Numerical Simulation of Monodisperse Droplet Generation in Nozzles

DFG – SPP 1423 „Prozess-Spray“

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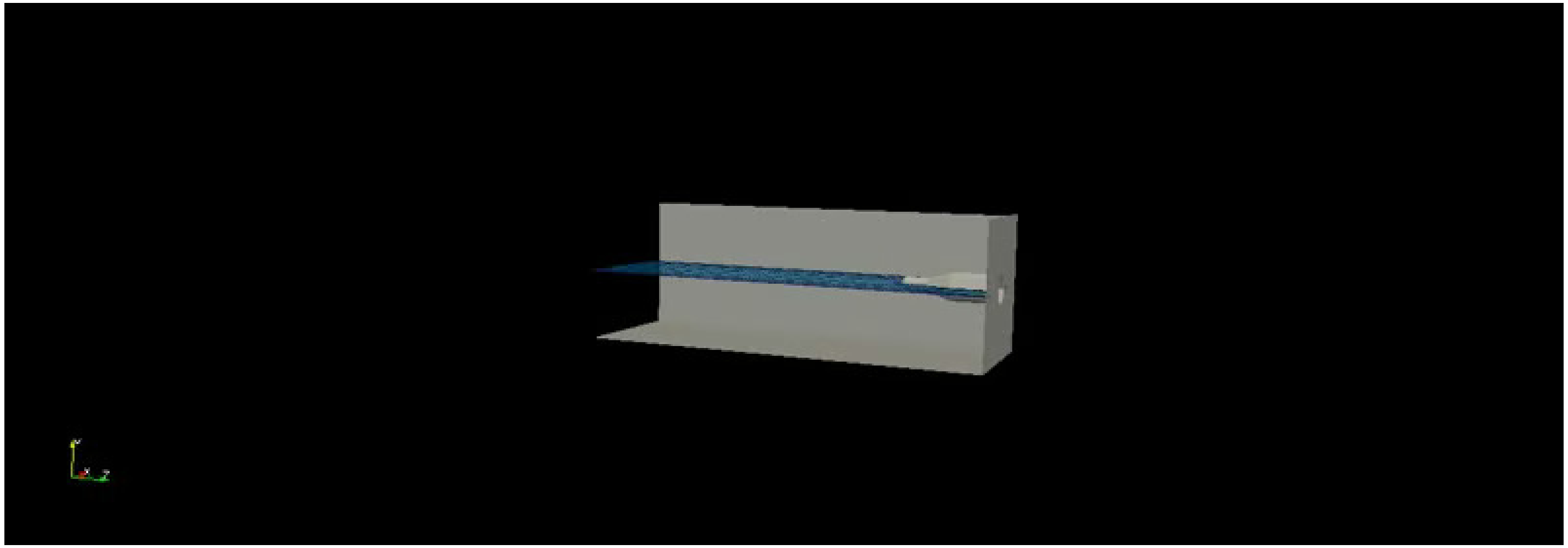
Motivation

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

Specific Application: droplet generation in pneumatic jets

Problem: The results (dispersity, droplet generation frequency, stream length) are due to many parameters, i.e., density (ratio), viscosity (ratio), rheological behaviour, surface tension, flow conditions,…



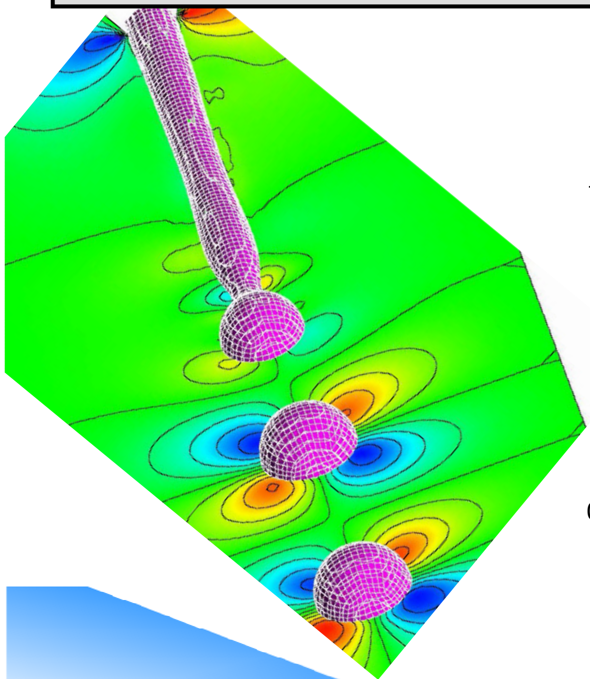
Methods

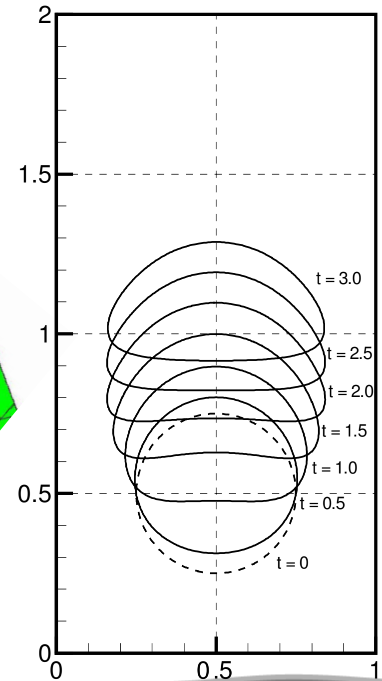
- Mass conservative FEM levelset approach with „exact“ interphase reconstruction. Implicit treatment of the surface tension force term

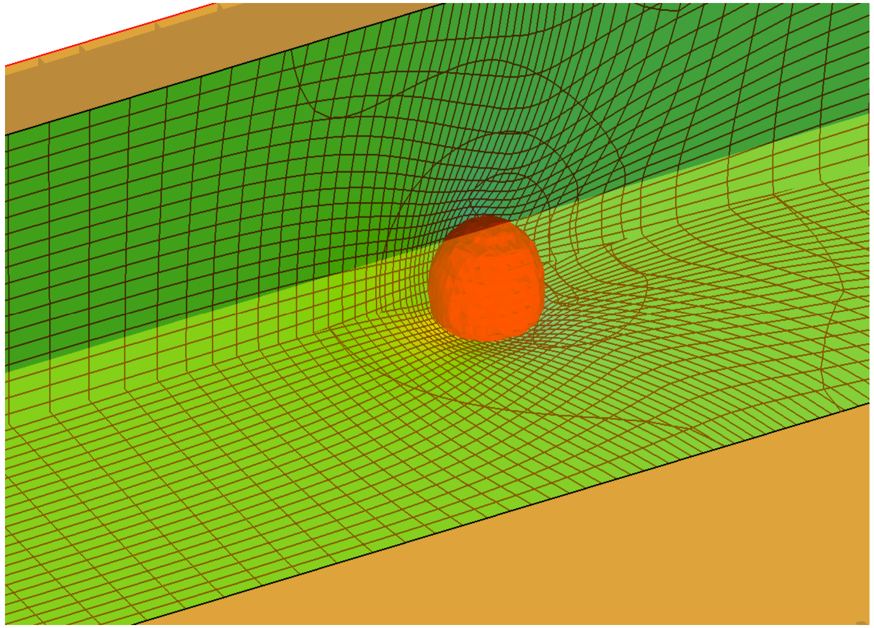
- Fast solvers (parallel multigrid) for scalar equations and for the Pressure-Poisson equation supporting large density jumps

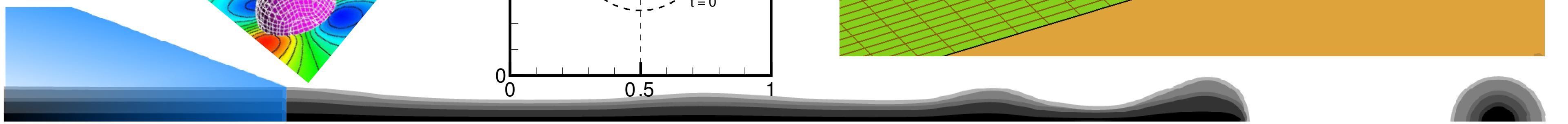
- Systematic validation and benchmarking (CFX, FEMLAB, FLUENT).

- Incorporation of adaptive grid deformation techniques (ALE approach)









Governing Equations

The incompressible Navier Stokes equation

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

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

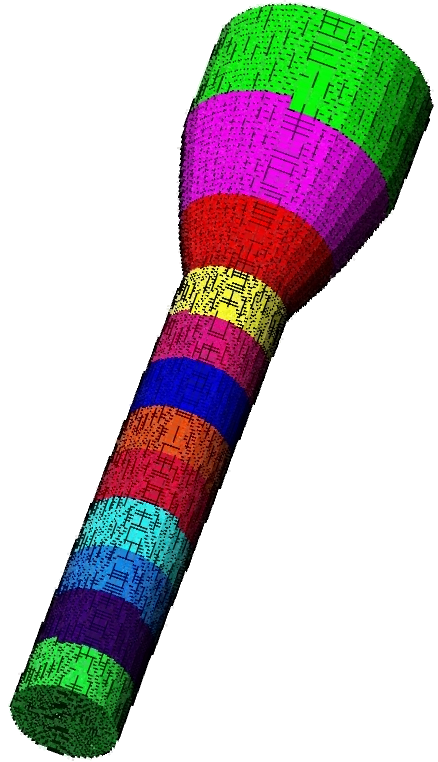
Interphase tension force

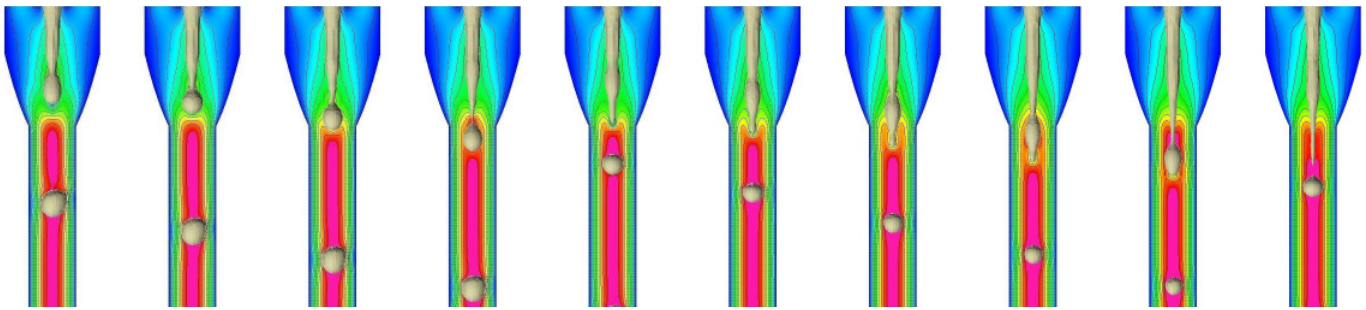
$$\mathbf{f}_{ST}=\sigma\kappa\mathbf{n},\quad \kappa=-\nabla\cdot\mathbf{n}\quad \text{on}\quad \Gamma$$

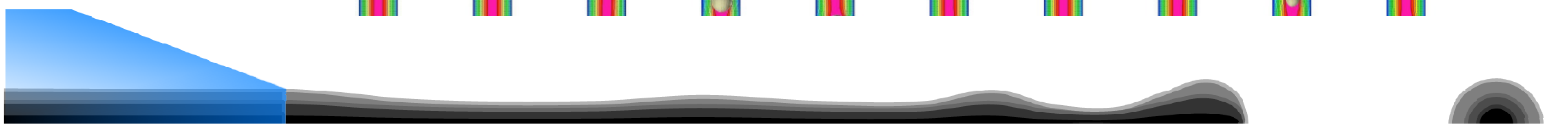
unknown interphase location

Dependency of physical quantities

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



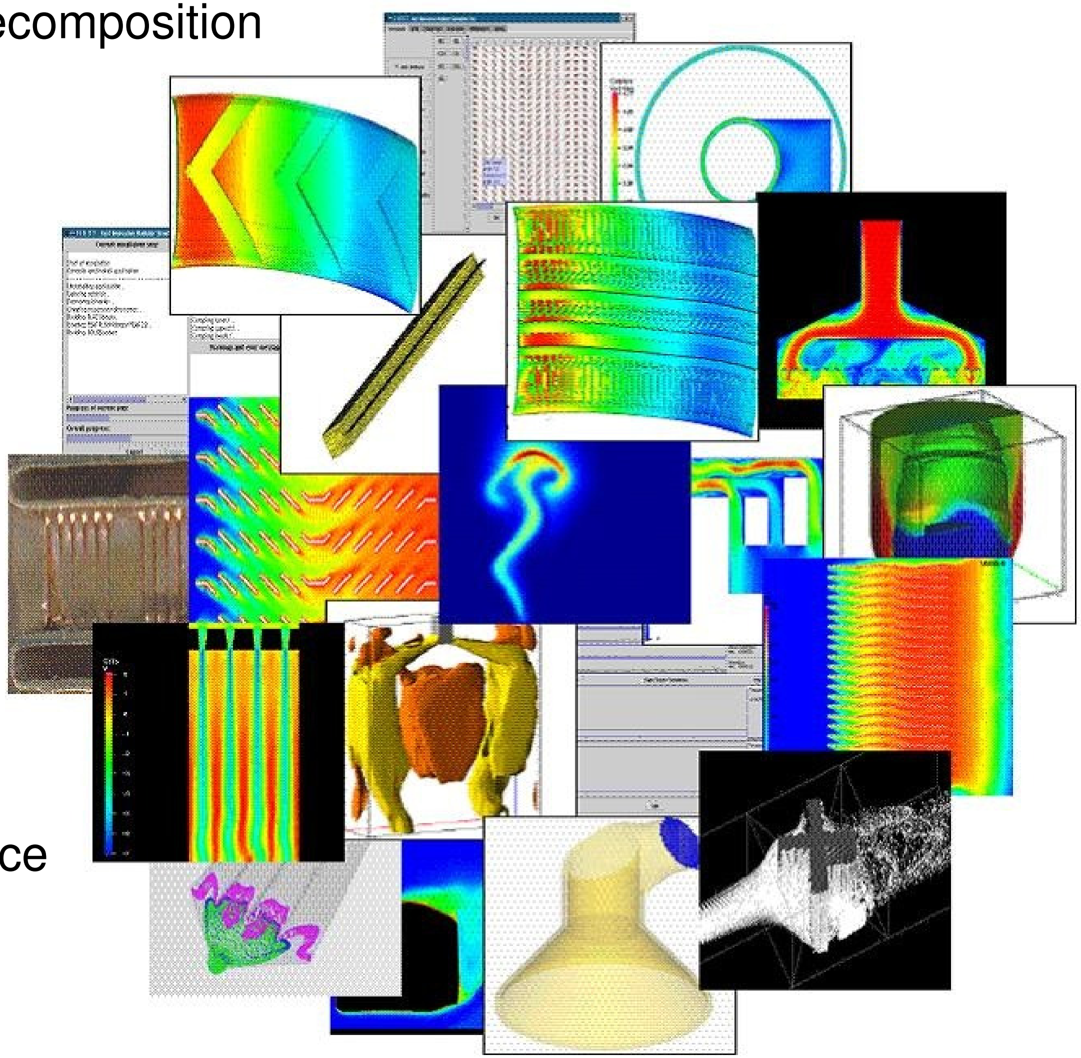




Efficient Flow Solver

Main features of the FeatFlow approach:

- Parallelization based on domain decomposition
- High order discretization schemes
- Use of unstructured meshes
- Newton-Multigrid solvers
- FCT & EO stabilization techniques
- Adaptive grid deformation



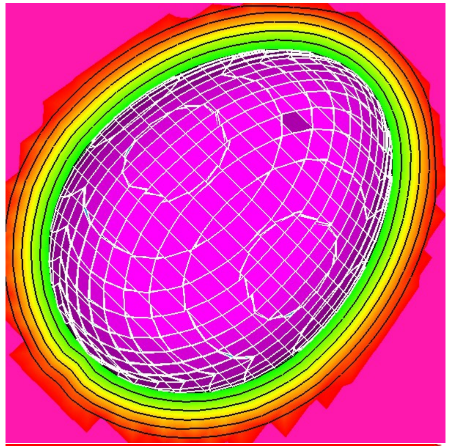
Discretization:

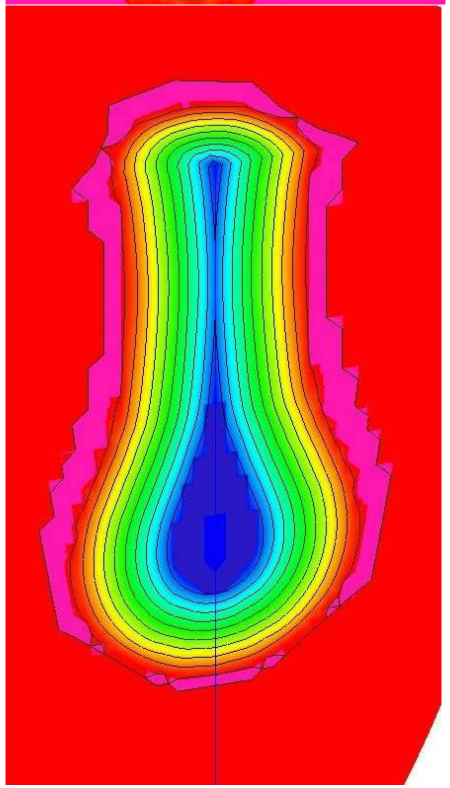
- Navier-Stokes: FEM Q_2/Q_1 in space
- Level Set: DG-FEM P_1
- Crank-Nicholson scheme in time

Efficient Interphase Capturing

Level Set Method (→“smooth“ distance function)

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





Benefits:

- Provides an accurate representation of the interphase
- Provides other auxiliary quantities (normal, curvature)
- Allows topology changes
- Treatment of viscosity, density and surface tension without explicit representation of the interphase
- Adaptive grid advantageous, but not necessary

Problems:

- It is not conservative → mass loss
- Needs to be reinitialized to maintain its distance property
- Higher order discretization: possible, but necessary?

Problems and Challenges

- **Steep gradients** of the velocity field and of other physical quantities near the interphase (oscillations!)

- **Reinitialization** (smoothed sign function, artificial movement of the interphase ($\rightarrow$ mass loss), how often to perform?)

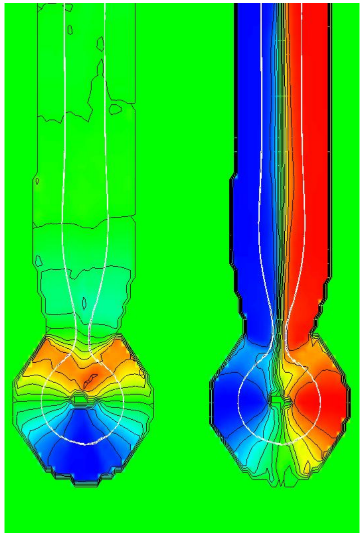
- **Mass conservation** (during advection and reinitialization of the Level Set function)

- Representation of **interphacial tension**: CSF, Line Integral, Laplace-Beltrami, Phasefield, *etc.*

- **Explicit** or **implicit** treatment ($\rightarrow$ *Capillary Time Step* restriction?)

Reinitialisation

<u>Alternatives</u>
- Brute force (introducing new points at the zero level surfaces)
- Fast sweeping (applying „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 interphase? (smoothing?)
- How often to perform? (expensive → steady state)

Fine-tuned reinitialisation

Our reinitialization is performed in combination of 2 ingredients:

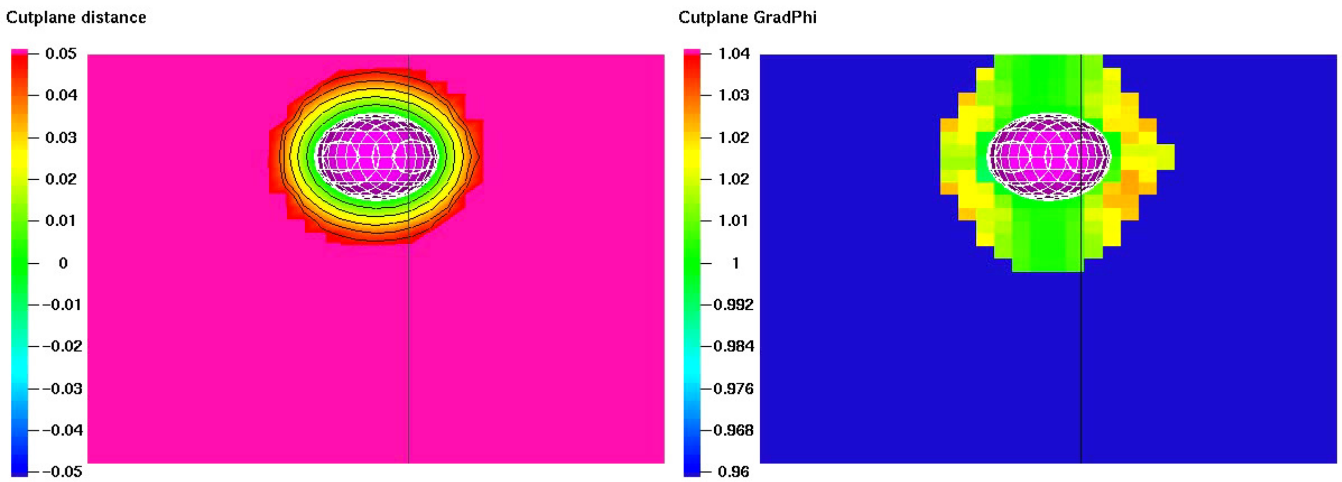
1) Elements intersected by the interphase are modified w.r.t. the slope of the distance distribution („Parolini trick") such that

$$\left|\nabla \phi\right| = 1$$

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 interphase (smoothening of the discontinuous P_1 based distance function)

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



Treatment of surface tension

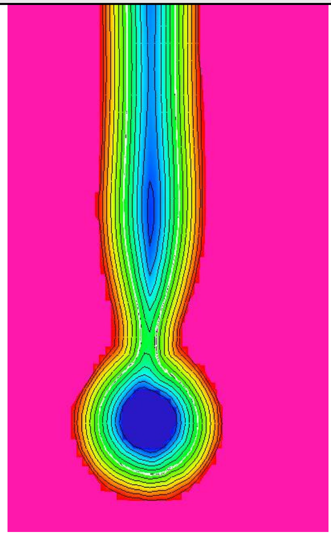
Continuum
Surface
Force

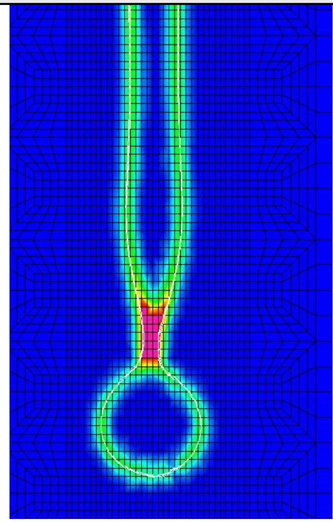
- Transformation of the surface integrals to volume integrals with the help of a <u>regularized</u> Dirac delta function δ
- Requires globally defined normals and curvature
- Reduction of spurious oscillations

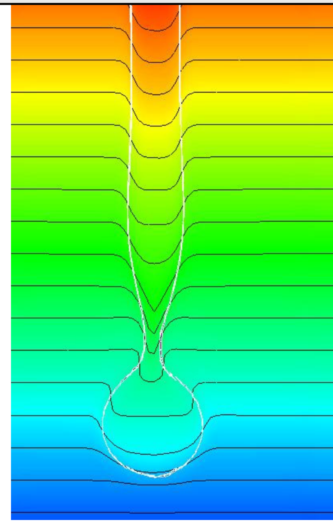
$$\mathbf{n}_{P_1} \xrightarrow{\mathrm{L}_2\ \text{projection}} \mathbf{n}_{Q_1}$$ continuous normal field

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

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


Level Set distribution

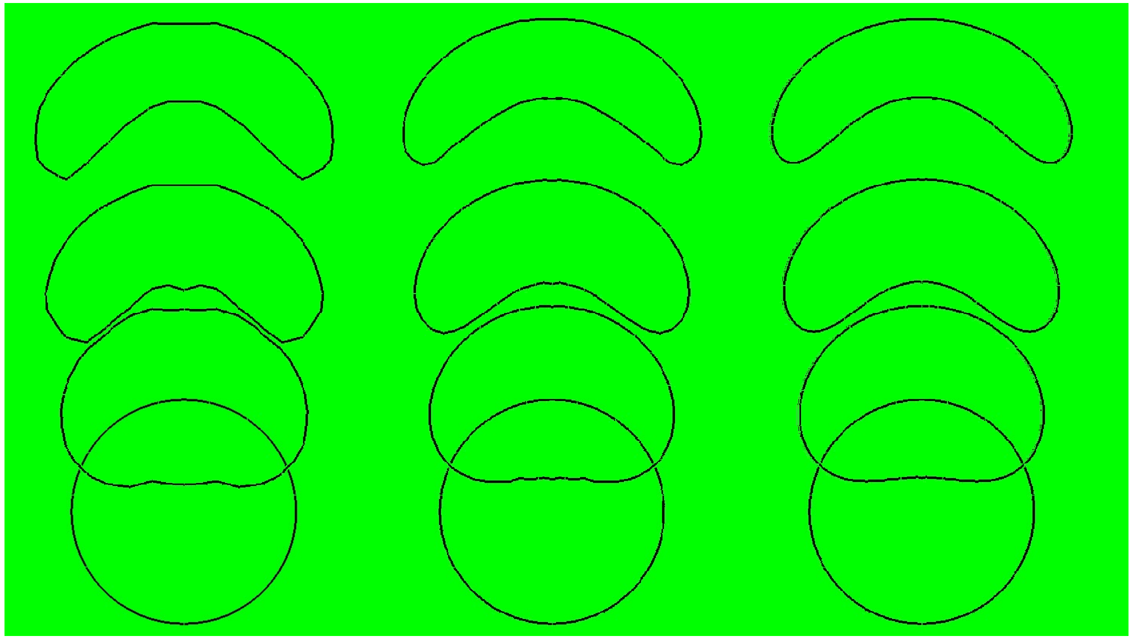

Distribution of the smoothed interphacial tension force $(\sigma\kappa\delta)_{Q_1}$

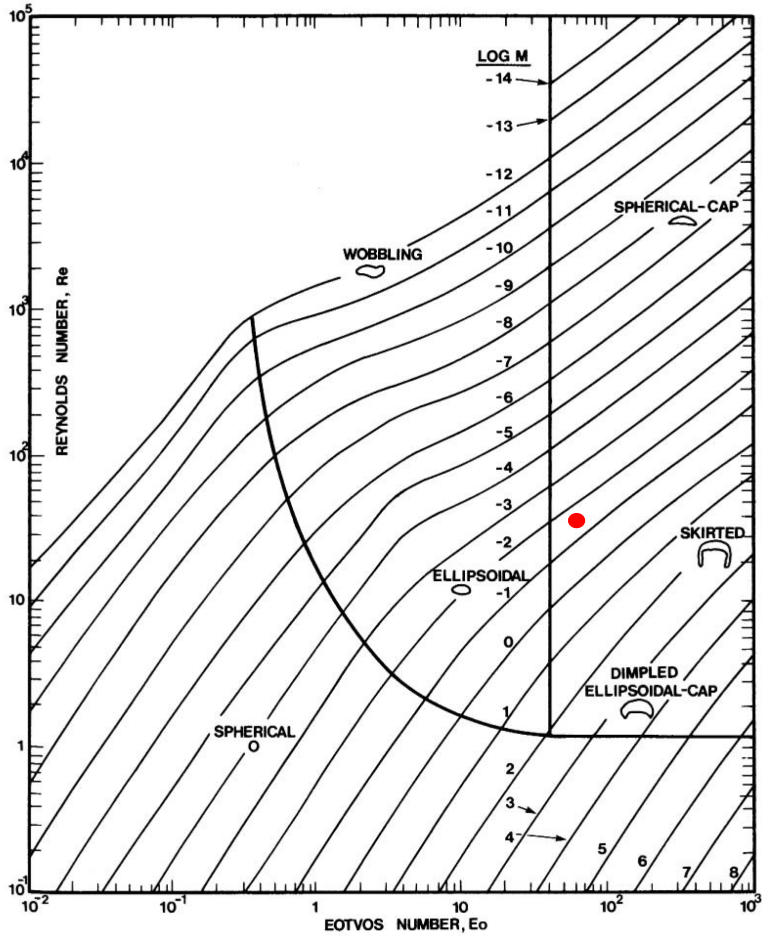

Resulting pressure distribution

Convergence analysis for density jumps

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

Level 2 Level 3 Level 4





Validation and benchmarking

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

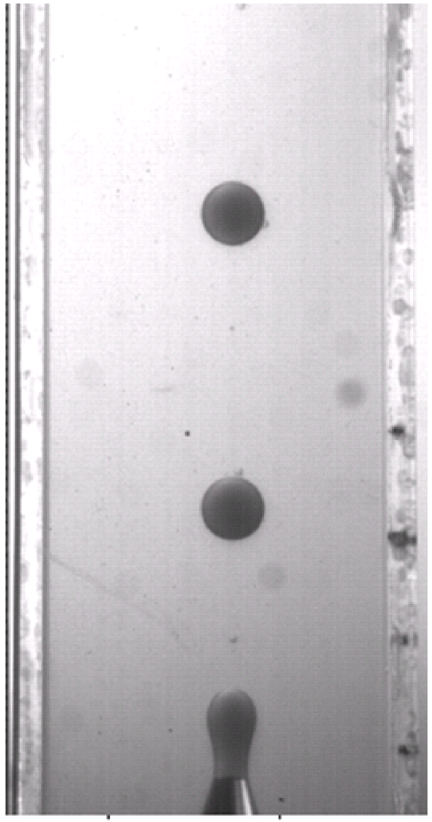
$\mu_C = 500\, mPa\, s$

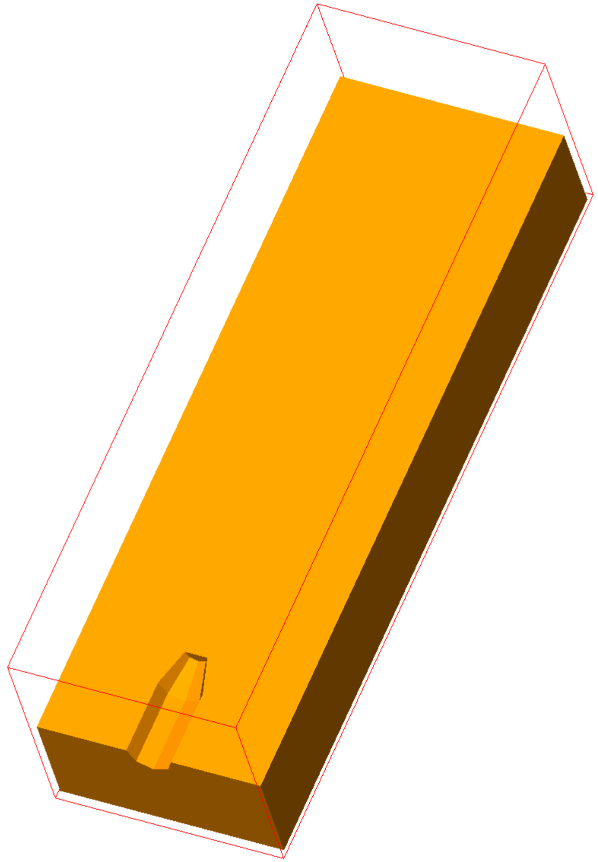
$\rho_C = 1340\; kg\, m^{-3}$

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

Dispersed phase:

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

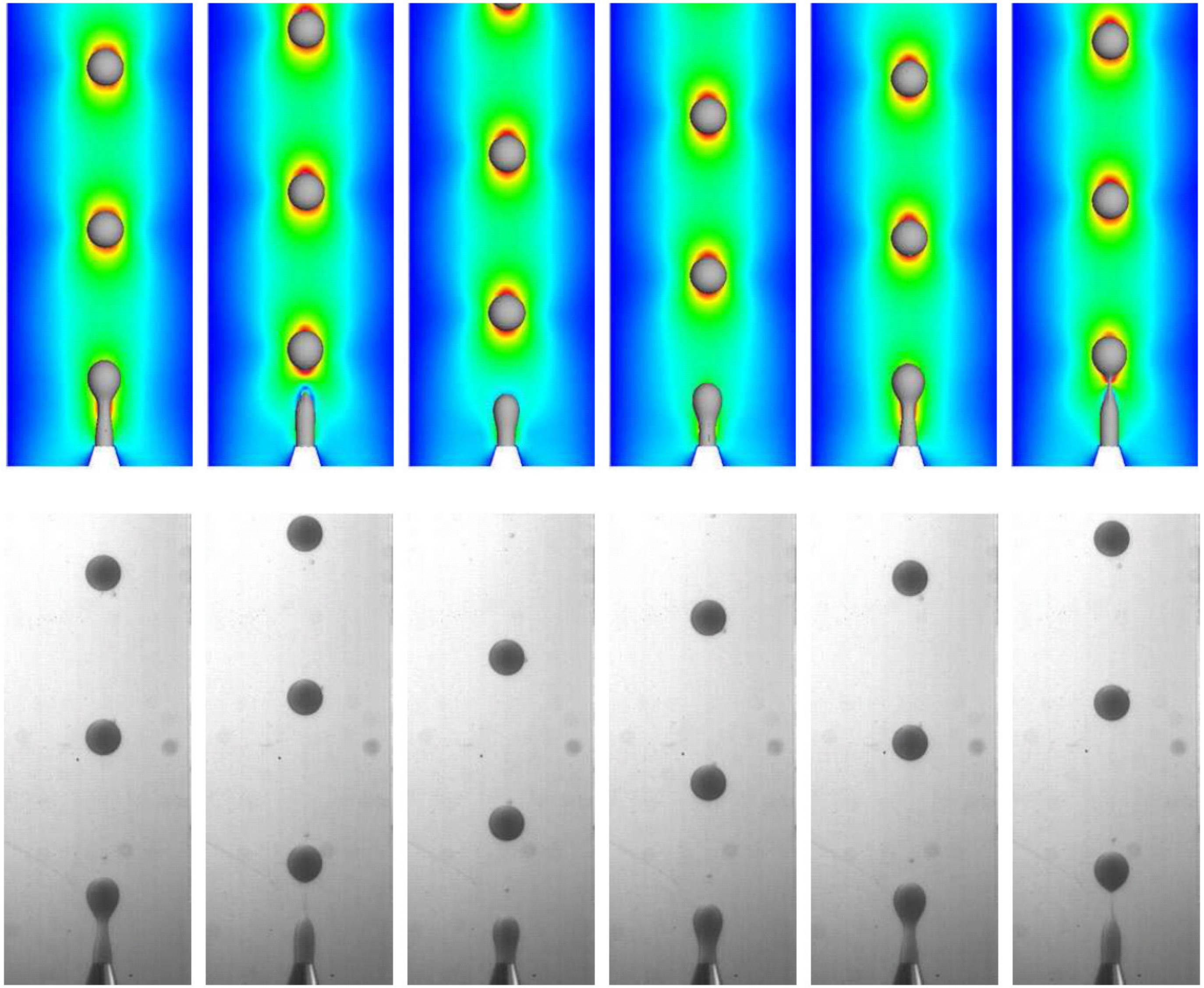




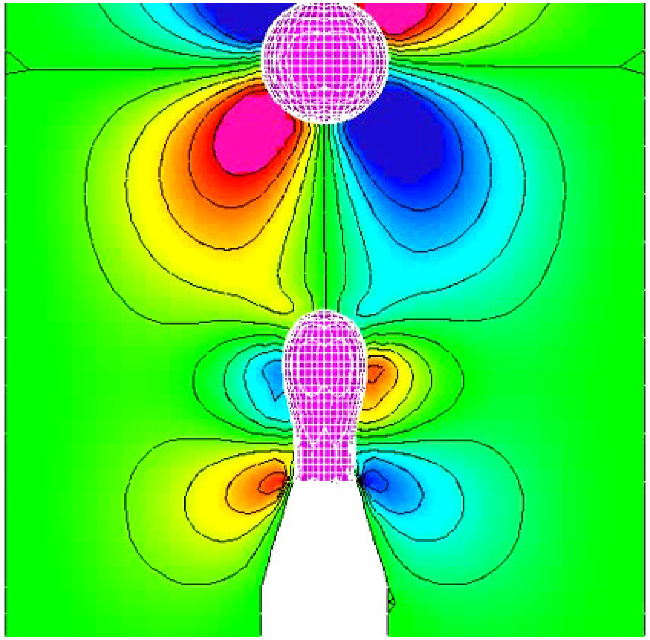
Validation parameters:

- frequency of droplet generation
- droplet size
- stream length

Benchmarking of the dripping mode

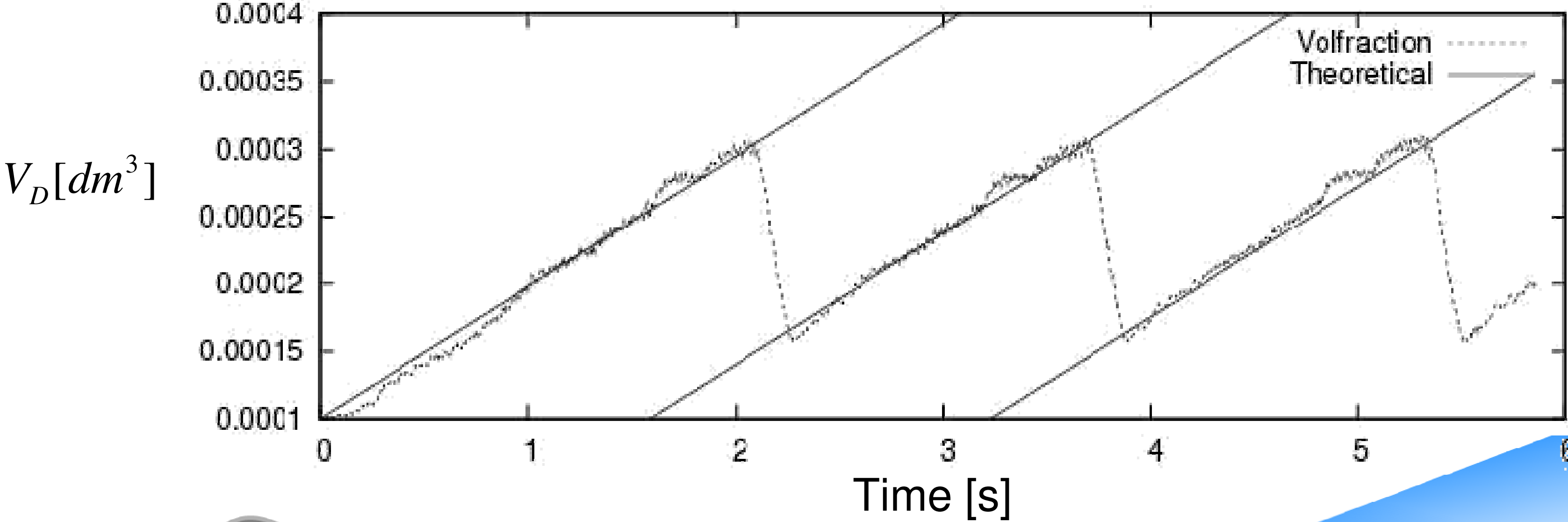


Benchmarking of the dripping mode



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

Accumulated volume of the dispersed phase in time



Jetting mode extension

Continuous phase:

Glucose-Water mixture

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

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

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

Silicon oil

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Dispersed phase:

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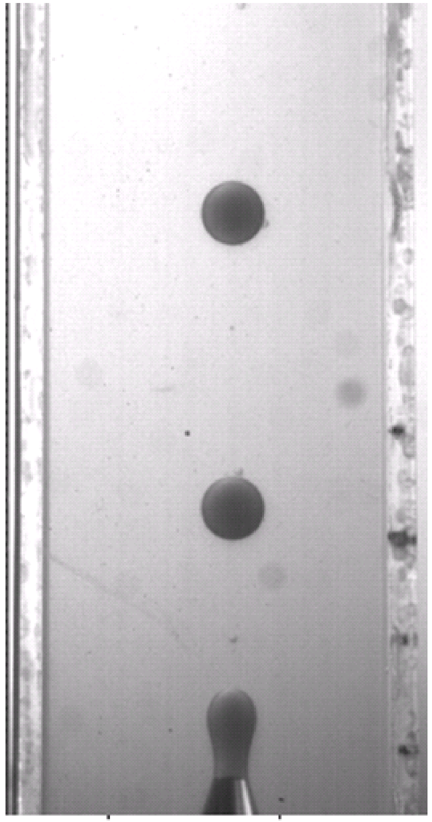
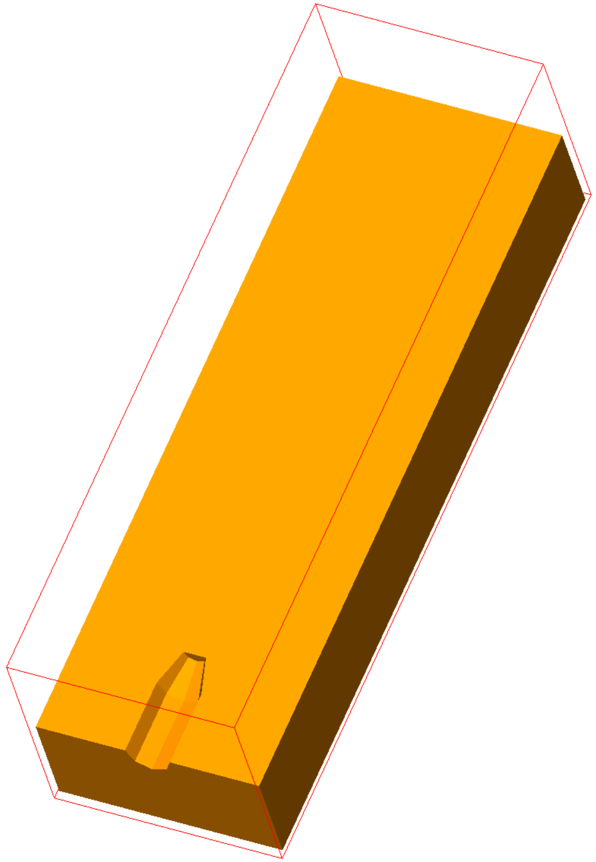




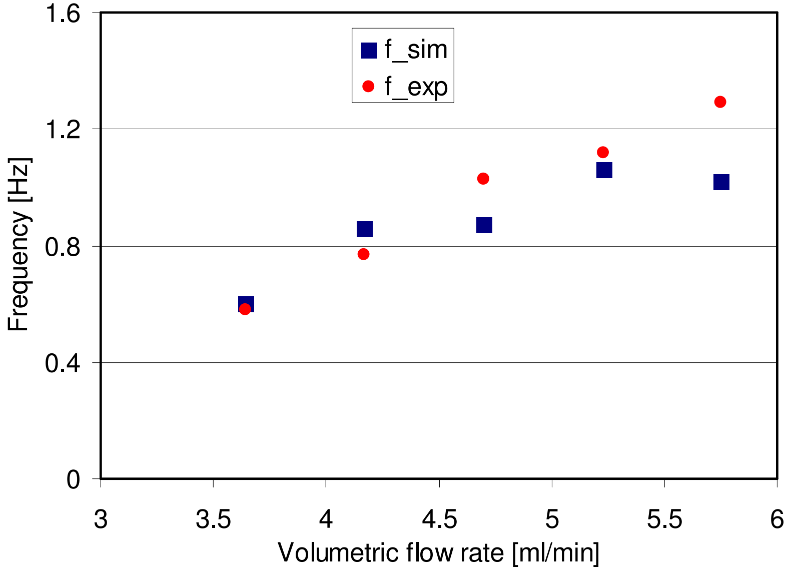
Operating conditions

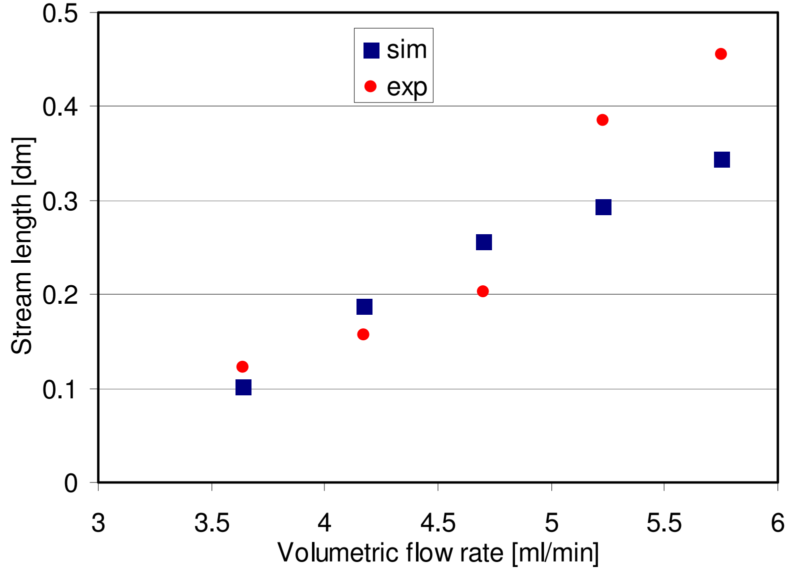
V_D [ml/min]	3,64	4,17	4,70	5,23	5,75
V_C [ml/min]	99,04	113,34	128,34	143,34	156,95

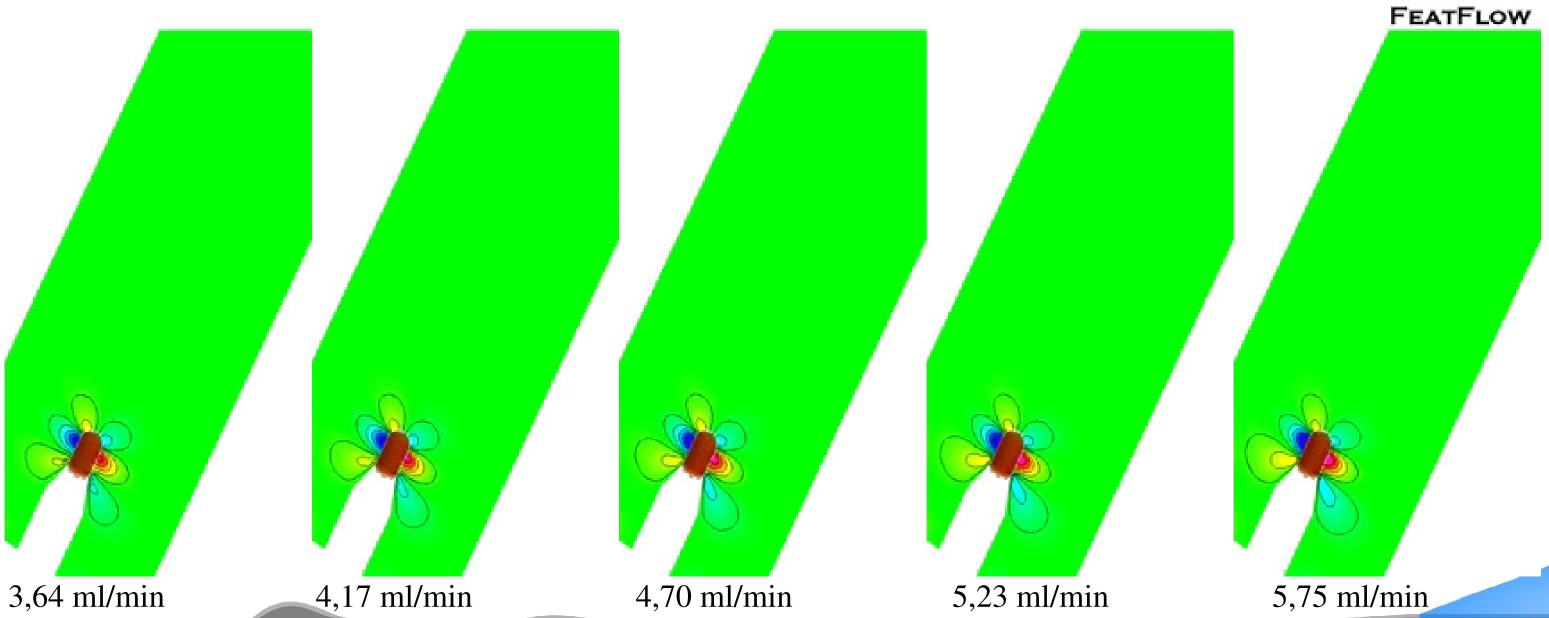
Validation parameters:

- frequency of droplet generation
- droplet size
- stream length

Comparison with experimental results





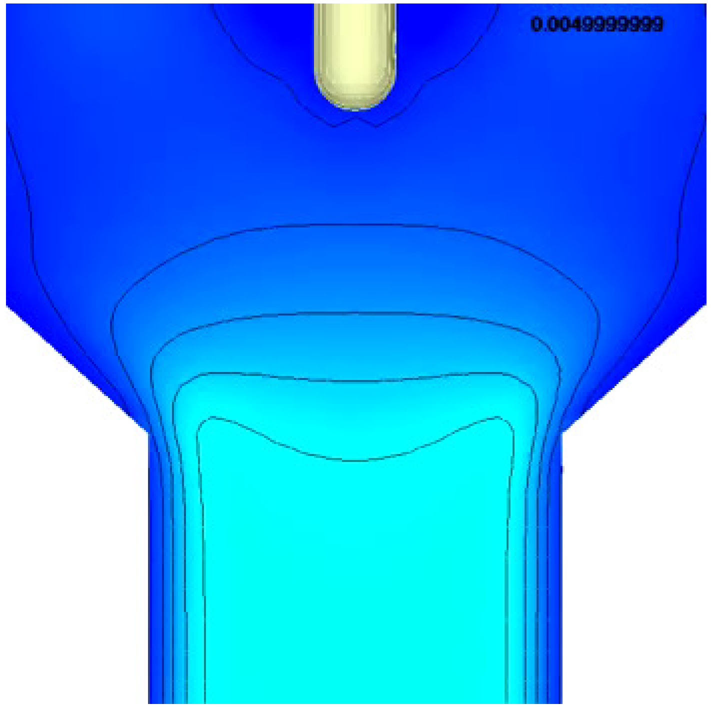


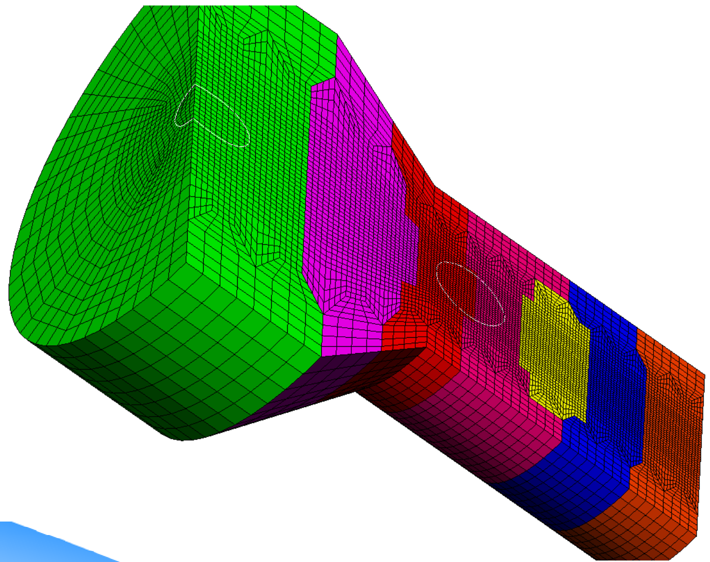
Monodisperse droplet generation in nozzles

In case of monodisperse droplets:

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

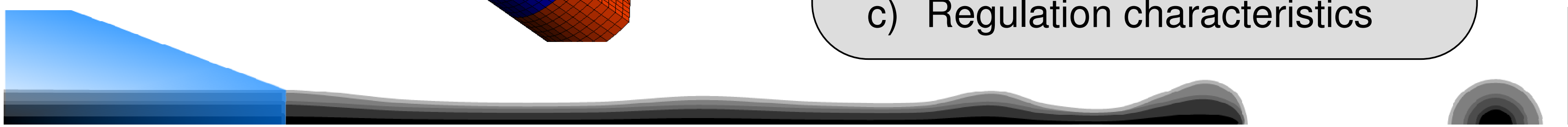
Geometrical parameters:
- Capillary diameter
- Outer pipe diameter
- Contraction ratio and angle





Alternatives of regulations:
- Dispersed phase
- Continuous phase

a) Mean flowrate
b) Regulation frequency
c) Regulation characteristics

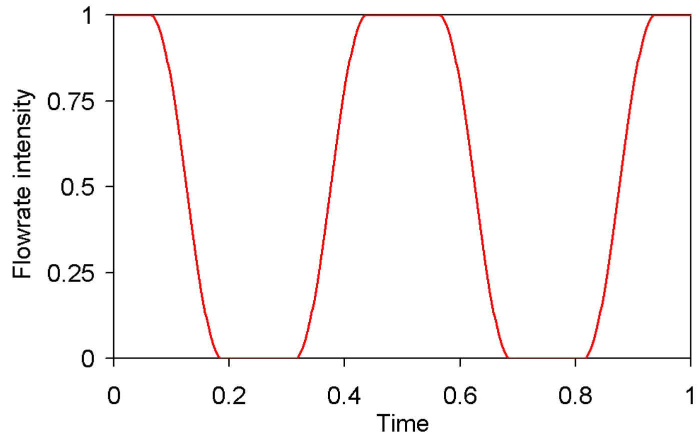


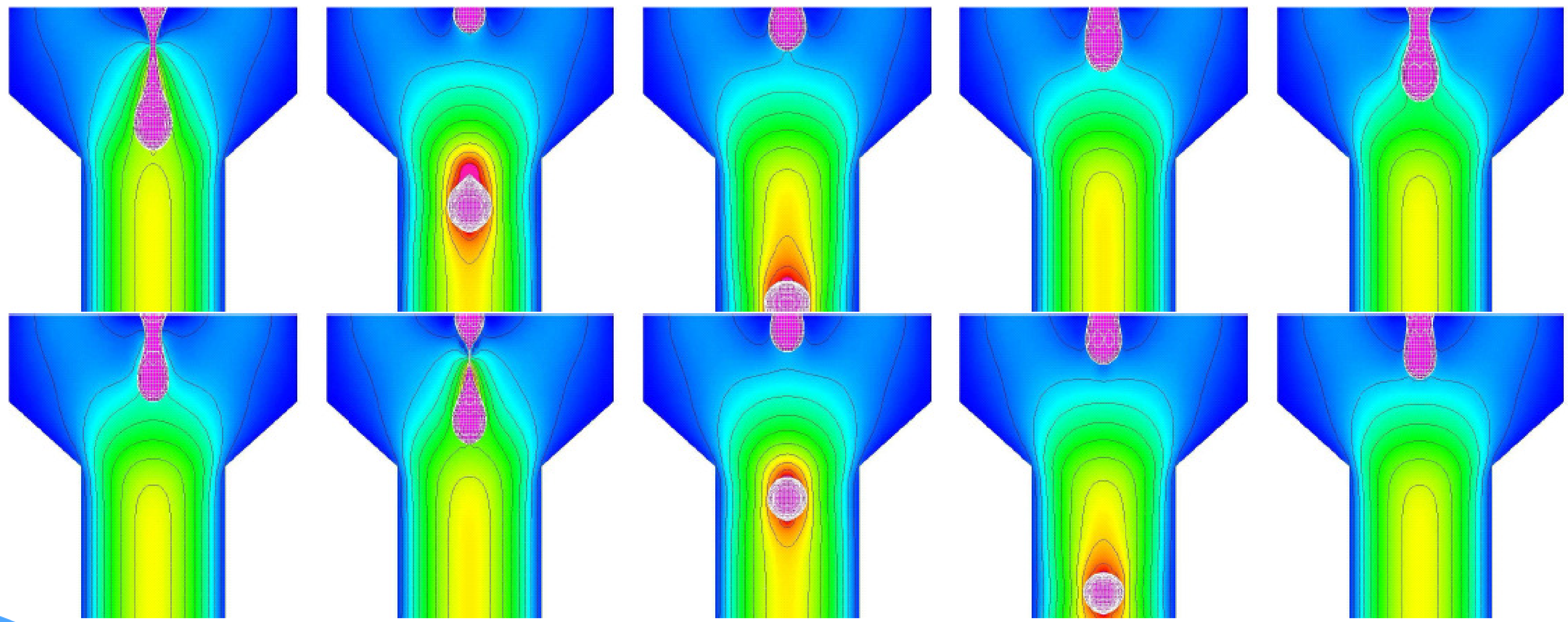
Monodisperse droplet generation in nozzles

In case of monodisperse droplets:

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

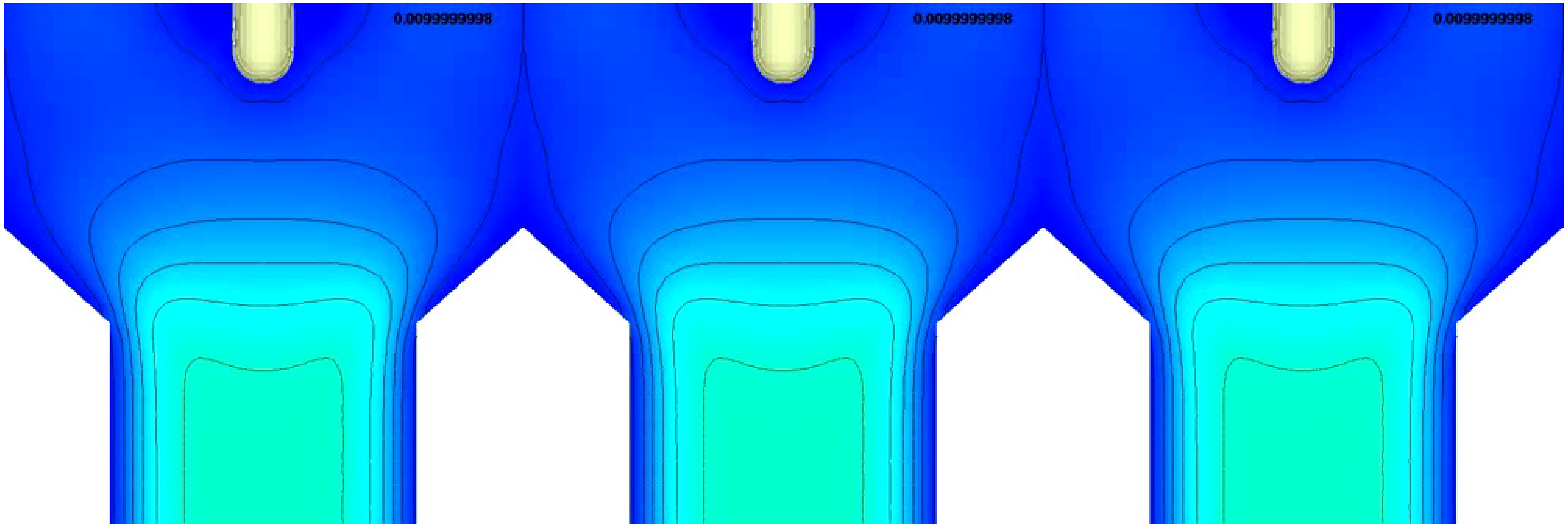
Can be influenced?



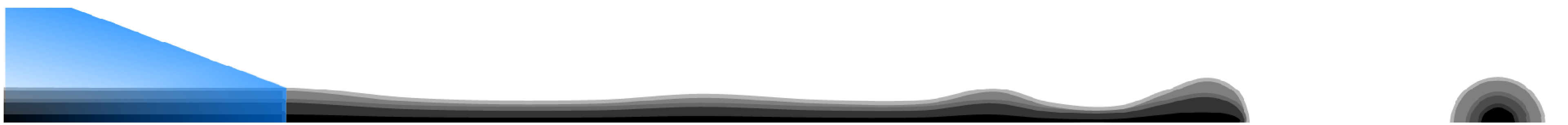


Monodisperse droplet generation in nozzles

With regulation	With regulation	No regulation
$\dot{V}_{D,\mathrm{mean}} = \dot{V}_{STD}$	$\dot{V}_{D,\mathrm{mean}} = 1.5\dot{V}_{STD}$	$\dot{V}_{D} = \dot{V}_{STD}$



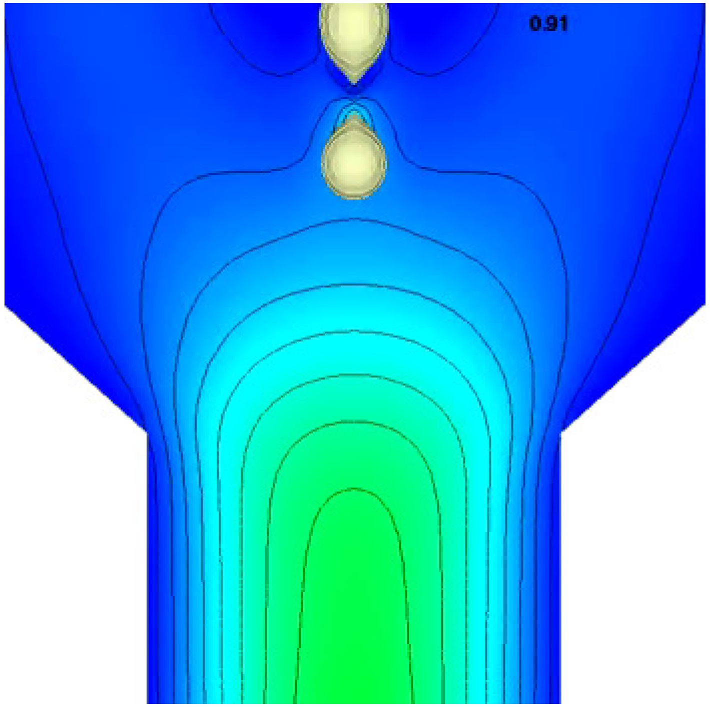
$d_{\mathrm{drop}} = 5.0\,mm$ $d_{\mathrm{drop}} = 5.7\,mm$ $d_{\mathrm{drop}} = 5.2\,mm$



Monodisperse droplet generation in nozzles

Small capillary

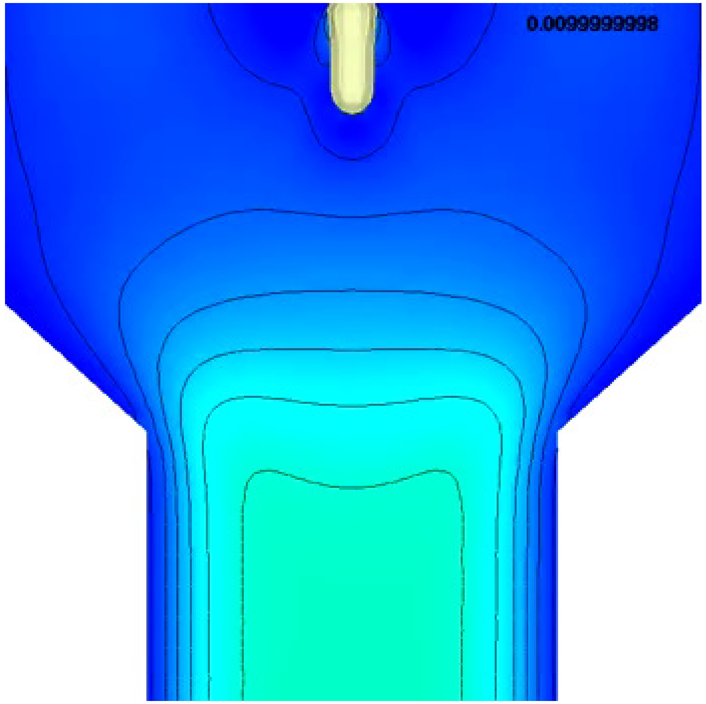
$$\dot{V}_{D,\mathrm{mean}} = 0.75\dot{V}_{STD}$$



Not monodisperse

Smaller capillary

$$\dot{V}_{D,\mathrm{mean}} = 0.75\dot{V}_{STD}$$



$$d_{\mathrm{drop}} = 4.5\,mm$$

Future tasks

Mathematical model

- Solver adjustment for large jump of physical paramters
- Grid deformation method
- Keep mass conservation under control
- Software performance (speed up)

Application

- Numerical experiments for cases with large jumps of the physical quantities
- Influence of the operation conditions on the performance of the process
- Influence of flowrate modulation of the phases
- Influence of non-Newtonian fluid models

Comparisons, validation, benchmarking