ERCOFTAC Spring Festival
Gdańsk, May 12-13, 2011

Multiphase flow modelling using particle methods

Group of Hydrodynamics and Multiphase Flow - selected research activities

Jacek Pozorski

with contributions of **Arkadiusz Grucelski,** **Mirosław Łuniewski** and **Kamil Szewc**

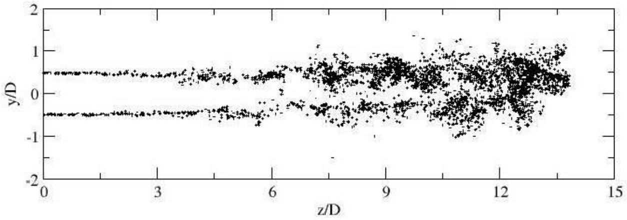
Institute of Fluid-Flow Machinery,
Polish Academy of Sciences, Gdańsk, Poland

Group of Hydrodynamics and Multiphase Flow in a nutshell

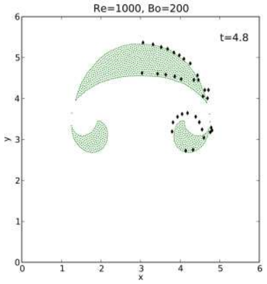
People: *2 research associates (Dr.), 1 research assistant, 4 PhD students*

Main areas of interest:

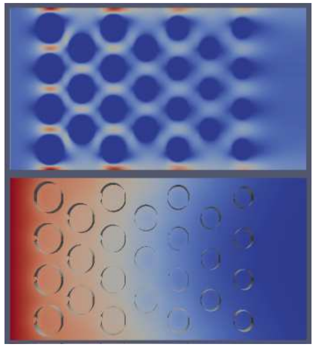
- Lagrangian stochastic approach (PDF) and hybrid particle methods
  (RANS/PDF, LES/FDF, POD/FDF):
  near-wall turbulence, flows with scalar variables



- **modelling turbulent dispersed flows***
  COST Actions: „LES AID”, „Particles in Turbulence”



- **developments of Smoothed Particle Hydrodynamics (SPH) for flows with interfaces***
  collaboration with EDF R&D, France



- **porous media flow and heat transfer with Lattice Boltzmann (LBM)***
  collaboration with the Inst. of Chemical Processing of Coal, Zabrze
- flow design (inverse problem solution or vortex methods),
- longer-term: *combustion, also in two-phase flow*

** topics addressed in this talk*

LES particle-laden turbulent flows

reconstruction of SGS flow velocity

In particle equation of motion,
fluid velocity at particle location is needed:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{U}_p$$
$$\frac{d\mathbf{U}_p}{dt} = f_D\frac{\mathbf{U}_f^* - \mathbf{U}_p}{\tau_p}$$
$$\frac{dT_p}{dt} = f_\theta\frac{T_f^* - T_p}{\tau_\theta}$$

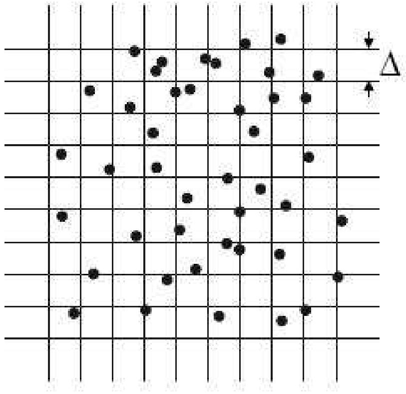
particle velocity $\mathbf{U}_p$; **fluid velocity** $\mathbf{U}_f$; **in LES:** $\mathbf{U}_f = \bar{\mathbf{U}}_f + \mathbf{u}_f$

fluid velocity along particle trajectory: $\mathbf{U}_f^* = \mathbf{U}_f(\mathbf{x}_p, t)$, **or** $\mathbf{U}_f^* = \bar{\mathbf{U}}_f(\mathbf{x}_p, t) + \mathbf{u}_f^*$

fluid temperature seen by particles: $T_f^* = T_f(\mathbf{x}_p, t)$, **in general** $T_f^* = \bar{T}_f(\mathbf{x}_p, t) + \theta_f^*$

LES filtering impacts on:

pref.conc., slip vel. → coolling rate
particle tke → wall deposition
slip vel., rel.temp. → cooling/heatig, evaporation



Langevin eq. for SGS fluid velocity along particle trajectories

$$d\mathbf{u}_i^* = -\frac{\mathbf{u}_i^*}{\tau_L^*}dt + \sqrt{\frac{4k_{sg}}{3\tau_L^*}}dW_i$$

[Pozorski et al., CTR SP 2004,
Shotorban & Mashayek, PoF 2006,
Pozorski & Apte, IJMF 2009]

LES results of particle-laden turbulent channel flow

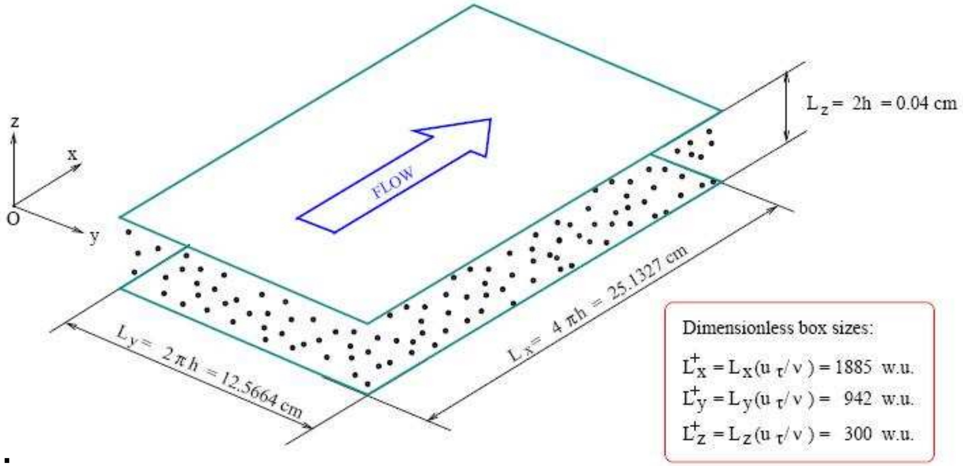
Flow case: turbulent channel flow at $\mathrm{Re}_\tau = 150$ (benchmark of COST Action LES-AID)

- domain size in streamwise (x), wall-normal (y) and spanwise (z) directions:

  $$4\pi h \times 2h \times (4/3)\pi h$$

- discretisation: $64 \times 84 \times 64$ FV meshes
- the mesh: uniform with $\Delta x^+ = 29.5$, $\Delta z^+ = 9.8$,

  $\Delta y^+ = 0.17$ at the wall up to $\Delta y^+ = 10$ at the CL

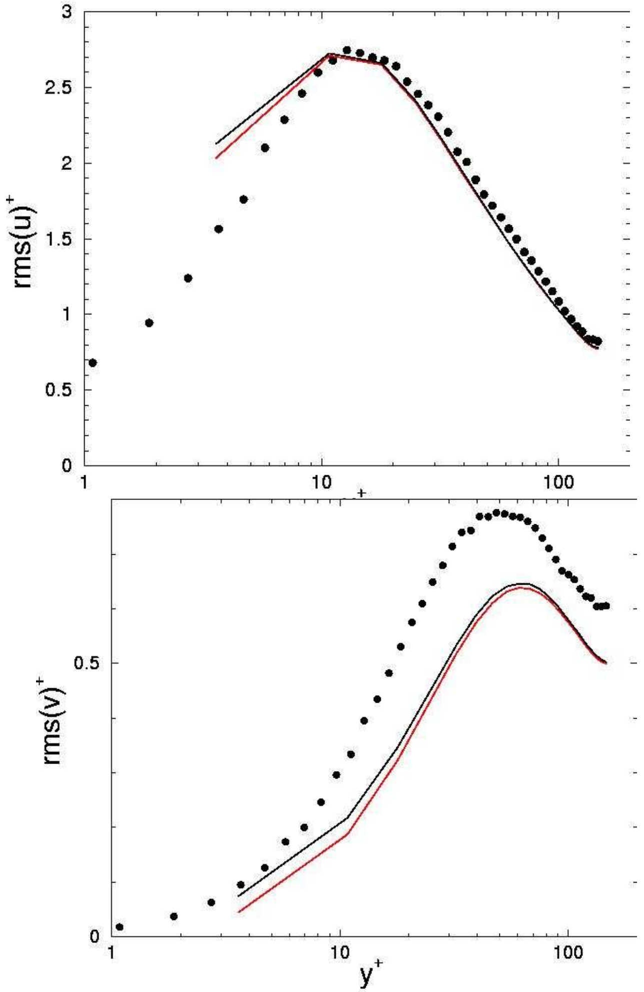


DNS data available for particle dynamics:

[Marchioli, Soldati, Kuerten et al., IJMF 2008]

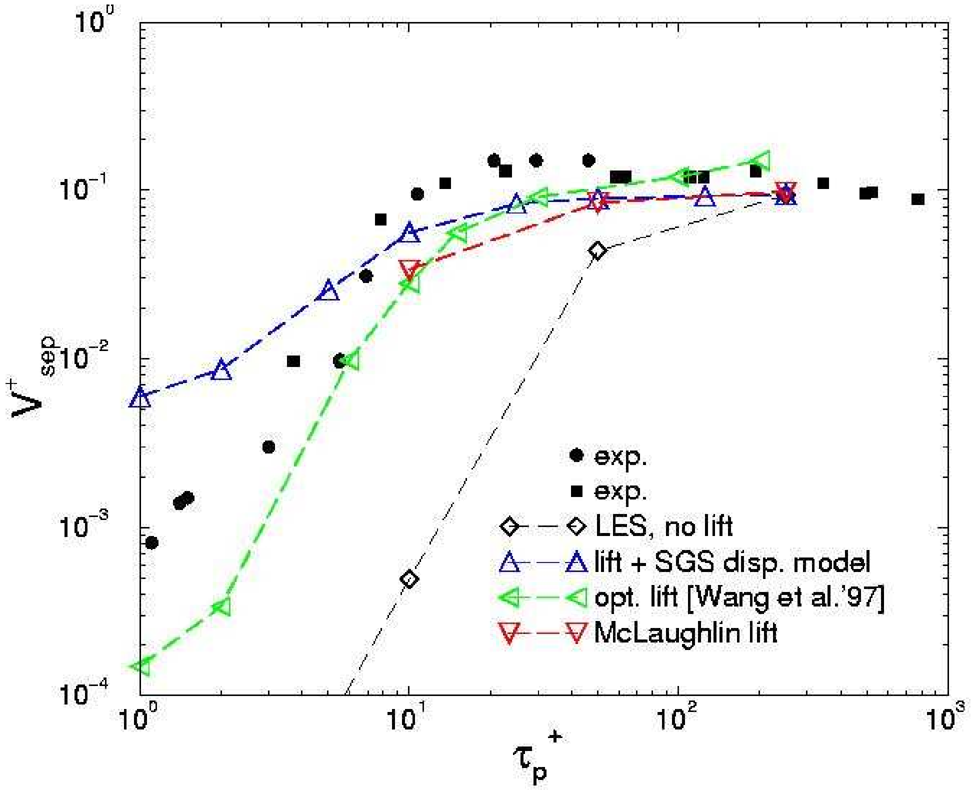
Channel flow:

intensity of particle velocity fluctuations, deposition rate



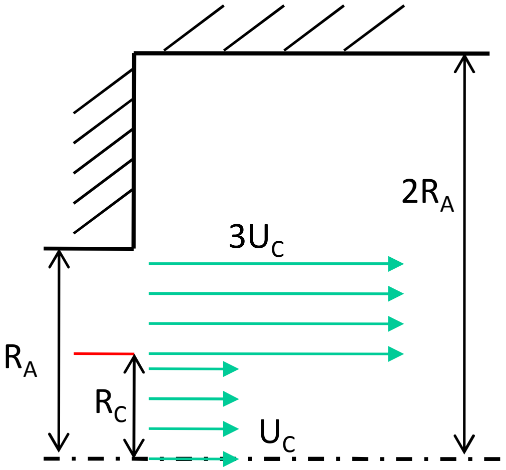
Particle rms velocity: a) streamwise, b) wall-normal. Particles of St=1. Symbols: DNS reference data; red lines: LES; black lines: LES with stochastic SGS particle dispersion model.

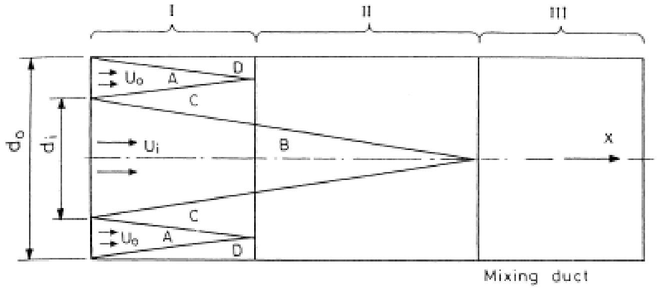
Deposition velocity
(mass flux of separating particles):



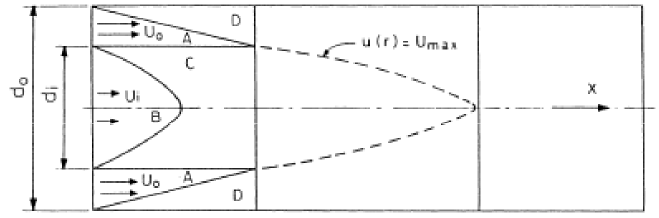
[Pozorski & Łuniewski, QLES 2007, 2009]

LES of coaxial jets



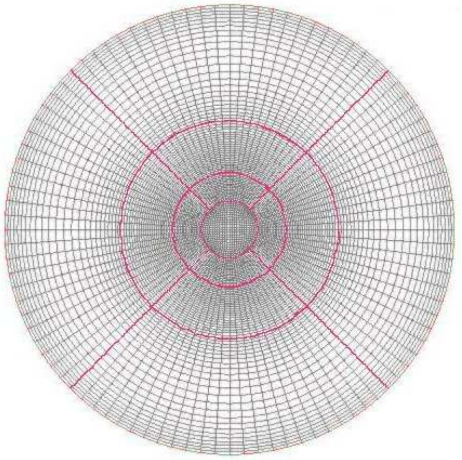


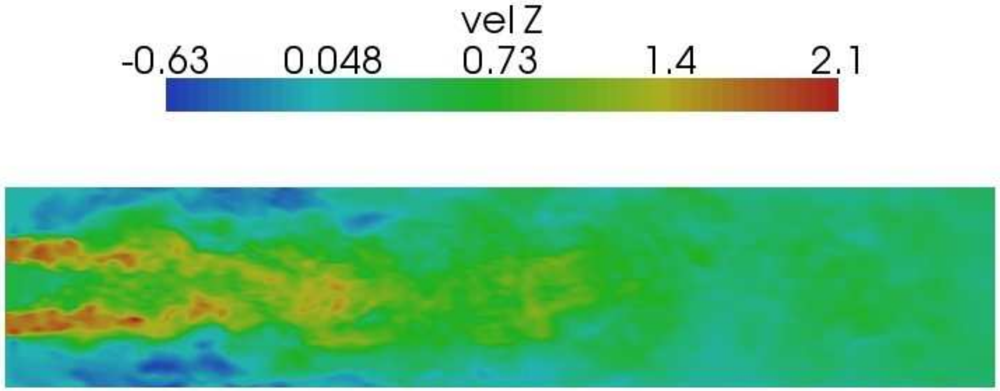
(a) $U_o/U_i = \lambda < 1$



(b) $U_o/U_i = \lambda > 1$

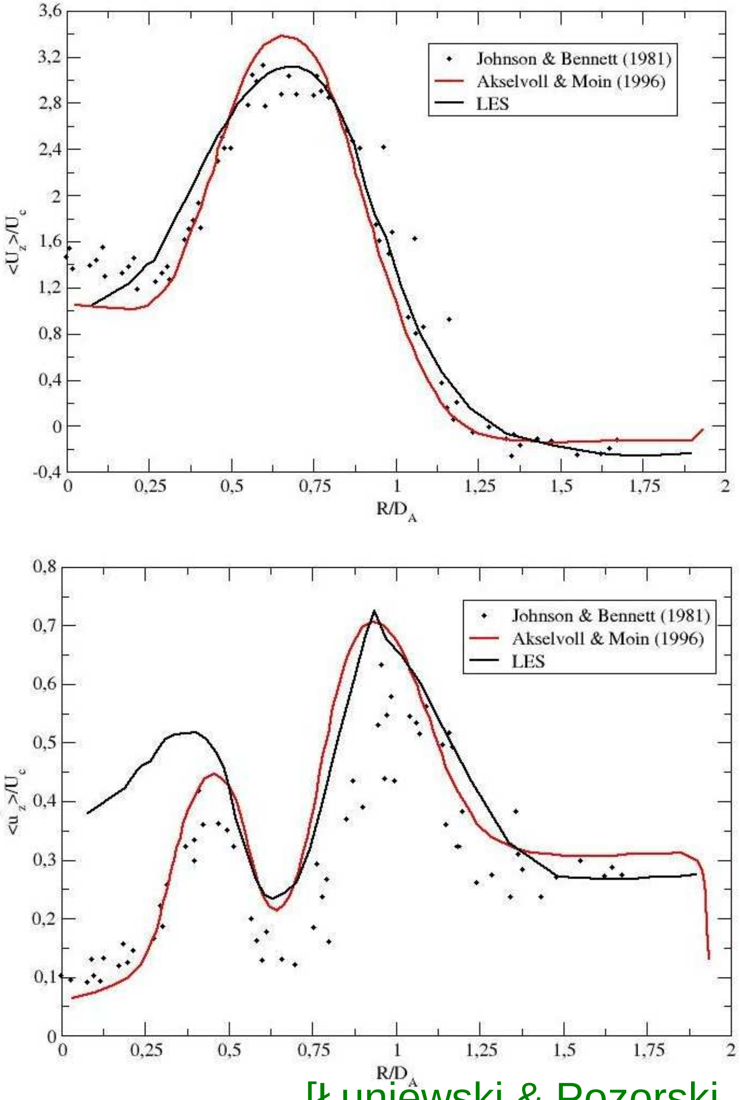
Computational domain in (r,θ,z) : $2D_A$ x 2π x $40D_A$
13-block structuralmesh, ~1.2M finite volumes,
academic solver Fastest3D + PTSOLV module



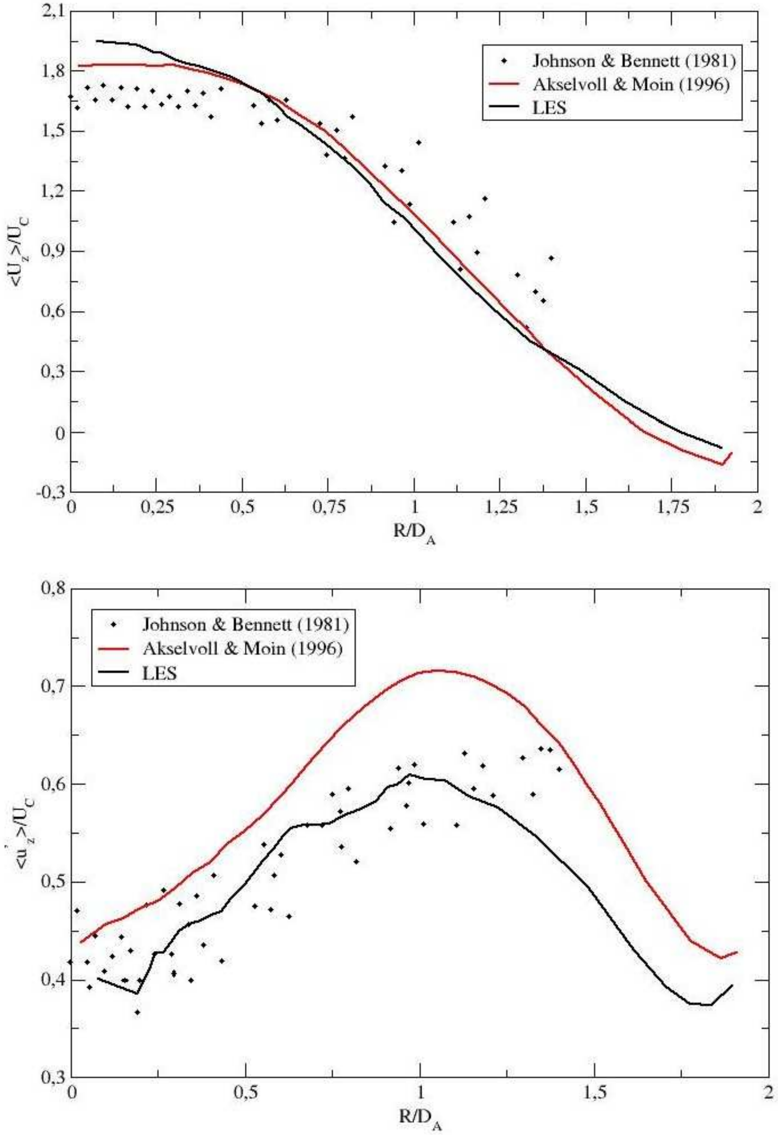


Coaxial jets: fluid velocity statistics

$z/D_A = 0.87$



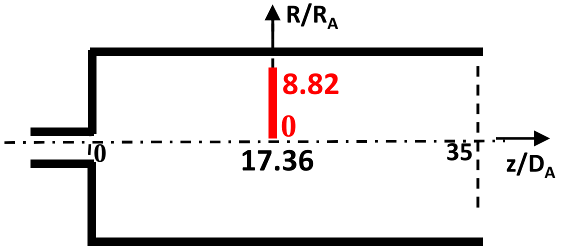
$z/D_A = 4.30$

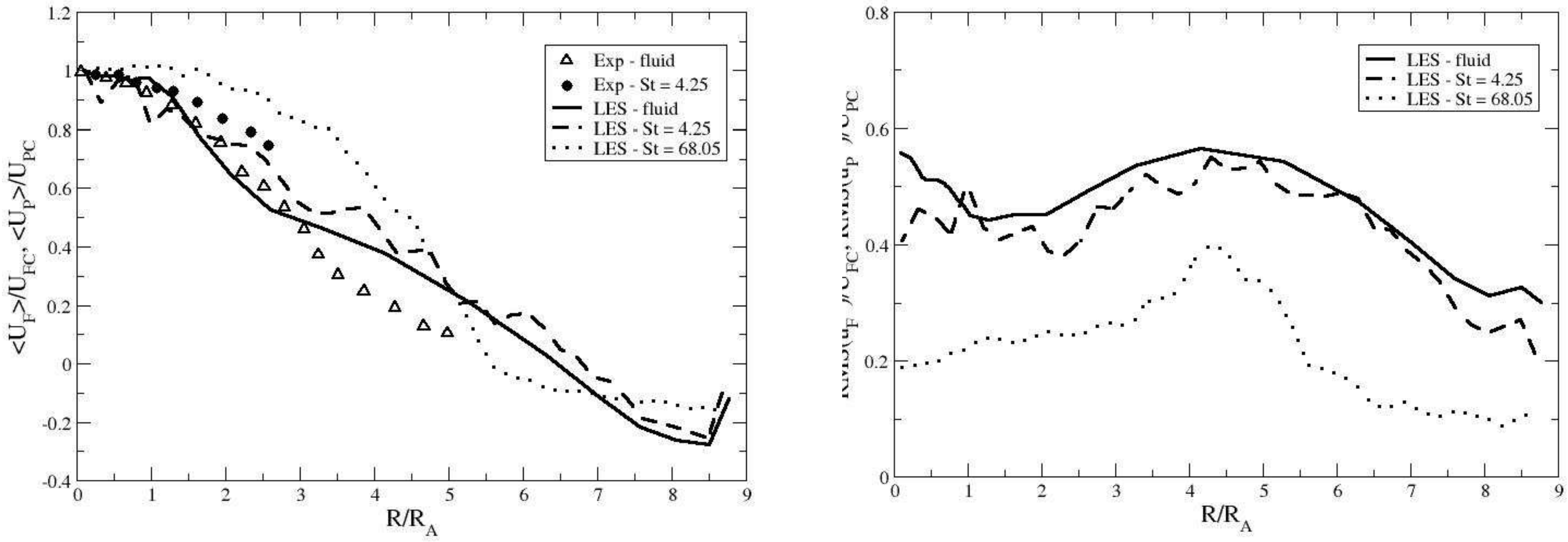


[Łuniewski & Pozorski, 2010]

Coaxial jets: fluid and particle velocity

Radial distribution of the axial velocity component at z/D_A = 17.36



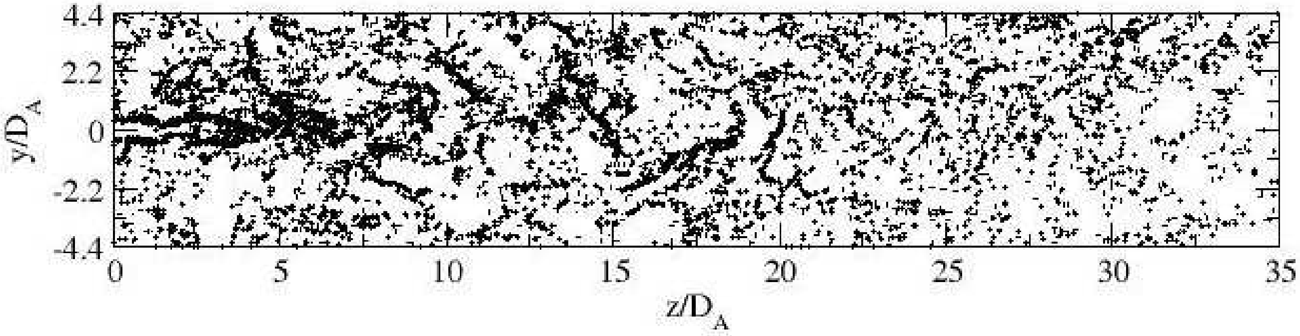


LES results for fluid and particles: (a) Mean axial velocity; (b) its fluctuation intensity.
Exp .: Fan, Zhao & Jin (*The Chemical Engineering Journal* 63, 1996)

[Łuniewski & Pozorski, 2010]

Coaxial jets: particle dispersion

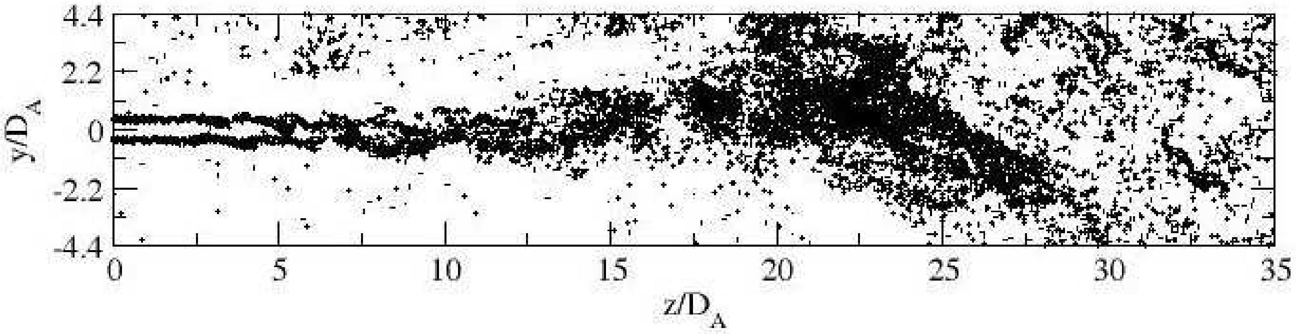
St = 4



$$St = \frac{\tau_p}{T_f} = \tau_p \frac{U_J}{D}$$

Stokes number

St = 68



Particle locations – Lagrangian tracking in the LES fluid field

[Łuniewski & Pozorski, 2010]

Smoothed Particle Hydrodynamics (SPH)

governing equations

The concepts of integral and summation interpolants:

$$\widetilde{A}(\mathbf{r}) = \int_{\Omega} A(\mathbf{r}')W(\mathbf{r} - \mathbf{r}', h)d\mathbf{r}'$$

$$\langle A \rangle (\mathbf{r}) = \sum_{b} A(\mathbf{r}_b)W(\mathbf{r} - \mathbf{r}_b, h)\Omega_b$$

SPH representation of the continuity equation:

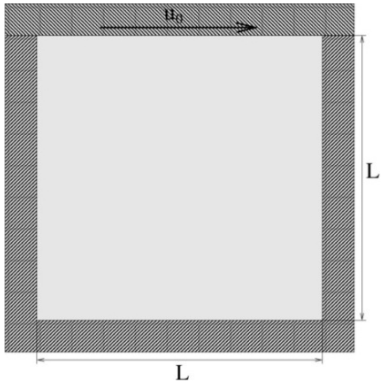
$$\frac{d\varrho_a}{dt} = -\varrho_a \sum_{b} \mathbf{u}_b \nabla_a W_{ab}(h) \frac{m_b}{\varrho_b}$$

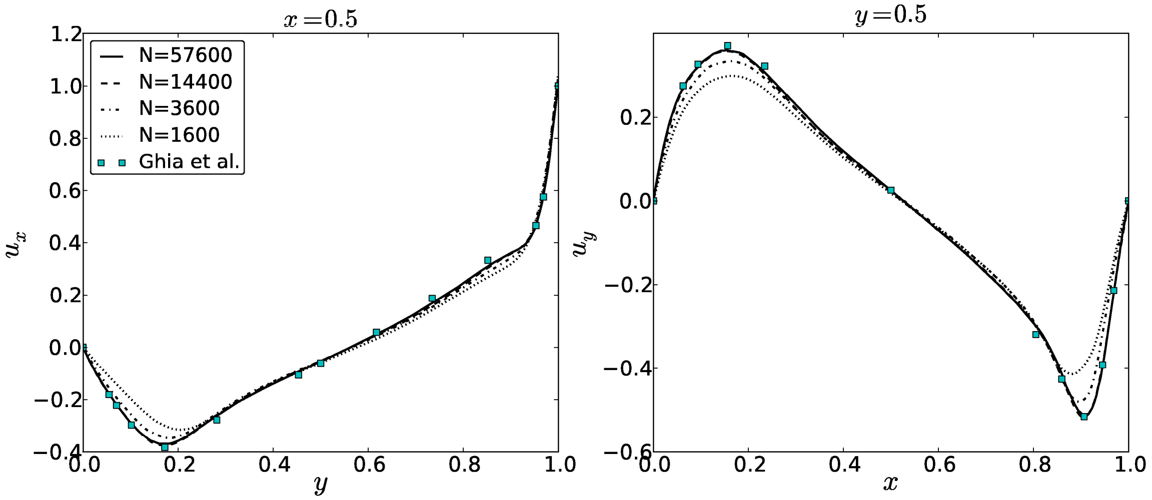
Smoothed Particle Hydrodynamics (SPH)

Incompressibility treatment; Validation case: lid-driven cavity

Developments in SPH: [Pozorski & Wawreńczuk & Szewc]

- truly incompressible formulation
- wall boundary conditions using ghost particles
- general (non-Boussinesq formulation) for buoyancy-driven flows
- modelling surface tension effects

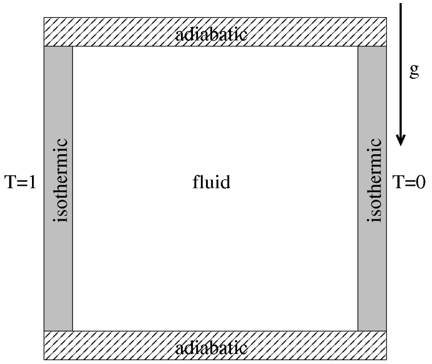




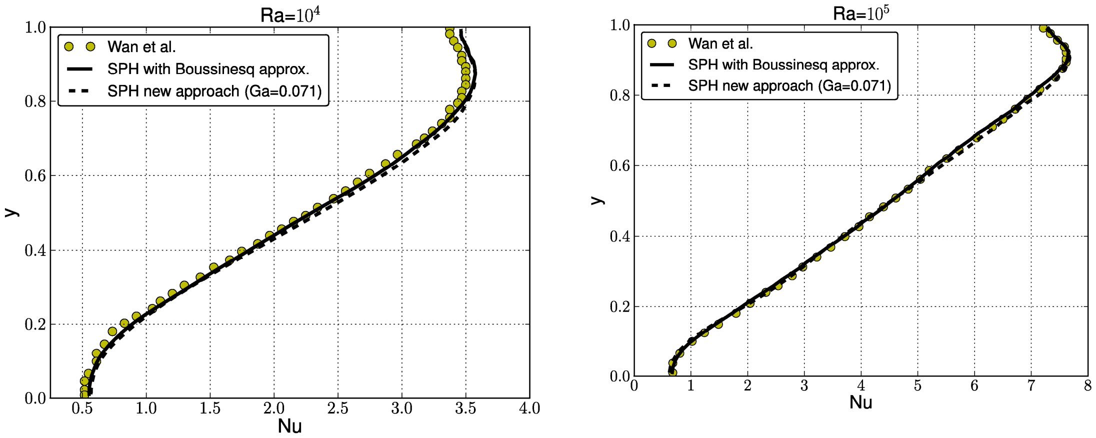
The lid-driven cavity flow at Re=1000:
ISPH with different number of particles
reference data: Ghia et. al. (JCP, 1982).

Smoothed Particle Hydrodynamics (SPH)

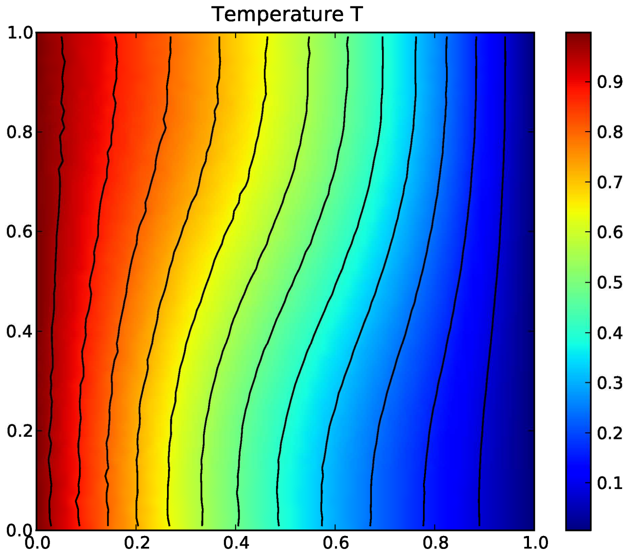
Buoyancy-driven flow: differentially-heated lid-driven cavity

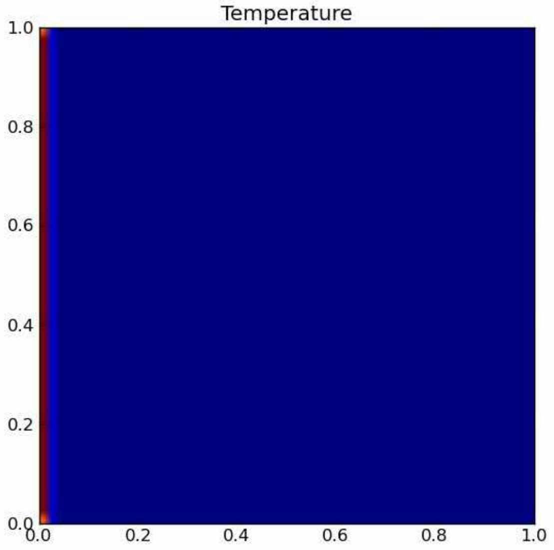


SPH simulation
of heated cavity flow:
Ra=1000 , Ra=10 000
[K. Szewc et al., 2011]



Vertical Nu distribution:SPH with/without Boussinesq approx.
[ref. data: Wan et al., Num. Heat Transfer B, 40 (2001),199-228





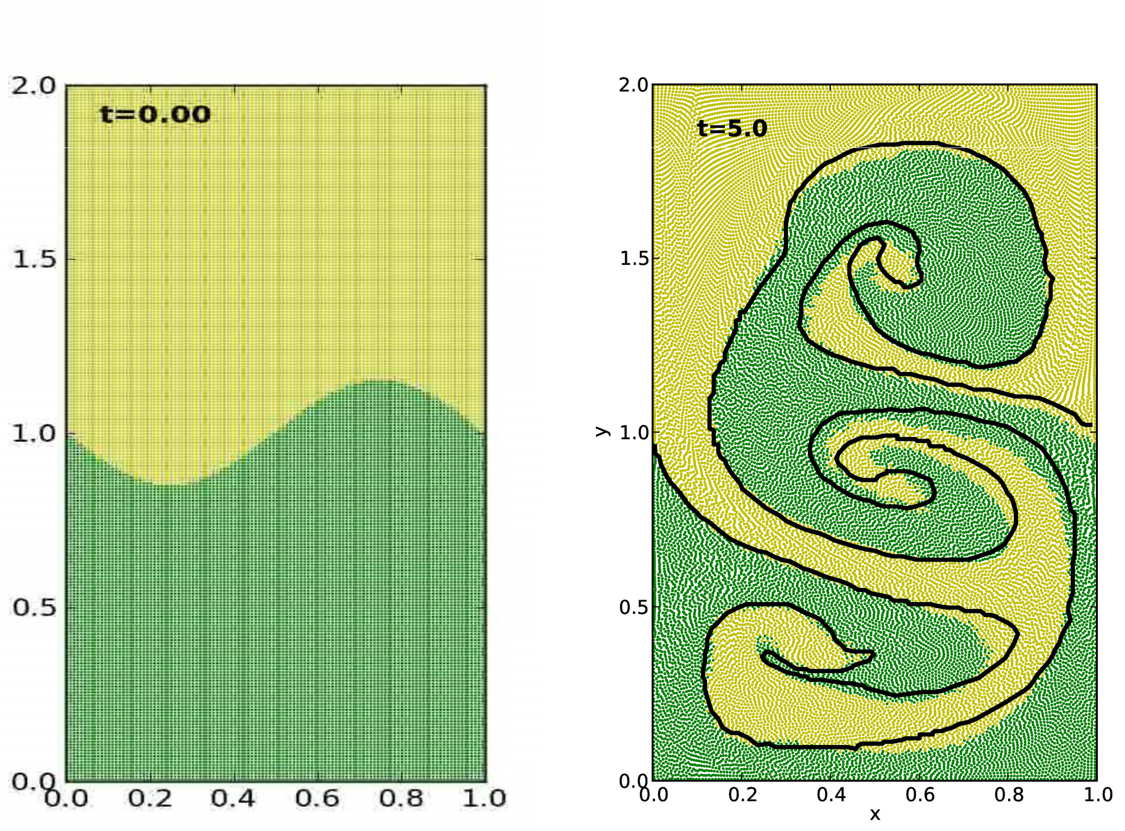
Smoothed Particle Hydrodynamics (SPH)

The Rayleigh-Taylor instability

Buoyancy-driven flow with surface tension effects

ISPH results for R-T instability (120x240 particles) at Re=420

[ref.data: Level Set results of Grenier et. al., JCP 228 (2009), 8380-8393]



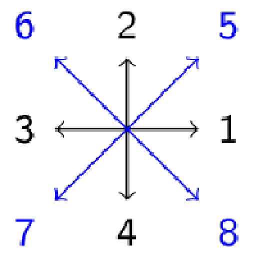
Flow and heat transfer in porous media

Aim: modelling the physics of two-phase, reactive flows
acquiring data for simplified, averaged description (1D/2D)

Tool: lattice Boltzmann method (LBM) for flow and heat transfer analysis in a complex-geometry domain (REV of a porous medium)

$$\boxed{f_i(\vec{r}+\mathbf{e}_i\delta t, t+\delta t) = f_i(\vec{r},t) - \tau^{-1}(f_i - f_i^{eq}),} \quad (*)$$

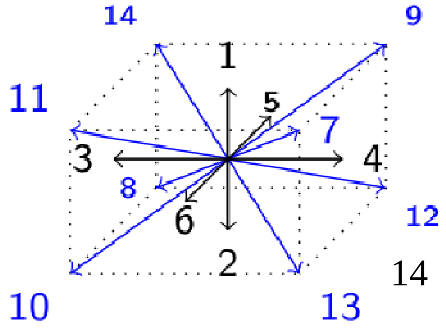
D2Q9 velocity scheme:
(i=0,1,2,…,8):



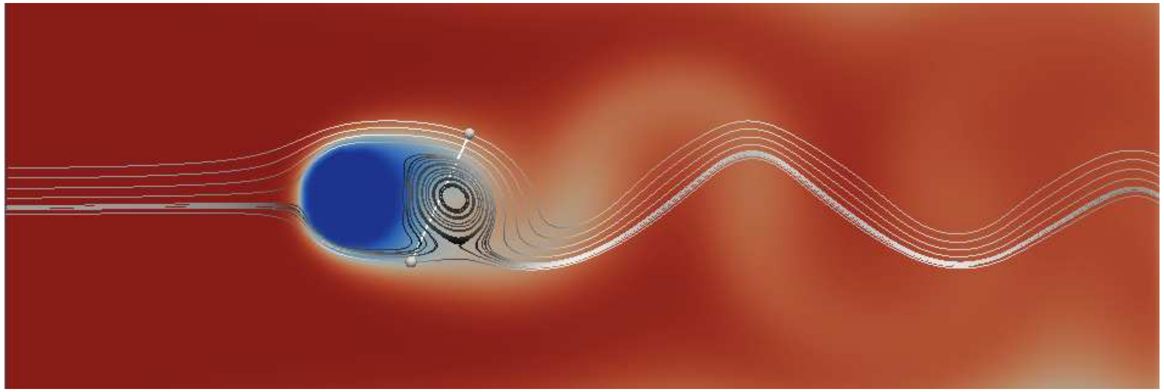
Idea of LBM:

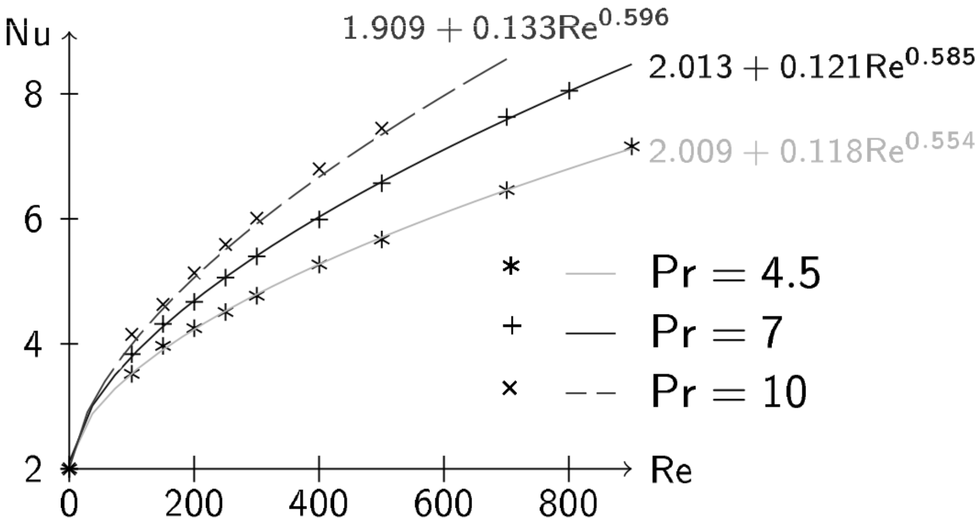
- simplified mesoscopic simulation on a **regular** mesh,
- discretisation of space, time and **velocity,**
- suitable closure of eq. (*) yields the correct form of macroscopic (averaged) flow equations
- additional distribution function for heat transfer

D3Q15 scheme:



LBM modelling of non-isothermal flows past obstacles





Non-isothermal flow past a cylinder

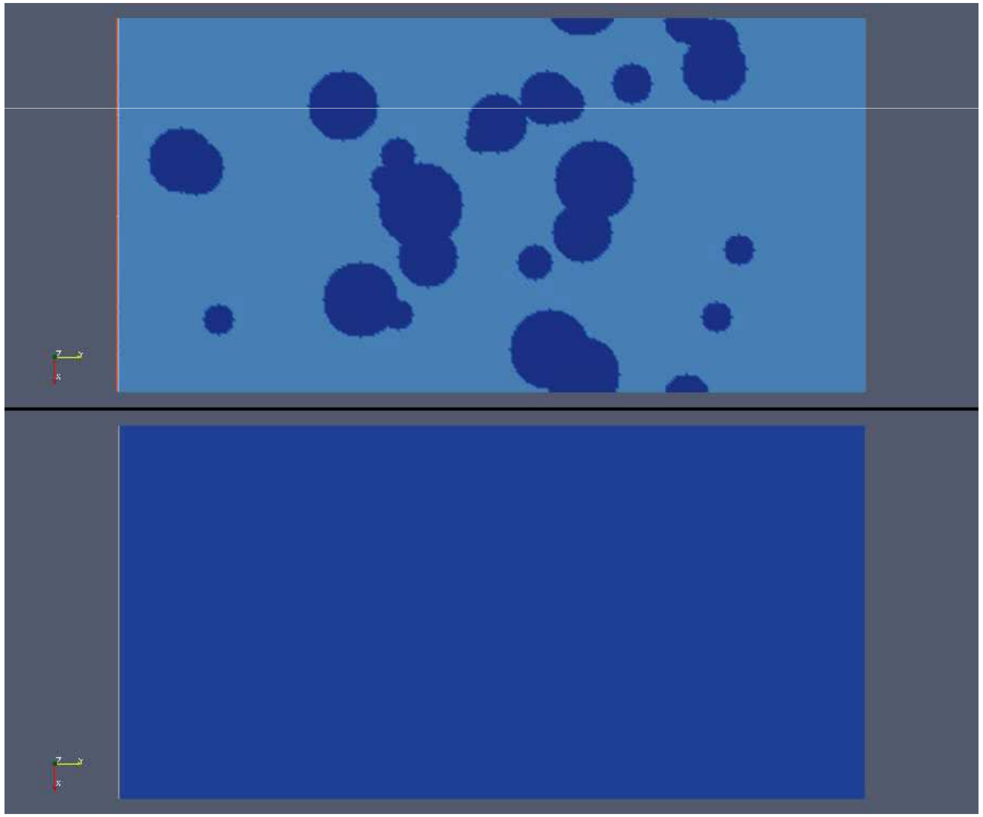
(the scale of gray corresponds to temperature, flow streamlines added).

[Grucelski & Pozorski, 2011 (submitted)]

LBM modelling of heat transfer in simulated porous media

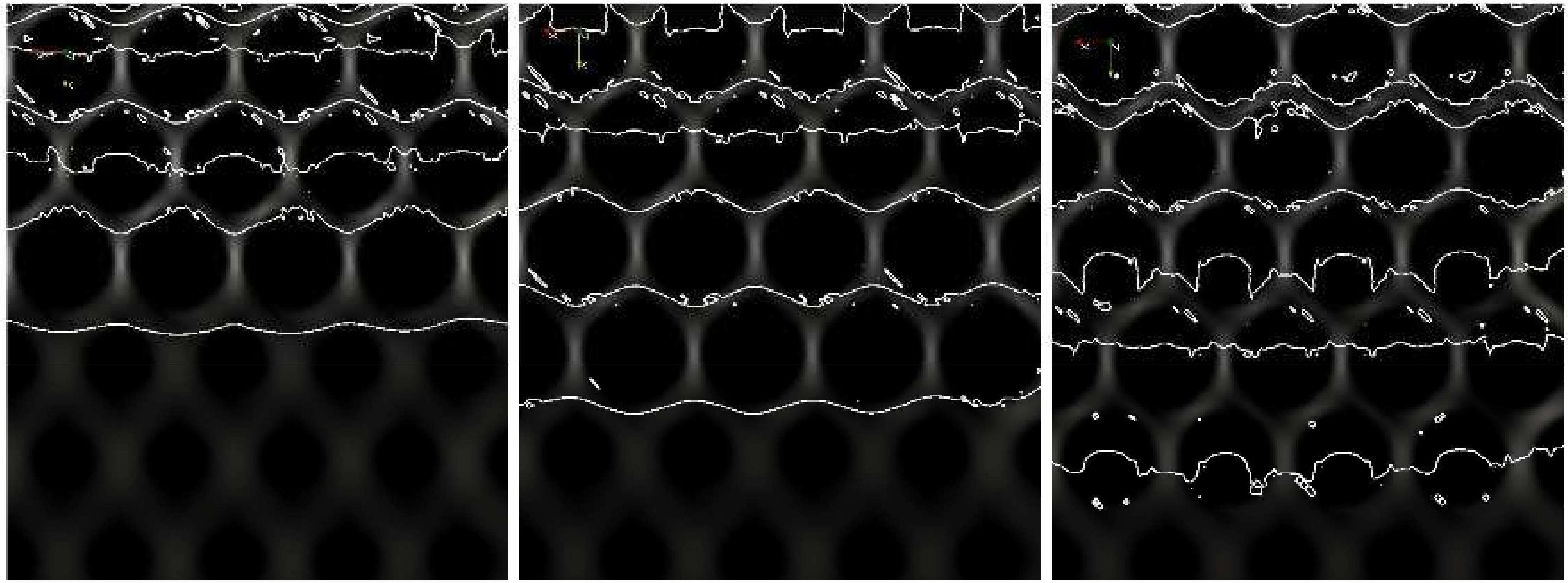
$$\frac{\partial\langle p\rangle}{\partial x} = -\frac{\varepsilon\nu}{K_{xx}}\langle u_x\rangle - \varepsilon^2\rho\beta_{xx}|\langle u_x\rangle|\langle u_x\rangle$$

Modelling difficulty:
implementation of boundary conditions
at the moving solid-fluid interface
(half-way bounce-back and on-site interpolation free b.c. tested)



Non-isothermal flow
through a system of obstacles
(approximation of a porous medium)
with thermal dilatation of grains
[A. Grucelski, 2011]

LBM modelling of heat transfer in simulated porous media



Non-isothermal flow through a system of obstacles
(approximation of a porous medium) with thermal dilatation of grains
(the scale of gray corresponds to flow velocity magnitude, temperature isolines added).

[A. Grucelski, 2010]

Conclusion

→LES of dispersed flows:

- importance of SGS particle dispersion demonstrated in wall bounded flows,
- simulation accomplished and validated for simple and coaxial, particle-laden jets,
- next aim: a better modelling of those effects.

→ SPH of multiphase flows:

- the incompressibility treatment studied and validated,
- non-Boussinesq formulation developed for heated flows,
- surface tension effects suiably modelled,
- next aim: a physically-sound modelling of interfaces, capillary effects, etc.

→ LBM of porous-media flows:

- approach validated for flows past obstacles and in the Darcy-Forchheimer regime,
- non-isothermal flows efficiently computed,
- variable geometry effects (thermal dilatability of grains) succesfully implemented,
- next aim: modelling of porous structure deformation.