On higher order FEM techniques for multiphase flow

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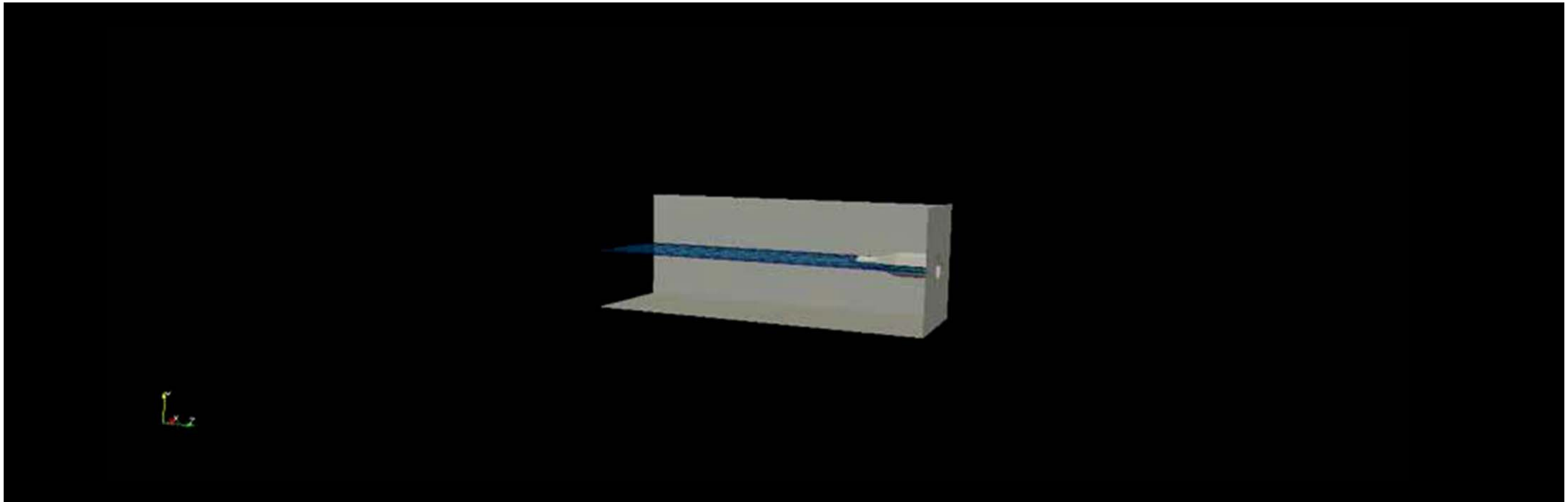
Overview & Motivation:

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

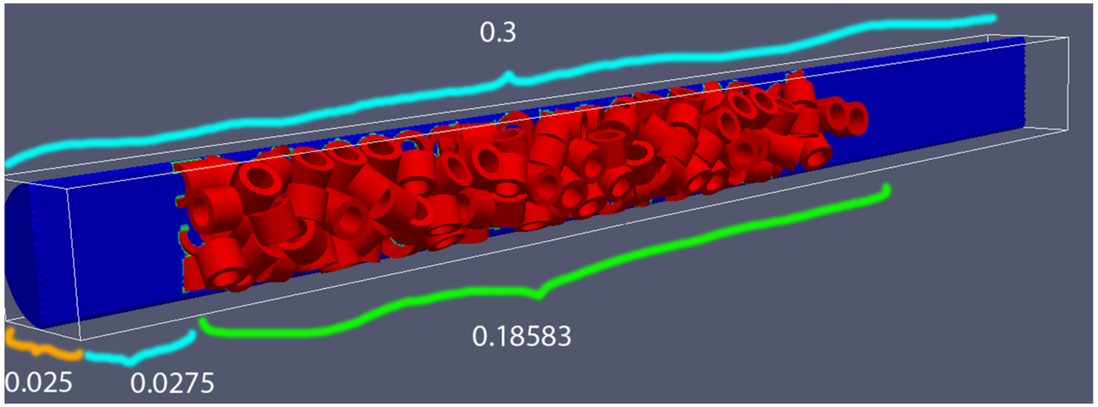
- Mathematical Modelling
- Numerics / CFD Techniques
- Validation / Benchmarking
- HPC Techniques / Software

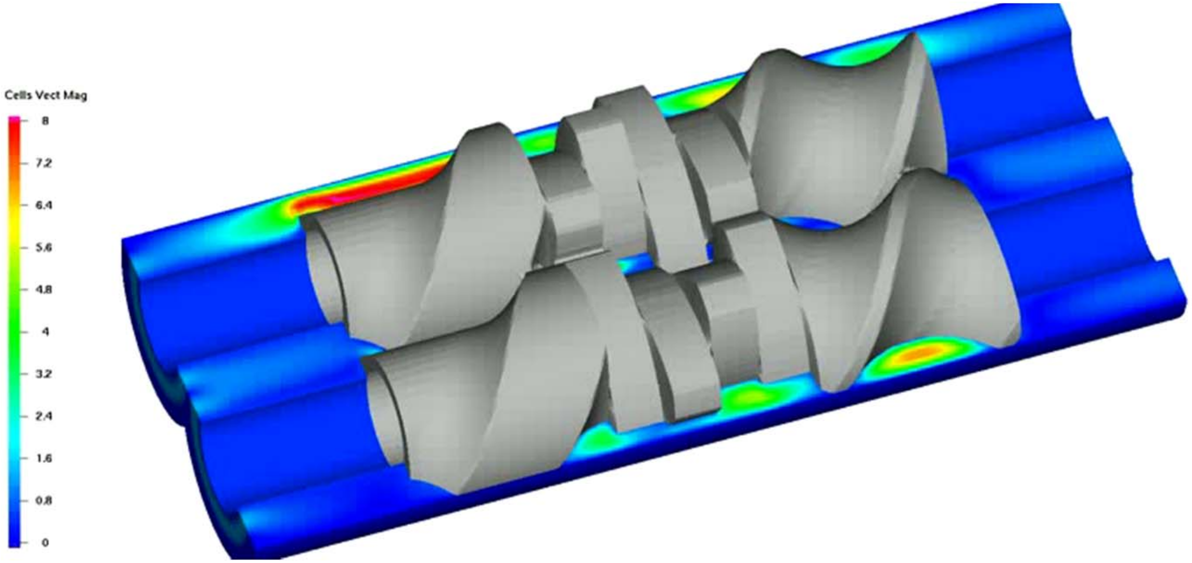
Vision: *Highly efficient, flexible and accurate „real life“ simulation tools based on modern Numerics and algorithms while exploiting modern hardware!*

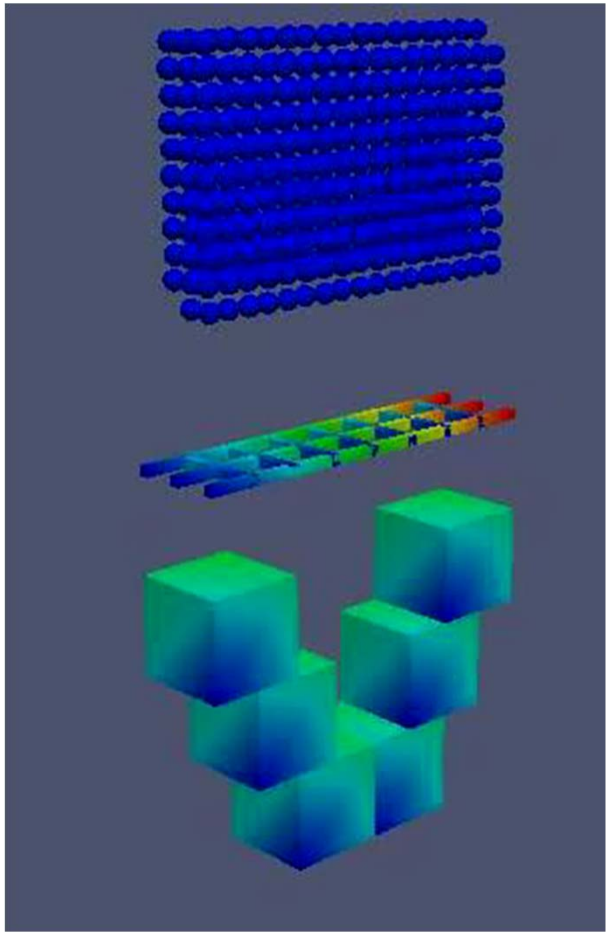
Realization: **FEATFLOW**



Typical applications require efficient basic flow solvers and techniques for liquid-liquid & liquid-solid interfaces in complex (time-dependent) domains



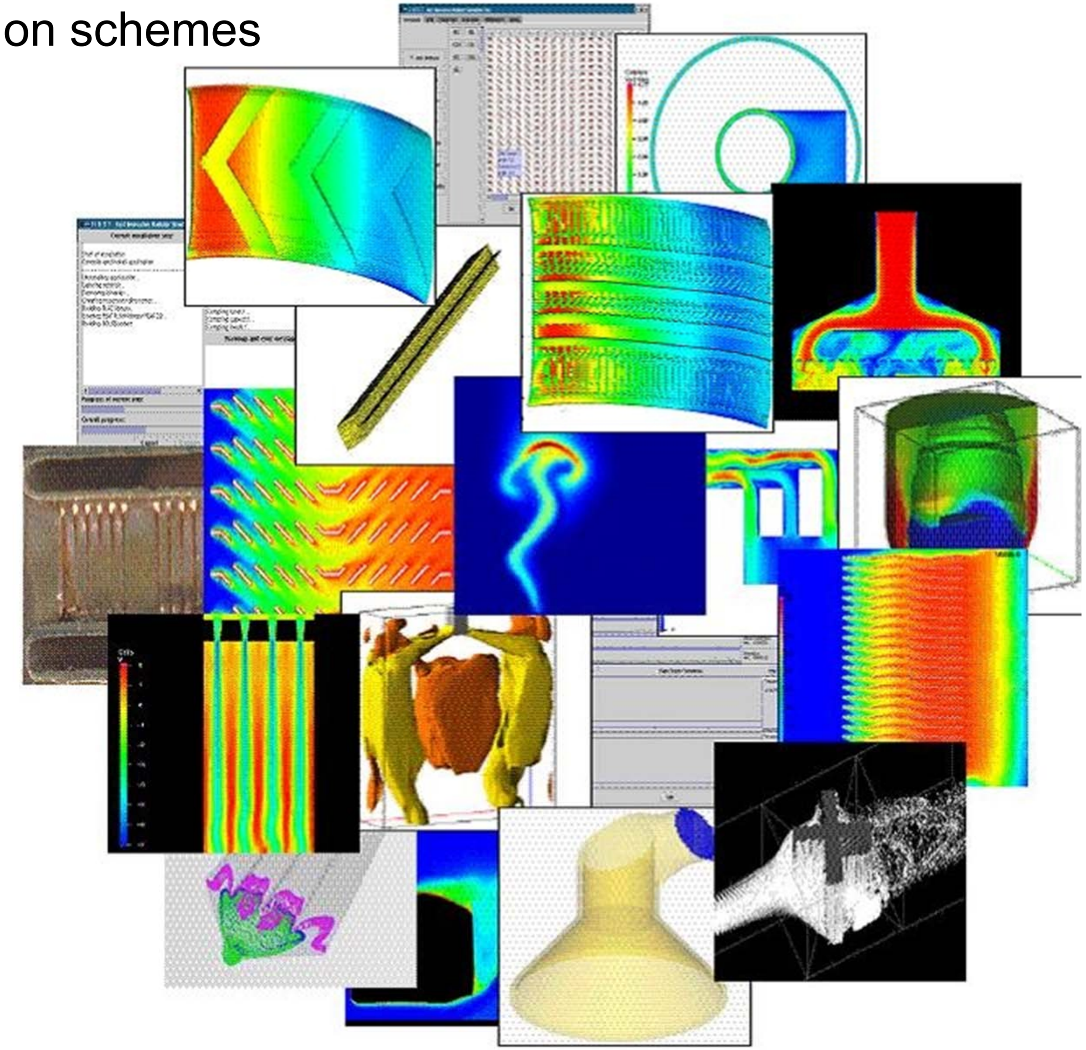




Basic Flow Solver: FeatFlow

<u>Numerical features:</u>

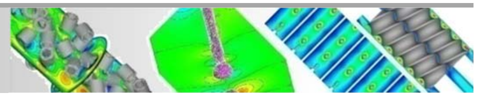
- High order FEM (Q2/P1) discretization schemes
- FCT & EO stabilization techniques
- Use of unstructured meshes
- Fictitious Boundary (FBM) methods
- Adaptive grid deformation
- Newton-Multigrid solvers



<u>HPC features:</u>

- Massive parallel
- GPUs/ARMs
- Open source

Hardware-oriented Numerics



Two phase flow (l-l) with resolved interfaces

The incompressible Navier Stokes equations

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

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

Interface tension force

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

unknown interface location

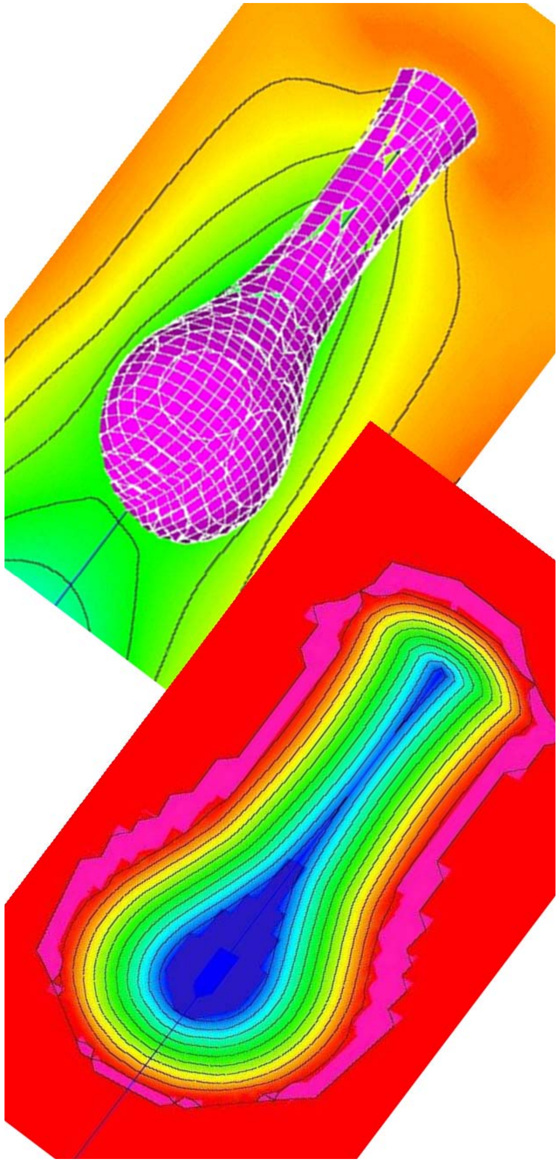
Dependency of physical quantities

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

Interface capturing realized by **Level Set method**

$$\boxed{\frac{\partial \phi}{\partial t} + \mathbf{v}\cdot\nabla\phi = 0}$$

- Exact representation of the interface
- Natural treatment of topological changes
- Provides derived geometrical quantities (**n,** κ)



Two phase flow (l-l) with resolved interfaces

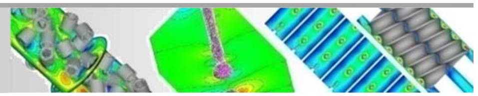
Problems and Challenges

- **Steep gradients** of the velocity field and of other physical quantities near the interface (oscillations!)
- **Reinitialization** w.r.t. distance field (artificial movement of the interface → mass loss, how often to perform?)
- **Mass conservation** (during advection and reinitialization of the Level Set function)
- Representation of **surface tension**: CSF, Line Integral, Laplace-Beltrami, Phasefield, etc.
- **Explicit** or **implicit** treatment (→ *Capillary Time Step* restriction?)
- **Fast multigrid solvers** for Q2/P1 via Discrete Projection Method

Two phase flow (l-l) with resolved interfaces

Steep changes of physical quantities:

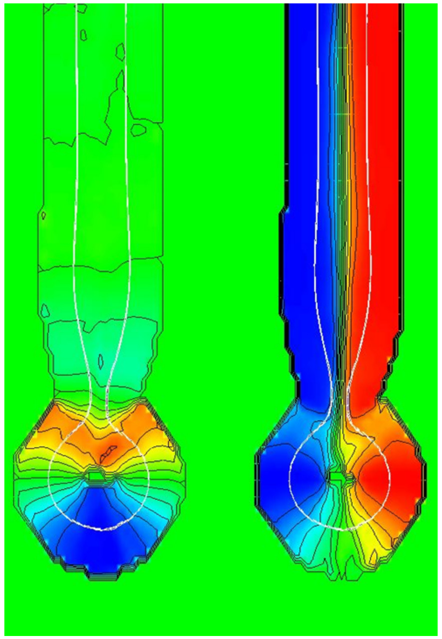
1) Elementwise averaging of the physical properties (prevents oscillations):
   $\rho_e = x\rho_1 + (1-x)\rho_2, \quad \mu_e = x\mu_1 + (1-x)\mu_2$ $\qquad$ *x* is the volume fraction
2) Flow part: Extension of nonlinear stabilization schemes (FCT, TVD, EO-FEM) for the momentum equation for LBB stable element pairs with discontinuous pressure (Q2/P1)
3) Interface tracking part with DG(1)-FEM: Flux limiters satisfying LED requirements



Two phase flow (l-l) with resolved interfaces

Reinitialization
- Mainly required in the vicinity of the interface
- How often to perform?
- Which realization to implement?
- Efficient parallelization (3D!)

Alternatives
- Brute force (introducing new points at the zero level set)
- Fast sweeping („advancing front“ upwind type formulas)
- Fast marching
- Algebraic Newton method
- **Hyperbolic PDE approach**
- many more…..



Globally defined normal vectors

Maintaining the signed distance function by PDE reinitialization

$$\frac{\partial \phi}{\partial \tau} + \mathbf{u} \cdot \nabla \phi = S(\phi) \qquad \mathbf{u} = S(\phi)\frac{\nabla \phi}{|\nabla \phi|} \quad \Leftrightarrow \quad |\nabla \phi| = 1$$

Problems:
- What to do with the sign function at the interface? (smoothing?)
- How to handle the underlying non-linearity?
- How often to perform? (expensive → steady state)

Two phase flow (l-l) with resolved interfaces

Fine-tuned reinitialization

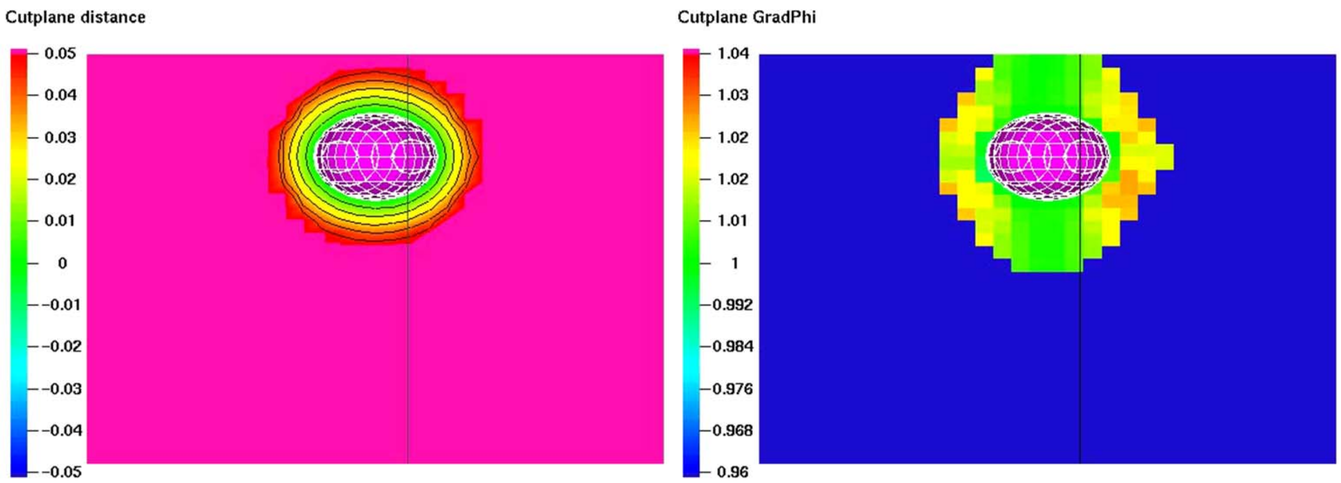
Our reinitialization is performed in combination of 2 ingredients:

1) Elements intersected by the interface are modified w.r.t. the slope of the distance distribution („Parolini trick“ for DG-P1) such that $|\nabla \phi| = 1$

2) Far field reinitialization: realization is based on the PDE approach („FBM“), but it does not require smoothening of the distance function!

In addition: continuous projection of the interface (smoothening of the discontinuous P_1 based distance function)

$$\phi_{P_1} \xrightarrow{L_2 \text{ projection}} \phi_{Q_1} \xrightarrow{L_2 \text{ projection}} \phi_{P_1}$$



Two phase flow (l-l) with resolved interfaces

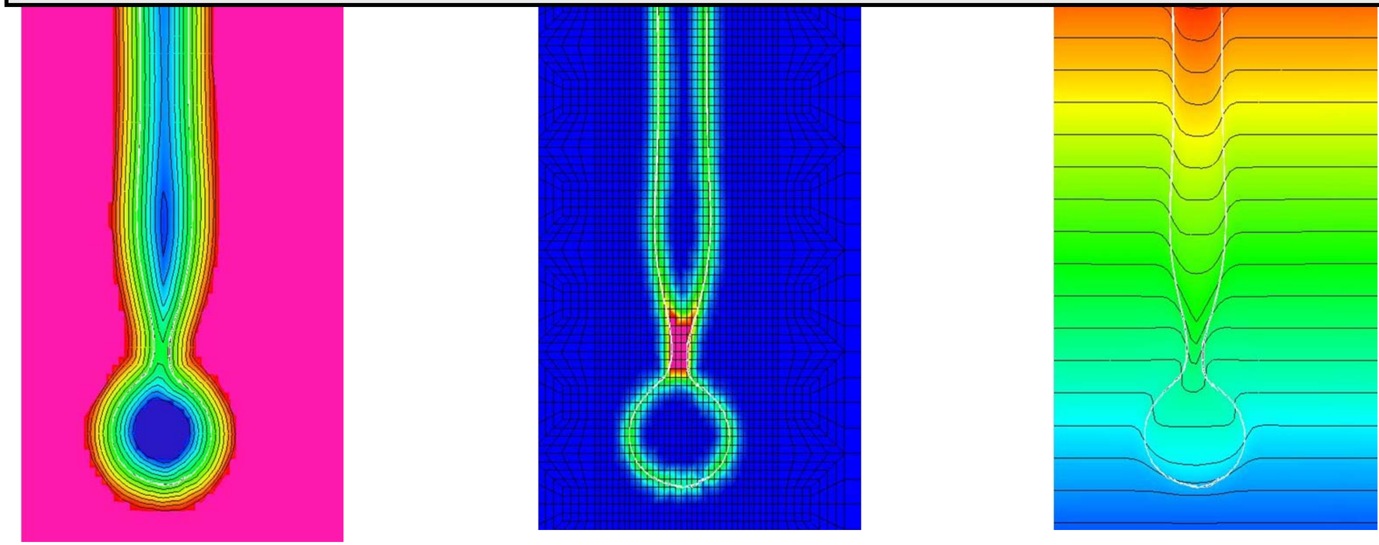
Continuum
Surface
Force

- Transformation of the surface integrals to volume integrals with the help of a <u>regularized</u> Dirac delta function δ
- Requires globally defined normals and curvature
- Reduction of spurious oscillations

$$\mathbf{f}_{\mathrm{ST}} = \sigma\kappa\mathbf{n}\delta(x,\varepsilon)$$

$$\mathbf{n}_{P_1} \xrightarrow{\mathrm{L}_2\text{ projection}} \mathbf{n}_{Q_1} \qquad \text{continuous normal field}$$

$$\kappa_{Q_1} = \frac{\int_\Omega \nabla\cdot\mathbf{n}_{Q_1}\,d\mathbf{x}}{\int_\Omega d\mathbf{x}} \qquad \text{continuous curvature field}$$



Level Set distribution

Distribution of the smoothed surface tension force $(\sigma\kappa\delta)_{Q_1}$

Resulting pressure distribution

Two phase flow (l-l) with resolved interfaces

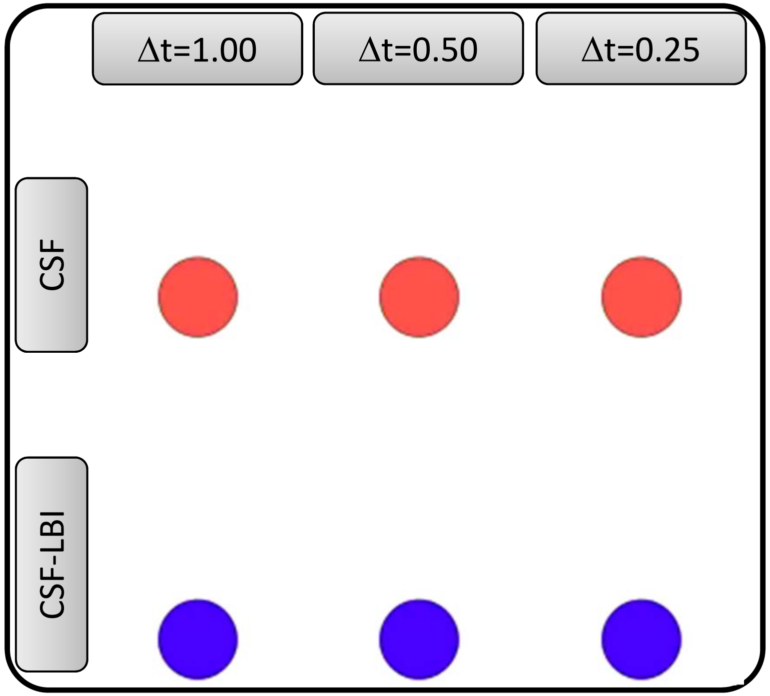
<u>Surface Tension</u>: Semi-implicit CSF formulation based on Laplace-Beltrami

$$\mathbf{f}_{\mathrm{ST}} = \int_\Omega \sigma \kappa \hat{\mathbf{n}} \cdot \mathbf{v}\, \delta(\Gamma, \mathbf{x})\, d\mathbf{x} \qquad = \int_\Omega \sigma \left(\underline{\Delta} \mathbf{x}|_\Gamma \right) \cdot \left(\mathbf{v}\, \delta(\Gamma, \mathbf{x}) \right) d\mathbf{x}$$

$$= -\int_\Omega \sigma \underline{\nabla} \mathbf{x}|_\Gamma \cdot \underline{\nabla} \left(\mathbf{v}\, \delta(\Gamma, \mathbf{x}) \right) d\mathbf{x} = -\int_\Omega \sigma \underline{\nabla} \mathbf{x}|_\Gamma \cdot \underline{\nabla} \mathbf{v}\, \delta(\Gamma, \mathbf{x})\, d\mathbf{x}$$

Application of the semi-implicit time integration yields $\quad \mathbf{x}|_{\Gamma^{n+1}} = \mathbf{x}|_{\Gamma^n} + \Delta t\, \mathbf{u}^{n+1}$

$$\Downarrow$$



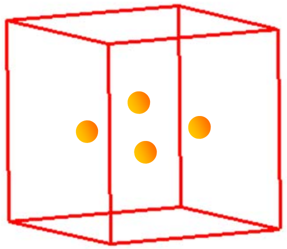
$$\mathbf{f}_{\mathrm{ST}} = -\int_\Omega \sigma\, \delta_\varepsilon \left(dist(\Gamma^n, \mathbf{x}) \right) \underline{\nabla} \tilde{\mathbf{x}}|_\Gamma^n \cdot \underline{\nabla} \mathbf{v}\, d\mathbf{x}$$

$$- \Delta t^{n+1} \int_\Omega \sigma\, \delta_\varepsilon \left(dist(\Gamma^n, \mathbf{x}) \right) \underline{\nabla} \mathbf{u}^{n+1} \cdot \underline{\nabla} \mathbf{v}\, d\mathbf{x}$$

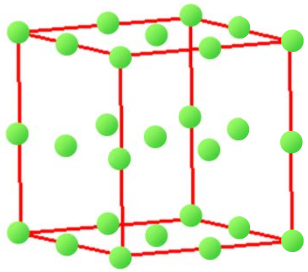
Advantages
- Relaxes *Capillary Time Step* restriction
- „Optimal“ for FEM-Level Set approach due to global information

Data Layout for Q2/P1 FEM

1 cell/4 dofs

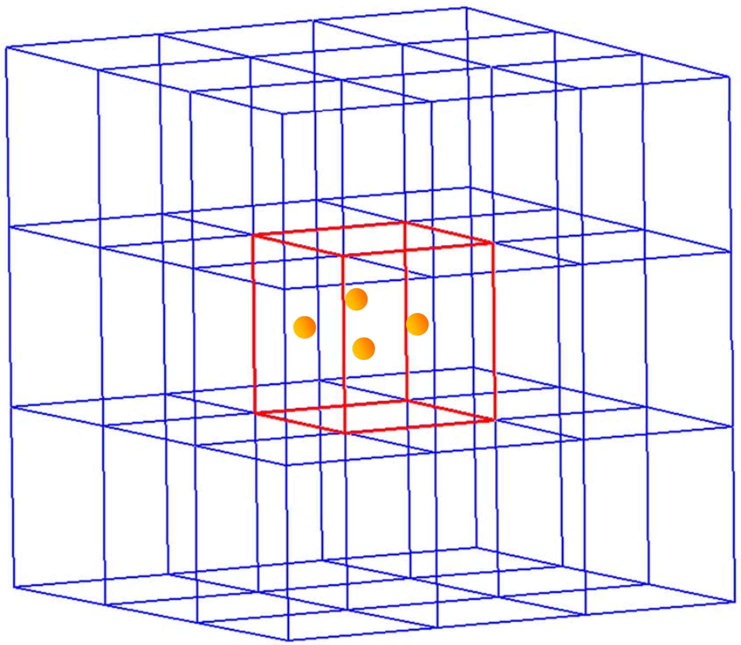


1 cell/27 dofs



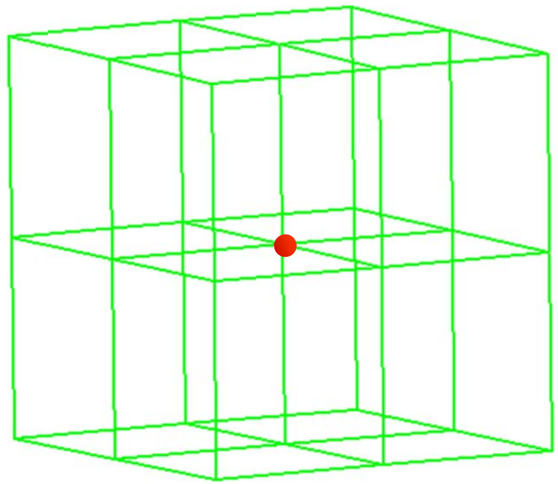
P_1 – stencil

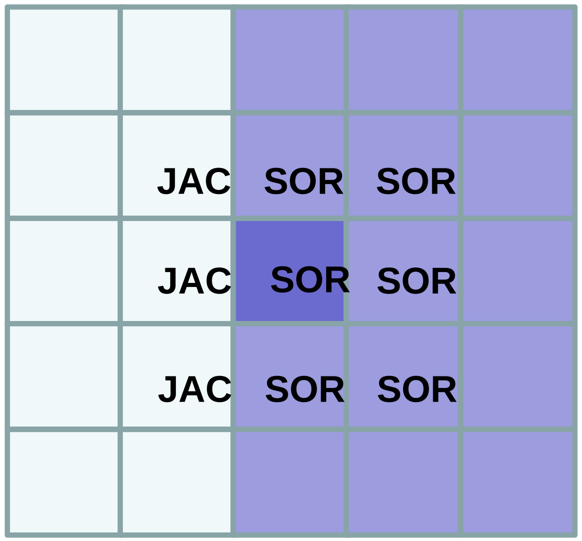
27 cells/108 (4x27) dofs



Q_2 – stencil

8 cells/125 (5x5x5) dofs





Numerical Analysis of the Multigrid Solvers

dt = 0.001 | nOfSmstepP(SOR) = 8,F,rlx = 1.0 | nOfSmstepV(SOR+JAC) = 4,V,rlx = 0.5

Level	# MG steps P	MG rates P	# NonLin/MG steps V	MG rates V
2	2.4	0.0425	2/1	3.6e-4
3	3.7	0.1324	2/1	1.3e-3
4	3.0	0.0947	2/1	2.2e-3

dt = 0.010 | nOfSmstepP(SOR) = 8,F, rlx = 1.0 | nOfSmstepV(SOR+JAC) = 4,V,rlx = 0.5

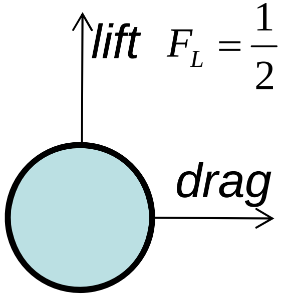
Level	# MG steps P	MG rates P	# NonLin/MG steps V	MG rates V
2	2.2	0.0330	2/1	1.3e-3
3	3.9	0.1439	2/1	6.4e-3
4	3.2	0.1064	2/1	8.5e-3

Convergence criterions	LinearDefectReductionP=1e-3	NonLinearDefectReductionV=1e-4 LinearDefectReductionV=1e-1

Benchmarking

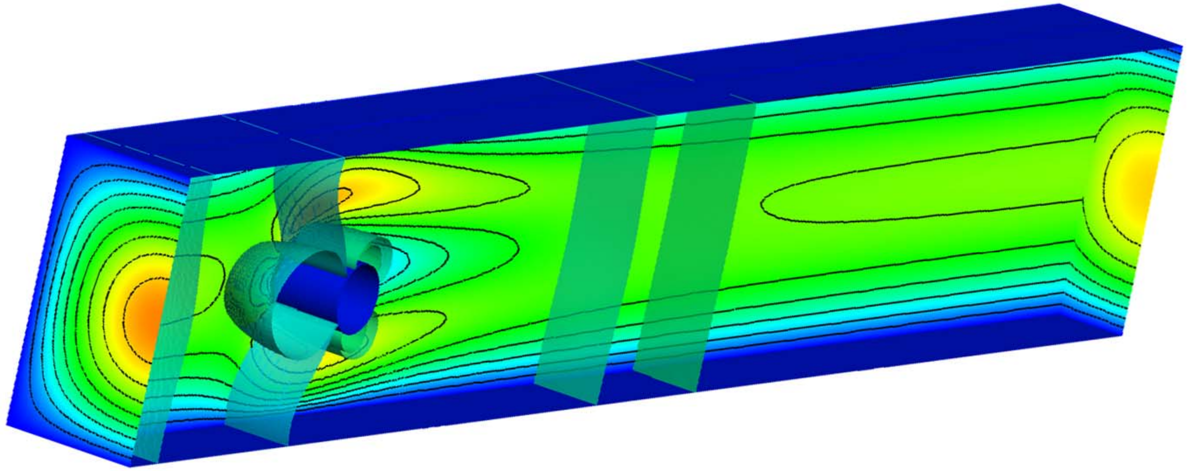
Flow Simulation with CFD software available on the market

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



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

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

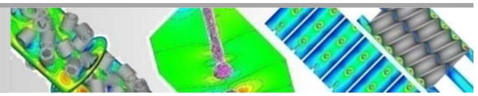


- Comparison of CFX 12.0, **OpenFoam 1.6** and **FeatFlow**
- Drag and lift coefficients behave very sensitive to mesh resolution

→ Ideal indicator for computational accuracy

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

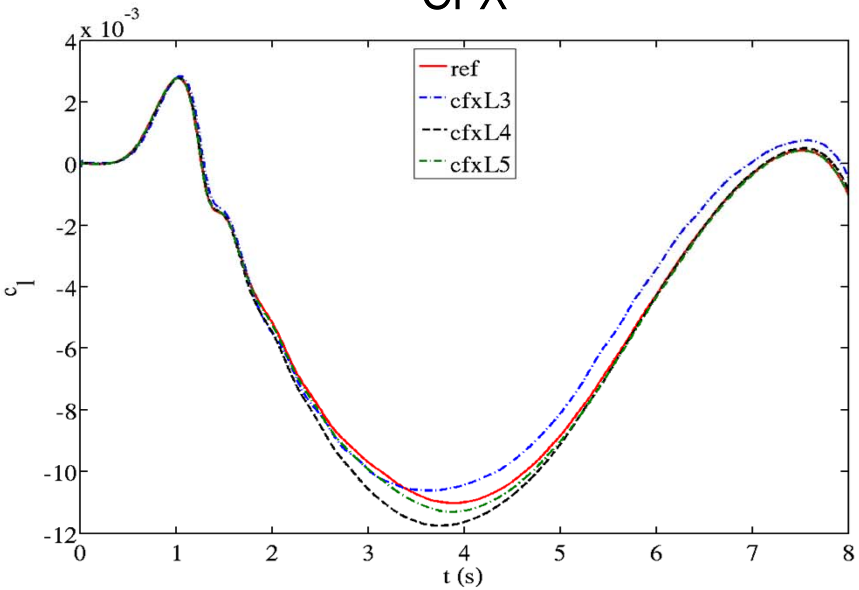
Mesh Level	**# Elements**
L2	6,144
L3	49,152
L4	393,216
L5	3,145,728



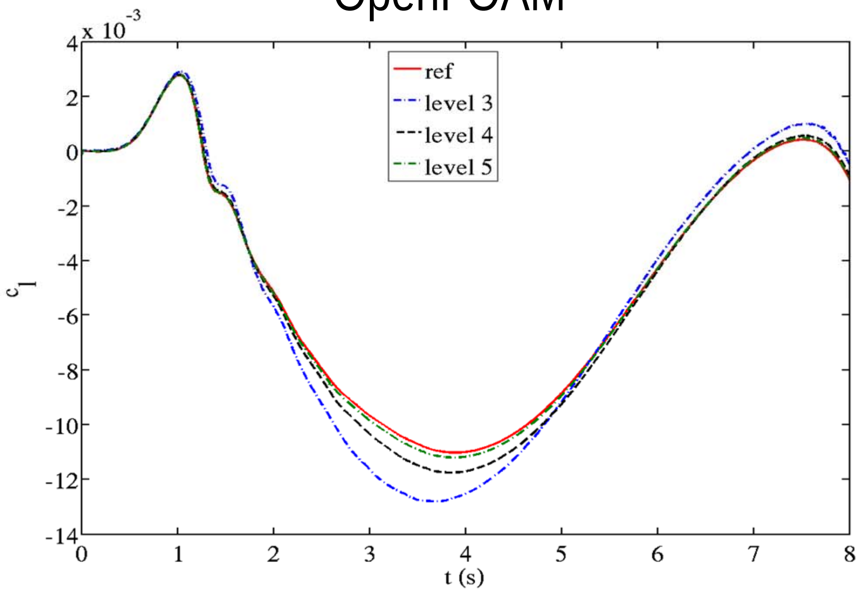
Benchmarking

Flow Simulation with CFD software available on the market

CFX



OpenFOAM



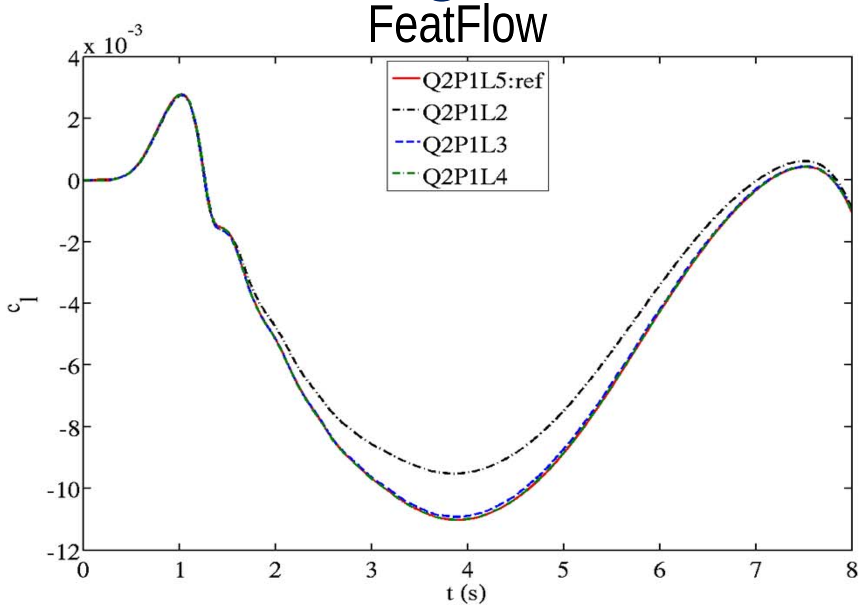
Case	L2 error		timing
	c_D	c_L	
CFX L3	0.0152	0.0781	13420
CFX L4	0.0098	0.0631	4 x 58680
CFX L5	0.0029	0.0224	8 x 205600

Case	L2 error		Timing
	c_D	c_L	
OF L3	0.0261	0.1449	5180
OF L4	0.0067	0.0591	4 x 19500
OF L5	0.0016	0.0147	8 x 595200

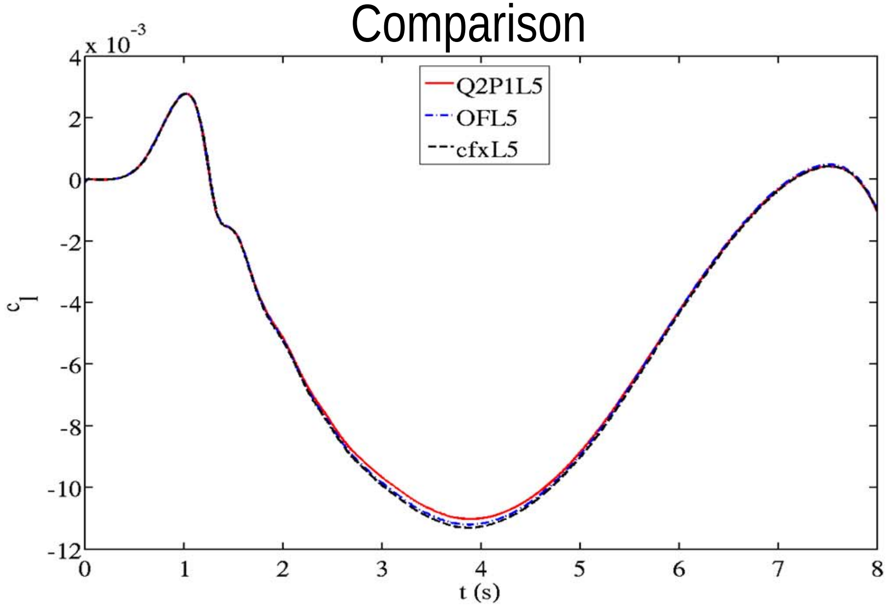
Benchmarking

Flow Simulation with FeatFlow

FeatFlow



Comparison



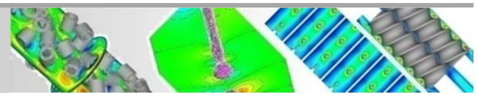
Case	L2 error		Timing
	c_D	c_L	
FF L2	0.0209	0.1378	2 x 5000
FF L3	0.0029	0.0109	3 x 25000
FF L4	0.0005	0.0015	20 x 32000
FF L5	(ref)	(ref)	23 x 242000

Case	L2 error		timing
	c_D	c_L	
FF L3	0.0029	0.0109	3 x 25000
OF L5	0.0016	0.0147	8 x 595200
CFX L5	0.0029	0.0224	8 x 205600

Less than 2 hours sim. time with adaptive time stepping on 3+1 processors

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

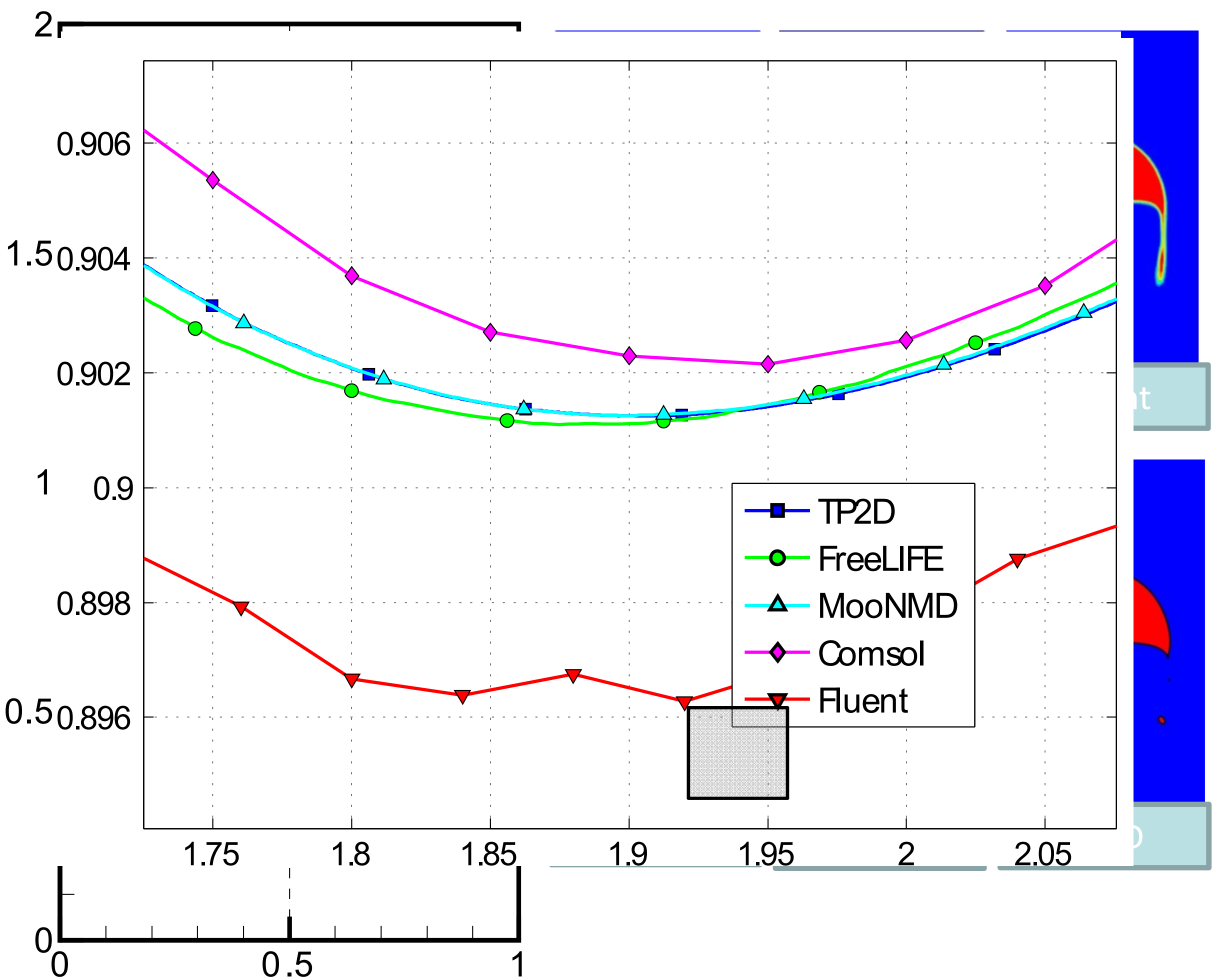
→ High order Q2/P1 FEM + (parallel) Multigrid Solver



Benchmarking

2D Bubble Benchmarks

http://www.featflow.de/beta/en/benchmarks/



Benchmark quantities

Center of mass $\mathbf{x}_c = \dfrac{\int_{\Omega_2} \mathbf{x}\, dx}{\int_{\Omega_2} 1\, dx}$

Mean rise velocity $\mathbf{U}_c = \dfrac{\int_{\Omega_2} \mathbf{u}\, dx}{\int_{\Omega_2} 1\, dx}$

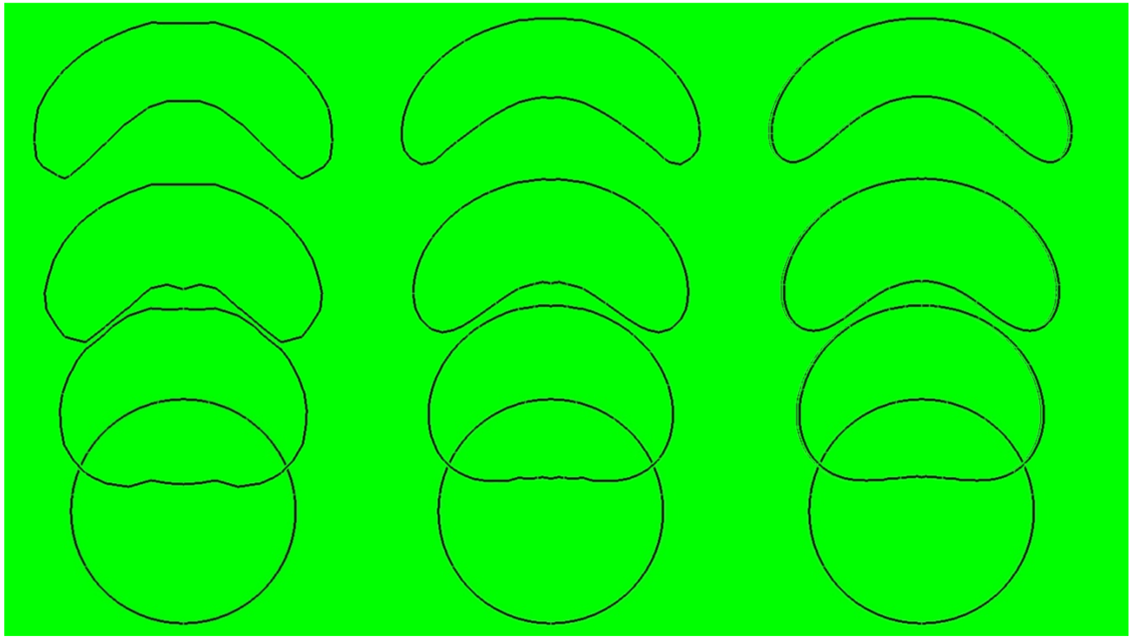
Circularity $¢ = \dfrac{P_a}{P_b} = \dfrac{\pi d_a}{P_b}$

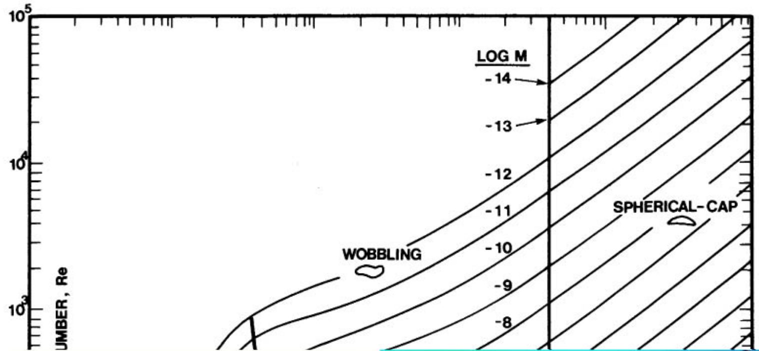
Hysing, S.; Turek, S.; Kuzmin, D.; Parolini, N.; Burman, E.; Ganesan, S.; Tobiska, L.: Quantitative benchmark computations of two-dimensional bubble dynamics, International Journal for Numerical Methods in Fluids, 2009

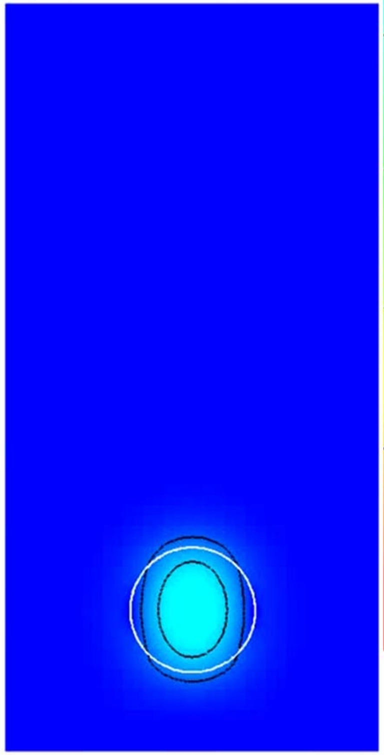
3D convergence analysis for large density jumps

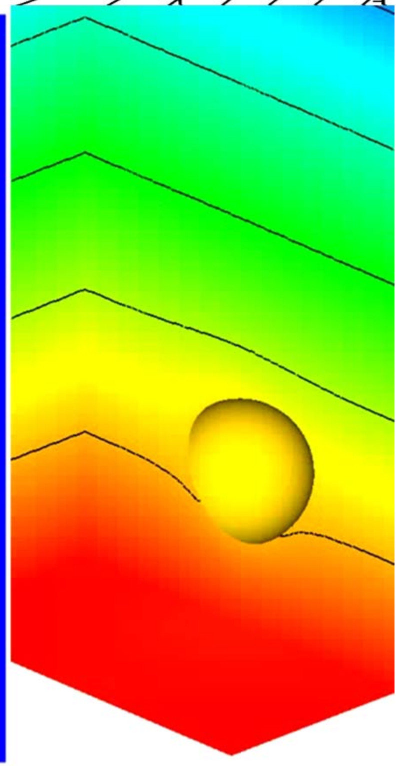
Rising bubble problem for Eo = 60, Re = 34
Density jump 1:100

Level 2 Level 3 Level 4









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

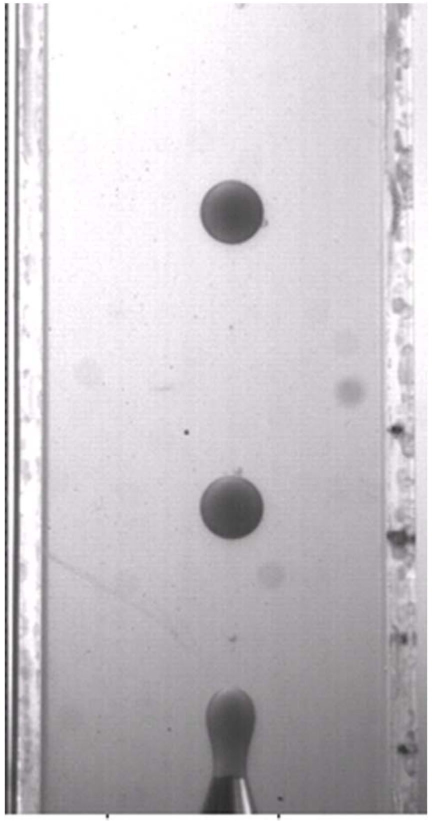
$\mu_C = 500\, mPa\, s$

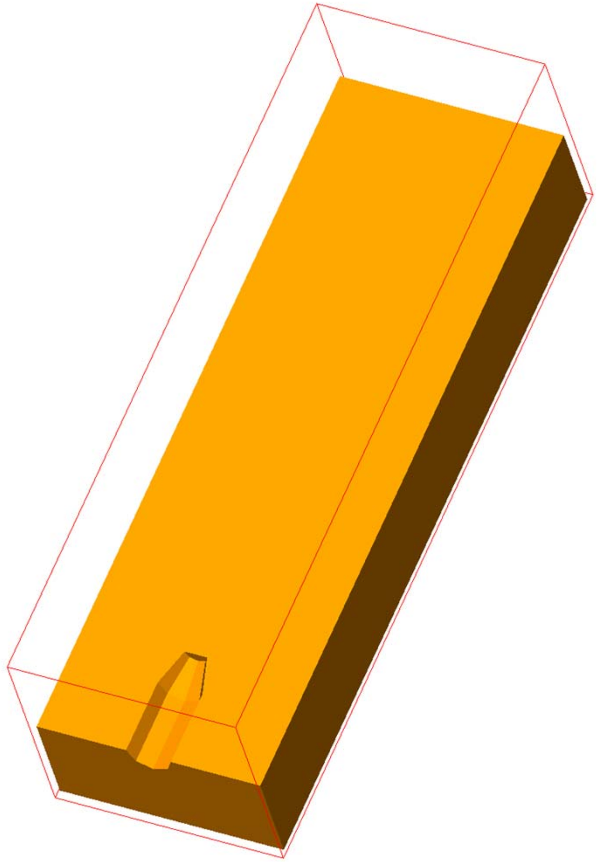
$\rho_C = 1340\, kg\, m^{-3}$

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

Dispersed phase:

Experimental setup with **AG Walzel** **(BCI/Dortmund)**

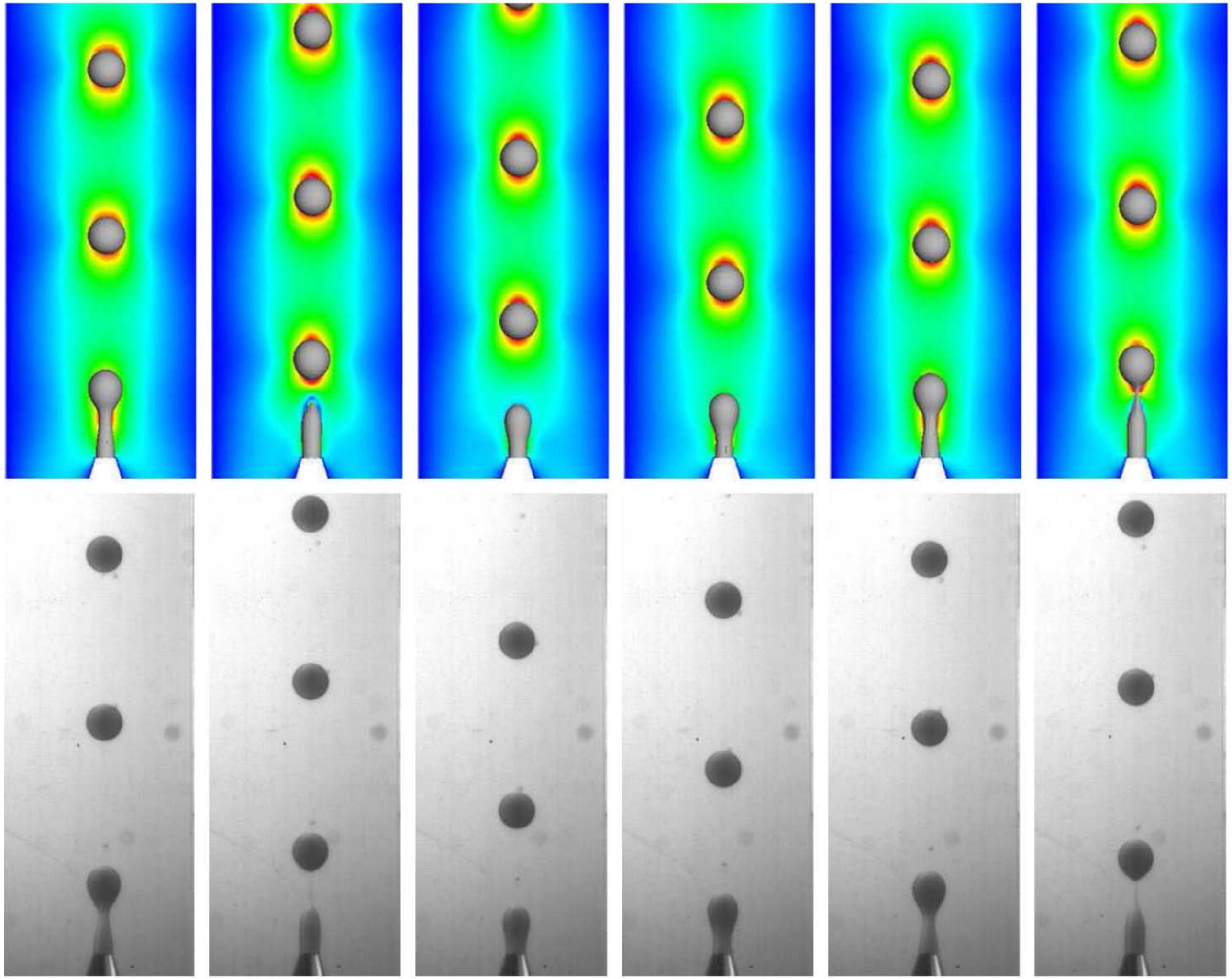


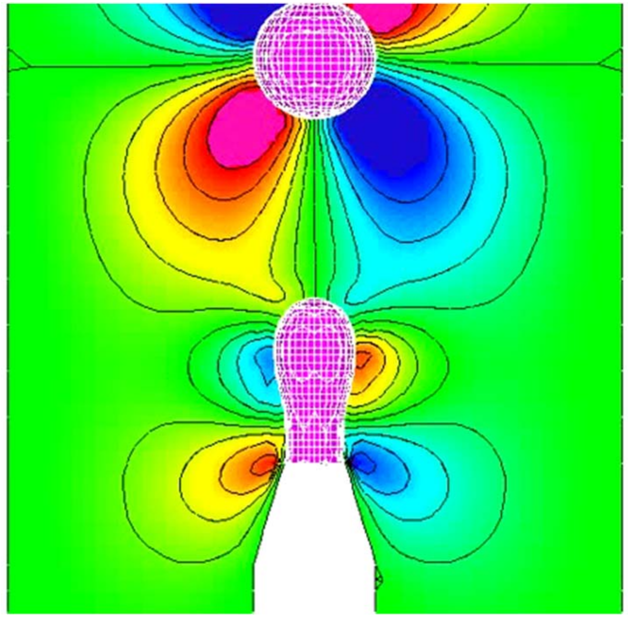


Validation parameters:

- 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

Tailored monodisperse droplets via modulation

In case of monodisperse droplet generation:

$$\dot{V}_D = f V_{\text{droplet}}$$

Influencable variables

On the level of the process:

- Flowrates
- Modulation frequency
- Modulation amplitude

Geometrical changes:

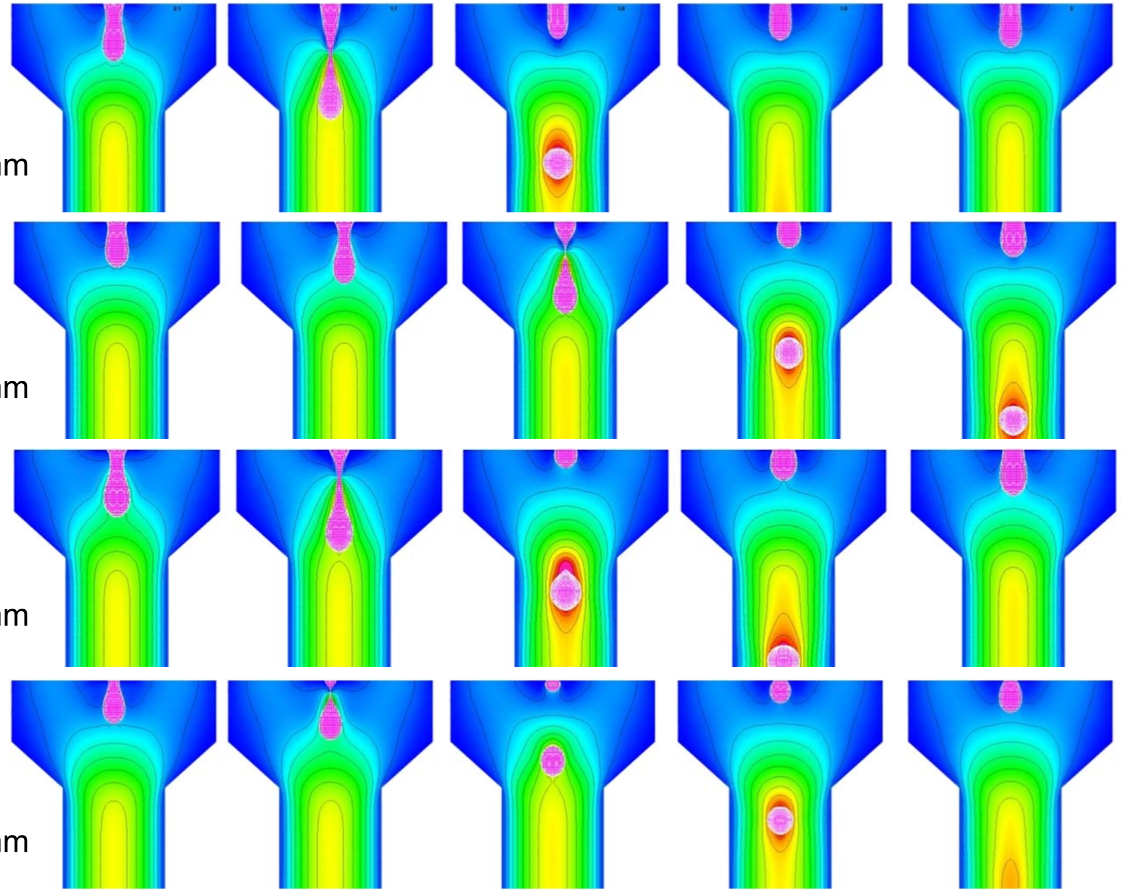
- Capillary size
- Contraction angle
- Contraction ratio

No Regulation
Flowrate: 100%
Capillary: STD
Droplet size: 5.2mm

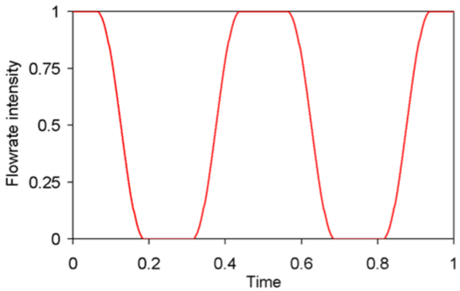
Regulated
Flowrate: 100%
Capillary: STD
Droplet size: 5.0mm

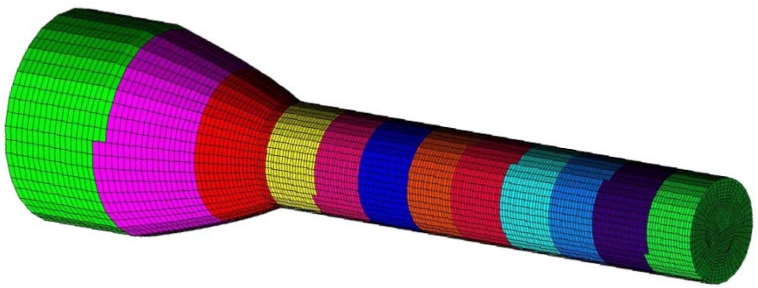
Regulated
Flowrate: 150%
Capillary: STD
Droplet size: 5.7mm

Regulated
Flowrate: 75%
Capillary: STD
Droplet size: 4.5mm



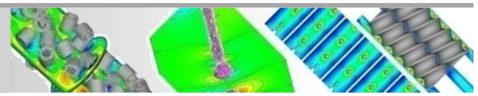
Modulation function



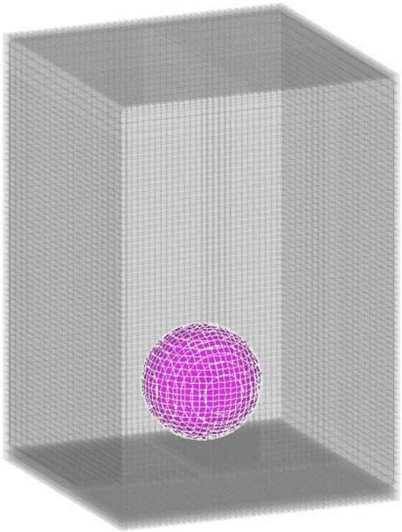


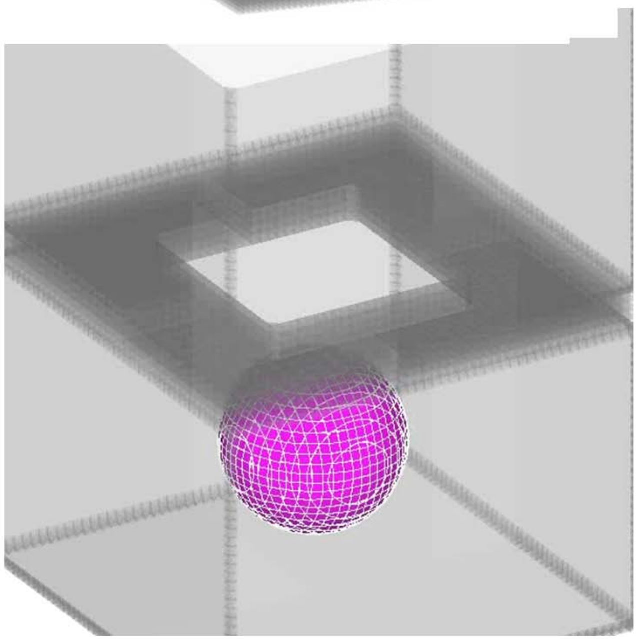
Resulting operation envelope:

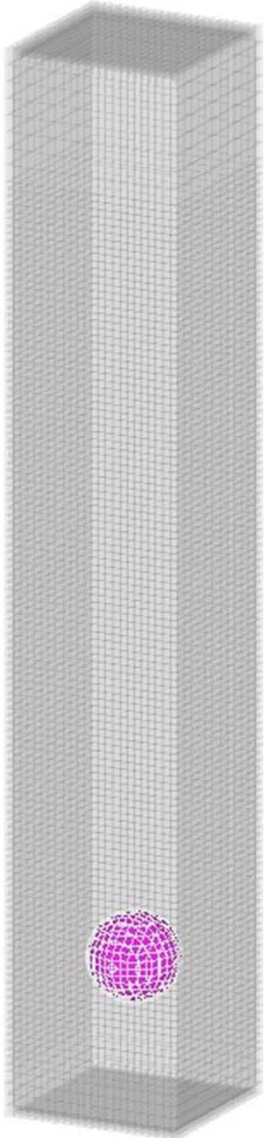
- Size: 4.5 mm – 5.7 mm
- Volume: 0.38 cm^3 – 0.77 cm^3

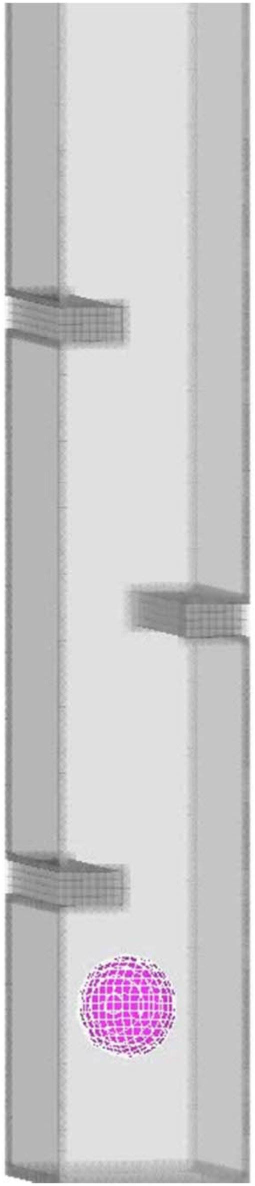


Preliminary Studies: Coupling FBM-LSFEM









Next Steps for Multiphase Flow

- Adaptive time stepping + adaptive grid alignment/ALE.
- Coupling with turbulence models.
- Coupling with rigid particles.
- Analysis of viscoelastic effects.
- Benchmarking and experimental validation for many particles/bubbles.