Lattice-Boltzmann vs. Navier-Stokes simulation of particulate flows

Amir Eshghinejadfard, Abouelmagd Abdelsamie, Dominique Thévenin

University of Magdeburg, Germany

14th Workshop on Two-Phase Flow Predictions
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CONTENT

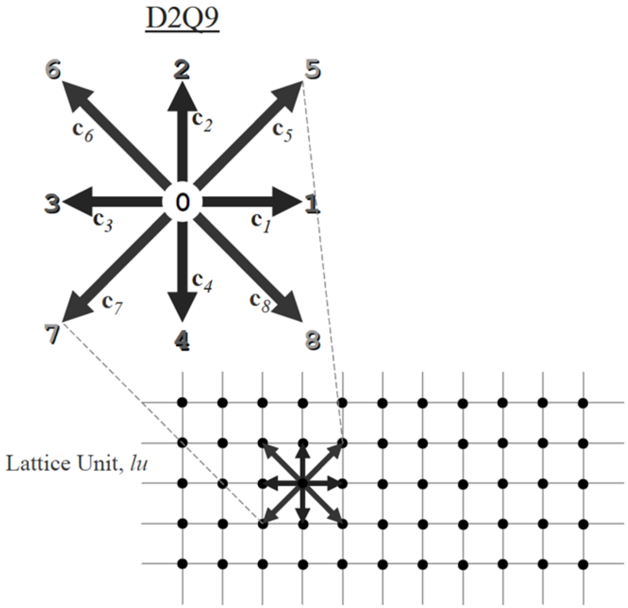
- Lattice Boltzmann method (LBM)
- Navier Stokes Equation (NSE)
- LBM vs. NSE
  - ➢ Cavity flow
  - ➢ Flow over stationary cylinder
  - ➢ Turbulent channel flow
- LBM applications in two-phase flows:
  - ➢ Spherical particles
  - ➢ Ellipsoid particles
  - ➢ Particulate flows with heat transfer

LATTICE BOLTZMANN METHOD (LBM)

- LBM is a mesoscopic method originated from LGA.

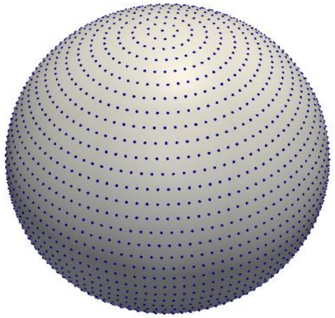
$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i(\mathbf{x},t) - \frac{\Delta t}{\tau}\left[f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)\right]$$

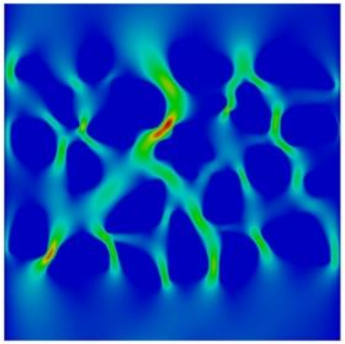
$$\rho = \sum_i f_i \qquad \rho\mathbf{u} = \sum_i \mathbf{c}_i f_i$$

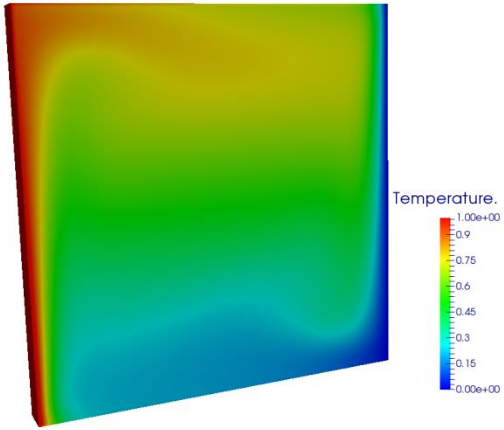


ALBORZ

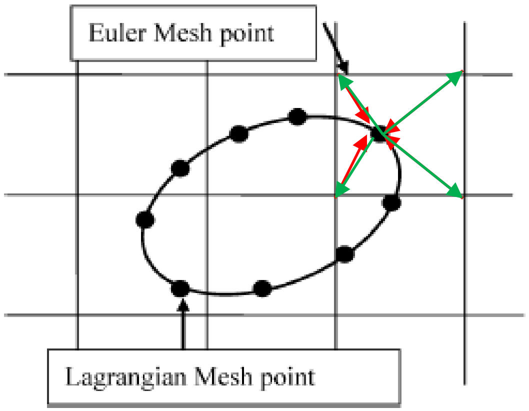
- ALBORZ: In-house code developed in LSS-OvGU, Magdeburg.
  - ➢ Particulate flows,
  - ➢ Turbulent flows,
  - ➢ Porous media,
  - ➢ Non-isothermal flows
- Single and Multi Relaxation time
- Parallelized on MPI.
- Particles: Immersed Boundary Method (IBM)
- Natural convection: Boussinesq approximation







IMMERSED BOUNDARY METHOD (IBM)



- Force at each Lagrangian node:

$$\mathbf{F}^n = \frac{\mathbf{U}^d - \mathbf{u}^{noF}}{\Delta t}$$

- U^d: desired Lagrangian node velocity;
- U^{noF}: velocity without force at each Lagrangian node.
- Interpolation: $\mathbf{u}^{noF} = \sum_b \mathbf{u}_{i,j} D(\mathbf{x}_{i,j} - \mathbf{X}_b)(\Delta h)^3,$
- Spread: $\mathbf{F}_{i,j} = \sum_b \mathbf{F}_b D(\mathbf{x}_{i,j} - \mathbf{x}_b)\Delta s_b$

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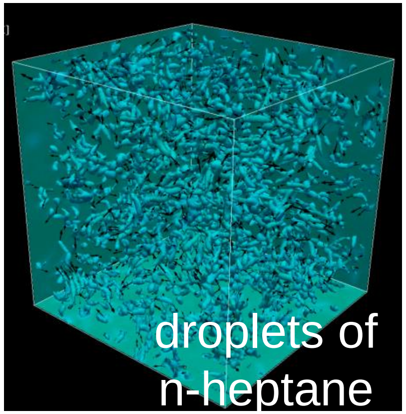
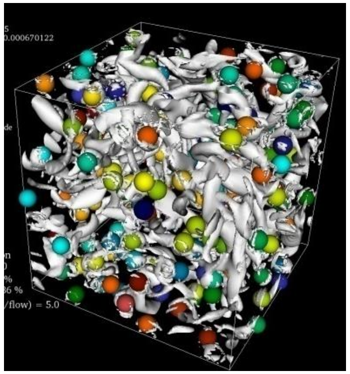
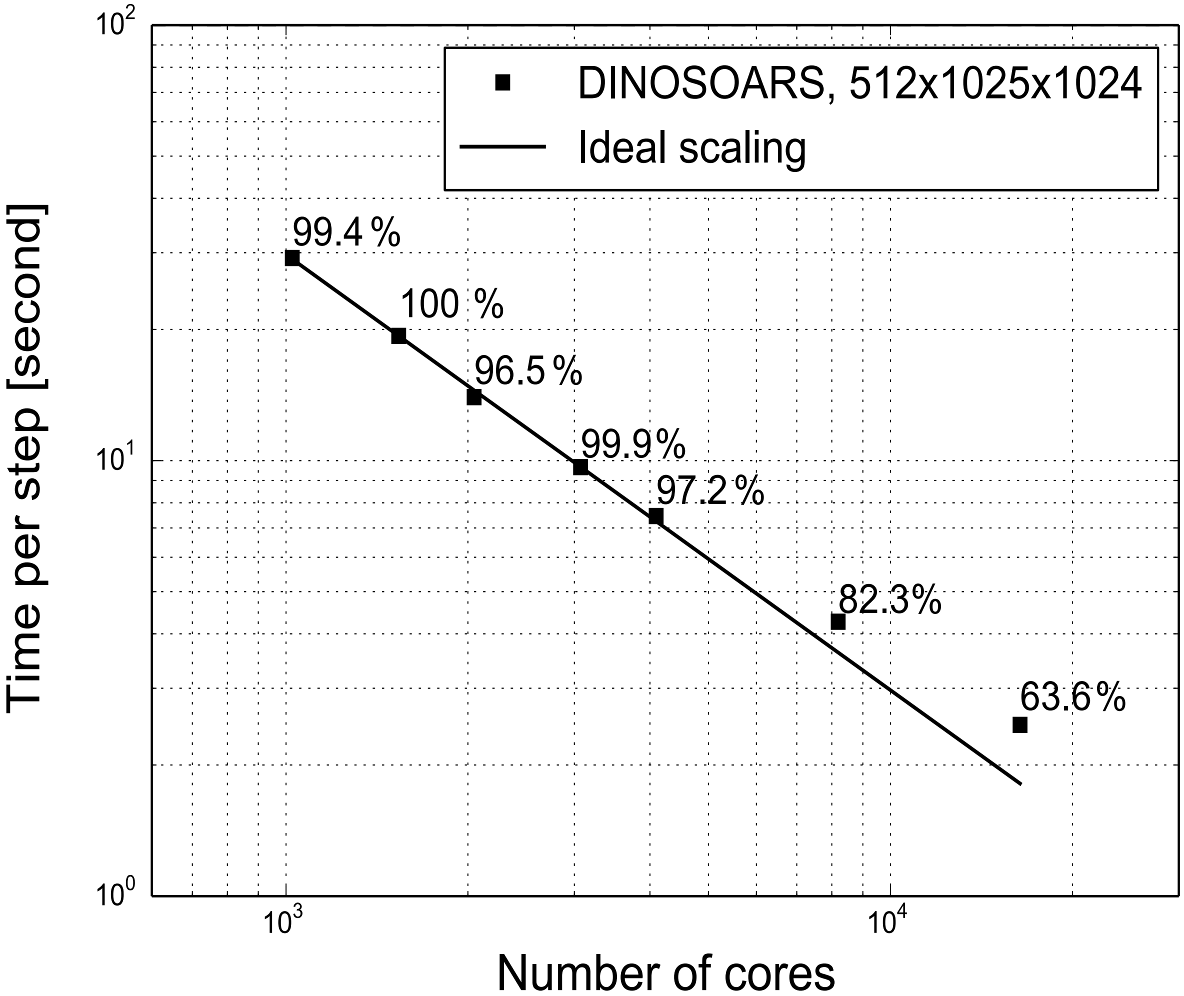
DNS: with DINOSOARS (A. Abdelsamie)

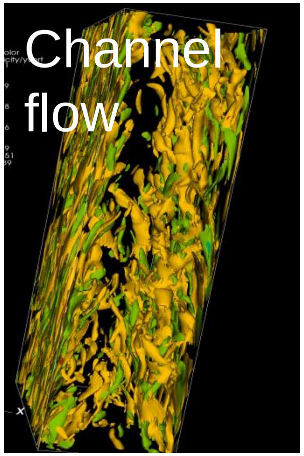
- Low Mach (for reacting cases) number or incompressible (for cold flow), 3-D parallel.
- 6th order in space (FDM) and 3rd/4th order in time (Runge-Kutta)
- Multiphase (Lagrangian) for spherical droplets/particles:
  - Inert or Reactive (evaporation, burning)
  - Point-particles or Resolved (Immersed Boundary, IBM)
- Includes Direct Boundary-IBM, for complex geometries
- Point-wise implicit integration for stiff chemistry
- Poisson equation solved by fully spectral method, even for non-periodic boundaries
- Full reactions schemes or tabulated chemistry (FPI)
- Kinetics, transport & thermodynamics: coupled to Cantera1.8 and Eglib3.4

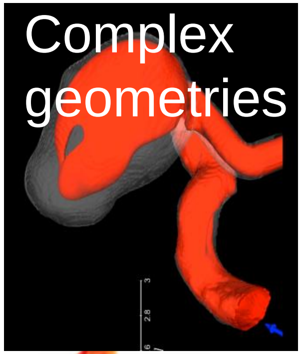




Code Scaling (SuperMuc)







Strong scaling of DINOSOARS on SuperMUC for reactive benchmark up to >10^4 cores.

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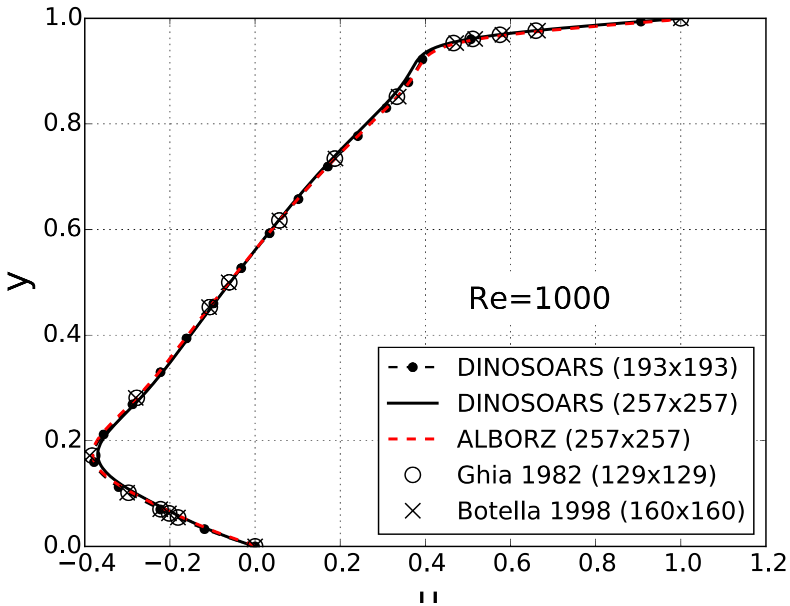
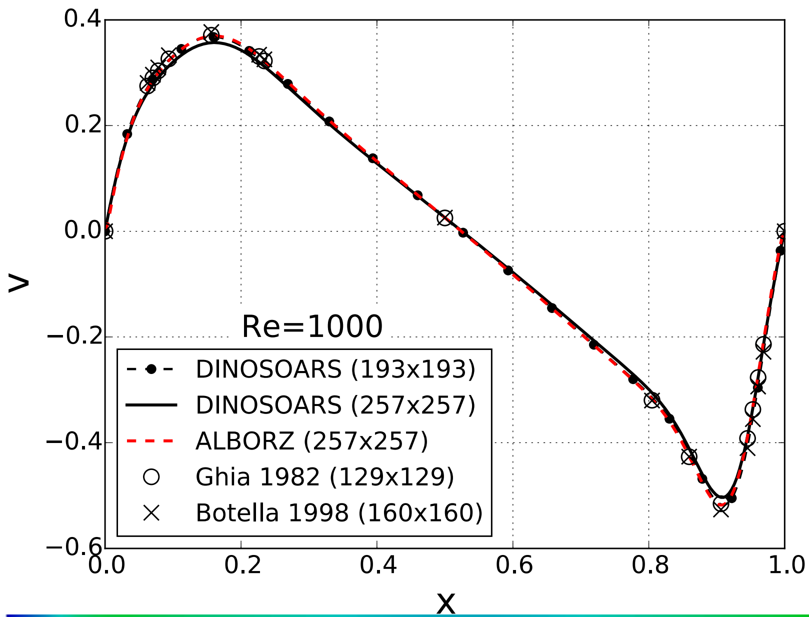
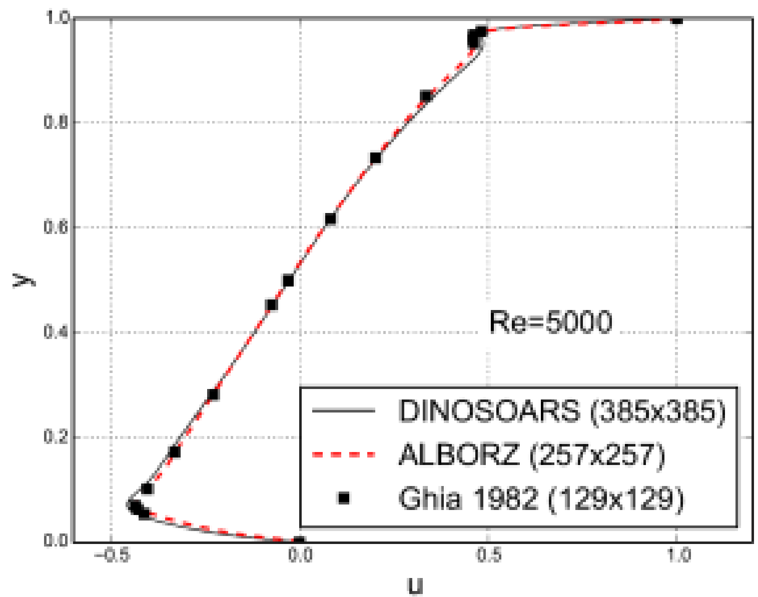
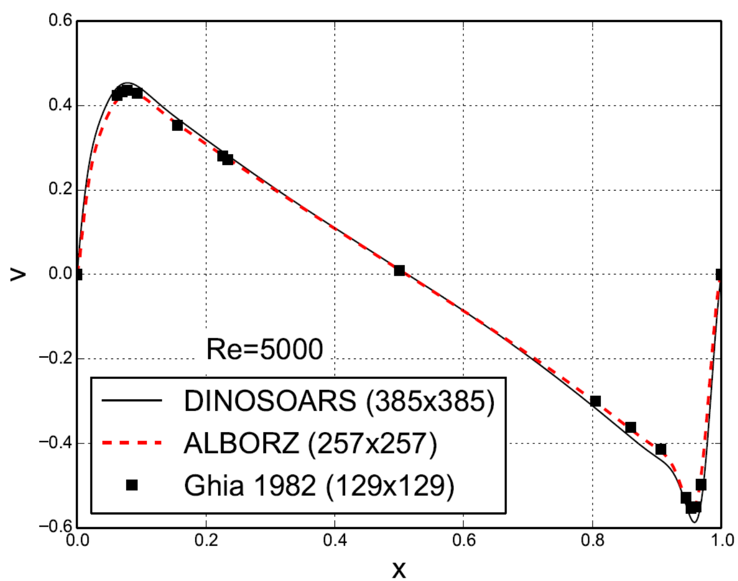
Lid driven cavity at Re=1000, 5000









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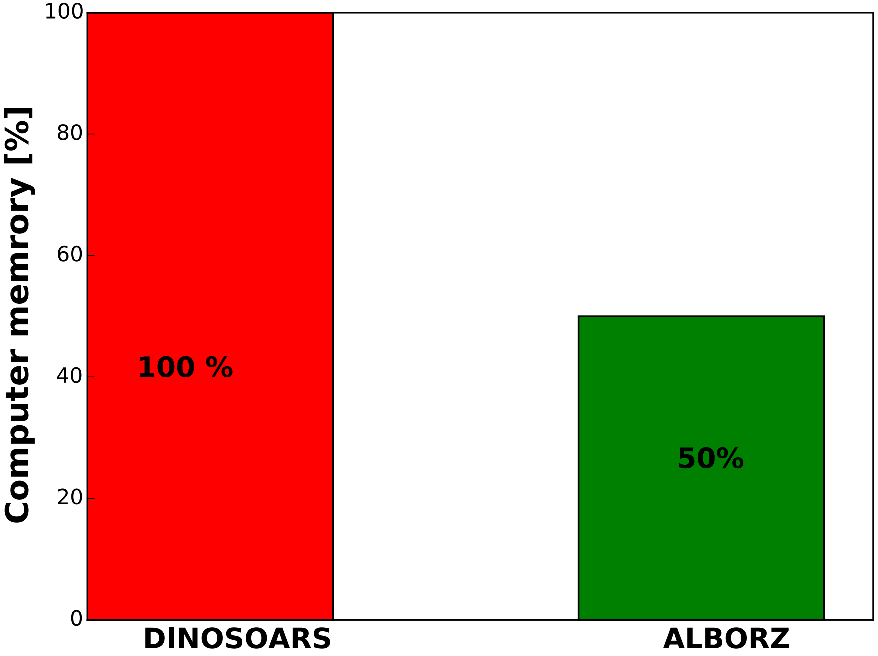
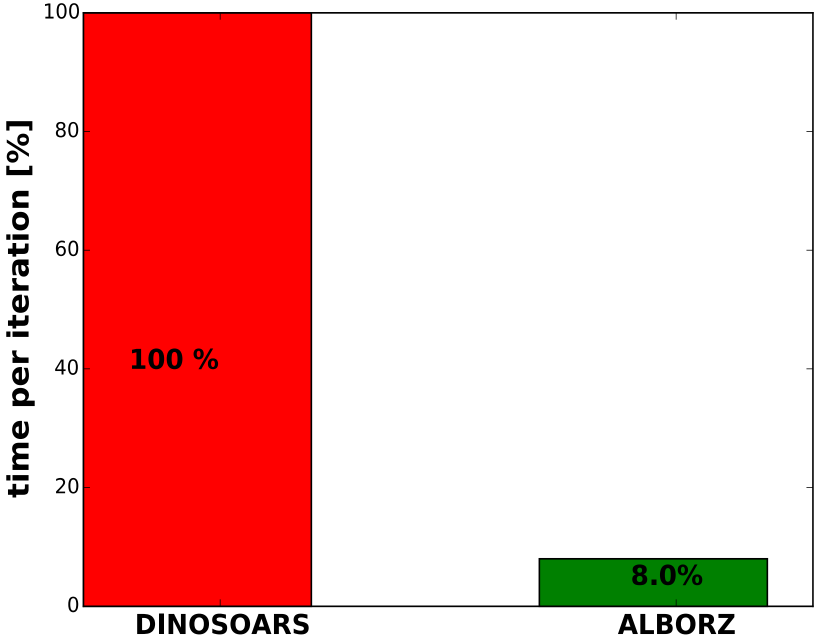
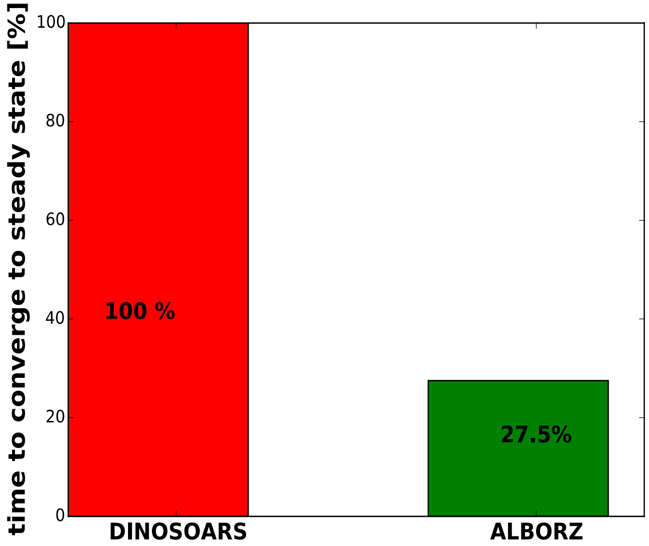


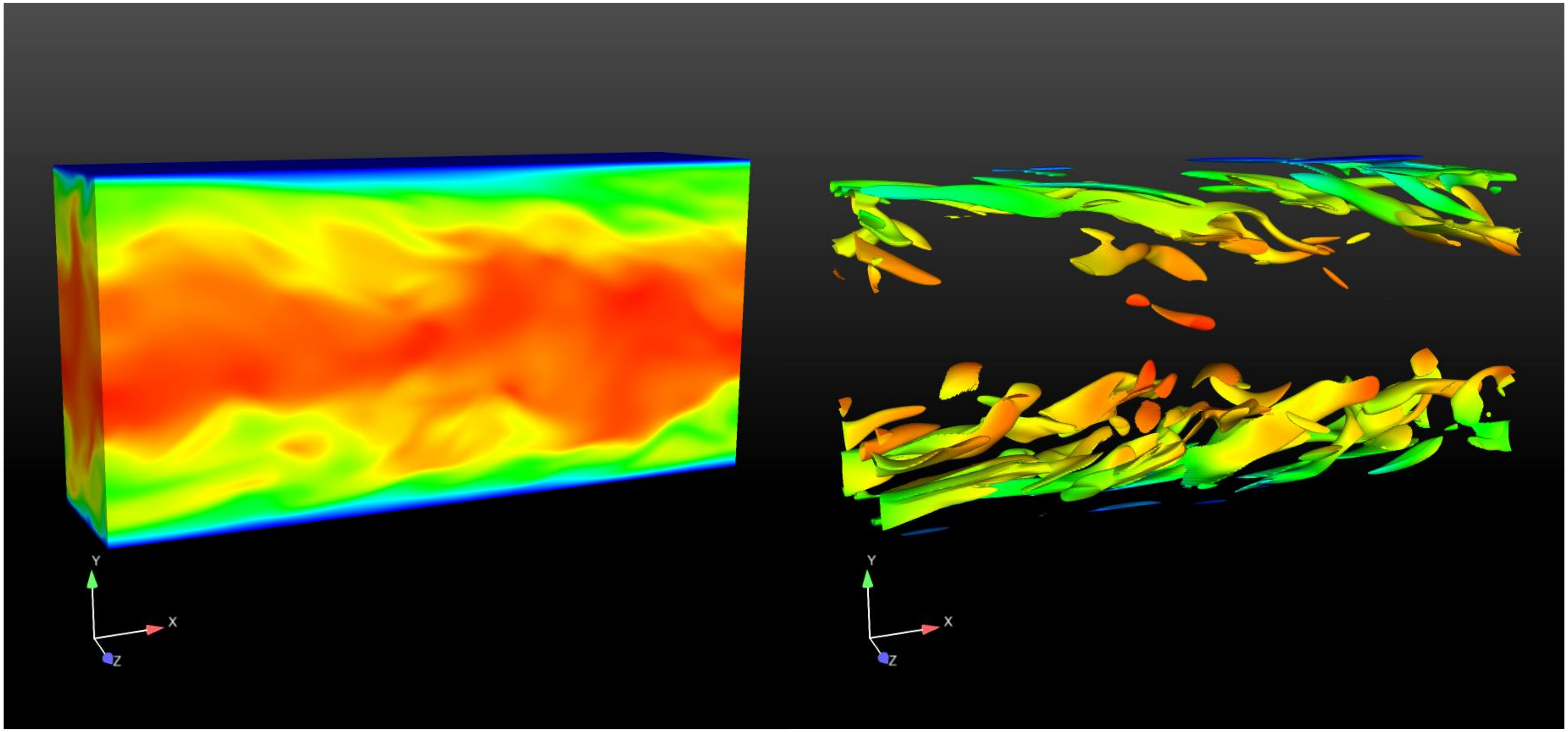




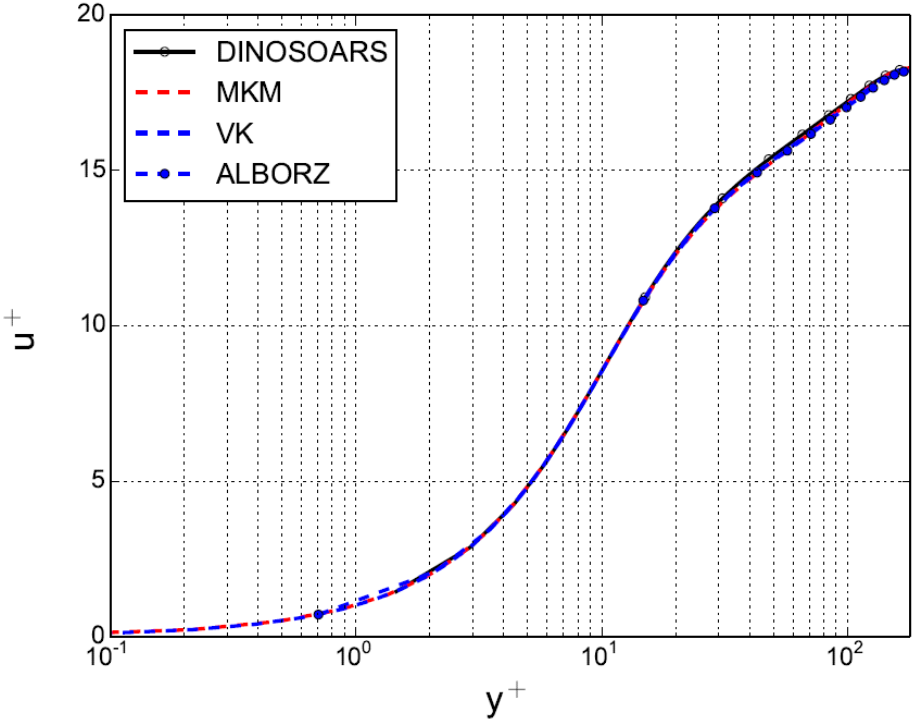
TURBULENT CHANNEL FLOW

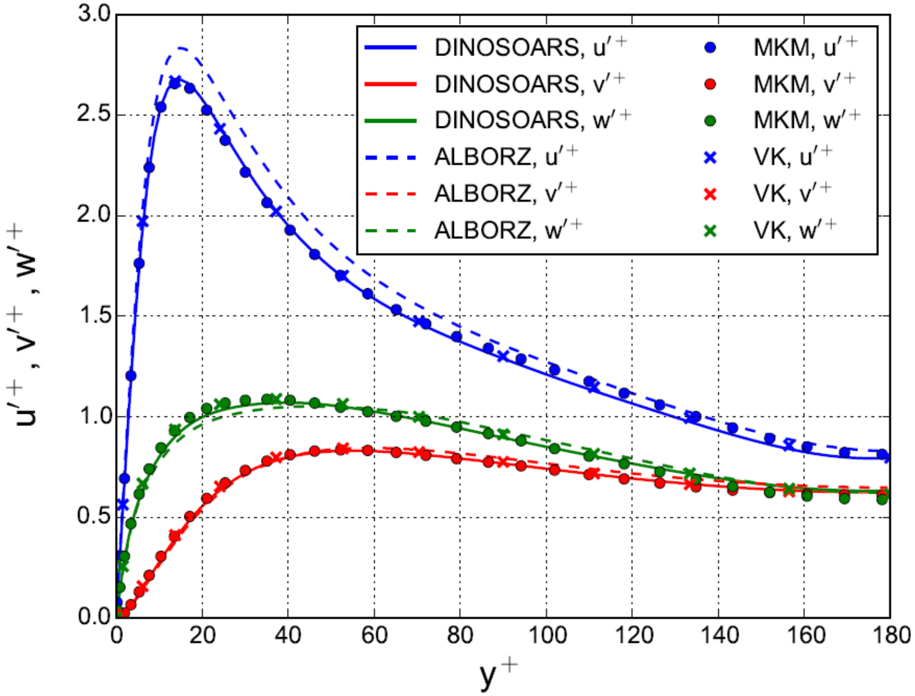
$$Re_\tau = \frac{u_\tau . H}{\upsilon} = 180 \quad , \quad u_\tau = \sqrt{\frac{\tau_w}{\rho}} \qquad Re_b = \frac{u_b . 2H}{\upsilon} = 5600$$

	L_x	L_y	L_z	N_x	N_y	N_z	Npoints
DINOSOARS	8δ	2δ	4δ	256	193	128	6.3 mil.
ALBORZ	4δ	2δ	4δ	512	256	256	33.6 mil.



TURBULENT CHANNEL FLOW

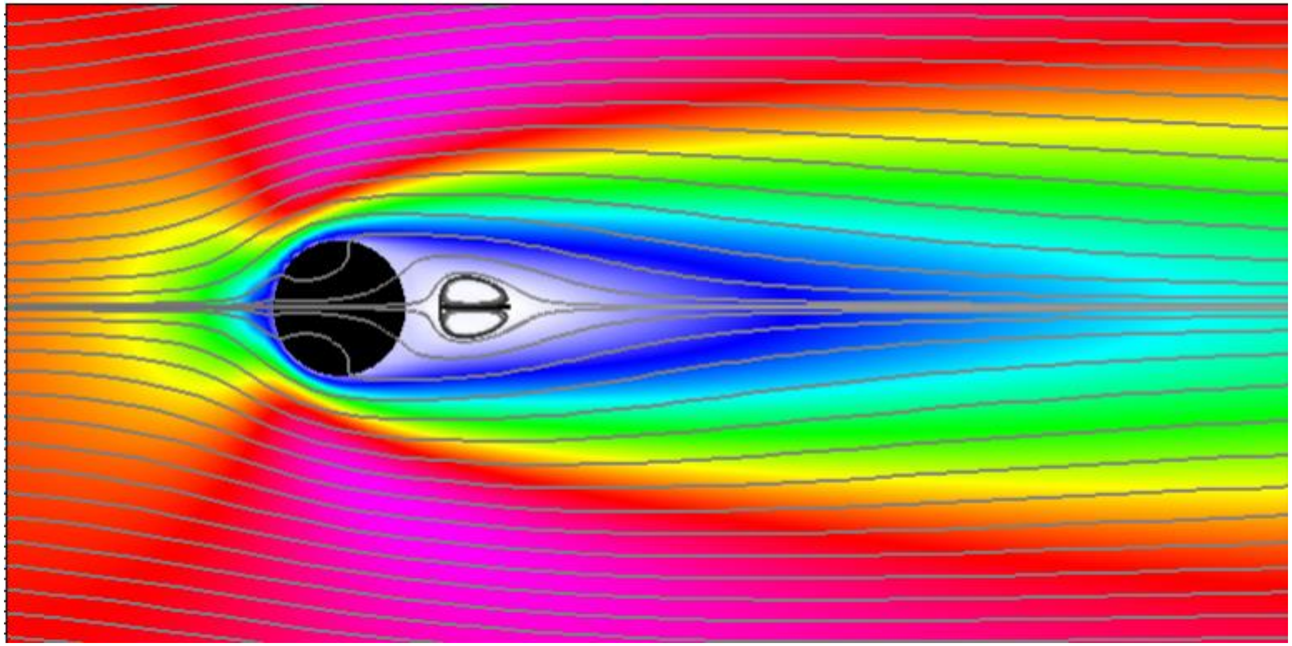




* Moser R., Kim J., Mansour N. N. (1999). Phys. Fluid, Vol. 11.
** Vreman A. W., and Kuerten J. G. M. (2014) Phys. Fluid, 2014, Vol. 26.

Flow over stationary cylinder at Re=20

- Domain: 768x768
- DINOSOARS, C_d = 2.14
- ALBORZ, C_d =2.16



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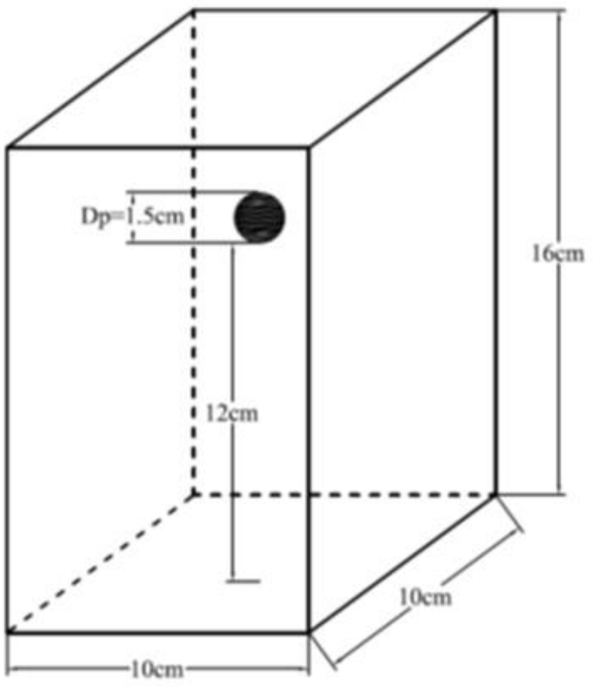
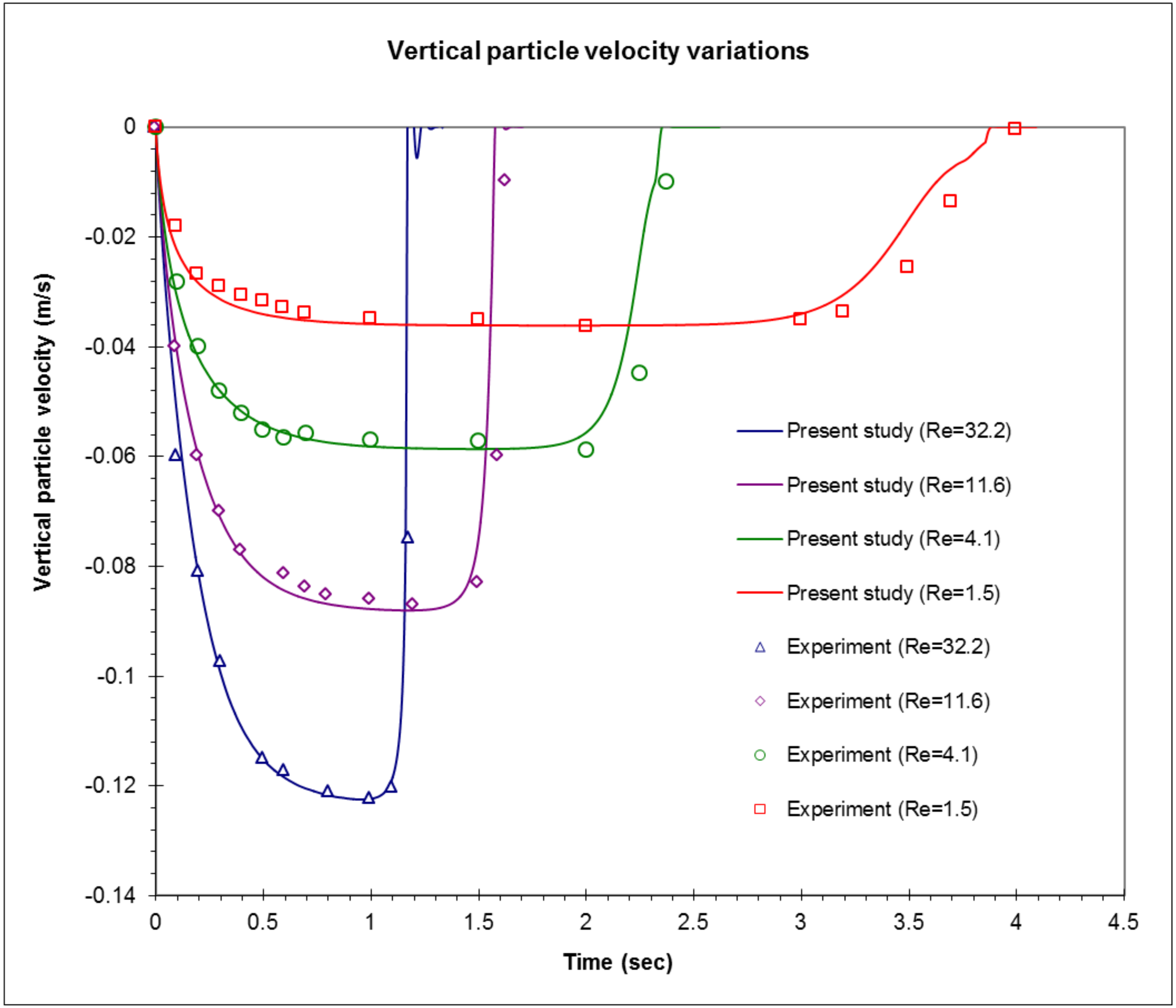
SPHERICAL PARTICLE SEDIMENTATION

- Dimensions of the box: $0.1 \times 0.16 \times 0.1\ m^3$.
- The sphere starts its motion at a height H_s=0.12m from the bottom of the box.
- Particle diameter: 15 mm
- Particle density: 1120 kg/m^3.
- $\mathrm{Re} = \frac{U_\infty D}{\upsilon} = 1.5;\ 4.1;\ 11.6;\ 32.2$



*ten Cate, A., Nieuwstad, C. H., Derksen, J. J., & Van den Akker, H. E. A. (2002).. *Phys. Fluids*, Vol. *14*.

SPHERICAL PARTICLE SEDIMENTATION RESULTS

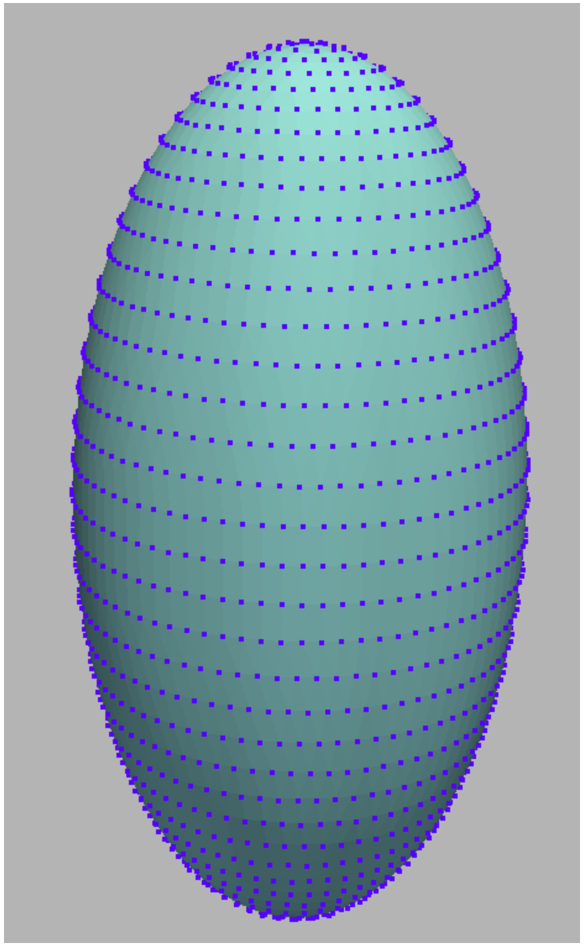


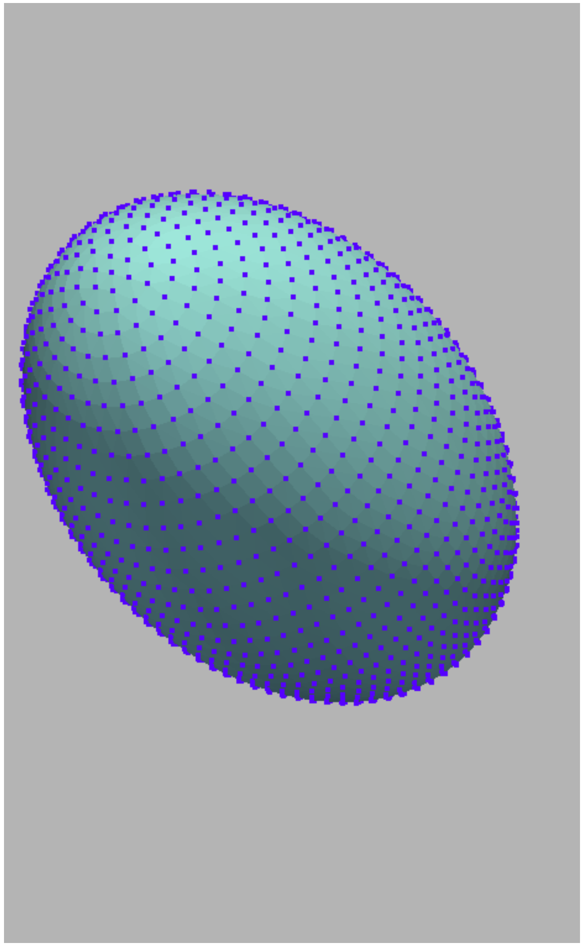
ELLIPSOID PARTICLES

- Differences with spherical particles:
  - *Lagrangian points distribution*
  - *Rotational velocity calculation*
  - *Particle-Particle and Particle-Wall collision force*

CREATING AN ELLIPSOID

- Lagrangian points *distribution and area calculation*



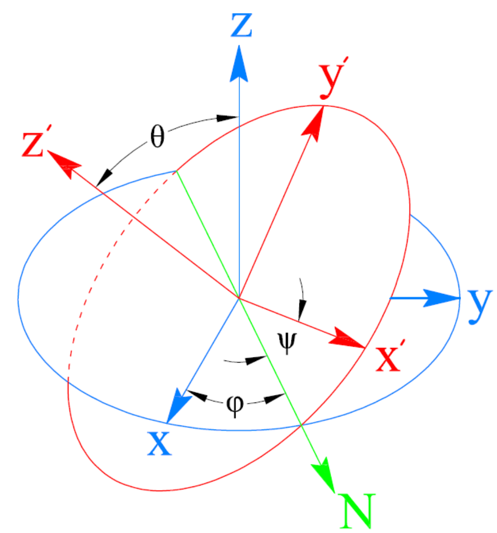


$$\frac{x'^2}{a^2}+\frac{y'^2}{b^2}+\frac{z'^2}{b^2}=1$$

$$S=2\pi b\int_{x_1}^{x_2}\sqrt{1-\frac{(a-b)(a+b)x^2}{a^4}}dx$$

Newton's equation of motion for moving particle

- For the simulation of a moving particle, we have to consider the equations of motion of the particle.



$$M_P \frac{d\mathbf{U}_P}{dt} = \int F_b dV + (\rho_P - \rho_f) V_P \mathbf{g} + \mathbf{F}^c$$

$$I'_{xx} \frac{d\Omega'_x}{dt} - \Omega'_y \Omega'_z (I'_{yy} - I'_{zz}) = T'_x$$

$$I'_{yy} \frac{d\Omega'_y}{dt} - \Omega'_z \Omega'_x (I'_{zz} - I'_{xx}) = T'_y$$

$$I'_{zz} \frac{d\Omega'_z}{dt} - \Omega'_x \Omega'_y (I'_{xx} - I'_{yy}) = T'_z$$

Body-fixed coordinate

Inertial coord.

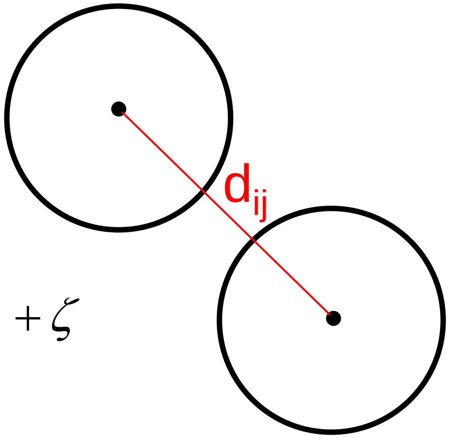
$$T' = MT,$$

$$M = \begin{pmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_0 q_1 + q_2 q_3) & 2(q_1 q_3 - q_0 q_2) \\ 2(q_1 q_2 - q_0 q_3) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(q_2 q_3 + q_0 q_1) \\ 2(q_1 q_3 + q_0 q_2) & 2(q_2 q_3 - q_0 q_1) & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{pmatrix}$$

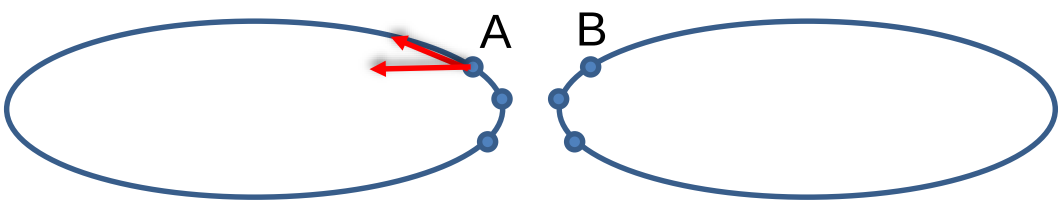
$$\dot{\mathbf{q}} = \begin{bmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{bmatrix} \begin{bmatrix} 0 \\ \Omega'_x \\ \Omega'_y \\ \Omega'_z \end{bmatrix} \Rightarrow \Omega = M^{-1} \Omega'$$

COLLISION FORCE

- Particle-Particle collision: Spring force model*



$$\mathbf{F}_{i,j}^{P} = \begin{cases} 0, & d_{ij} > R_i + R_j + \zeta \\ \dfrac{c_{ij}}{\varepsilon_p}\left(\dfrac{d_{ij} - R_i - R_j - \zeta}{\zeta}\right)^2 \left(\dfrac{\mathbf{x}_i - \mathbf{x}_j}{d_{ij}}\right), & R_i + R_j < d_{ij} \le R_i + R_j + \zeta \end{cases}$$

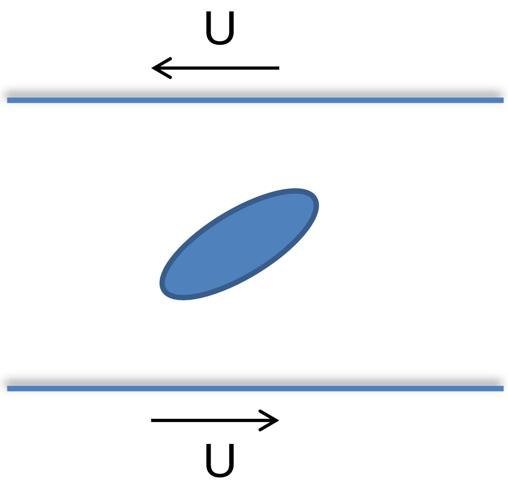


- Each Lagrangian point may have collision with one or more points of other particles.

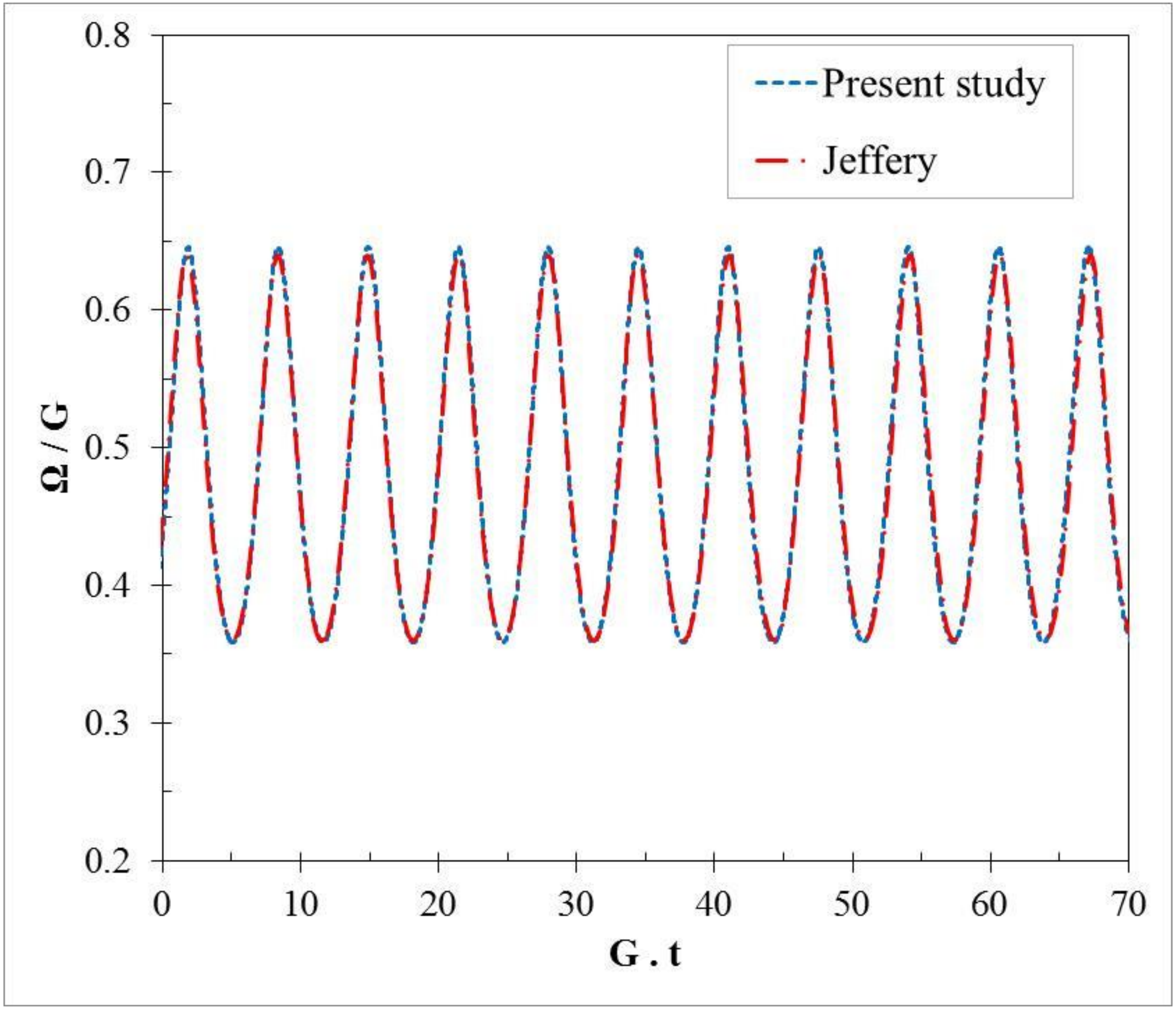
*Feng, Z. G., & Michaelides, E. E. (2004) J. Comput. Physi., Vol. 195.

SPHEROIDAL PARTICLE IN COUETTE FLOW

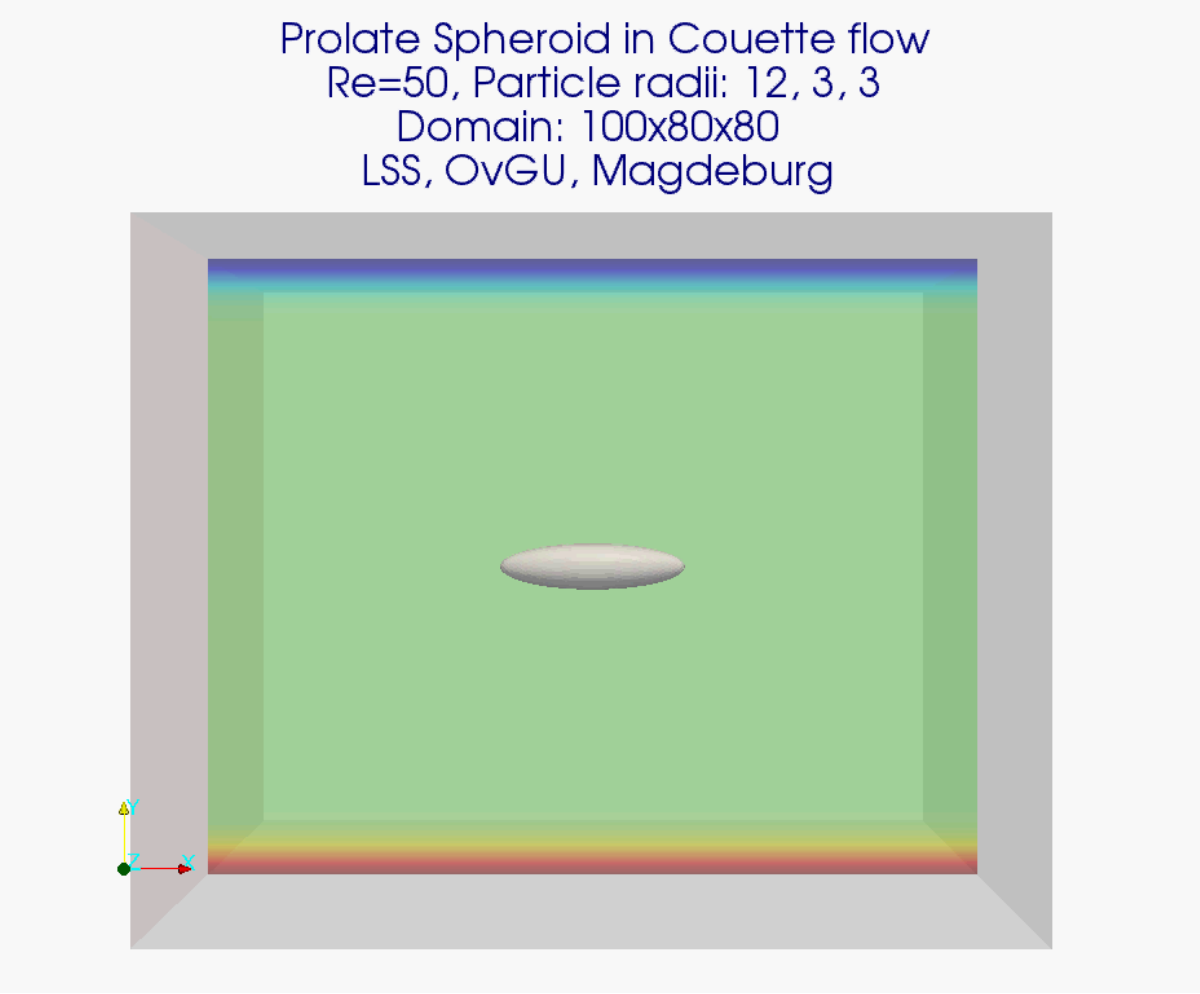
- Computational domain: 120×120×60 lattice nodes.
- Reynolds number=0.5
- Neutrally buoyant
- Particle radii: 6.0 ; 4.5; 4.5
- Shear rate is $G=2U/N_y=1/8640$
- $\mathrm{Re} = \frac{4G.D^2}{\upsilon}$



ELLIPSOID PARTICLE IN COUETTE FLOW

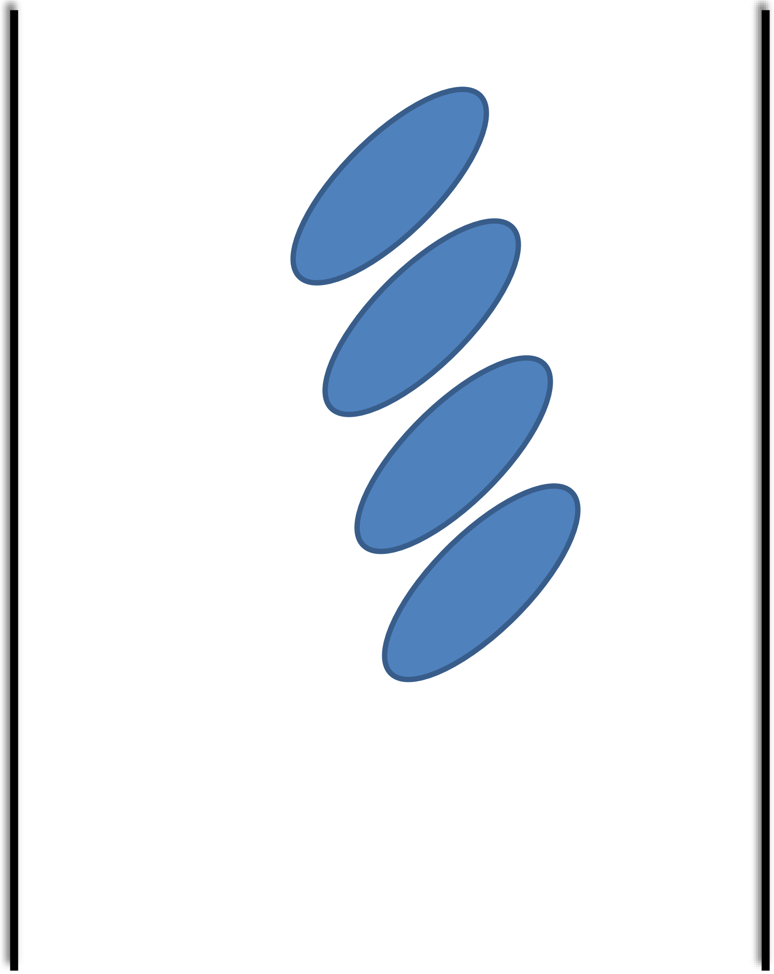


SPHEROID ROTATION



Multiple particles

- Dimensions of the box: 0.1×0.16×0.1 m^3.
- The upper particle is at height H_s=0.12m from the bottom of the box.
- Particle major diameter: 15 mm
- Particle minor diameter: 7.5 mm
- Particle density: 1120 kg/m^3.
- Fluid density: 960 kg/m^3
- Fluid viscosity: 58e-3 Pa.s



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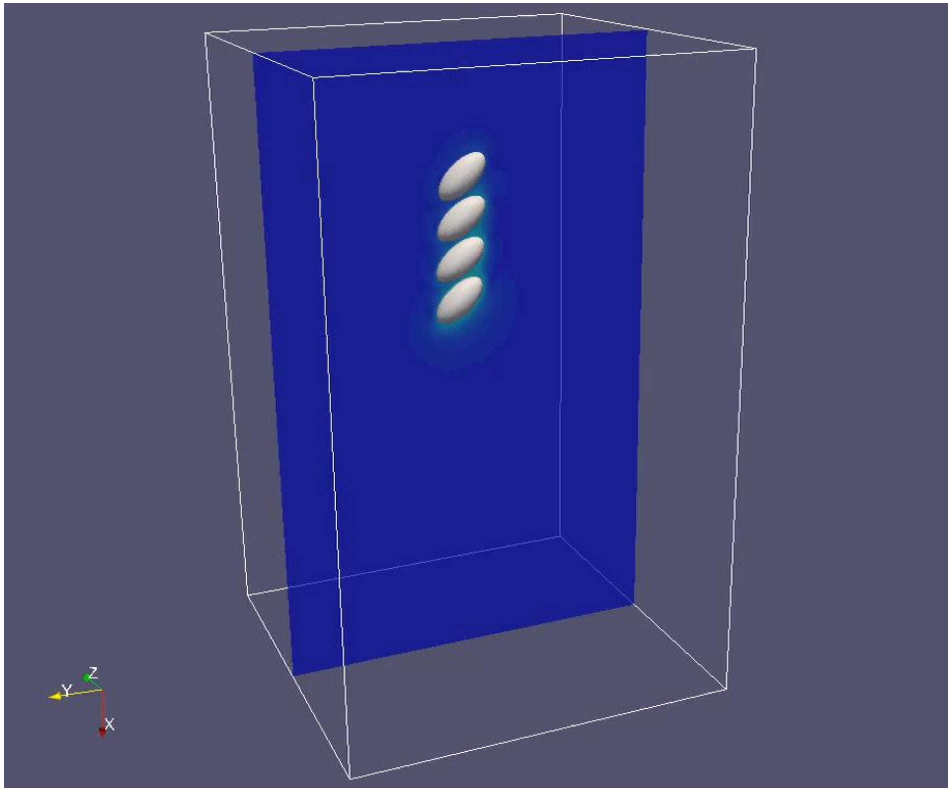

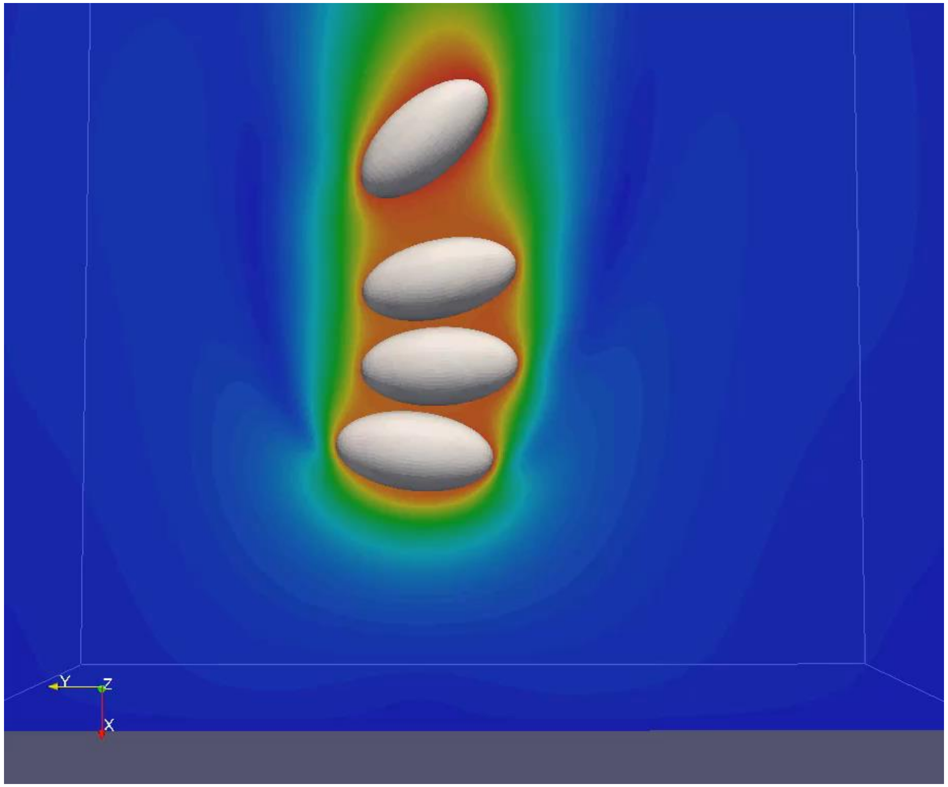

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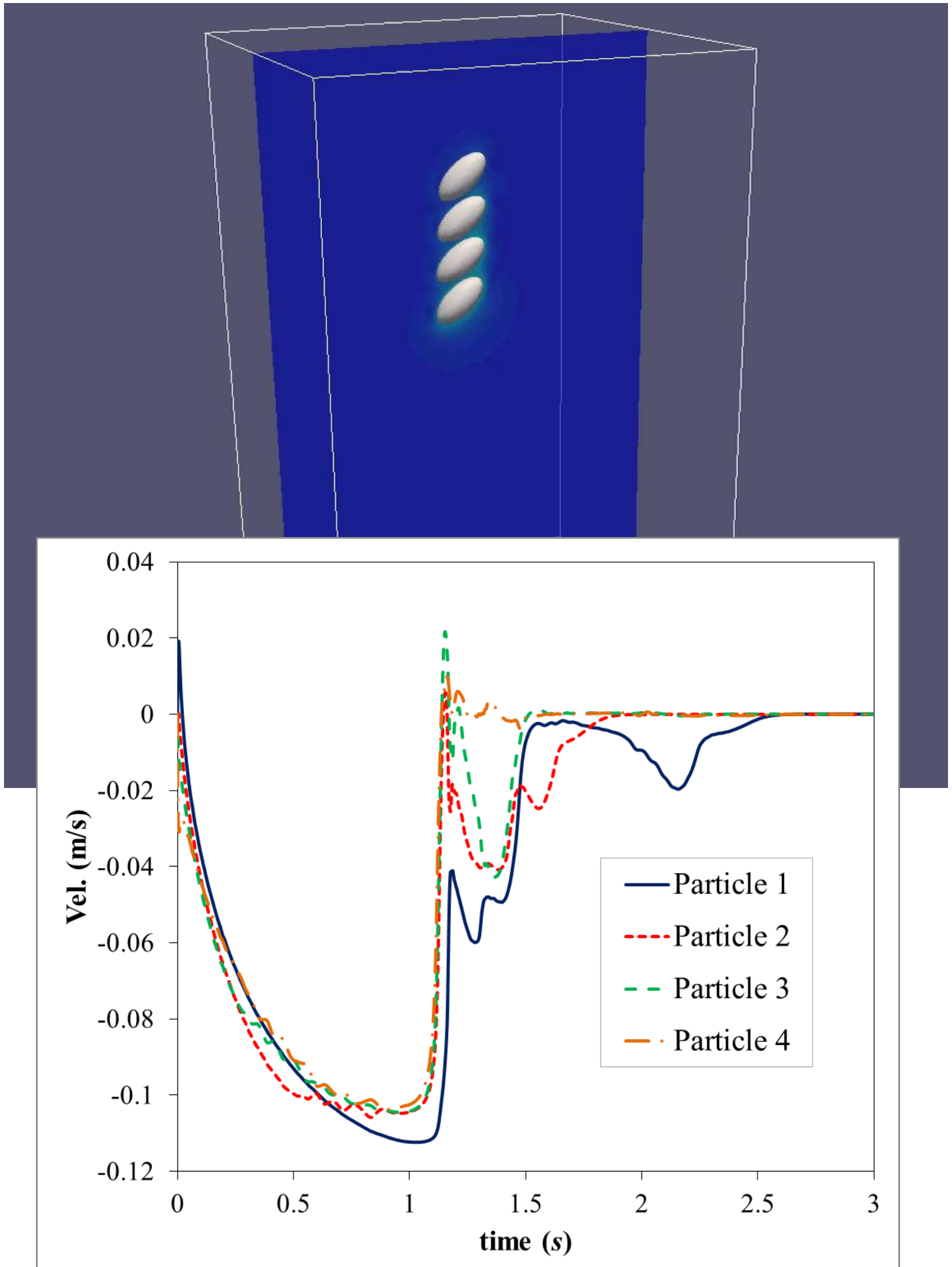
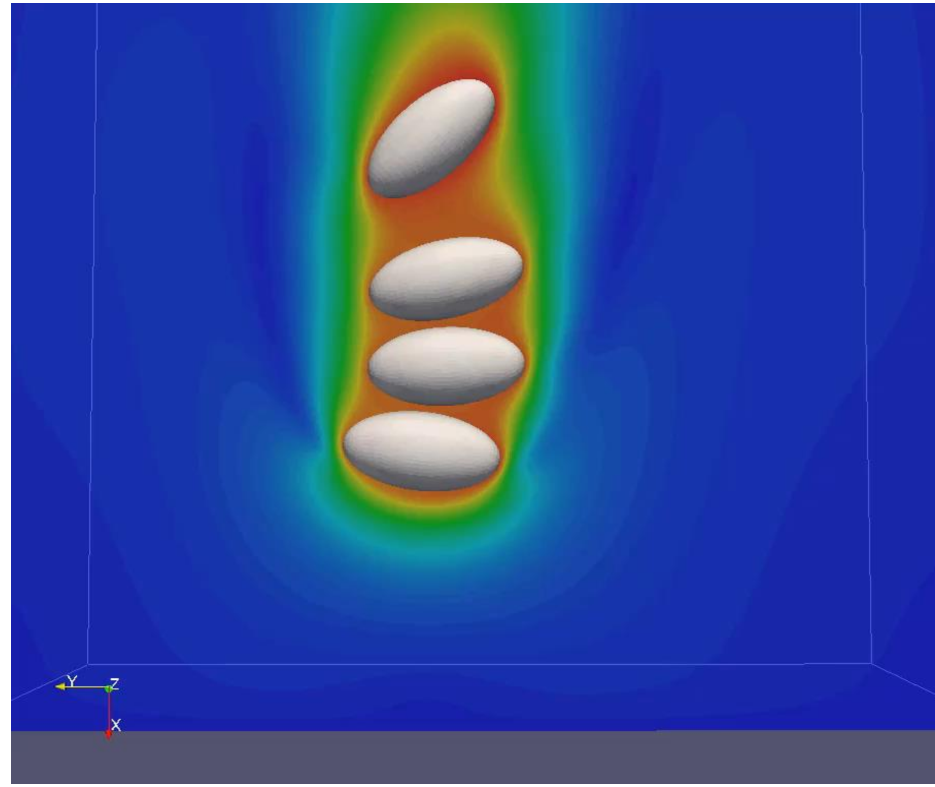
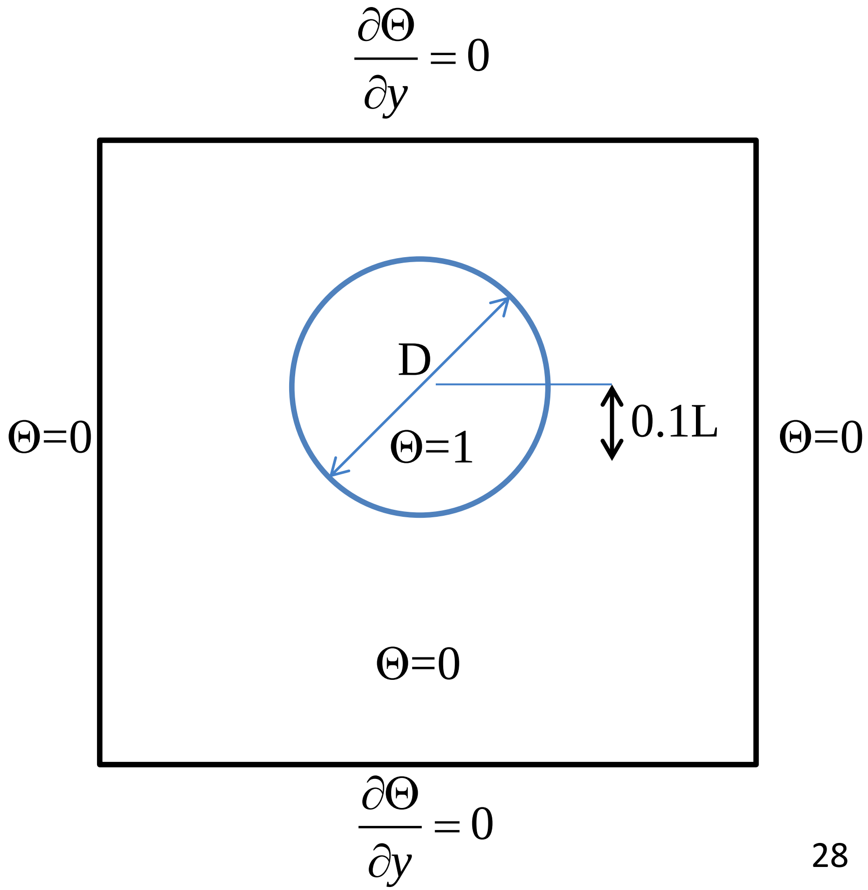




Hot circular cylinder in a square enclosure

- *Hot eccentric cylinder in a square box*
- $D = 0.4L$
- $Gr = \dfrac{g\beta(\Theta_h - \Theta_c)L^3}{\upsilon^2} = 100,000$
- $\Pr = 10$



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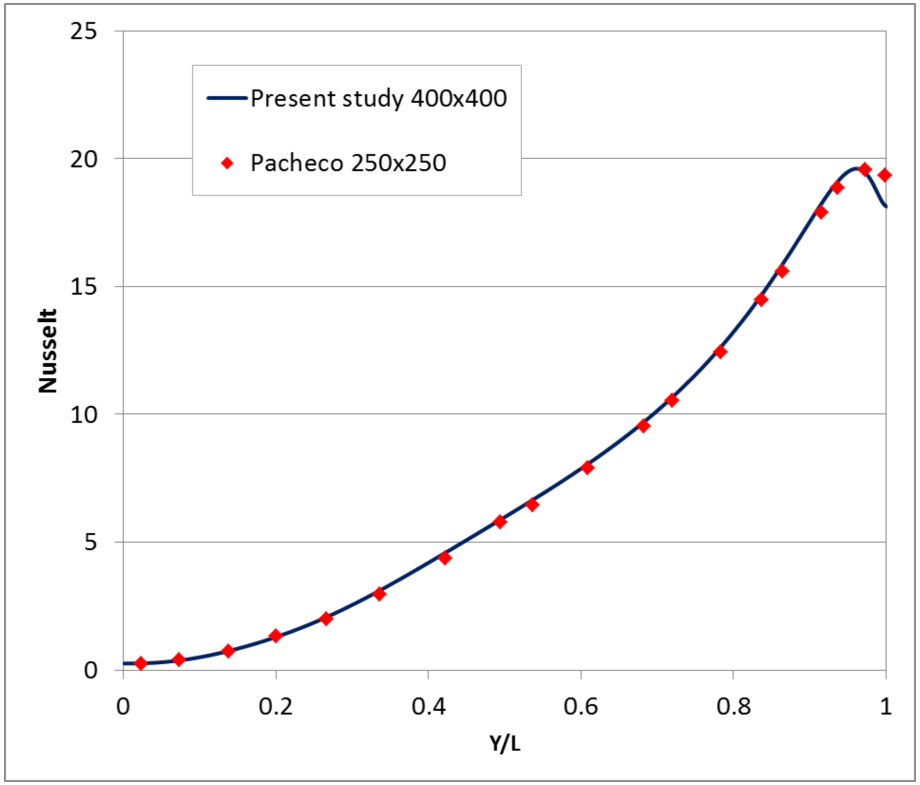
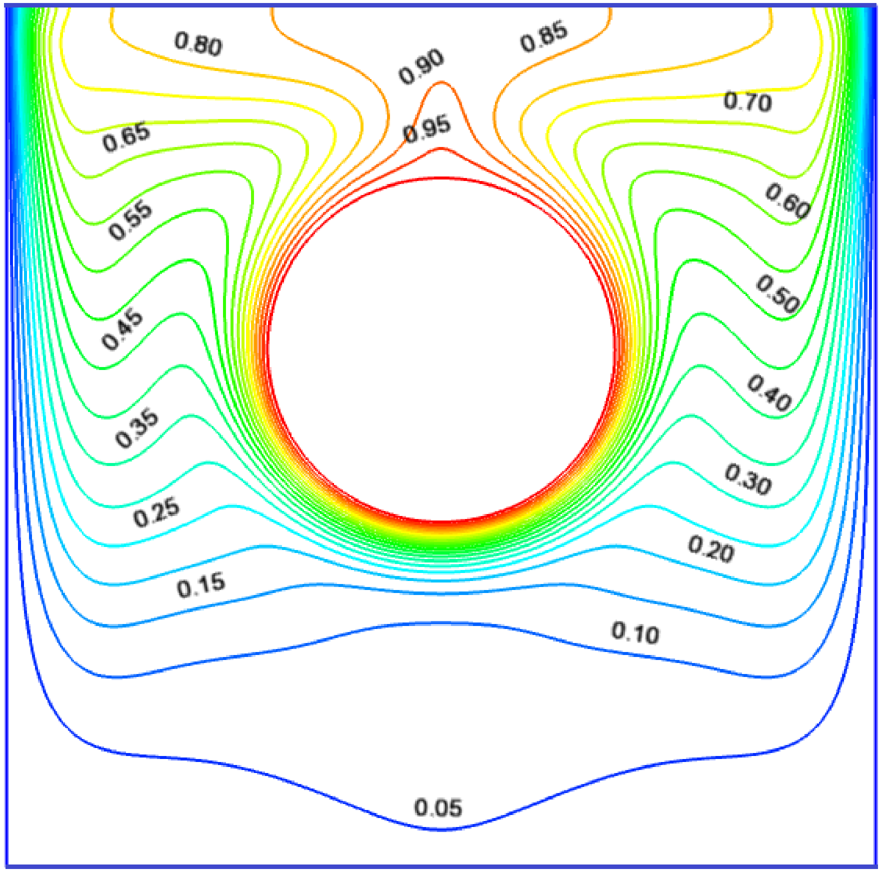
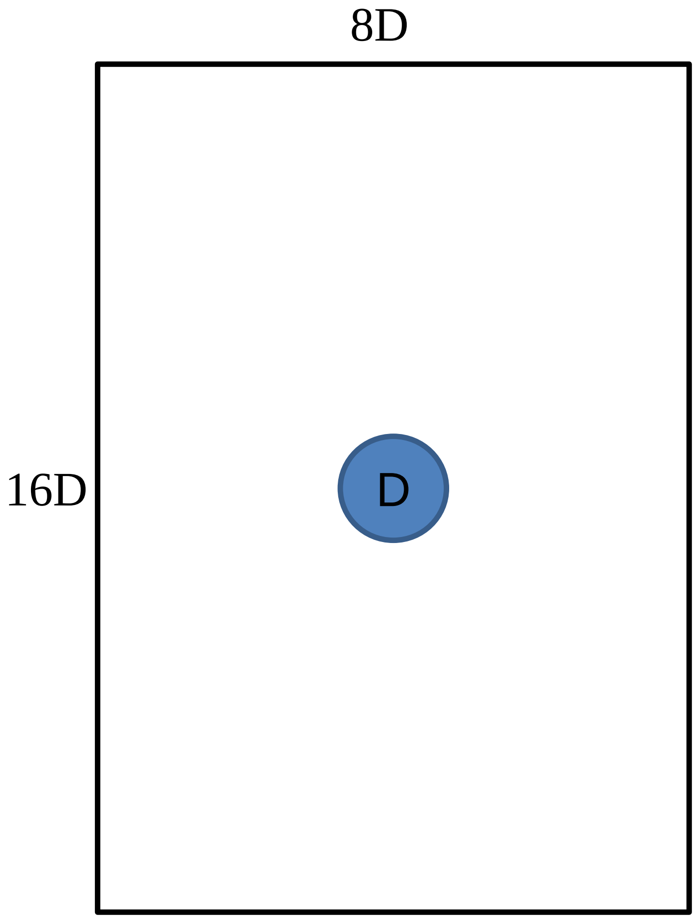




Catalyst particle with varied temperature

- Catalyst particle is located in an enclosure
- Particle temperature changes with time
- $\rho_r = 1.1$
- $C_{P,r} = 1$
- $\mathrm{Re} = 40$
- $Gr = 1000$
- $\mathrm{Pr} = 0.7$
- $\bar{Q} = 1$



* Wachs A., (2011). Comput. Chem. Eng. Vol. 3511.

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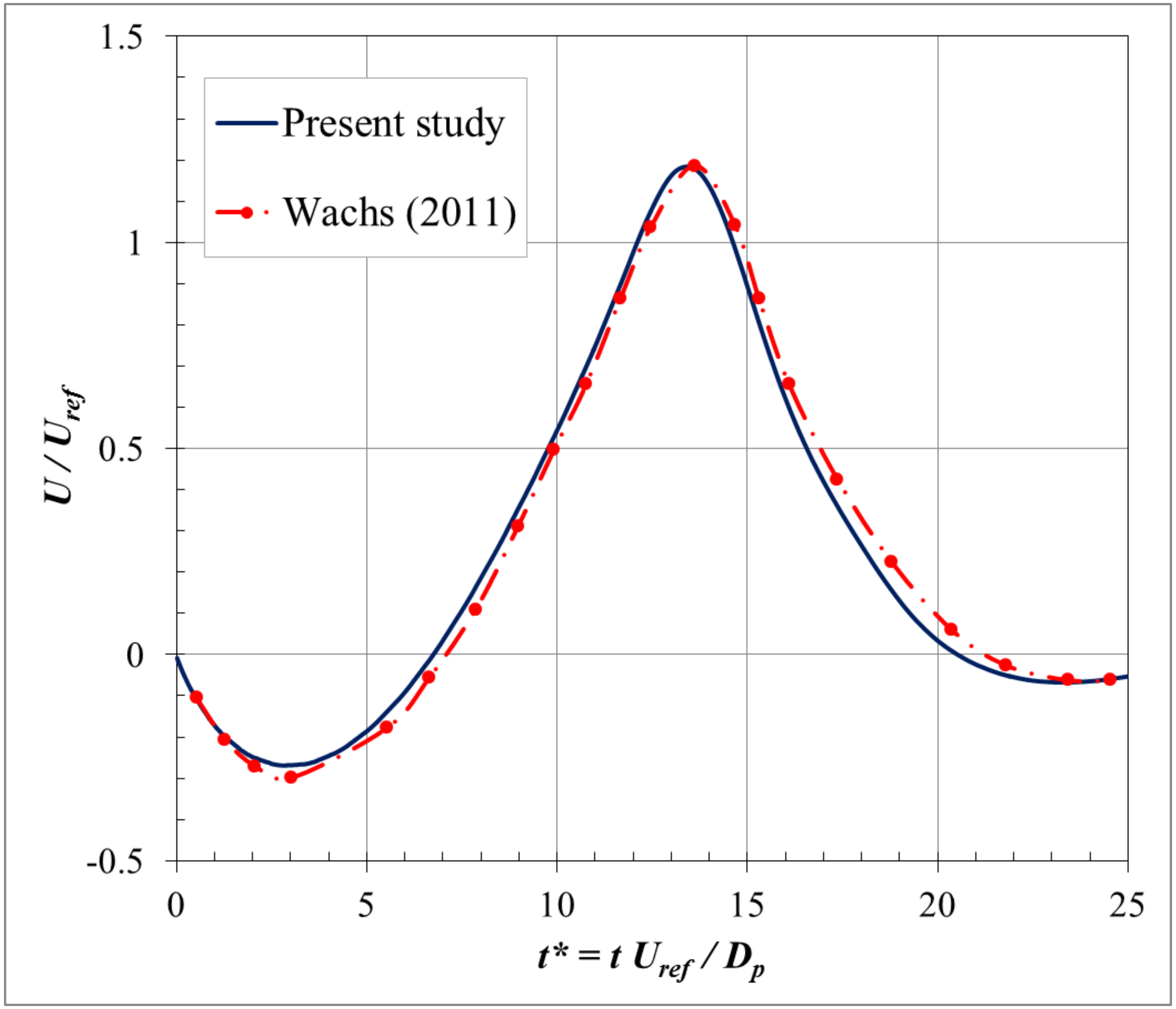

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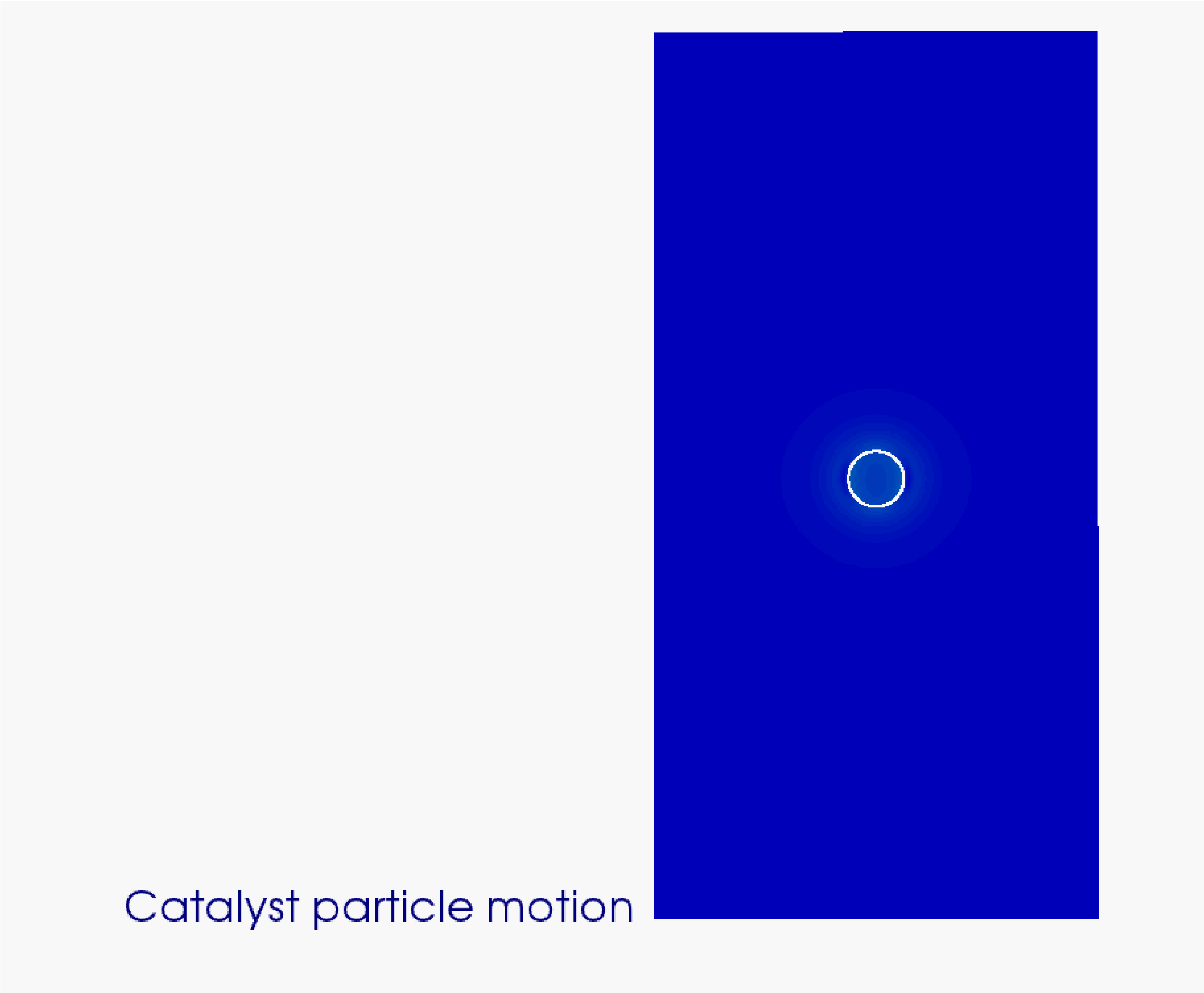
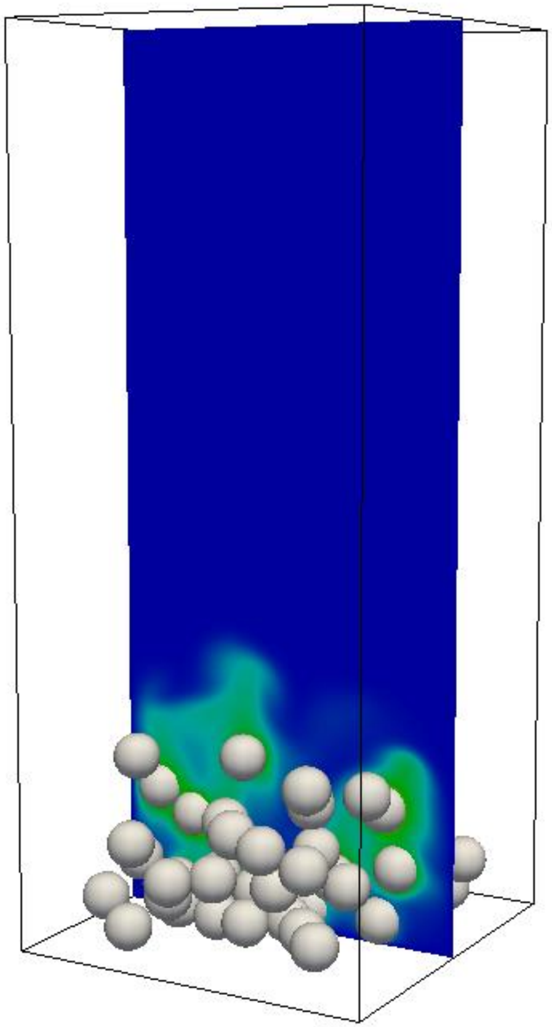


60 Catalyst particles with varied temperature

- 60 Catalyst particles are located in an enclosure
- Particle temperature changes with time
- Domain: 8*D*×8*D*×19*D*
- $\rho_r = 1.1$
- $C_{P,r} = 1$
- $\mathrm{Re} = 40$
- $\mathrm{Pr} = 0.7$
- $Gr = 1000$
- $\bar{Q} = 3.88$



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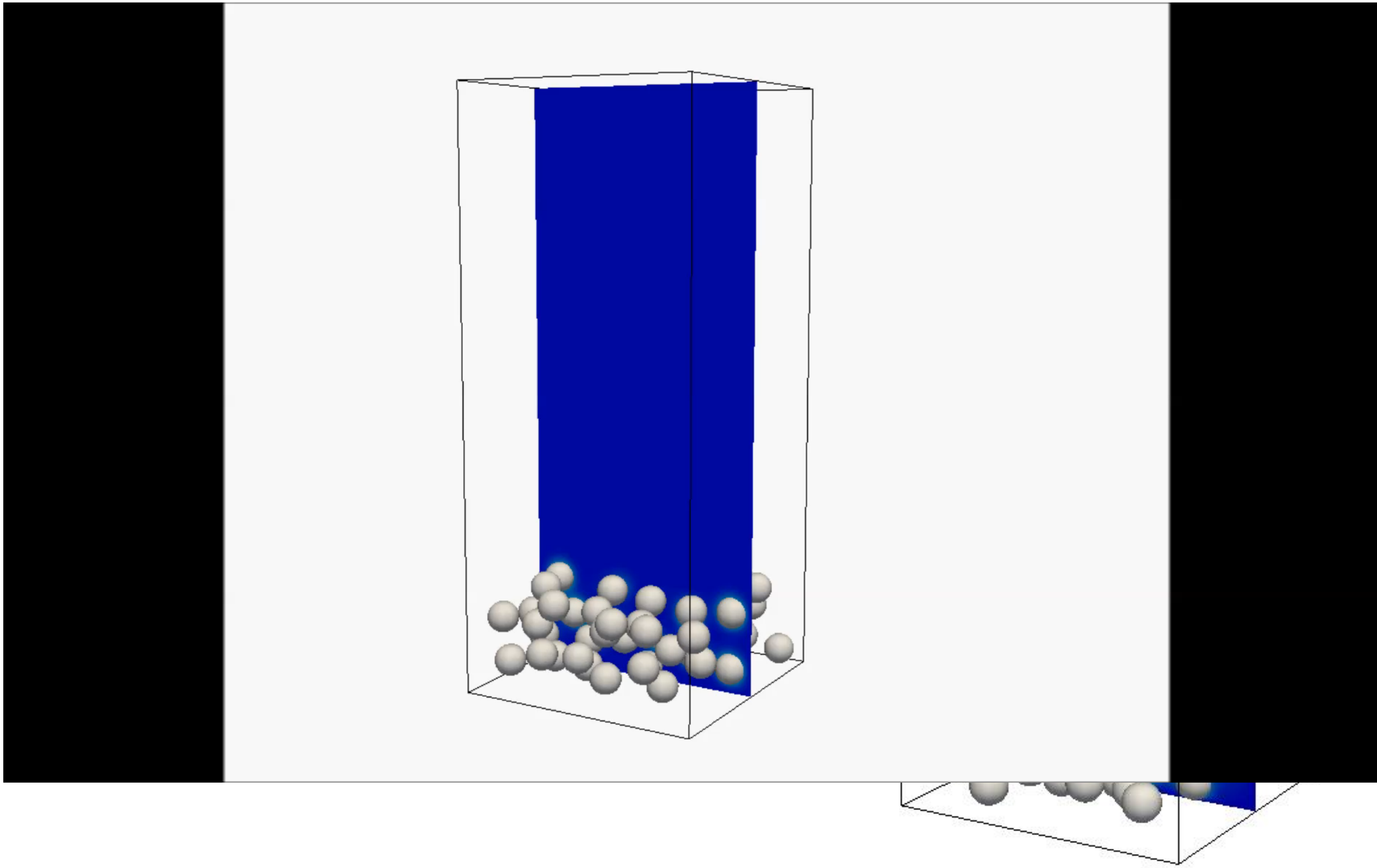

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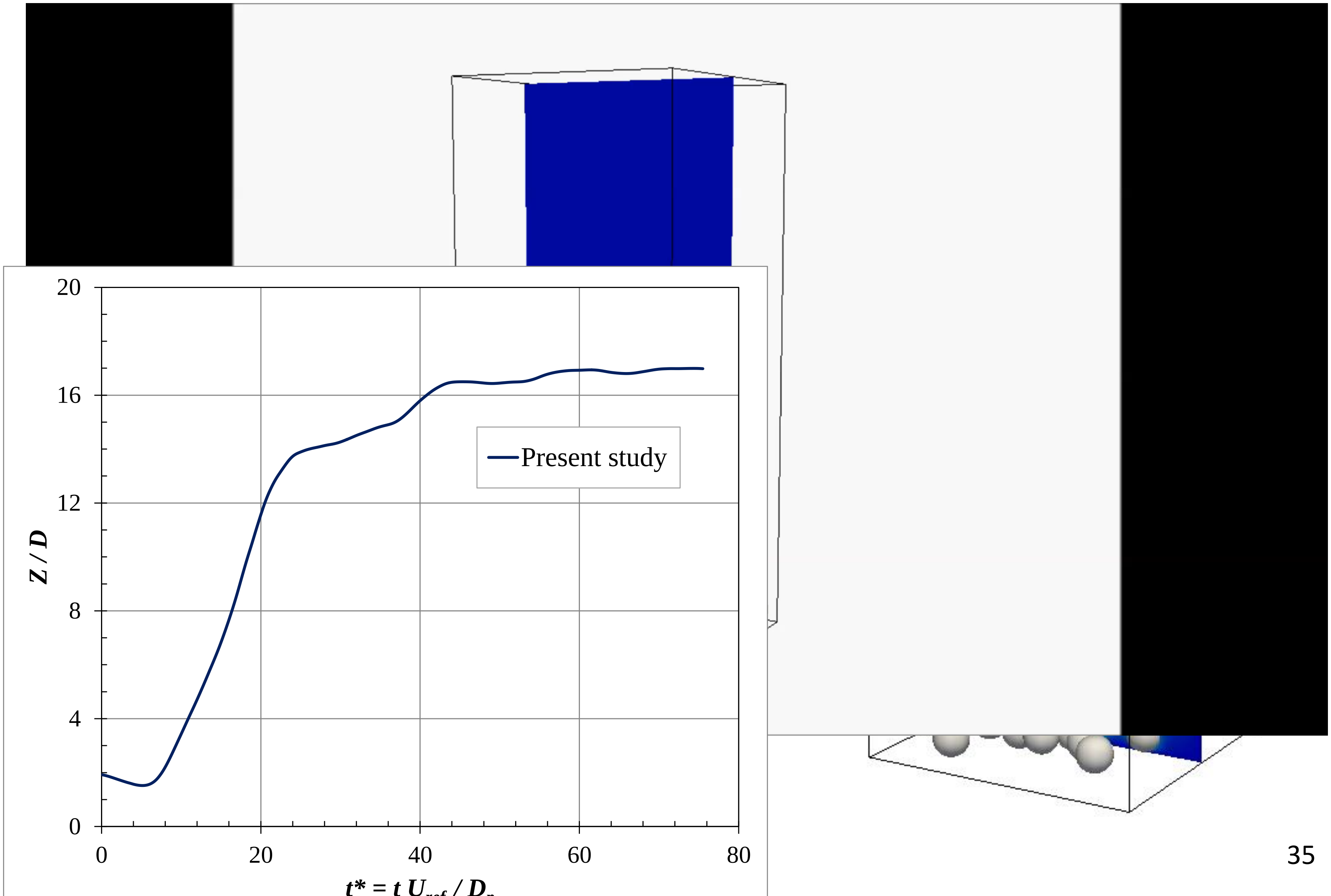

CONCLUSIONS & OUTLOOK

- LBM is a promising approach for multiphase flow simulation.
- Motion of particles of different shapes is successfully modeled by LBM
- Thermal effect can be considered by IB-LBM.
- LBM required less memory and computational time for lid-driven cavity flow.
- In case of turbulent flow the current 6th order NSE code can capture the vortices structure and predict fluctuations better than LBM.

THANK YOU FOR YOUR ATTENTION!