Numerische Simulation zur Herstellung monodisperser Tropfen in pneumatischen Ziehdüsen

(DFG-SPP 1423 `Prozess-Spray‘, Bremen 2009)

Stefan Turek, Otto Mierka

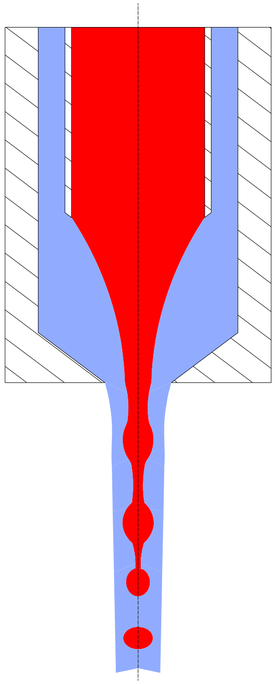
Institut für Angewandte Mathematik, TU Dortmund
http://www.mathematik.tu-dortmund.de/LS3
http://www.featflow.de

- **Ausgangssituation**
  Monodisperse Tropfen aus laminaren Flüssigkeitsfäden mittels Ziehdüsen
  → **oft verwendetes Verfahren**

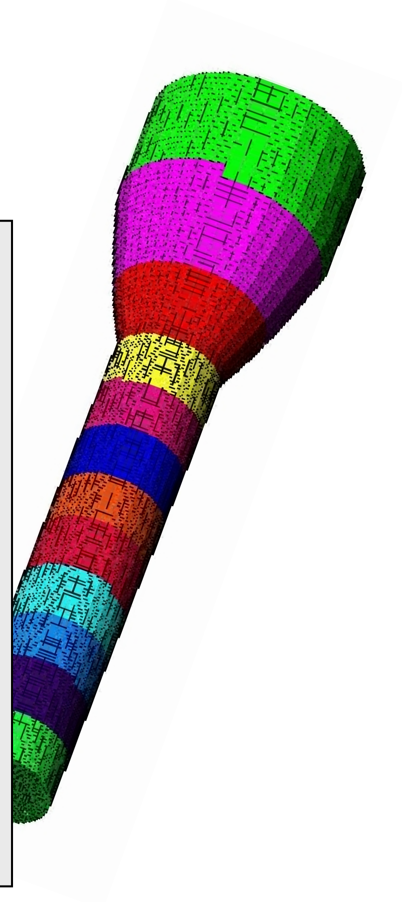
  Aber: Vielzahl möglicher Parameter wie Dichteverhältnis, Viskosität, Rheologie, Grenzflächenspannung und Strömungsbedingungen
  → **Grundlagenuntersuchungen notwendig**

- **Ziele**
  →Detaillierte numerische CFD-Simulationen (mit **FEATFLOW)**
  →**Nicht-newtonsche** Fluide + **mehrkomponentige** Suspensionen
  →**Optimierung** zur gezielten Steuerung (2./3.Phase)

- **Methoden / Arbeitsprogramm**
  → **Effiziente CFD-Techniken** (adaptive Gitter, implizite Level-Set, TVD, parallele Mehrgitterlöser, HPC)
  → **Detaillierte Untersuchungen** zu Düsenformen + Strömungsanregung



- **Einbindung in das SP-Programm**
  Zusammenarbeit mit AG Walzel (Experimente), Benchmarking



The incompressible Navier Stokes equation

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

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

unknown interphase location

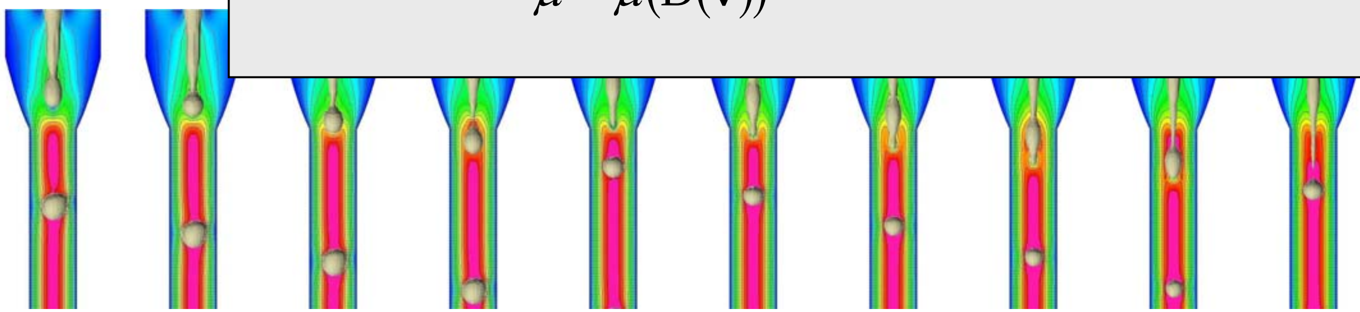
Interphase tension force

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

$$-\nabla\cdot\mathbf{n} \quad \text{on} \quad \Gamma$$

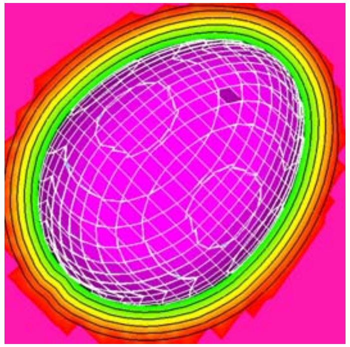
Dependency of physical quantities

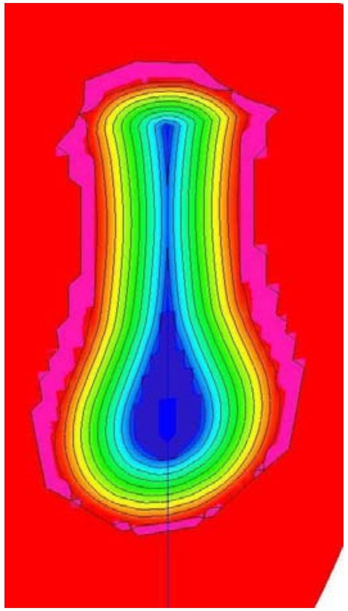
$$\mu = \mu(\mathrm{D}(\mathbf{v}))$$



Levelset method (→"smooth" distance function)

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





Problems:
- It is not conservative
- Needs to be reinitialized to maintain its distance property

Benefits:
- Provides the accurate representation of the interphase
- Provides other auxiliar quantities (normal, curvature)
- Allows topology changes

Maintaining the distance function by PDE-based reinitialization

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = S(\phi) \qquad \mathbf{u} = S(\phi) \frac{\nabla \phi}{|\nabla \phi|}$$

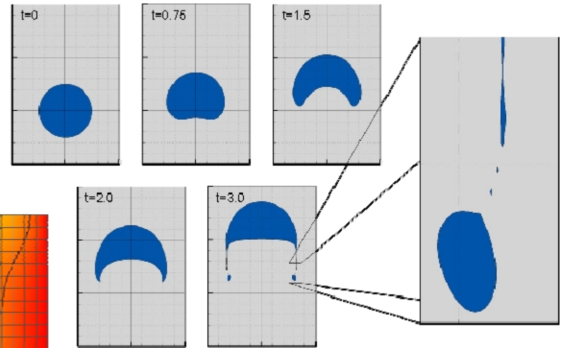
Problems:
- What to do with the sign function at the interphase? (smoothing?, DG?)
- How often to perform? (expensive→steady state)

technische universität
dortmund

Flow solver is based on FeatFlow using the Pressure Schur Complement method

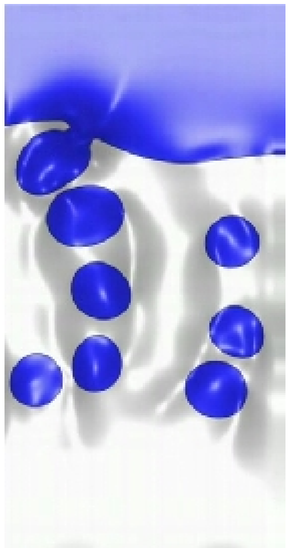
Discretization:

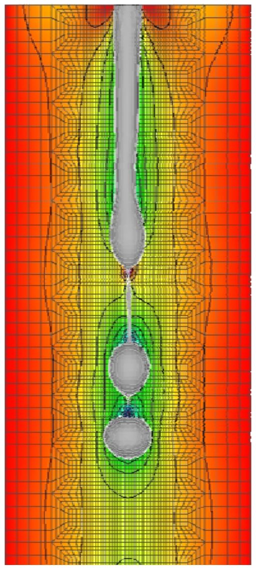
- a) Navier-Stokes: FEM Q_2/P_1 in space + stabilization (TVD,EO-FEM)
- b) Levelset: **DG FEM P_1** in space no stabilization !
- Crank-Nicholson scheme in time



Main features of the FeatFlow approach:

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





Problems and challenges

technische universität dortmund

- Steep gradients of the velocity field and of physical properties (such as μ and ρ) near the interphase (oscillations!)

- Representation of interphacial surface tension: CSF, Line Integral, Laplace-Beltrami, Phasefield, *etc.* (oscillations!), explicit or implicit treatment?

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

- Mass conservation (during Levelset advection and reinitialization)

Steep changes of physical quantities:

- Elementwise averaging of the physical properties (prevents oscillations):

$$\rho_e = x\rho_1 + (1-x)\rho_2, \quad \mu_e = x\mu_1 + (1-x)\mu_2$$ *x* is the volume fraction

- Extension of nonlinear stabilization schemes (AFC, TVD) for the momentum equation

Smoothening of interphacial tension (reduction of spurious oscillations):

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

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

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

$(\sigma\kappa\delta)_{Q_1}$ originates from the same space as the pressure (!)

Reinitialization is performed in combination of three ingredients:

1) Elements intersected by the interphase are modified w.r.t. the slope of the distance distribution such that

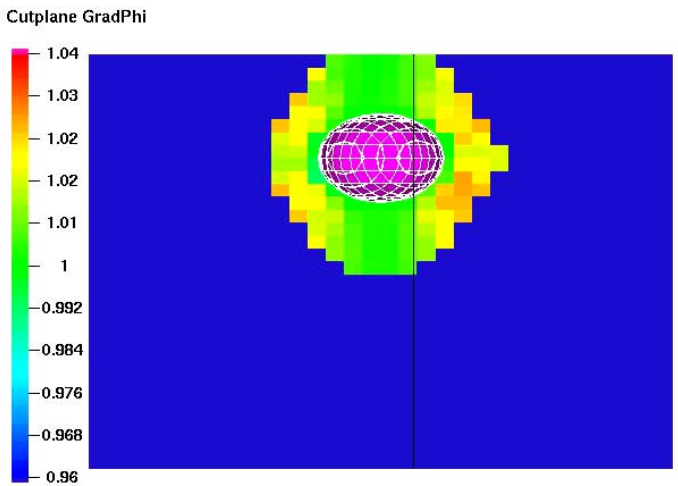
$$\left|\nabla \phi\right| = 1$$

2) Far field reinitialization

Realization is based on the PDE approach, but it does not require smoothening of the distance function!

3) Continuous projection of the interphase (smoothening of the discontinuous P_1 based distance function)

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



technische universität dortmund

Mass conservation

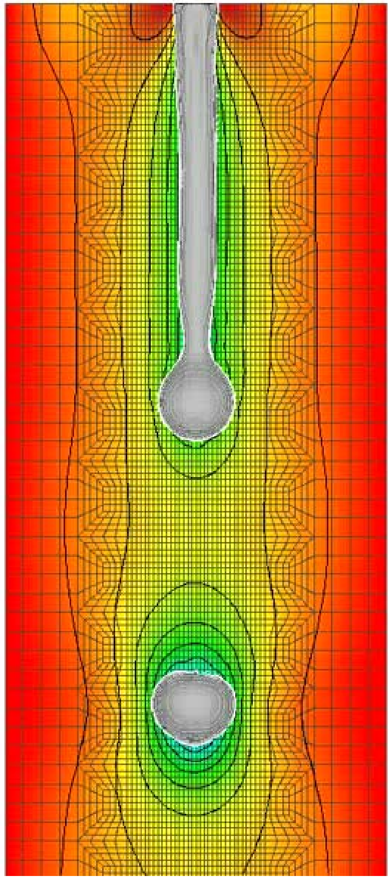
Must be satisfied on the continuous and discrete level as well!

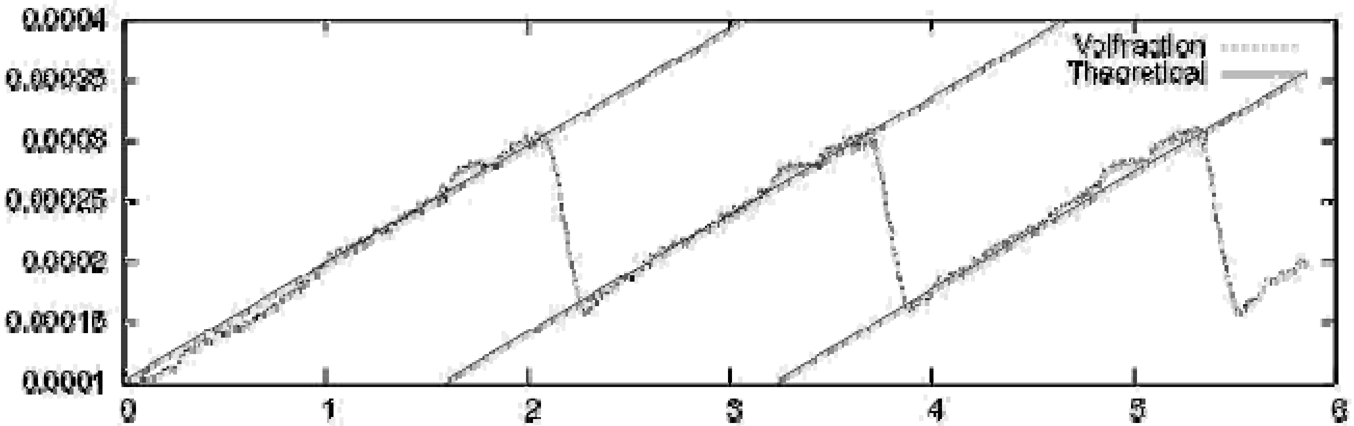
Combination of:

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0, \quad \text{with} \quad \frac{\partial \rho(\phi)}{\partial t} + \nabla \cdot (\rho(\phi)\mathbf{v}) = 0$$

Nonlinear system of PDEs!

No stabilization! (distance function should be smooth anyway)

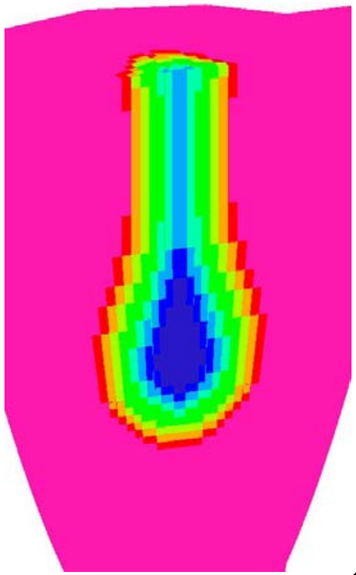




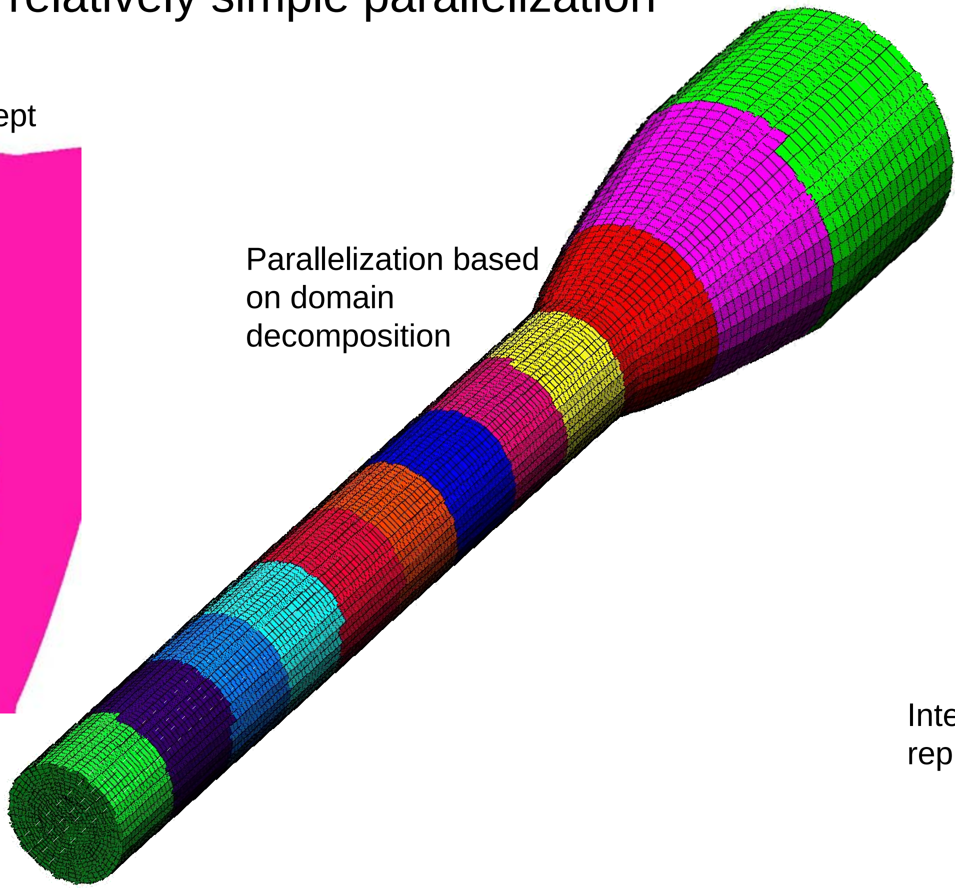
Benefits of DG FEM for levelset

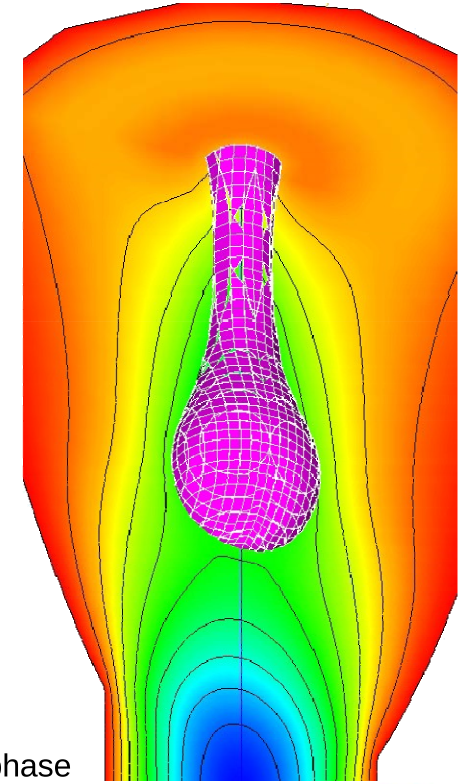
- possibility of reduction of the computational domain (only for levelset)
- mass preserving (interphase preserving!) reinitialization
- exact localization of the interphase (polygons)
- exact evaluation of volume fractions
- relatively simple parallelization

Layering concept



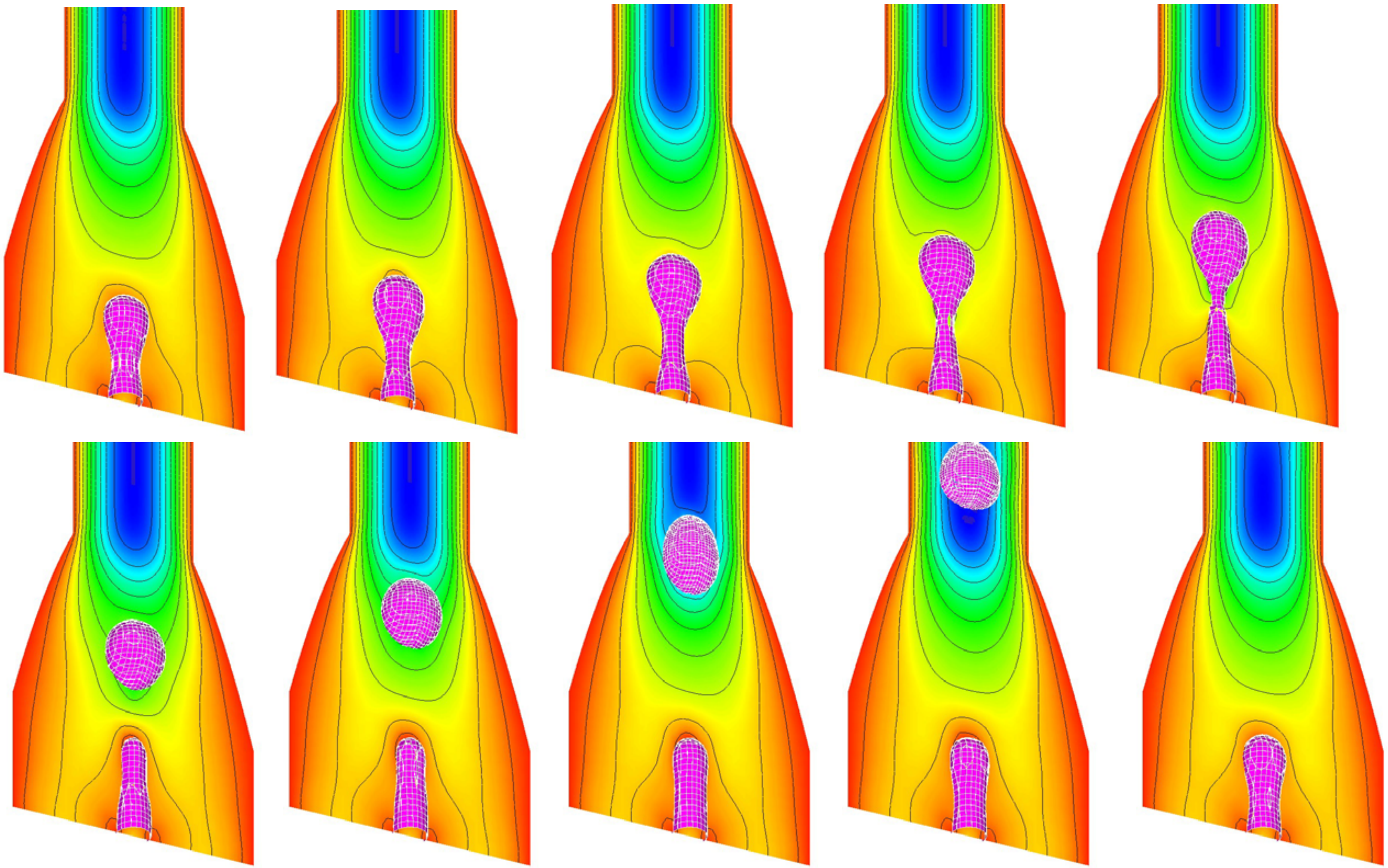
Parallelization based on domain decomposition





Interphase representation by polygons

Droplet jetting application



Ausblick

- Validierung der Komponenten mittels Benchmarks und Experimenten (mit AG Walzel) ➔ 1.Phase
- Anpassung der Geometrie ➔ 1.Phase
- Versuche mit Strömungsanregung ➔ 1.Phase
- Optimierung der numerischen Komponenten ➔ 1.Phase

- Verbesserte Numerik für realistische Dichteunterschiede ➔ 2.Phase
- Weiterentwicklung für Nichtnewtonsche Fluide ➔ 2.Phase
- Partikelbehaftete Suspensionen ➔ 2./3.Phase
- Ankopplung von Optimierungswerkzeugen ➔ 3.Phase