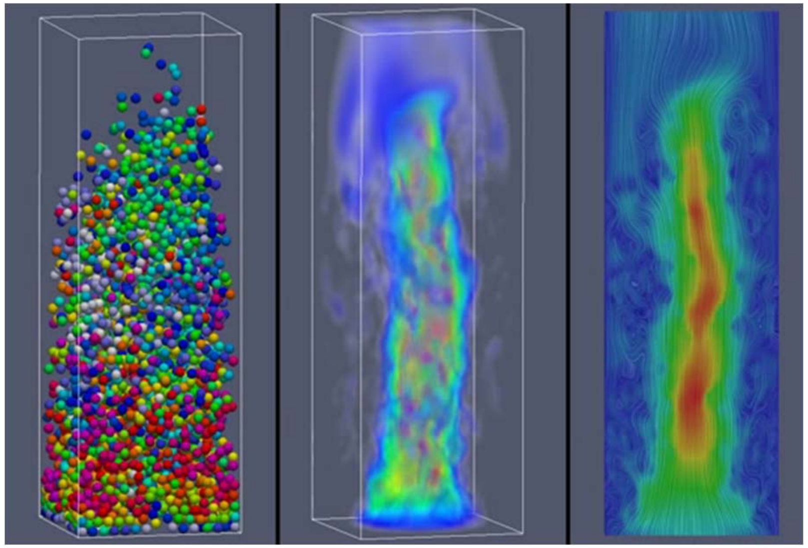
Finite Element-Fictitious Boundary Methods for the Numerical Simulation of Complex Particulate Flows



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http://www.mathematik.tu-dortmund.de/LS3
http://www.featflow.de

Basic Flow Solver

Basic CFD tool – **FEATFLOW**
(robust, parallel, efficient)

HPC features:
- Massively parallel
- GPU computing
- Open source


Numerical features:
- Higher order Q2P1 FEM schemes
- FCT & EO FEM stabilization techniques
- Use of unstructured meshes
- **Fictitious Boundary (FBM) methods**
- Dynamic adaptive grid deformation
- Newton-Multigrid solvers

Non-Newtonian flow module:
- generalized Newtonian model (Power-law, Carreau, ... etc.)
- viscoelastic model (Giesekus, Oldroyd B, …etc.)

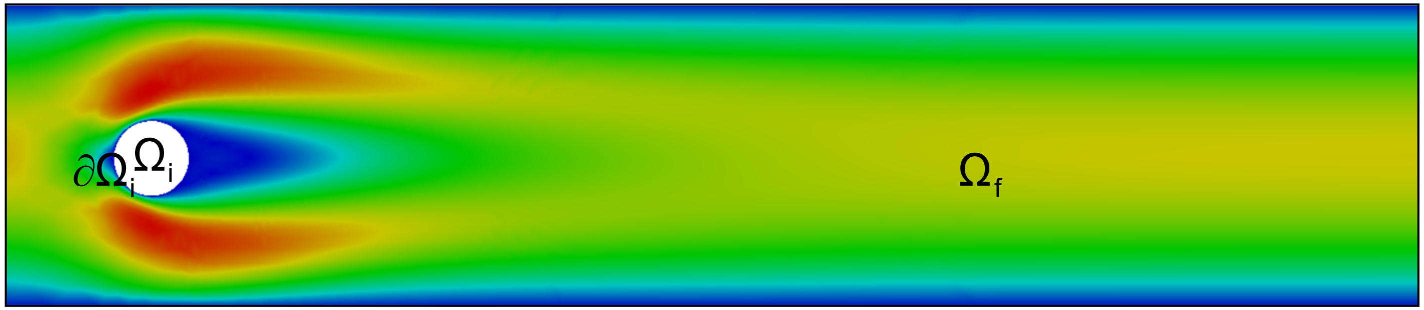
Multiphase flow module (resolved interfaces):
- l/l – interface tracking (Level Set)
- s/l – interface capturing (FBM)
- $s/l/l$ – combination of l/l and s/l

Engineering aspects:
- Geometrical design
- Modulation strategy
- Optimization

FEM-based simulation tools for the accurate prediction of multiphase flow problems, particularly with liquid-solid interfaces

Liquid– (Rigid) Solid Interfaces

Consider the flow of N solid particles in a fluid with density ρ and viscosity μ. Denote by $\Omega_f(t)$ the domain occupied by the fluid at time t, by $\Omega_i(t)$ the domain occupied by the ith-particle at time t and let $\overline{\Omega} = \overline{\Omega}_f \cup \overline{\Omega}_i$.



The fluid flow is modelled by the **Navier-Stokes equations**:

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

where σ is the total stress tensor of the fluid phase:

$$\sigma(X,t) = -pI + \mu[\nabla u + (\nabla u)^T]$$

Equations of Motion (I)

The motion of particles can be described by the **Newton-Euler equations**.
A particle moves with **a translational velocity** U_i and **angular velocity** ω_i which satisfiy:

$$M_i \frac{dU_i}{dt} = F_i + F_i' + (\Delta M_i) g, \qquad I_i \frac{d\omega_i}{dt} + \omega_i \times (I_i \omega_i) = T_{i,}$$

- M_i : mass of the i-th particle (i=1,...,N)
- I_i : moment of inertia tensor of the i-th particle
- ΔM_i : mass difference between M_i and the mass of the fluid
- F_i : hydrodynamic force acting on the i-th particle
- T_i : hydrodynamic torque acting on the i-th particle

Equations of Motion (II)

The position and orientation of the i-th particle are obtained by integrating the **kinematic equations**:

$$\frac{dX_i}{dt} = U_i\,, \quad \frac{d\theta_i}{dt} = \omega_i\,, \quad \frac{d\omega_i}{dt} = I_i^{-1} T_i$$

which can be done numerically by an explicit Euler scheme:

$$X_i^{n+1} = X_i^n + \Delta t U_i^n \qquad \omega_i^{n+1} = \omega_i^n + \Delta t\left(I_i^{-1} T_i^n\right) \qquad \theta_i^{n+1} = \theta_i^n + \Delta t \omega_i^n$$

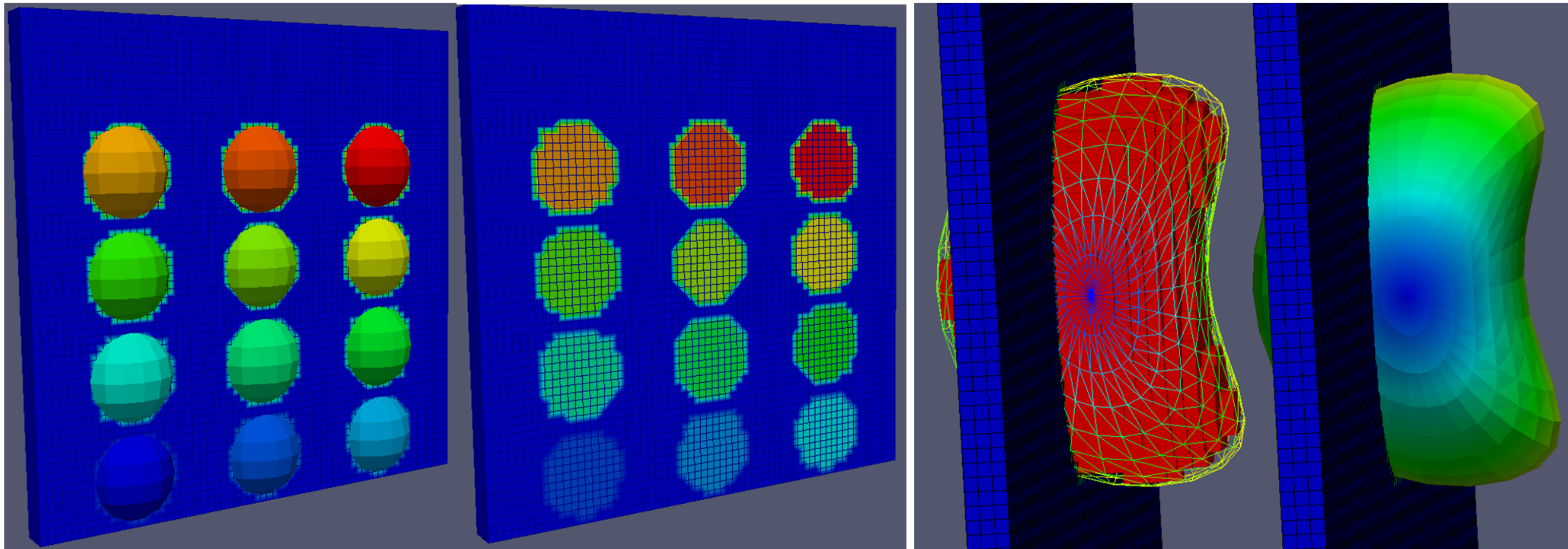
Boundary Conditions

We apply the velocity u(X) as no-slip boundary condition at the interface $\partial\Omega_i$ between the i-th particle and the fluid, which for $X \in \Omega_i$ is defined by:

$$u(X) = U_i + \omega_i \times (X - X_i)$$

Eulerian Approach:

- Internal objects are represented as a boolean (in/out) function on the mesh
- Use of a fixed mesh possible
- Complex shapes are possible (surface triangulation, implicit functions)
- Higher accuracy possible by using mesh adaptation techniques



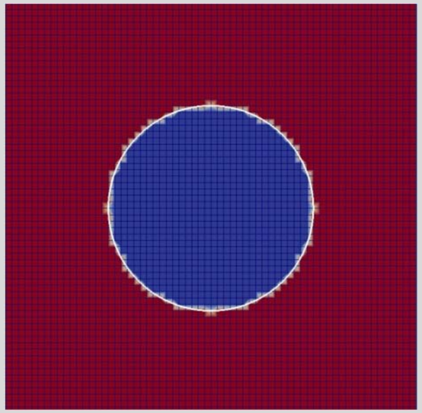
Hydrodynamic force and torque acting on the i-th particle

$$F_i = -\int_{\partial\Omega_i} \sigma \cdot n_i d\Gamma_i, \qquad T_i = -\int_{\partial\Omega_i} (X - X_i) \times (\sigma \cdot n_i) d\Gamma$$

Force Calculation with Fictitious Boundary Method

The FBM can only decide:

- \`INSIDE\`(1) and \`OUTSIDE\`(0)
- Only first order accuracy



Alternative:

Replace the surface integral by a volume integral

Numerical Force Evaluation (I)

Define an ***indicator function*** α_i:

$$\alpha_i(X) = \begin{cases} 1 & \text{for } X \in \Omega_i \\ 0 & \text{for } X \in \Omega_f \end{cases}$$

Remark: The gradient of α_i is zero everywhere except at the surface of the i-th Particle and approximates the normal vector (in a weak sense), allowing us to write:

$$F_i = -\int_{\Omega_T} \sigma \cdot \nabla \alpha_i \, d\Omega \,, \qquad T_i = -\int_{\Omega_T} (X - X_i) \times (\sigma \cdot \nabla \alpha_i) \, d\Omega$$

On the finite element level we can compute this by:

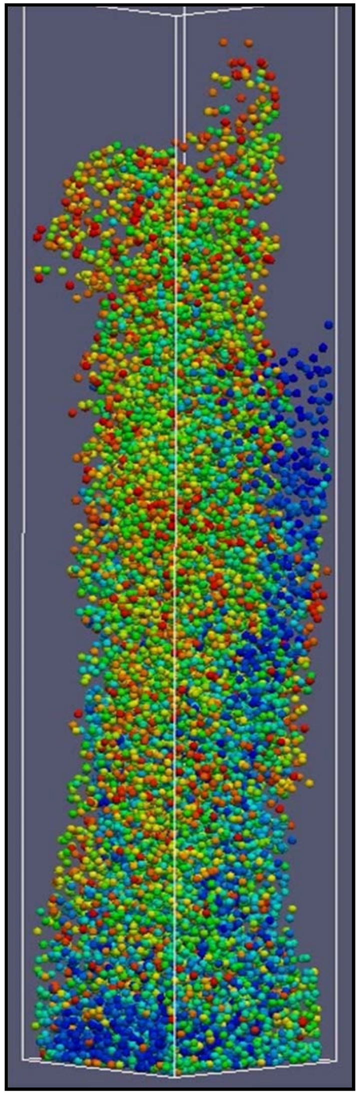
$$F_i = -\sum_{T \in T_{h,i}} \int_{\Omega_T} \sigma_h \cdot \nabla \alpha_{h,i} \, d\Omega \,,$$

$$T_i = -\sum_{T \in T_{h,i}} \int_{\Omega_T} (X - X_i) \times (\sigma_h \cdot \nabla \alpha_{h,i}) \, d\Omega$$

$\alpha_{h,i}(x)$: finite element interpolant of $\alpha(x)$

$T_{h,i}$: elements intersected by i-th particle

Large-scale FBM-Simulations



Integration over Ω_T *too* expensive:

- Gradient is non-zero on $\partial\Omega_i$
- Information available from FBM
- Evaluate boundary cells only
- Visit each cell only once

$$F_i = -\sum_{T \in T_{h,i}} \int_{\Omega_T} \sigma_h \cdot \nabla \alpha_{h,i} \, d\Omega ,$$

$$T_i = -\sum_{T \in T_{h,i}} \int_{\Omega_T} (X - X_i) \times (\sigma_h \cdot \nabla \alpha_{h,i}) \, d\Omega$$

Numerical Solution Scheme

Solve for velocity and pressure applying FBM-conditions

$$NSE\left(u_f^{n+1}, p^{n+1}\right) = BC\left(\Omega_i^n, u_i^n\right)$$

Calculate hydrodynamic force, torque and apply

$$F_i^{n+1} \qquad T_i^{n+1}$$

Contact force calculation

$$F_{c,i}^{n+1}$$

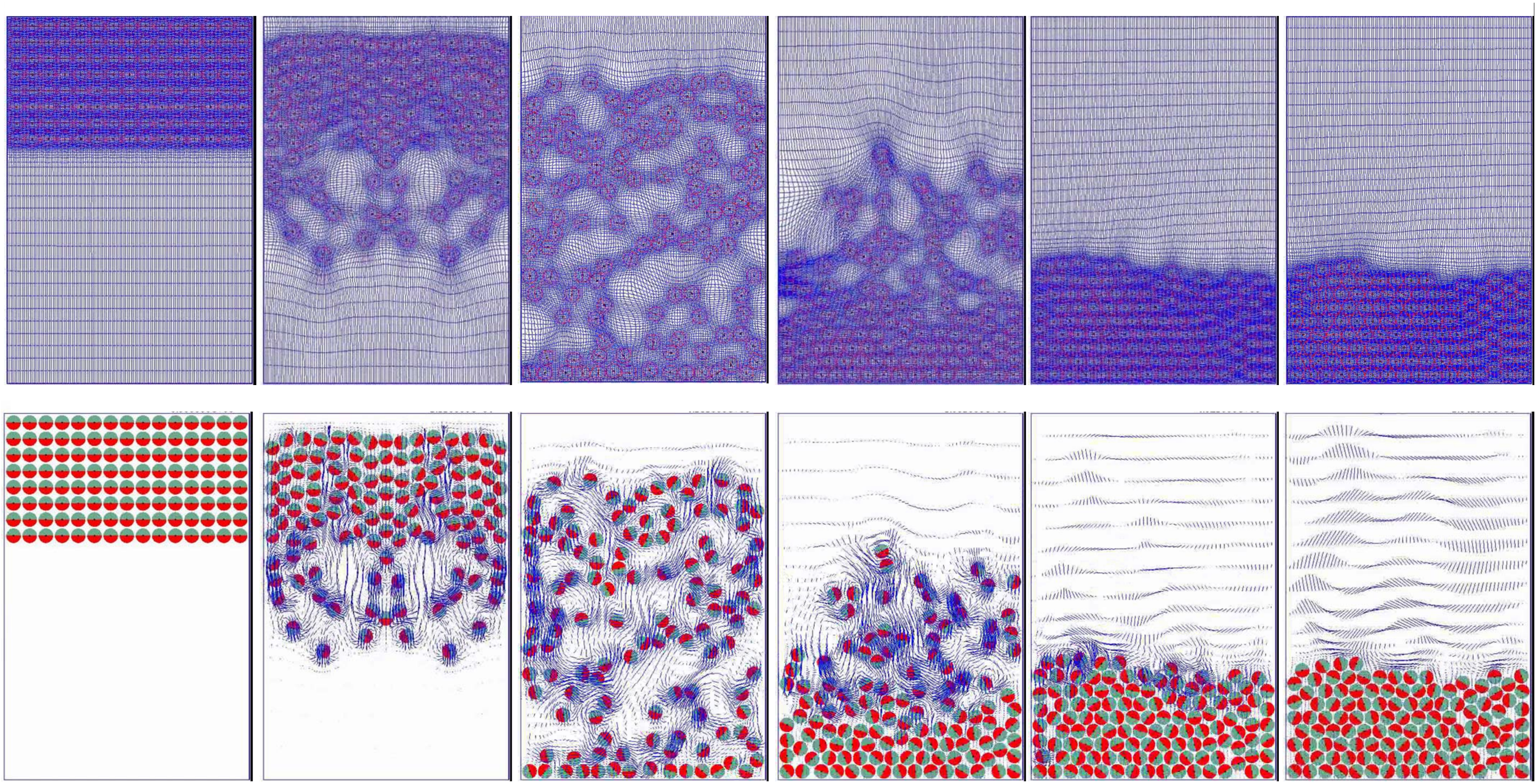
Compute new velocity and angular velocity

$$u_i^{n+1} = u_i^n + \Delta t \left(F_{c,i}^{n+1}/M_i\right) \quad \omega_i^{n+1} = \omega_i^n + \Delta t I_i^{-1}\left(r \times F_{c,i}\right)$$

Position update

$$X_i^{n+1} = X_i^n + \Delta t u_i^n \qquad \theta_i^{n+1} = \theta_i^n + \Delta t \omega_i^n$$

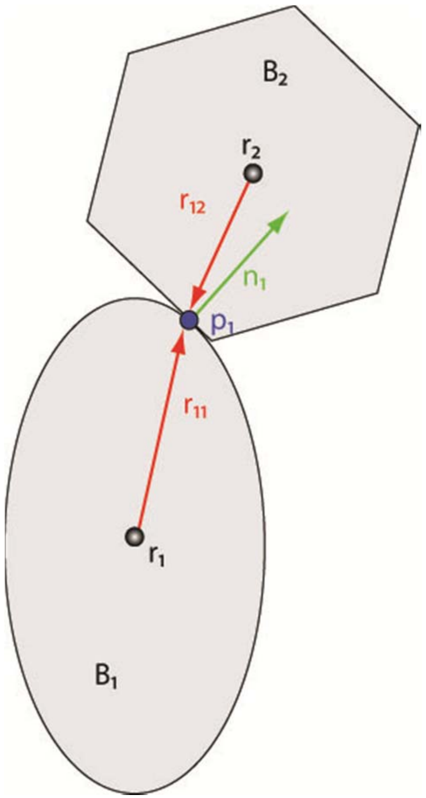
Grid Deformation Method



Further improvement via adaptive Grid Deformation which preserves the (local) logical structure (→ GPU)

Contact Force Calculation

- Contact force calculation realized as a three step process
  - → Broadphase
  - → Narrowphase
  - → Contact/Collision force calculation
- Worst case complexity for collision detection is $O(n^2)$
  - → Computing contact information is expensive
  - → Reduce number of expensive tests → Broad Phase
- *Broad phase*
  - → Simple rejection tests exclude pairs that cannot intersect
  - → Use hierarchical spatial partitioning
- *Narrow phase*
  - → Uses Broadphase output
  - → Calculates data neccessary for collision force calculation



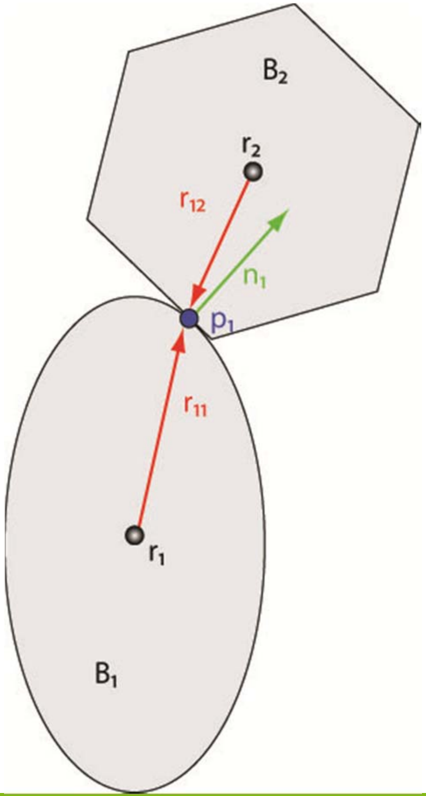
For a single pair of colliding bodies we compute the impulse f that causes the velocities of the bodies to change:

$$f = \frac{-(1+\varepsilon)\left(n_1(v_1 - v_2) + \omega_1(r_{11} \times n_1) - \omega_2(r_{12} \times n_1)\right)}{m_1^{-1} + m_2^{-1} + (r_{11} \times n_1)^T I_1^{-1}(r_{11} \times n_1) + (r_{12} \times n_1)^T I_2^{-1}(r_{12} \times n_1)}$$

Using the impulse f, the change in linear and angular velocity can be calculated:

$$v_1(t+\Delta t) = v_1(t) + \frac{fn_1}{m_1}, \omega_1(t+\Delta t) = \omega_1(t) + I_1^{-1}(r_{11} \times fn_1)$$

$$v_2(t+\Delta t) = v_2(t) - \frac{fn_1}{m_2}, \omega_2(t+\Delta t) = \omega_2(t) - I_2^{-1}(r_{12} \times fn_1)$$



Multi-Body Collision Model

In the case of **multiple colliding bodies** with ***K* contact points** the impulses influence each other. Hence, they are combined into a **system of equations** that involves the following matrices and vectors:

- N: matrix of contact normals
- C: matrix of contact conditions
- M: rigid body mass matrix
- f: vector of contact forces ($f_i \geq 0$)
- f^{ext}: vector of external forces(gravity, etc.)

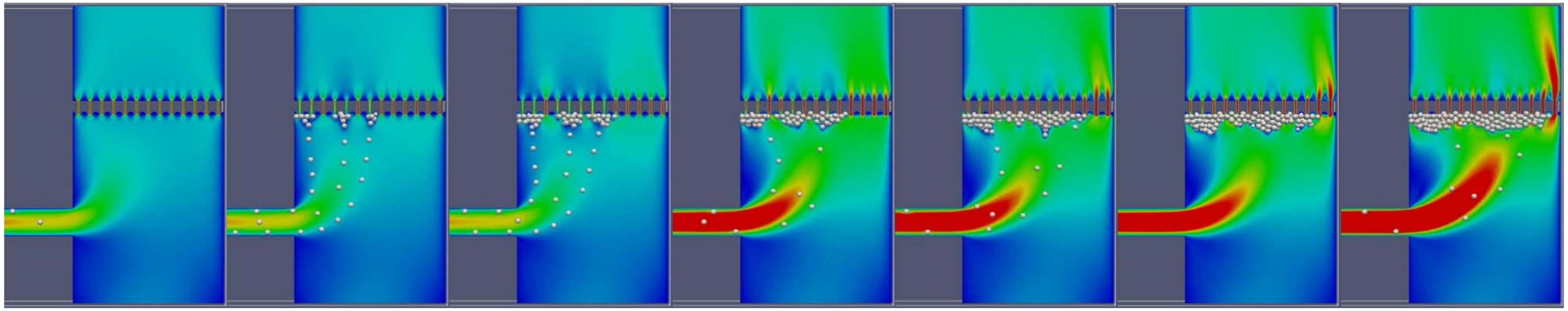
$$\underbrace{N^T C^T M^{-1} C N}_{A} \cdot \underbrace{\Delta t f^{t+\Delta t}}_{x} + \underbrace{N^T C^T \left(u^t + \Delta t M^{-1} + f^{ext}\right)}_{b} \geq 0, f \geq 0$$

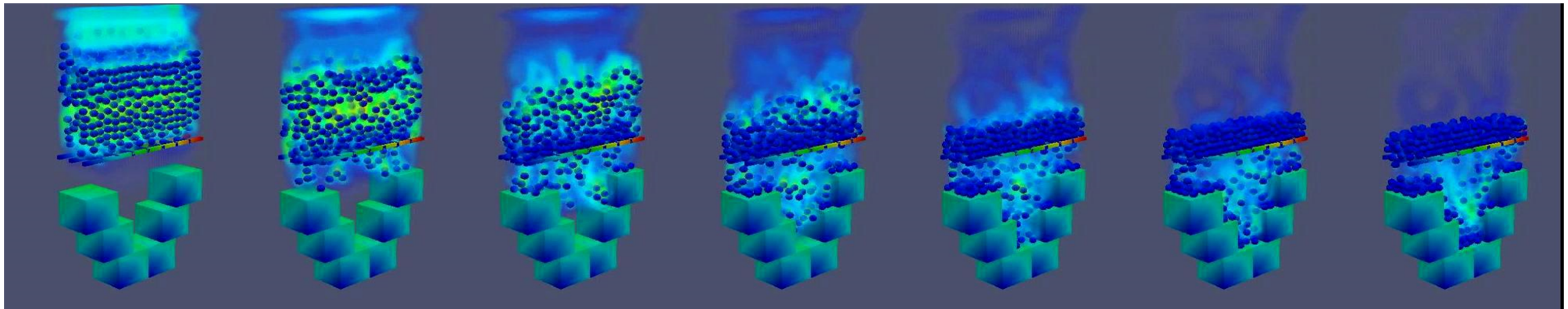
A problem of this form is called a **linear complementarity problem (LCP)** which can be solved with efficient iterative methods like the **Projected Gauss-Seidel solver (PGS)**.

Kenny Erleben, *Stable, Robust, and Versatile Multibody Dynamics Animation*

Examples

- Flows with complex geometries
- Fluidized bed
- Particulate flow demonstrating incompressibility
- GPU sedimentation example
- Numerical results and benchmark test cases
- Comparison of results with other groups

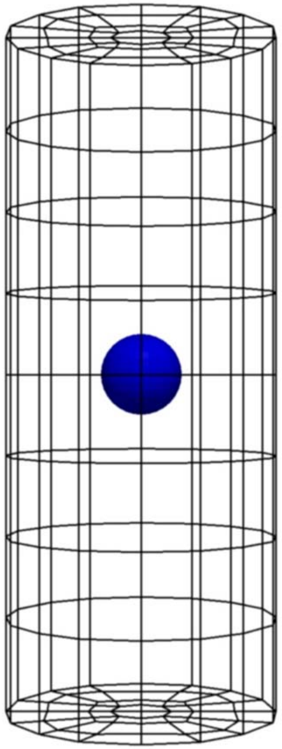


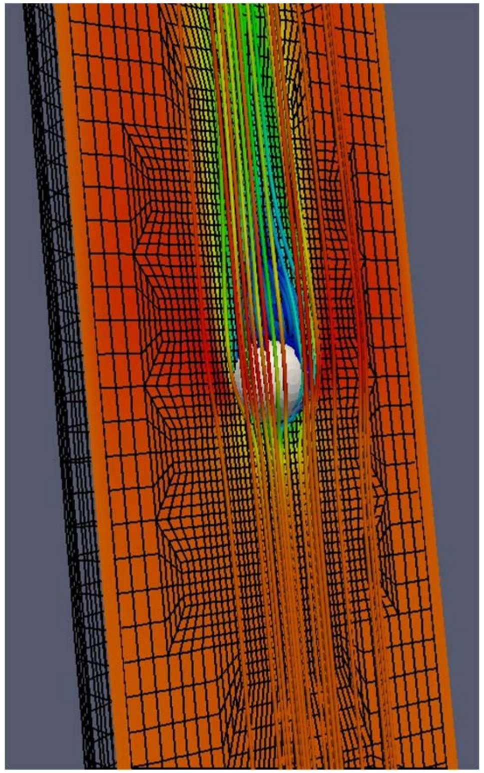


Benchmarking and Validation (I)

Free fall of particles:

- Terminal velocity
- Different physical parameters
- Different geometrical parameters





Münster, R.; Mierka, O.; Turek, S.: Finite Element fictitious boundary methods (FEM-FBM) for 3D particulate flow, IJNMF, 2011

$d_s = 0.3, \quad \rho_s = 1.14$

ν	$U_{featflow}$	U_{exp}	Relative error (%)
0.02	5.885	6.283	6.33
0.05	4.133	3.972	4.05
0.1	2.588	2.426	6.66
0.2	1.492	1.401	6.50

$d_s = 0.2, \quad \rho_s = 1.14$

ν	$U_{featflow}$	U_{exp}	Relative error (%)
0.02	4.370	4.334	0.83
0.05	2.699	2.489	8.44
0.1	1.649	1.552	6.25
0.2	0.946	0.870	8.74

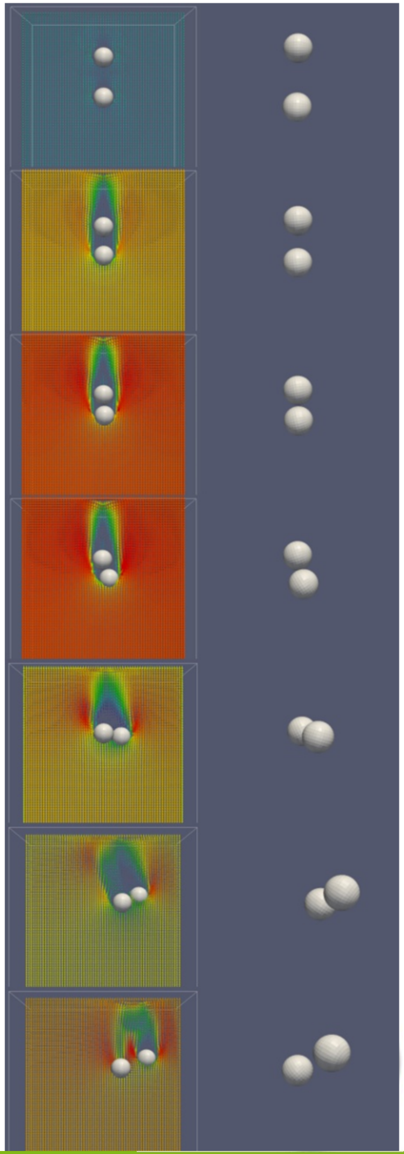
$d_s = 0.3, \quad \rho_s = 1.02$

ν	$U_{featflow}$	U_{exp}	Relative error (%)
0.01	2.167	2.107	2.84
0.02	1.495	1.436	4.11
0.05	0.809	0.749	8.01
0.1	0.402	0.404	0.44
0.2	0.218	0.216	1.02

$d_s = 0.2, \quad \rho_s = 1.02$

ν	$U_{featflow}$	U_{exp}	Relative error (%)
0.01	1.4660	1.4110	3.90
0.02	0.9998	0.9129	9.52
0.05	0.4917	0.4603	6.82
0.1	0.2637	0.2571	2.57
0.2	0.1335	0.1317	1.37

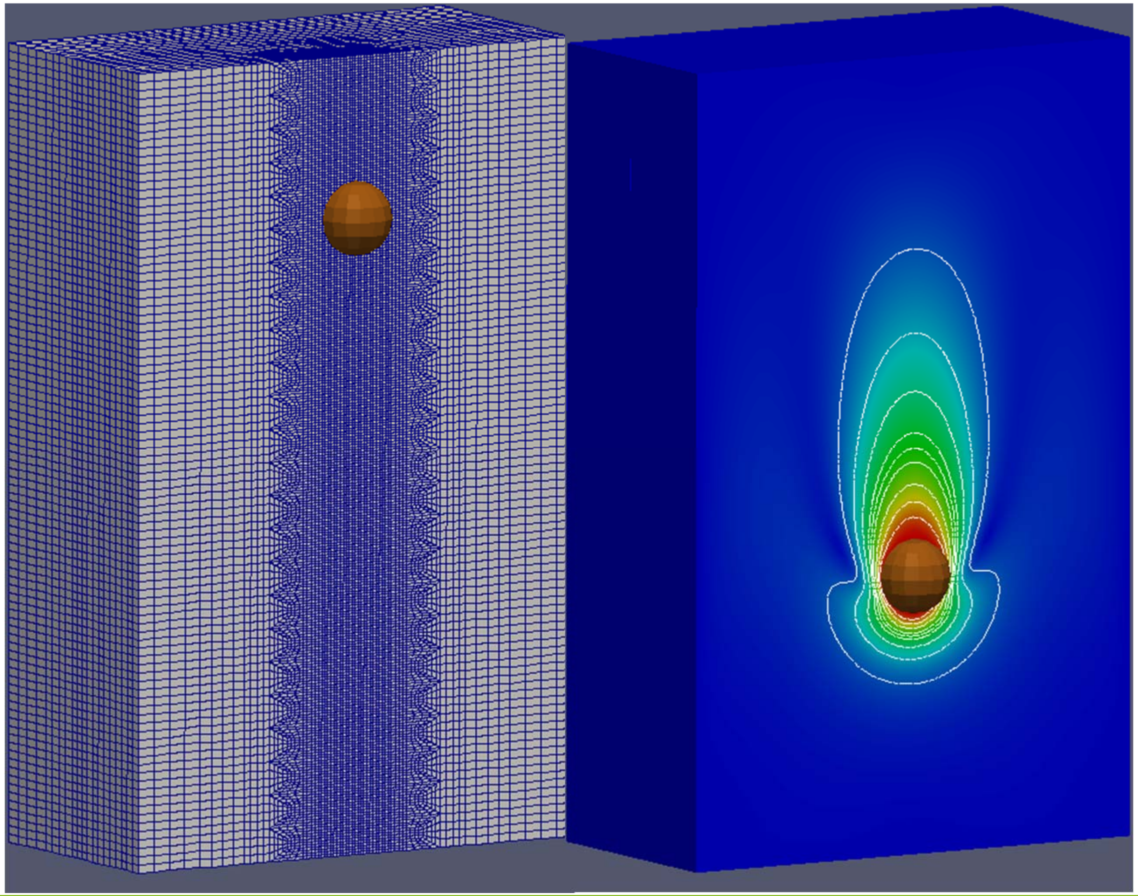
Source: Glowinski et al. 2001



Benchmarking and Validation (II)

Settling of a sphere towards a plane wall:

- Sedimentation Velocity
- Particle trajectory
- Kinetic Energy
- Different Reynolds numbers



Setup

Computational mesh:

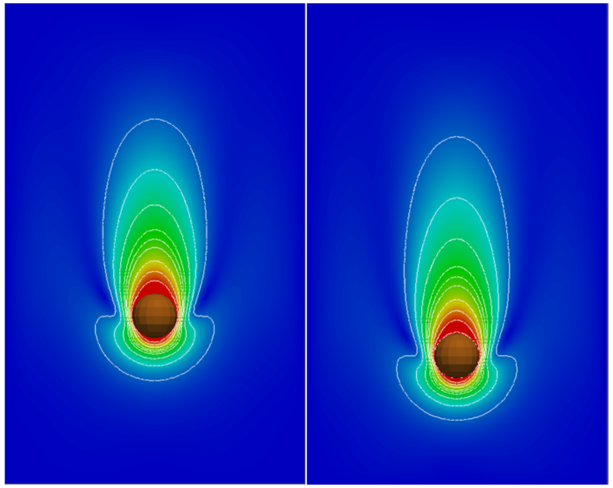
- 1.075.200 vertices
- 622.592 hexahedral cells
- Q2/P1:
  → 50.429.952 DoFs

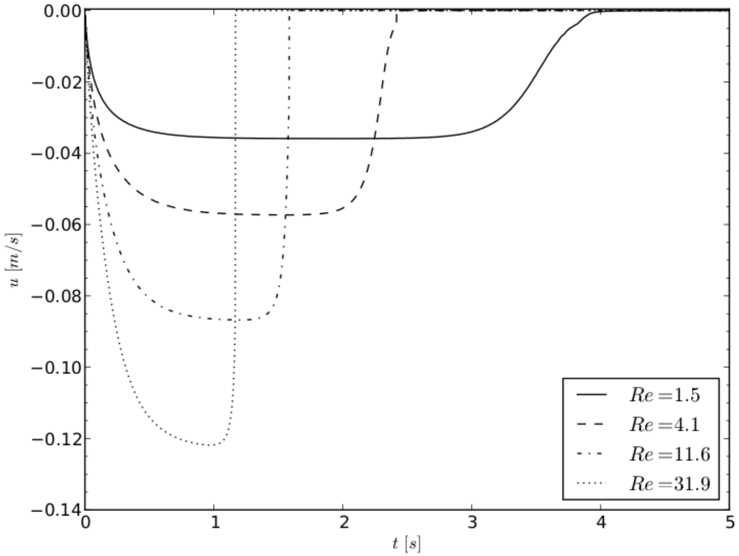
Hardware Resources:

- 32 Processors

Observations

- Velocity profiles compare well to ten Cate‘s data
- Maximum velocity close to experiment
- Flow features are accurately resolved

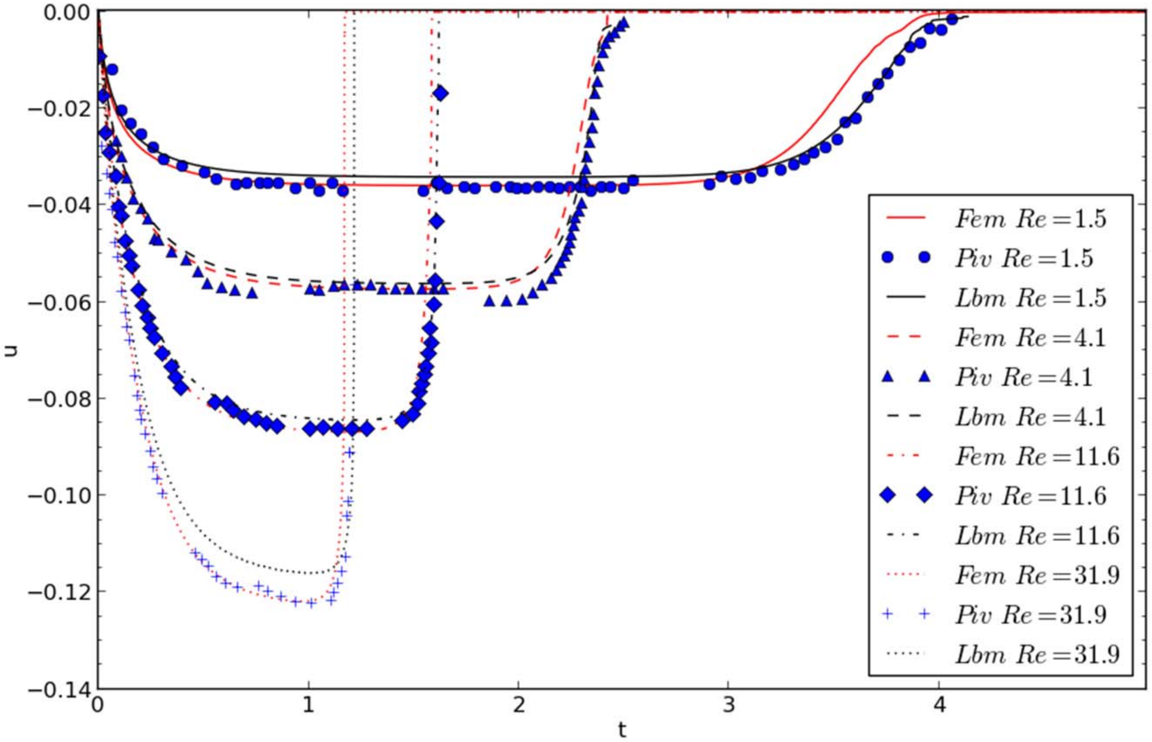




Re	u_{max}/u_∞	u_{max}/u_∞ ten Cate	u_{max}/u_∞ exp
1.5	0.945	0.894	0.947
4.1	0.955	0.950	0.953
11.6	0.953	0.955	0.959
31.9	0.951	0.947	0.955

Tab. 1 Comparison of the u_{max}/u_∞ ratios between the FEM-FBM, ten Cate's simulation and ten Cate's experiment

Comparison



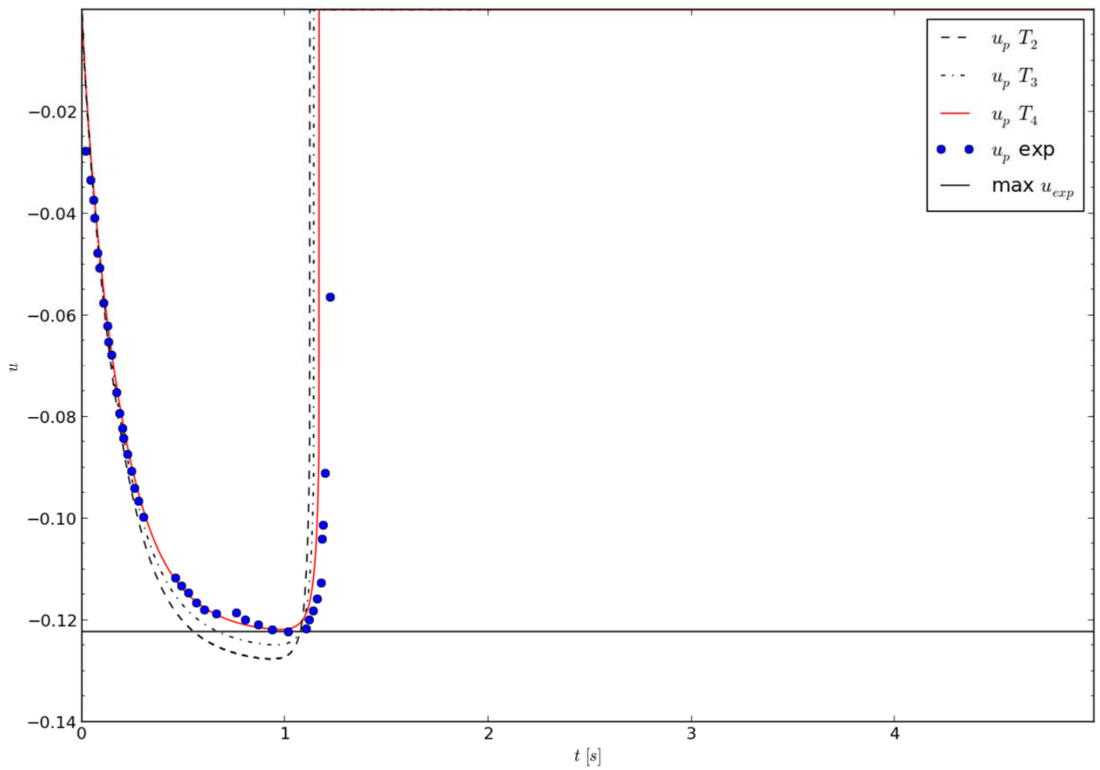
Comparison of FEM-FBM and the experimental values and the LBM results of the group of Sommerfeld

Source: 13th Workshop on Two-Phase Flow Predictions 2012
Acknowledgements: Ernst,M., Dietzel,M., Sommerfeld,M.

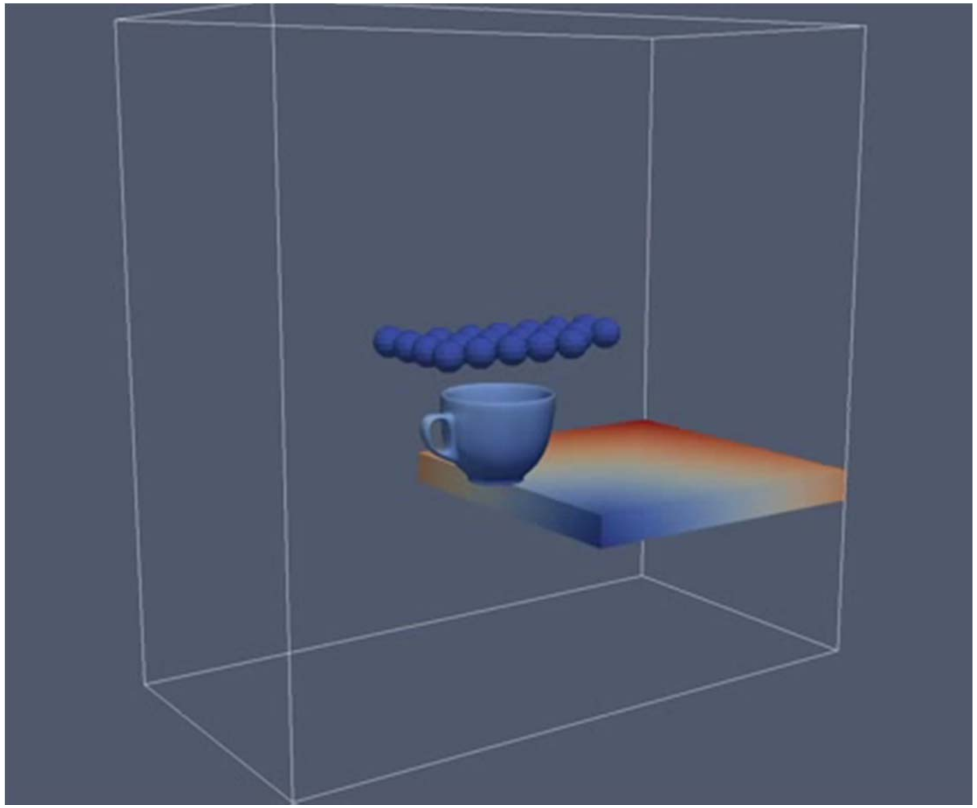
FEM-Multigrid Framework

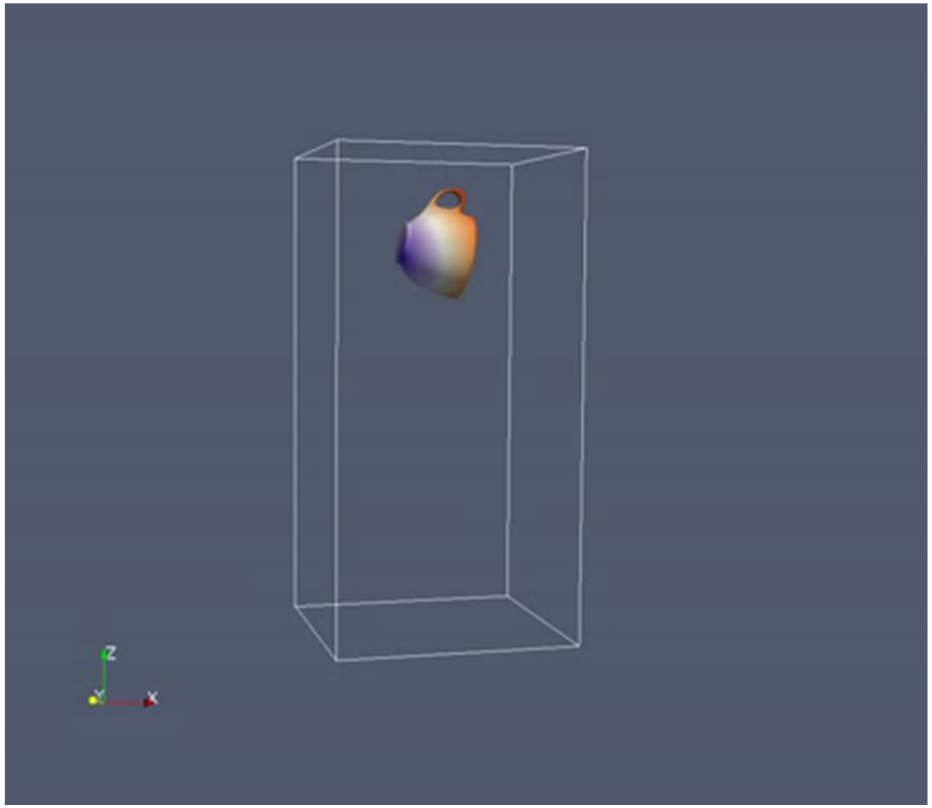
- *Increasing the mesh resolution produces more accurate results*

  Test performed at different mesh levels
  - Maximum velocity is approximated better ✓
  - Shape of the velocity curve matches better ✓

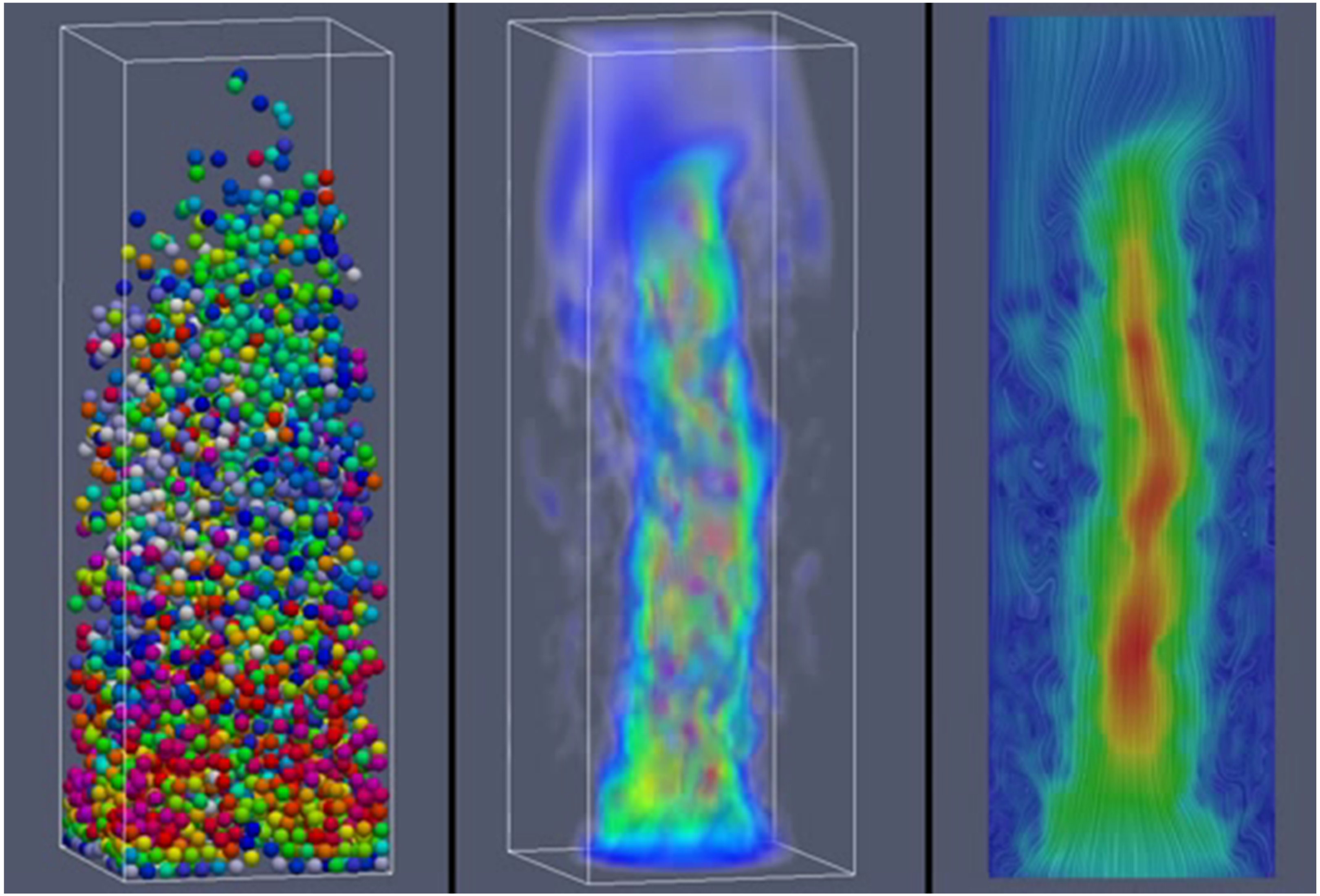


Complex Geometry Examples

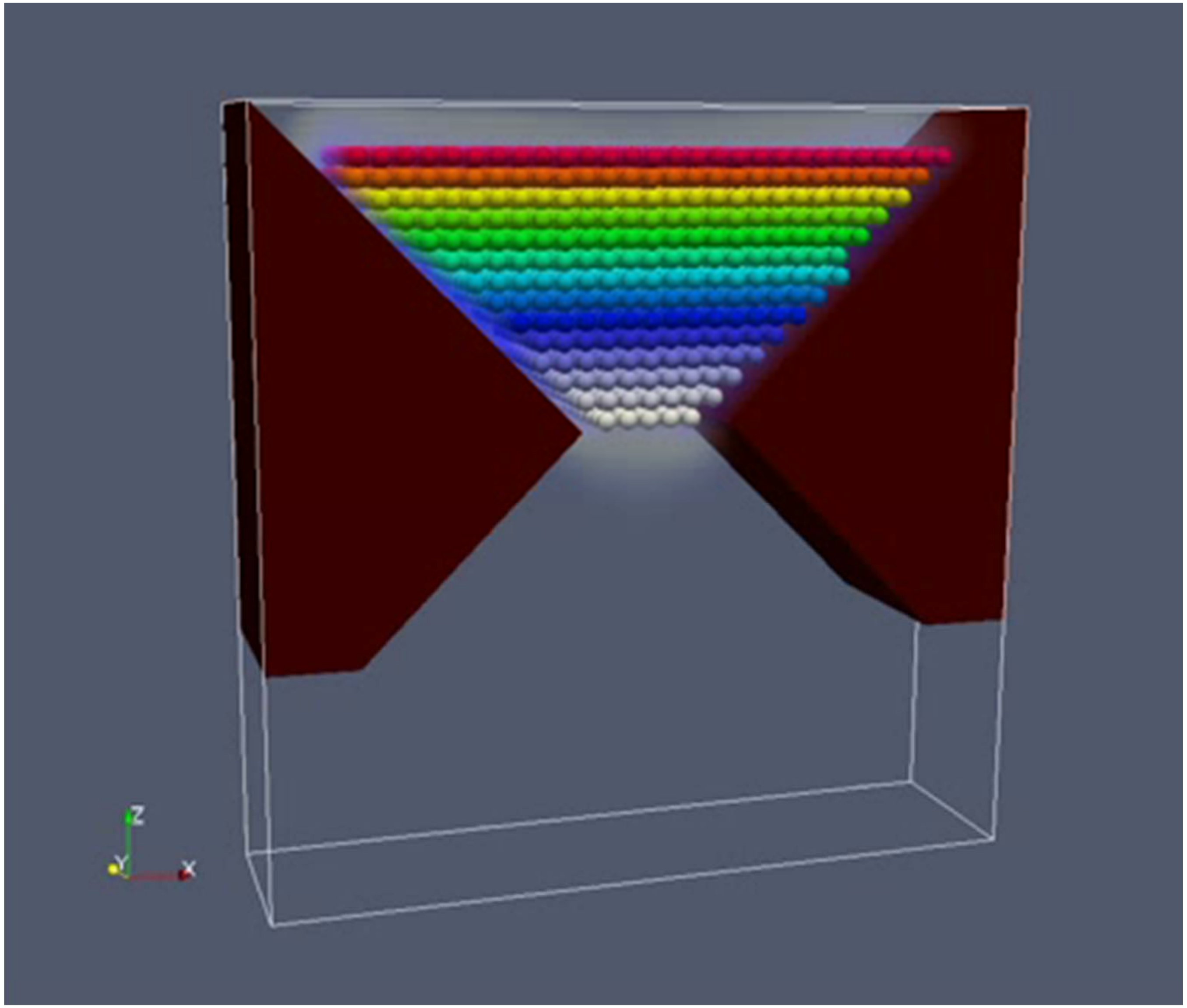




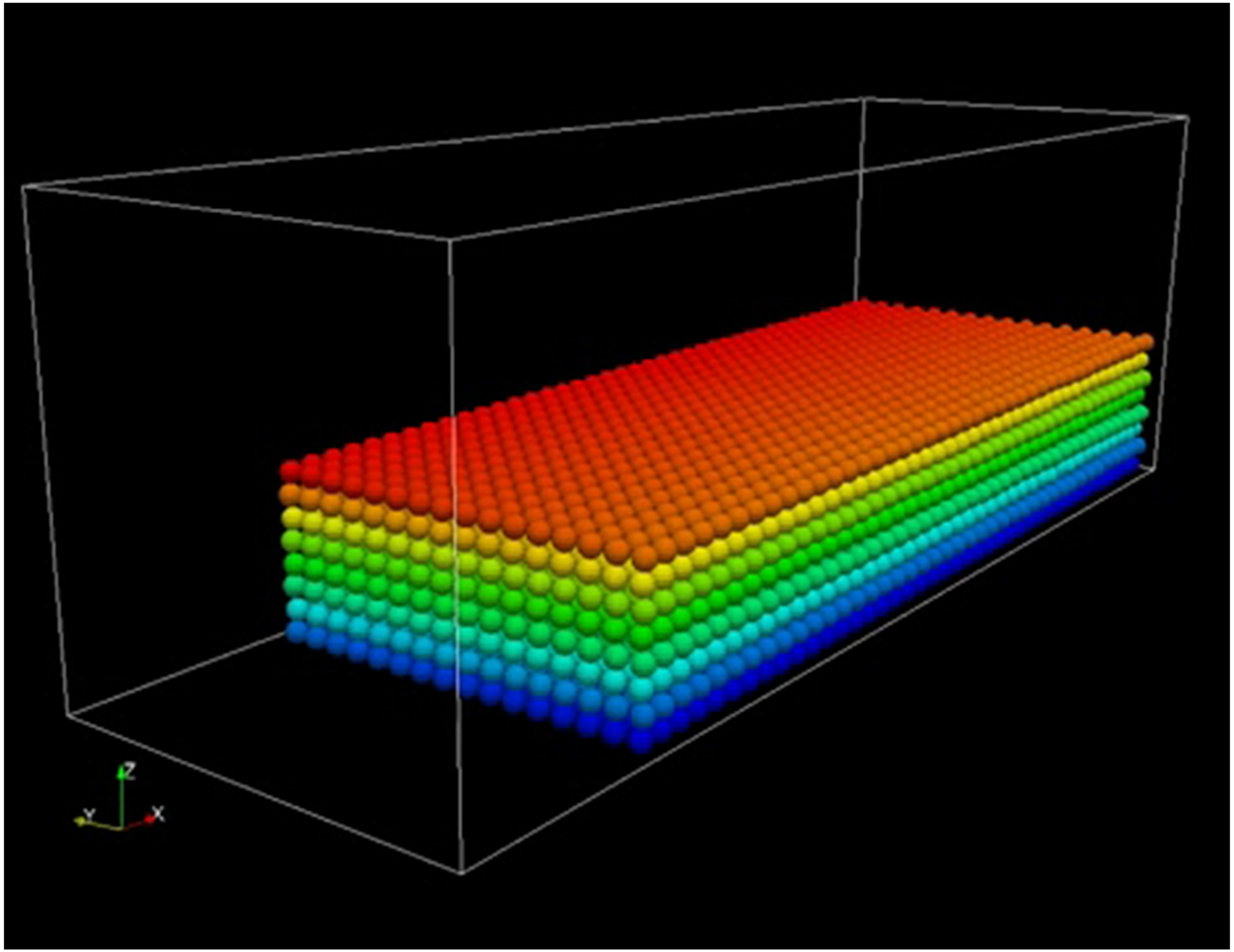
Fluidized Bed Example



DGS Configuration

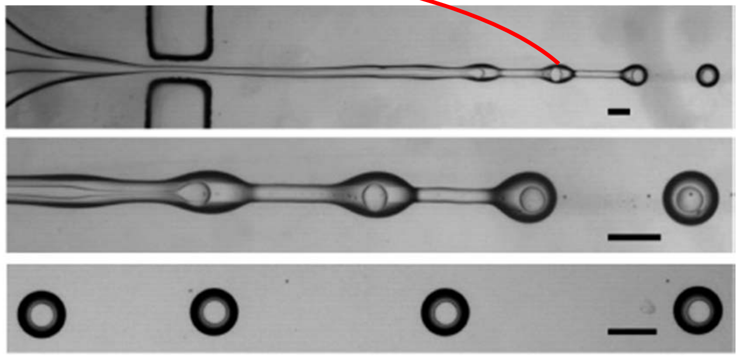


Large-Scale Examples



Fluidics

Embedded particles



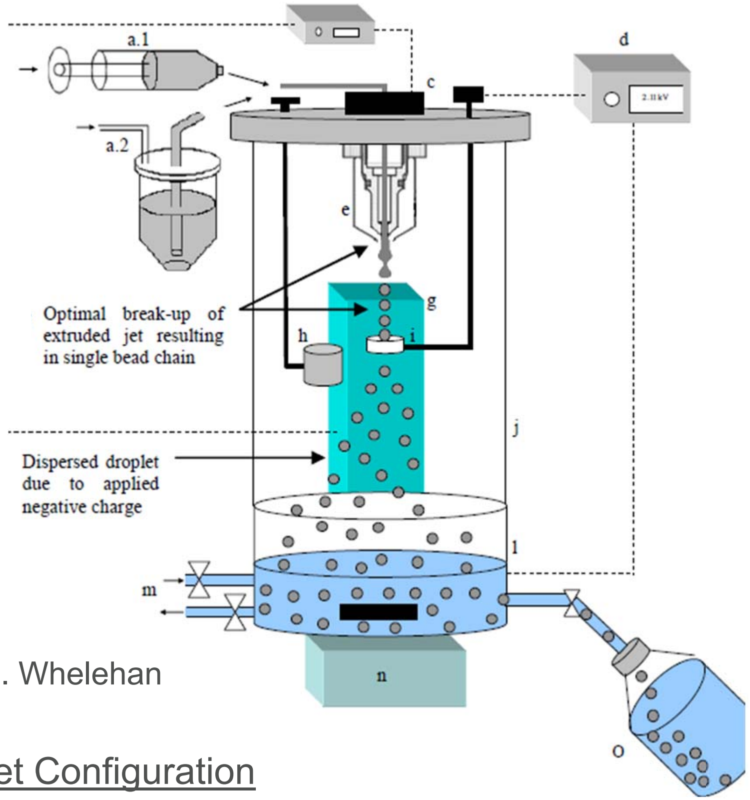
- Viscoelastic fluids
- Multiphase problems
  - → Liquid-Liquid-Solid
  - → Liquid-Gas-Solid

Hardware-Oriented Numerics

- Improve parallel efficiency of collision force computation
- Further develop collision detection and collision force computation on GPUs

Fluid Prilling and Encapsulation (I)

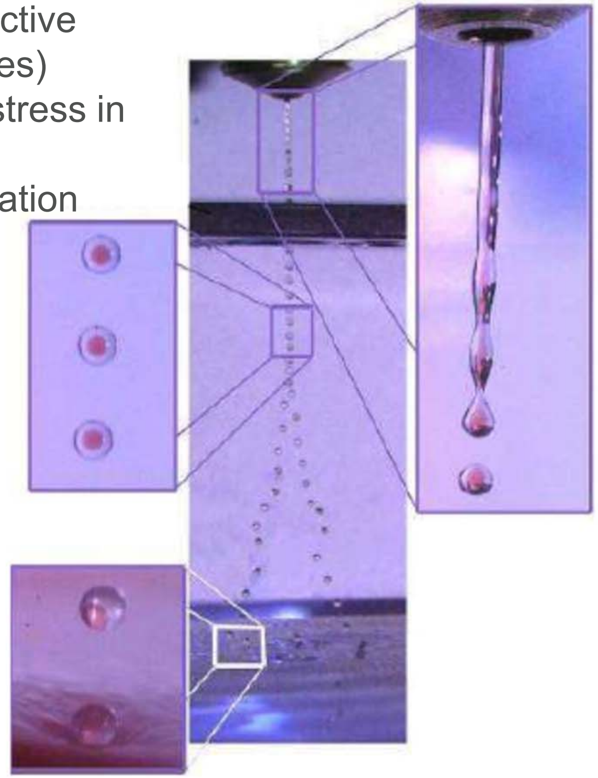
- Numerical simulation of *micro-fluidic drug encapsulation ("monodisperse compound droplets")*
- Polymeric "bio-degradable" outer fluid with generalized Newtonian behaviour
- Optimization w.r.t. boundary conditions, flow rates, droplet size, geometry



M. Whelehan

In Pharmaceutics

- Controlled drug release
- Protection of chemically active ingredients (from both sides)
- Protection against shear stress in stirred reactors
- Protection against evaporation
- Taste or odor masking



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Jet Configuration

- Core material is defined as the specific material that requires to be coated (liquid, emulsion, colloid or solid)
- Shell material is present to protect and stabilize the core (Alginate, Chitosan, Gelatin, Pectin, Waxes, Starch)

Fluid Prilling and Encapsulation (II)

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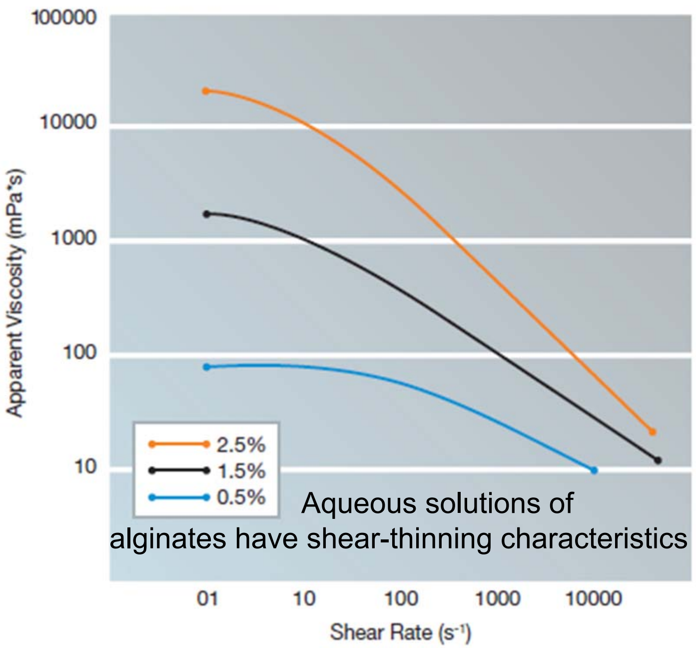
	Tasks related to code development	Tasks related to applicatio
mgLS[(2)]-FBM-FEM flow module	• Multiple Level Set fields for simulation of liquid core encapsulation - l/l/g • Fictitious boundary method for particle encapsulation - s/l/g	• Validation via experimental results • Modulation for monodisperse compound drops



Aqueous solutions of alginates have shear-thinning characteristics

Preliminary simulation results for encapsulation of solid particles