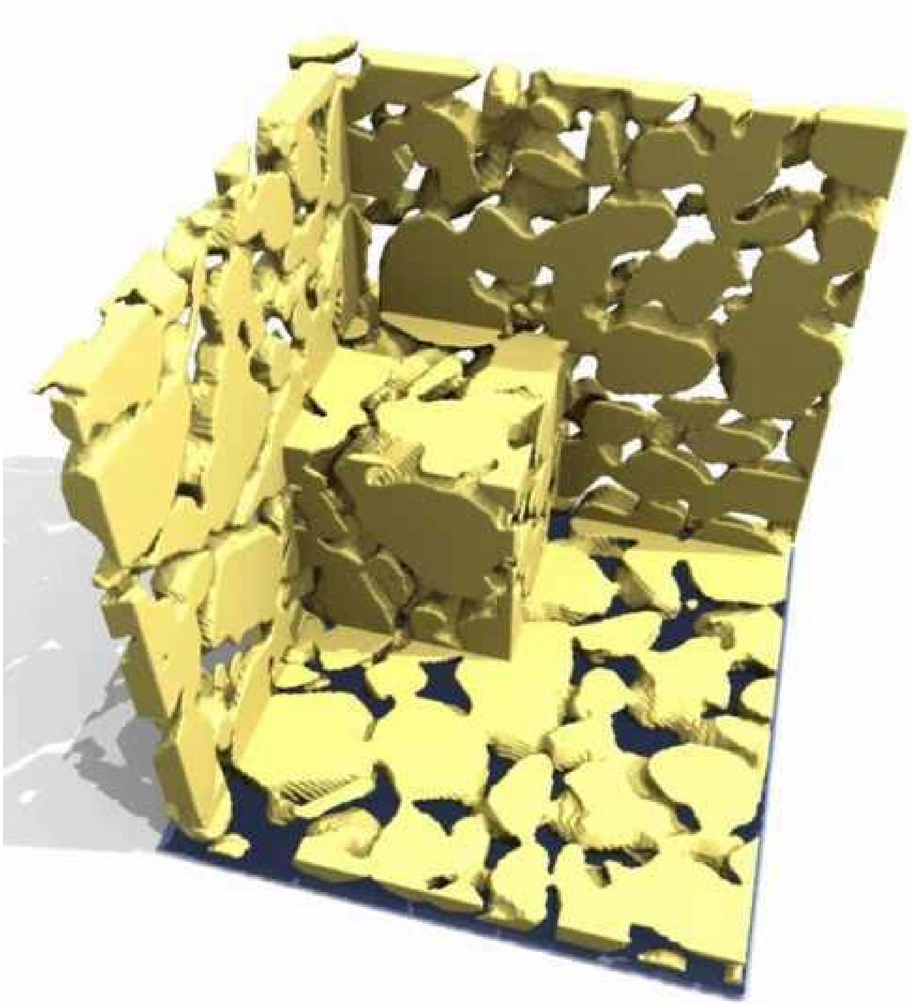


basic properties of block grid

- zoning of a flow field by blocks of various sizes to adapt the mesh size to local flow characteristic length
- uniform Cartesian mesh in each block for efficient computations (2nd order sub grid incl.)
- same grid size in all blocks to simplify connectivity

Numerical examples I: multiphase flows in porous media
a) drainage

Non wetting phase (air) displaces
wetting phase (water)
when subjected to pressure gradient



Application

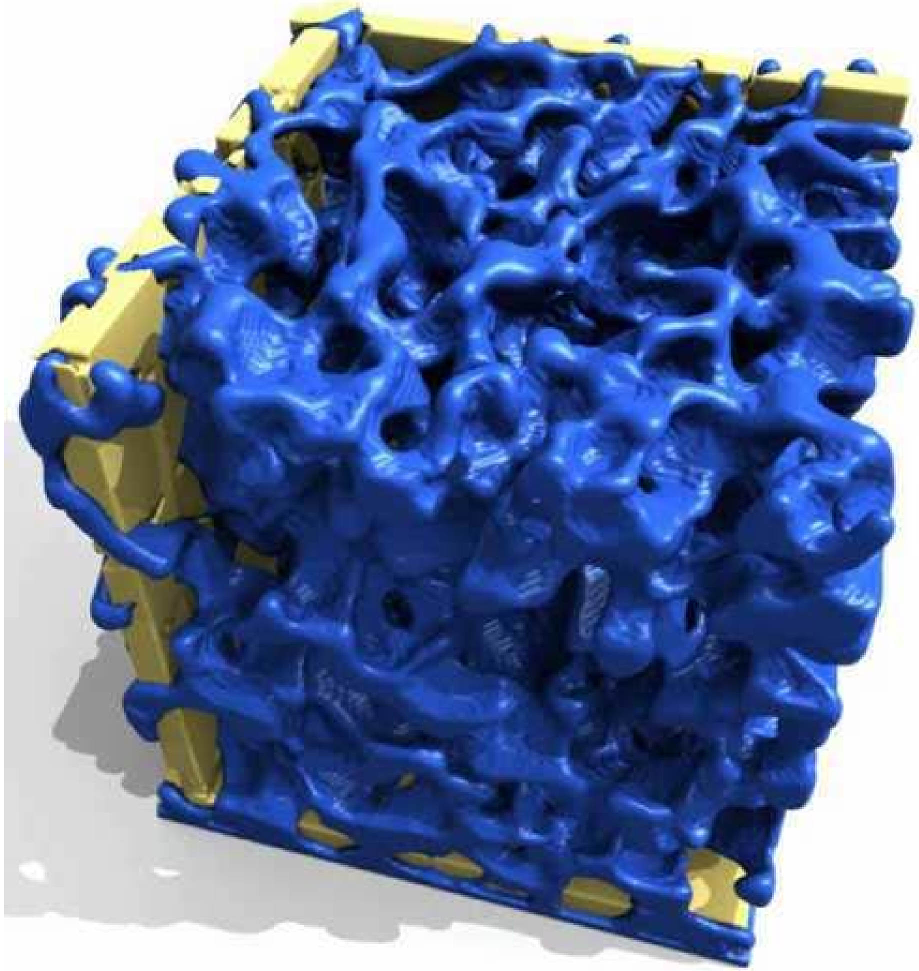
- Determination of transport properties, e.g. relative permeabilities (which depends on saturation)
- Gaining input data for upscaling processes: microscale → mesoscale → macroscale

Numerical examples I: multiphase flows in porous media
b) imbibition

Inverse process – wetting phase displaces the non-wetting phase.

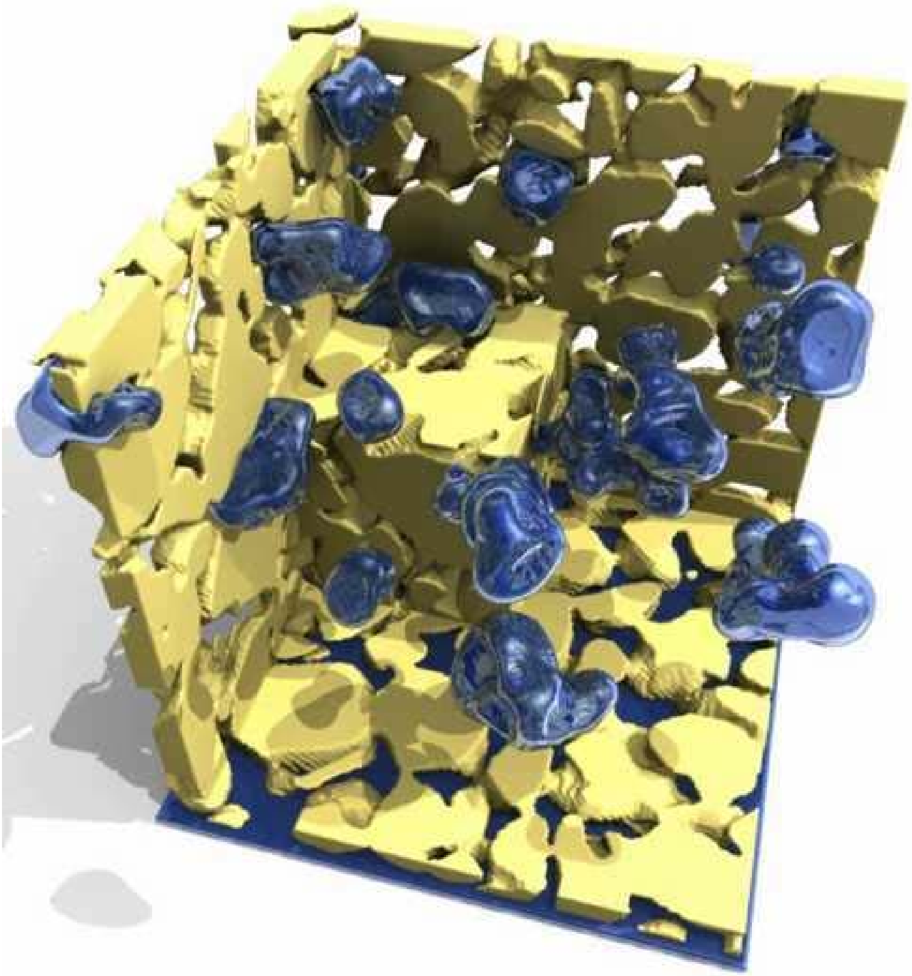
Relevance

- Imbibition is not a simple inverse process of drainage
- Appearance of hysteretic effects



Numerical examples I: multiphase flows in porous media
c) secondary drainage

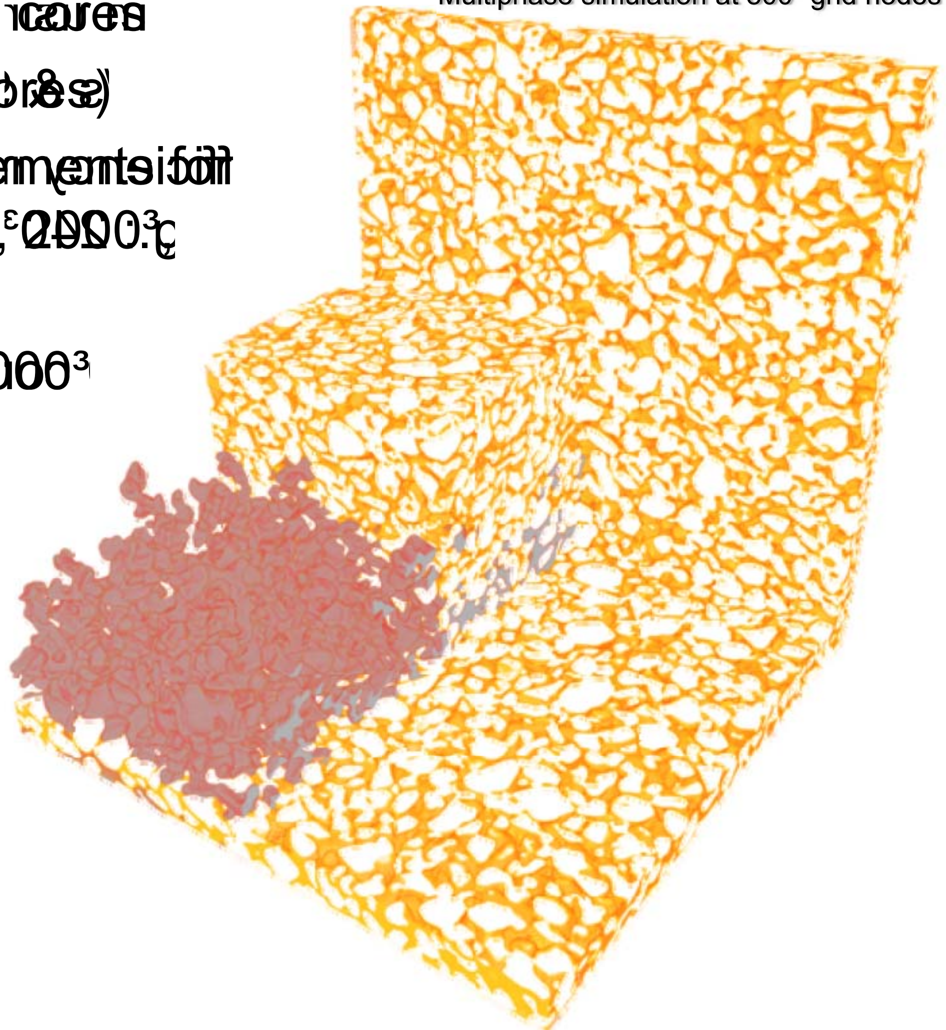
- A second drainage closes the cycle
- The history of drainage and imbibition has an impact of the systems behaviour
- Drainage and imbibition are two complementary but different processes



Parallel efficiency I

- 10^{12} Degrees of freedom using 4080 cores
- SGI Altix 4700 (62TFlop/s & 9728 Cores)
- Performance and efficiency measurements for different grid sizes, e.g.: 240³, 1000³, 2000³, 4000³ nodes
- parallel efficiency at 4080 cores & 4000³ nodes: **92%**

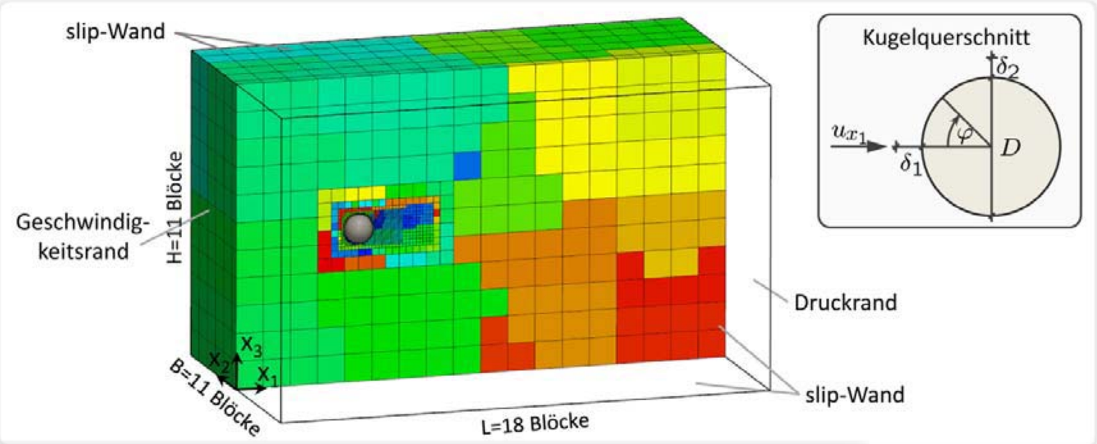
Multiphase simulation at 800³ grid nodes

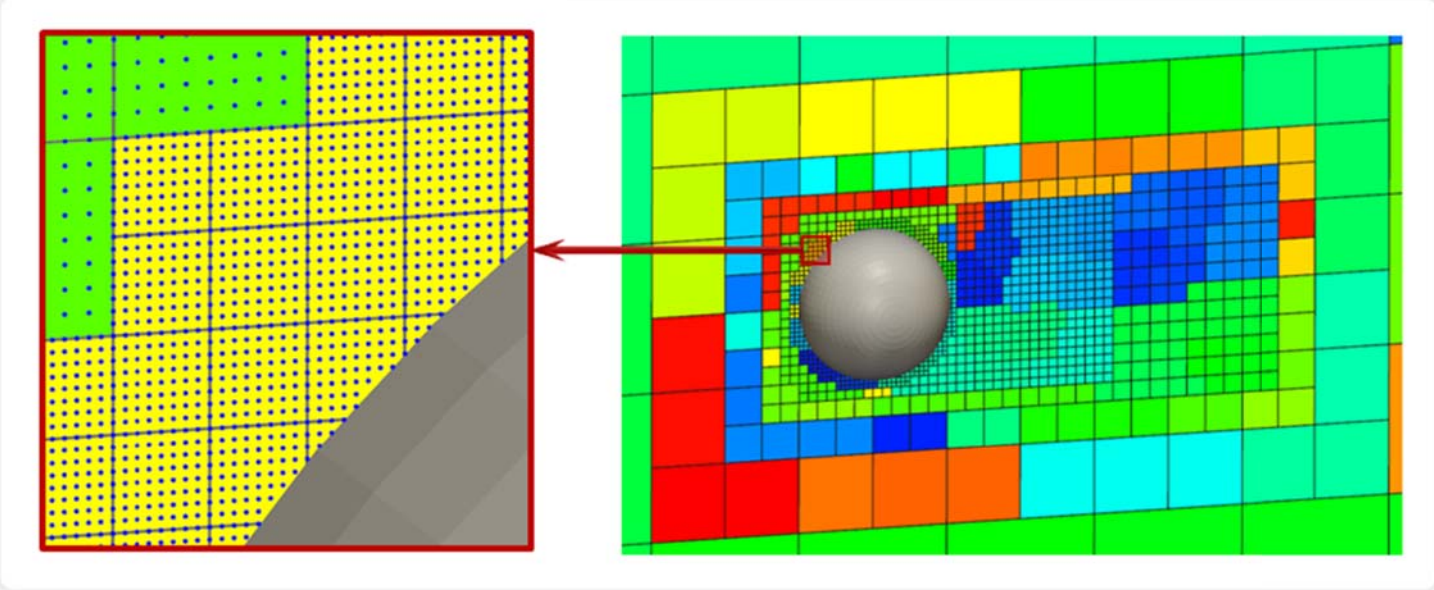


SGI Altix 4700 at LRZ in Munich

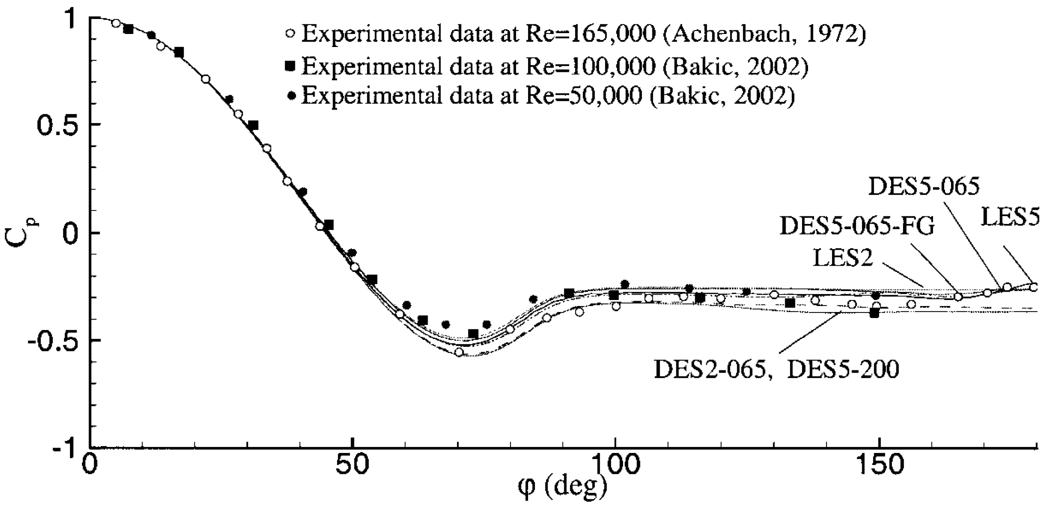
Numerical examples II: Turbulent flows

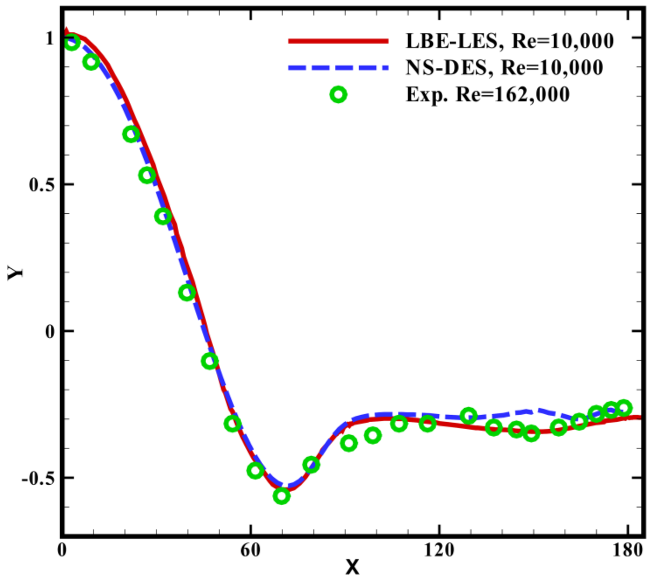
Transitional flow around a sphere:
Re= 10^3 -10^4
Ma=0.02
Cs=0.1
6 grid levels
2x 10^7 grid nodes
70 procs, 80% par. efficiency

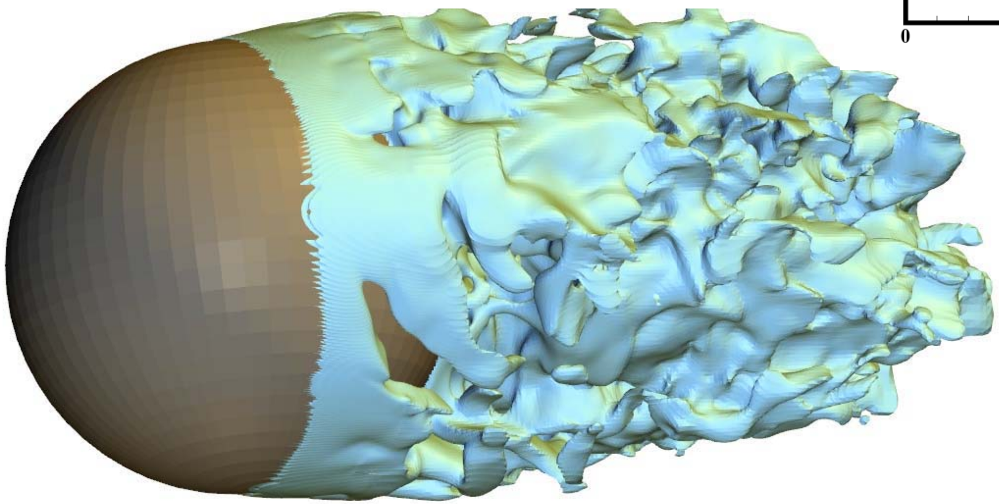




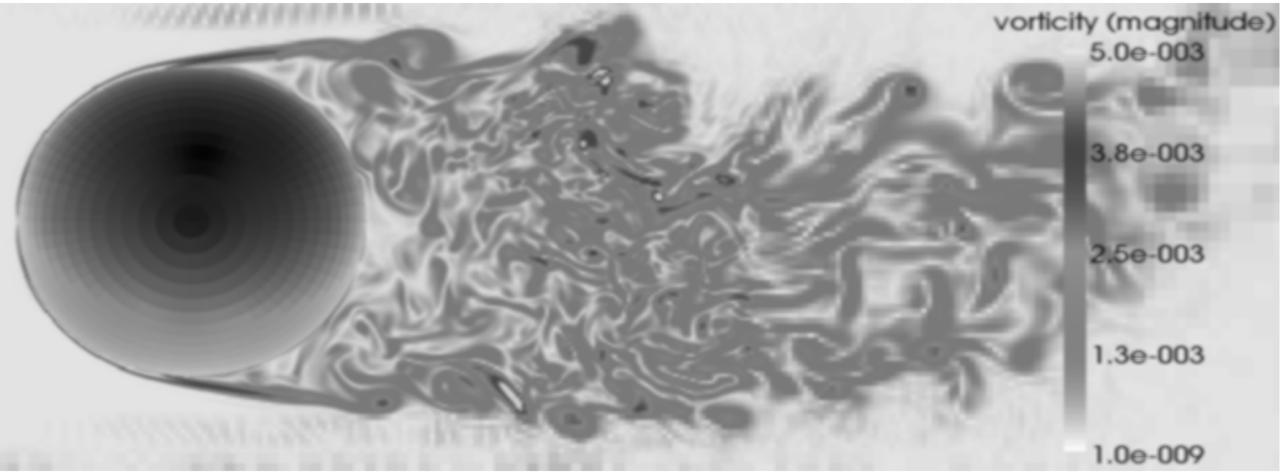
Numerical examples II: Turbulent flows

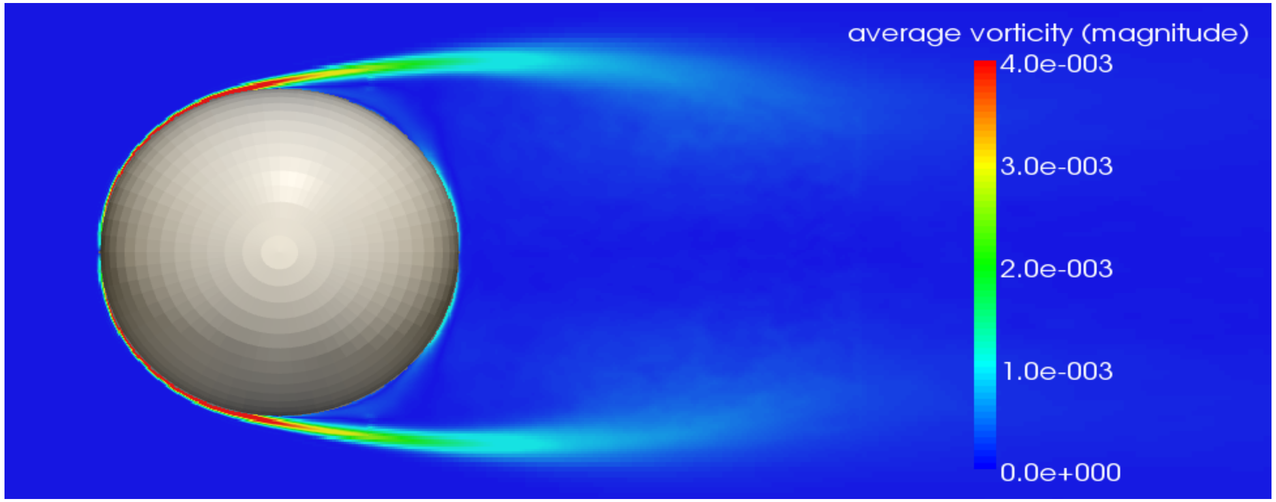






Numerical examples II: Turbulent flows

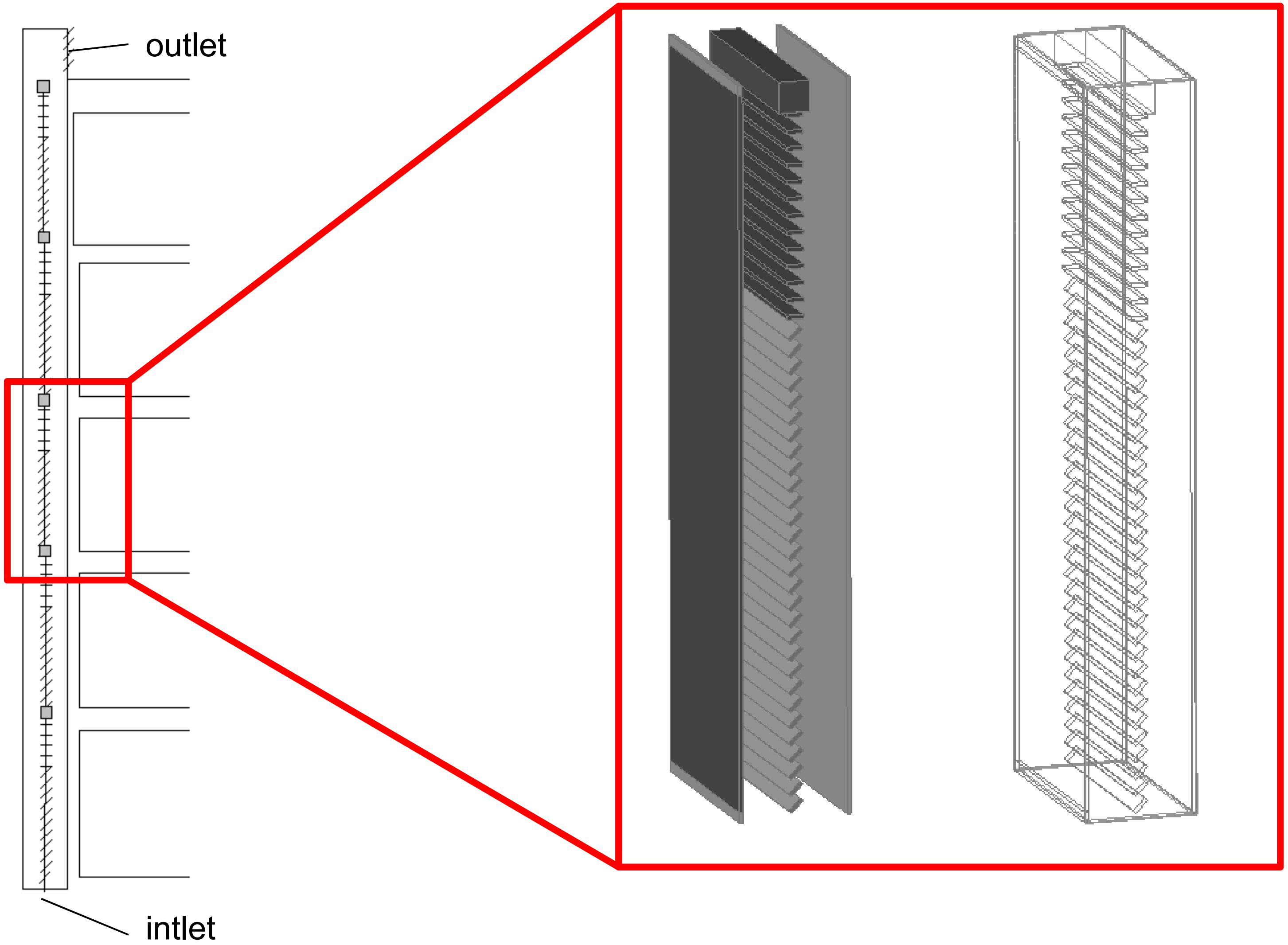




(laminar) boundary layer separation:
Achenbach: 82.5° Re=10^4,
Bakic : 80° – 83° at Re=5*10^4

This simulation: 83

Numerical examples III: Heat flux in double skin facade



Numerical examples III: Heat flux in double skin facade

Solar Radiation:

Diffuse Radiation: 200 [W/m²]

Direct Radiation: 571 [W/m²]

Outside air temperature: 35 °C

Wind:

0,0 m/s

Outside glazing:

Surface temperature: T: 40 [°]

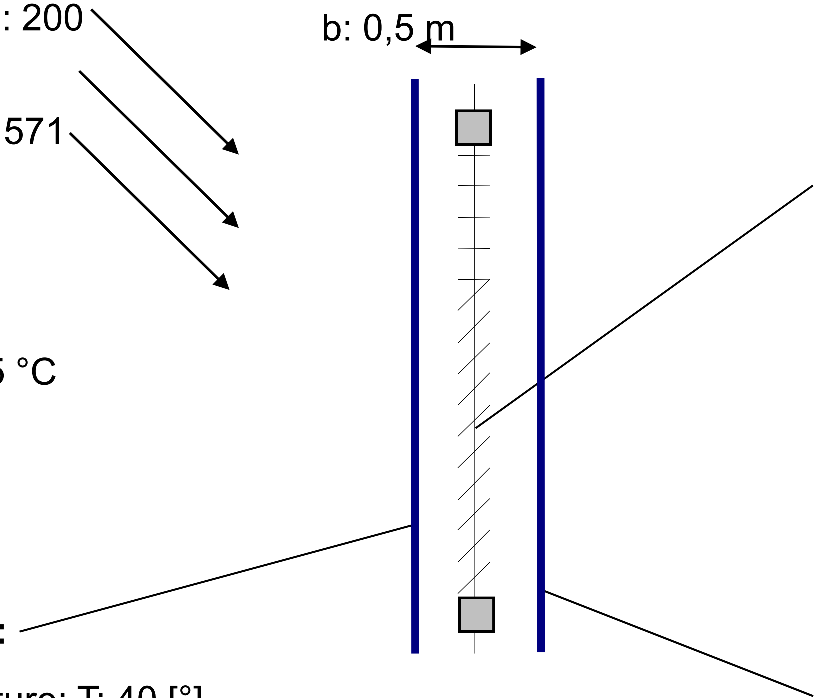
ρ: 2550 [kg/m³]

c: 0,70 [kJ/(kg K)]

g: 0,86 [-]

Double skin facade:

b: 0,5 m



Pressure:

P_0 = 0,0 [hPa]

Simulation
$3x10^8$ DOF -> dx=1cm
time: 5 min
Ra: $4 \cdot 10^{11}$ [-]
Large-Eddy model

Fins:

Surface temperature : T: 55 [°]

ρ: 2710 [kg/m³]

c: 0,90 [kJ/(kg K)]

α: 0,40 [-]

ρ_{RAD}: 0,60 [-]

Inside glazing:

Surface temperature: T: 30 [°]

ρ: 2550 [kg/m³]

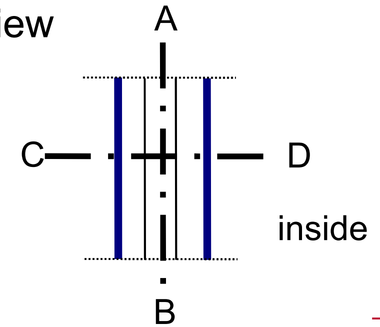
c: 0,7 [kJ/(kg K)]

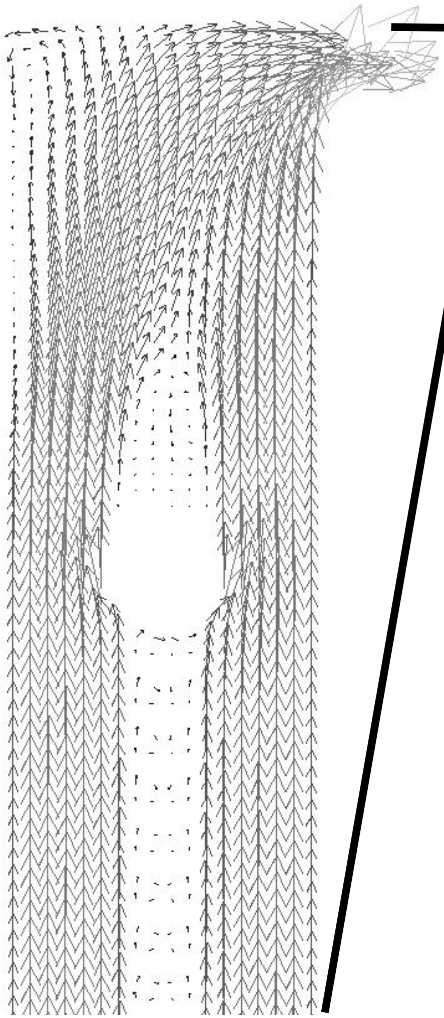
g: 0,59 [-]

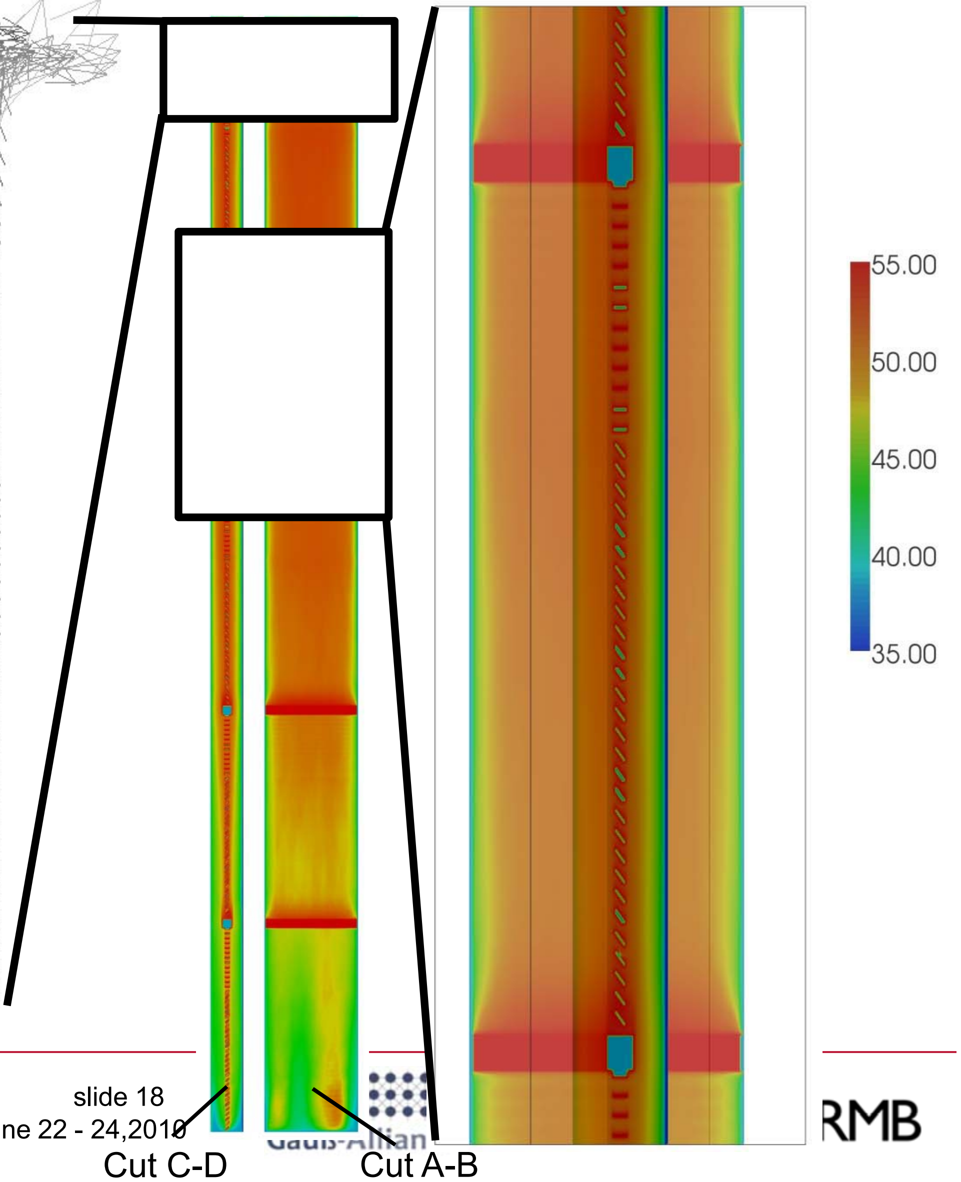
Numerical examples III: Heat flux in double skin facade

Variant d) 0.25 m outlet

Flux	0.74	[m^3/s]
T_{EG}	42.57	[°C]
T_{OG1}	45.19	[°C]
T_{EOG2}	46.63	[°C]
T_{OG3}	47.36	[°C]
T_{OG4}	47.61	[°C]



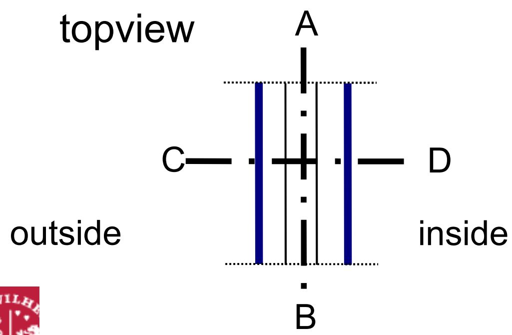


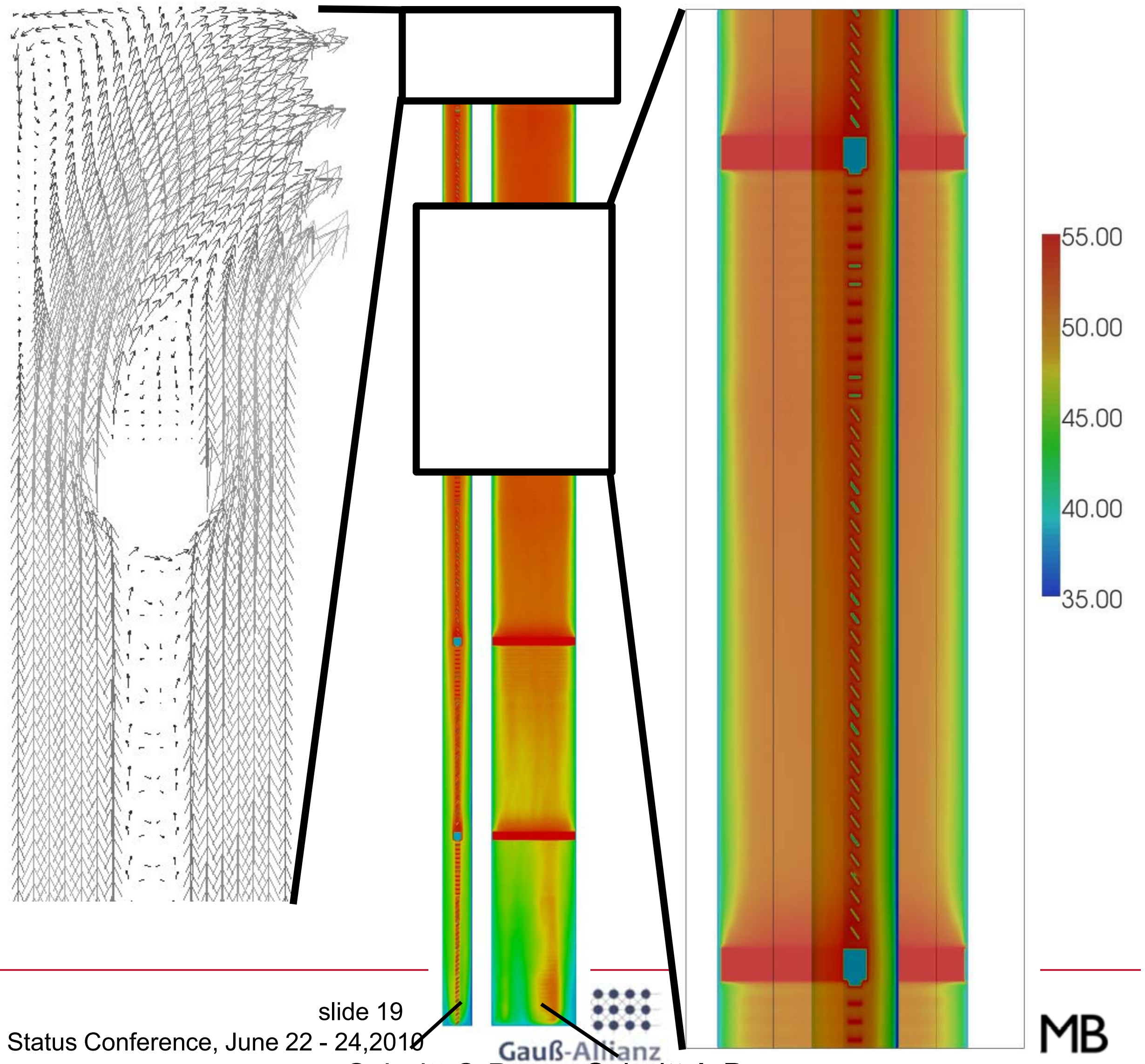


Numerical examples III: Heat flux in double skin facade

Variant d) 0.5 m outlet

flux	1.05	[m^3/s]
T_{EG}	42.18	[°C]
T_{OG1}	44.86	[°C]
T_{EOG2}	46.64	[°C]
T_{OG3}	47.50	[°C]
T_{OG4}	47.76	[°C]

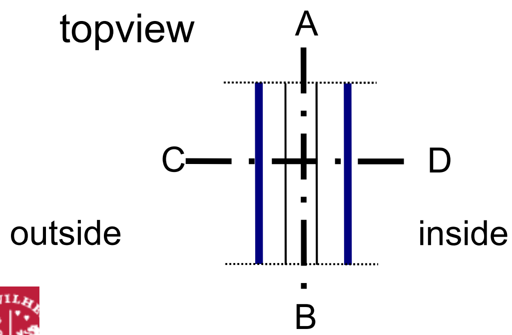


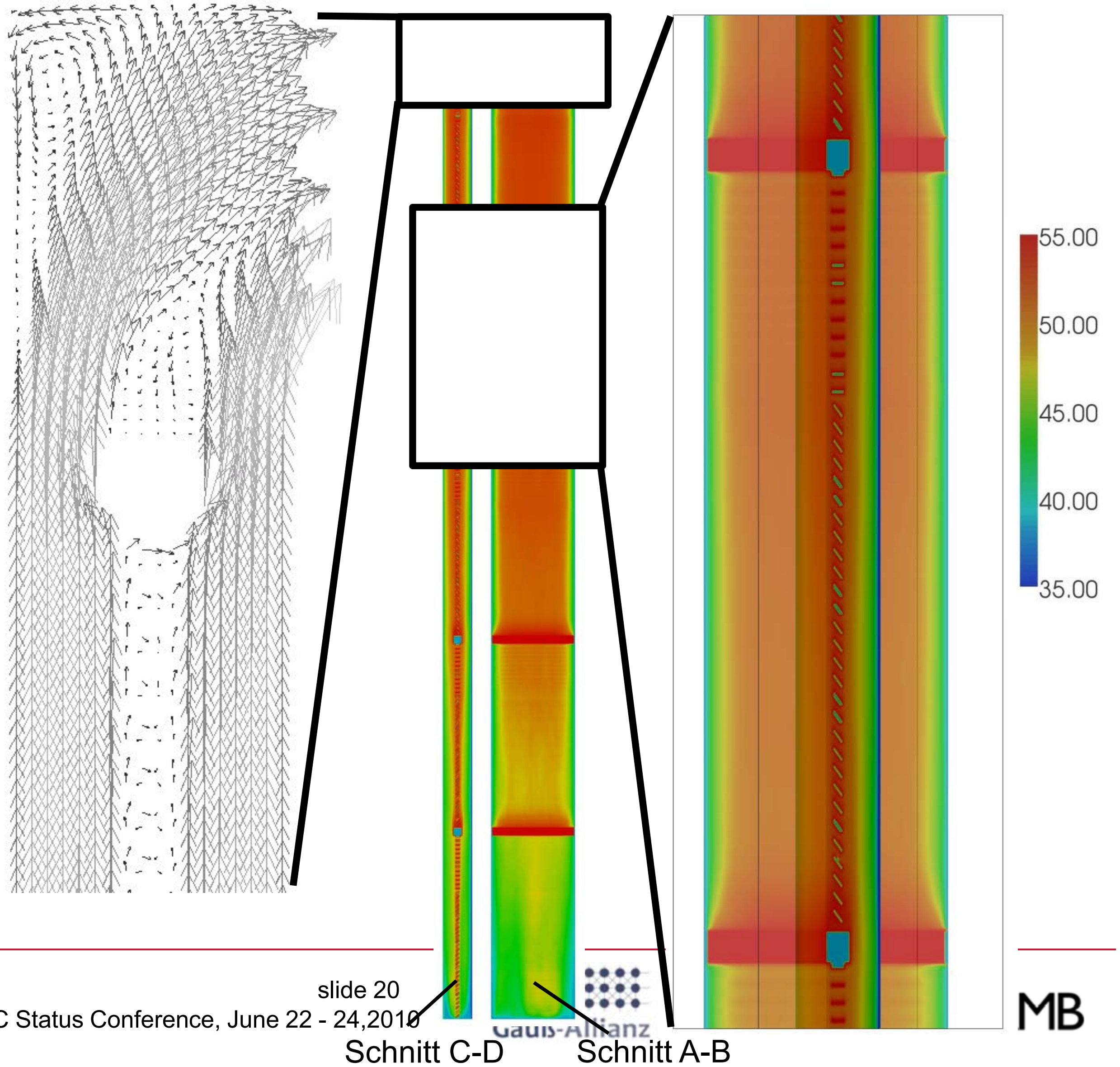


Numerical examples III: Heat flux in double skin facade

Variant d) 0.75 m outlet

flux	1.13	[m³/s]
T_{EG}	41.87	[°C]
T_{OG1}	44.74	[°C]
T_{EOG2}	46.55	[°C]
T_{OG3}	47.43	[°C]
T_{OG4}	47.70	[°C]

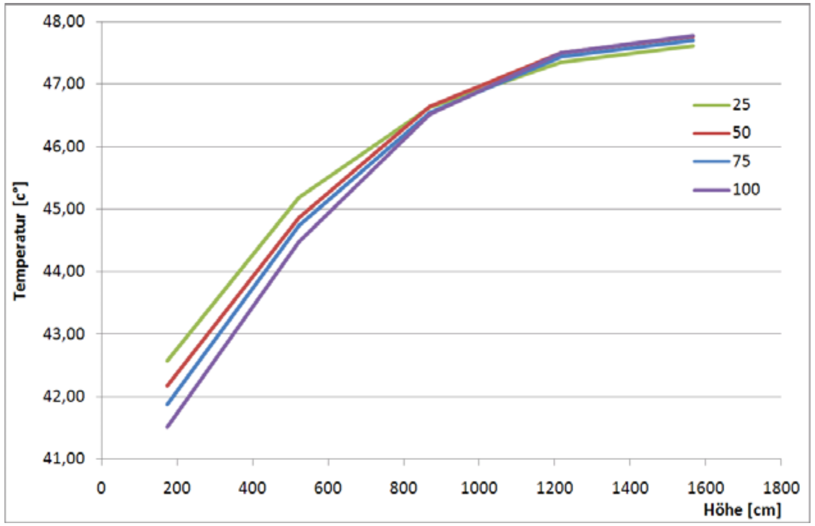


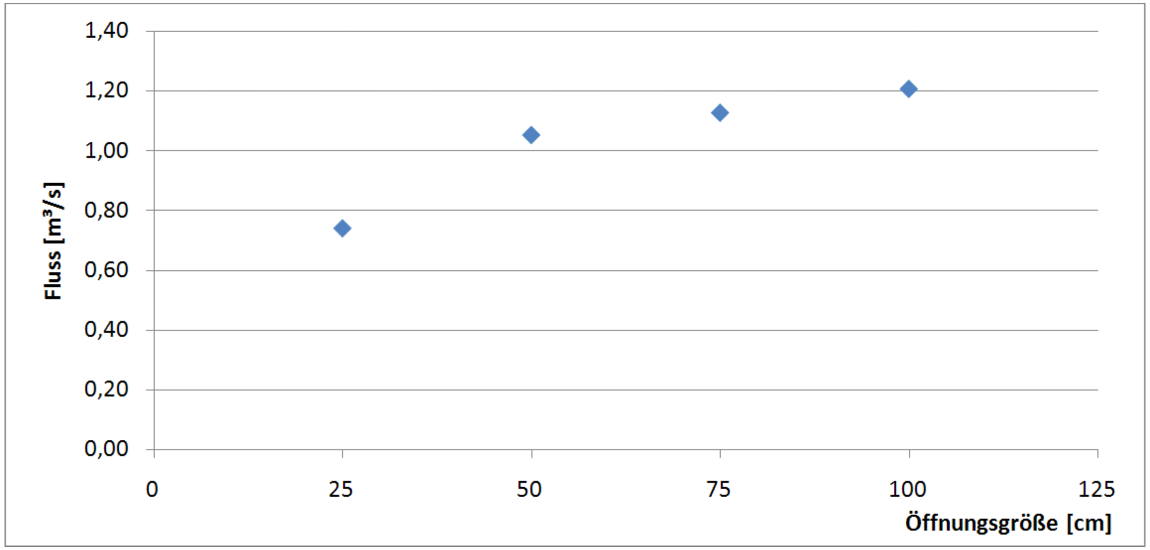


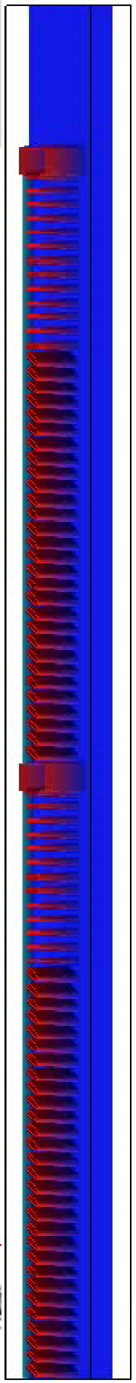
Numerical examples III: Heat flux in double skin facade

Variant d) 1.0 m outlet

flux	1.21	[m³/s]
T_{EG}	41.51	[°C]
T_{OG1}	44.48	[°C]
T_{EOG2}	46.52	[°C]
T_{OG3}	47.51	[°C]
T_{OG4}	47.78	[°C]







VirtualFluids

Parallel efficiency II

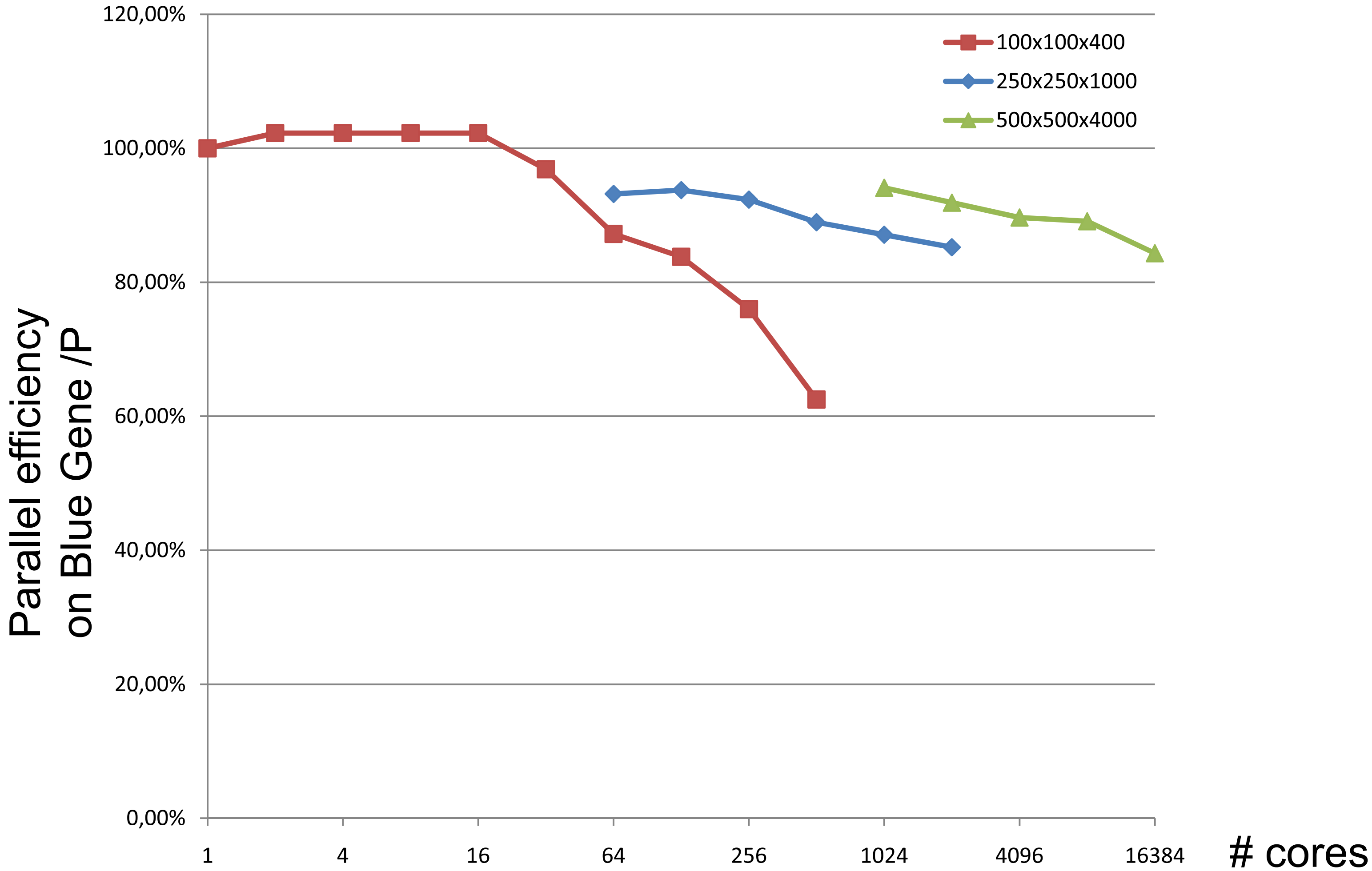
Babel, IBM Blue Gene/P at IDRIS-CNRS, Orsay, France

- 40.960 cores PowerPC 450
- 20 Tbytes of memory
- 139 Tflops total peak performance

Hardware Description:

- 10 racks Blue Gene/P (10240 compute nodes, 40960 cores PowerPC 450,
- 20 Tbytes of memory for a total peak performance of : 139 Tflops)
- Disk space :
- 800 Tbytes shared between the Blue Gene/P and the Power6.

Parallel efficiency II

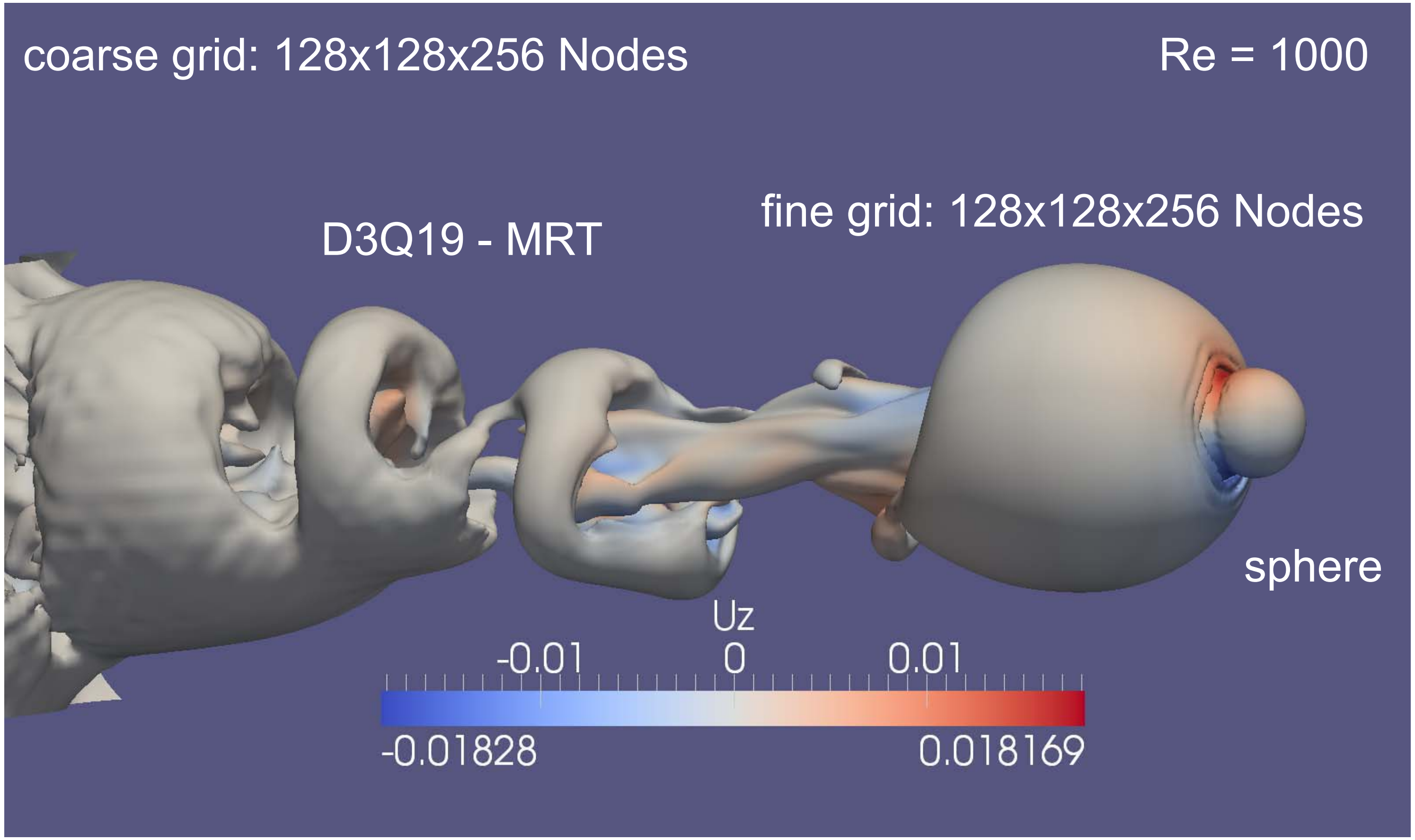


General Purpose Graphics Processing Unit (GPGPU)

- TESLA C1060
- 30 multiprocessors with 8 processors each = 240 Processors
- Cores running at 1,3 GHz
- 4 GB device memory
- Memory bandwidth = 102 GB/sec
- 933 GFlops of theoretical single precision floating point performance
- CUDA –SDK

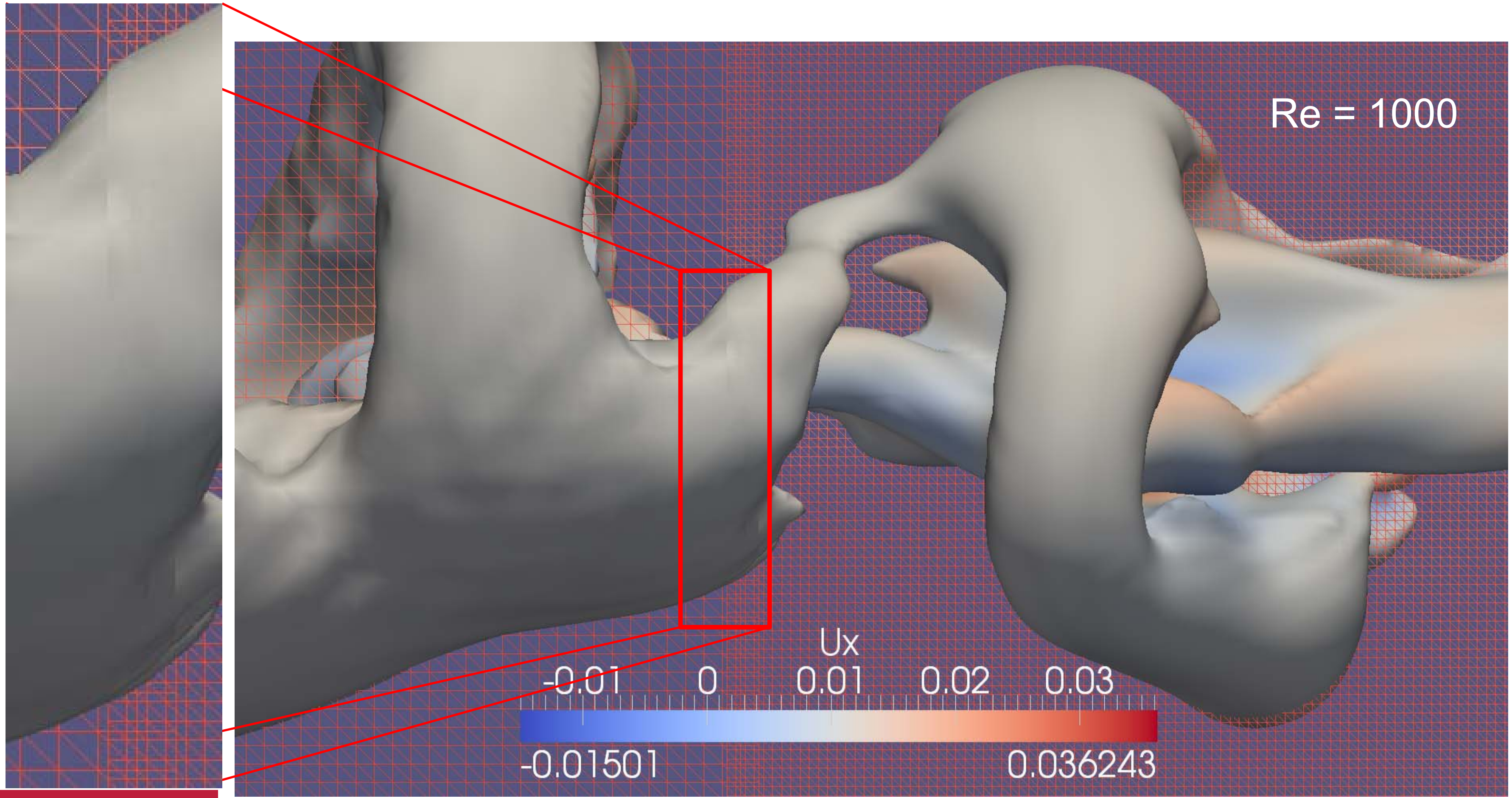
3D grid refinement on GPUs

Smooth transition between coarse and fine grid



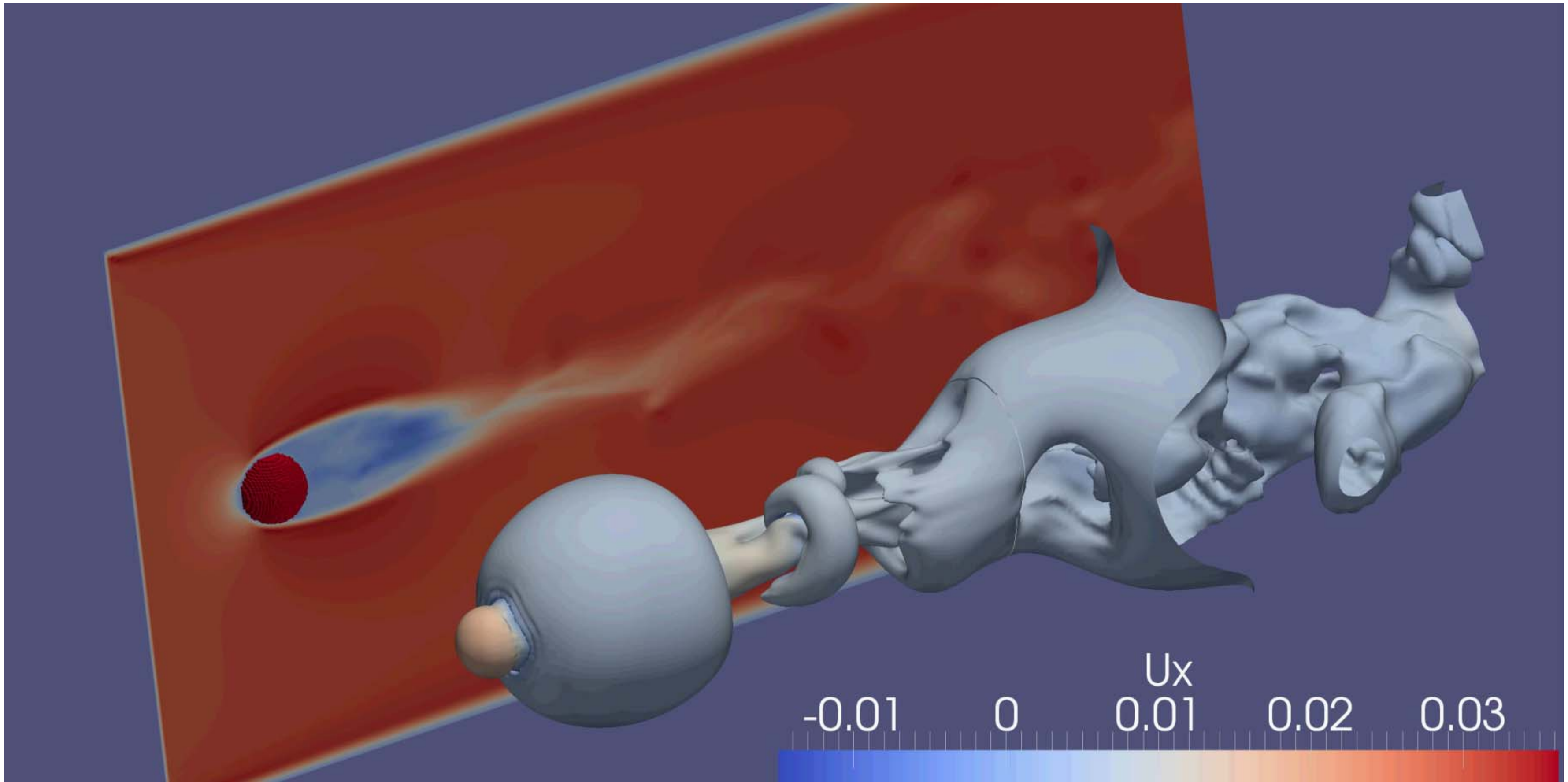
Quality of results

Testcase: channelflow around a sphere (velocity in x direction)



Quality of results

Simulation: Smoothly data transfer at the grid interface $\frac{\Delta x_{coarse}}{\Delta x_{fine}} = 2$



Performance Analysis

	Resolution [nodes]	NUPS [x10^6]	NUPS [%]
Uniform	256x256x144	280.81	100.00
Non-uniform	2x256x192x96	242,57	86.38
Non-uniform*	2x256x192x96	212,25	75.58
Uniform	256x128x144	281.53	100.00
Non-uniform	2x256x96x96	233.59	82.97
Non-uniform*	2x256x96x96	204.39	72.60
Uniform	128x128x144	255.42	100.00
Non-uniform	2x128x96x96	201.84	79.02
Non-uniform*	2x128x96x96	176.61	69.14

* effective number of NUPS - no coarse nodes in fine grid

Department cluster *Ludwig* at TU Braunschweig:

- 48 TByte LUSTRE file system
- 160 compute nodes:
  - » 2x2,6 GHz Intel Quad X5550
  - » 12 GByte DDR3 RAM
  - » 1 Gbyte Ethernet / 2.5 Gbyte InfiniBand network
  - 1280 cores -> app. ***20 TFlops***

- 24 hybrid GPU-nodes
  - » as above +
  - » 4 Nvidia Tesla C 1060 with 0.5 Tflops each
  - » 16 GByte DDR5 RAM
  - ->96 GPUs summing up to 23.040 cores ->app. ***40 Tflops***

- **Price 900 k€**
- **power consumption 78 kW**

GPU – Nodes (Ludwig)

1 GPU - Node

4 GPUs = 960 Cores

(2 CPUs,12 GB RAM)

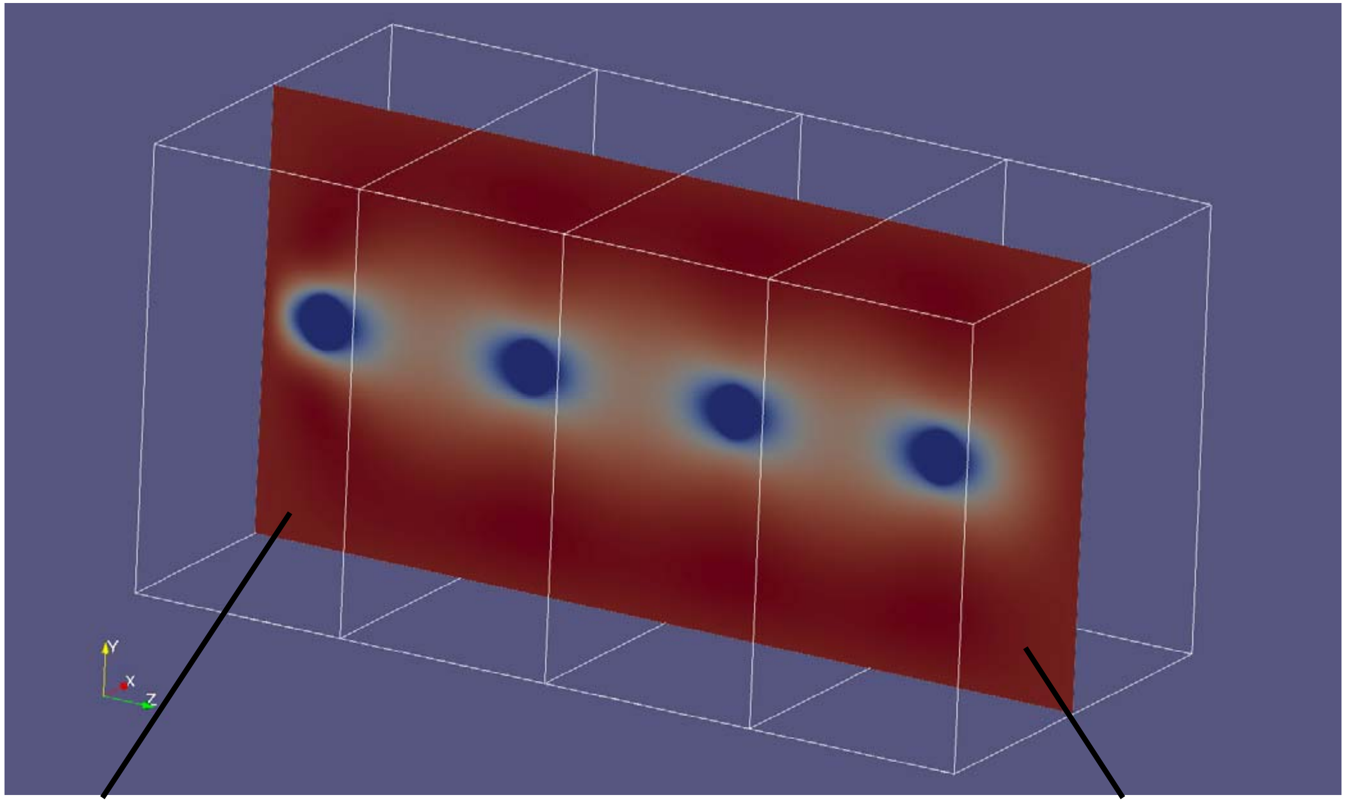
24 GPU - Nodes

96 GPUs = 23.040 Cores, 384 GB RAM)

(48 CPUs, 288 GB RAM)

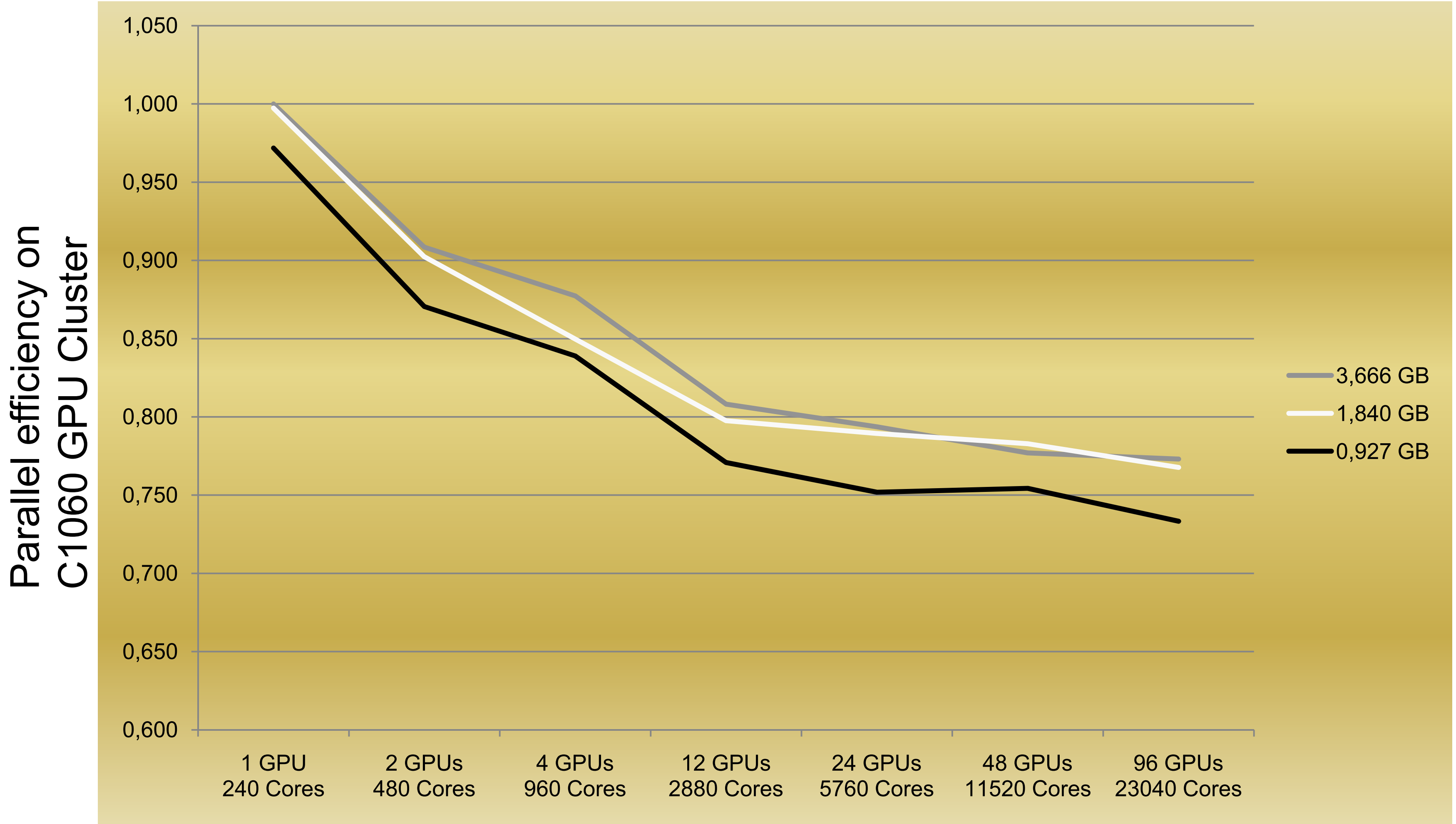
Parallel efficiency III (GPU-Cluster)

Resolution 256x512x256 grid nodes = 3,66 GB/GPU



No. 1 … **No. 96**

Results for 3 Resolutions



Preliminary comparison Blue-Gene/P – GPU-Cluster

	#cores	precision	# grid nodes	absolute performance
Blue-Gene/P	16.384	double	10^9	~20 GNUPS
Ludwig (96 GPUs)	23.040	single	3.2×10^9	~45 GNUPS

preliminary result:

outstanding FLOPS/€ and FLOPS/W ratio for GPU-cluster

Outlook

2do:

•Multi-level parallelization on mixed CPU/GPU-systems

•Adaptivity requires dynamic loadbalancing on massively parallel systems:

- •purely local load redistribution based on anisotropic load diffusion model (NO master-slave)

•fault tolerant parallel computations

- •requires MPI 2.x + additional functionality
- •frequent dumps of subdomains‘ hydrodynamic moments using space-trees + interpolations

Acknowledgments

The following agencies have made this research possible:

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  Konsistente Multiskalenströmungsmechanik mit der kaskadierten Lattice Boltzmann Methode

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