

LBM for coupled transport problems

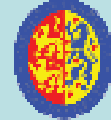
Manfred Krafczyk, Benjamin Ahrenholz, Sebastian
Bindick, Sören Freudiger, Martin Geier, Sebastian
Geller, Christian Janßen, Konstantin Kucher, Jannis
Linxweiler, Martin Schönherr, Maik Stiebler, Sonja
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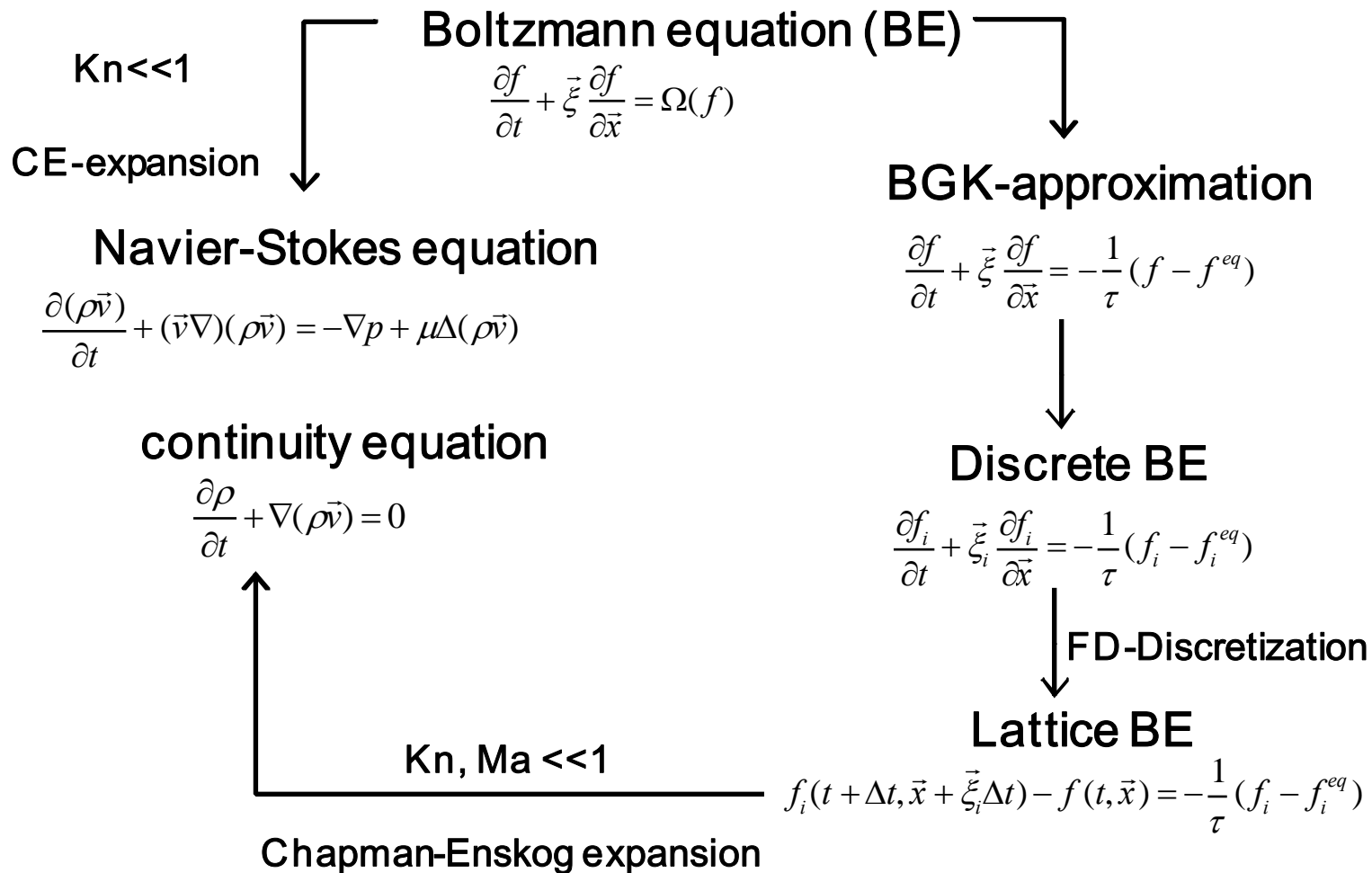
www.irmb.tu-bs.de

Outline

- The modeling map
 - BGK vs. MRT et al.
 - Virtual Fluids
 - coupled problems: the scale map concept
 - FSI
 - GPU-acceleration
 - turbulent LES flows on non-uniform grids
 - Turbulent thermal flow driven by radiation
 - flow acoustics
 - Free surface flows
 - Turbulent multiphase flow
-
- outlook



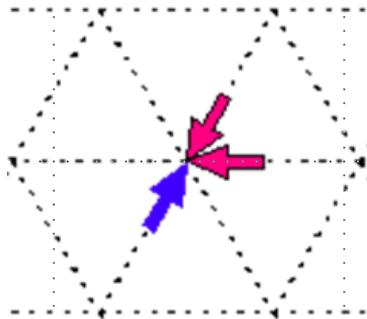
Boltzmann, Navier-Stokes + continuity eq.



Lattice Boltzmann Equation (LBE)

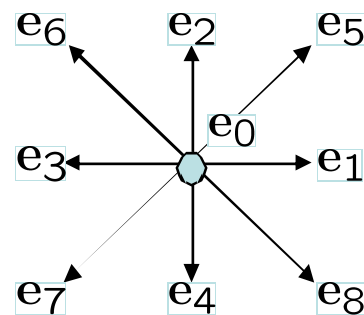
$$f_i(t + \Delta t, \mathbf{x} + \mathbf{e}_i \Delta t) = f_i(t, \mathbf{x}) + \Omega_i, \quad i = 0, \dots, b-1$$

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



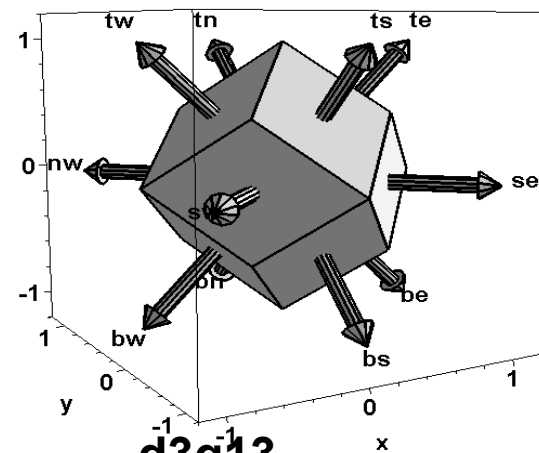
d2q6-Model

Wolfram 86, Hasslacher 86



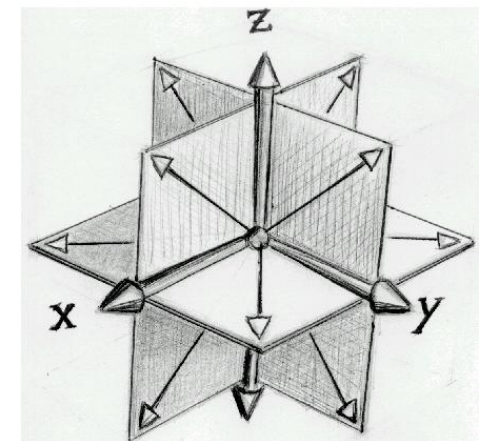
d2q9-Model

Qian 92



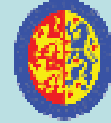
**d3q13-
Model**

d'Humieres 01



**d3q19-
Model**

Qian 92



Lattice Boltzmann Equation (LBE)

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

**Collision
operator:**

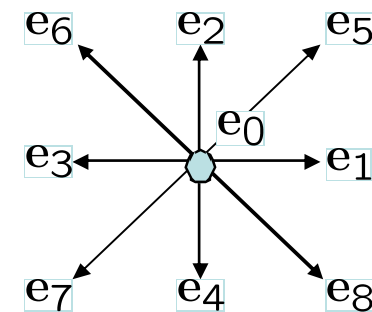
$$\Omega = M^{-1} k$$

transformation into moment space:

$$m = Mf := (\rho, \rho u_x, \rho u_y, e, p_{xx}, p_{xy}, h_x, h_y, \epsilon)$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & c & 0 & -c & 0 & c & -c & -c & c \\ 0 & 0 & c & 0 & -c & c & c & -c & -c \\ -2c^2 & c^2 & c^2 & c^2 & c^2 & 4c^2 & 4c^2 & 4c^2 & 4c^2 \\ 0 & c^2 & -c^2 & c^2 & -c^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & c^2 & -c^2 & c^2 & -c^2 \\ 0 & -c^3 & 0 & c^3 & 0 & 2c^3 & -2c^3 & -2c^3 & 2c^3 \\ 0 & 0 & -c^3 & 0 & c^3 & 2c^3 & 2c^3 & -2c^3 & -2c^3 \\ c^4 & -2c^4 & -2c^4 & -2c^4 & -2c^4 & 4c^4 & 4c^4 & 4c^4 & 4c^4 \end{bmatrix}$$

d2q9-Model



Collision operator

Relaxation rates: $s_\nu, s_e, s_h, s_\epsilon$

MRT: *Humieres 92, Lallemand 00*

$$\begin{aligned} k_0 &= k_1 = k_2 = 0 \\ k_3 &= k_e = s_e (e - 3\rho(u_x^2 + u_y^2)) \\ k_4 &= k_{xx} = s_\nu (p_{xx} - \rho(u_x^2 - u_y^2)) \\ k_5 &= k_{xy} = s_\nu (p_{xy} - \rho u_x u_y) \\ k_6 &= k_{hx} = s_h h_x \\ k_7 &= k_{hy} = s_h h_y \\ k_8 &= k_\epsilon = s_\epsilon \epsilon, \end{aligned}$$

TRT: *Ginzburg 03*

even moments: $s_\nu = s_e = s_\epsilon$
odd moments: s_h

LBGK: *Quian 92*

$$s_\nu = s_e = s_h = s_\epsilon$$

CLBM:

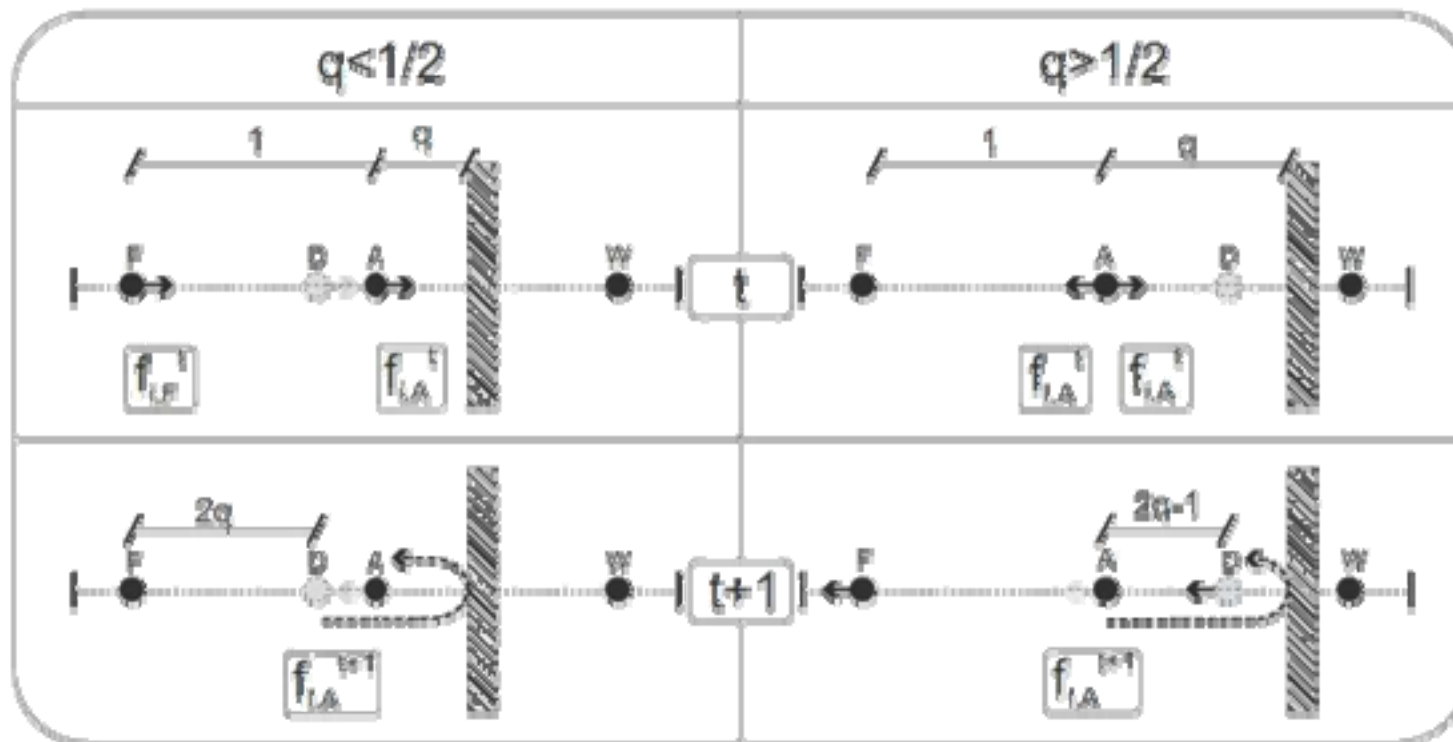
M. Geier, A. Greiner, and J. G. Korvink,
Physical Review E, vol. 73, no. 6, p. 066705,
2006.

$$\begin{aligned} k_0 &= k_1 = k_2 = 0 \\ k_e &= s_e (e - 3\rho(u_x^2 + u_y^2)) \\ k_{xx} &= s_\nu (p_{xx} - \rho u_x u_y) \\ k_{xy} &= s_\nu (p_{xx} - \rho(u_x^2 - u_y^2)) \\ k_{hx} &= s_h \left(h_x - 6u_y k_{xy} \left(\frac{1}{s_\nu} - \frac{1}{s_h} \right) \right) \\ &\quad + s_h \left(-u_x \left(\frac{1}{2} \left(e - \frac{k_e}{s_h} \right) - \frac{3}{2} \left(p_{xx} - \frac{k_{xx}}{s_h} \right) \right) \right) \\ k_{hy} &= s_h \left(h_y - 6.0u_x k_{xy} \left(\frac{1}{s_\nu} - \frac{1}{s_h} \right) \right) \\ &\quad + s_h \left(-u_y \left(\frac{1}{2} \left(e - \frac{k_e}{s_h} \right) + \frac{3}{2} \left(p_{xx} - \frac{k_{xx}}{s_h} \right) \right) \right) \\ k_\epsilon &= s_\epsilon \left(\epsilon - 27u_x^2 u_y^2 + k_e \left(\frac{1}{s_e} - \frac{1}{s_\epsilon} \right) + \frac{3}{2} (u_x^2 + u_y^2) \left(e - \frac{k_e}{s_\epsilon} \right) \right) \\ &\quad + s_\epsilon \left(-\frac{9}{2} (u_x^2 - u_y^2) \left(p_{xx} - \frac{k_{xx}}{s_\epsilon} \right) + 36u_x u_y \left(p_{xy} - \frac{k_{xy}}{s_\epsilon} \right) \right) \\ &\quad + s_\epsilon \left(-6u_x \left(h_x - \frac{k_{hx}}{s_\epsilon} \right) - 6u_y \left(h_y - \frac{k_{hy}}{s_\epsilon} \right) \right) \end{aligned}$$

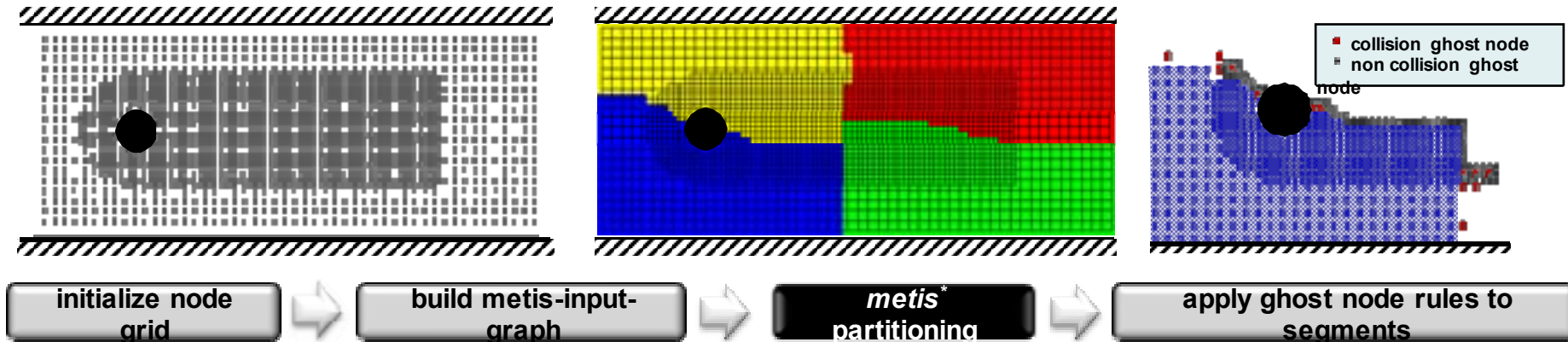
Interpolation based scheme for no-slip BC [Bouzidi, et al., 2001]

$$f_{iA}^{t+1} = (1-2q) \cdot f_{iF}^t + 2q \cdot f_{iA}^t - 6 \frac{e_{iW}^{t+1}}{c^2}, \quad 0.0 < q < 0.5$$

$$f_{iA}^{t+1} = \frac{2q-1}{2q} \cdot f_{iA}^t + \frac{1}{2q} \cdot f_{iF}^t - 3 \frac{e_{iW}^{t+1}}{qc^2}, \quad 0.5 \leq q \leq 1.0$$



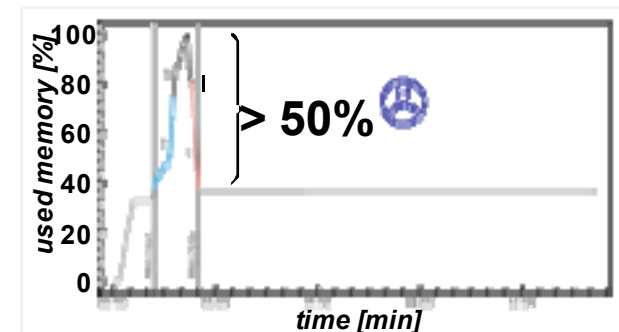
Virtual Fluids



* [<http://glaros.dtc.umn.edu/gkhome/views/metis/>]]

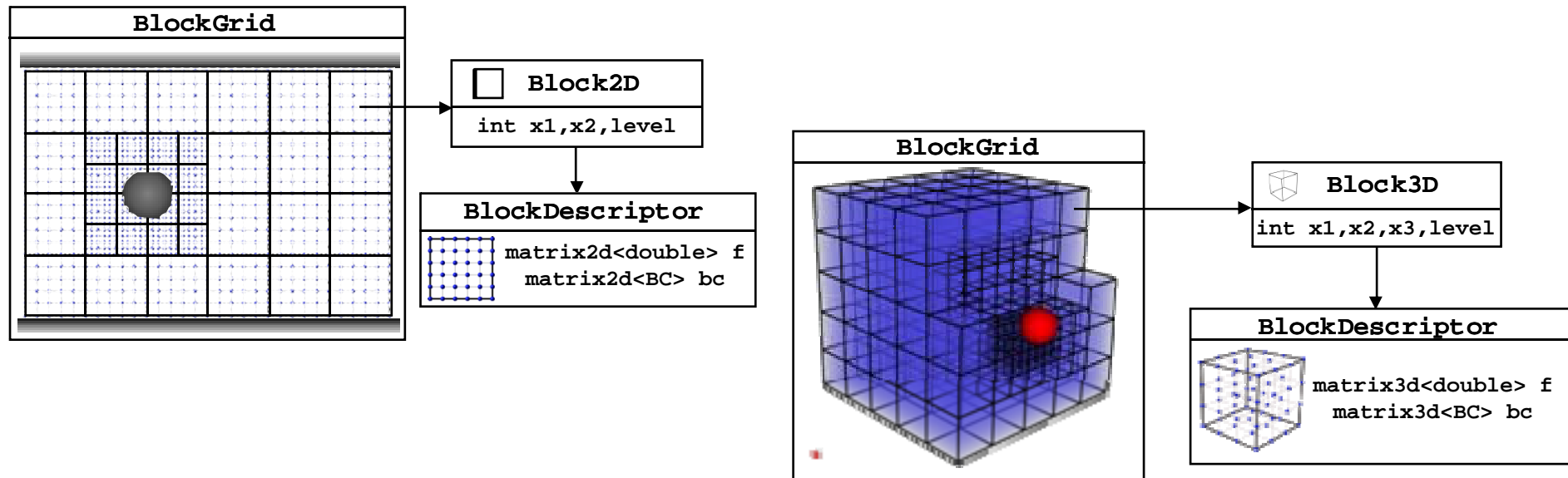
disadvantages of node grids in respect of distributed (, adaptive) computations:

- segmentation for a huge number of nodes
→ preprocess costs a lot of time and memory
- arbitrary shapes of refined areas
→ many possible ghost node configurations



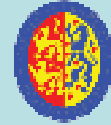
▶ **switch to block grid structure**

VirtualFluids reloaded: block grid



basic strategies of block grid

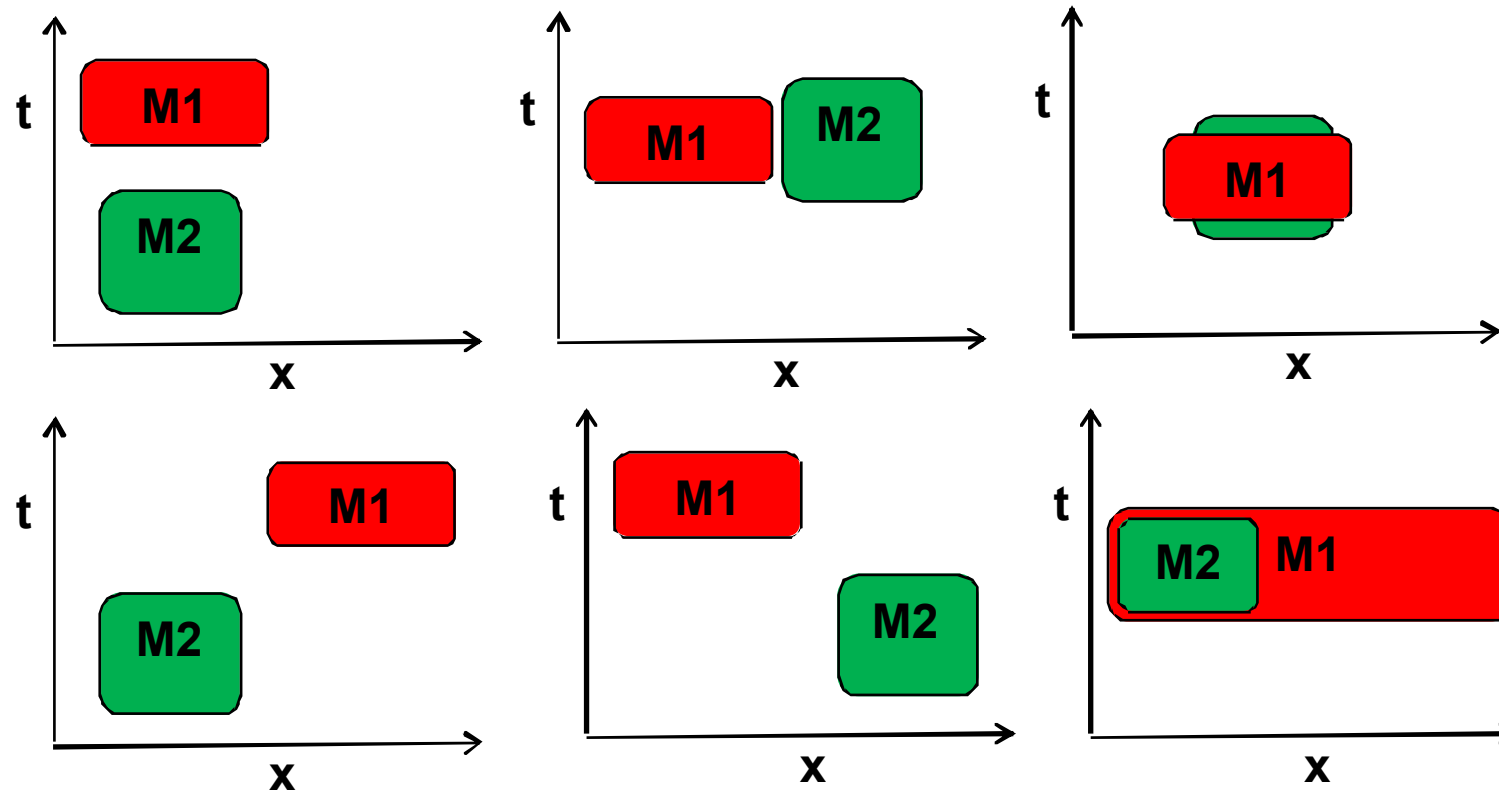
- zoning of a flow field by blocks of various sizes to adapt the mesh size to local flow characteristic length
- uniform Cartesian mesh in each block for efficient computations
- same grid size in all blocks to simplify connectivity



Coupled problems: the scale separation map

Alfons Hoekstra, Eric Lorenz, Jean-Luc Falcone and Bastien Chopard

Towards a Complex Automata Framework for Multi-scale Modeling: Formalism and the Scale Separation Map, [Lecture Notes in Computer Science](#) Springer Berlin, pp. 922-930, 2007



How far can you get with simple LES-LB turbulence modeling ?

$$V = V_0 + V_T$$

M. Krafczyk, J. Tölke, and L.-S. Luo,
Int. J. of M. Phys. B 17(1/2):33-39 (2003)

Smagorinsky:

$$\nu_t = (C_S \Delta_x)^2 \bar{S}, \quad \bar{S} = \sqrt{\sum_{i,j} S_{ij} \cdot S_{ij}},$$

$$C_s \in \{0.05, 0.2\}$$

$$P_{ij} = \sum_{\alpha} e_{\alpha i} e_{\alpha j} f_{\alpha} = c_s^2 \rho \delta_{ij} + \rho u_i u_j - \frac{1}{S_{xx}} 2c_s^2 \rho S_{ij}$$

strain rate tensor is local quantity !

$$Q_{mn} \equiv \frac{1}{3} \delta \rho \delta_{mn} + j_m j_n - P_{mn}, \quad m, n \in \{x, y, z\},$$

$$P_{xx} = \frac{1}{3} [(e + 2\delta\rho) + 3p_{xx}],$$

$$P_{yy} = \frac{1}{3} \left[(e + 2\delta\rho) + \frac{1}{2} (3p_{ww} - 3p_{xx}) \right] = P_{xx} + \frac{1}{2} (p_{ww} - 3p_{xx})$$

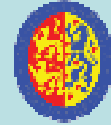
$$P_{zz} = P_{yy} - p_{ww},$$

$$P_{xy} = p_{xy}, \quad P_{yz} = p_{yz}, \quad P_{zx} = p_{zx},$$

$$\nu_t = 3(C_S \Delta_x)^2 \bar{S} = \frac{3}{2} s_{xx} (C_S \Delta_x)^2 \bar{Q},$$

$$\tau_t = 3\nu_t = \frac{1}{2} \left(\sqrt{\tau_0^2 + 18C_s^2 \Delta_x^2 \bar{Q}} - \tau_0 \right), \quad \bar{Q} = \sqrt{\sum_{i,j} Q_{ij} \cdot Q_{ij}}$$

$$\tau_0 = 3 \frac{UL}{\text{Re}} + \frac{1}{2}, \quad s_{xx} = \frac{1}{\tau_0 + \tau_t},$$



Transitional flow around a sphere:

$Re=10^3-10^4$

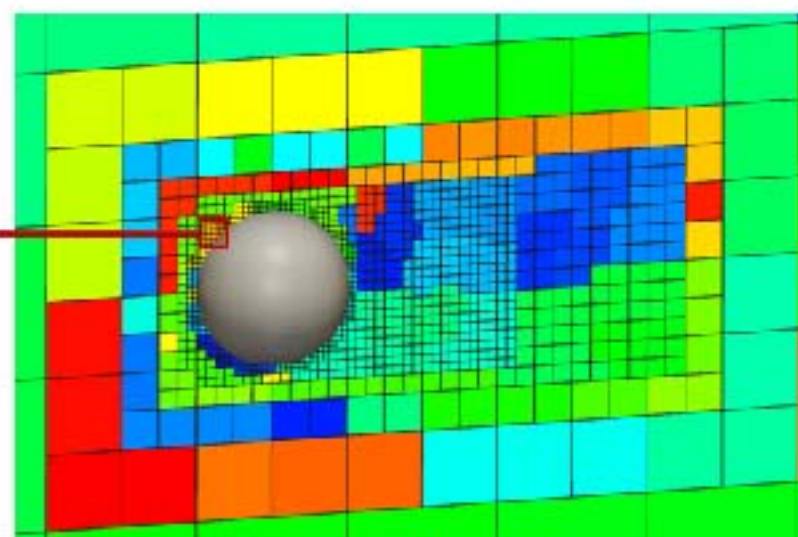
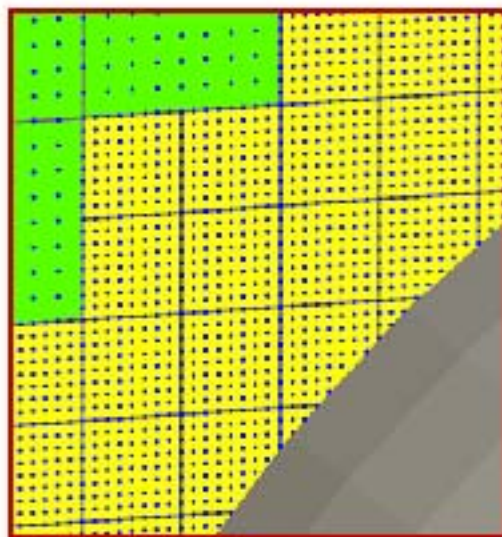
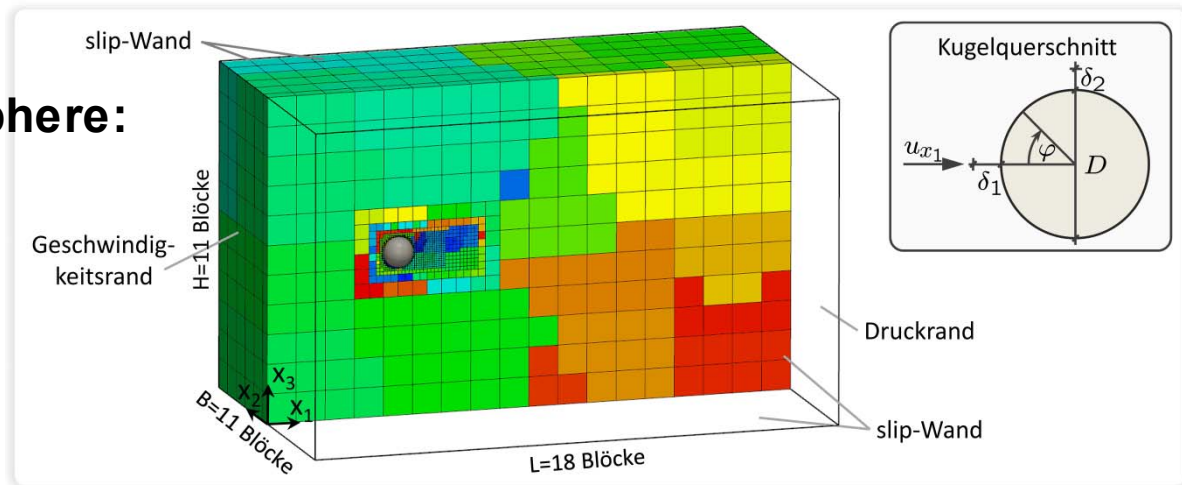
$Ma=0.02$

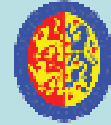
$Cs=0.18$

6 grid levels

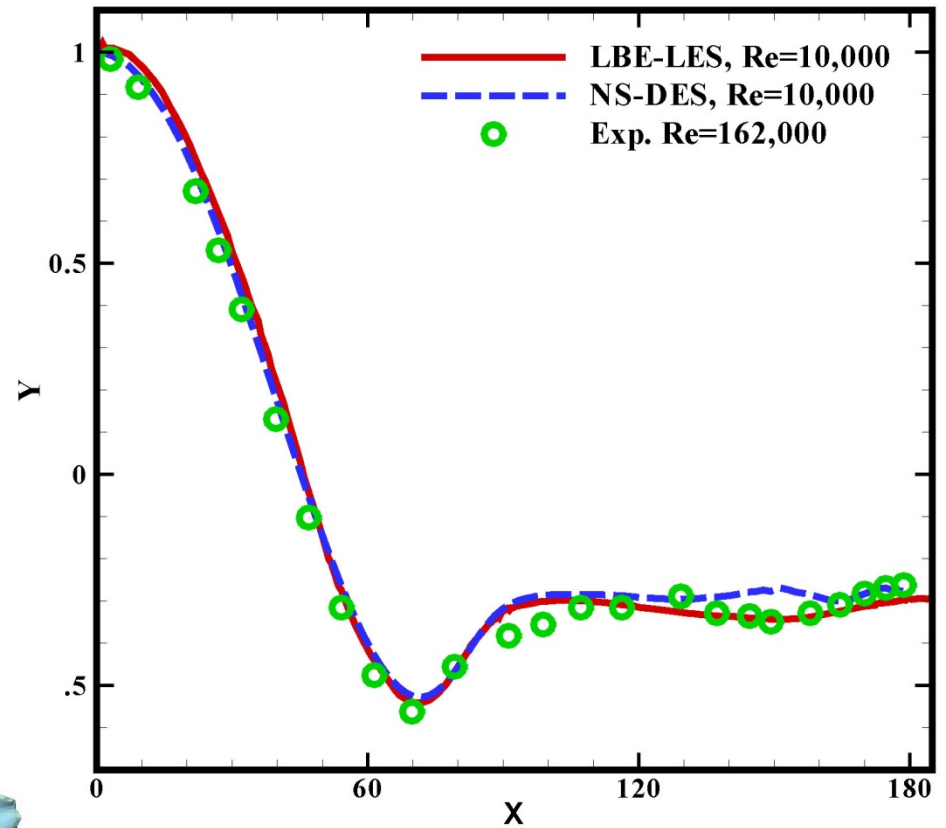
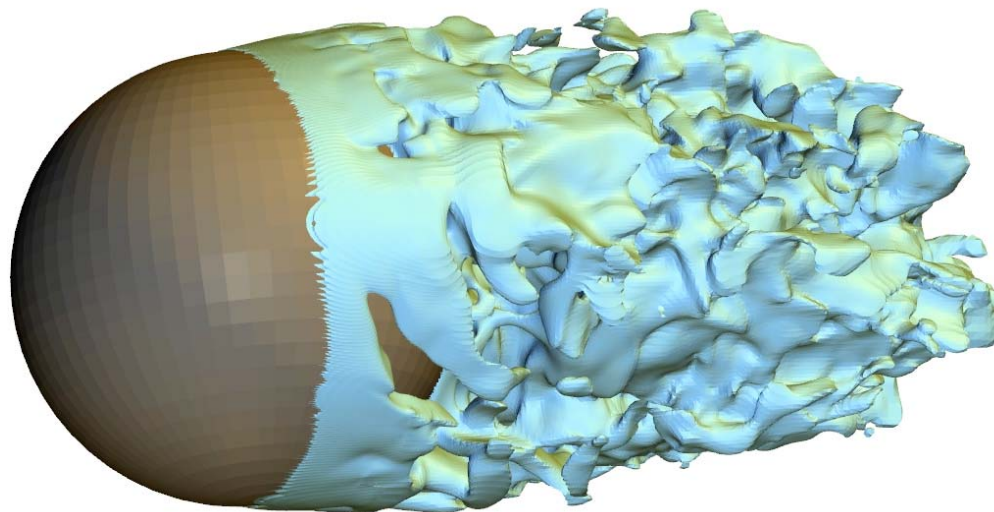
2×10^7 grid nodes

70 procs, 80% par. efficiency

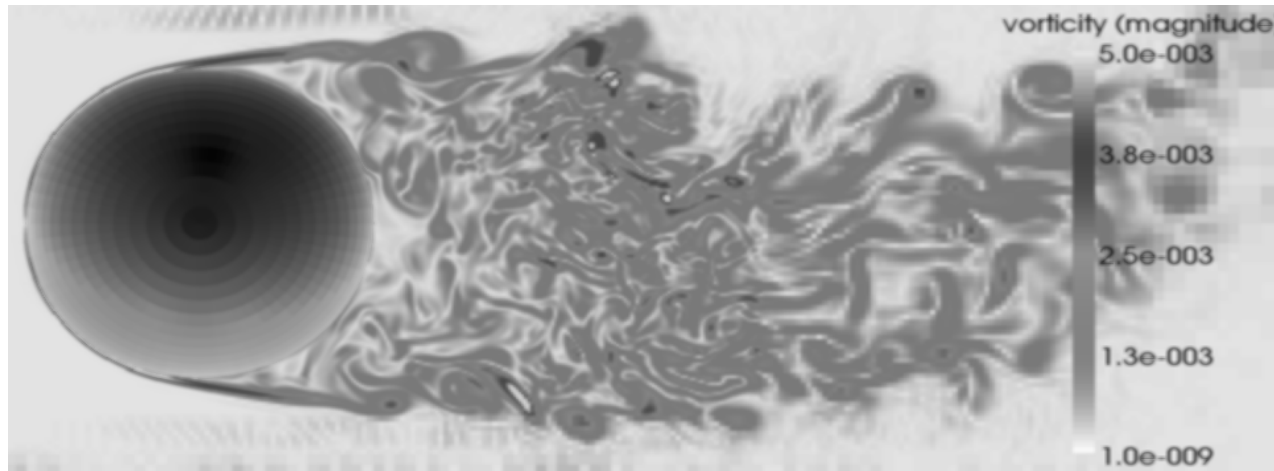




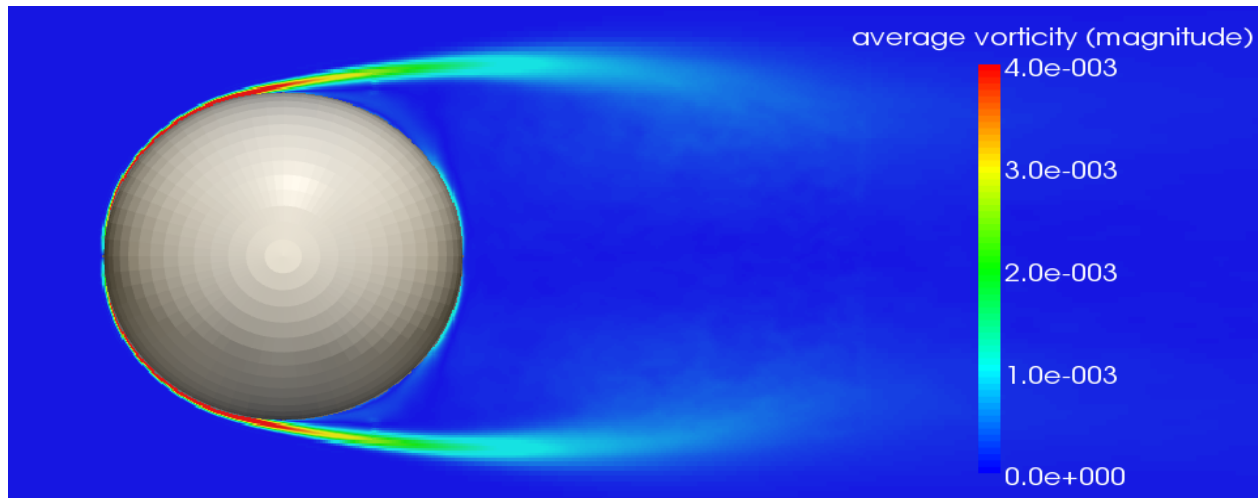
Results I:



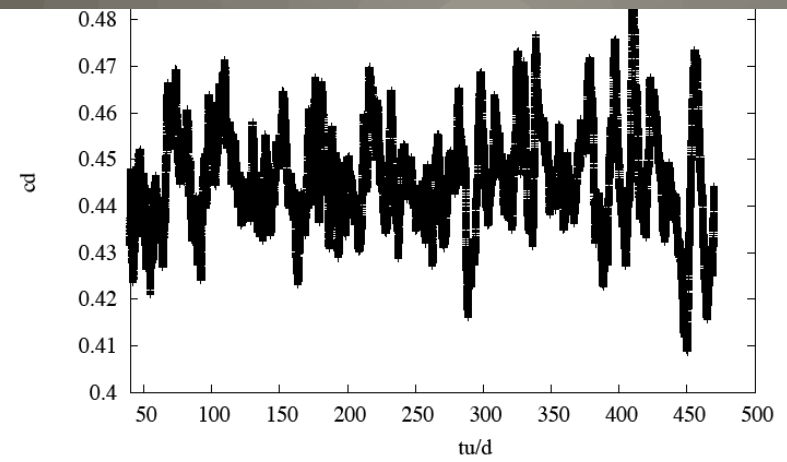
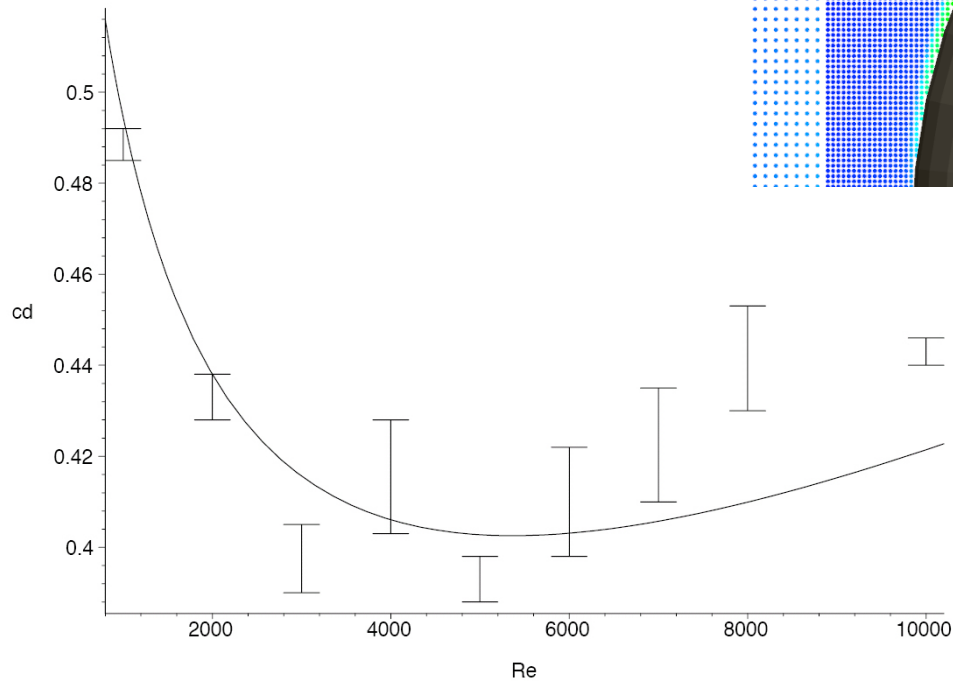
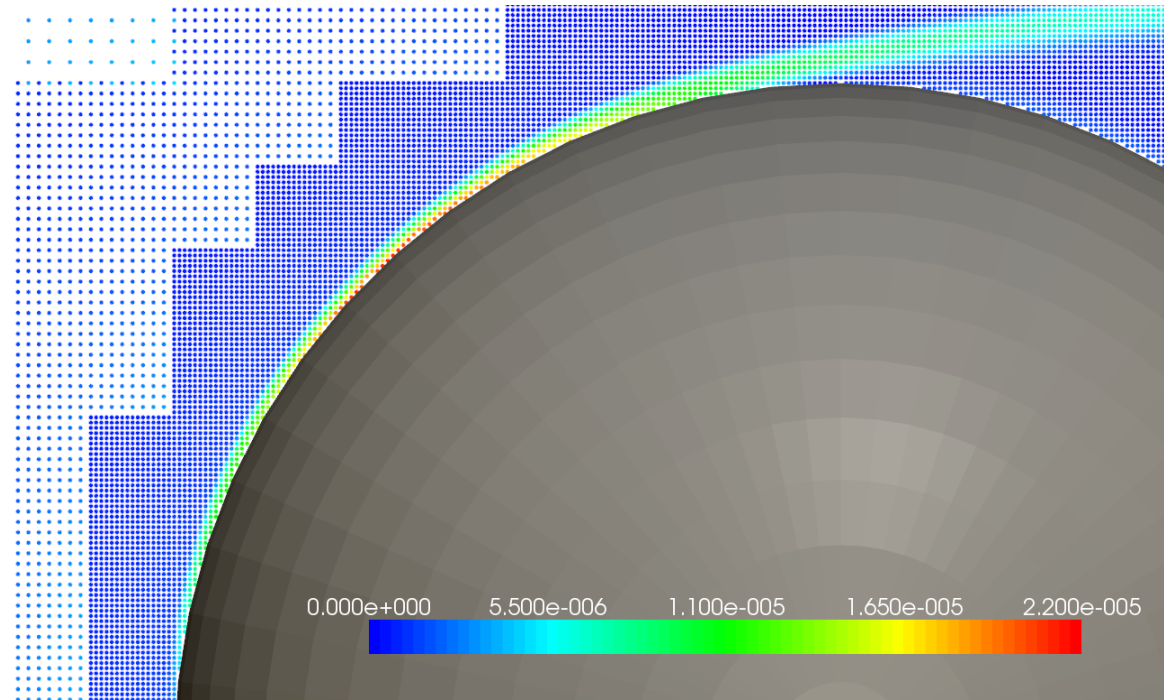
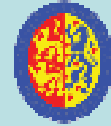
Results II:



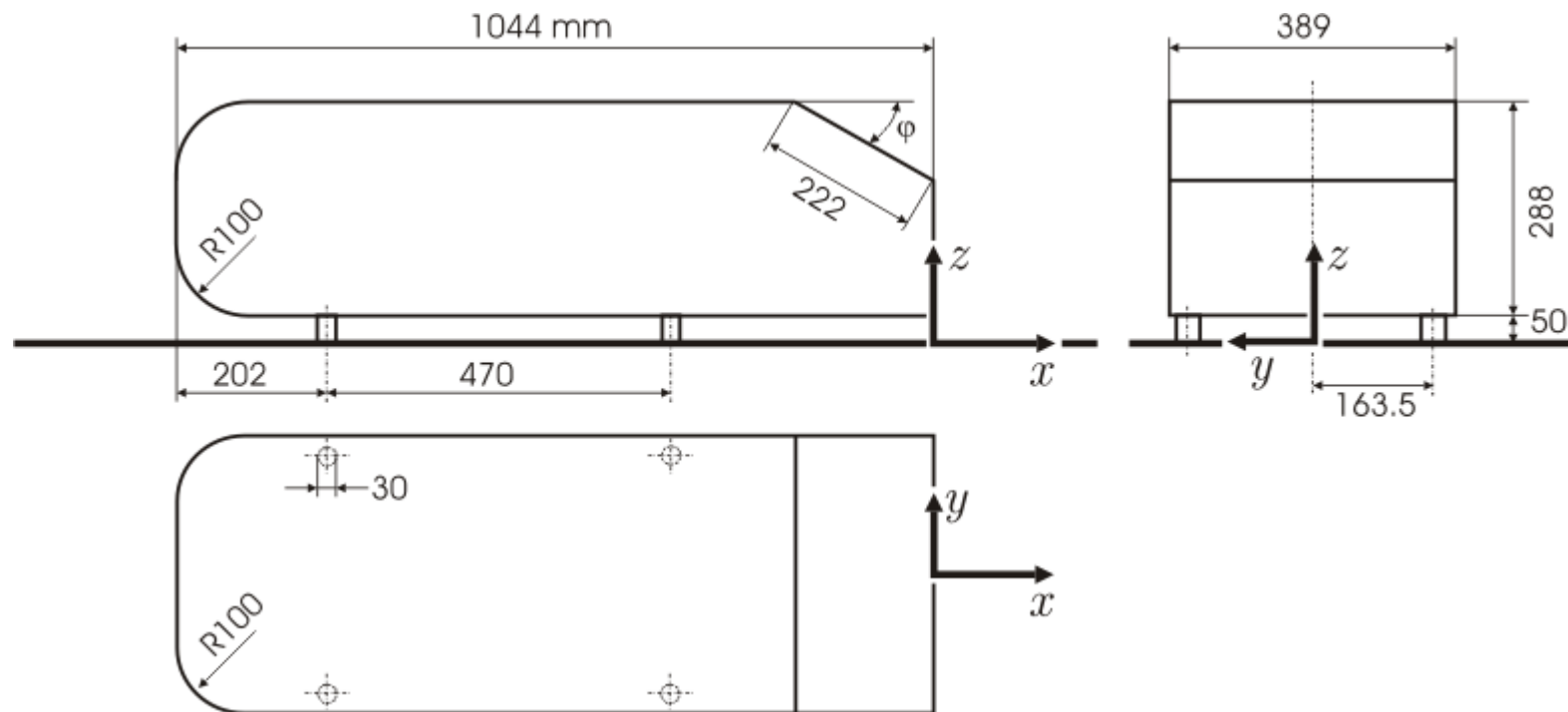
(laminar) boundary layer
separation:
Achenbach: 82.5° $Re=10^4$,
Bakic : $80^\circ - 83^\circ$ at $Re=5 \cdot 10^4$



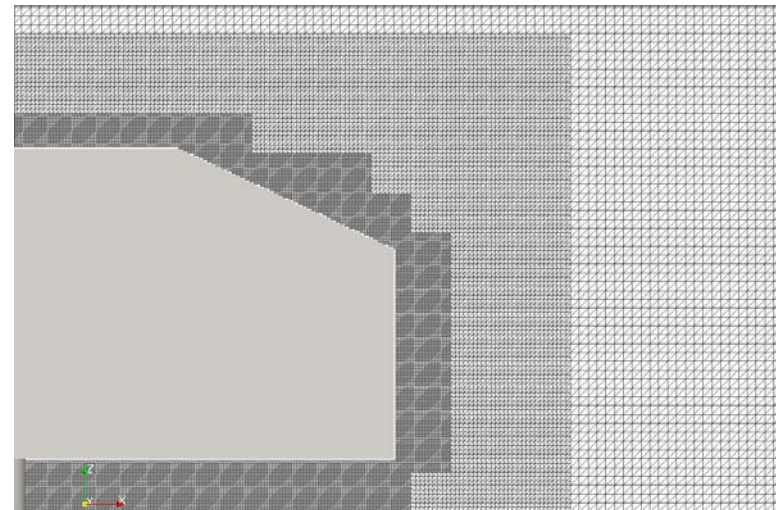
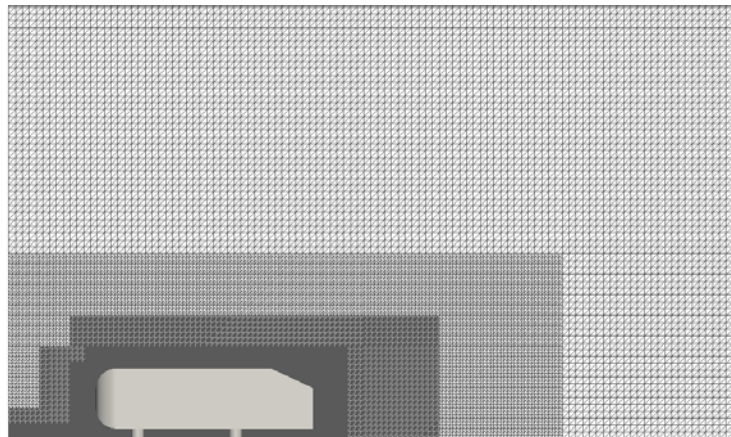
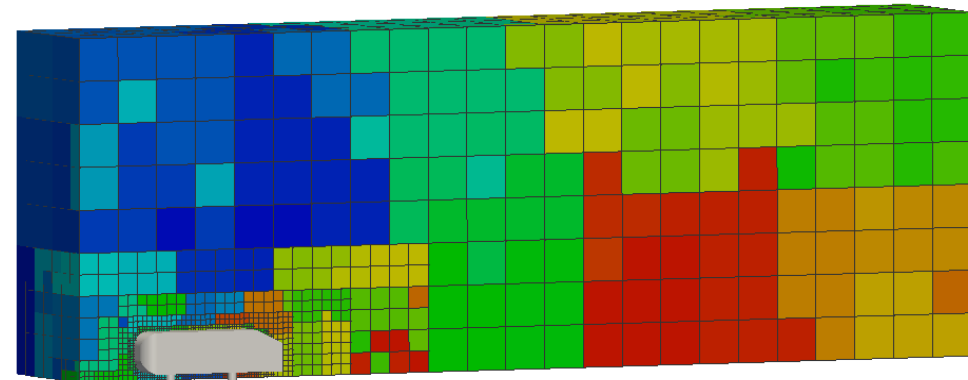
This simulation: 84°

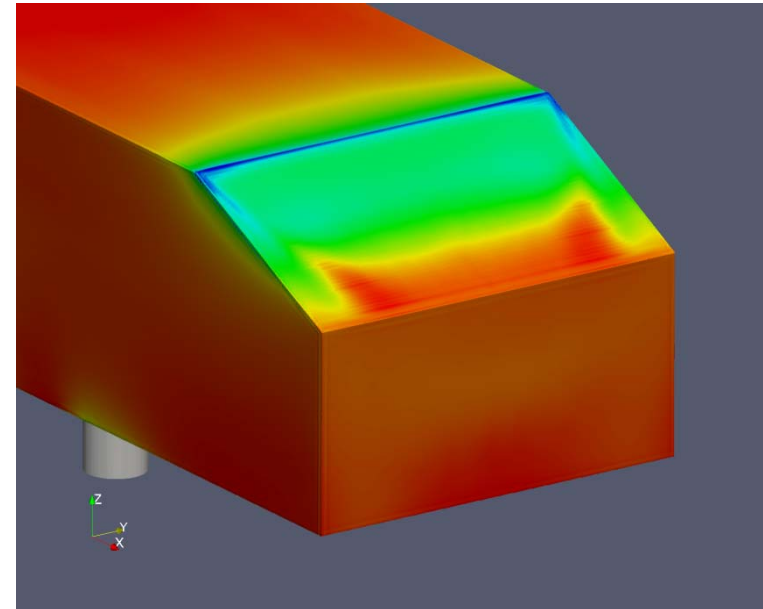
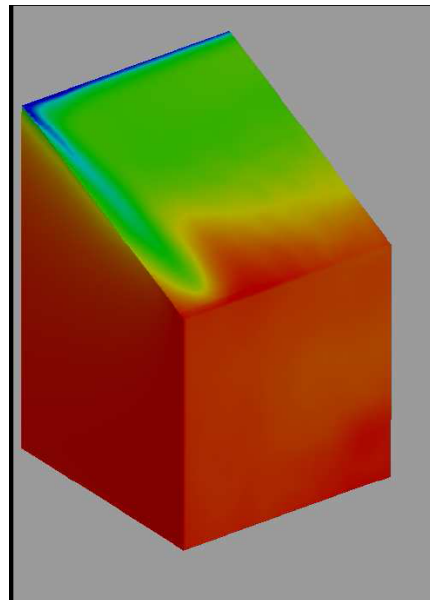
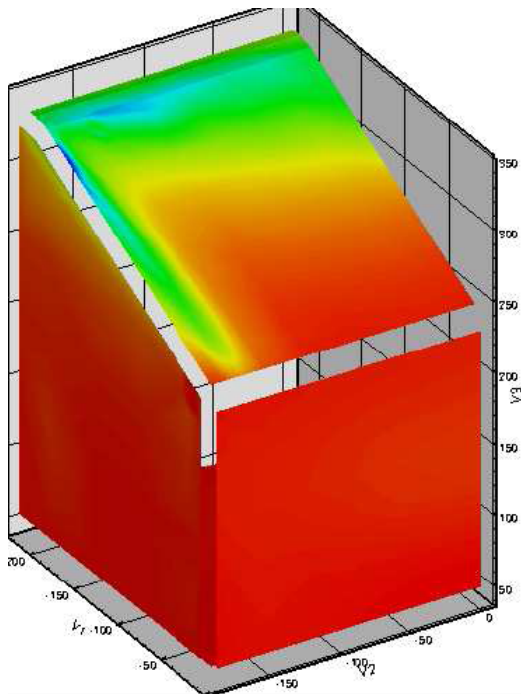


Ahmed body (http://www.cfd-online.com/Wiki/Ahmed_body):

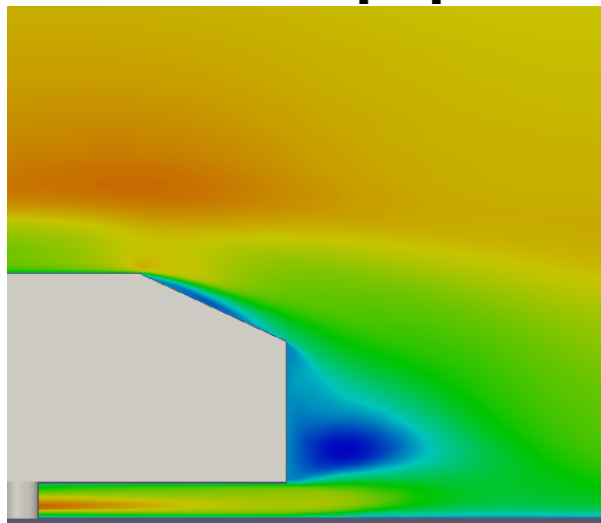
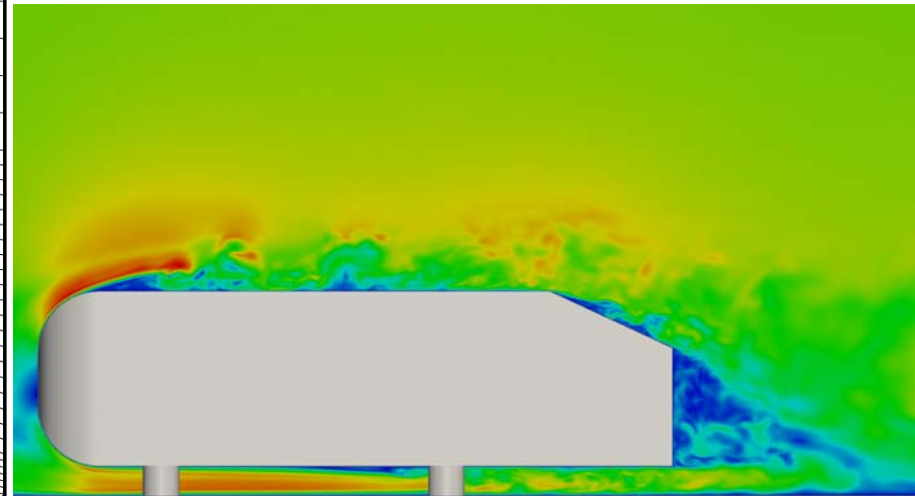
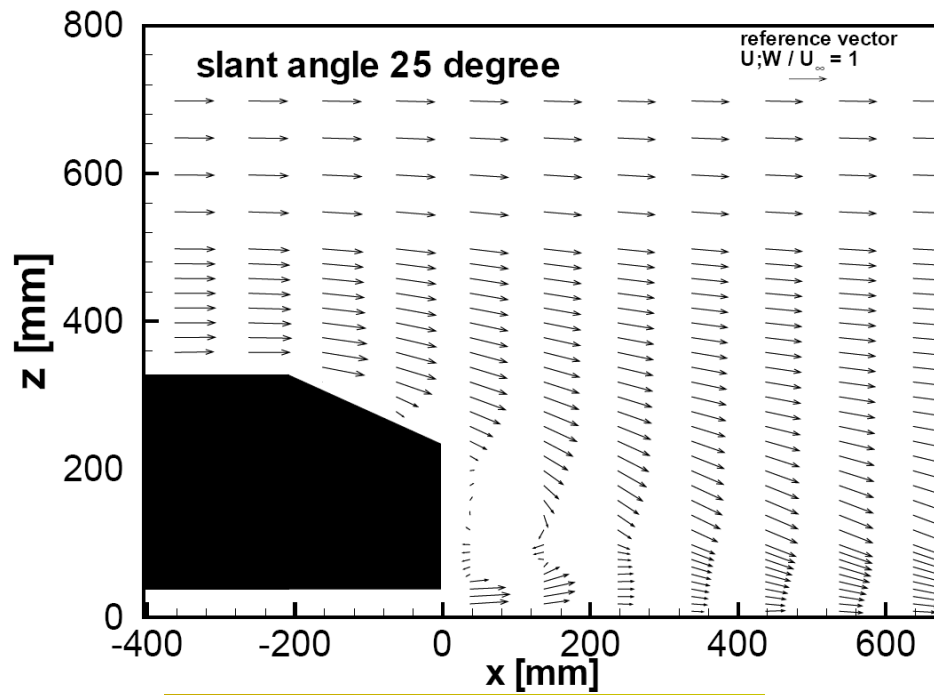
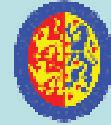


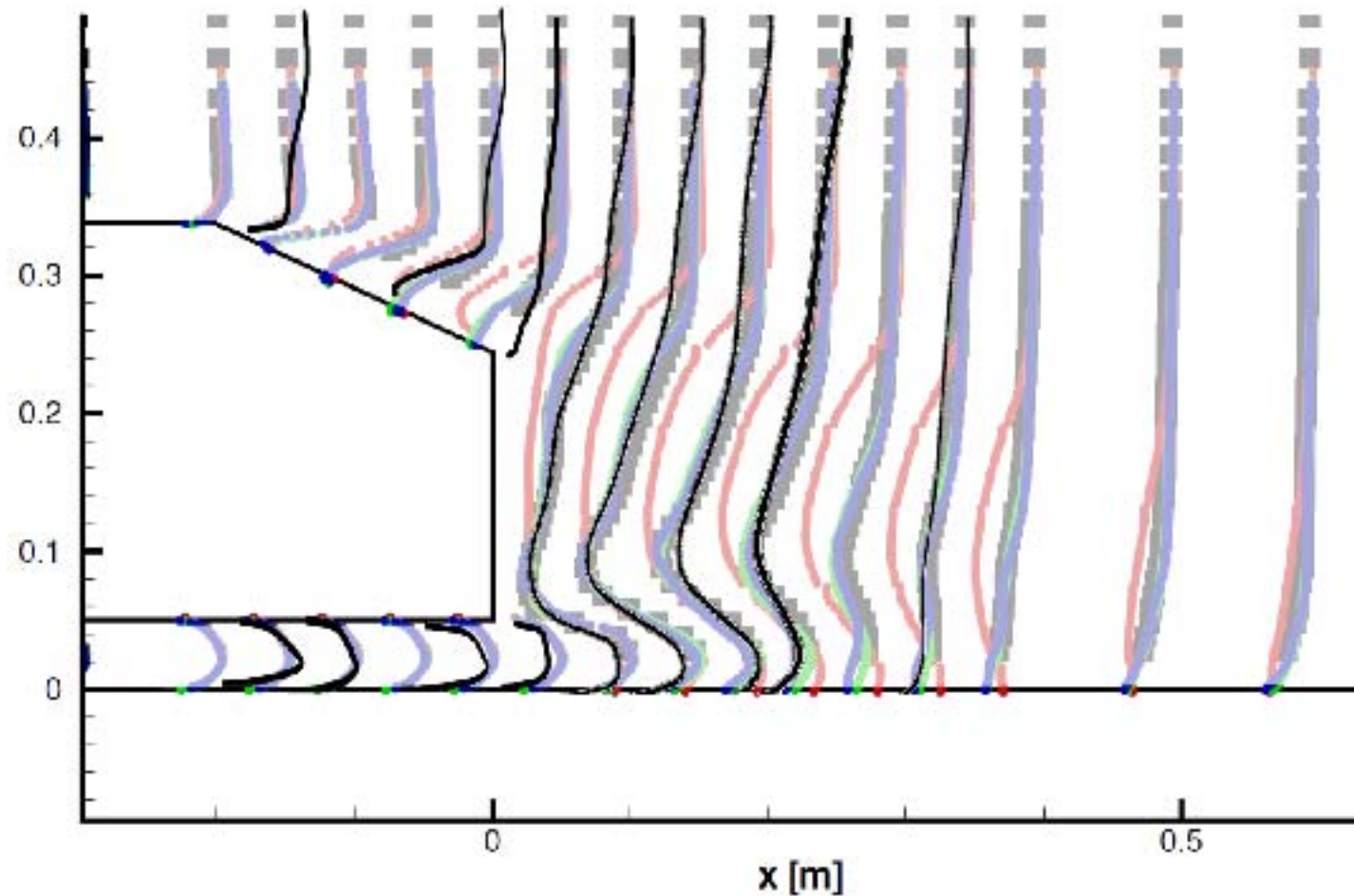
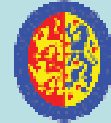
Re=10⁶
Ma=0.02
Cs=0.18
5 grid levels
1.7x10⁷ grid nodes
64 procs, 80% par. efficiency





Pressure distribution for rear slant angle 25° :
left: exp (Lienhart et al.), mid: E. Fares (Powerflow,EXA), right: VirtualFluids





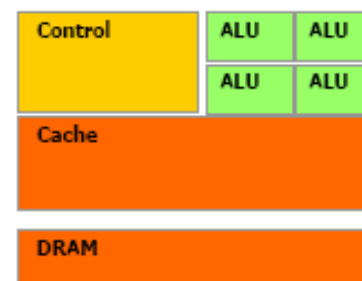
Velocity profiles for rear slant angle 25° :

dots: exp (Lienhart et al.), grey lines: E. Fares (Powerflow, EXA), black lines: VirtualFluids

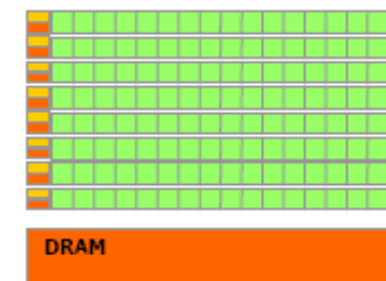
nVIDIA - G80/G92/GT200: the parallel stream processor

GTX 280: 1.4 billion transistors

Montecito: 1.7 (1.5 are L3



CPU



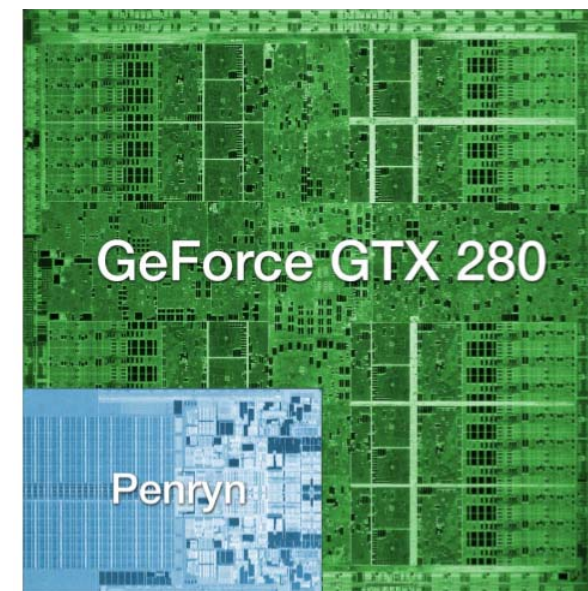
GPU

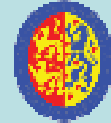
Hardware:

- GeForce
- Tesla
- Quadro

Software:

- Compute Unified Device Architecture (CUDA 2.0, Compiler+SDK)

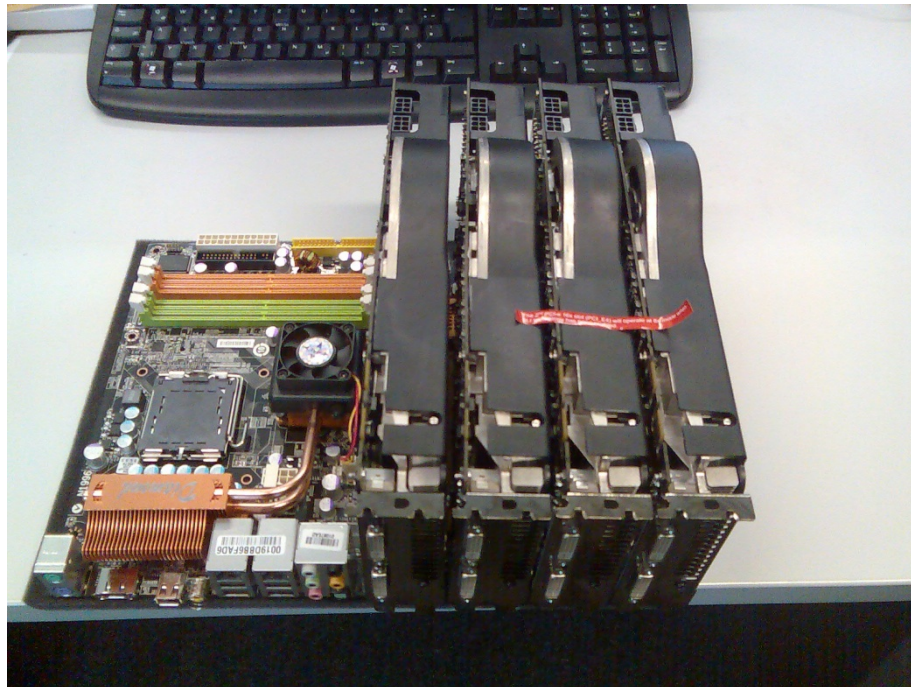




Comparison CPU-GPU

Platform	Memory [MB]	Peak [GFLOPS]	BW [GB/s]	price [Euro]
Intel Core 2 Duo (3.0 GHz)	4 000	48	7.0	1000
NEC SX-8R A (8 CPUs)	128 000	281	563	expensive
nVIDIA GTX280	1 024	624	142	500

Multi-GPU: Supercomputer on the Desktop -Teraflop Computing



Hardware cost:

- 5000 \$

Communication between GPUs:

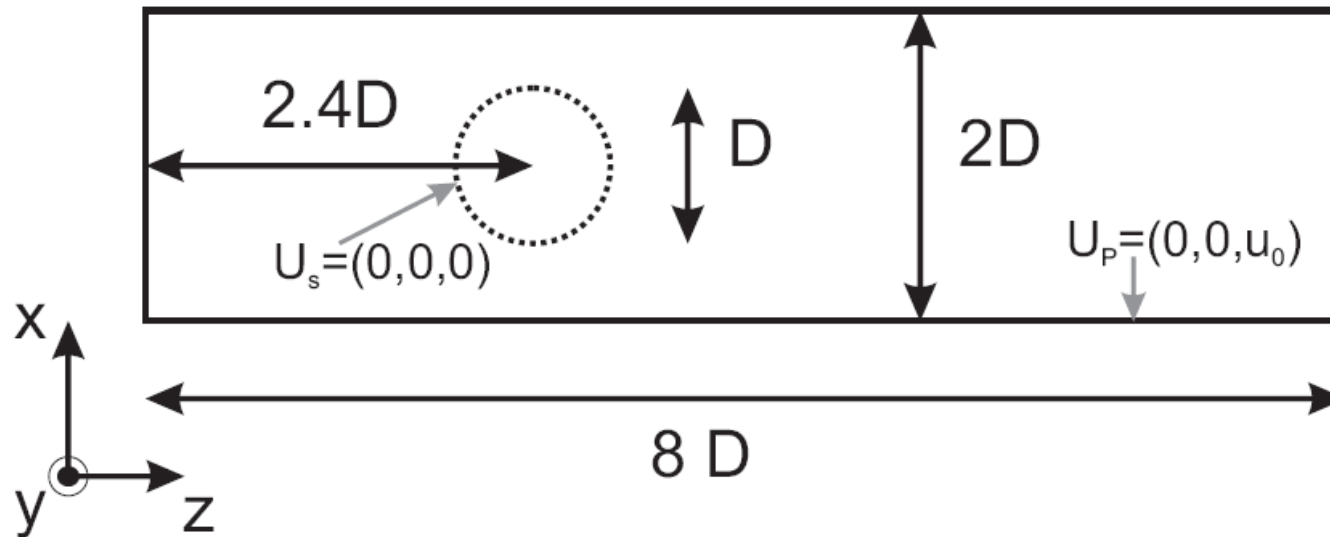
- 4 PCI Express slots
- Bandwidth Host↔Device
200-3000 MB/sec
- Latency like Front Side Bus (266 MHz)
- PThreads
- CUDA

Mainboard:
P6N Diamond MSI

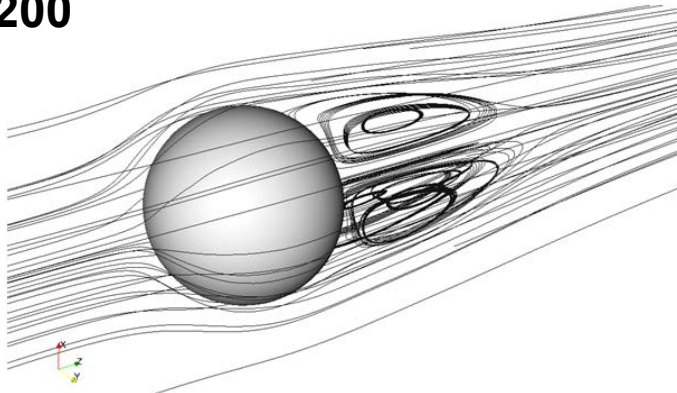
→**512 Cores!**

	Bandwidth [MB/s]	Latency [ns]
PCI-E/FSB	300-3000	10
Infiniband	312-7500	5 000
G-Ethernet	125	80 000

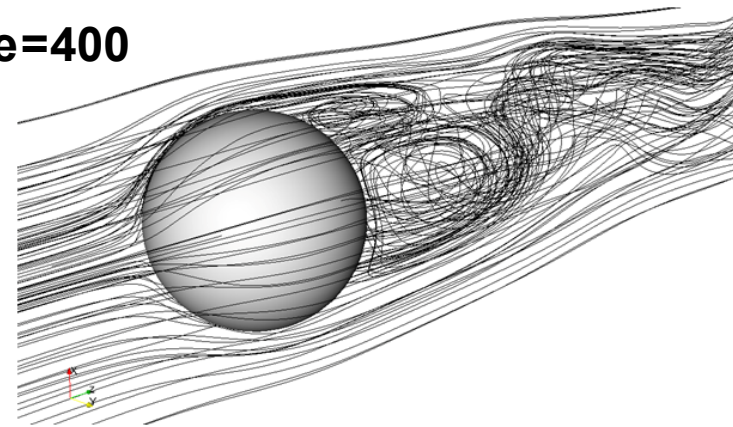
Example: moving sphere in a pipe



Re=200



Re=400



Moving Sphere in a pipe: Results (1 GPU)

$(2n_x, n_y, n_z) = 128 \times 128 \times 512$

R. Clift, J. R. Grace, M. E. Weber:
Bubbles, Drops and Particles,
Academic Press, 1978

Re [-]	ν [m ² s ⁻¹]	WCT [s]	# iter[-]	$c_{d,W}$ [-]	$c_{d,W,Ref.}$ [-]	$\frac{p.drag}{v.drag}$	Rel. Err. [-]
10	0.121920	106	15 000	14.74	15.84	0.93	6.9%
50	0.024384	415	59 000	3.697	3.876	1.15	4.6%
100	0.012192	520	74 000	2.380	2.312	1.43	2.9%
200	0.006096	774	110 000	1.679	1.706	1.90	1.6%
300	0.004064	2100 ¹	300 000	1.440 ²	1.448	2.35	0.6%
400	0.003048	2800 ¹	400 000	1.305 ³	1.296	2.82	0.7%

¹ nonstationary flow field, time required to reach oscillatory state from initial uniform flow field (no disturbance imposed)

² average value, $t = 280 \dots 2000 T_{ref}$

³ average value, $t = 200 \dots 3000 T_{ref}$

Moving Sphere in a pipe: Performance Single GPU

Tesla test sample (GT200)

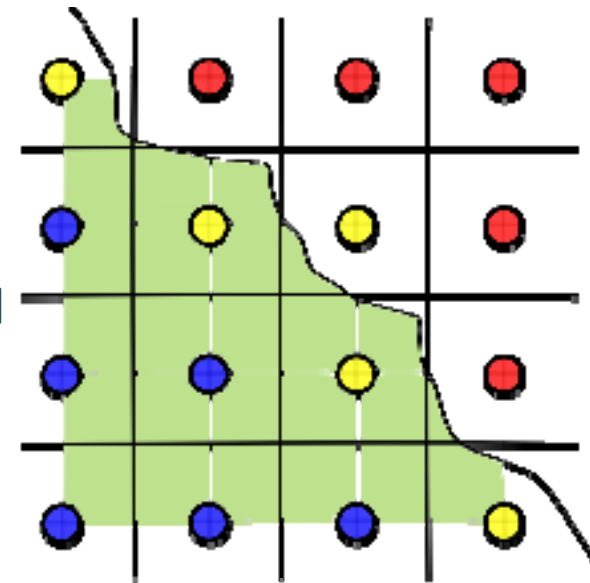
- 192 cores (1.1GHz)
- 101 GB/s throughput
- supports double precision

Results for grid 64(128)x128x512 (single prec.)

- **690 MLUPS**
- **72 % Throughput (!)** (83 % pure MemCpy)
- **43 % peak perf.**

Extensions for free surface flows

- fluid ●, interface ● and inactive gas ● nodes
- pressure boundary condition at the interface ● [Körner2005]
- initialization of new interface nodes needed ● → ●



Extensions for free surface flows

- fluid ●, interface ● and inactive gas ● nodes
- pressure boundary condition at the interface ● [Körner2005]
- initialization of new interface nodes needed ● → ●

- VOF approach to capture the interface [Körner2005] [Thürey2008]

- introduce fill level $\varepsilon = \frac{V_{fluid}}{V_{cell}}$

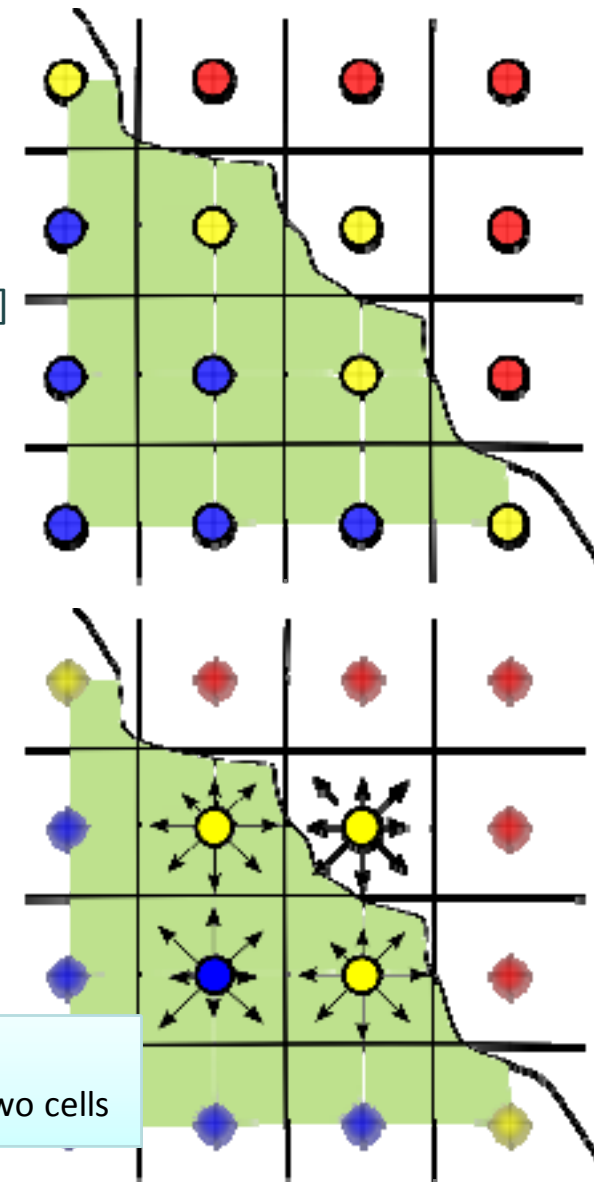
gas:	0.0
interface:]0.0 – 1.0 [
fluid:	1.0

- flux calculation in terms of LB distribution functions

$$\Delta m_i = [f_i(\vec{x} + \vec{e}_i \Delta t, t) - f_i(\vec{x}, t)] \cdot A_i$$

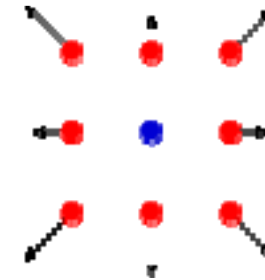
- calculate new fill level ε^{t+1}

I: inverse direction to i
A: wet area between two cells



Basic free surface algorithm

- Compute the flow field
 - Collision (local)
 - Add body force (local)
 - Propagation (non-local)
 - Apply boundary conditions (local)

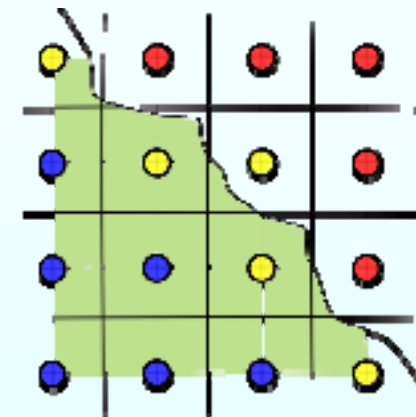


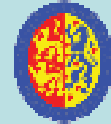
- Free surface part on interface nodes
 - Apply pressure boundary condition (**non-local**)
 - Evaluate mass fluxes and new fill levels (**non-local**)
 - Detect cell changes (local)
 - Assure closed interface cell layer (**non-local**)
 - Initialize new fluid nodes (**non-local**)

$$f_i(t, \mathbf{x}) = -f_{inv}(t, \mathbf{x}) + f_i^{eq}(\rho, \mathbf{v}) + f_{inv}^{eq}(\rho, \mathbf{v})$$


$$\overline{\rho(\mathbf{x})} = \sum_i w_i \rho(\mathbf{x} + \mathbf{e}_i) \quad \overline{\mathbf{v}(\mathbf{x})} = \sum_i w_i \mathbf{v}(\mathbf{x} + \mathbf{e}_i)$$

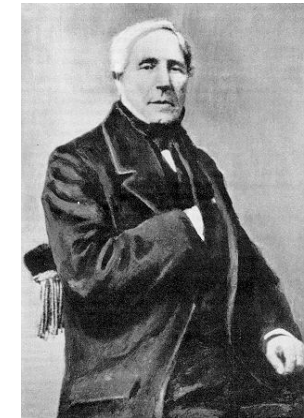
[Körner2005, Thürey2008]





Performance of D3Q19 model: Poiseuille flow

- Nvidia GTX 275 
 - 1024MB device memory, which corresponds to a maximum of 6 million nodes
 - 240 cores with 1.4 GHz each

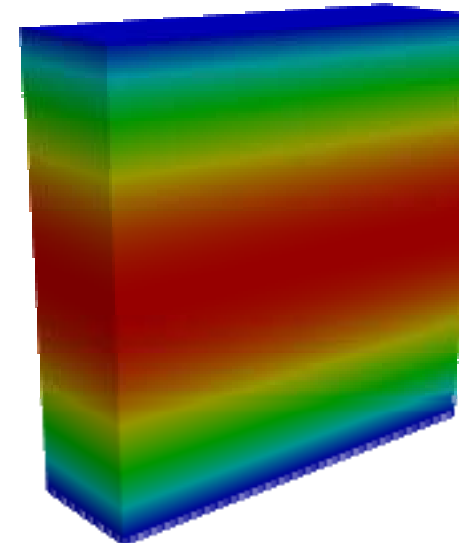


- Resulting performance in MNUPS

NUPS = node updates per second

Threads (nx, flow dir.)

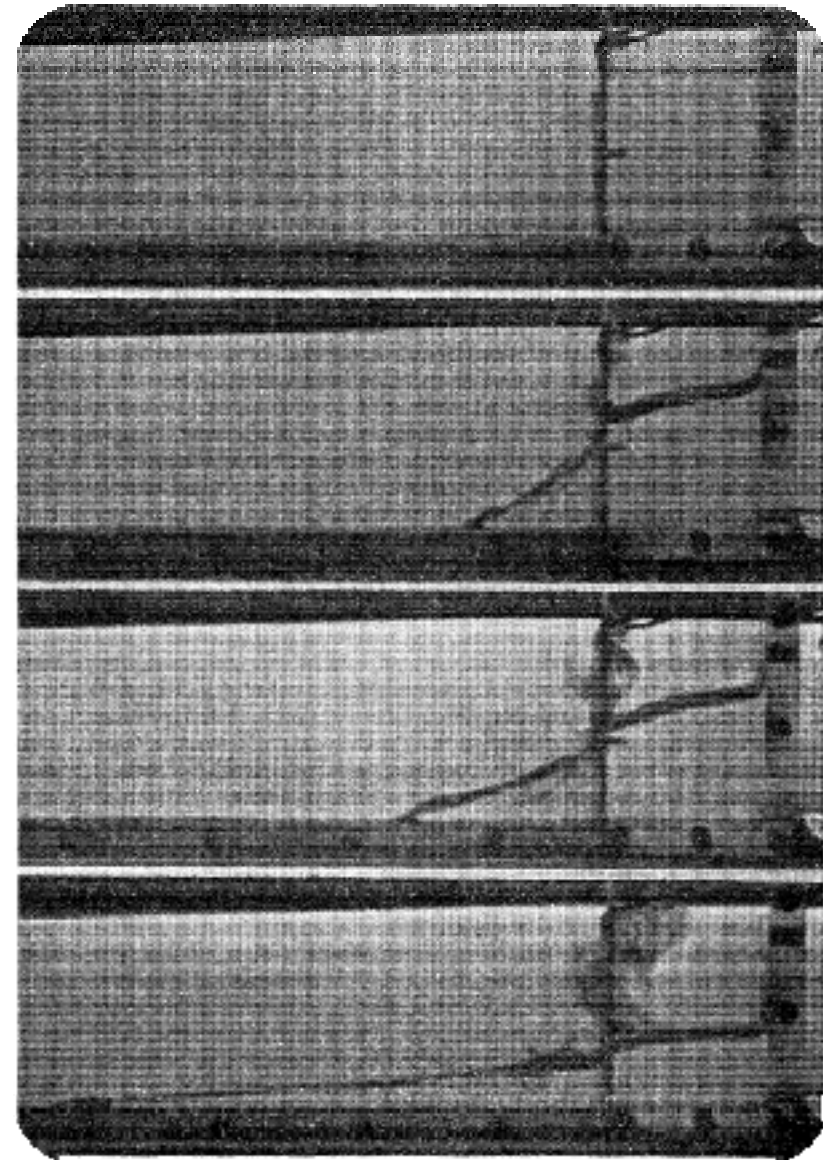
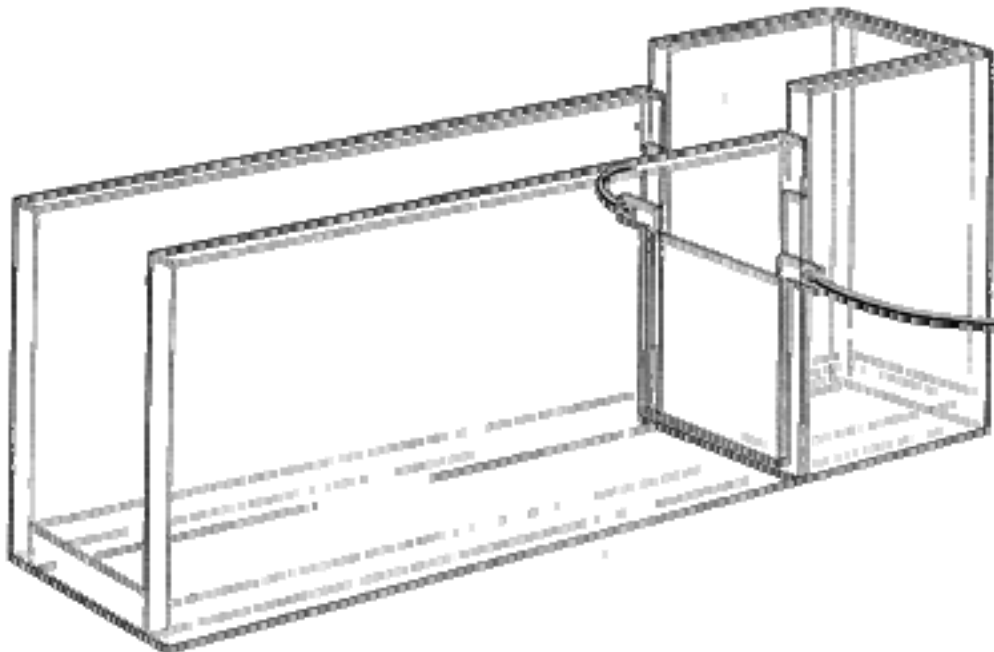
ny x nz	32	64	128	256
32x32	318	352	289	287
64x64	295	357	306	284
128x128	353	372	295	--
256x256	317	357	--	--



- Maximum performance:
 - 372 MNUPS, 1 million nodes → 372 time steps per second

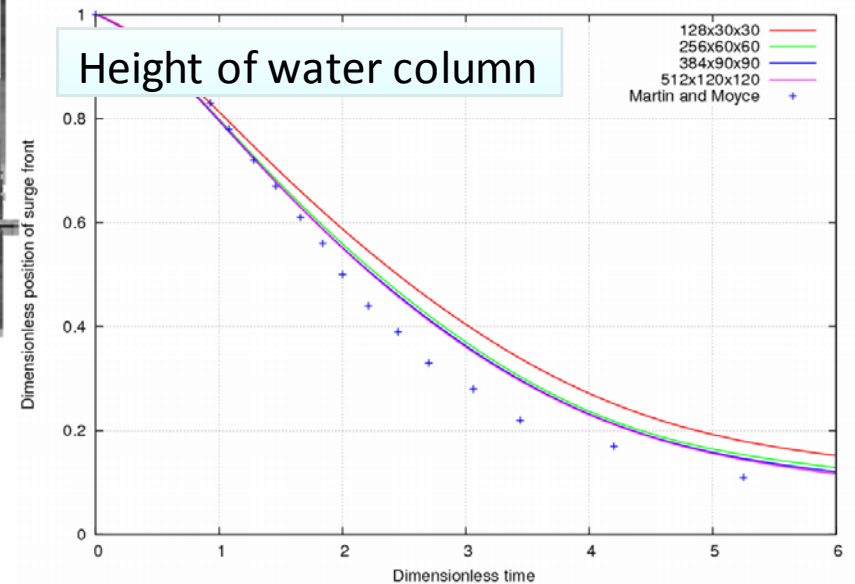
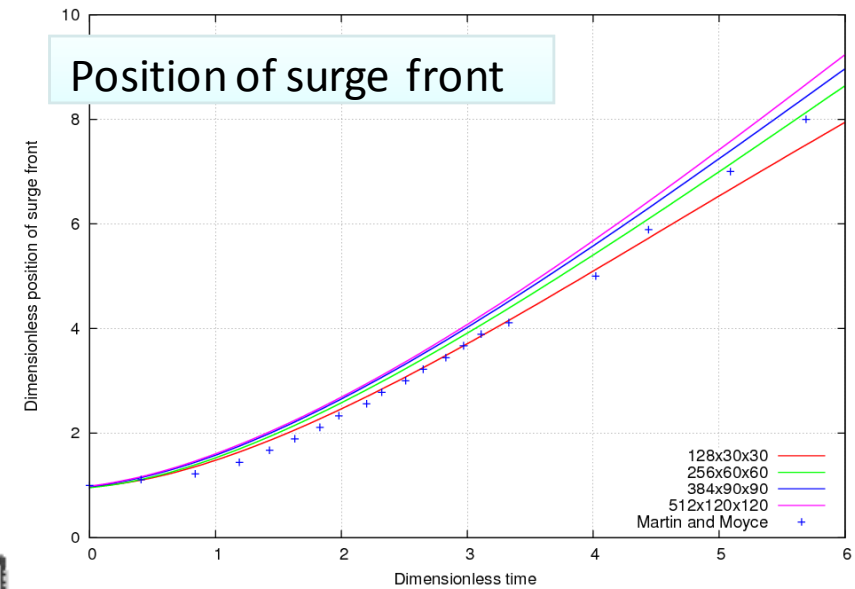
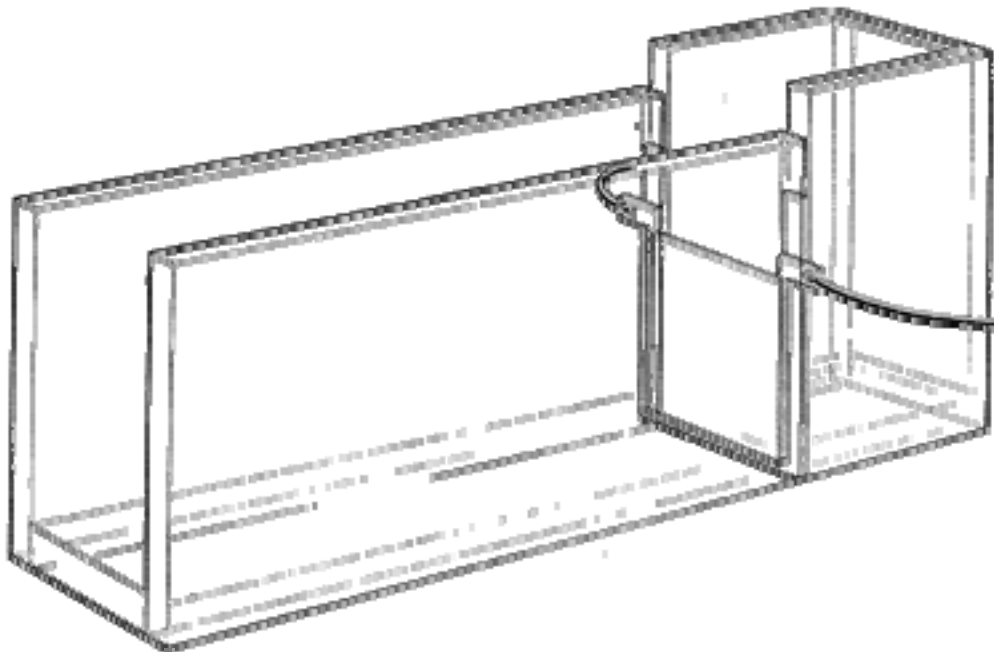
Dam break test case [Martin1952]

- Observe collapsing water column
 - position of the surge front
 - height of the water column
- $Re\ 100\ 000$, $Fr\ 2.4$
- D3Q19, MRT collision operator



Dam break test case [Martin1952]

- Observe collapsing water column
 - position of the surge front
 - height of the water column
- Re 100 000, Fr 2.4
- D3Q19, MRT collision operator

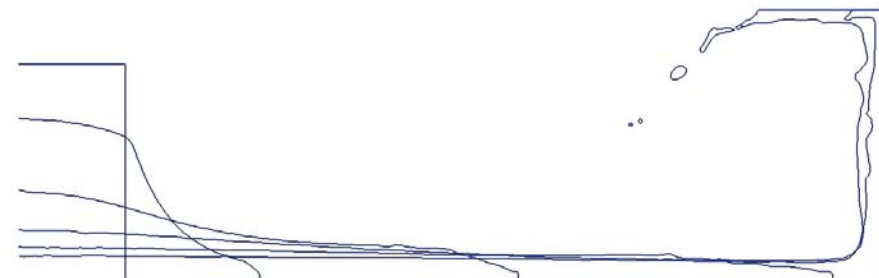


Dam break test case - Performance

- Average performance of 75 MNUPS
 - 20% of the maximum performance of a singlephase kernel
- Good agreement between experimental and numerical results
- See „Free surface flow simulations on GPUs“, C. Janßen, M. Krafczyk, 2010

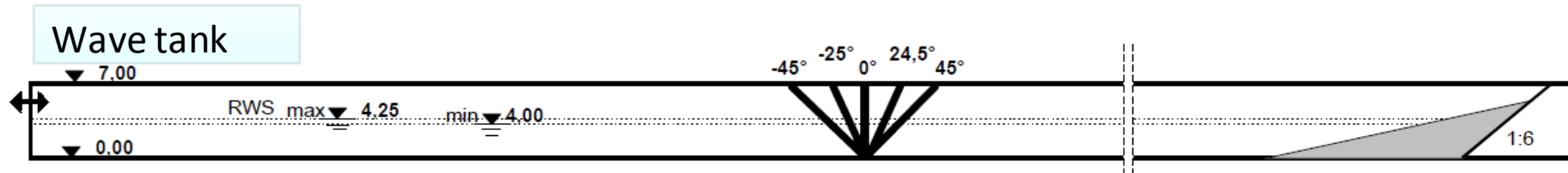
nx,ny,nz	Nodes	Time steps	Comp. time
128x30x30	115200	4000	6s
256x60x60	921600	8000	102s

Simulation details

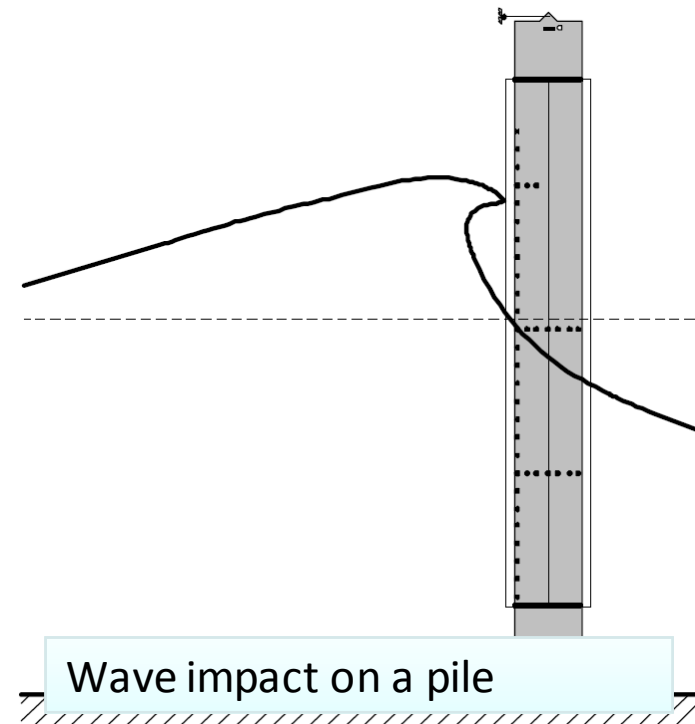


Time series

Wave impact on lean structures [Wienke2001]

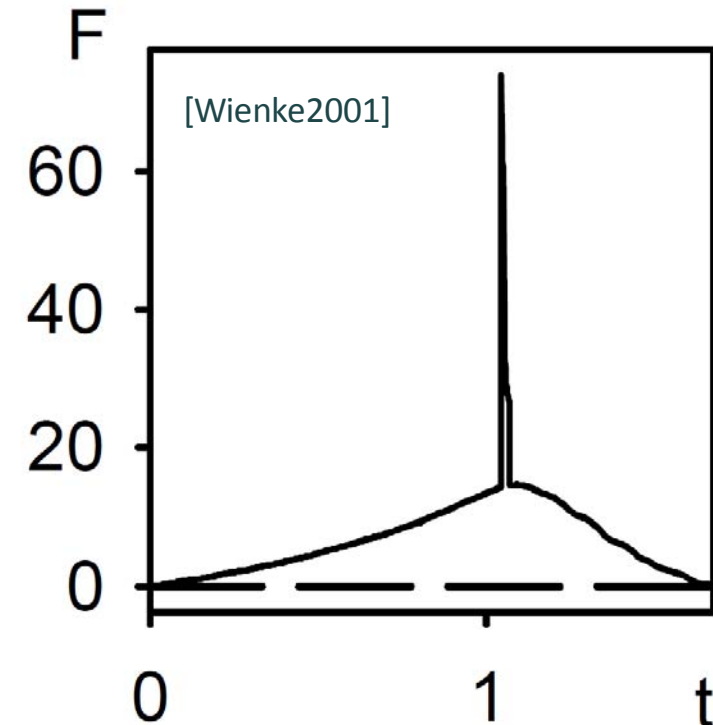
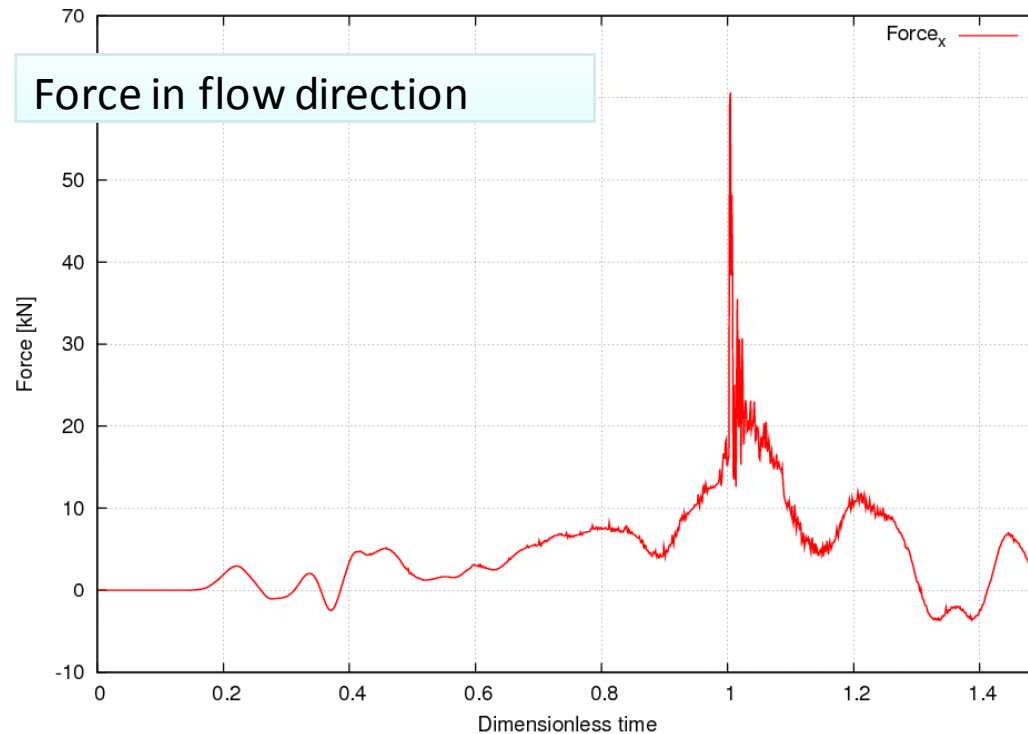


Experimental setup



Wave impact on a pile

Wave impact on lean structures – Force evaluation



- Grid resolution 256x64x64 (1 million nodes)
- Re 1 000 000, Fr 1.0
- D3Q19, MRT collision operator, Smagorinsky LES
- Momentum exchange method for force evaluation

65 MNUPS (GTX 275)
10 000 time steps
160 seconds computational time
(corresponds to 16 seconds real time)

Multiphase LB-simulations on non-uniform grids

Starting from the classical Gunstensen model:

Gunstensen, A. K., Rothman, D. H., Zaleski, S., and G. Zanetti, "Lattice Boltzmann model of immiscible fluids", [Phys. Rev. A](#) 43(8) (1991):4320-4327.

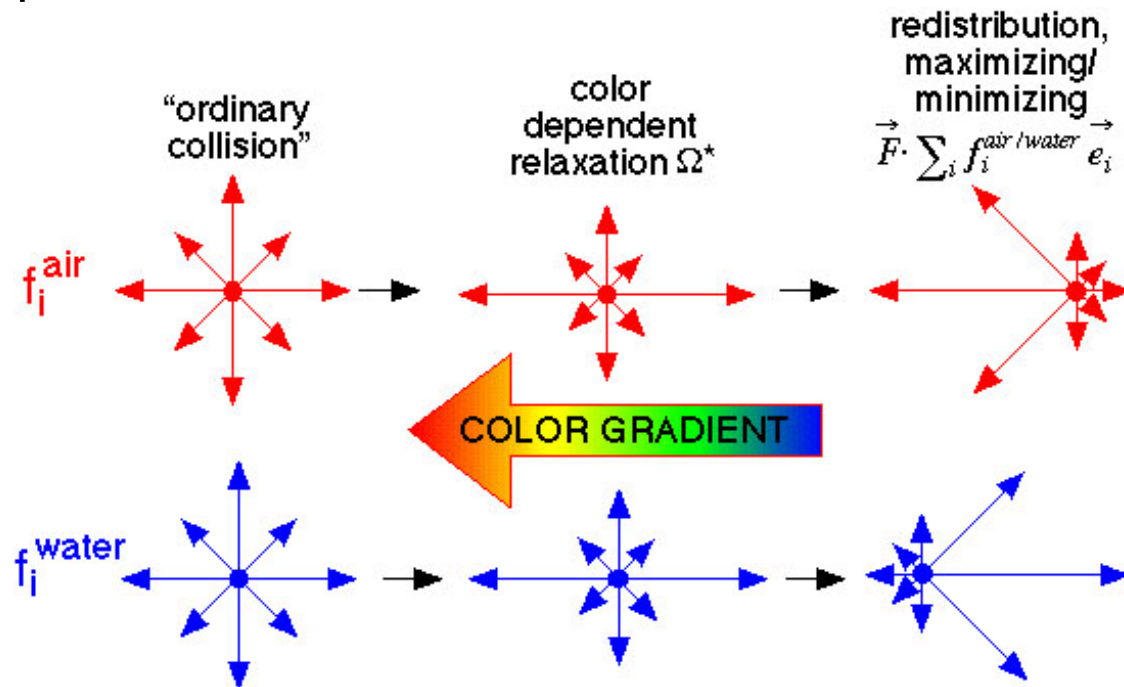
- two sets of distributions f_i^{air} and f_i^{water}
- Collision operator for each phase has two contributions

$$\Omega = \Omega^{(1)} + \Omega^{(2)}$$

$$\Omega^{(2)} = \frac{A_k}{2} |\vec{F}| \left[\frac{(\vec{e}_i \vec{F})^2}{|\vec{F}|^2} - \frac{1}{2} \right]$$

With a 'phase' gradient

$$\vec{F}(\vec{x}) = \sum_i \vec{e}_i [\rho^{air}(\vec{x} + \vec{e}_i) - \rho^{water}(\vec{x} + \vec{e}_i)]$$



implementation of a new extension of the Rothmann-Keller model

- one set of distributions










- phase parameter $\theta = \frac{\rho_{red} - \rho_{blue}}{\rho_{red} + \rho_{blue}} \in [-1; +1]$

- surface tension

[Kehrwald, Numerical Analysis of Immiscible Lattice BGK, PhD, Kaiserslautern, 2004]

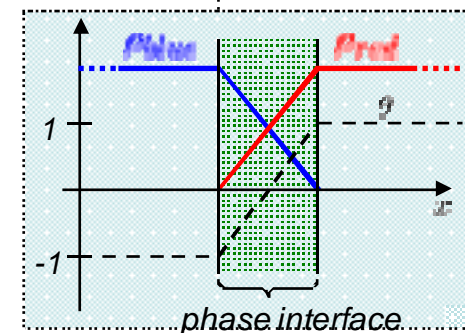
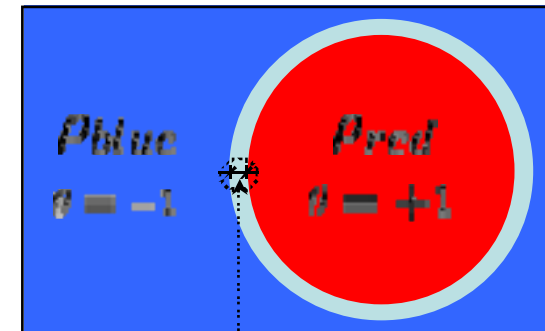
[Tölke et. al., An adaptive scheme using hierarchical grids for lattice Boltzmann multi-phase flow simulations, Computers and Fluids, 35:820-830, 2005]

$$m_i^{oq,l} = m_i^{oq,l} + m_i^{SI,l}$$

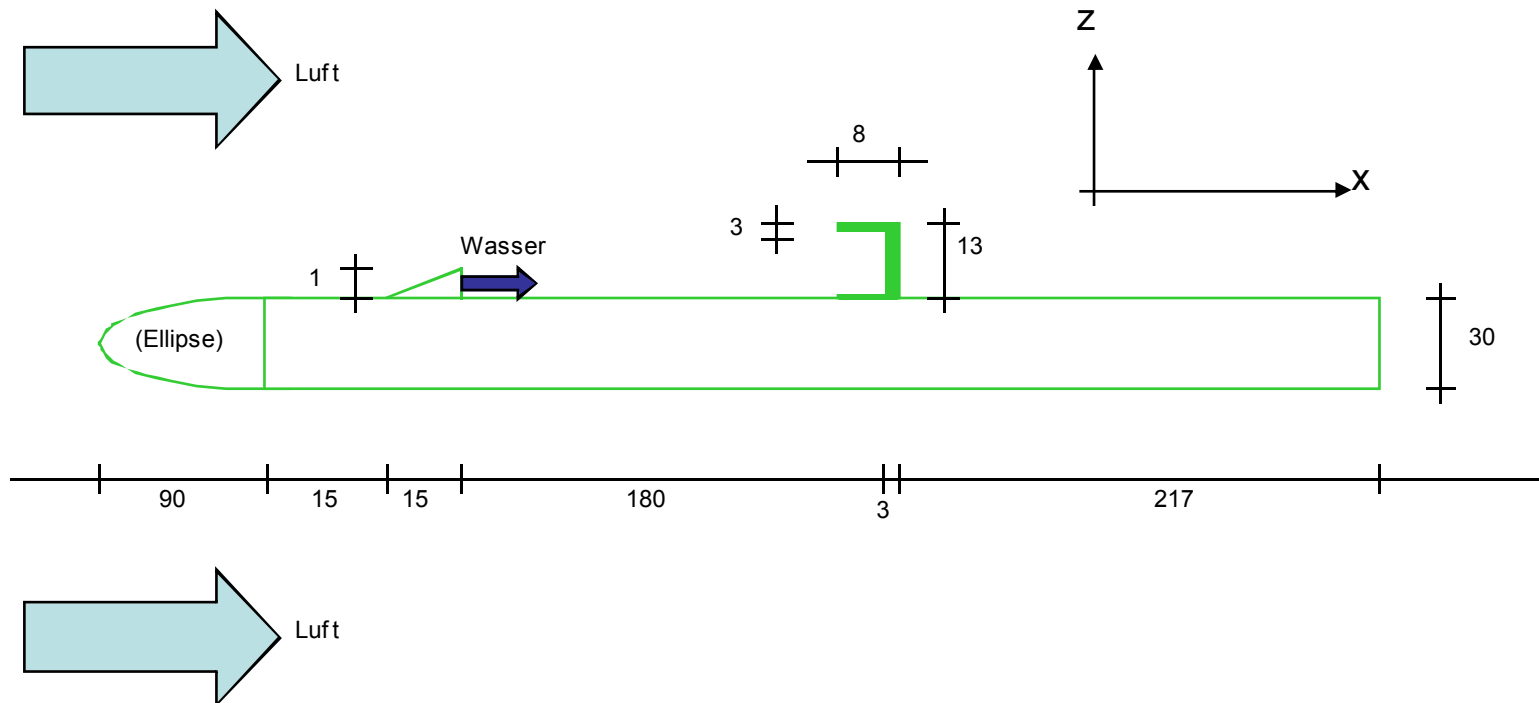
			$m_1^{SI,l} = -\sigma C_1 (n_{l,x}^2 + n_{l,y}^2 + n_{l,z}^2)$
			$m_9^{SI,l} = -\sigma C_9 (2n_{l,x}^2 - n_{l,y}^2 - n_{l,z}^2)$
			$m_{11}^{SI,l} = -\sigma C_{11} (n_{l,y}^2 - n_{l,z}^2)$
			$m_{13}^{SI,l} = \sigma C_{13} (n_{l,x} n_{l,y})$
			$m_{14}^{SI,l} = \sigma C_{14} (n_{l,y} n_{l,z})$
			$m_{18}^{SI,l} = -\sigma C_{18} (n_{l,x} n_{l,z})$

gradient of phase field $C_i^l(t, x) = \frac{3}{2\sigma \Delta t} \sum_i w_i \frac{r_i}{c} \theta(t, x + r_i \Delta t_i)$

vector normal to phase field $n_{i,n} = \frac{C_{i,n}}{|C_i^l|}$



Test case car roof L-ledge

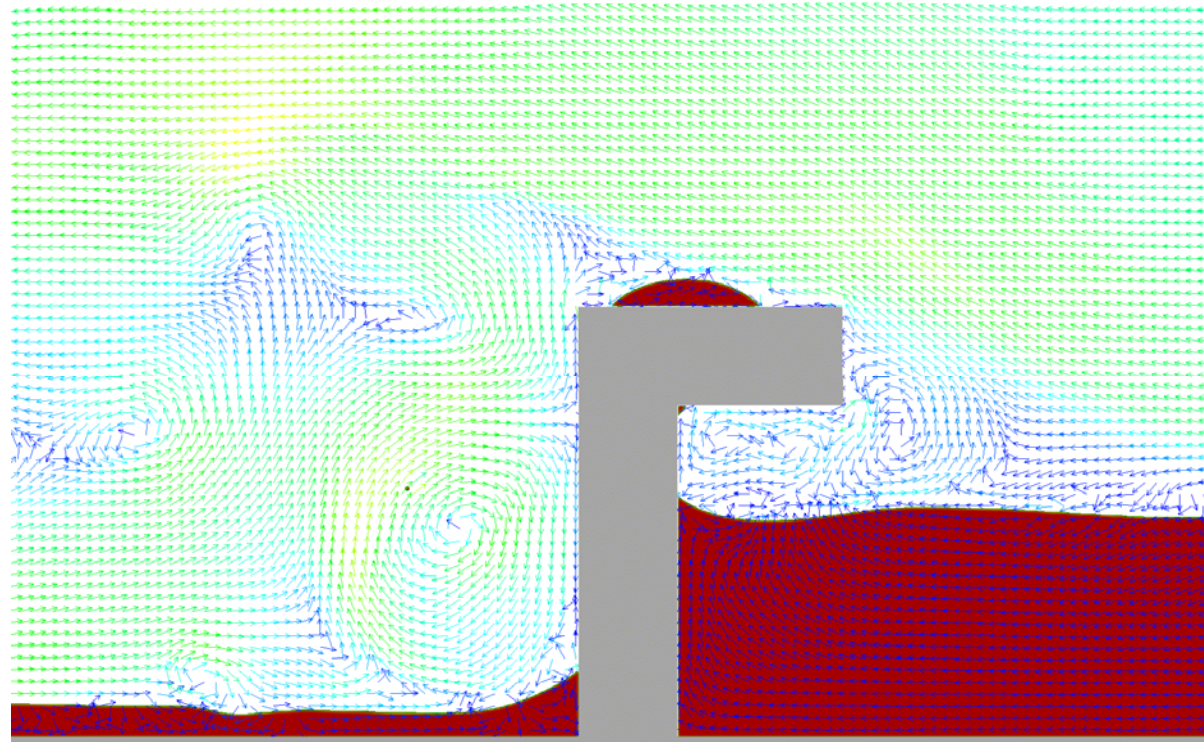
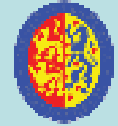


$$\text{Re} = \frac{U_\infty L_R}{\nu_L} = \frac{11.44 \cdot 0.18}{1.8E-5} = 114400$$

$$\text{Ca} = \frac{U_\infty \mu_L}{\sigma} = \frac{11.44 \cdot 1.5E-5}{0.072} = 0.0028$$

$$\text{Bo} = \frac{2 \rho_W g H_R^2}{3\sigma} = \frac{2 \cdot 1000 \cdot 9.81 \cdot 0.013^2}{3 \cdot 0.072} = 15.4$$

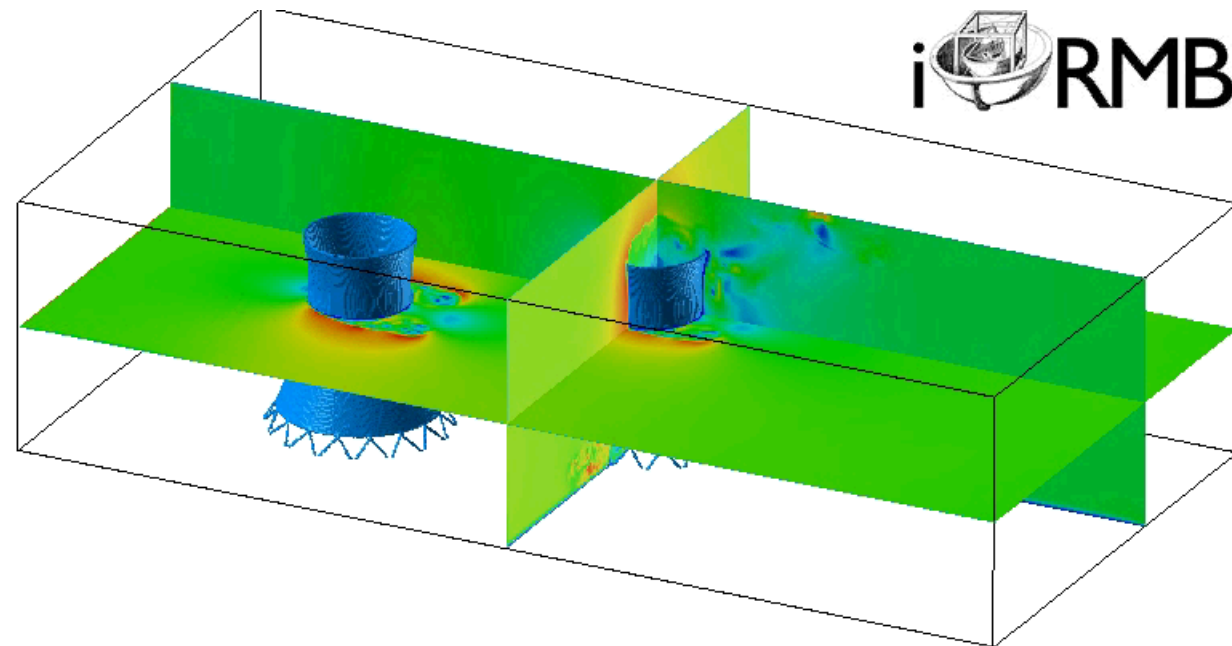
$$\frac{\mu_W}{\mu_L} = \frac{1E-3}{1.8E-5} = 55$$



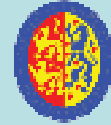
Fluid-Structure-Interaction



Ferrybridge, England 1965

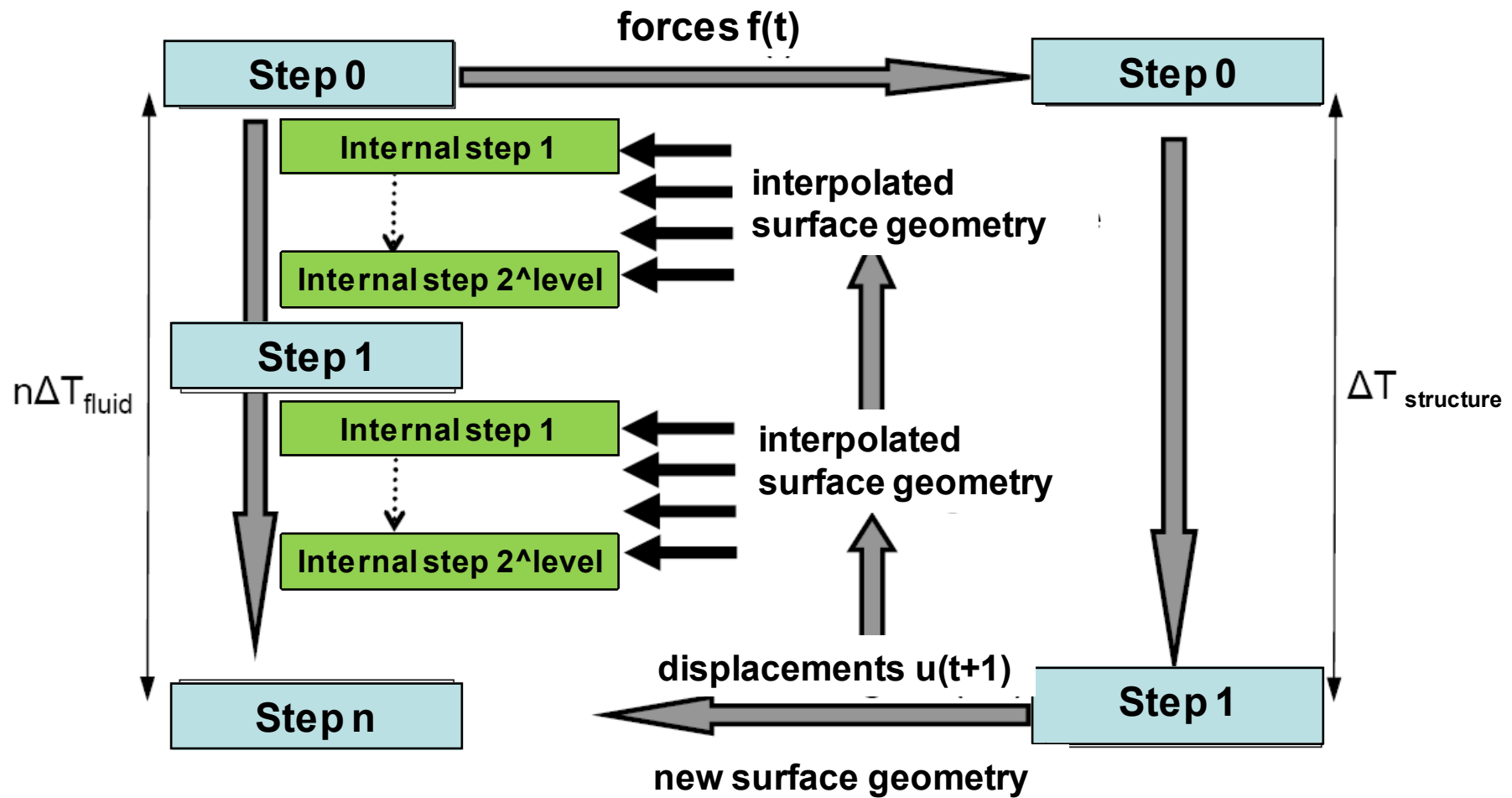


512 cores, 2×10^9 DOF LES simulation



LBM solver

structural FEM solver



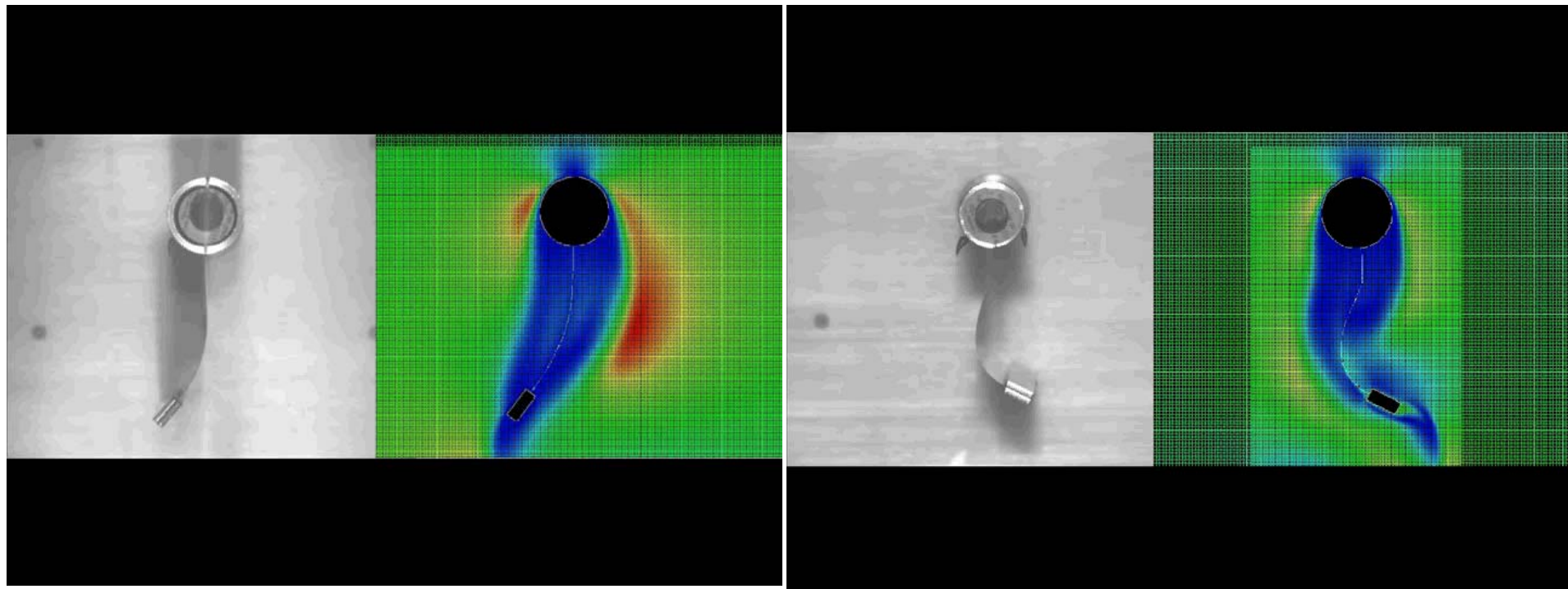
Experimental Benchmark

EXPERIMENTAL STUDY ON A FLUID-STRUCTURE INTERACTION REFERENCE TEST CASE

Jorge P. Gomes and Hermann Lienhart

Fluid-Structure Interaction: Modeling, Simulation,
Optimisation

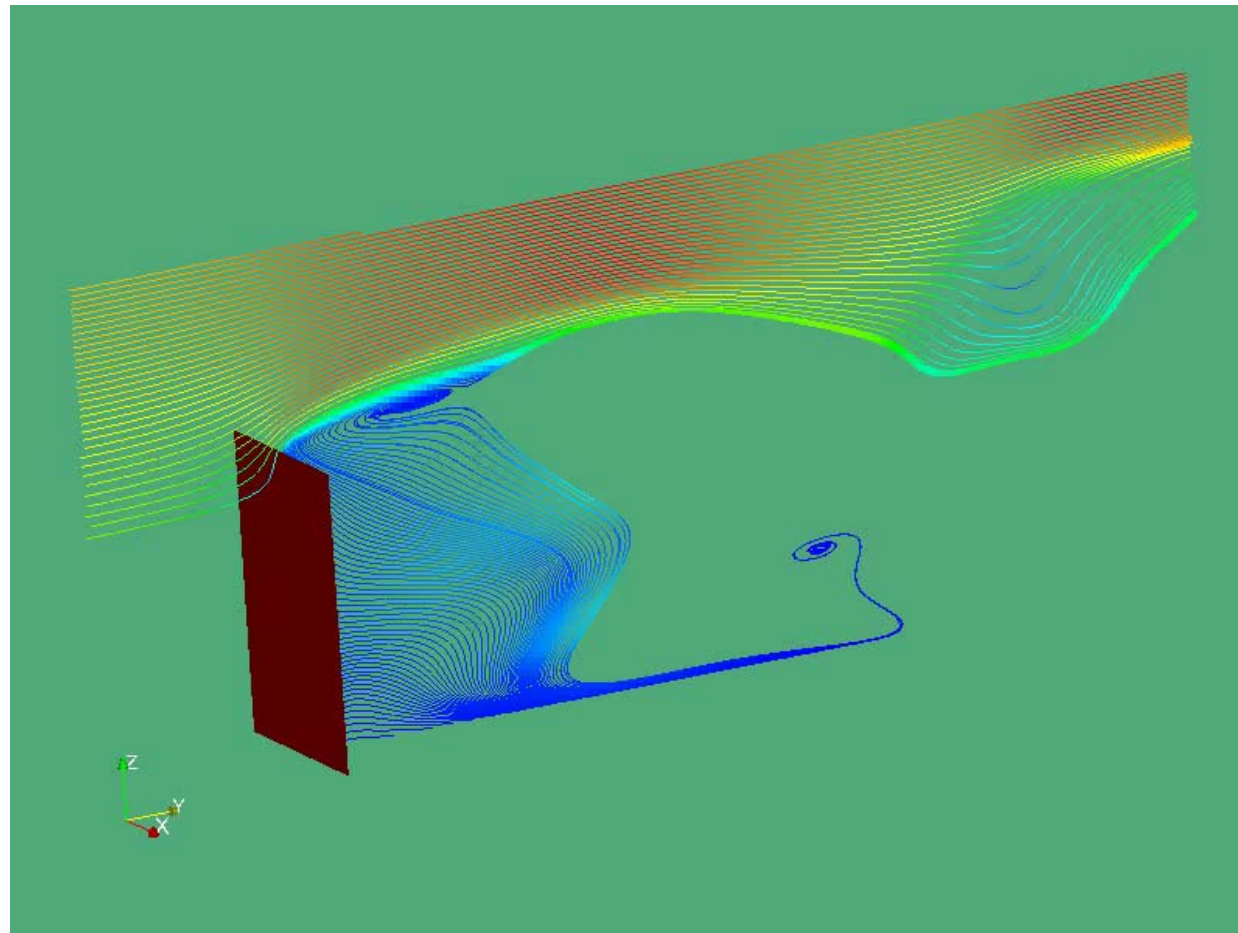
Lecture Notes in Computational Science and Engineering ,
Vol. 53, pages 356 - 370



Re=140

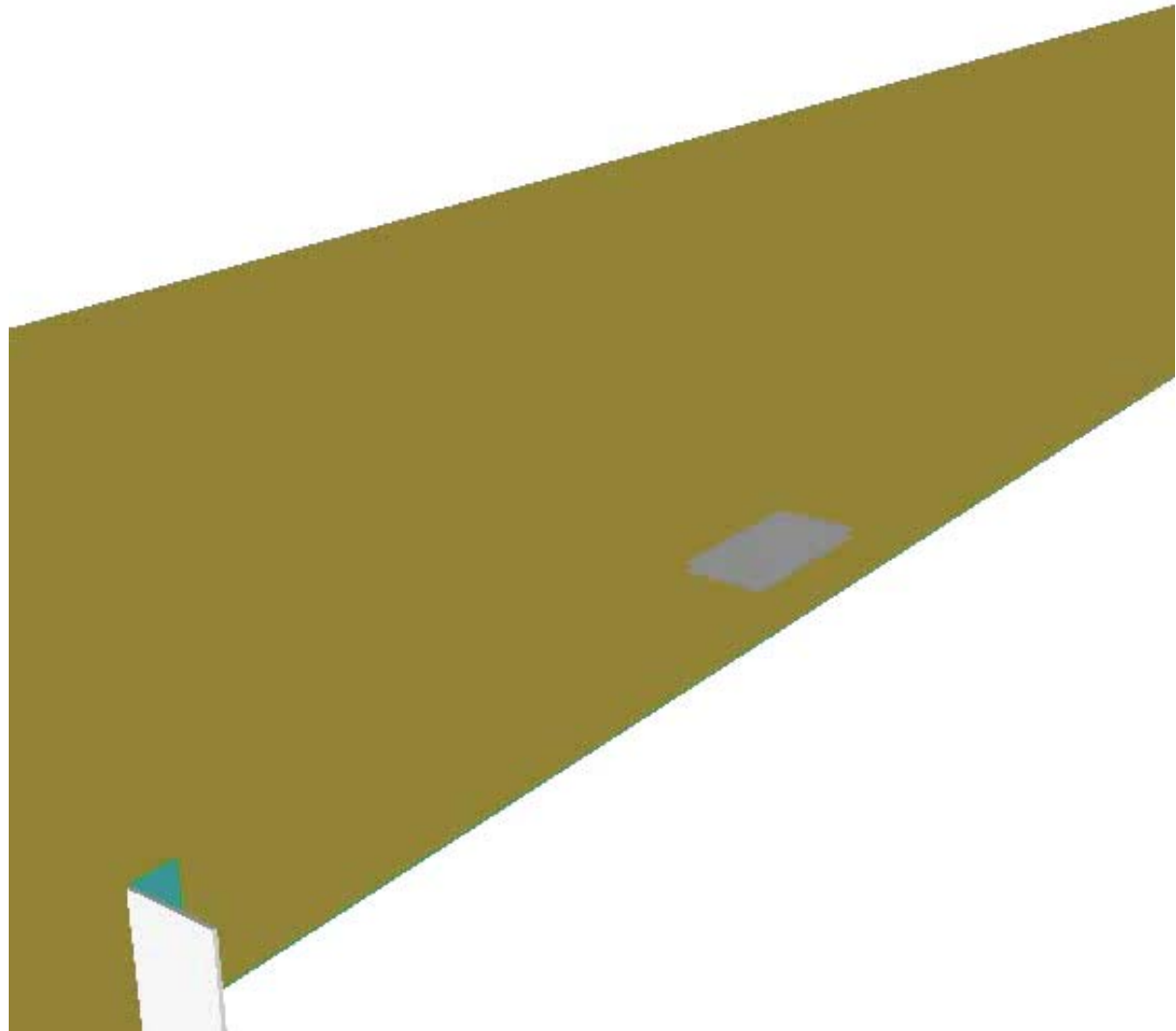
Re=190

3D FSI
Re=2500

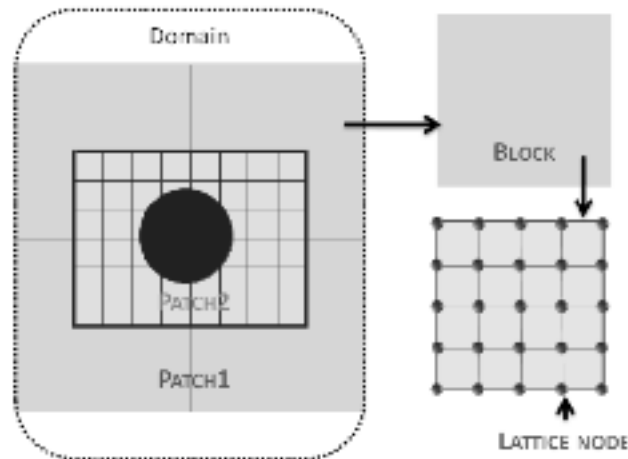


Oscillating Membrane in flow field

- **Re=6000**
- **lattice size: 128x128x512**
- **3 GPUs**
- **> 1E9 LUPS**
- **250 time steps in 1 sec**
- **LES**
- **Compt. Steering**
- **500 000 time steps**
- **2000 sec total time**
- **dt_s=10 dt_f**
- **Membrane: Eigenmodes**



Grid refinement on GPU



```

L_max := maximum number of grid levels;
l := grid level
dT_l0 := coarse grid time step;
dX_l0 := coarse grid node distance;
endtime := maximum number of time steps;

```

```

updateGrid(l, endtime )

```

```

begin

```

```

    dT := 2(-l) * dT_l0;

```

```

    dX := 2(-l) * dX_l0;

```

```

    dX_temp := 2(-(l+1)) * dX_l0;

```

```

    for l=0 to l <= endtime step l+=dT

```

```

    begin

```

```

        if(l+1 < -l_max) updateGrid(l+1, 1);

```

```

        collision(l);

```

```

        propagation(l);

```

```

        applyBoundaryConditions(l)

```

```

        if( l != l_max) then interpolateGridInterface(l, l+1);

```

```

    end;

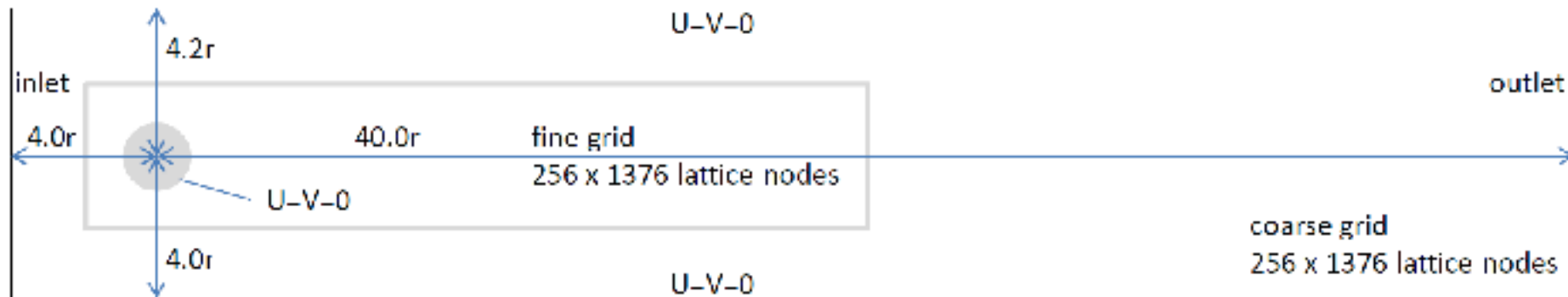
```

```

end;

```

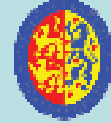
2D-benchmark



$Re = 100$	present method	Crouse [3]	Schäfer and Turek [12]
C_D	3.19	3.2645-3.2650	3.22-3.24
C_L	0.94	0.9492-1.0709	0.99-1.01
St	0.322	0.3050-0.3076	0.295-0.305

Computational Efficiency

	Resolution	NUPS	NUPS	processing time for $10^5 \Delta t$
	[nodes x nodes]	$[\times 10^6]$	[%]	[s]
uniform	2048 x 15360	911.62	100.00	3450.73
non-uniform (raw)	2 x 1024 x 15360	903.35	99.09	5223.46
non-uniform (effective)	2 x 1024 x 15360	828.07	90.84	5223.46
uniform	1024 x 7680	920.59	100.00	854.27
non-uniform (raw)	2 x 512 x 7680	911.20	99.02	1294.6
non-uniform (effective)	2 x 512 x 7680	835.27	90.73	1294.62
uniform	512 x 3840	902.55	100.00	217.83
non-uniform (raw)	2 x 256 x 3840	837.50	92.79	352.13
non-uniform (effective)	2 x 256 x 3840	767.71	85.06	352.13



Thermal flows

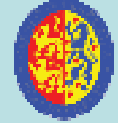
the temperature equation is discretized by a finite difference (FD) scheme:

$$\frac{T_{i,j,k}(t + \Delta t^{FD}) - T_{i,j,k}(t)}{\Delta t^{FD}} = -\vec{j}_{i,j,k}(t) \nabla_{i,j,k}^{(h)} T_{i,j,k}(t) + \alpha \Delta_{i,j,k}^{(h)} T_{i,j,k}(t)$$

J. Tölke: A thermal model based on the lattice Boltzmann method for low Mach number compressible flows, *Journal of Computational and Theoretical Nanoscience*, 3(4): 579–587 (2006).

Mezrhab A, Bouzidi M, Lallemand P. Hybrid lattice-Boltzmann finite-difference simulation of convective flows. *Comput. Fluids*, 2004;33:623–41.

van Treeck, C., Rank, E., Krafczyk, M., Tölke, J., and Nachtwey, B. Extension of a hybrid thermal LBE scheme for Large-Eddy simulations of turbulent convective flows. *Computers & Fluids* 35, 8–9 (2006), 863–871.

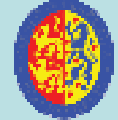


Boundary Conditions

- Same lattice for MRT and FD scheme
- Dirichlet condition: quadratic polynomial extrapolation
- Neumann condition: cubic polynomial extrapolation

$$T = T_{bc} \Big|_{r=\frac{1}{2}} \Rightarrow T(r=0) = \frac{8}{3} T_{bc} - 2T(1) + \frac{1}{3} T(2)$$

$$\frac{\partial T}{\partial r} = 0 \Big|_{r=\frac{1}{2}} \Rightarrow T(r=0) = \frac{21}{23} T(1) + \frac{3}{23} T(2) - \frac{1}{23} T(3)$$



Coupling of LBE and Thermal Model

The coupling of the temperature field to the energy mode of the LB model is done by inserting the temperature into the equilibrium moments:

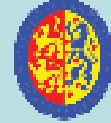
HTLBE – Hybrid thermal lattice Boltzmann equation

$$m_1^{eq} = ((3T - 1) + (u_x^2 + u_y^2 + u_z^2)) \rho_0$$

$$m_2^{eq} = (1 - 18T) \rho_0$$

$$T = T(t, i, j, k)$$

P. Lallemand, L. Luo,
Phys. Rev. E 68, 036706 (2003)



Characteristic Quantities

Rayleigh, Prandtl and Nusselt Numbers

$$Ra = \frac{Pr g_z \beta (T_s - T_\infty) L^3}{\nu^2} \quad Pr = \nu / \alpha \quad Nu \equiv \frac{hL}{k} = \frac{\partial(T_s - T) / \partial y|_{y=0}}{(T_s - T_\infty) / L}$$

L = characteristic length

k_f = thermal conductivity of the fluid

h = convective heat transfer coefficient

T_s = surface temperature

α = thermal diffusivity

β = thermal expansion coefficient

Validation study:

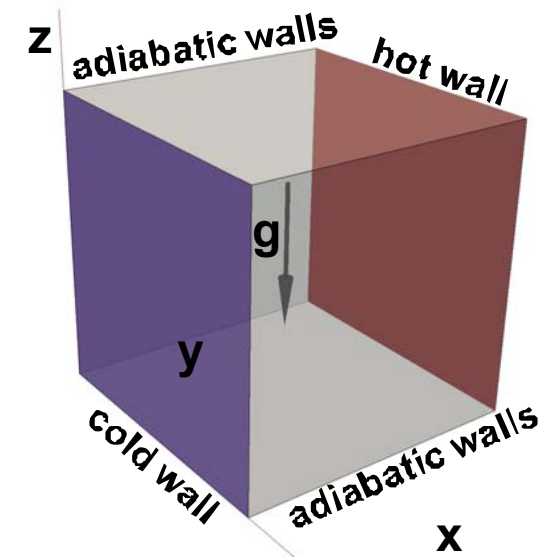
Rayleigh-Benard convection in a closed cavity
for Rayleigh numbers $> 1e9$ LES is applied

$$1e5 < Ra < 2e7 \Rightarrow Nu \approx 0.54 Ra^{1/4}$$

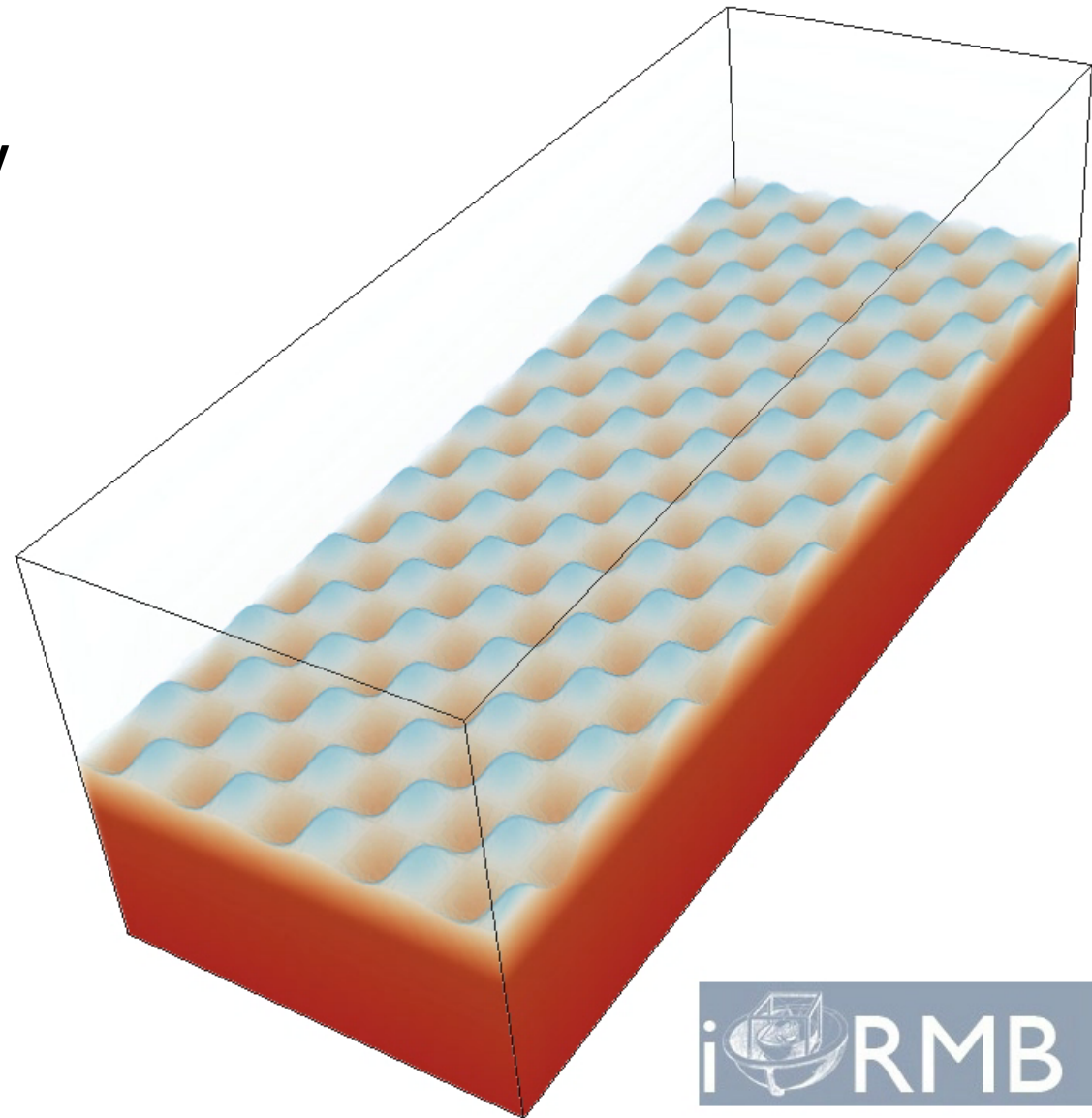
$$2e7 < Ra < 3e10 \Rightarrow Nu \approx 0.14 Ra^{1/3}$$

$$Ra < 1e13 \Rightarrow Nu \approx 0.825 + \left\{ \frac{0.387 Ra^{1/6}}{\left[1 + (0.492/Pr)^{9/16} \right]^{8/27}} \right\}^2$$

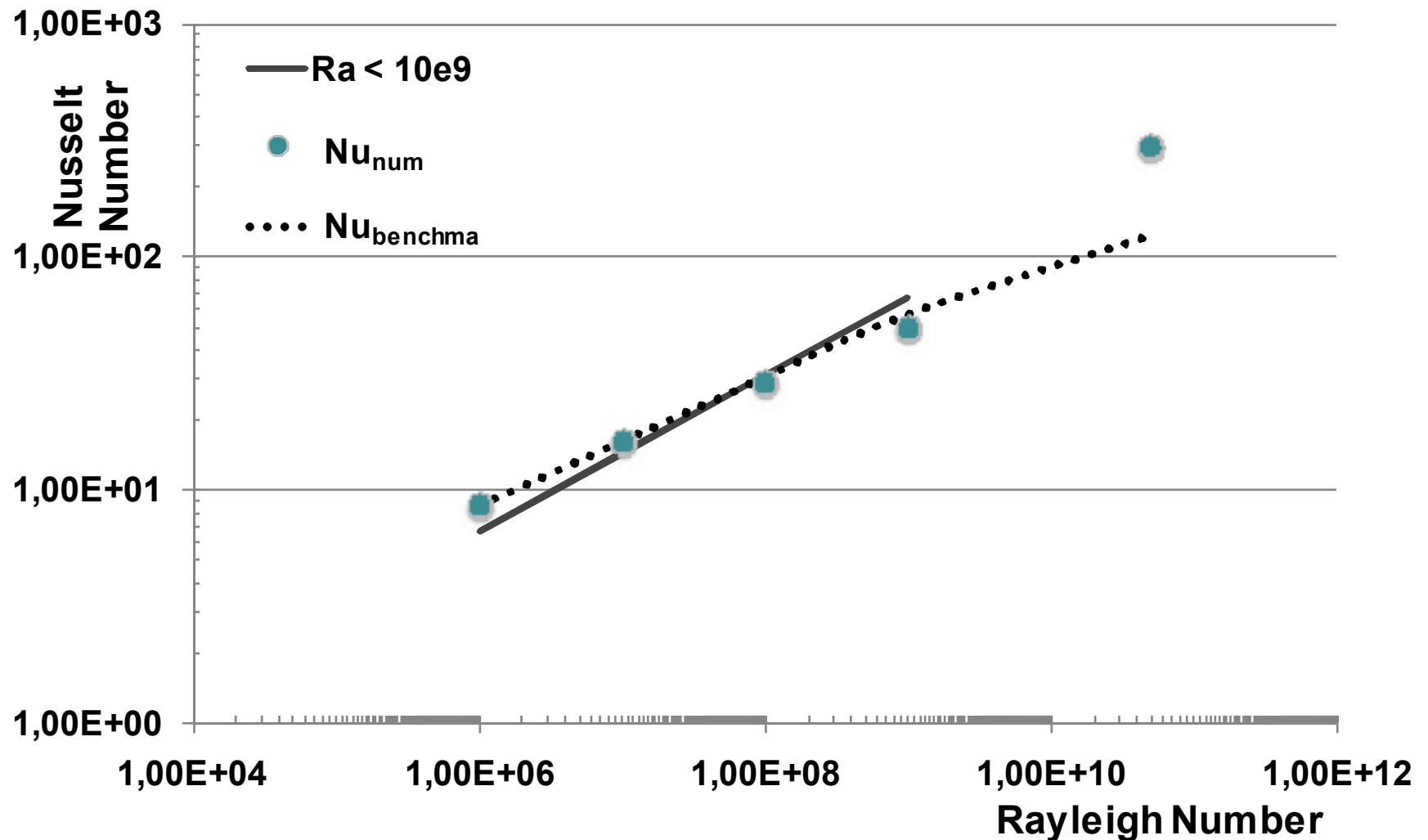
$$Ra < 1e9 \Rightarrow Nu \approx 0.68 + \frac{0.670 Ra^{1/4}}{\left[1 + (0.492 / Pr)^{9/16} \right]^{4/9}}$$



Rayleigh-Benard instability
 $Ra=2 \times 10^{10}$
400x150x150 grid nodes



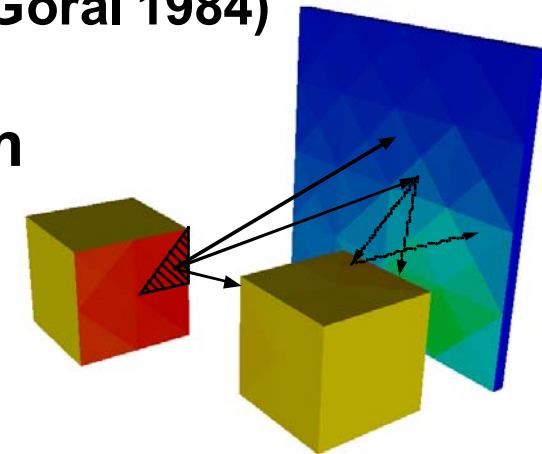
Comparison of theoretical prediction, benchmark data and numerical results:



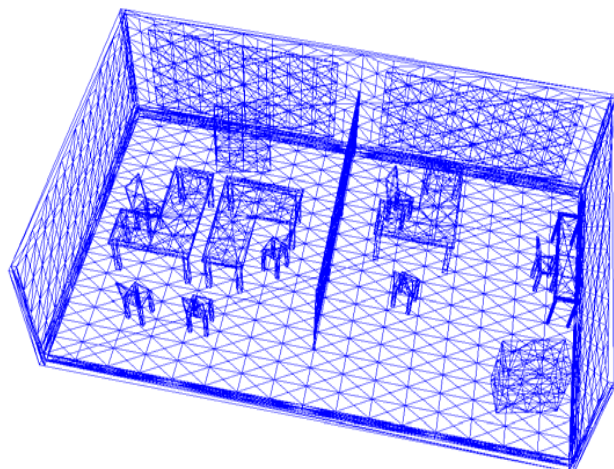
The Radiosity equation for radiative heat transfer (Goral 1984)

$$B_i = E_i + \rho_d \sum_{j=1}^n B_j F_{ij} \quad \text{heat flux equilibrium}$$

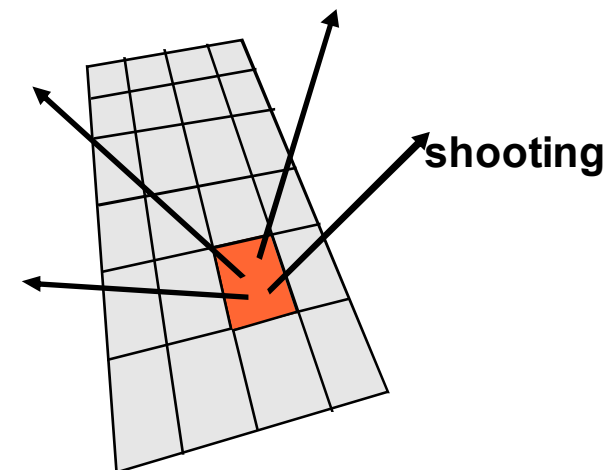
$$\begin{pmatrix} B_1 \\ B_2 \\ \dots \\ B_n \end{pmatrix} = \begin{pmatrix} E_1 \\ E_2 \\ \dots \\ E_n \end{pmatrix} + \begin{pmatrix} \rho_1 F_{11} & \rho_1 F_{12} & \dots & \rho_1 F_{1n} \\ \rho_2 F_{21} & \rho_2 F_{22} & \dots & \rho_2 F_{2n} \\ \dots & \dots & \dots & \dots \\ \rho_n F_{n1} & \rho_n F_{n2} & \dots & \rho_n F_{nn} \end{pmatrix} \cdot \begin{pmatrix} B_1 \\ B_2 \\ \dots \\ B_n \end{pmatrix}$$



radiation exchange



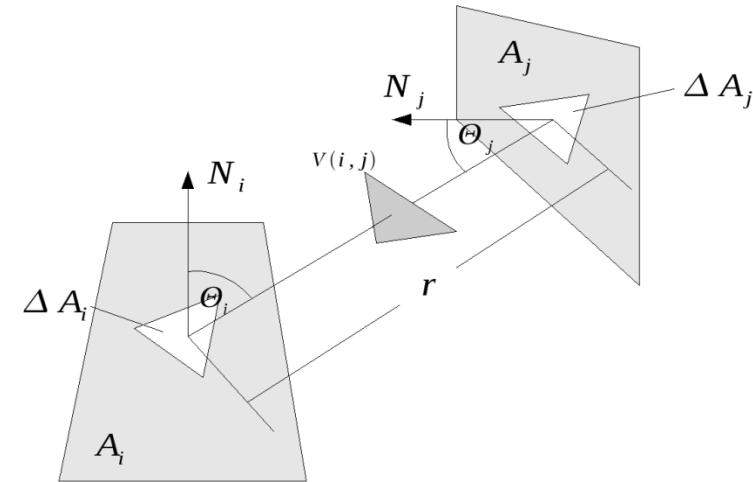
surface mesh



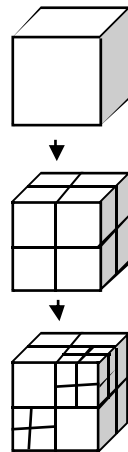
shooting

Formfactor

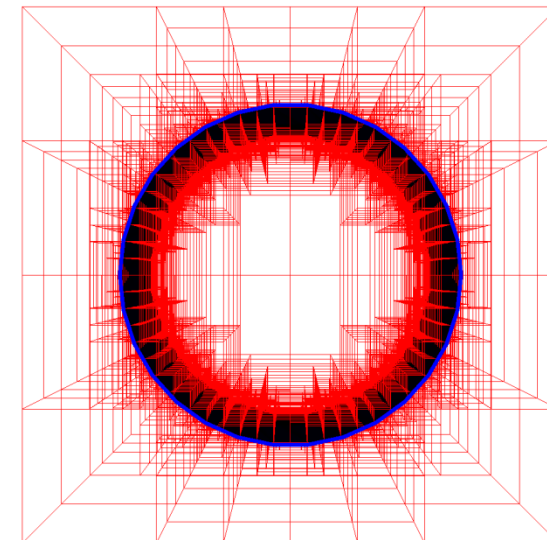
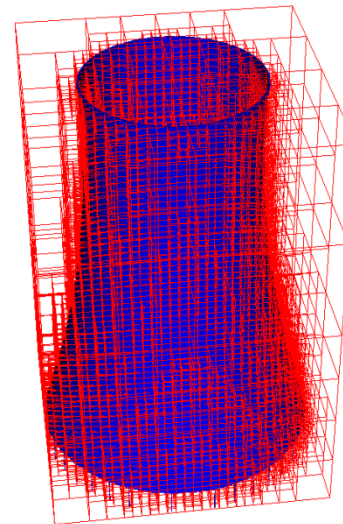
$$F_{ij} = \frac{\cos \Theta_i \cos \Theta_j}{\Pi r^2} V(p_i, p_j) A_i$$



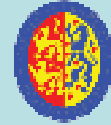
Efficient hierarchical visibility test



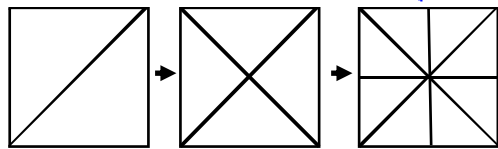
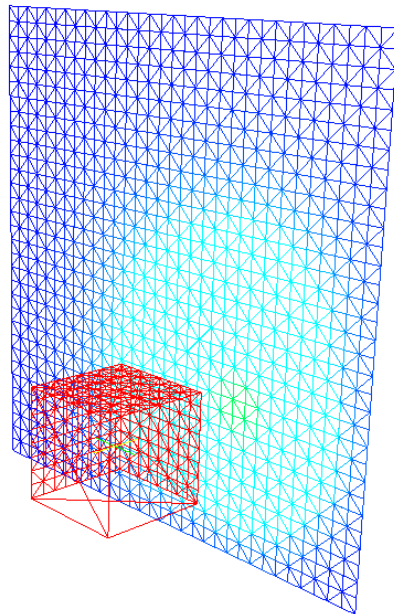
recursive subdivision into octants



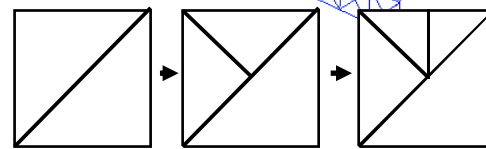
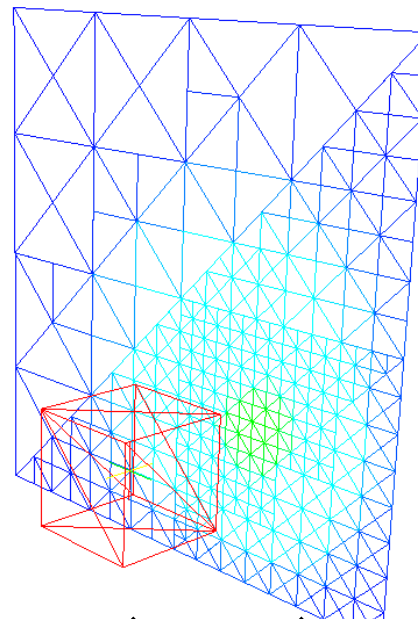
octree



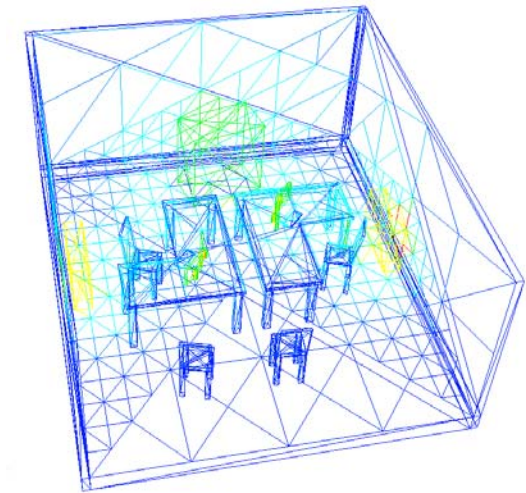
Mesh generation



a-priori mesh refinement



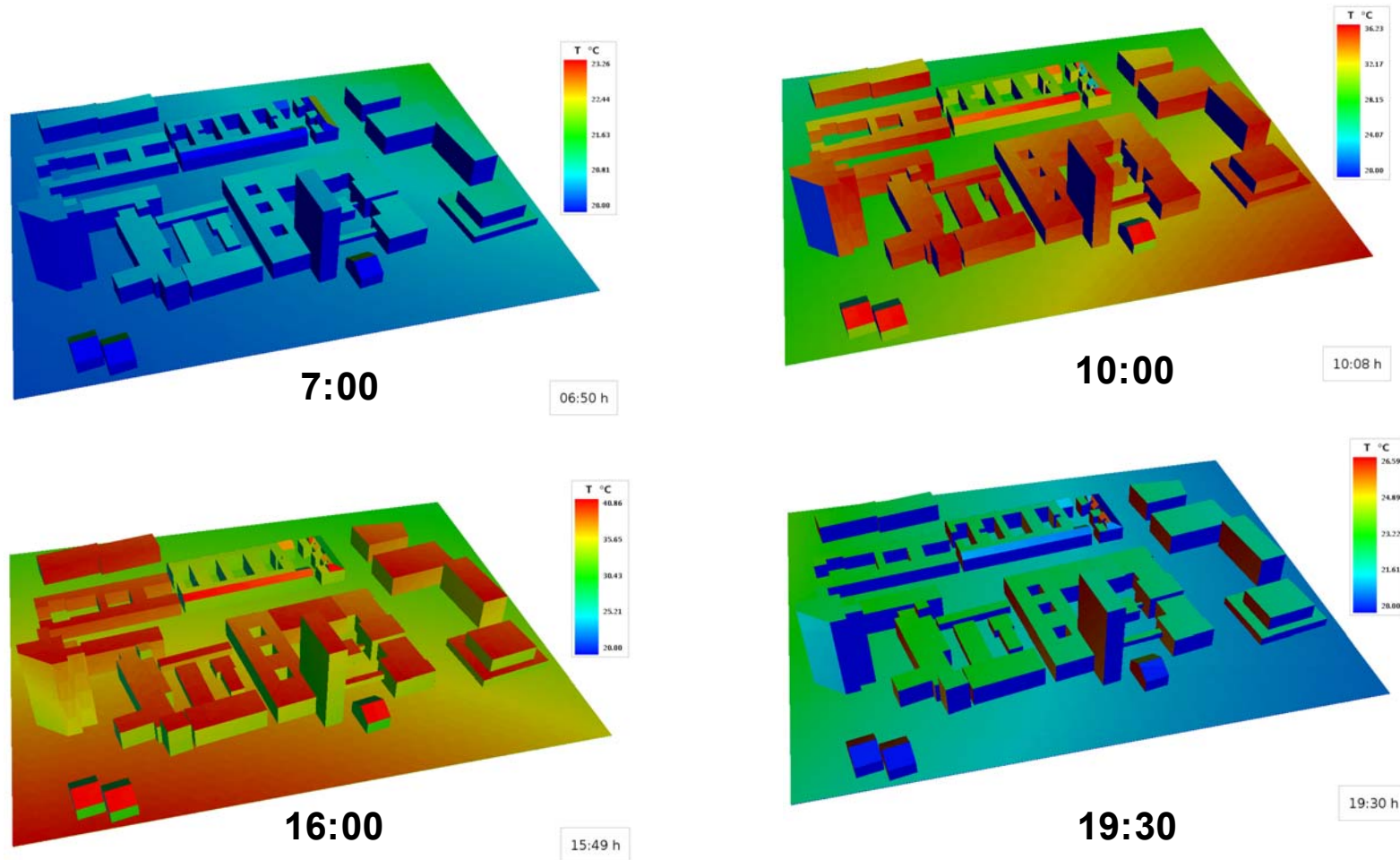
adaptive mesh refinement

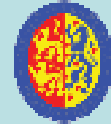


**office with adaptively
refined mesh**

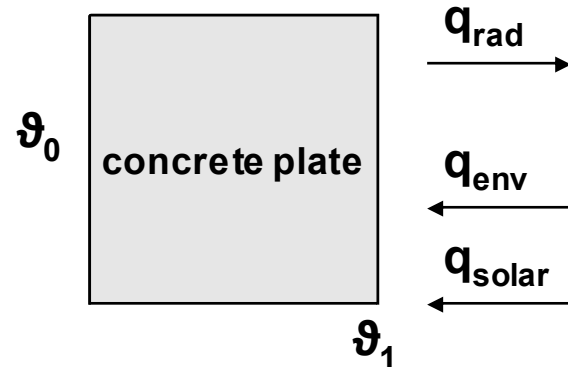
Examples

Surface temperature induced by solar radiation (Campus TU Braunschweig)





Coupling radiative heat transfer and heat conduction

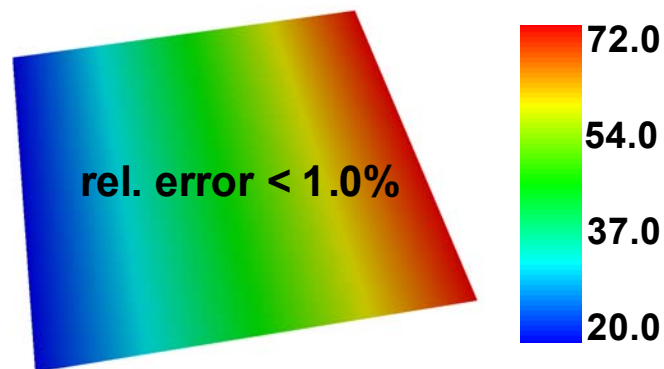


heat equation for stationary temperature fields in isotropic bodies

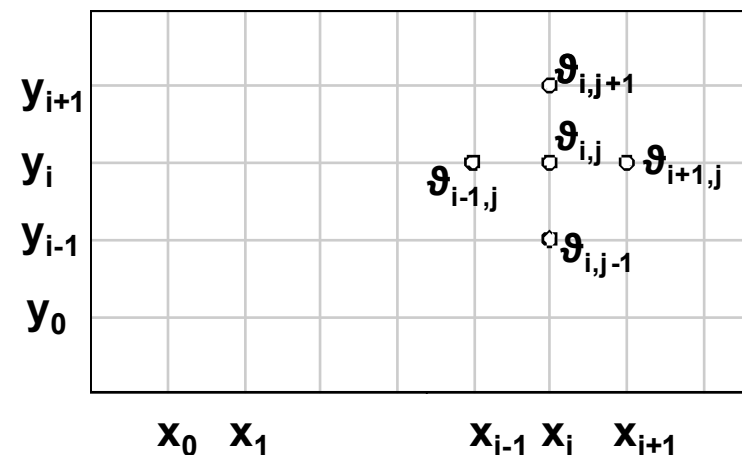
$$q = \frac{\lambda}{dx} (\vartheta_1 - \vartheta_0)$$

heat equation for non-stationary temperature fields with heat sources

$$\frac{\partial \vartheta}{\partial t} = \frac{\lambda}{c\rho} \left(\frac{\partial^2 \vartheta}{\partial x^2} + \frac{\partial^2 \vartheta}{\partial y^2} \right) + \frac{\dot{W}(x,y,t,\vartheta)}{c\rho}$$



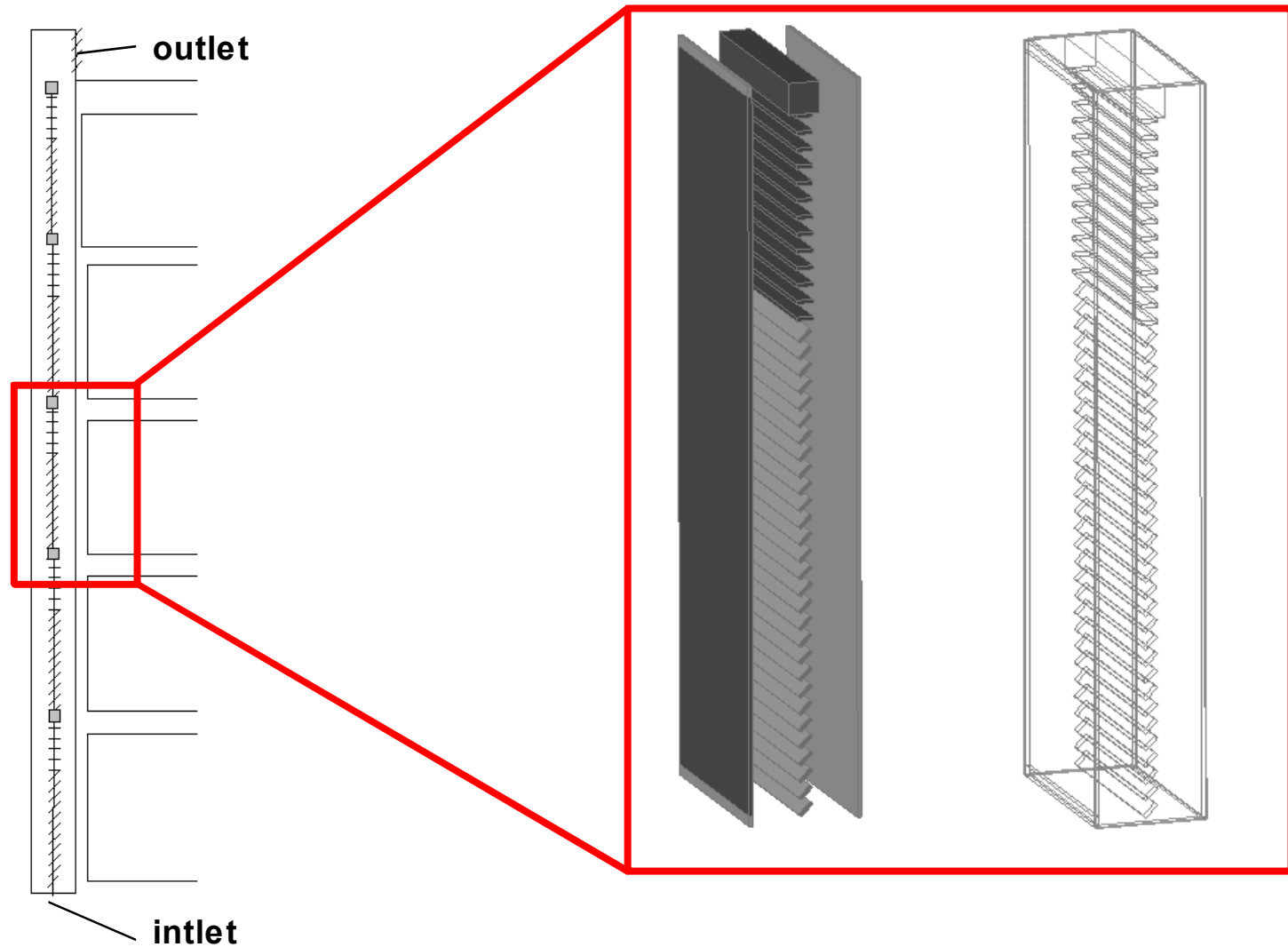
grid discretization



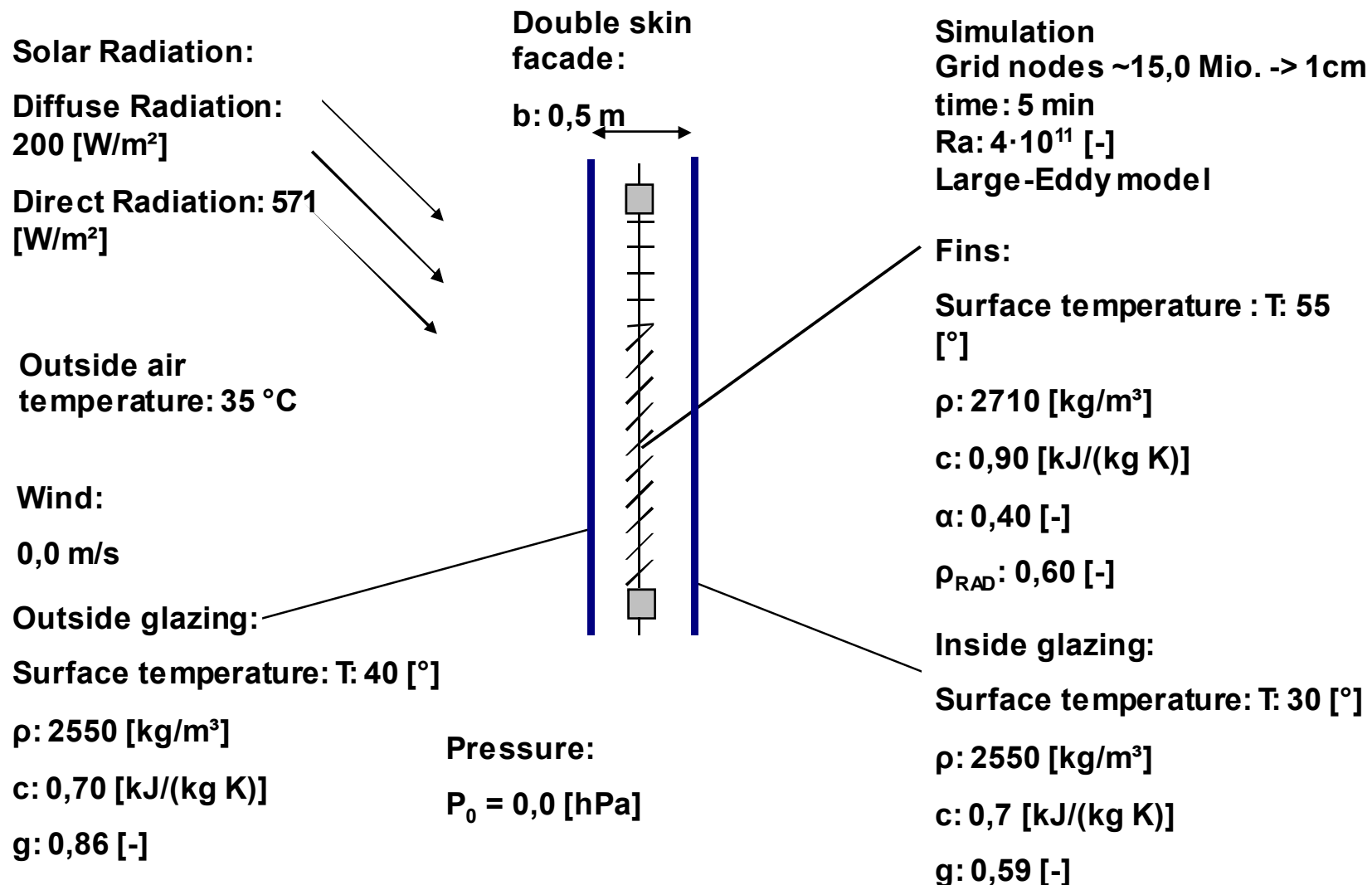
$$\vartheta_{i,j}^{k+1} = (1 - 2M_x - 2M_y) \vartheta_{i,j}^k + M_x (\vartheta_{i-1,j}^k + \vartheta_{i+1,j}^k) + M_y (\vartheta_{i,j-1}^k + \vartheta_{i,j+1}^k) + \frac{\Delta t}{c\rho} \dot{W}_{i,j}^k$$

$$M_x := \frac{a\Delta t}{\Delta x^2} \quad \wedge \quad M_y := \frac{a\Delta t}{\Delta y^2}$$

Heat flux in double skin facade

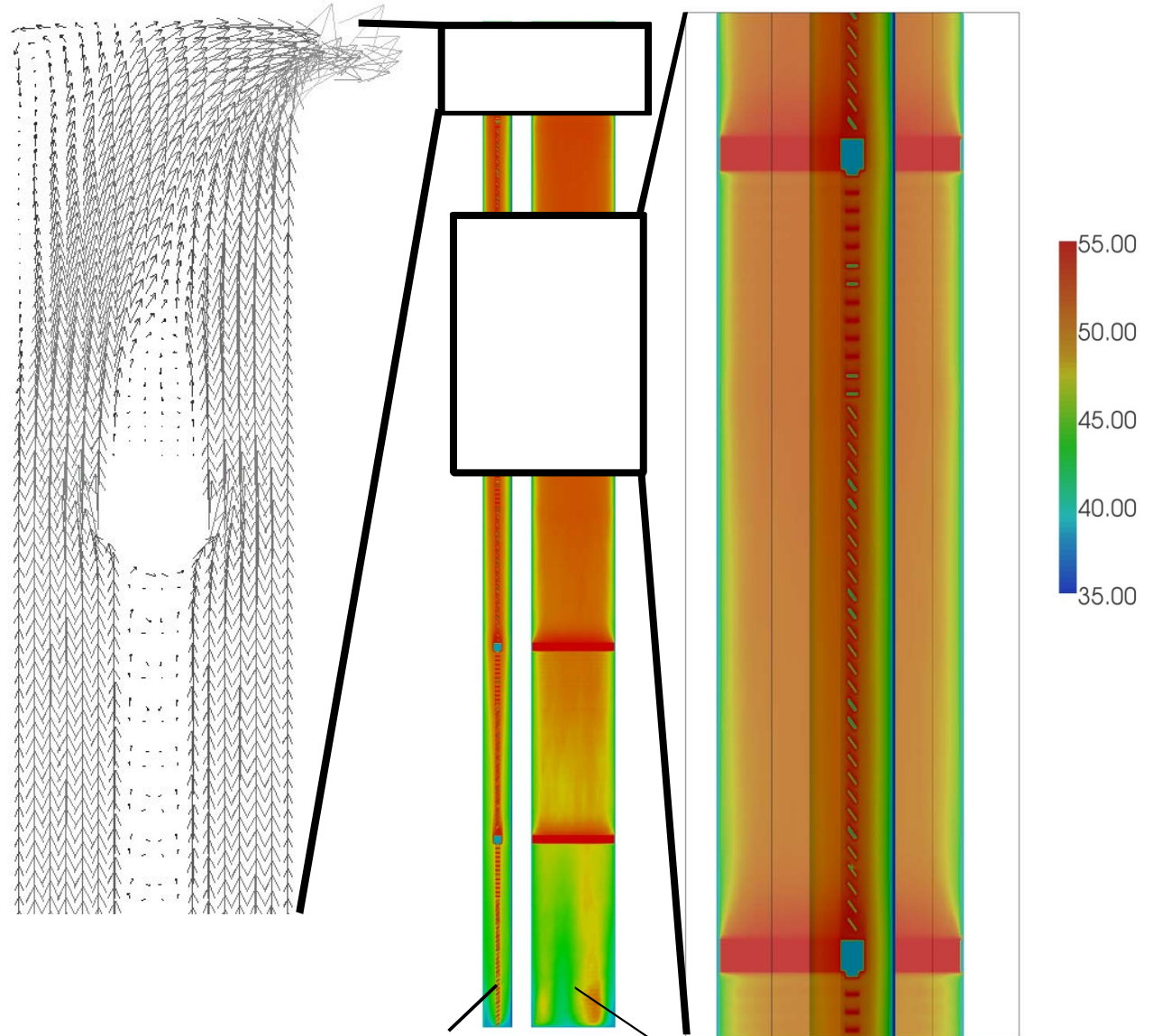
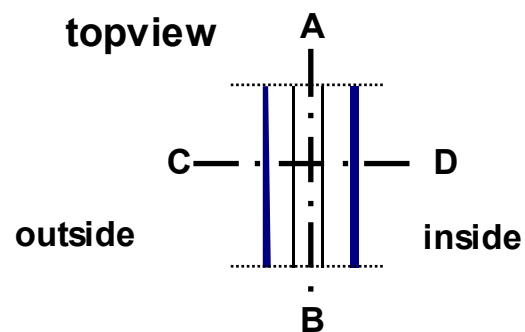


Thermal Fluid Simulation – Boundary Conditions



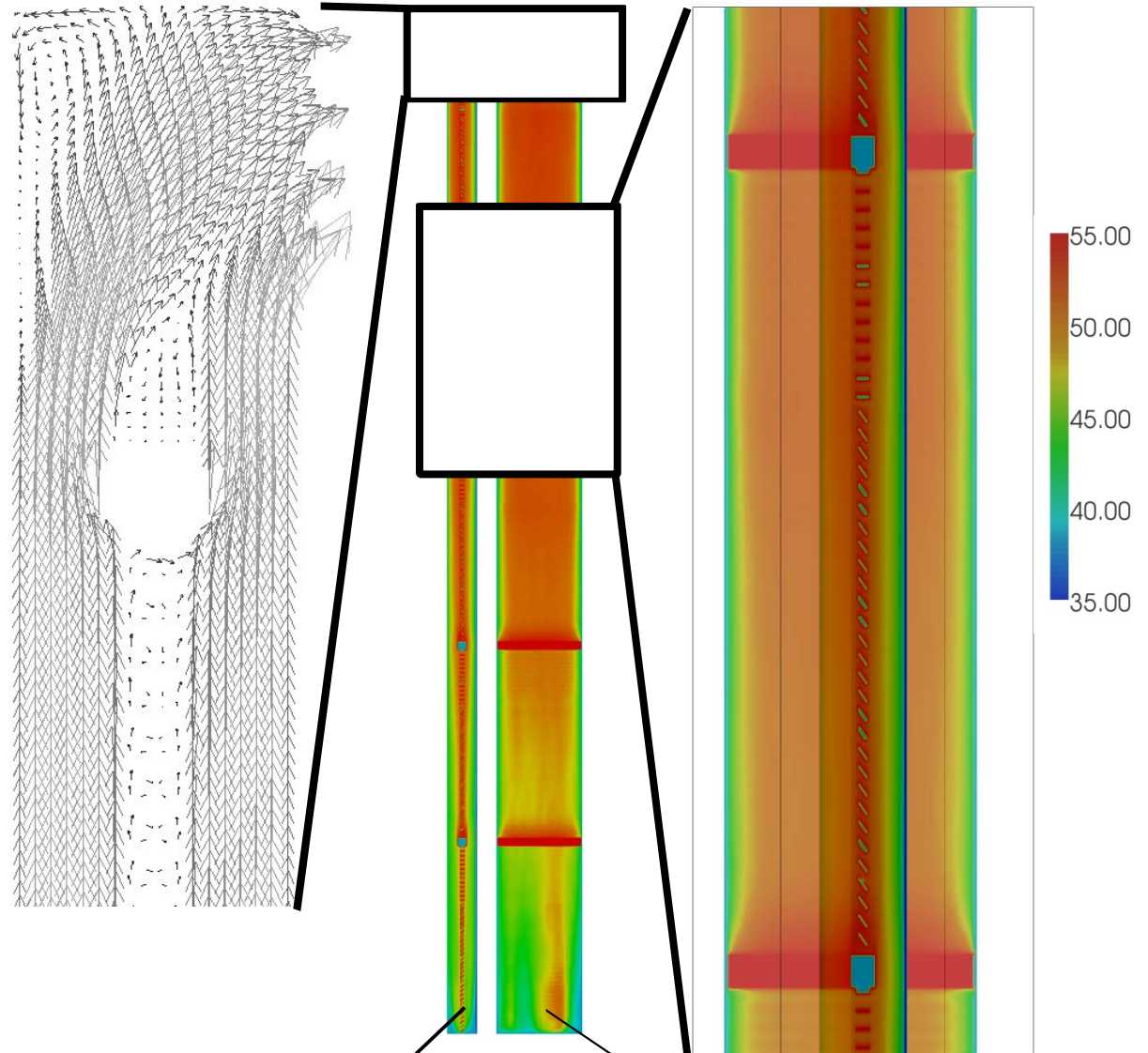
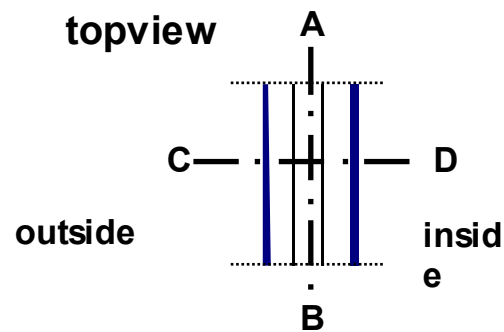
Variant d) 0.25 m outlet

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]



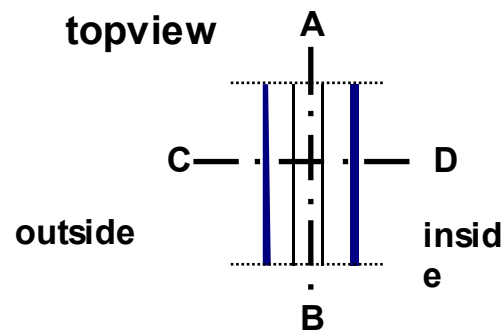
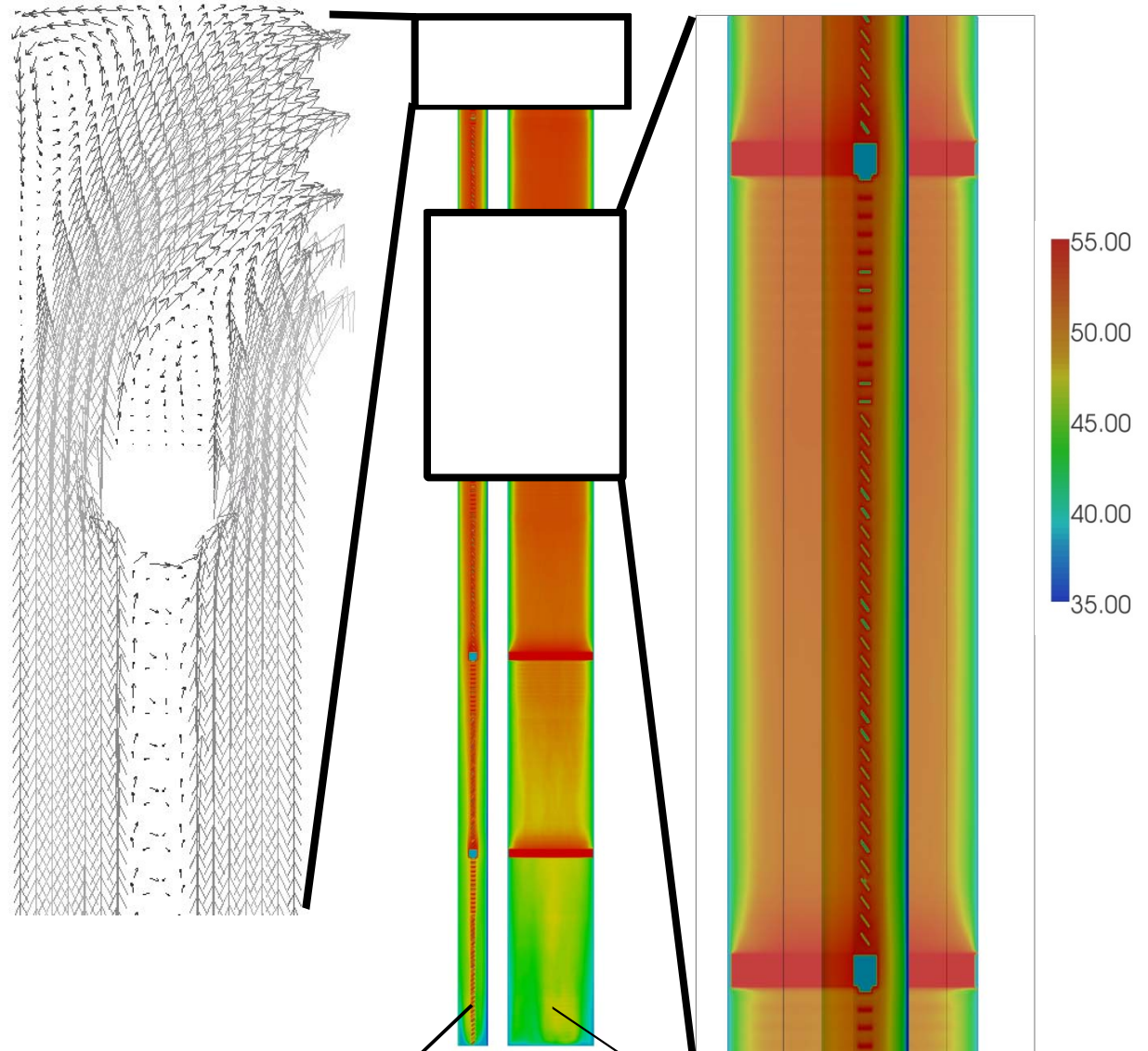
Variant d) 0.5 m outlet

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]



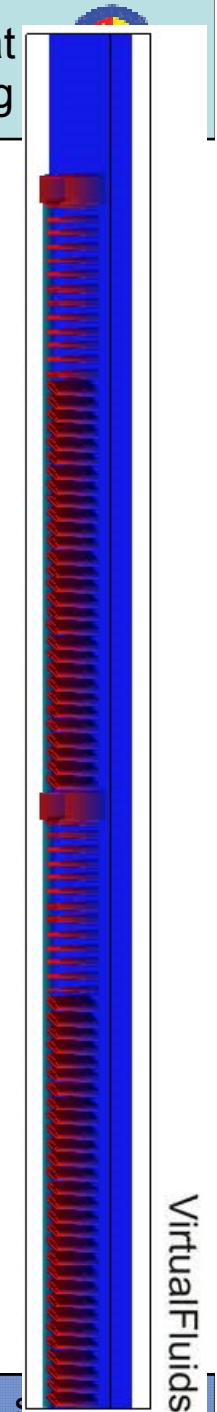
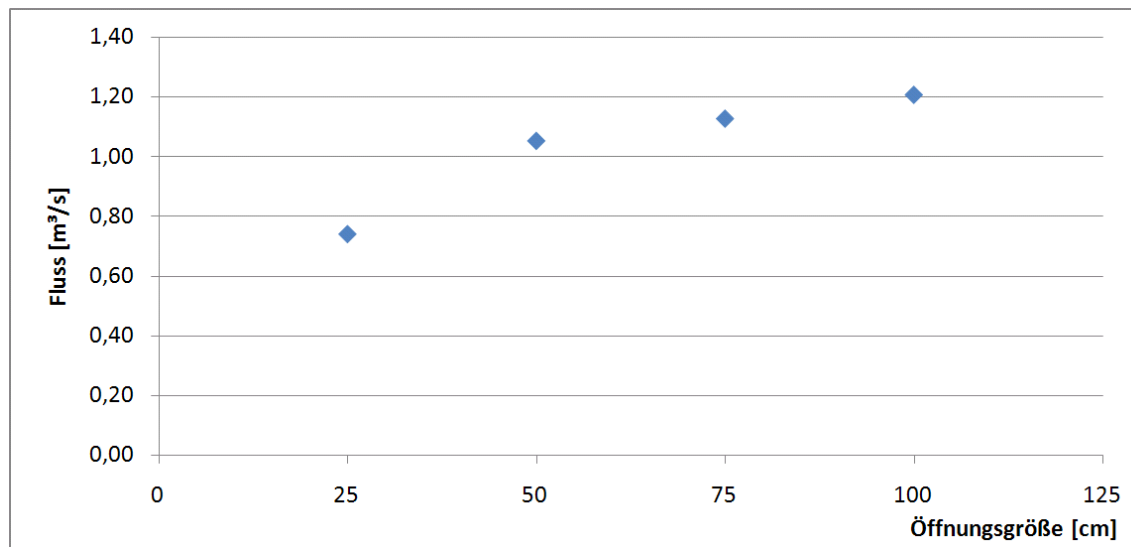
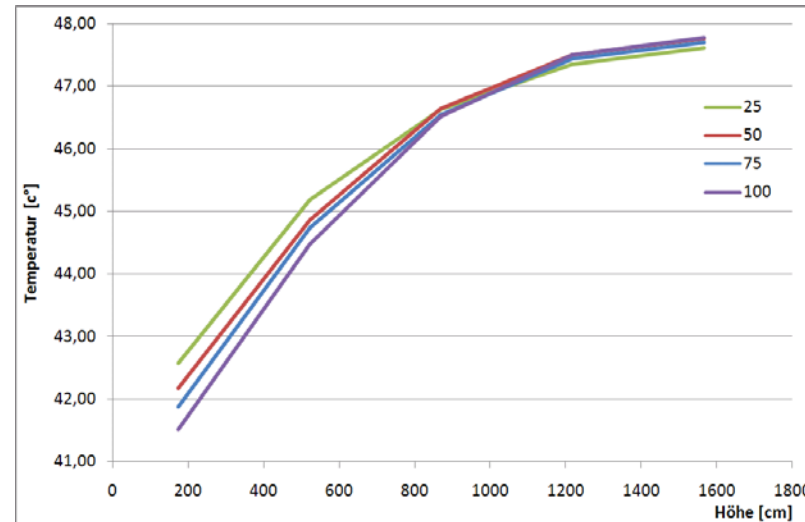
Variant d) 0.75 m outlet

flux	1.13	[m ³ /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]



Variant d) 1.0 m outlet

flux	1.21	[m ³ /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]

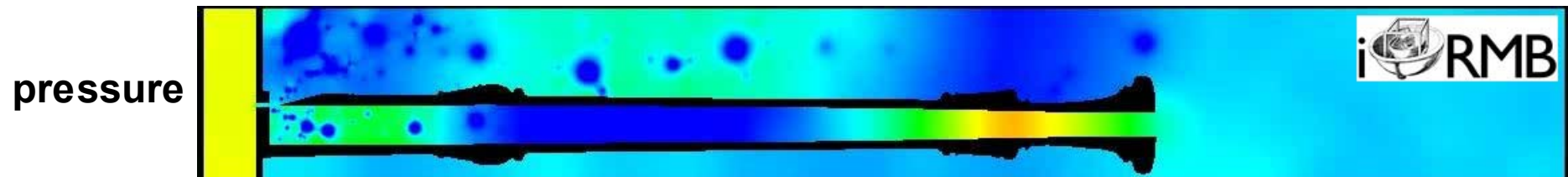


Flow acoustics

LB-solution of the wave equation
$$\frac{\partial^2 v'}{\partial t^2} - \left(c_0^2 + \left(\frac{4}{3} \nu + \nu' \right) \frac{\partial}{\partial t} \right) \frac{\partial^2 v'}{\partial x^2} = 0$$

Flute: $Re=6000$, air, $f_0=415$ Hz

Simulation: 8×10^6 grid nodes, 10^6 dt, 6 h on single GPU: **$f_0=413$ Hz**



LODI BCns for LB: Izquierdo & Fueyo, Phys. Rev. E 78, 046707 (2008)

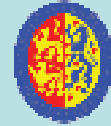
Conclusions

- Coupled problems: feasible with LBM
- Required: MRT, 2nd order BCns, grid refinement, HPC
- GPU 😊

Outlook

- Improved turbulence models (WALE), wall functions
- 3D-grid refinement (also for GPU)
- local BCns in 3D
- Multi-level parallelization CPU/GPU, fault tolerance, postprocessing
- Improved multiphase models
- further validation studies for coupled problems

... and the best news is ...



... some work is still left to do !

