Institut für
Kontinuumsmechanik

Leibniz
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Modeling and Simulation of Particles in Fluids

7^{th} Colloquium on Unilateral Problems in Structural Mechanics, 17 June 2010

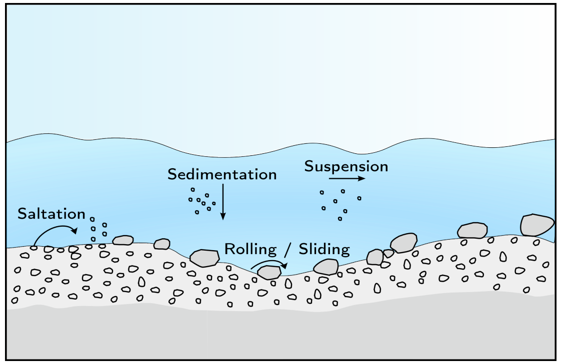
Peter Wriggers & Bircan Avci

▷ Motivation

- **Goal: Theoretical and numerical description of fluid-particle interaction**

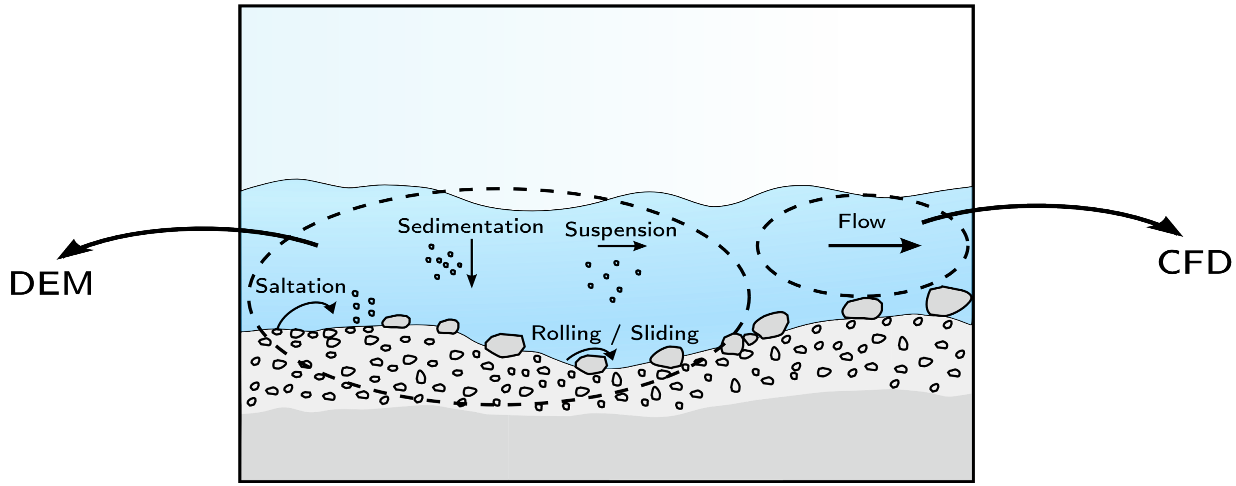
Elbe flood 2002
(www.wwf.de)

River sedimentation
(www.anra.gov.au)



- ∗ Direct numerical simulation of three dimensional particulate flows
- ∗ Sedimentation and erosion processes in river engineering
- ∗ Homogenization strategies
- ∗ Multiscale methods for sediment transport

▷ Multiphase system

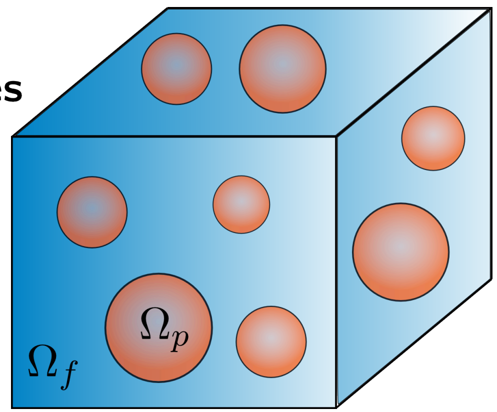


- DEM
  - ∗ Spherical quasi-rigid particles
  - ∗ Contact forces
  - ∗ Rolling / sliding / sticking
  - ∗ Adhesion
  - ∗ Gravity
- CFD
  - ∗ Incompressible viscous flow
  - ∗ Nonstationary flow field

COUPLING

▷ Fluid-solid particle system

- Multiphase field
  - n solid particles ($p = 1, \ldots, n$) in a fluid (density ρ_f, viscosity μ)
  - Domain occupied by the fluid at time t: $\Omega_f(t)$
  - Domain occupied by the particle p at time t: $\Omega_p(t)$
- Fluid phase
  - Nonstationary incompressible *Navier-Stokes*
  - Finite Element Method (FEM)
- Particle phase
  - *Newton-Euler* equations for solid particles
  - Discrete Element Method (DEM)



Motivation

Multiphase System

DEM

Coupling

Numerical Examples

Summary & Challenges

- The fluid constituents
  - *Navier-Stokes* equations in $\Omega_f(t)$

$$\rho_f\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) - \nabla\cdot\boldsymbol{\sigma} = \boldsymbol{0} \quad , \quad \nabla\cdot\boldsymbol{u} = 0$$

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \mu\left[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right]$$

where $\boldsymbol{\sigma}$: stress tensor

- The particle constituents
  - *Newton-Euler* equations in $\Omega_p(t)$

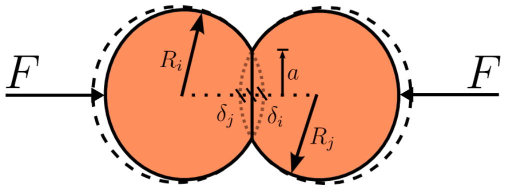
Translation: $$M\frac{d\boldsymbol{U}}{dt} = (\rho - \rho_f)V\boldsymbol{g} + \boldsymbol{F}^p + \boldsymbol{F}^f$$

Rotation: $$\boldsymbol{I}\frac{d\boldsymbol{\omega}}{dt} + \boldsymbol{\omega}\times(\boldsymbol{I}\boldsymbol{\omega}) = \boldsymbol{T}^p + \boldsymbol{T}^f$$

where $\boldsymbol{F}^{(\cdot)}$: Forces, $\boldsymbol{T}^{(\cdot)}$: Torque

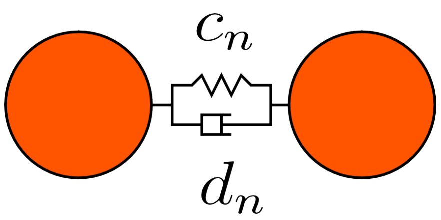
▷ Models for DEM

- **Normal contact**
  - $*$ Penalty force approach
  - $*$ *Hertz* contact law [*Hertz*, 1896]



$$F_{ij} = c_n \delta^{3/2} + d_n \dot{\delta}$$

where F_{ij} : contact force



$$c_n = \frac{4}{3\pi(k_i + k_j)} \sqrt{R}$$

$$k_l = \frac{1 - \nu_l^2}{\pi E_l} \ , \ l = i, j$$

$$\delta = \delta_i + \delta_j \ , \ R = \frac{R_i R_j}{R_i + R_j}$$

contact radius: $a = \frac{F}{c_n} R^{3/2}$

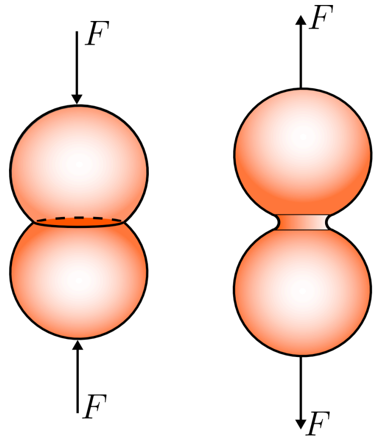
- **Normal contact with adhesion: JKR contact model** [*Johnson*, *Kendall* & *Roberts*, 1971]

  * Force between two spheres

$$F = \frac{4Ea^3}{3R} - 2\pi a^2 \sqrt{\frac{2WE}{\pi a}}$$

with: $\frac{1}{E} = \frac{1-\nu_i}{E_i} + \frac{1-\nu_j}{E_j}$

and W : (underwater) work of adhesion [e.g. *Loskofsky* et. al. , 2006]



  * Contact radius

$$a = \left[\frac{3R}{4E}\left(F + 3\pi WR \pm\sqrt{(2\pi WR)^2 + 6\pi WRF}\right)\right]^{1/3}$$

* Equilibrium contact area

$$a_o = \left(\frac{6\pi W R^2}{K}\right)^{1/3} \quad \text{with: } K = \frac{4}{3}E$$

* Separation force and separation contact radius

$$F_s = \frac{3}{2}\pi R W \quad , \quad a_s^3 = \frac{1}{4}a_o^3$$

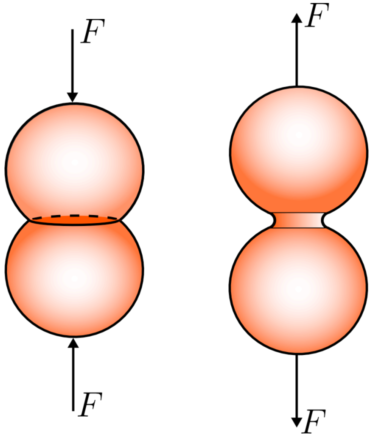
* Force-contact radius relation

$$\frac{F}{F_s} = 4\left(\frac{a}{a_o}\right)^3 - 4\left(\frac{a}{a_o}\right)^{3/2}$$

* Displacement-contact radius relation

$$\frac{\delta}{\delta_s} = 6^{1/3}\left[2\left(\frac{a}{a_o}\right)^3 - \frac{4}{3}\left(\frac{a}{a_o}\right)^{1/2}\right]$$

critical separation distance : $\delta_s = \dfrac{1}{2}\dfrac{a_o^2}{(6^{1/3}R)}$



- **Tangential contact with static / dynamic friction** [*Cundall* & *Strack*, 1979; *Wriggers*, 1987; *Luding*, 2005]

  * Total relative velocity of the contact surfaces

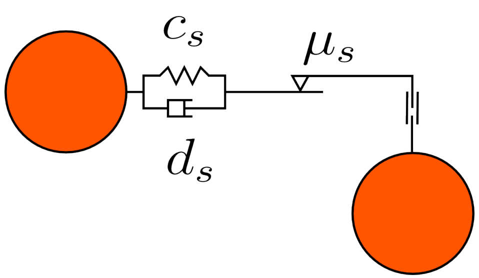
$$\boldsymbol{U}_{ij} = \boldsymbol{U}_i - \boldsymbol{U}_j + R_i \boldsymbol{n} \times \boldsymbol{\omega}_i + R_j \boldsymbol{n} \times \boldsymbol{\omega}_j$$

  * Tangential velocity at the contact point

$$\boldsymbol{U}_t = \boldsymbol{U}_{ij} - (\boldsymbol{U}_{ij} \cdot \boldsymbol{n})\boldsymbol{n}$$

  * Projection of the tangential spring

$$\boldsymbol{g} = \boldsymbol{g}' - (\boldsymbol{g}' \cdot \boldsymbol{n})\boldsymbol{n}$$



  * Tangential test force

$$\boldsymbol{F}_t^o = -c_s \boldsymbol{g} - d_s \boldsymbol{U}_t$$

Coulomb-criteria	Tang. force	Tang. spring
Sticking: $\lvert\boldsymbol{F}_t^o\rvert <= \mu_s F_n$	$F_t = \lvert\boldsymbol{F}_t^o\rvert$	$\boldsymbol{g}' = \boldsymbol{g} + \boldsymbol{U}_t \Delta t$
Sliding: $\lvert\boldsymbol{F}_t^o\rvert > \mu_s F_n$	$F_t = \mu_d F_n$	$\boldsymbol{g}' = -(1/c_s)(F_t \boldsymbol{t} + d_s \boldsymbol{U}_t)$

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- **Rolling resistance** [*Iwashita* & *Oda*, 1998; *Marshall*, 2008]

  * Rolling velocity

$$\boldsymbol{U}_r = -R(\boldsymbol{\omega}_i - \boldsymbol{\omega}_j) \times \boldsymbol{n} - \frac{1}{2}\Big(\frac{R_j - R_i}{R_i + R_j}\Big)\boldsymbol{U}_t$$

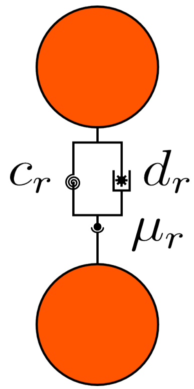
  * Rolling resistance torque

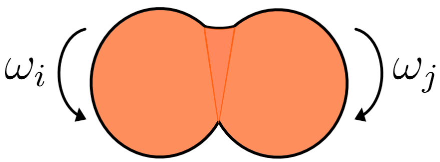
$$M_r = -c_r\Big(\int_{t_0}^{t} \boldsymbol{U}_r(\tau)d\tau\Big) \cdot \boldsymbol{t}_r - d_r\boldsymbol{U}_r \cdot \boldsymbol{t}_r$$

with: $\boldsymbol{t}_r = \boldsymbol{U}_r / |\boldsymbol{U}_r|$

and $|M_r| <= M_{r,crit}$

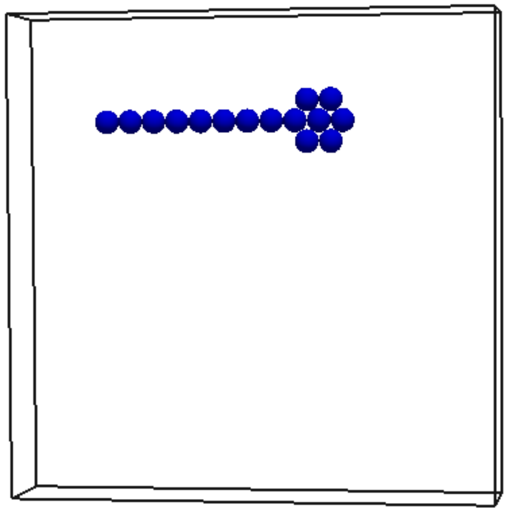
where $M_{r,crit}$: threshold value



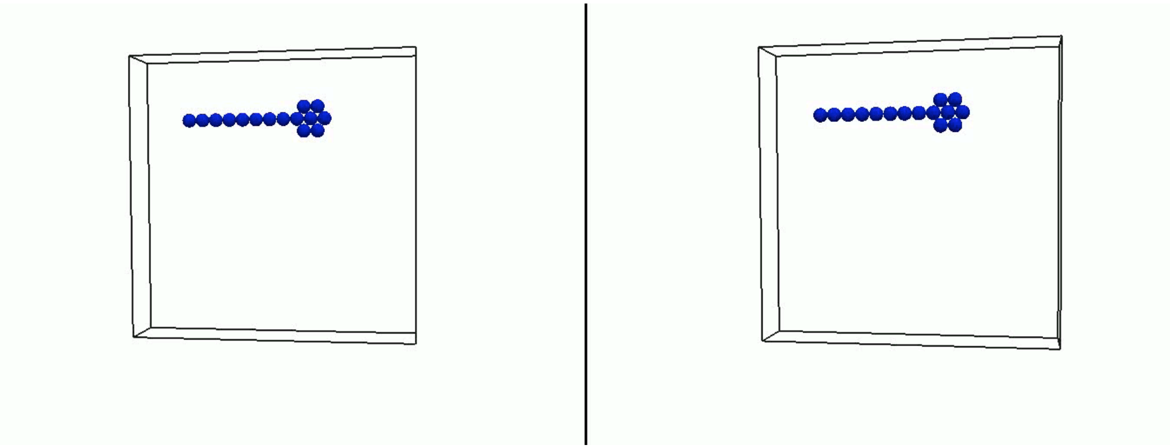


▷ Numerical Example

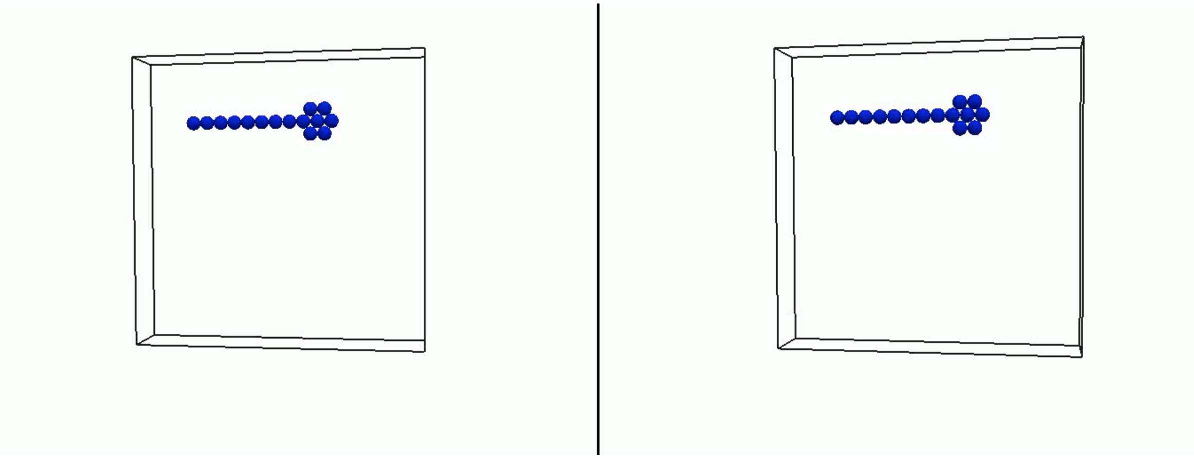
- **Pendular under dead load**



effects of adhesive forces



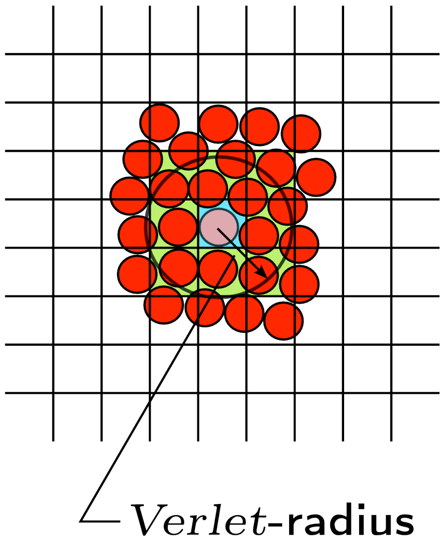
effects of rolling resistance



▷ Contact detection

- **Cell index method** [*Quentrec* & *Brot*, 1973]
  - ∗ Subdivision of the domain in cells
  - ∗ Sorting of the particles into cells
- **Verlet neighbour list** [*Verlet*, 1967]
  - ∗ Neighbour if:

    R_i+pair separation+R_{max} <= *Verlet*-radius
  - ∗ Possible neighbours in neighbour cells
  - ∗ Contact check only with neighbours
  - ∗ Reconstruction of the list from time to time [e.g. *Pöschel*, 2005]



▷ Efficient force computation

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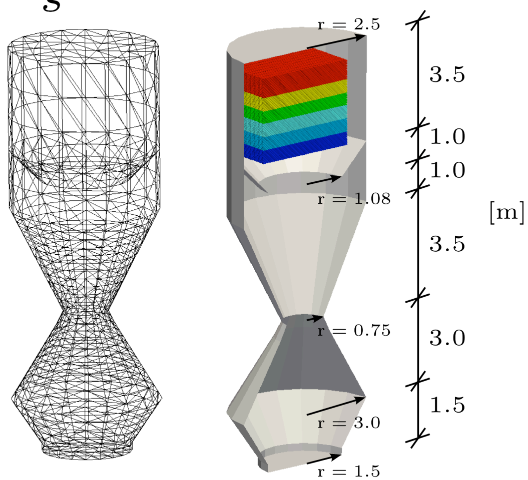
▷ Numerical Example

- **Filling of a hopper with particles**

  * No. of particles: $n = 505750$
  * Radius: $r = 0.02\,\mathrm{m}$
  * Density: $\rho = 10\,\mathrm{kg/m^3}$
  * E-modulus: $c_n = 1 \times 10^7\,\mathrm{N/m^2}$
  * Poisson's ratio: $\nu = 0.00$
  * Damping: $d_n = 1 \times 10^{-5}\,\mathrm{N/(m}$
  * Gravitational acc.: $g = 9.81\mathrm{m/s^2}$
  * Time step: $\Delta t = 1 \times 10^{-5}\,s$
  * Simulation time: $t_s = 6\,s$
  * No friction: $\mu_s = 0.0$



▷ Coupling of the phases

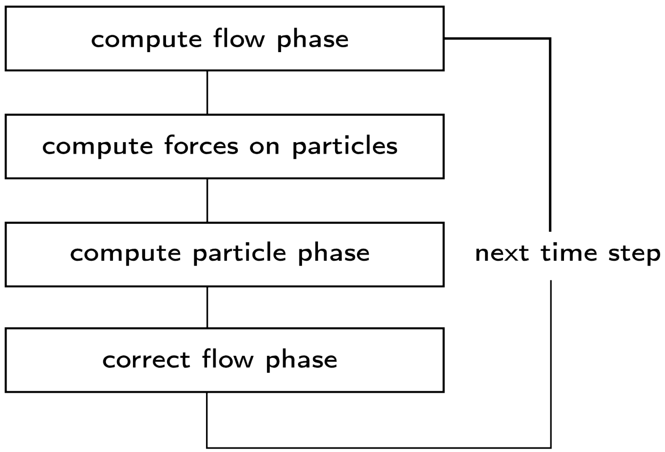
- Different approaches
  - ∗ ALE-technique with body-fitted grid
    [*Johnson* & *Tezduyar*, 1996]
  - ∗ Fictitious domains

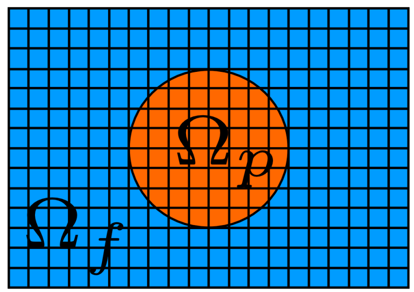
    Implicit Coupling

    [*Glowinski et. al.*, 1999; *Patankar et. al.*, 2000]

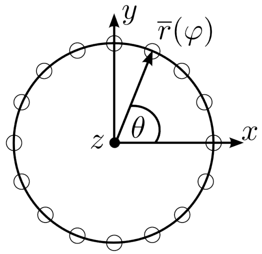
    Explicit Coupling

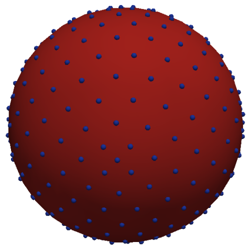
    [*Duchanoy* & *Jongen*, 2003; *Wan* & *Turek*, 2003]

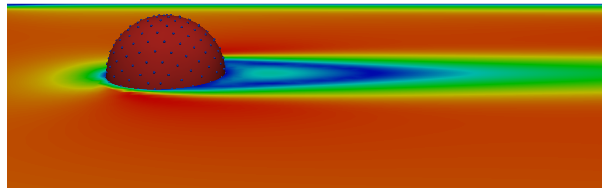




- Hydrodynamic forces
  - ∗ Lagrangian force points







  - ∗ Finite elements:

    nonconforming rotated trilinear elements with mean values on element faces for the velocitiy [*Rannacher* & *Turek*, 1992] and constant pressure in elements

  - ∗ Translational forces [*Lebedev* & *Laikov*, 1999]

$$d\boldsymbol{F} = \langle \boldsymbol{\sigma} \rangle \, \boldsymbol{n} \, dA = \boldsymbol{t} \, dA \quad , \quad \langle \nabla \boldsymbol{u} \rangle = \frac{1}{V} \int \boldsymbol{u} \otimes d\boldsymbol{A}$$

$$\boldsymbol{F}^f = \int \boldsymbol{t} \, dA = \sum_i (d\boldsymbol{F})_i = J \sum_i \omega_i \boldsymbol{t}_i \quad , \quad J = 4\pi r^2$$

  - ∗ Torque

$$\boldsymbol{T}^f = \sum_i \left((\boldsymbol{x} - \boldsymbol{x}_p) \times d\boldsymbol{F} \right)_i$$

- Interaction between particle and fluid phase

  * Rigid-body movement enforcing

    Additional constraint to the *Navier-Stokes* equations

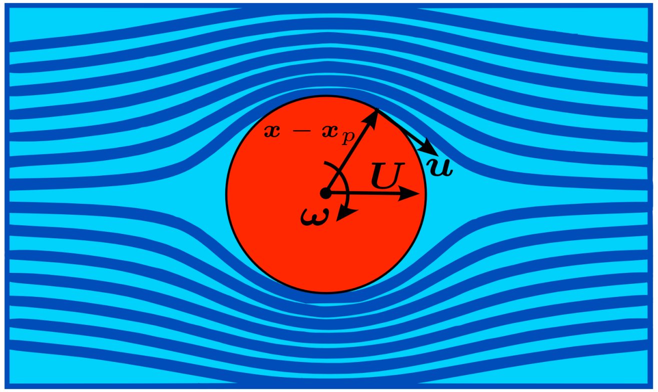
    $$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{U} + \boldsymbol{\omega} \times (\boldsymbol{x} - \boldsymbol{x}_p) \quad \forall\, \boldsymbol{x} \in \Omega_p$$

  * Smooth flow velocity transition

    Nonlinear weighted velocity update [*Luo* et al., 2007]

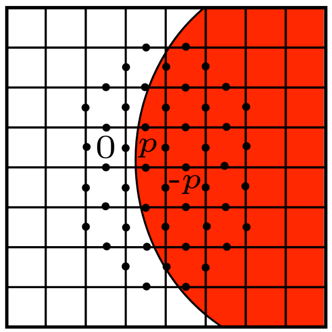
    $$\boldsymbol{u} = (1-\varphi)\boldsymbol{u} + \varphi \boldsymbol{U}$$

    where: $\varphi = e^{-\alpha \cdot Re_p}$



  * Level set method

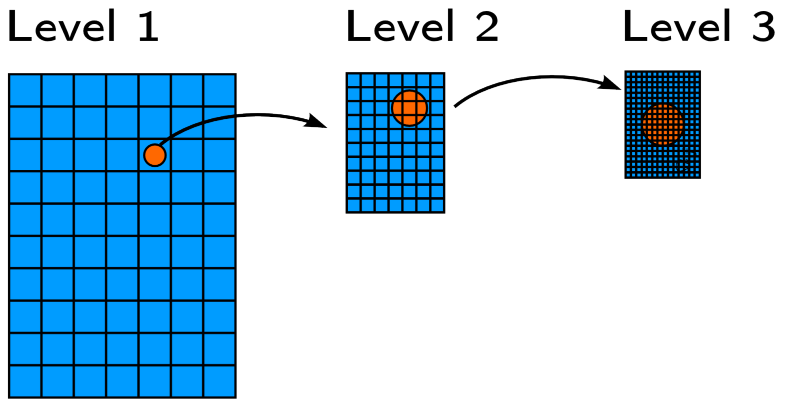
p	=: no. particle
$\langle 0 \rangle$	=: outer
$\langle p \rangle$	=: boundary
$\langle -p \rangle$	=: inner



- Coupling of FEM-DEM on the time level
  - ∗ Two different time scales
    with $\Delta t_F > \Delta t_D$
  - ∗ Subcycling time integration [$Feng$ & $Owen$, 2007]
  - ∗ Reduce Δt_D to $\Delta \tilde{t}_D$
    where: $\Delta \tilde{t}_D = \dfrac{\Delta t_F}{n_s}$, $n_s = int(\Delta t_F / \Delta t_D) + 1$
  - ∗ constant hydrodynamic forces during n_s subcycles

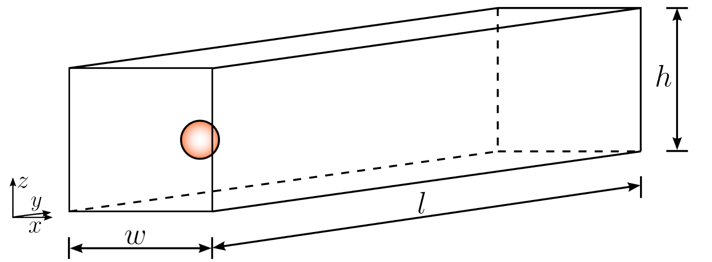
▷ Efficient computation of particulate flows

- Instationary flow solver *FEATFLOW*
  - ∗ Multigrid techniques as *Navier-Stokes* solver [*Turek*, 1998]
- Computation of particle-particle contact
  - ∗ Efficient force computation, e.g. *Verlet*-lists [*Verlet*, 1967]
  - ∗ Efficient integration scheme for DEM, e.g. *Gear*-algorithmus [*Gear*, 1971; *Allen* & *Tildesley*, 1987]
- Computation of the hydrodynamic forces
  - ∗ Efficient element assignment by using hierarchical techniques [*Wan* & *Turek*, 2007]



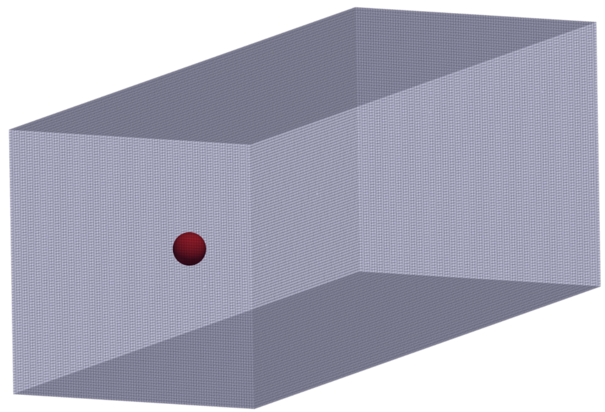
▷ Validation of fluid-particle coupling

- **Drag coefficient**
  - ∗ Numerical model

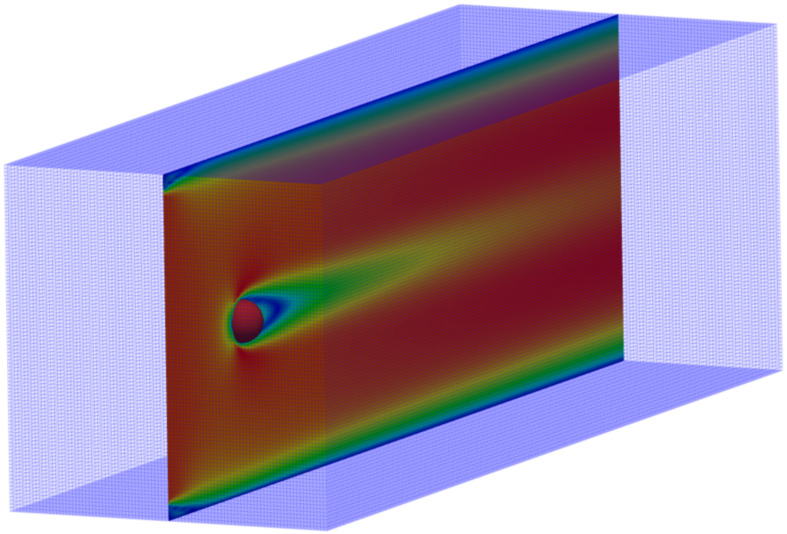


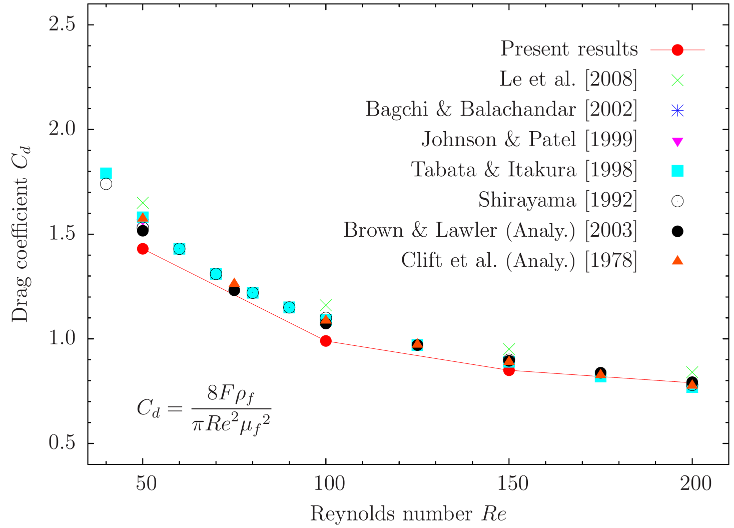
Computational domain			
Dimensions:	$h \times w \times l$	=	$2 \times 2 \times 6$
Particle location:	(x, y, z)	=	$(1, 1, 1)$
Particle diameter:	d	=	0.25
Inflow boundary at:	y	=	0.00

MG-Level	Discretization	No. Cells	Vertices	Cell Faces	D.o.f.'s
Level 1	$12 \times 12 \times 36$	5 184	6 253	16 560	54 864
Level 2	$24 \times 24 \times 72$	41 472	45 625	128 448	426 816
Level 3	$48 \times 48 \times 144$	331 776	348 145	1 011 456	3 366 144
Level 4	$96 \times 96 \times 288$	2 654 208	2 719 201	8 027 136	26 735 616

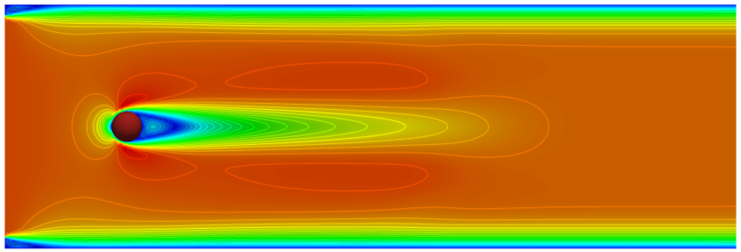


* **Numerical results**
Contour plots at Re= 150



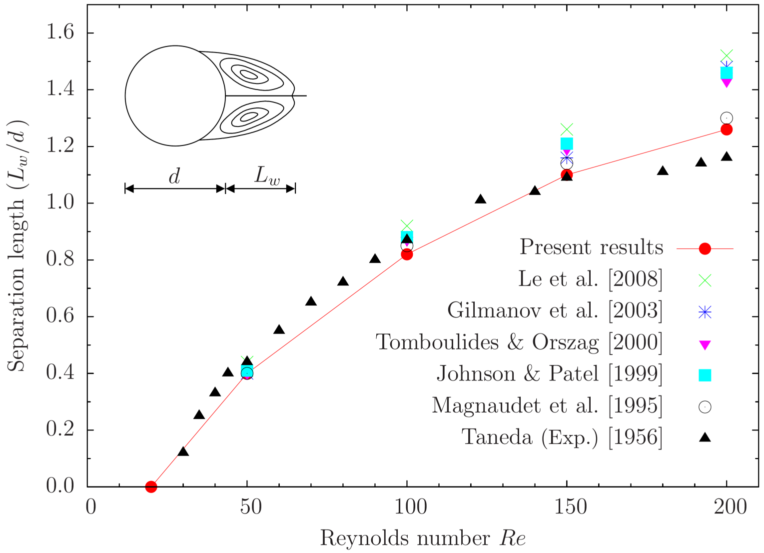


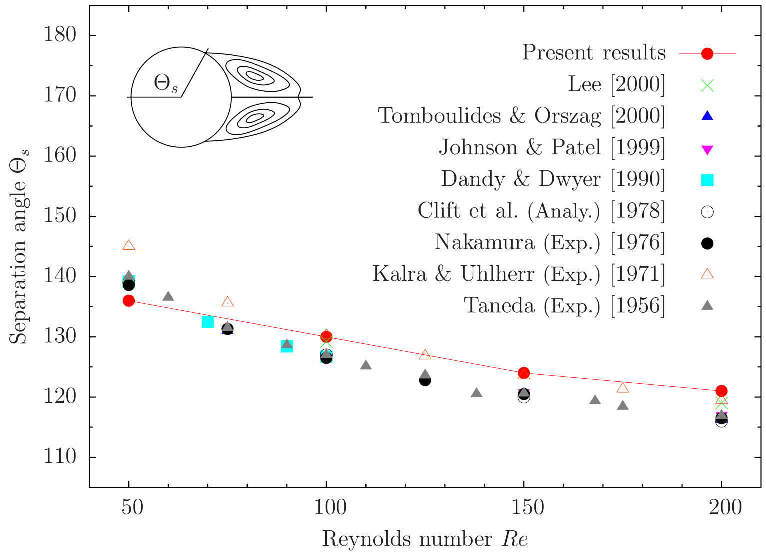
velocity



pressure

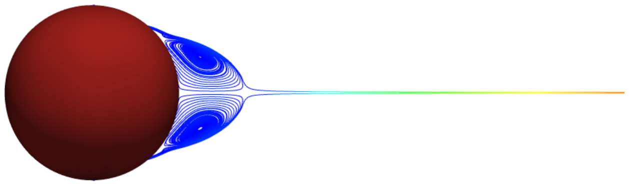
- **Wake length and wake separation angle**
  - ∗ Numerical results



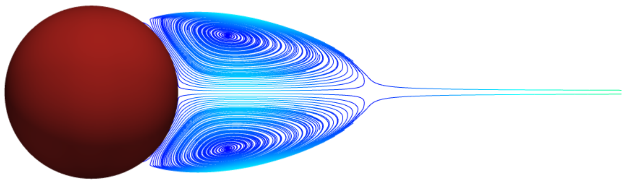


Wake behind a sphere at:

$Re = 50$



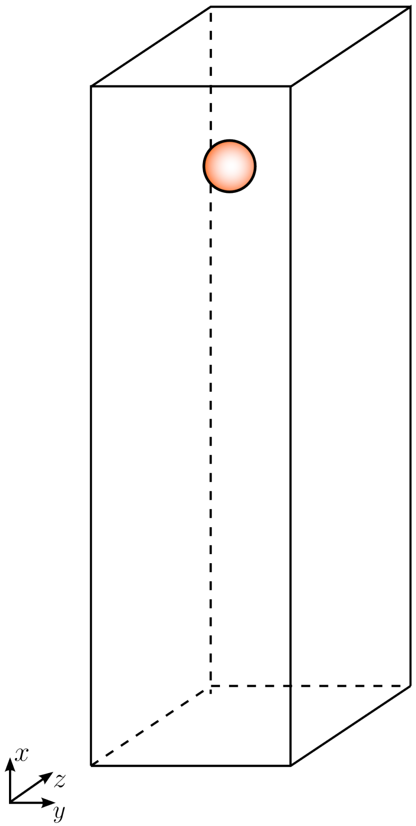
$Re = 150$



▷ A single sedimenting sphere

- **Physical parameters**

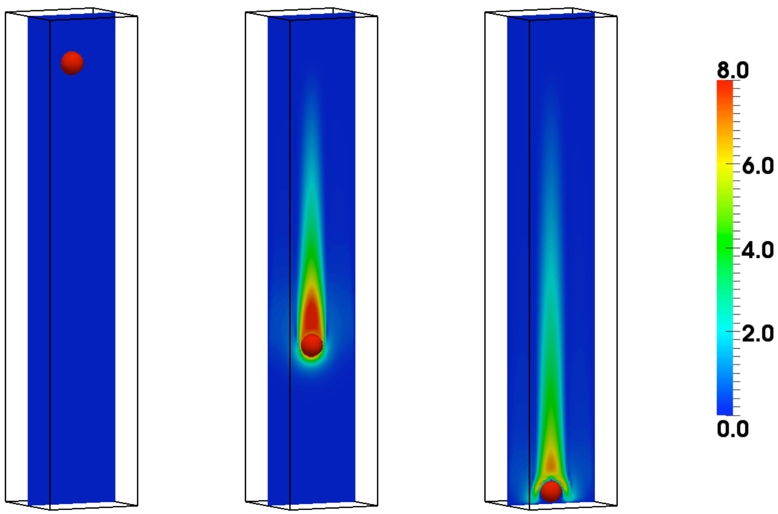
  - Domain size: $\Omega = [0,0,0] \times [10,2,2]$
  - Sphere radius: $r = 0.25$
  - Sphere location: $\boldsymbol{x} = (9,1,1)$
  - Density ratio: $\rho/\rho_f = 1.05$
  - Gravitational acc.: $\boldsymbol{g} = (-980,0,0)$
  - Fluid viscosity: $\nu = 0.01$
  - Time step fluid: $\Delta t_F = 1 \times 10^{-4}$
  - Time step DEM: $\Delta t_D = 1 \times 10^{-5}$

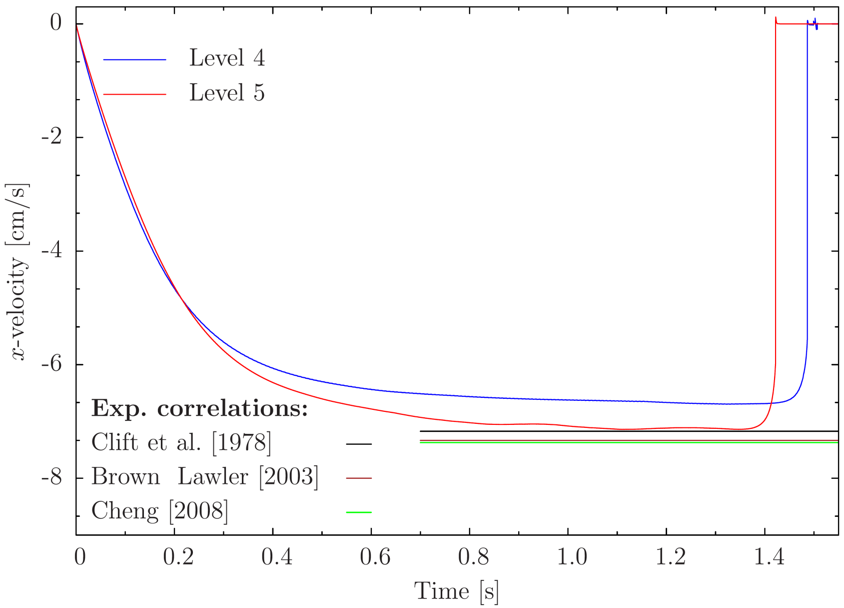


MG-Level	Discretization	No. Cells	Vertices	Cell Faces	D.o.f.'s
Level 1	5 × 5 × 25	625	936	2 150	7 075
Level 2	10 × 10 × 50	5 000	6 171	16 100	53 300
Level 3	20 × 20 × 100	40 000	44 541	124 400	413 200
Level 4	40 × 40 × 200	320 000	337 881	977 600	3 252 800
Level 5	80 × 80 × 400	2 560 000	2 630 961	7 750 400	25 811 200

- **Numerical results**

  Velocity contour plots for $y = 1$





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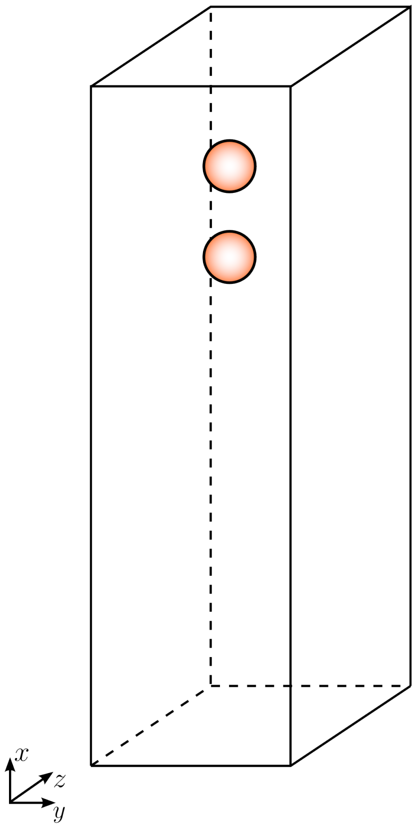
▷ Drafting, kissing and tumbling case

- **Physical parameters**

  * Domain size: $\Omega = [0,0,0] \times [10,2,2]$
  * Sphere radius: $r = 0.25$
  * Sphere location: $\boldsymbol{x} = (9,1,1); (8,1,1)$
  * Density ratio: $\rho/\rho_f = 1.05$
  * Gravitational acc.: $\boldsymbol{g} = (-980, 0, 0)$
  * Fluid viscosity: $\nu = 0.01$
  * Time step fluid: $\Delta t_F = 1 \times 10^{-4}$
  * Time step DEM: $\Delta t_D = 1 \times 10^{-5}$



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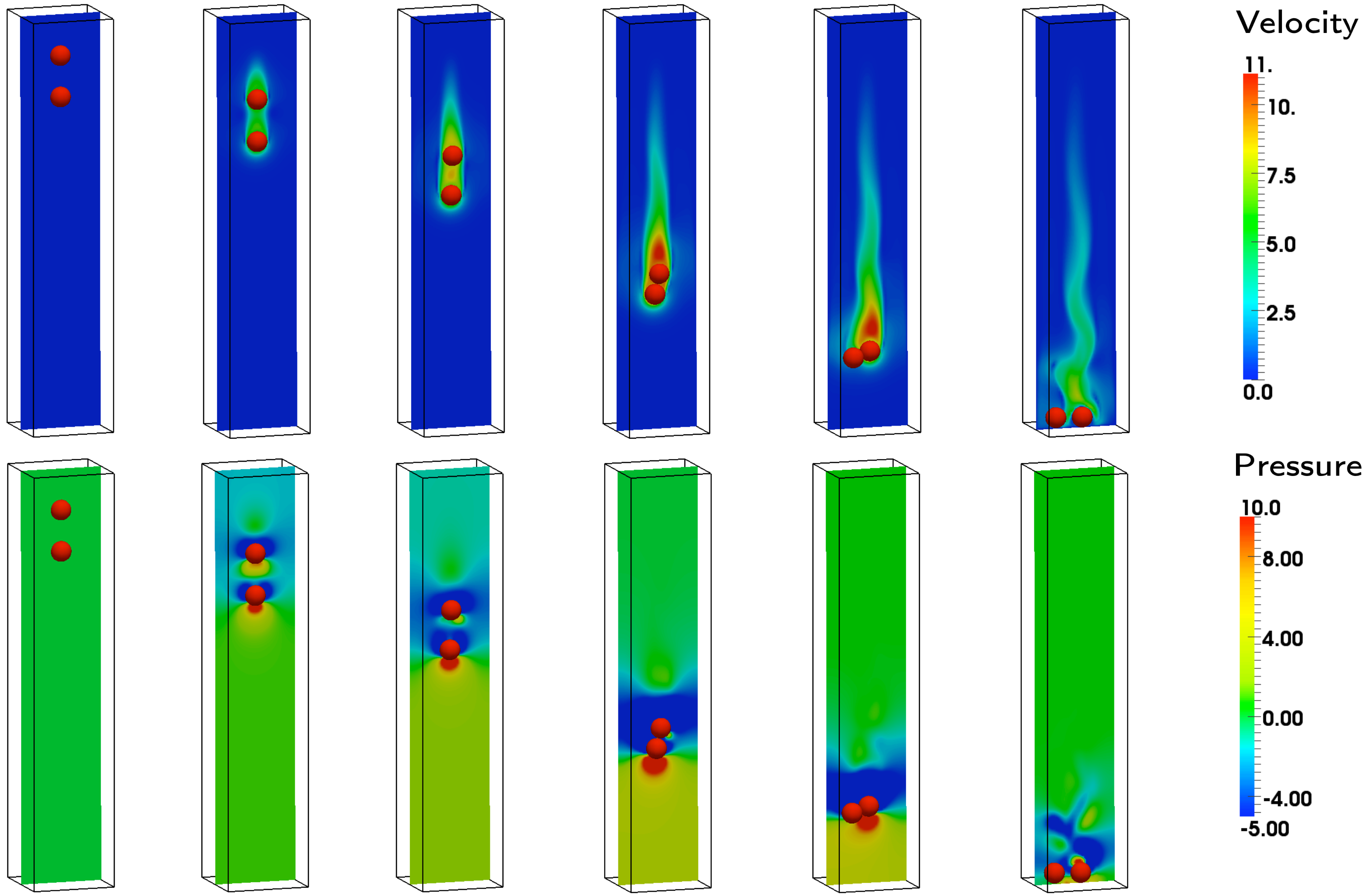
Level 3	$20 \times 20 \times 100$	40 000	44 541	124 400	413 200
Level 4	$40 \times 40 \times 200$	320 000	337 881	977 600	3 252 800
Level 5	$80 \times 80 \times 400$	2 560 000	2 630 961	7 750 400	25 811 200

- **Numerical results**

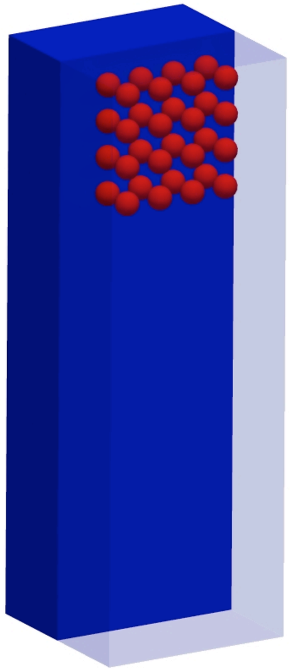
  Velocity and pressure contour plots for $y = 1$



▷ Sedimentation of 64 spheres

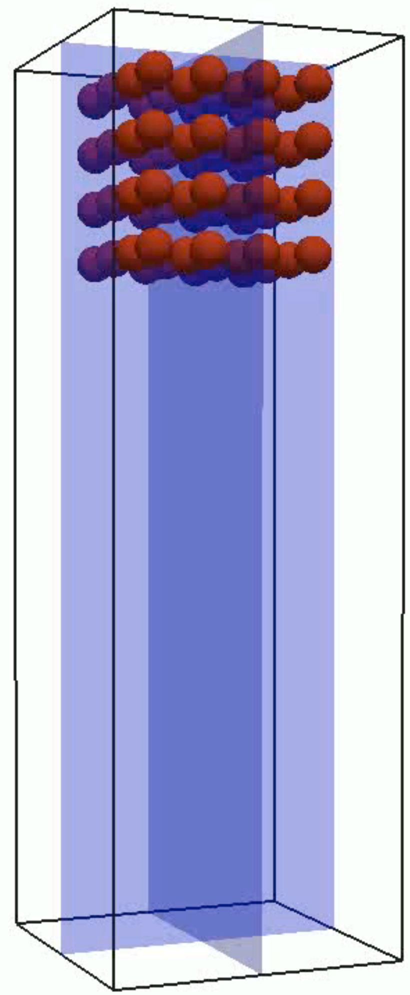
- **Physical parameters**

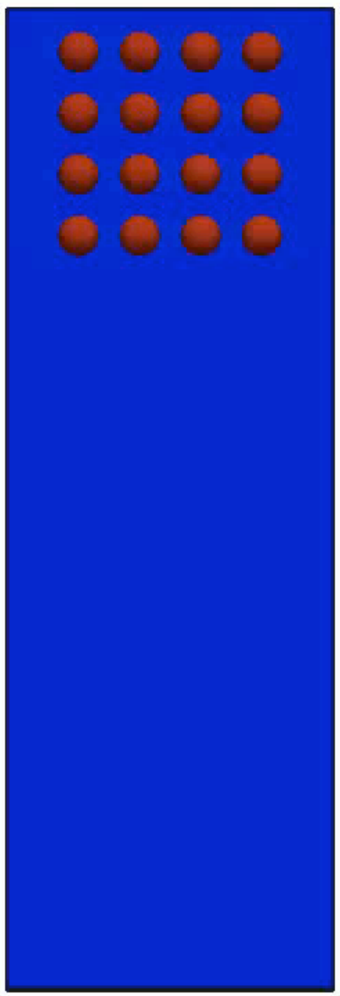
  - ∗ Domain size: $\Omega = [0,0,0] \times [2,2,6]$
  - ∗ Sphere radius: $r = 0.25$
  - ∗ Density ratio: $\rho/\rho_f = 1.50$
  - ∗ Gravitational acc.: $\boldsymbol{g} = (0,0,-980)$
  - ∗ Fluid viscosity: $\nu = 0.01$
  - ∗ Time step fluid: $\Delta t_F = 1 \times 10^{-4}$
  - ∗ Time step DEM: $\Delta t_D = 1 \times 10^{-6}$



▷ Sedimentation of 64 spheres

- **Particle positions**





▷ Numerical Example

- **Sedimentation with adhesion effects**

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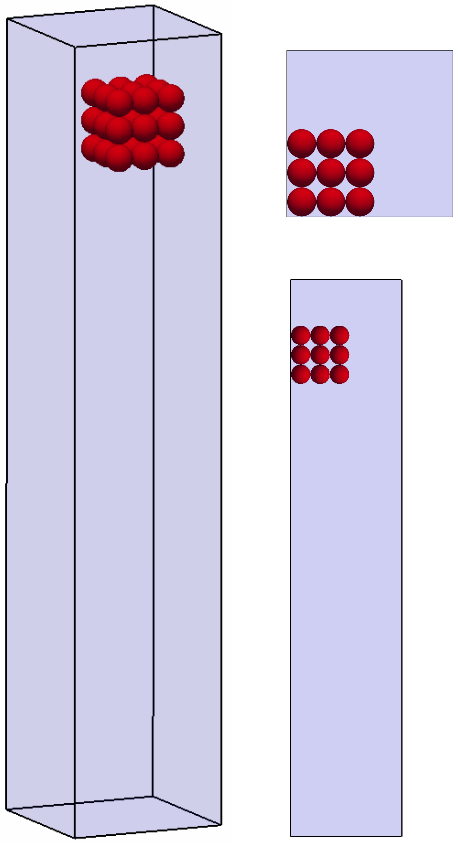
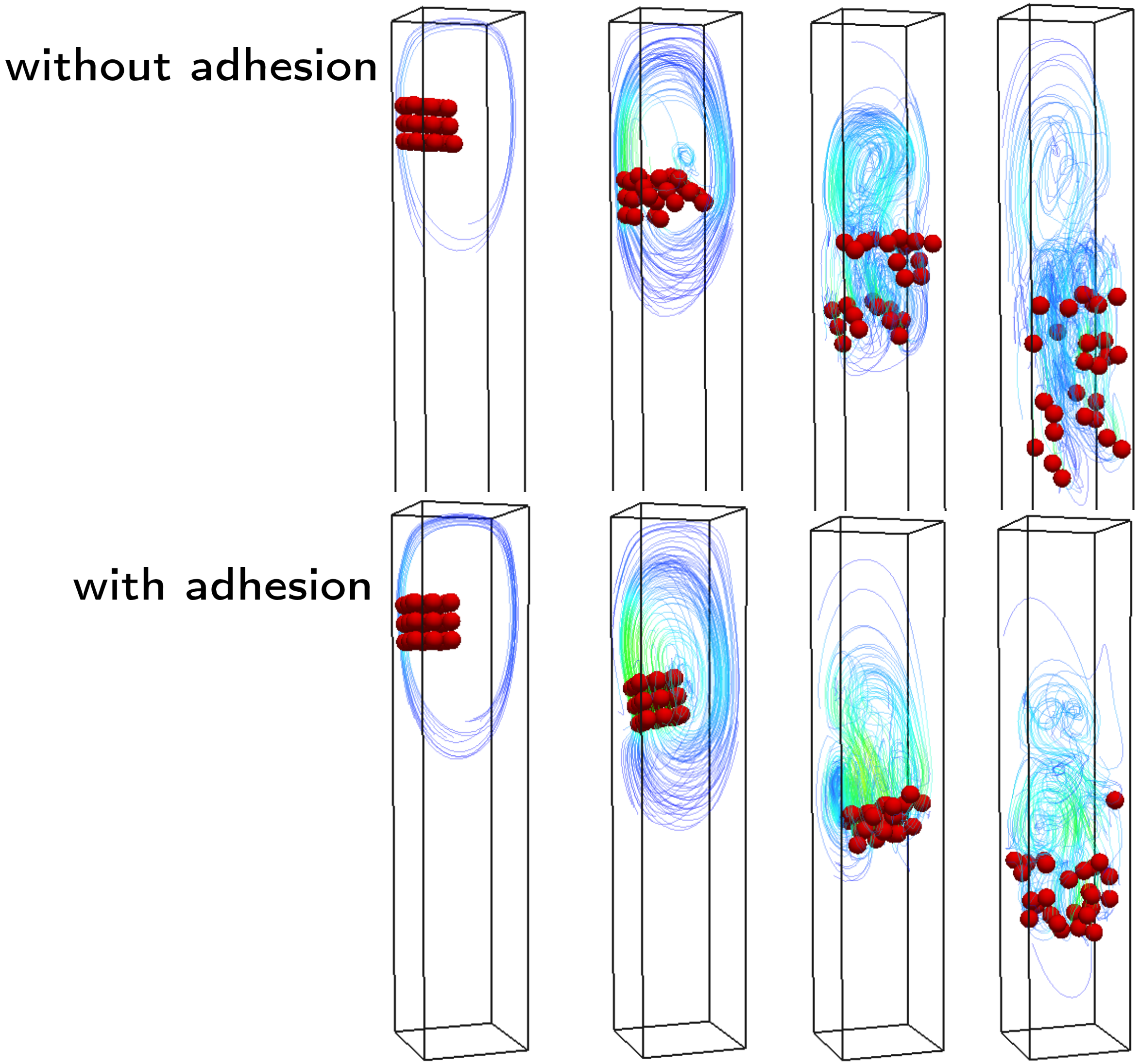
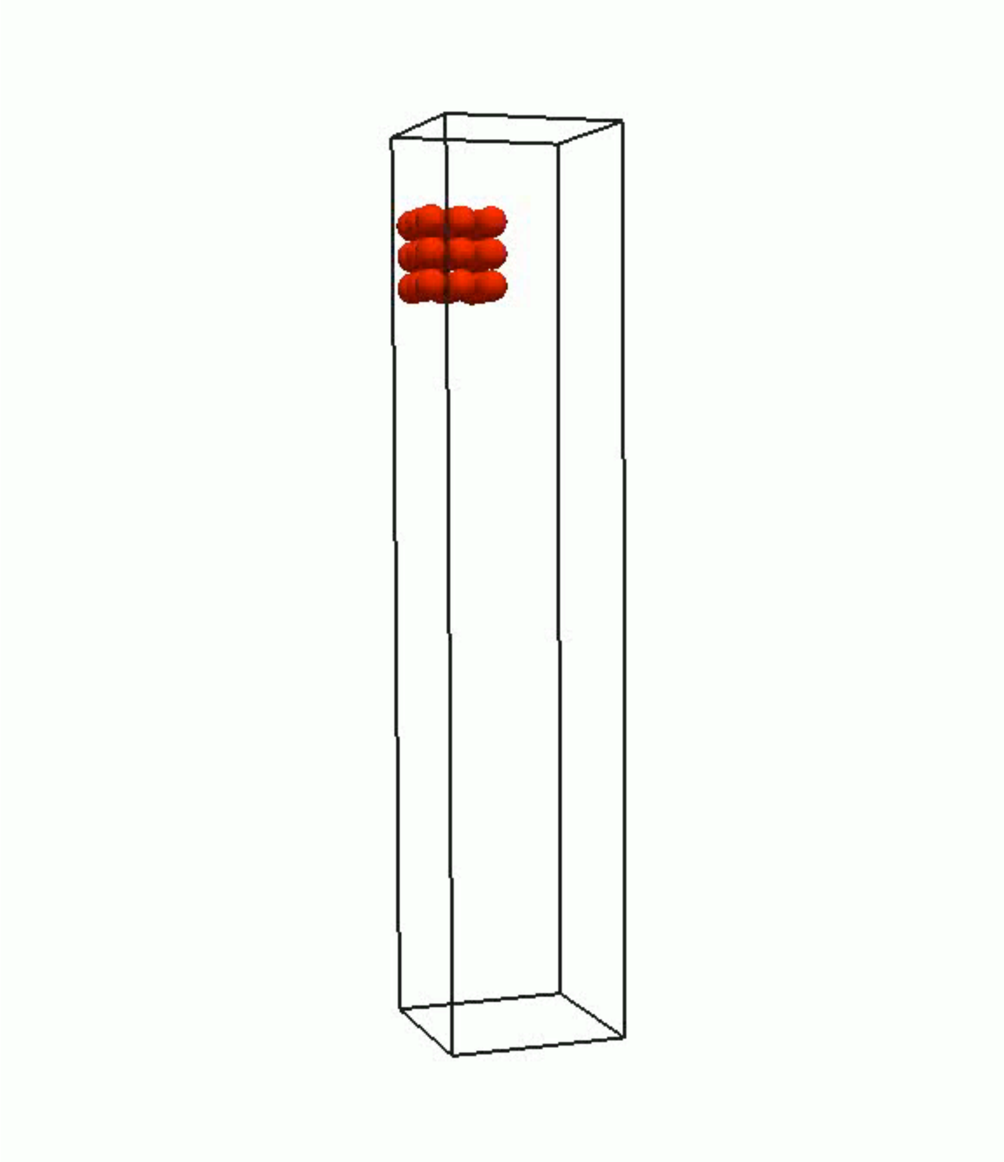
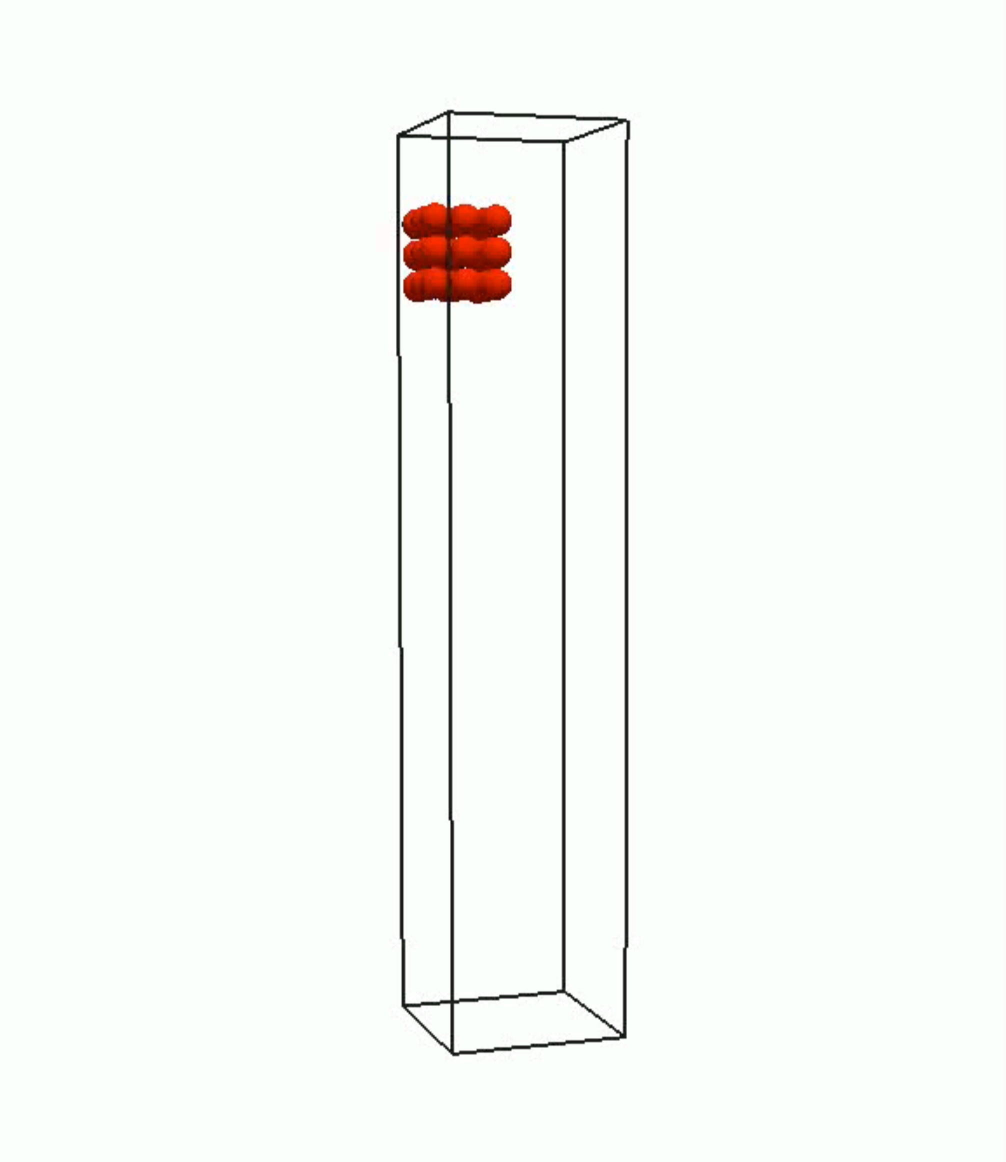




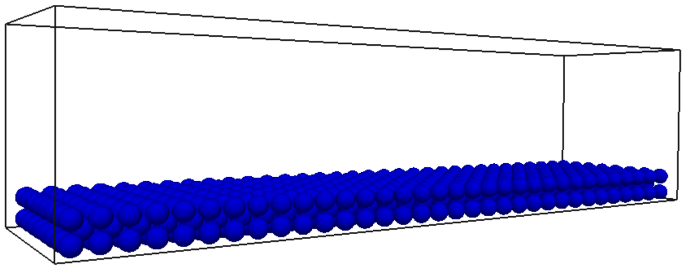


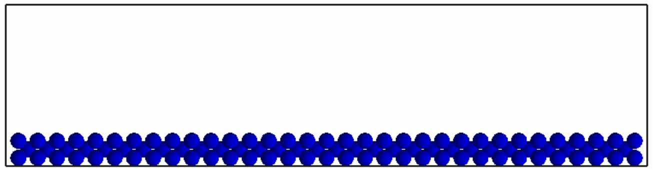


▷ Lid-driven cavity flow with particles

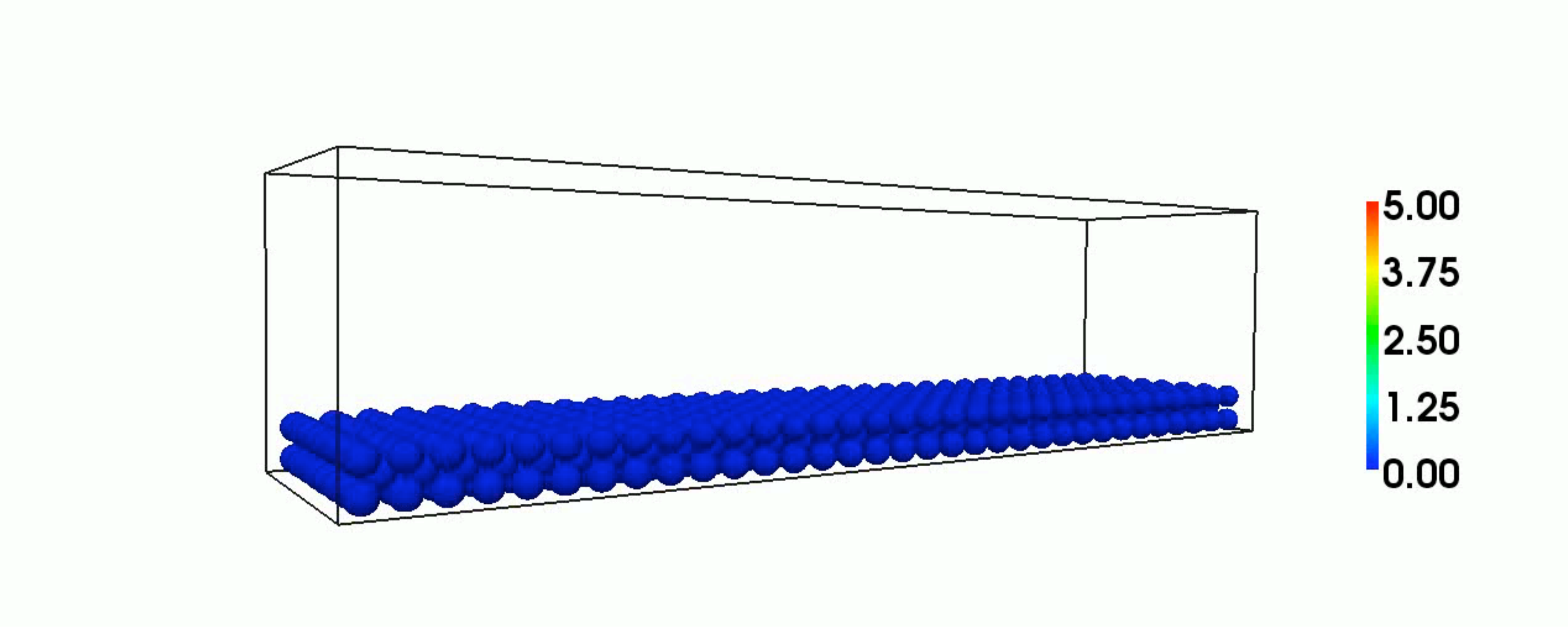
- **Physical parameters**

  * Domain size: $\Omega = [0, 0, 0] \times [0.5, 0.5, 2]$
  * No. particles: $n = 752$
  * Particle radius: $r = 0.025$
  * Density ratio: $\rho/\rho_f = 1.001$
  * Gravitational acc.: $\boldsymbol{g} = (0, 0, -980)$
  * Lid-driven velocity: $\boldsymbol{u} = (5, 0, 0)$
  * Fluid viscosity: $\nu = 0.01$
  * Time step fluid: $\Delta t_F = 1 \times 10^{-4}$
  * Time step DEM: $\Delta t_D = 1 \times 10^{-6}$

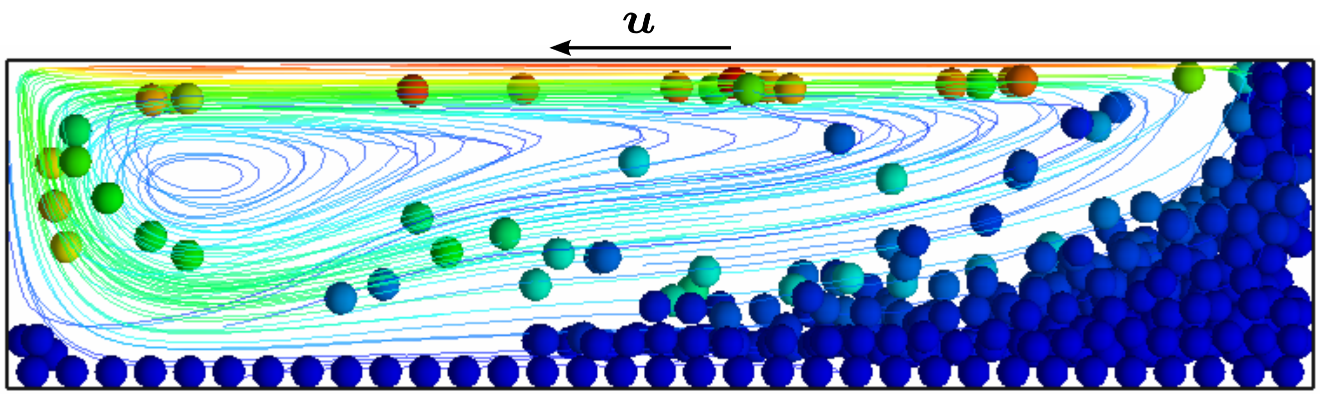


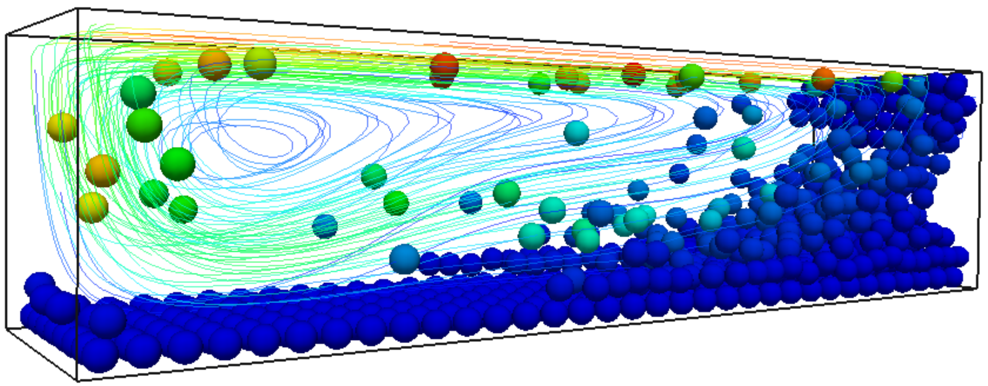


▷ Lid-driven cavity flow with particles



▷ Lid-driven cavity flow with particles





Videoclip

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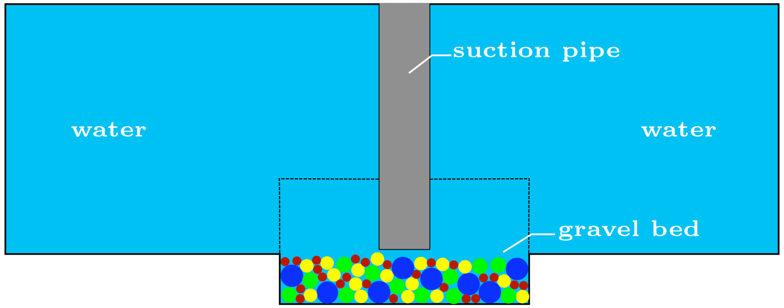
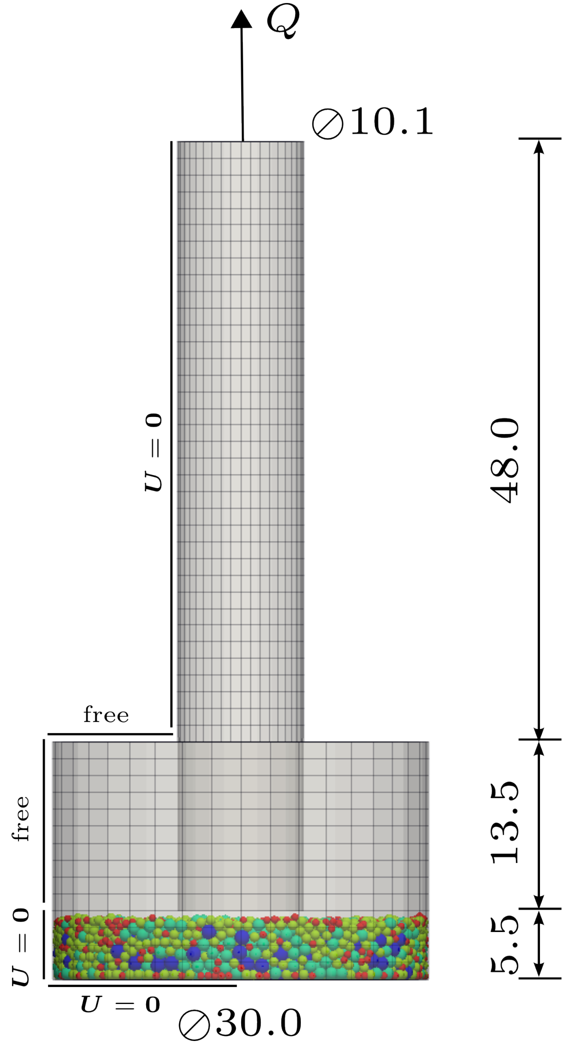
▷ Suction extraction of particles [*Feng, Han & Owen*, 2009]

- **Physical parameters**

  - ∗ No. particles: $n = 5000$
  - ∗ Particle radius: $r = 0.3 - 0.6$
  - ∗ Density ratio: $\rho/\rho_f = 2.65$
  - ∗ Gravitational acc.: $\boldsymbol{g} = (0, 0, -981)$
  - ∗ Fluid viscosity: $\nu = 0.01$
  - ∗ Time step fluid: $\Delta t_F = 1 \times 10^{-4}$
  - ∗ Time step DEM: $\Delta t_D = 1 \times 10^{-6}$



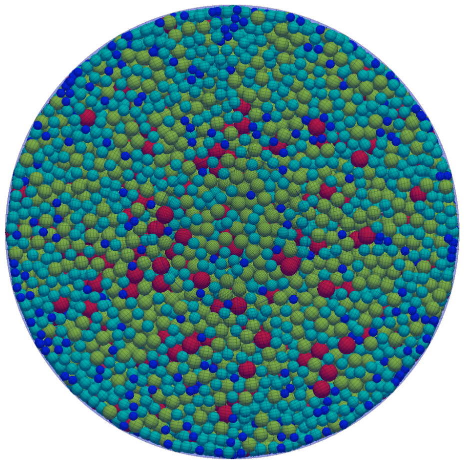


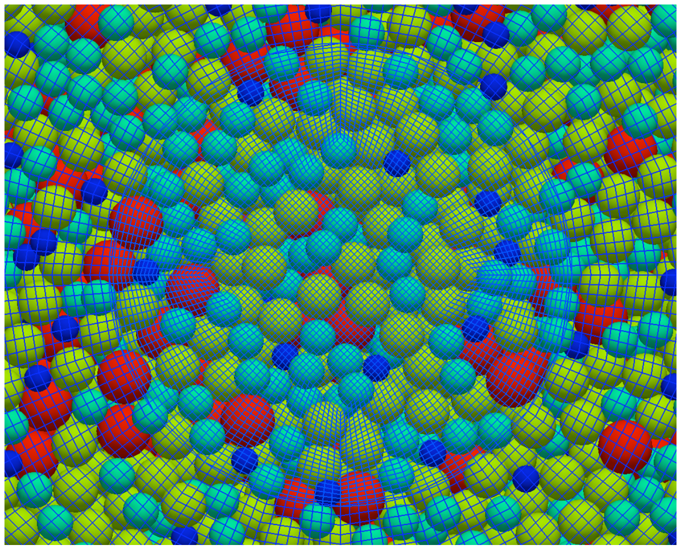
Particle size distribution

Particle size:	1.2	1.0	0.8	0.6
Distribution:	10%	40%	40%	10%

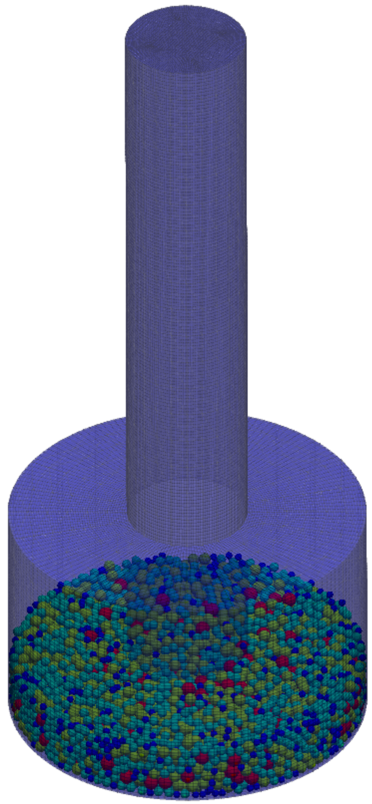
- **Discretization**

Top view



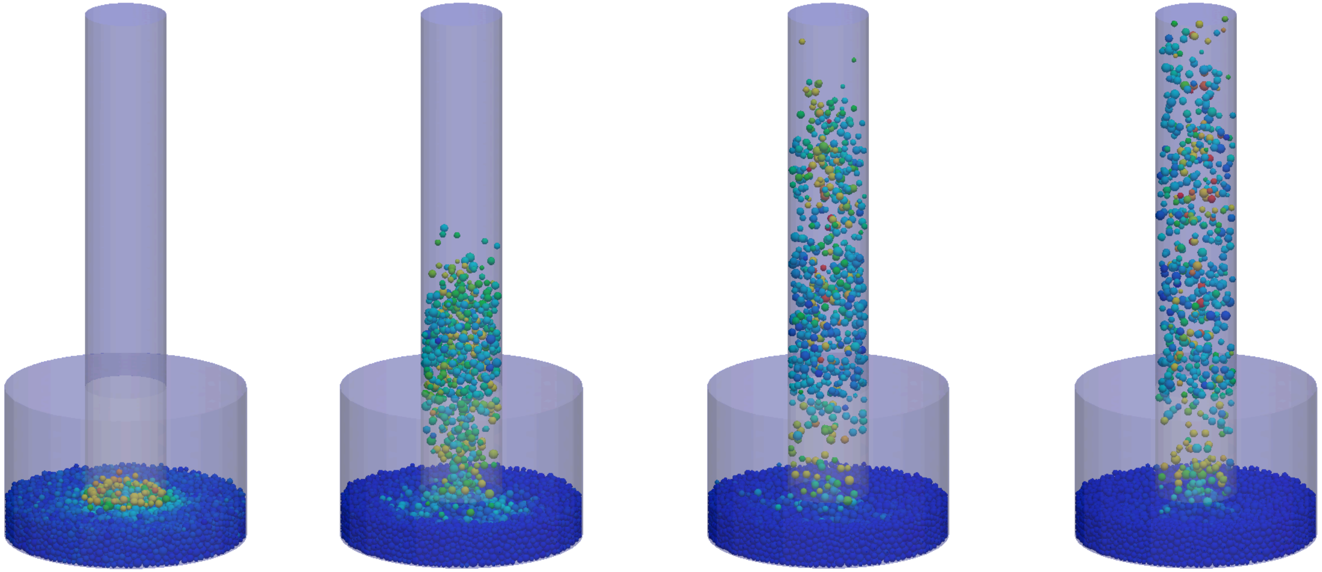


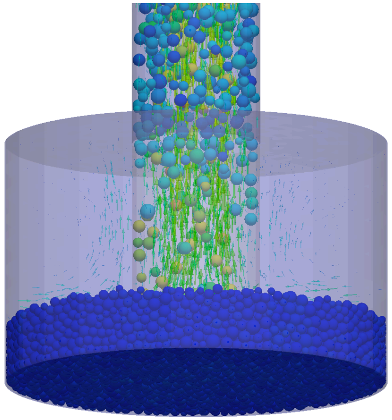
Isometric view

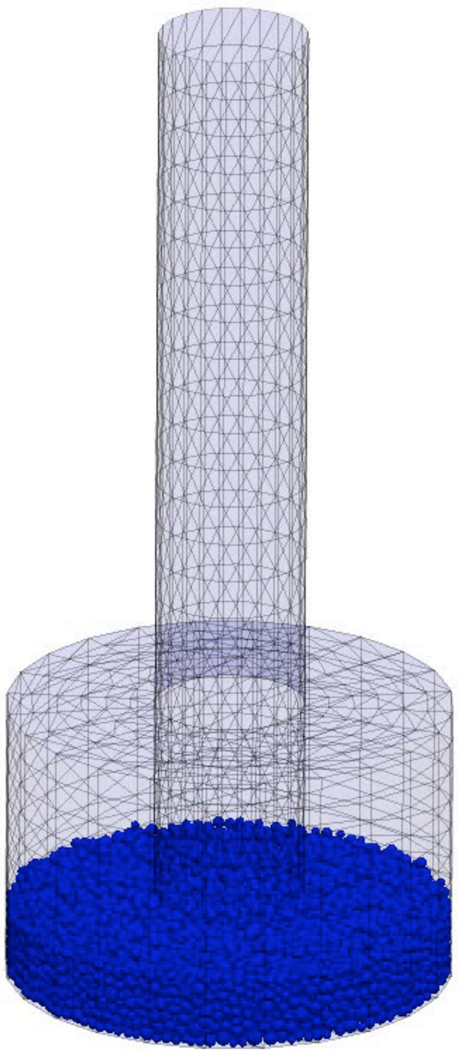


MG-Level	No. Cells	Vertices	Cell Faces	D.o.f.'s
Level 1	2 965	3 456	9 350	31 015
Level 2	23 720	25 611	72 980	242 660
Level 3	189 760	197 181	576 560	1 919 440
Level 4	1 518 080	1 547 481	4 583 360	15 268 160

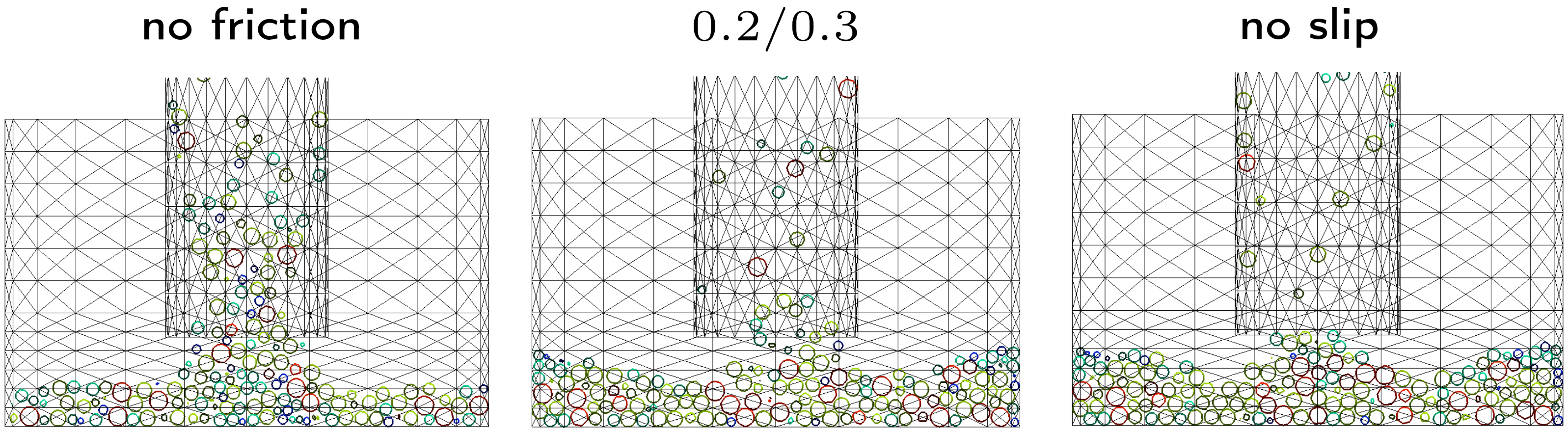
- **Fluid velocity at pipe outlet:** $v = 100$







- **Excavation profiles depending on the friction coefficient**
- **Friction coefficient μ_d/μ_s :**



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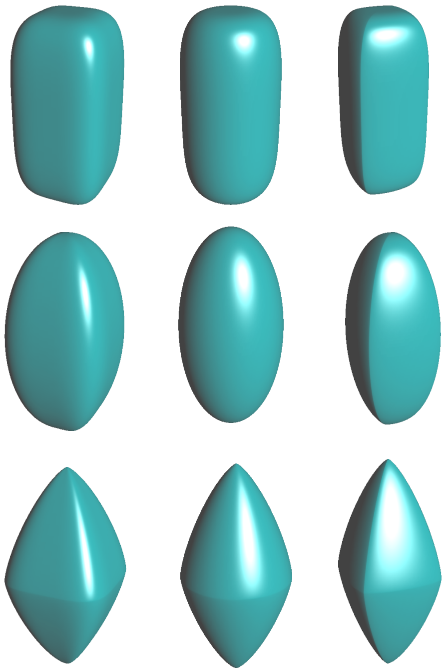
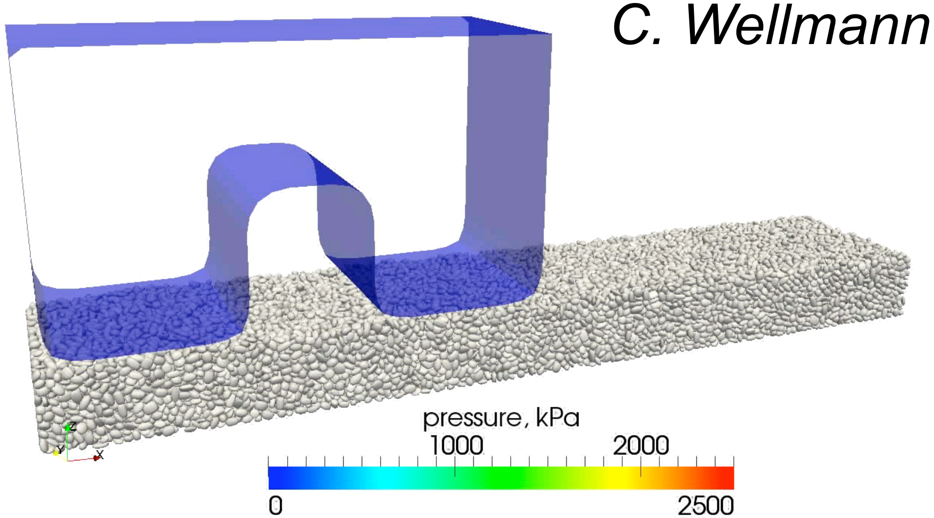
- scour genesis in front of bridge piers and bank constructions



- use differently shaped particles
- lubricated contact analysis

C. Wellmann



▷ Summary & Challenges

- Summary
  - ∗ Explicit direct numerical simulation of particulate flows
  - ∗ Particle interaction in a flow field with adhesion
  - ∗ Accurate enough to describe particulate flows on adequate fine background mesh
  - ∗ Simple to implement (coupling of existing DEM and CFD codes)

- Challenges
  - ∗ Particulate flow with turbulence models
  - ∗ Locally adaptive grid alignement
  - ∗ Parallelization of the flow solver