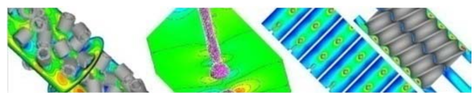
# Finite Element-Fictitious Boundary Methods (FEM-FBM) for time-dependent mixing processes in complex geometries

Stefan Turek, Otto Mierka, Raphael Münster
Institut für Angewandte Mathematik , LS III
Technische Universität Dortmund
ture@featflow.de

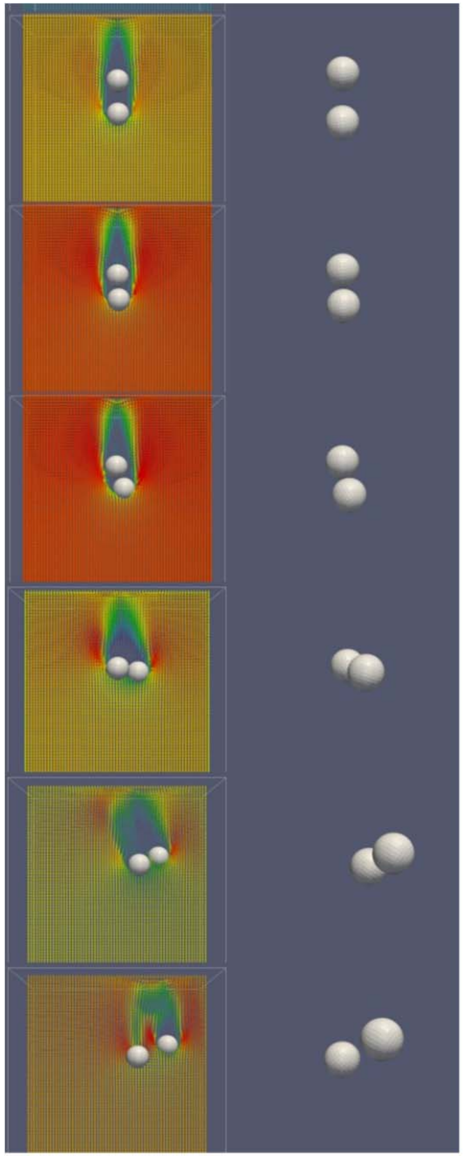
http://www.featflow.de
http://www.mathematik.tu-dortmund.de/LS3

technische universität
dortmund



# Motivation: Numerical & Algorithmic Challenges

***Accurate, robust, flexible and efficient simulation of multiphase problems with dynamic interfaces and complex geometries, particularly in 3D, is still a challenge!***



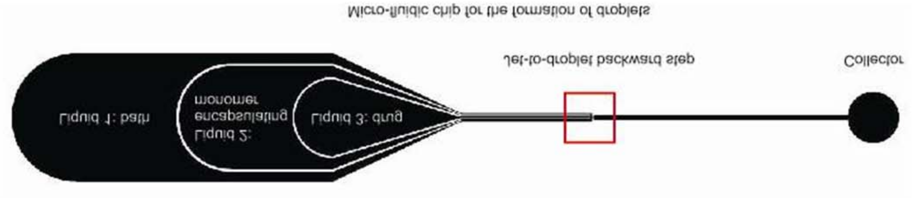
- Mathematical Modelling of Dynamic Interfaces
- Numerics / CFD Techniques
- HPC Techniques / Software
- Validation / Benchmarking

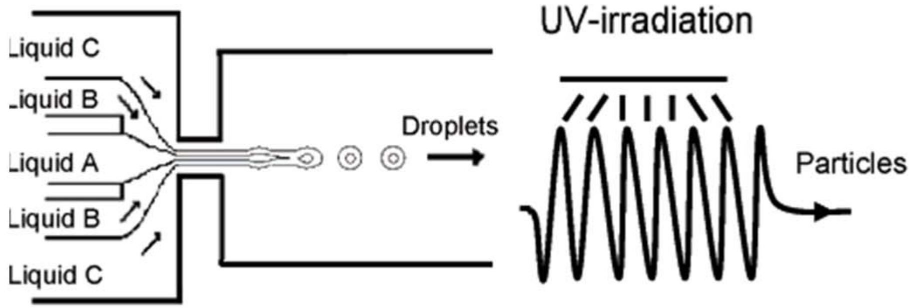
**Aim:** *Highly efficient, flexible and accurate „real life“ simulation tools based on modern numerics and algorithms while exploiting modern hardware!*

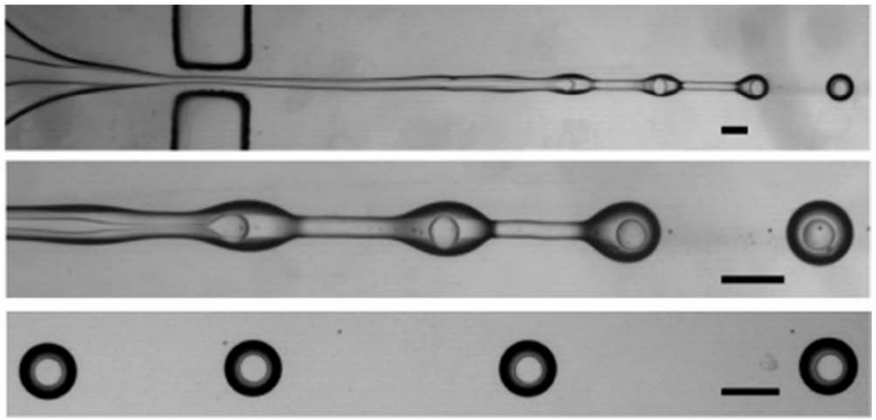
**Realization:** FEATFLOW

# Motivation: Target Application I

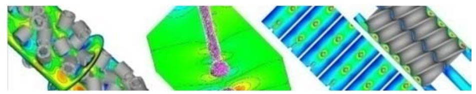
- Numerical simulation of *micro-fluidic drug encapsulation ("monodisperse compound droplets")* for application in lab-on-chip and bio-medical devices
- Polymeric "bio-degradable" outer fluid with viscoelastic effects
- Optimization of chip design w.r.t. boundary conditions, flow rates, droplet size, geometry



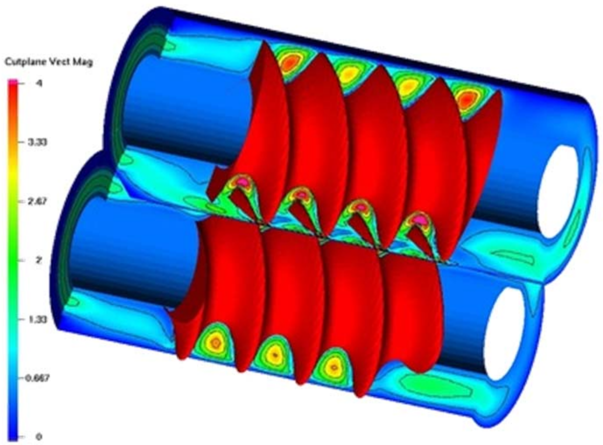



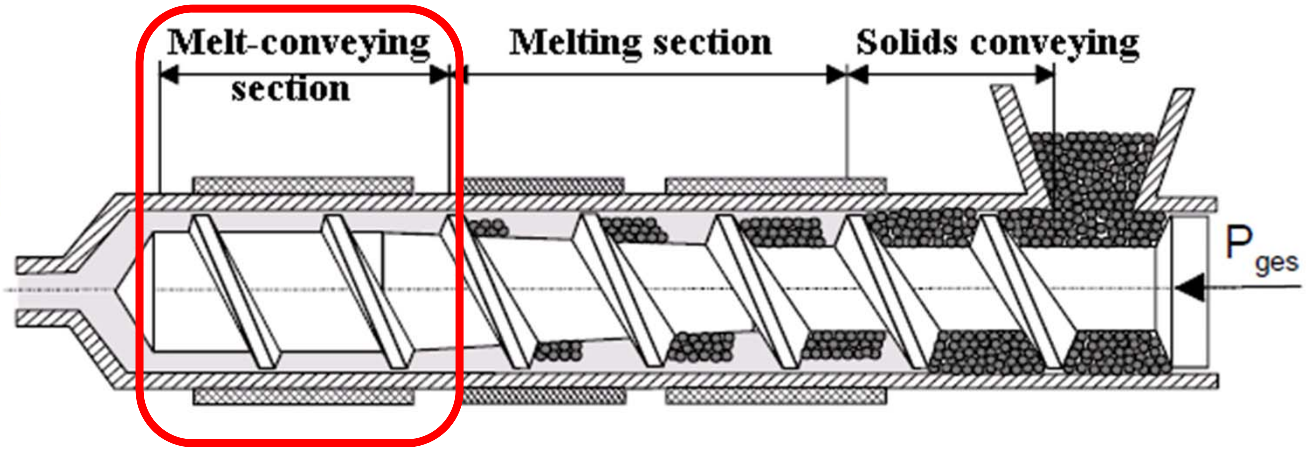


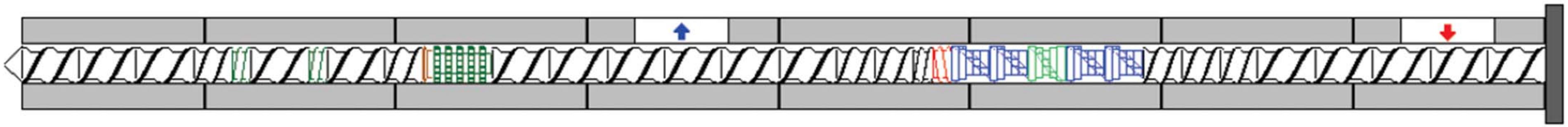


# Motivation: Target Application II

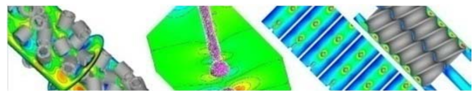
- Non-Newtonian rheological models (shear & temperature dependent)
- Non-isothermal flow conditions (cooling from outside, heat production)
- Evaluation of torque acting on the screws, resulting energy consumption
- Influence of local characteristics on global product quality
- Influence of gaps on back-mixing



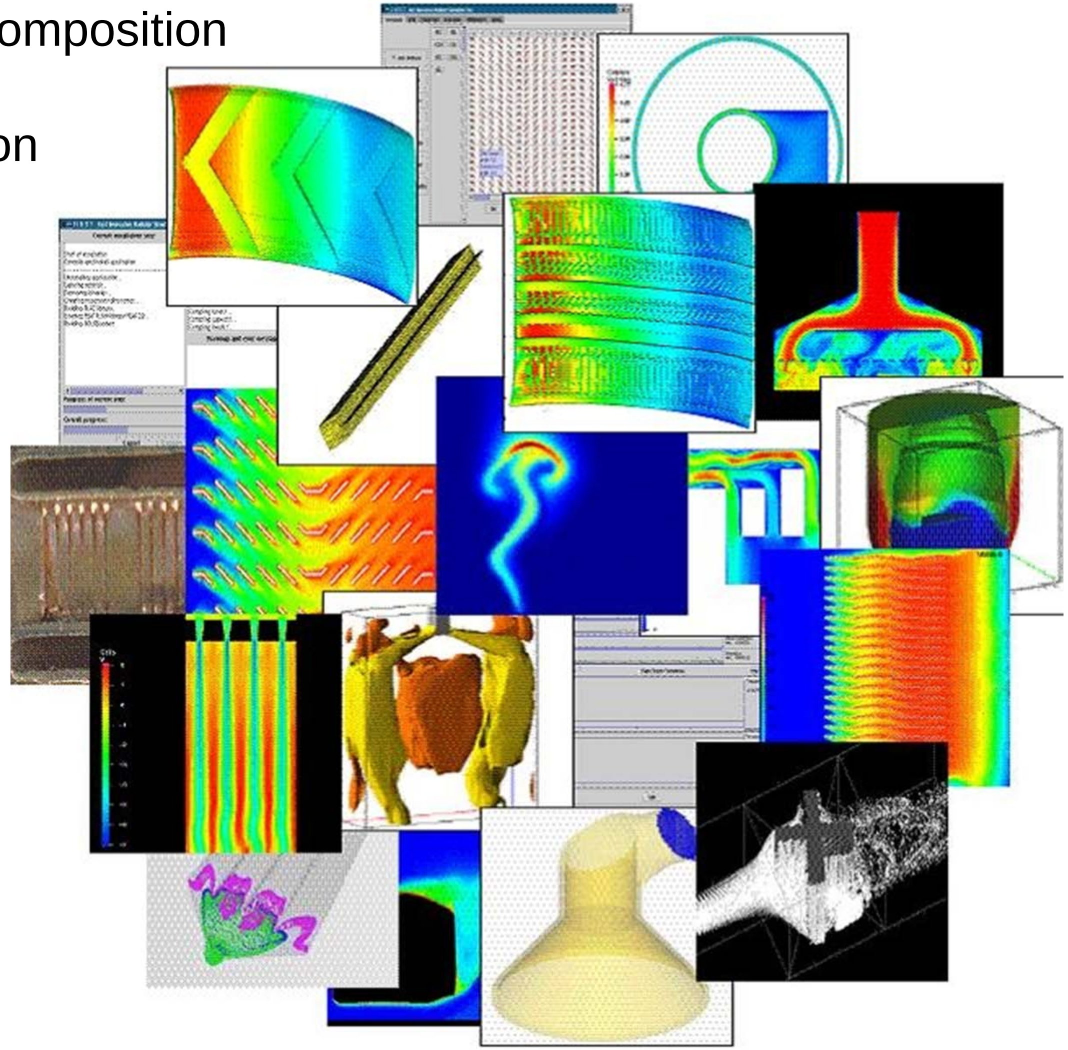




# Basic Flow Solver: FEATFLOW

**Numerical features:**

- Parallelization based on domain decomposition
- FCT & EO stabilization techniques
- High order FEM (Q2/P1) discretization
- Use of unstructured meshes
- Adaptive grid deformation
- Newton-Multigrid solvers

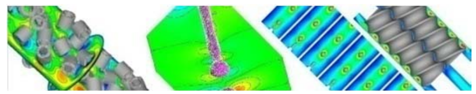


**HPC features**

- Massive parallel
- GPU computing
- Open source

**Hardware-oriented Numerics**





# Two phase flow (l-l) with resolved interphases

**The incompressible Navier Stokes equation**

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) - \nabla\cdot\left(\mu\left[\nabla\mathbf{v} + (\nabla\mathbf{v})^{T}\right]\right) + \nabla p = \mathbf{f}_{ST} + \rho\mathbf{g}$$

$$\nabla\cdot\mathbf{v} = 0$$

Interphase tension force

$$\mathbf{f}_{ST} = \sigma\kappa\mathbf{n}, \quad \kappa = -\nabla\cdot\mathbf{n} \quad \text{on} \quad \Gamma$$

unknown interphase location

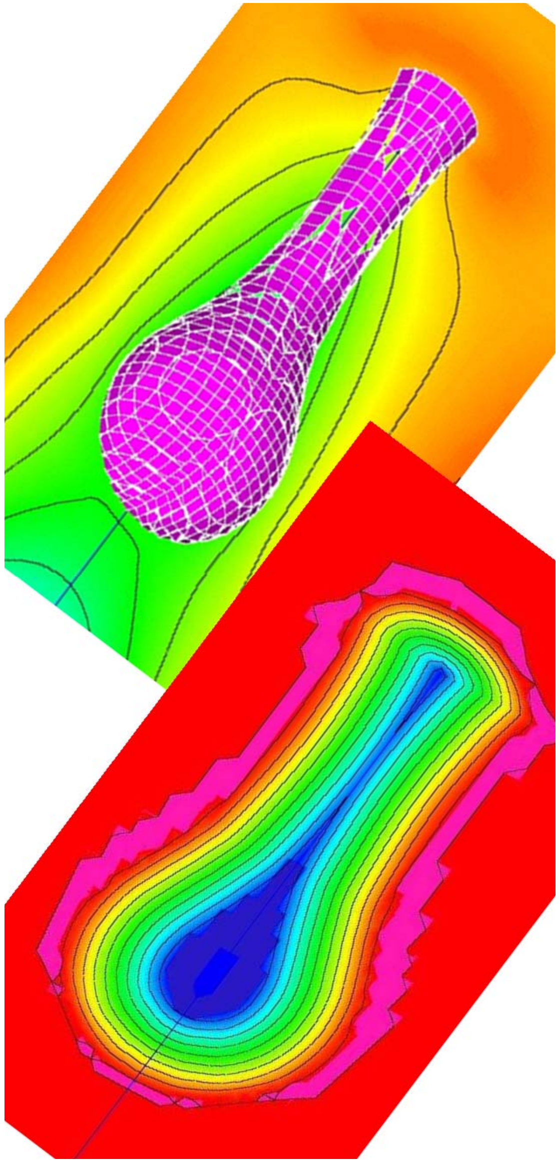
Dependency of physical quantities

$$\mu = \mu(D(\mathbf{v}),\Gamma), \quad \rho = \rho(\Gamma)$$

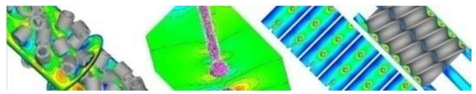
**Interphase capturing** realized by **Level Set method**

$$\frac{\partial \phi}{\partial t} + \mathbf{v}\cdot\nabla\phi = 0 \quad + \quad \frac{\partial \phi}{\partial \tau} + \mathbf{n}\cdot\nabla\phi = S(\phi) \qquad \mathbf{n} = S(\phi)\frac{\nabla\phi}{|\nabla\phi|}$$

- Exact representation of the interphase
- Natural treatment of topological changes
- Provides derived geometrical quantities (**n,** κ )
- Requires reinitializion w.r.t. distance field
- Can lead to mass loss → dG(1) discretization!







# Two phase flow (s-l) with resolved interphases

- **Fluid** motion is governed by the **Navier-Stokes equations**
- **Particle** motion is described by **Newton-Euler equations**

$$M_p \frac{dU_p}{dt} = F_p + F_{ex,col} + (\Delta M_p) g, \qquad I_p \frac{d\omega_p}{dt} = T_p - \omega_p \times (I_p \omega_p)$$

Hydrodynamic force

Torque

$$F_p = -\int_{\Gamma_p} \sigma \cdot n_p \, d\Gamma_p$$

Postprocessing the actual flow field

$$T_p = -\int_{\Gamma_p} (X - X_p) \times (\sigma \cdot n_p) \, d\Gamma_p$$

## Fictitious Boundary Method

- Surface integral is replaced by volume integral
- Use of monitor function (liquid/solid)

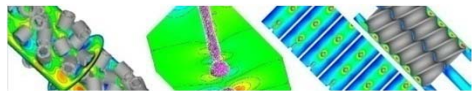
$$\alpha_p(X) = \begin{cases} 1 & \text{for} \quad X \in \Omega_p \\ 0 & \text{for} \quad X \in \Omega_f \end{cases}$$

- Normal to particle surface vector is non-zero only at the surface of particles $n_p = \nabla \alpha_p$

$$F_p = -\int_{\Gamma_p} \sigma \cdot n_p \, d\Gamma_p = -\int_{\Omega_T} \sigma \cdot \nabla \alpha_p \, d\Omega_T$$

$$T_p = -\int_{\Gamma_p} (X - X_p) \times (\sigma \cdot n_p) \, d\Gamma_p = -\int_{\Omega_T} (X - X_p) \times (\sigma \cdot \nabla \alpha_P) \, d\Omega_T$$





# Two phase flow (s-l) with resolved interphases

**Fictitious Boundary Method**

For computed

$$U_p^{n+1},\ \omega_p^{n+1}$$

→

Position update:

$$\frac{dX_p}{dt} = U_p,$$

Angle update:

$$\frac{d\theta_p}{dt} = \omega_p$$

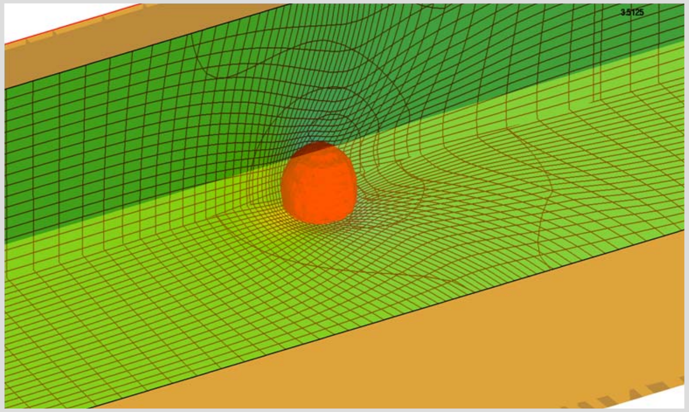
→

$$X_p^{n+1},\ \theta_p^{n+1}$$

Velocity "boundary condition" imposed for particles:

$$u(X) = U_p + \omega_p \times (X - X_p)$$

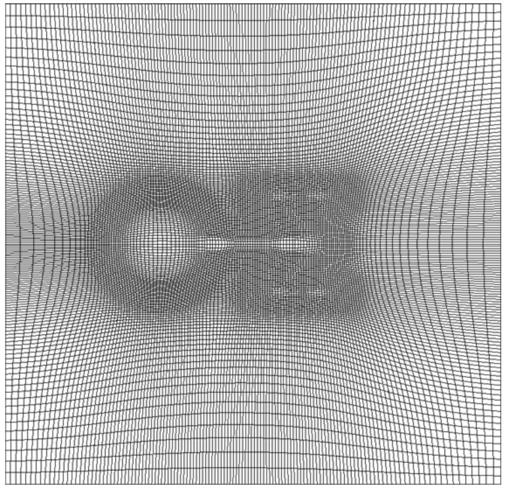
- supports HPC concepts (no computational overhead, constant data structures, optimal load balancing)
- reduces dramatically requirements put on the computational mesh
- relatively low resolution
  - Brute force → Finer mesh resolution
  - High resolution interpolation functions
  - Grid deformation (via Level-Set function)

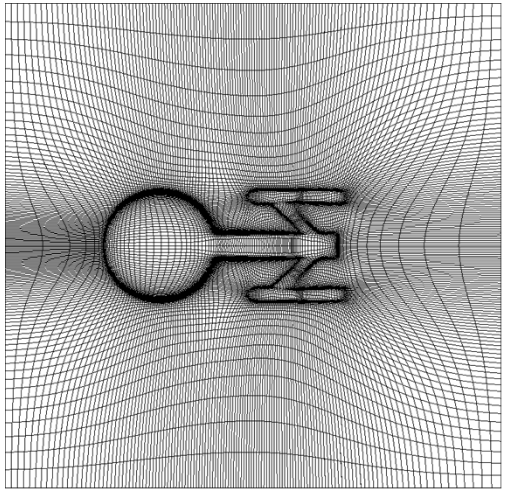


# Grid Deformation Method

**idea** : construct transformation $\phi$, $x = \phi(\xi, t)$ with $\det \nabla \phi = f$

⟹ local mesh area $\approx f$





1. Compute monitor function $f(x,t) > 0,\ f \in C^1$ and

$$\int_\Omega f^{-1}(x,t)\,dx = |\Omega|, \quad \forall t \in [0,1]$$

2. Solve $(t \in [0,1])$

$$\Delta v(\xi,t) = -\frac{\partial}{\partial t}\left(\frac{1}{f(\xi,t)}\right), \quad \left.\frac{\partial v}{\partial n}\right|_{\partial\Omega} = 0$$

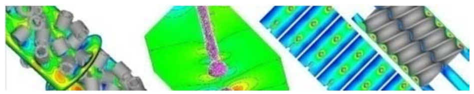
3. Solve the ODE system

$$\frac{\partial}{\partial t}\phi(\xi,t) = f(\phi(\xi,t),t)\nabla v(\phi(\xi,t),t)$$

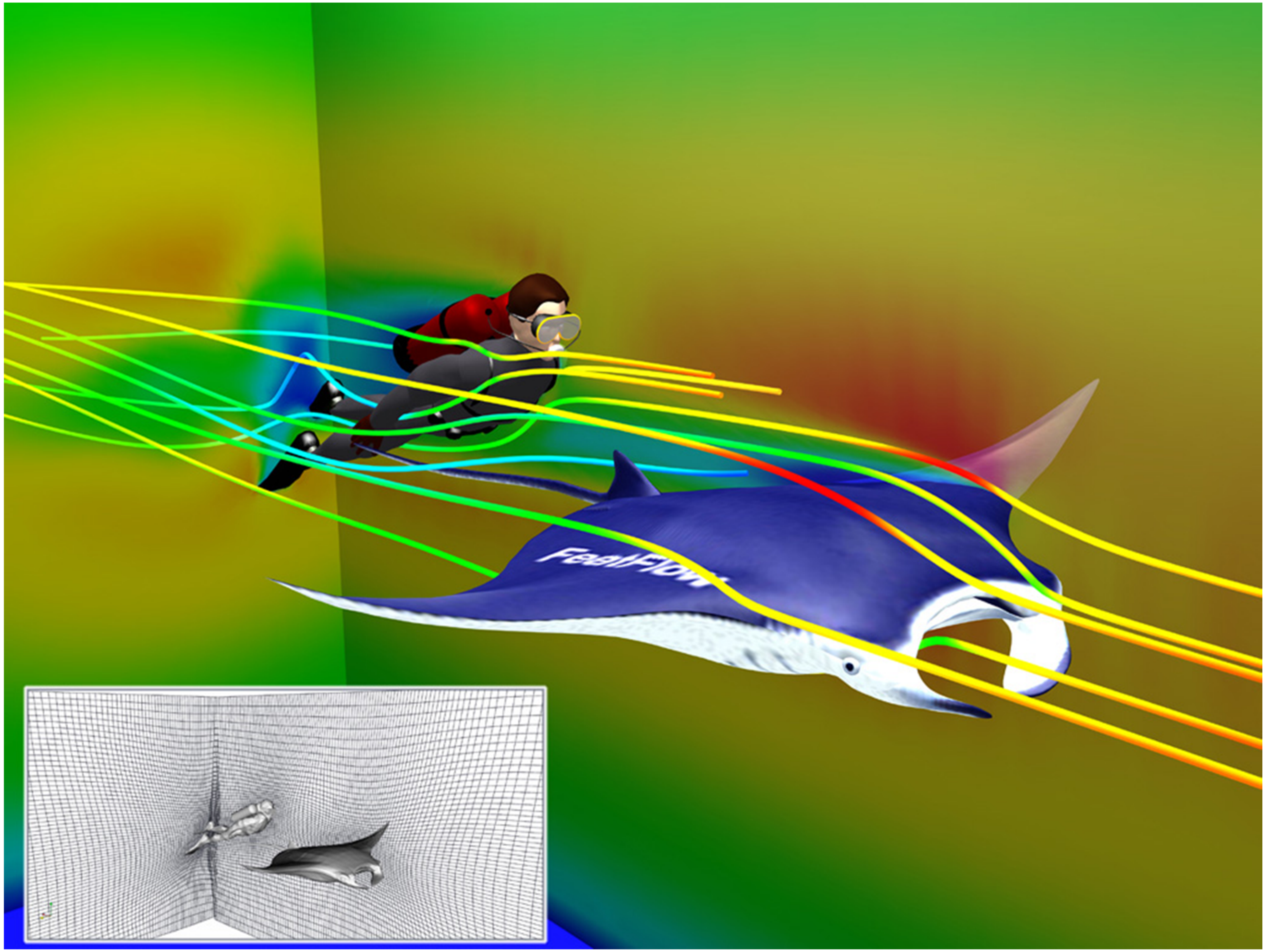
new grid points: $x_i = \phi(\xi_i, 1)$

**Grid deformation preserves the (local) logical structure of the grid**

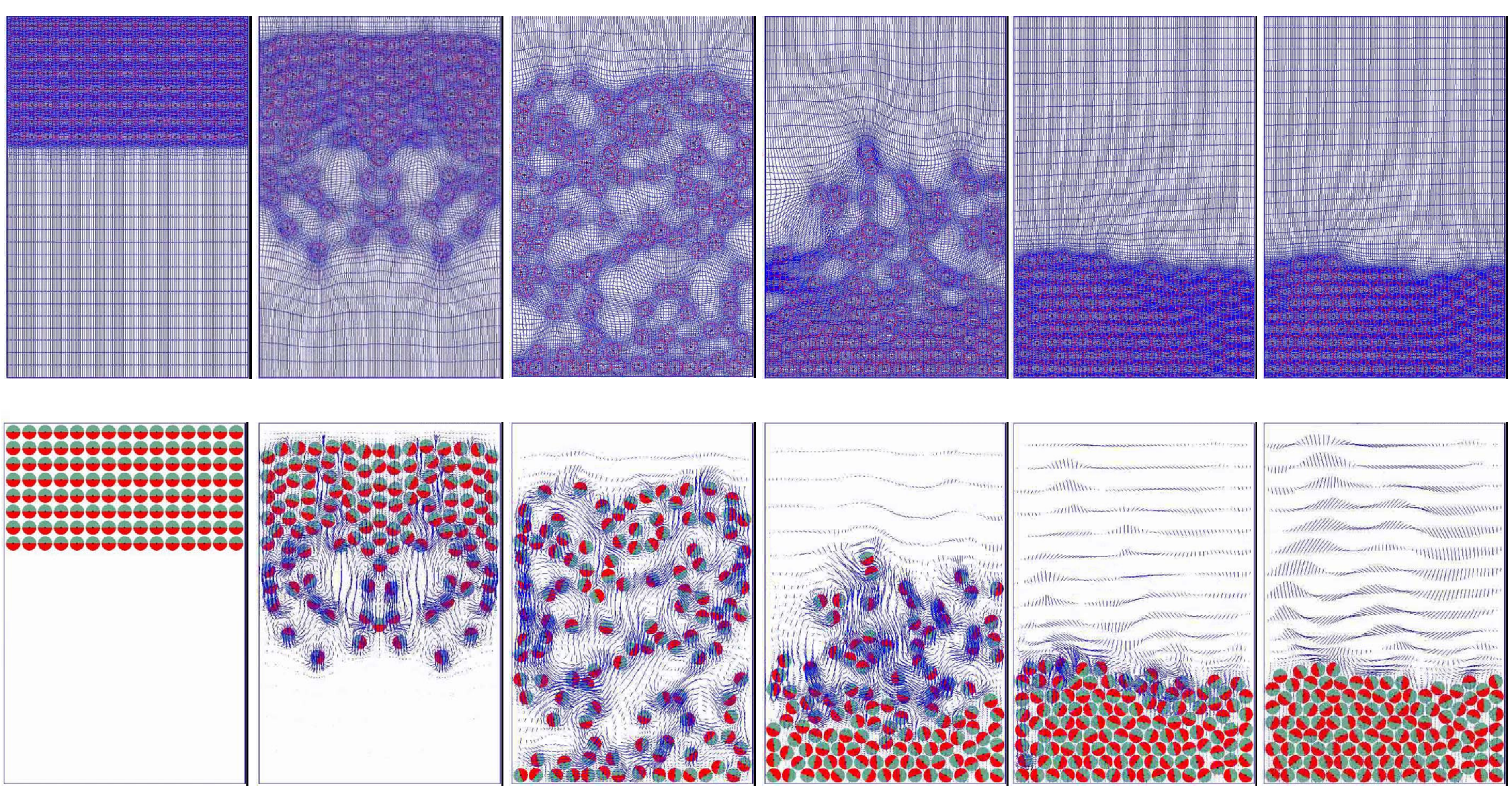




# Generalized Tensorproduct Meshes



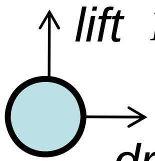
# Sedimentation of many Particles



# Benchmarking and Validation

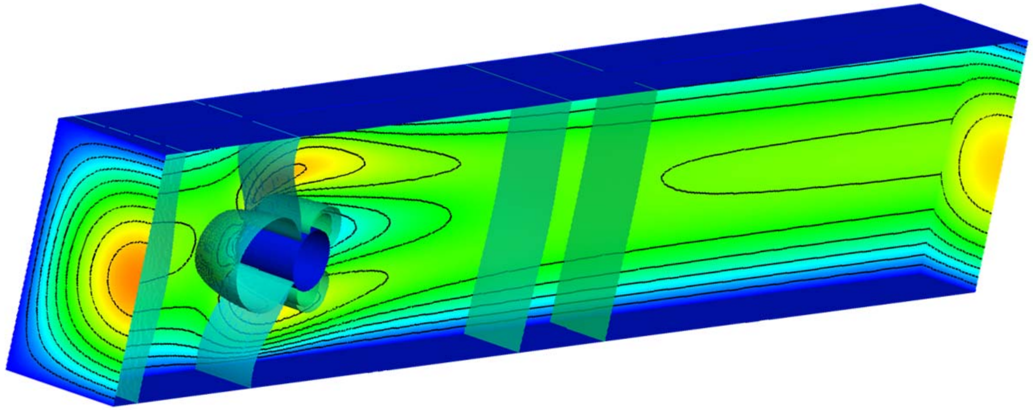
## Flow Simulation for the Flow Around Cylinder problem

### Known benchmark problem (DFG) in the CFD community




*lift* $F_L = \frac{1}{2}\rho v^2 A C_L$

*drag* $F_D = \frac{1}{2}\rho v^2 A C_D$



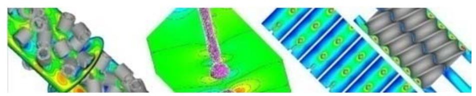
- Comparison of CFX 12.0, OpenFoam 1.6 and FeatFlow
- Drag and lift coefficients behave very sensitive to mesh resolution

→ Ideal indicator for computational accuracy

- Five consequently refined meshes L1 (coarse), …, L5 (fine)
- Same meshes and physical models used in all three codes

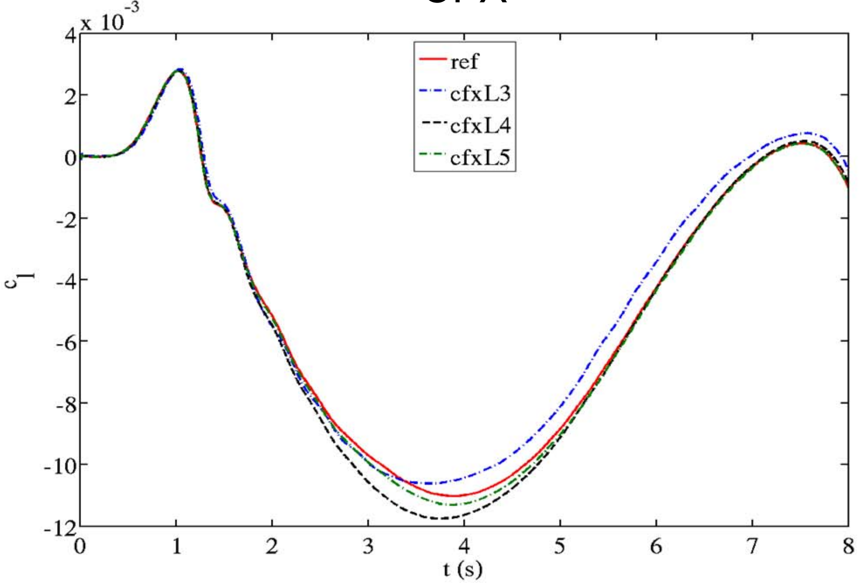
| Mesh Level | # Elements |
|---|---|
| L2 | 6,144 |
| L3 | 49,152 |
| L4 | 393,216 |
| L5 | 3,145,728 |



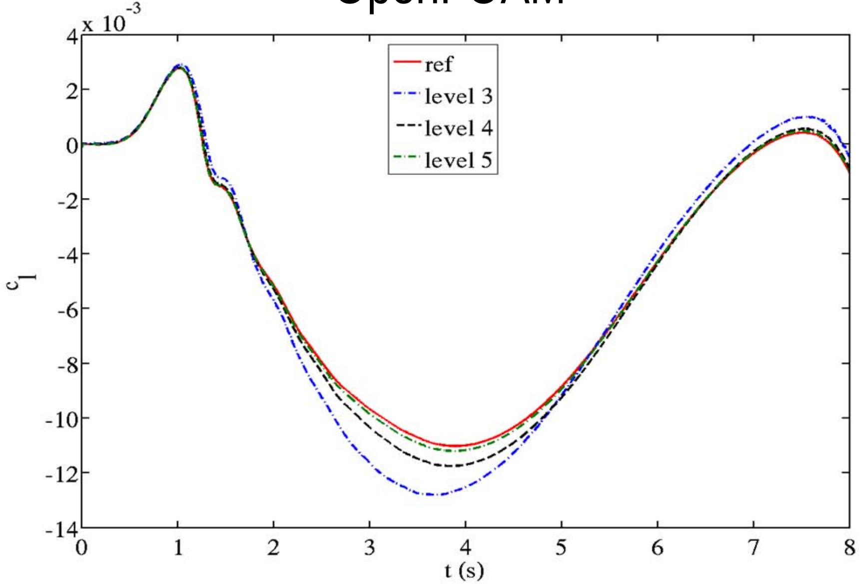


# Benchmarking and Validation

CFX



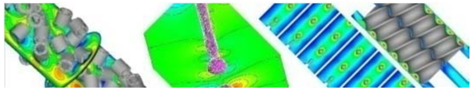

OpenFOAM




| Case | $L_2$Err | |
|---|---|---|
| | $c_D$ | $c_L$ |
| cfxL3 | 0.0152 | 0.0781 |
| cfxL4 | 0.0098 | 0.0631 |
| cfxL5 | 0.0029 | 0.0224 |

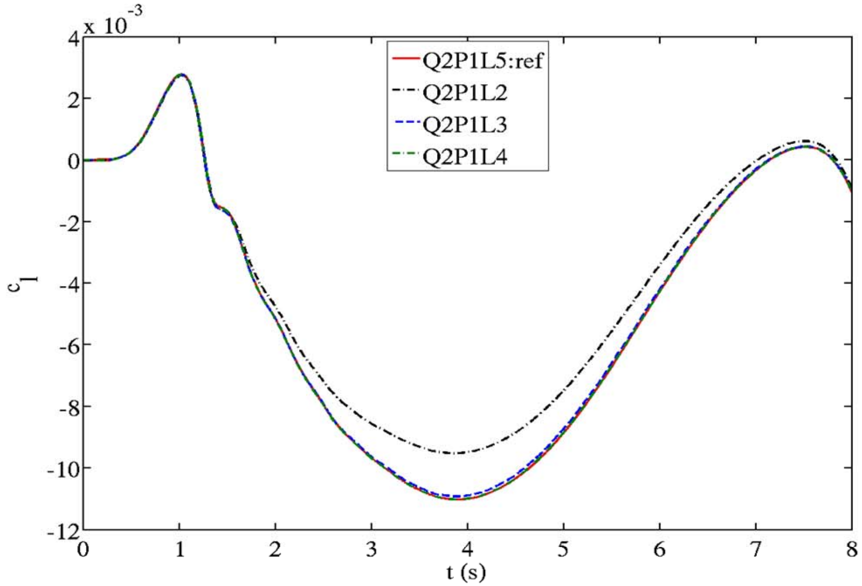
| Case | $L_2$Err | |
|---|---|---|
| | $c_D$ | $c_L$ |
| OFL3 | 0.0261 | 0.1449 |
| OFL4 | 0.0067 | 0.0591 |
| OFL5 | 0.0016 | 0.0147 |





# Benchmarking and Validation

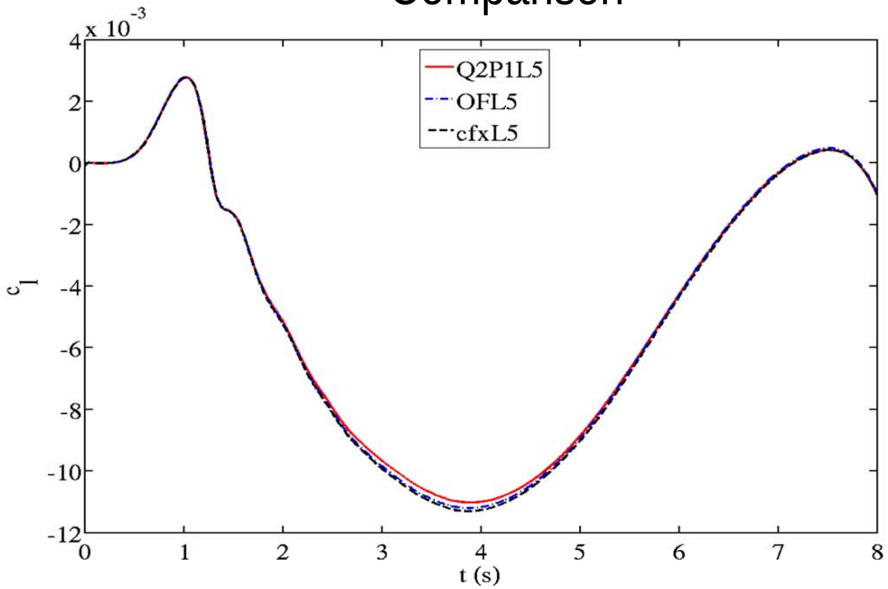
FeatFlow




| Case | $L_2$Err | |
|---|---|---|
| | $c_D$ | $c_L$ |
| Q2P1L2 | 0.0209 | 0.1378 |
| Q2P1L3 | 0.0029 | 0.0109 |
| Q2P1L4 | 0.0005 | 0.0015 |

Less then 2 hours sim. time on 3+1 processors

Comparison

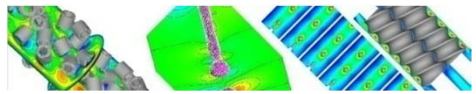



| Case | $L_2$Err | |
|---|---|---|
| | $c_D$ | $c_L$ |
| Q2P1L3 | 0.0029 | 0.0109 |
| OFL5 | 0.0016 | 0.0147 |
| cfxL5 | 0.0029 | 0.0224 |

→ Same order of accuracy with FeatFlow on L3 as L5 with CFX and OpenFOAM on L5!

→ High order Q2/P1 FEM + (parallel) Multigrid Solver

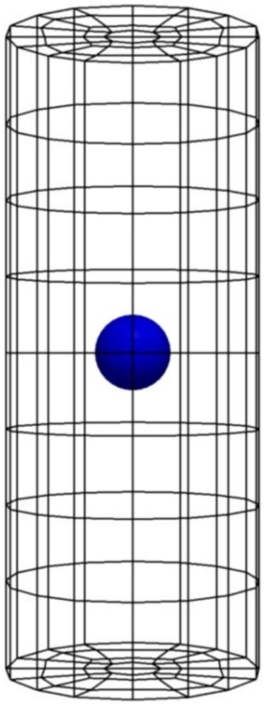


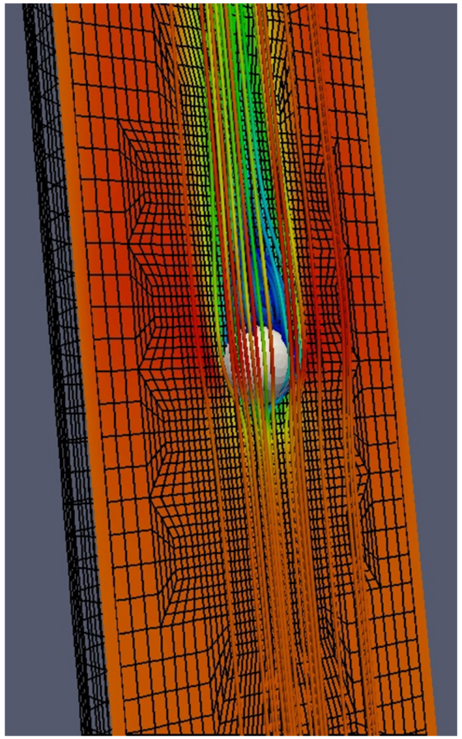


# Benchmarking and Validation

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, 2010, accepted

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

| $\nu$ | $U_{featflow}$ | $U_{exp}$ | 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 |

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

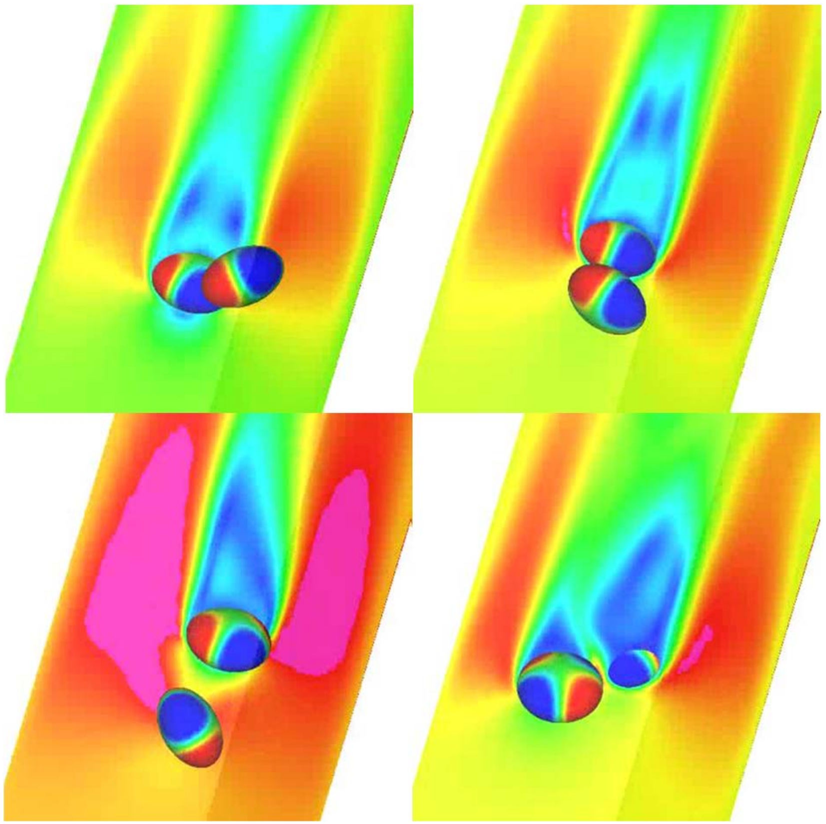
| $\nu$ | $U_{featflow}$ | $U_{exp}$ | Relative error (%) |
|---|---|---|---|
| 0.02 | 4.370 | 4.334 | 0.83 |
| 0.05 | 2.699 | 2.489 | 8.44 |
| 0.1 | 1.649 | 1.552 | 6.25 |
| 0.2 | 0.946 | 0.870 | 8.74 |

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

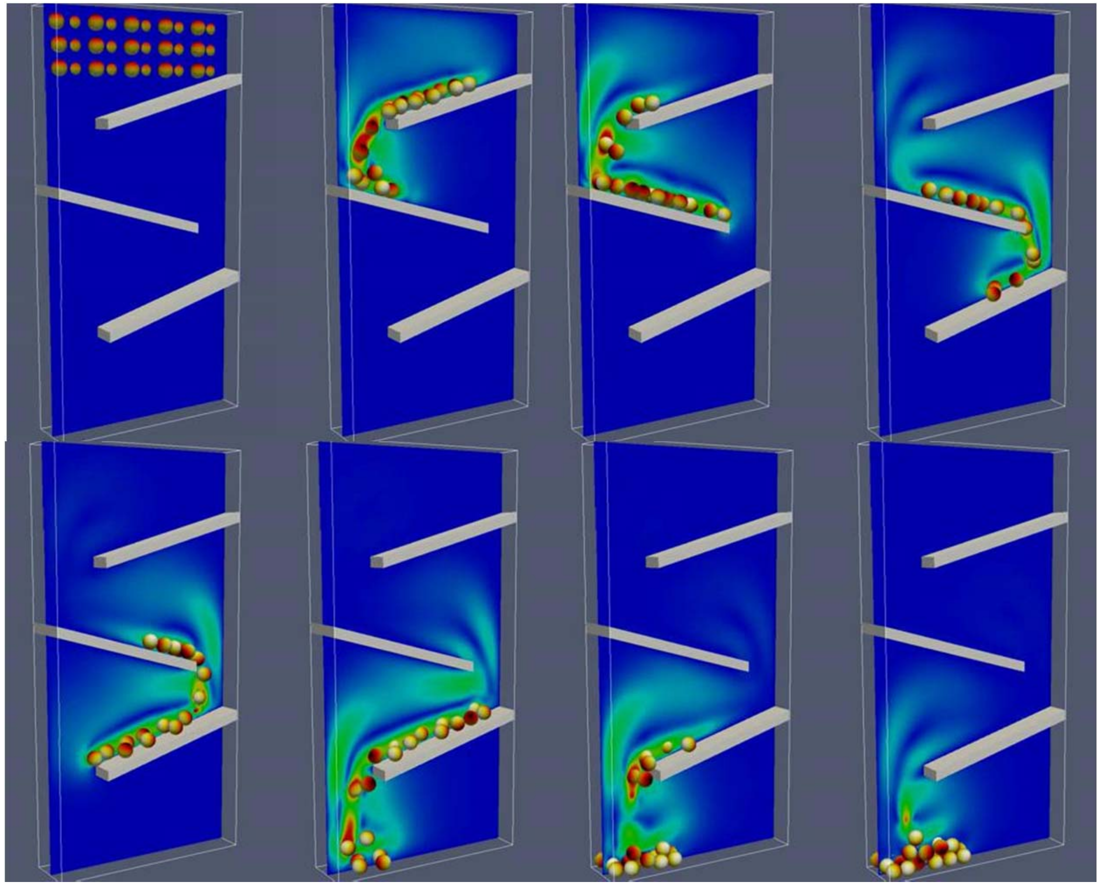
| $\nu$ | $U_{featflow}$ | $U_{exp}$ | Relative error (%) |
|---|---|---|---|
| 0.01 | 1.4660 | 1.4110 | 3.90 |
| 0.02 | 0.9998 | 0.9129 | 9.52 |
| 0.05 | 0.4917 | 0.4603 | 6.82 |
| 0.1 | 0.2637 | 0.2571 | 2.57 |
| 0.2 | 0.1335 | 0.1317 | 1.37 |

# 3D simulations with complex shapes

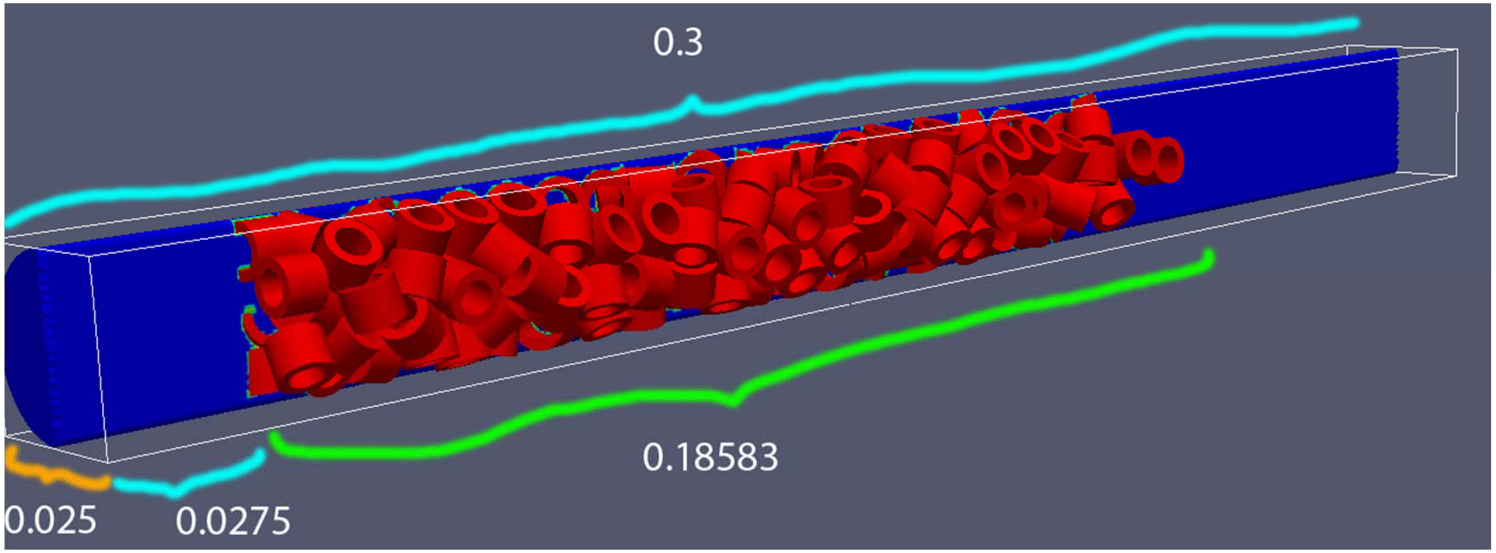
‘Kissing, Drafting, Thumbling’



Sedimentation of particles in a complex domain



# Absorber packing simulations

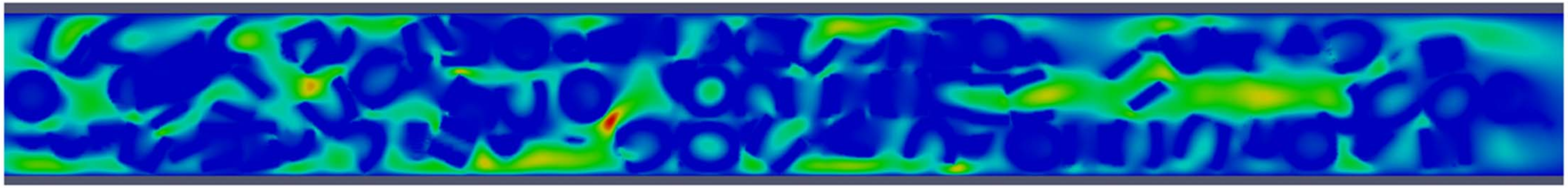



$v_{mean} = (1|0.1|0.01)\ ms^{-1}$

$\rho = 1.25\ g\ cm^{-3}$

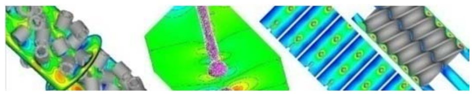
$\mu = 17.57\ 10^{-6}\ Pa\ s$

Velocity distribution



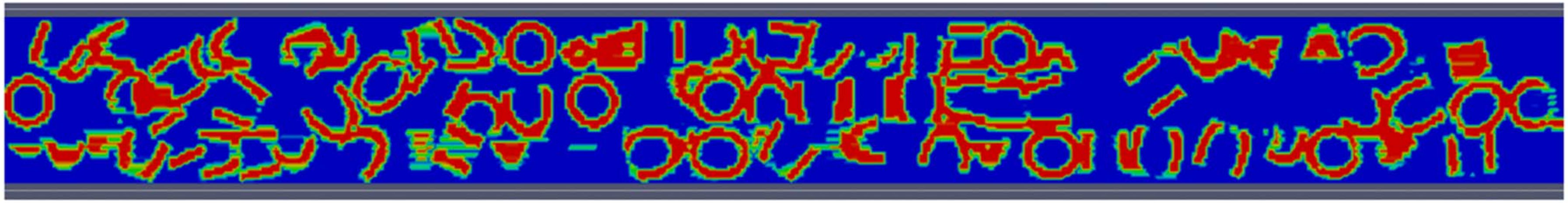
Pressure distribution





# Absorber packing simulations

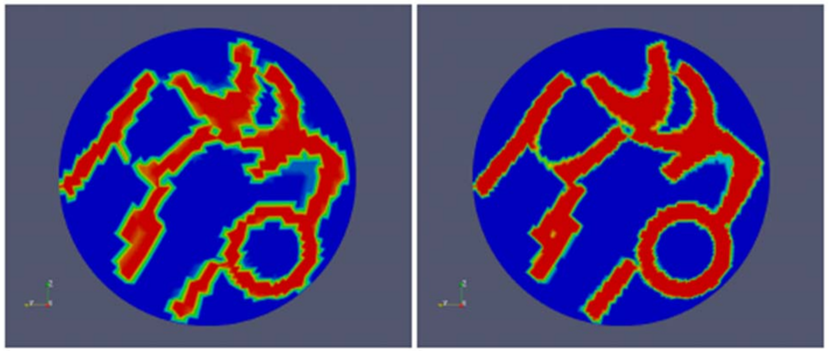
| Level | Mesh points | | | Velocity DOFs | | | Pressure DOFs | | |
|---|---|---|---|---|---|---|---|---|---|
| | $n_x$ | $n_{yz}$ | $n_{xyz}$ | $n_x$ | $n_{yz}$ | $n_{xyz}$ | $n_x$ | $n_{yz}$ | $n_{xyz}$ |
| 2 | 155 | 109 | 16,895 | 308 | 409 | 126,381 | 154(*4) | 96(*4) | 59,136 |
| 3 | 309 | 409 | 126,381 | 617 | 1,585 | 977,945 | 308(*4) | 384(*4) | 473,088 |
| 4 | 617 | 1,585 | 977,945 | 1,233 | 6,241 | 7,695,153 | 616(*4) | 1,536(*4) | 3,784,704 |

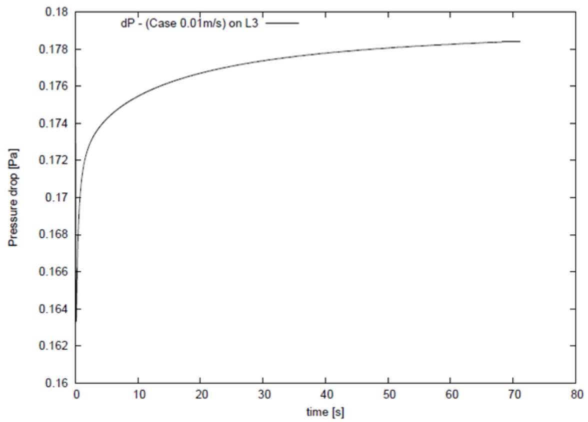


L3

L4

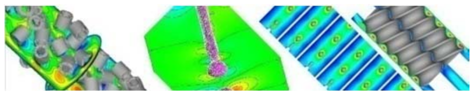
L3 L4





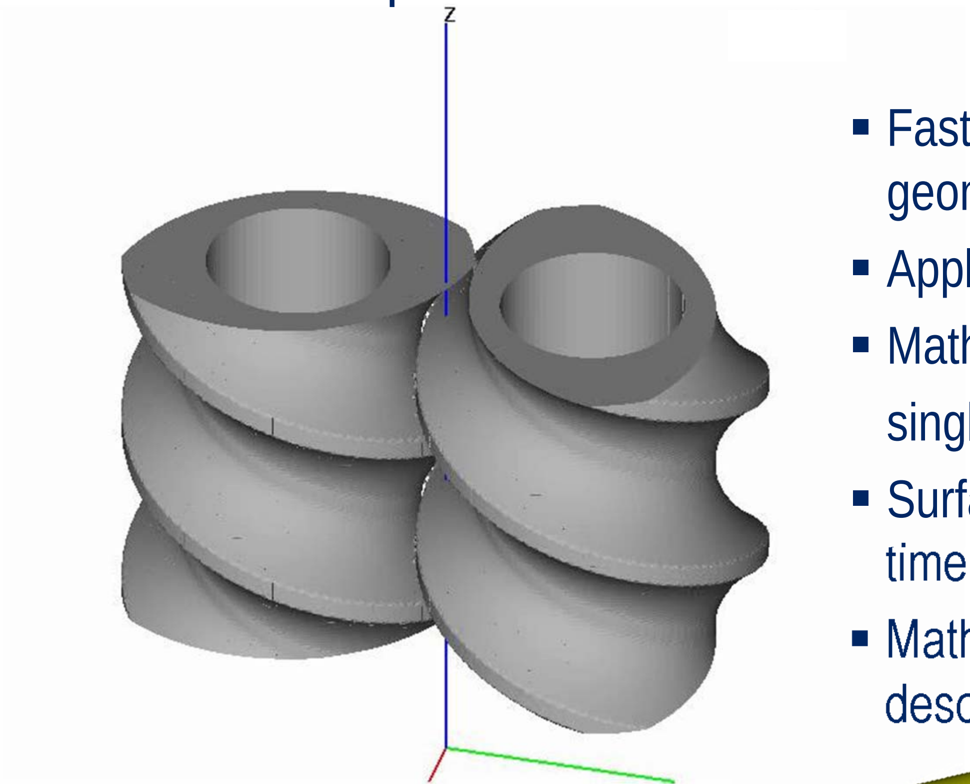

Stefan Turek

technische universität
dortmund

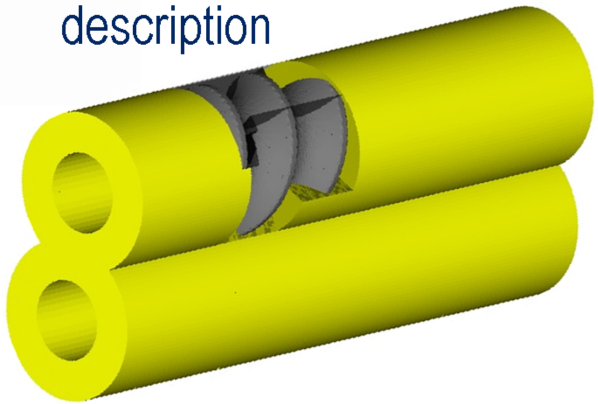


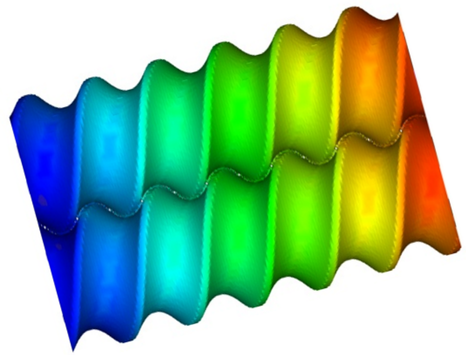
# Twinscrew Flow Simulations

## Geometrical representation of the twinscrews → Fictitious Boundary Method




- Fast and accurate description of the rotating geometry (screws)
- Applicable for conveying and kneading elements
- Mathematical description available for single, double- or triplet-flighted screws
- Surface and body of the screws are known at any time
- Mathematical formulation replaces external CAD-description



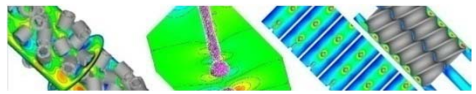


In cooperation with:

UNIVERSITÄT PADERBORN
Die Universität der Informationsgesellschaft

IANUS Simulation

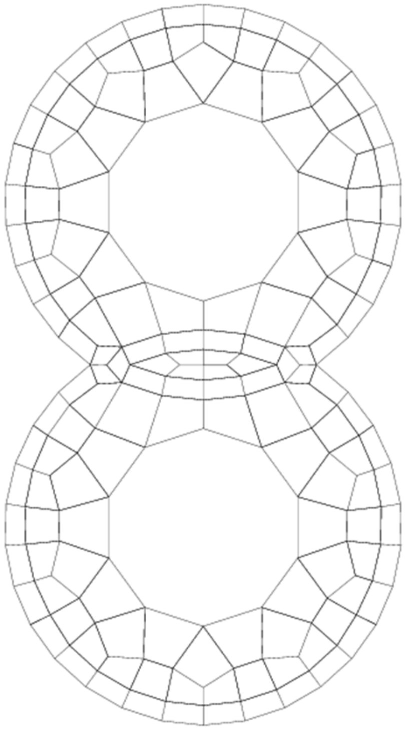


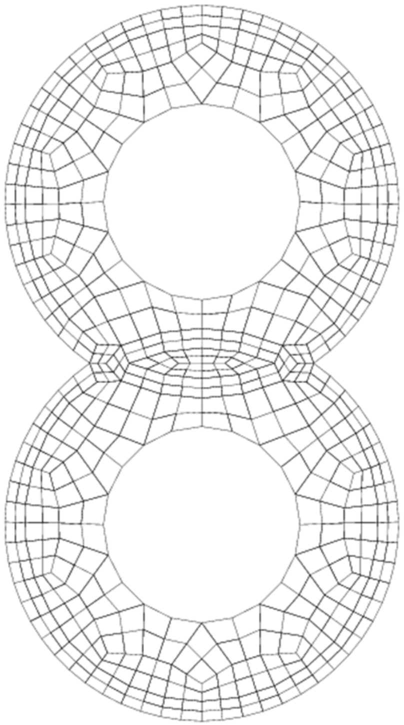


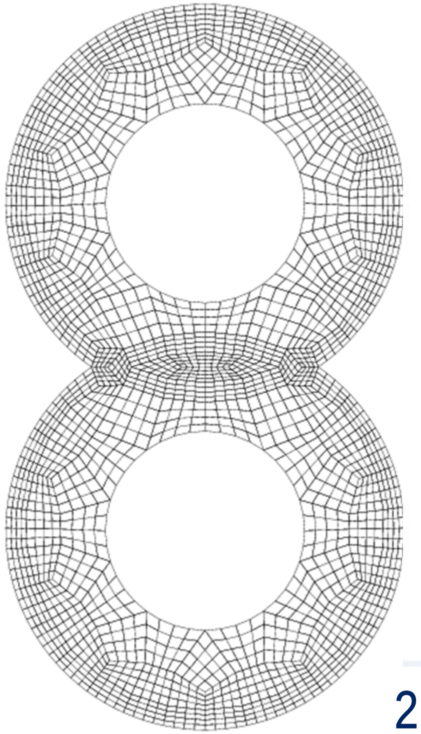
# Twinscrew Flow Simulations

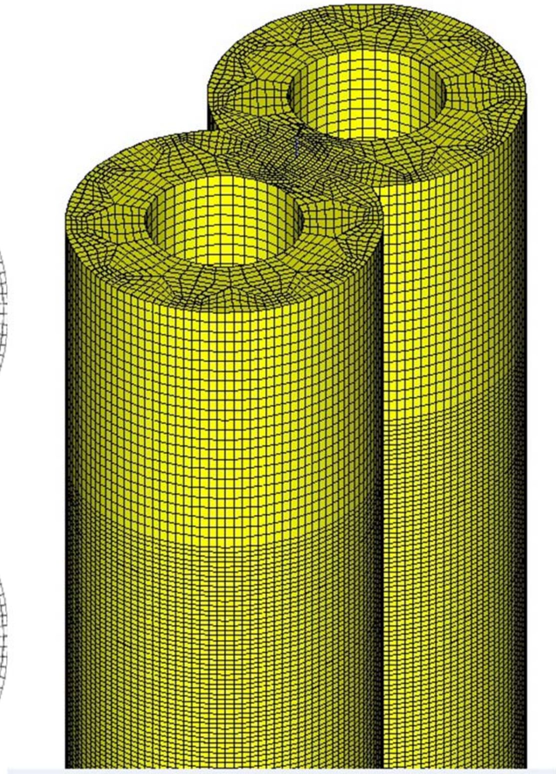
## Meshing strategy – Hierarchical mesh refinement

level 1 level 2 level 3





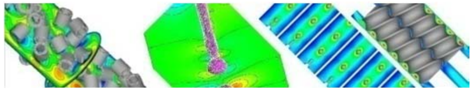




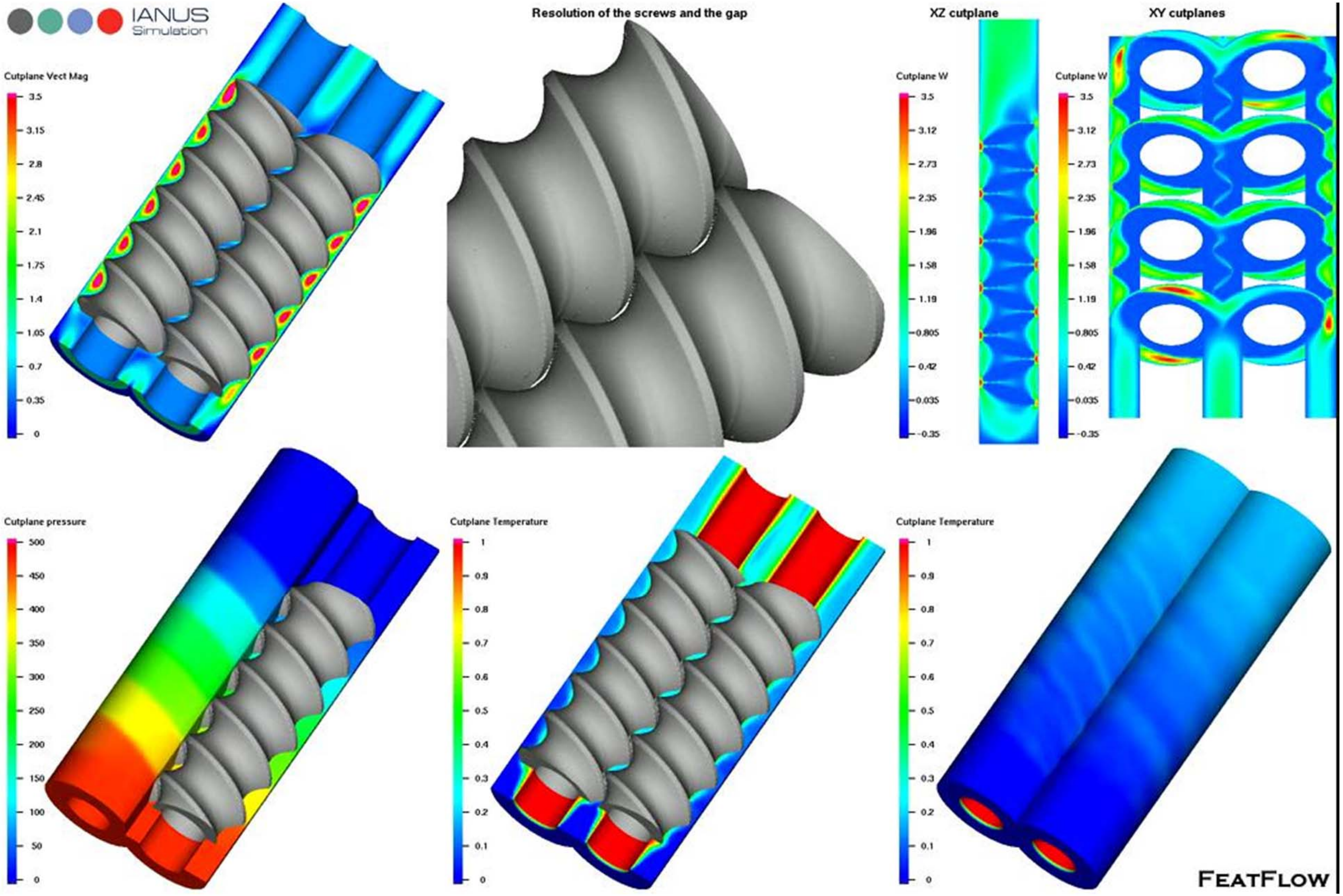
2D mesh extrusion into 3D

Pre-refined regions in the vicinity of gaps

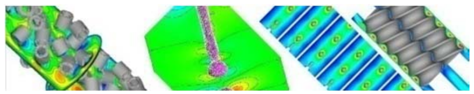




# Twinscrew Flow Simulations





Vielen Dank!

# Benchmarking with experimental results

Continuous phase:

Glucose-Water mixture

$\mu_D = 500\, mPa\, s$

$\rho_D = 972\; kg\; m^{-3}$

$\dot{V}_D = 3{,}64\, ml\; min^{-1}$

$\sigma_{CD} = 0{,}034\, N\; m^{-1}$

Silicon oil

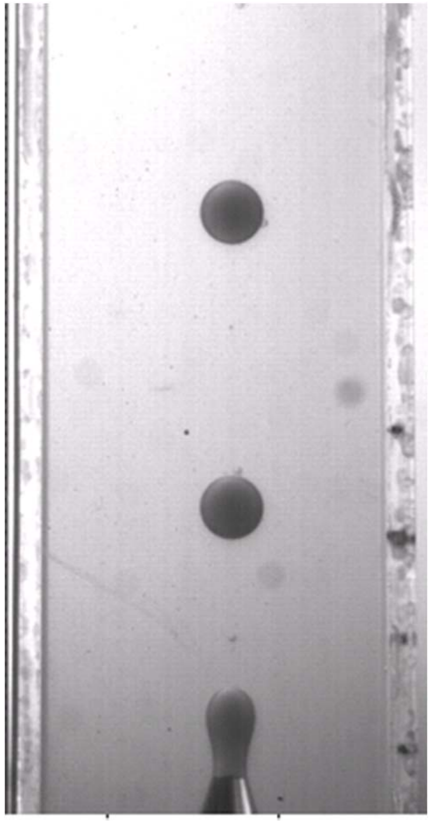
$\mu_C = 500\, mPa\, s$

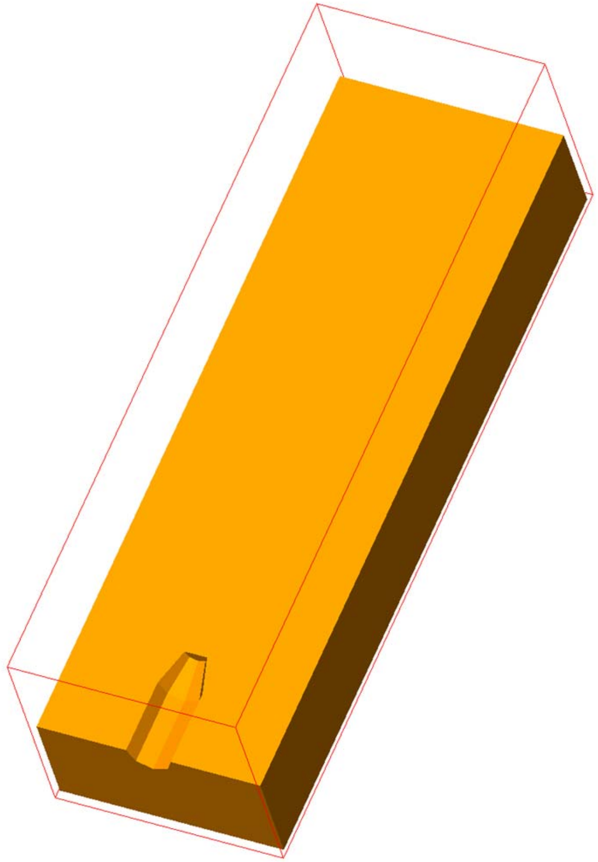
$\rho_C = 1340\; kg\; m^{-3}$

$\dot{V}_C = 99{,}04\, ml min^{-1}$

Dispersed phase:

Experimental Set-up with **AG Walzel (BCI/Dortmund)**

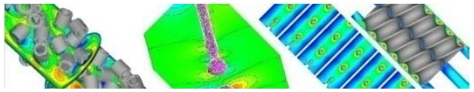




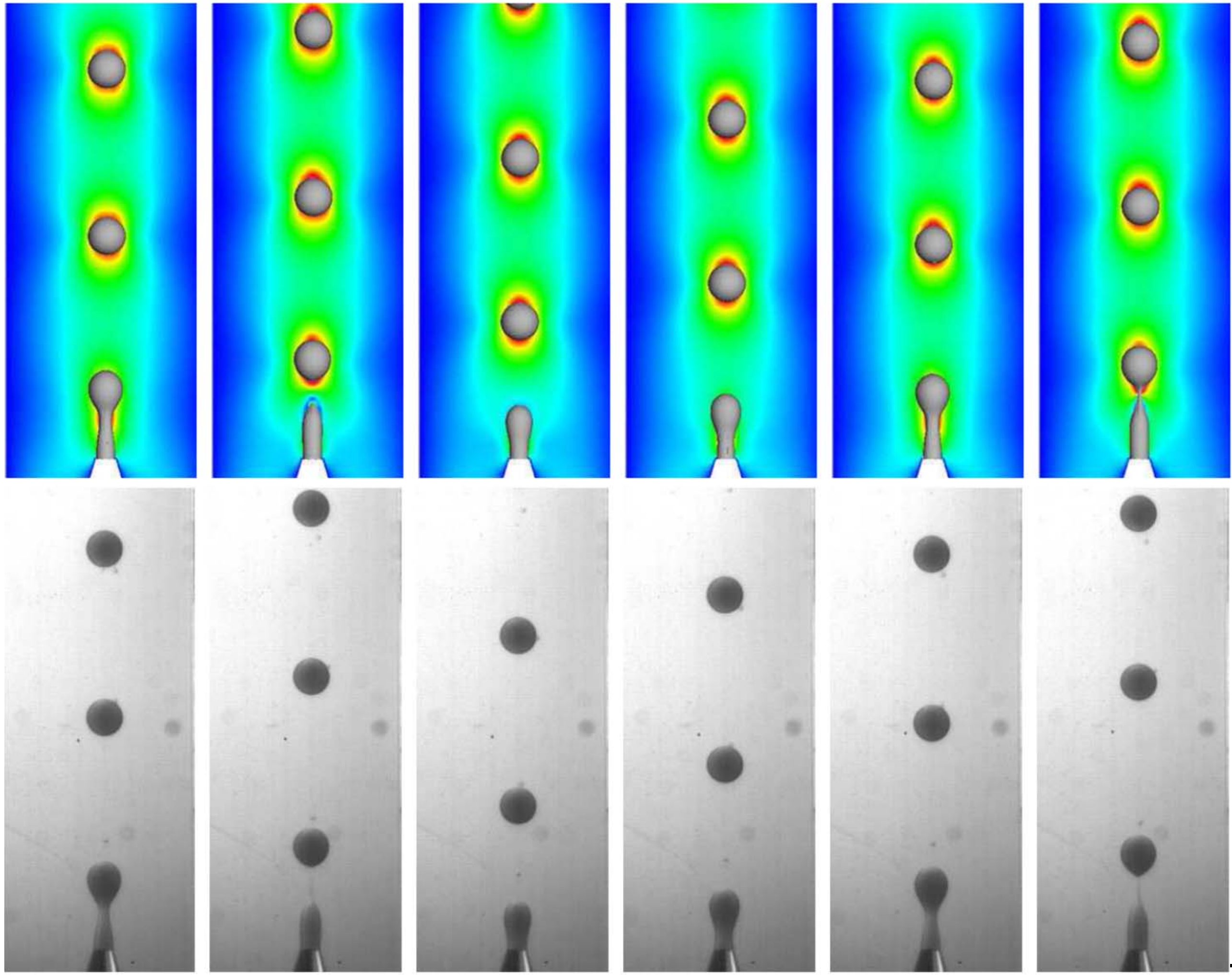
**Validation parameters:**

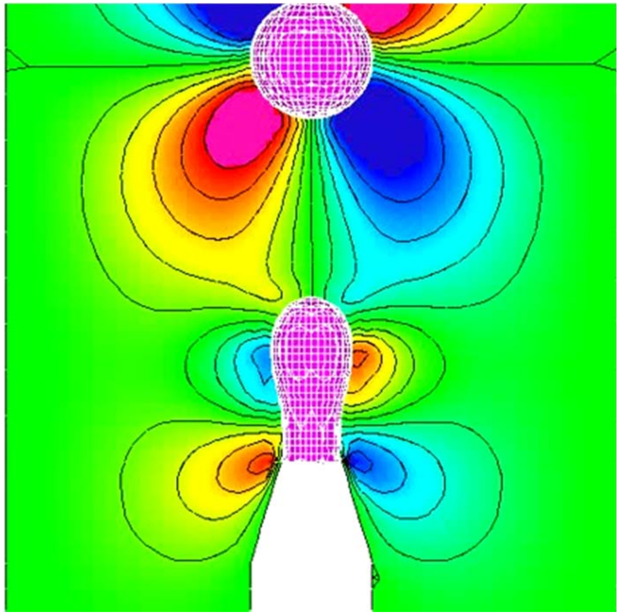
- frequency of droplet generation
- droplet size
- stream length





# Benchmarking with experimental results





| | Separation frequency [Hz] | Droplet size [dm] | Stream Length [dm] |
|---|---|---|---|
| Exp | 0,58 | 0,062 | 0,122 |
| Sim | 0,6 | 0,058 | 0,102 |

Exp. results → Group of Prof. Walzel BCI/Dortmund