Numerische Simulation zur Herstellung monodisperser Tropfen in pneumatischen Ziehdüsen

DFG – SPP 1423 „Prozess-Spray“

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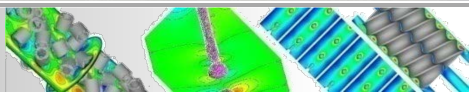
http://www.featflow.de
http://www.mathematik.tu-dortmund.de/LS3

Main objectives of the project

- Development of a fast and accurate CFD-based simulation tool suitable for non-Newtonian multiphase problems. Extension of the standard FeatFlow solver with additional packages
  - Level Set Method for interface capturing
  - Generalized Newtonian rheological models
  - ALE Method with dynamic mesh deformation

- Multistage validation of the simulation tool w.r.t experimental measurements or computational benchmarks

- Simulation of encapsulation (3-phase) processes:
  - under modulated conditions
  - materials obeying shear thinning rheological models



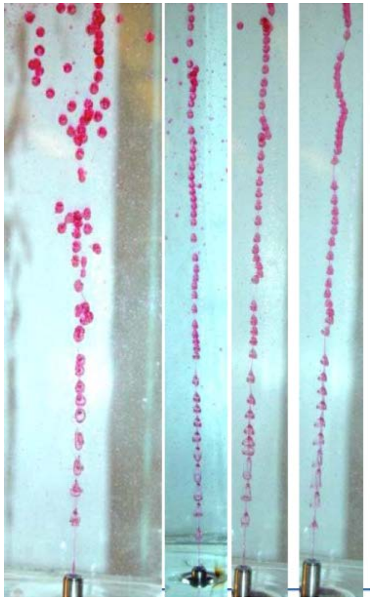
Continuity of development within SPP 1423

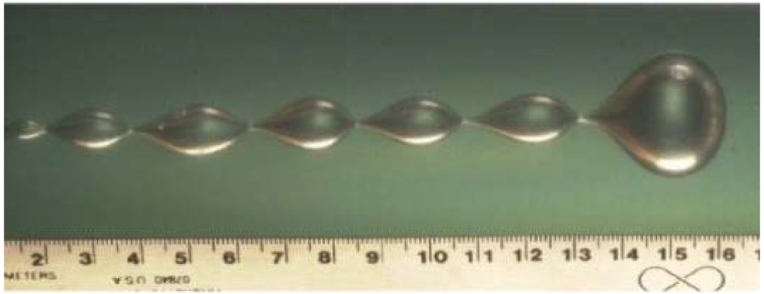
CFD simulation of monodisperse droplet generation by means of jet break-up
→ Geometry, material parameters, rheological properties, modulation

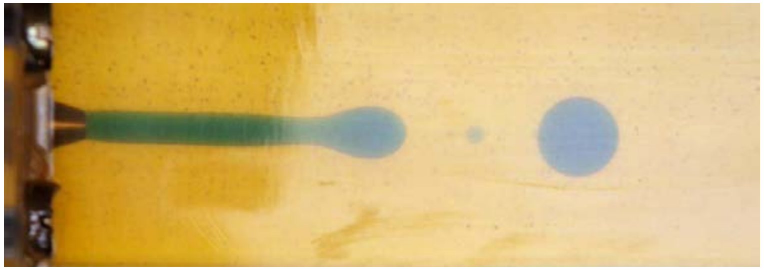
1st period
- LS-FEM
- Benchmarking and Validation
- Droplet dripping
- Modulation

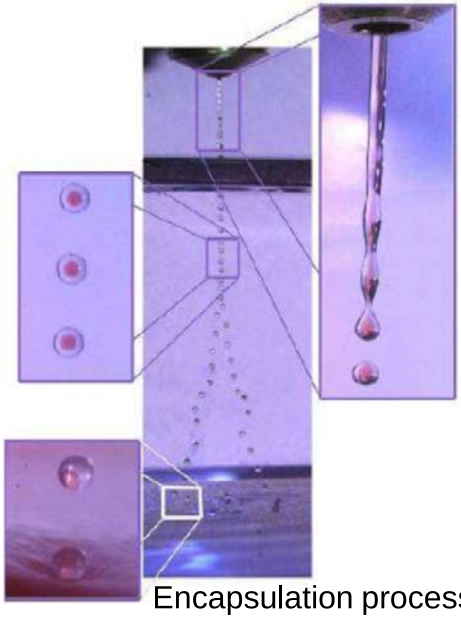
2nd period
- mgLS-FEM
- Gas/liquid-like systems
- Non-Newtonian models
- Jetting regime
- Wider range of Op. Cond.

3rd period
- mgLS$^{(2)}$-FEM
- Gas/liquid/solid systems with Non-Newtonian fluids
- Multiple Level Set
- Modulation


Modulation example

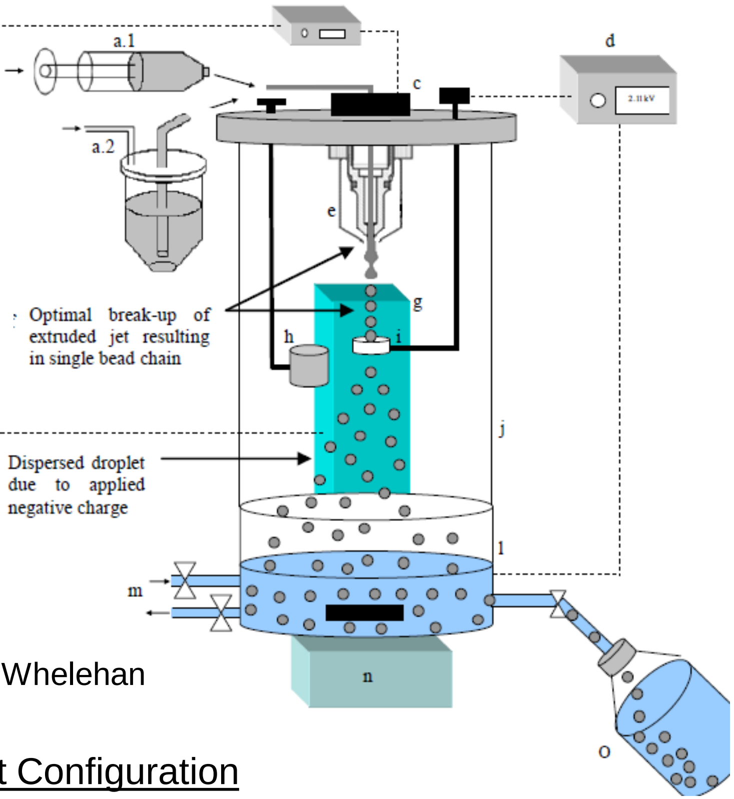

Non-Newtonian two phase flow


Newtonian jetting example


Encapsulation process

Encapsulation processes

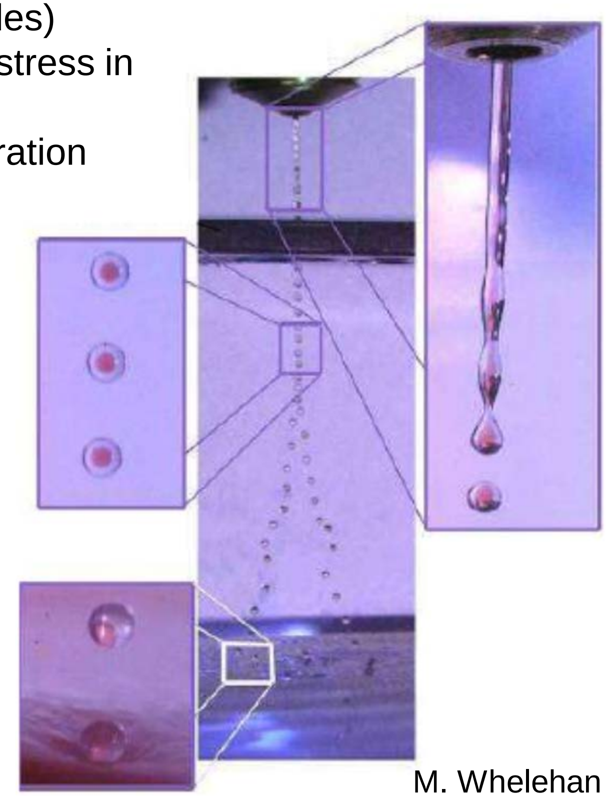
- Numerical simulation of *micro-fluidic drug encapsulation ("monodisperse compound droplets")*
- "Bio-degradable" outer liquid with generalized Newtonian behaviour
- Optimization w.r.t. boundary conditions, flow rates, droplet size, geometry, modulation



M. Whelehan

<u>In Pharmaceutics</u>

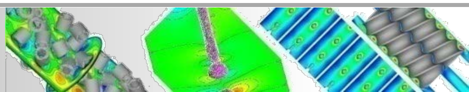
- Controlled drug release
- Protection of chemically active ingredients (from both sides)
- Protection against shear stress in stirred reactors
- Protection against evaporation
- Taste or odor masking



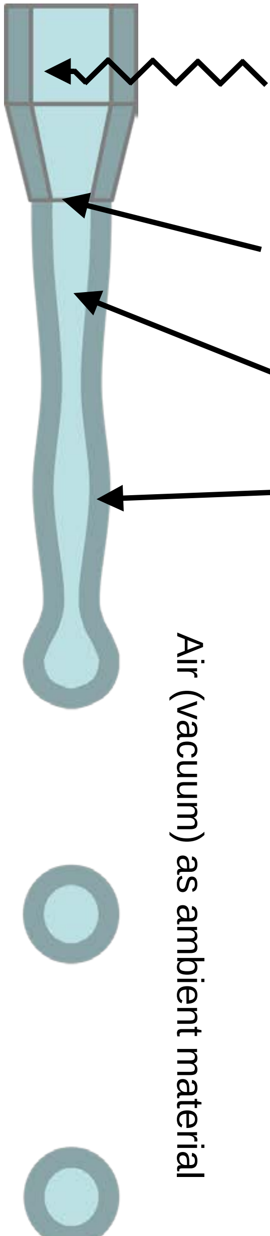
M. Whelehan

<u>Jet Configuration</u>

- 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)



Numerical challenges of the encapsulation process



Excitation of the nozzle with the aim of modulation

Coaxial arrangement of the nozzles

Inner core material (drugs, special agents)

Outer carrier shell (alginate)

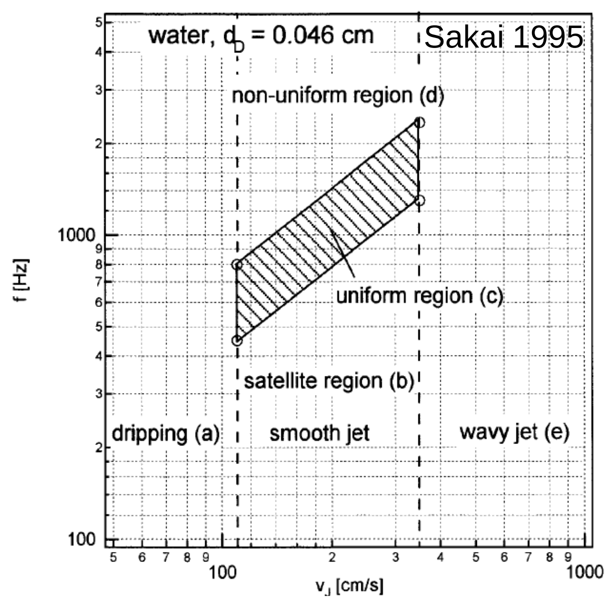
Individual difficulties:

- Moving interfaces (*g-l-l*)
- Large ratios of physical properties
- Surface tension effects
- Non-Newtonian fluids

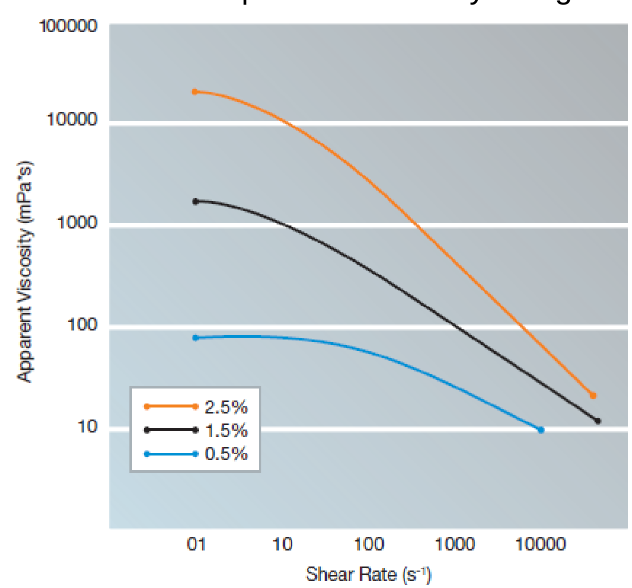
Numerical techniques:

- Level Set for tracking of multiple interfaces
- Mesh deformation with ALE for optimal resolution of the interface
- Complex rheological fluid properties:
  - Generalized Newtonian models (shear thinning)

Operation envelopes for modulation



Shear dependent viscosity of alginate



Modular structure of mgLS(2)-FEM

<u>Numerical features of FEATFLOW:</u>
- Higher order Q2P1 FEM schemes
- FCT & EO FEM stabilization techniques
- Use of unstructured meshes
- Fictitious Boundary (FBM) methods
- Newton-Multigrid solvers
- Parallel (domain decomposition)

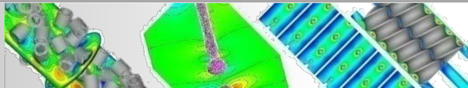
ALE based mesh deformation :
- Fast, due to PDE free implementation
- Use of monitor function (distance, gradients, triangulation)
- Dynamic performance for transient problems
- Artificial solver acceleration due to the reduced computational cost w.r.t. the given interface resolution

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

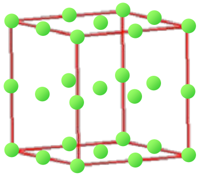
Multiphase flow module (resolved interfaces):
- ℓ/ℓ interface tracking method (Level Set)
- s/ℓ interface capturing method (FBM)
- $(s,\ell)/\ell/g$ composite jets of ℓ/ℓ and/or s/ℓ

Engineering aspects:
- Geometrical design
- Modulation strategy
- Optimization

FEM-based simulation tool for the accurate prediction of „tailor-made“ droplet generation within encapsulation processes



Practical realization – interface reconstruction



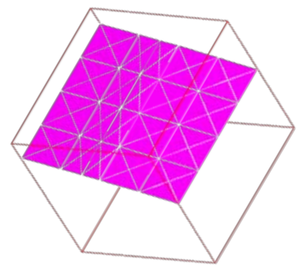
High order Q2 discretization of the Level Set equation $\dfrac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0$

Stability requirement: ϕ should be smooth!

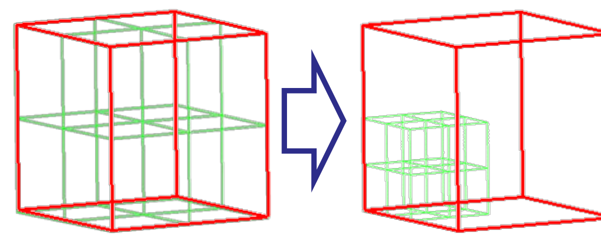
Reinitialization / Accurate distance computation / Interface reconstruction

<u>The key is to fully exploit the high order resolution of the interface</u>

- Triangulation of the arising surface

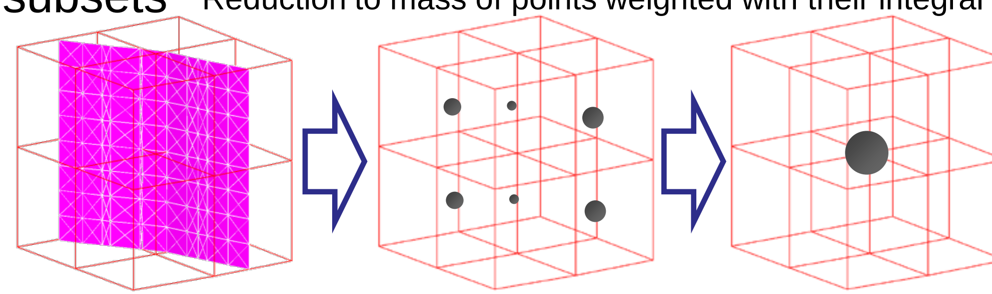


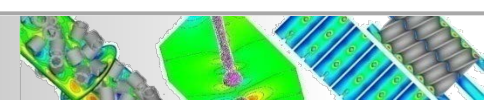
- Recursive subdivision of interface intersected elements (downward direction)



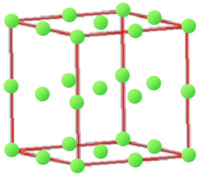
- Hierarchical storage of triangulated subsets (upward direction)

Reduction to mass of points weighted with their integral area





Practical realization – interface reconstruction



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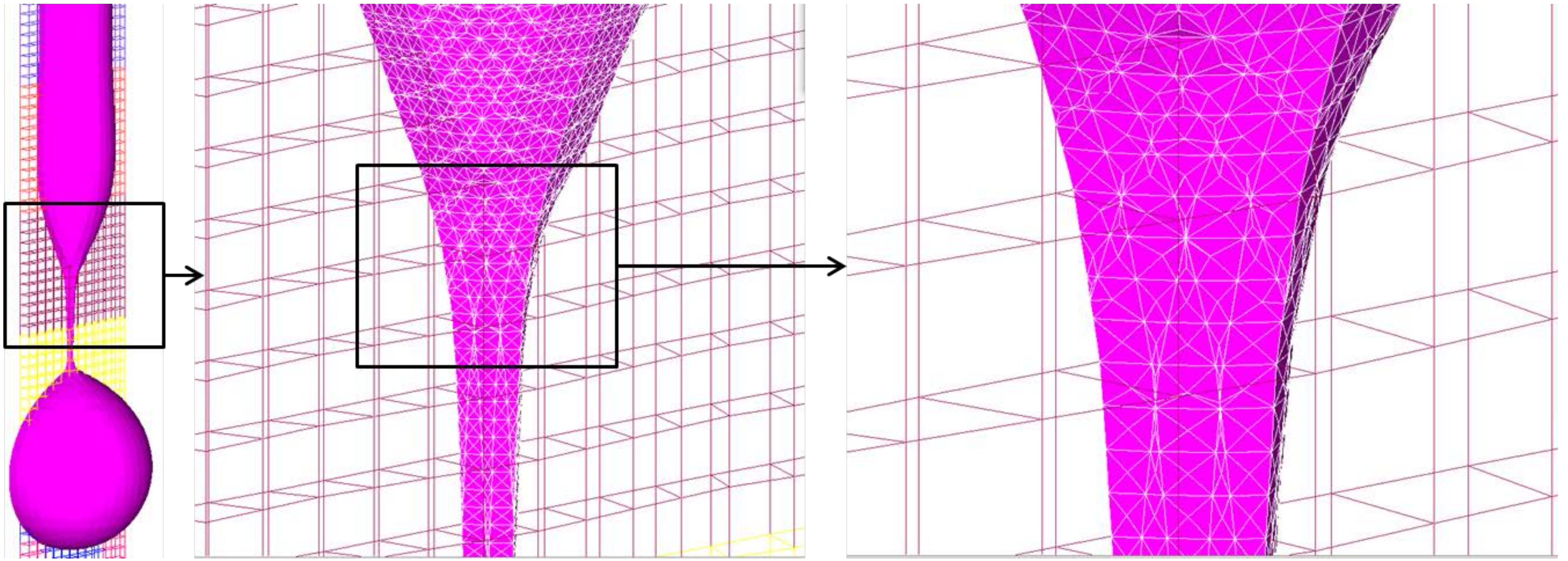
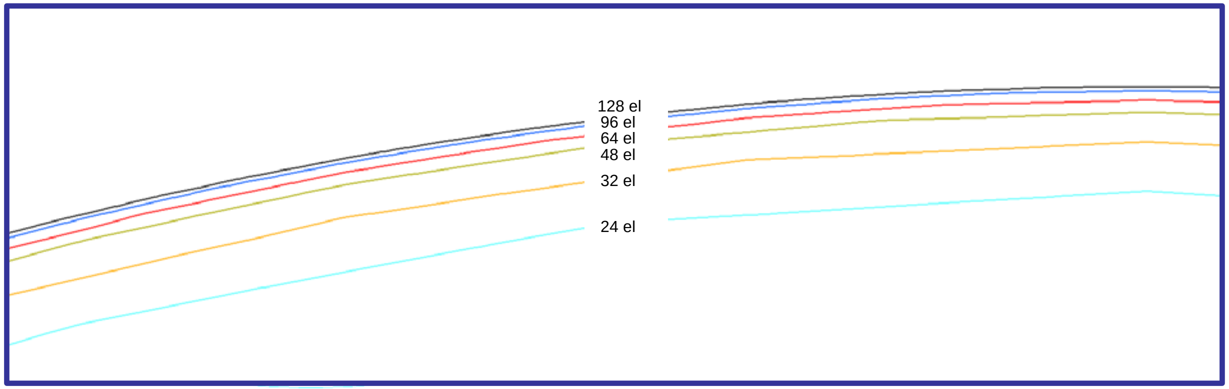


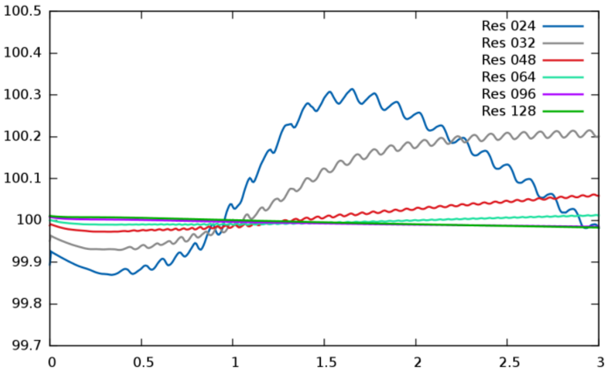
Validation and convergence of the flow solver

3D Rising Bubble benchmark initiative:

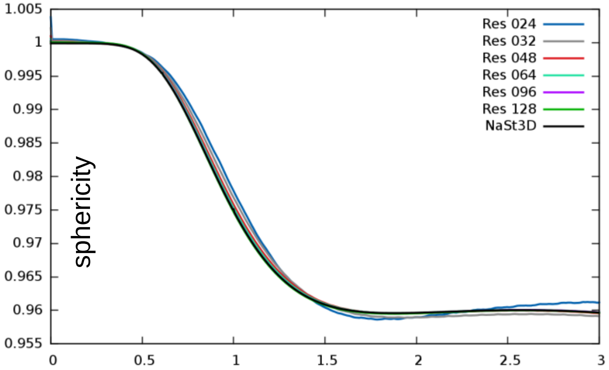
http://wissrech.ins.uni-bonn.de/research/projects/risingbubblebenchmark/



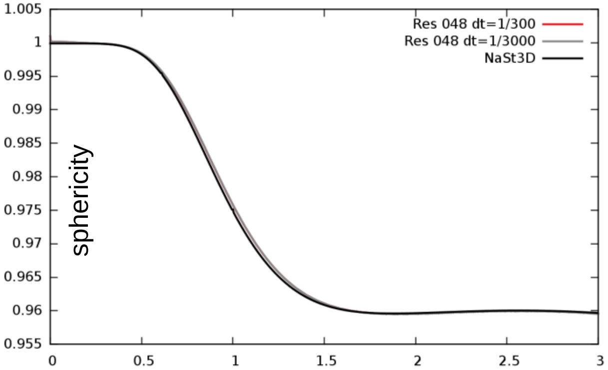
Mass loss evolution in time



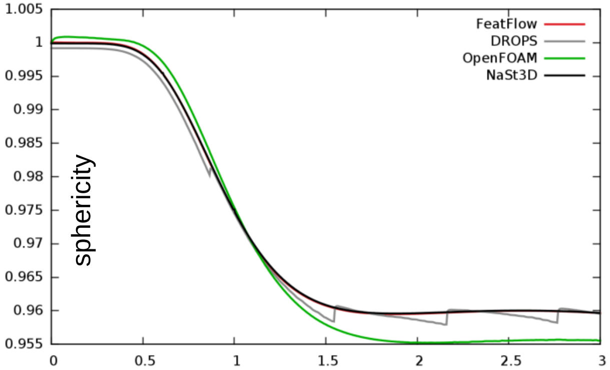
Spatial convergence: FEATFLOW vs Ref



Temporal convergence: FEATFLOW vs Ref



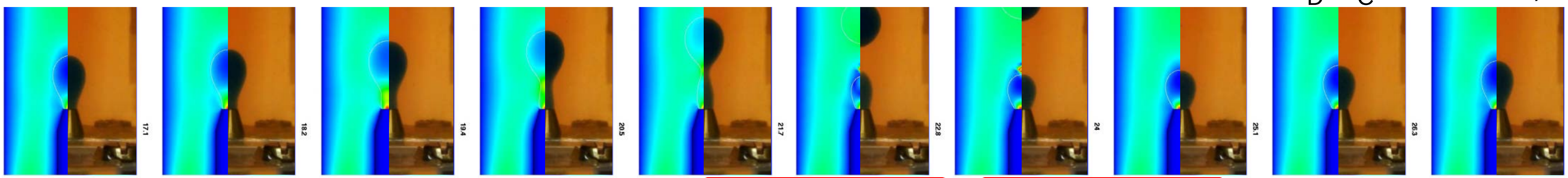
FEATFLOW vs other discret. techniques



Validation of droplet generation w.r.t. experiments

Cooperation with the group of Prof. Walzel / TU Dortmund

V_D/V_C = 2.5:123,1

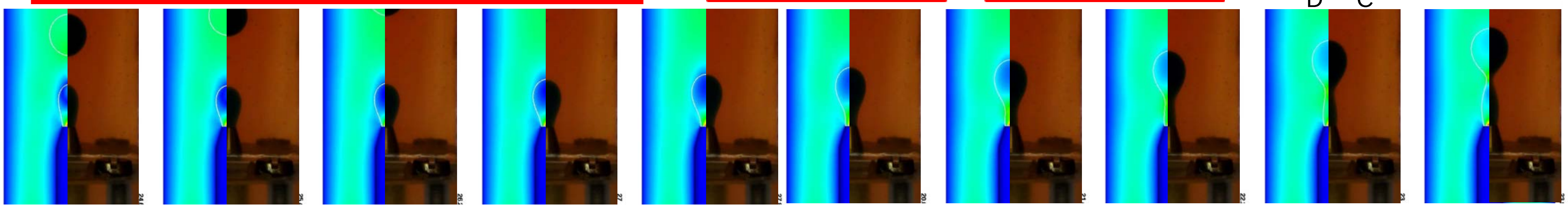


σ_{CD} = 0.025 N/m (+/- 0.001 N/m)

$\mu_1 : \mu_2 \sim 1.0$

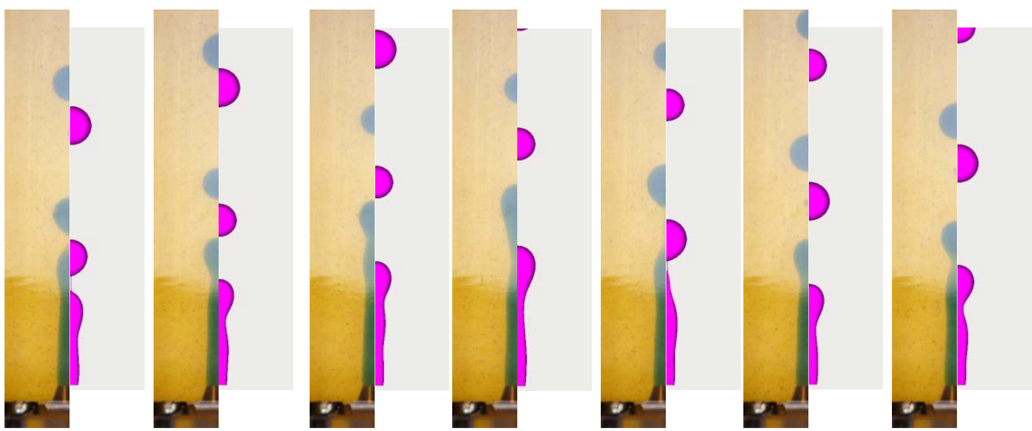
$\rho_1 : \rho_2 \sim 1.0$

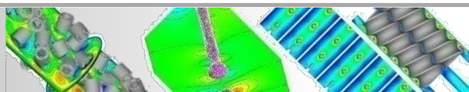
V_D/V_C = 3.0:148.7



V_D/V_C = 4.0:197.0

- Dripping shows an excellent agreement with experiments
- Increasing sensitivity of the process for higher flowrates leading to jetting!
- Introduction of controlled source of disturbances in terms of modulation



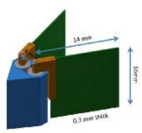


Recent development: Grid deformation and ALE

Advantages:
- Constant mesh/data structure
- Increased resolution in regions of interest
- Nonlinear PDE approach is **not** necessary → anisotropic Laplace smoother
- Straightforward usage for 3D unstructured meshes

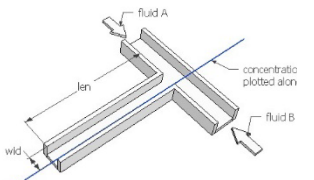
Intelligence of the method depends on the construction of the monitor function
- Geometrical description (solid body, interface triangulation)
- Field oriented description (steep gradients, fronts) → numerical stabilization

<u>Microfish dynamics</u>
Cooperation with:
Prof. Fischer @ MPI IS Stuttgart
Work published in:
Nature Communications, 2014

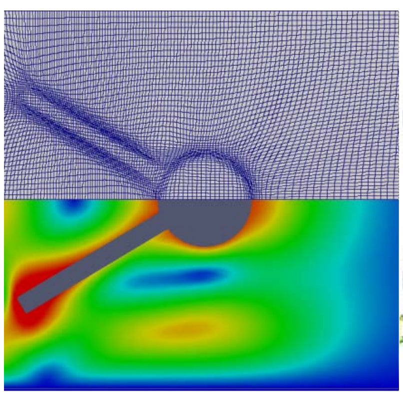


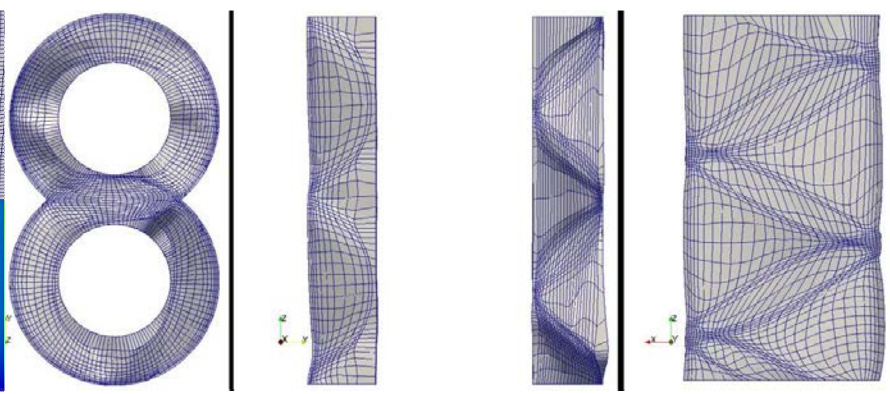
<u>Twinscrew extruders</u>
Cooperation with:
Prof. Schöppner @ KTP Paderborn
Work submitted to:
Comp. Meth. In Appl. Math. & Eng. , 2015

<u>Microreactors</u>

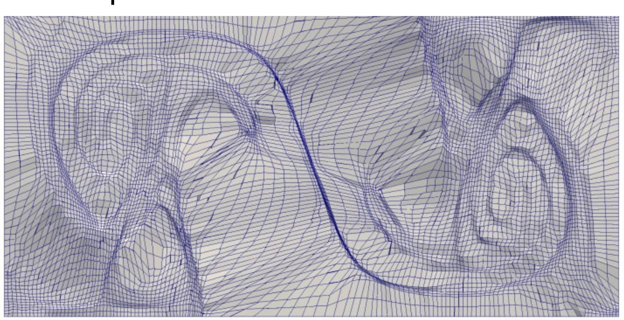


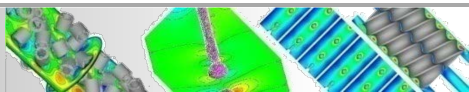
Cooperation with:
Prof. Schlüter @ TUHH Hamburg





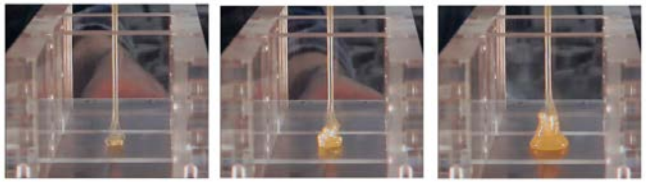
Computational mesh after deformation





Simulation of viscous liquid jets

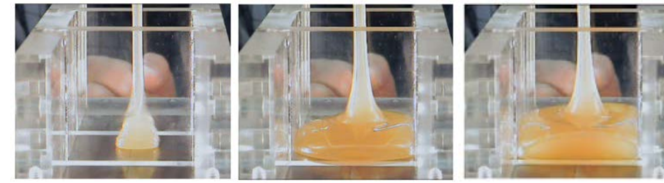
J. M. Nóbrega et al.: The phenomenon of jet buckling: Experimental and numerical predictions

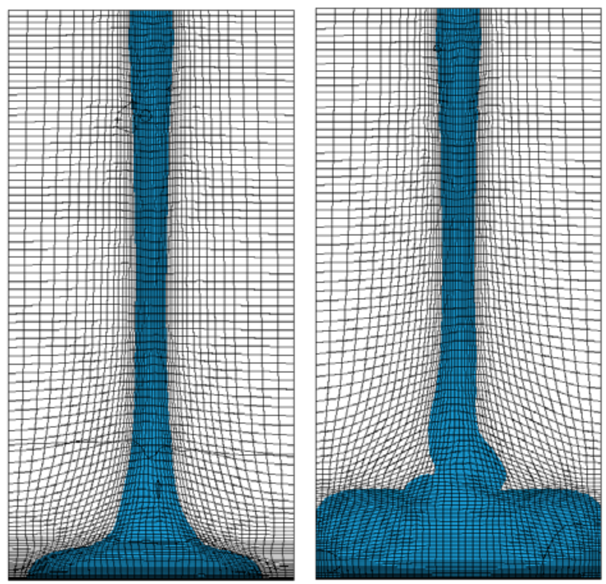


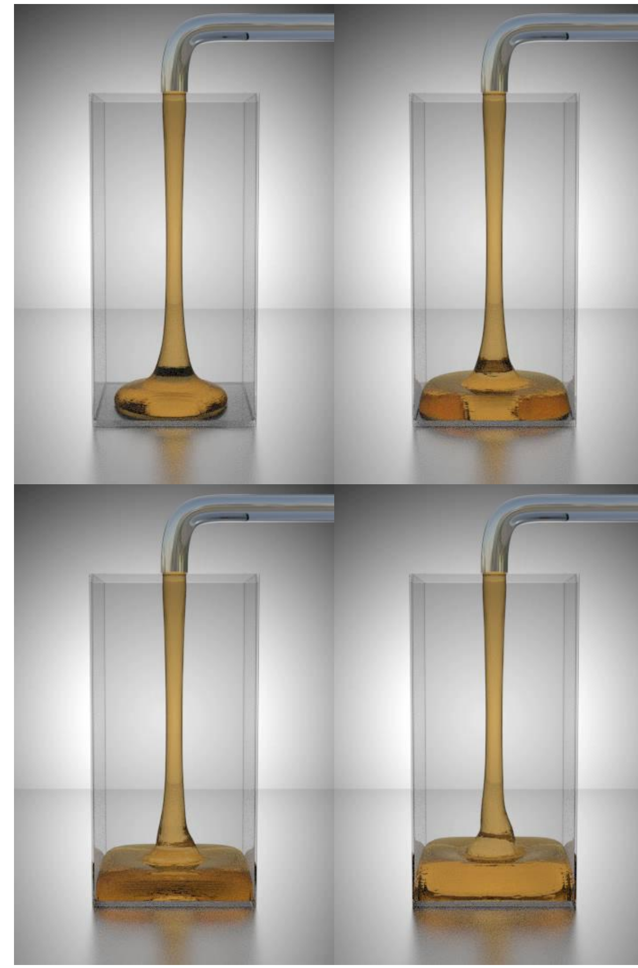
Corn syrup - air system

24x24x48 mesh

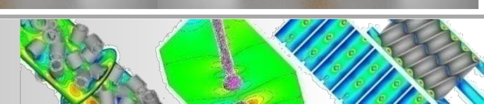
Interface triangulation:
T_0: ~100,000 triangles
T_N: ~300,000 triangles







Rendering: Raphael Münster / Blender



Encapsulation via modulation

<u>Reference case:</u>

Newtonian inner/outer liquid

Physical parameters for the simulation set-up:

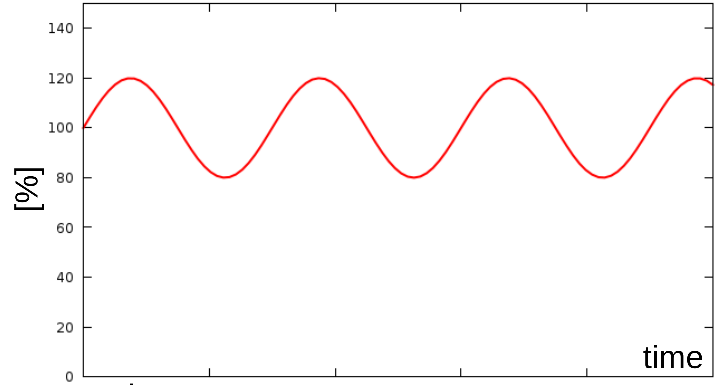
$$\mu_1 : \mu_2 : \mu_3 = 1 : 100 : 100$$

$$\rho_1 : \rho_2 : \rho_3 = 1 : 1000 : 1000$$

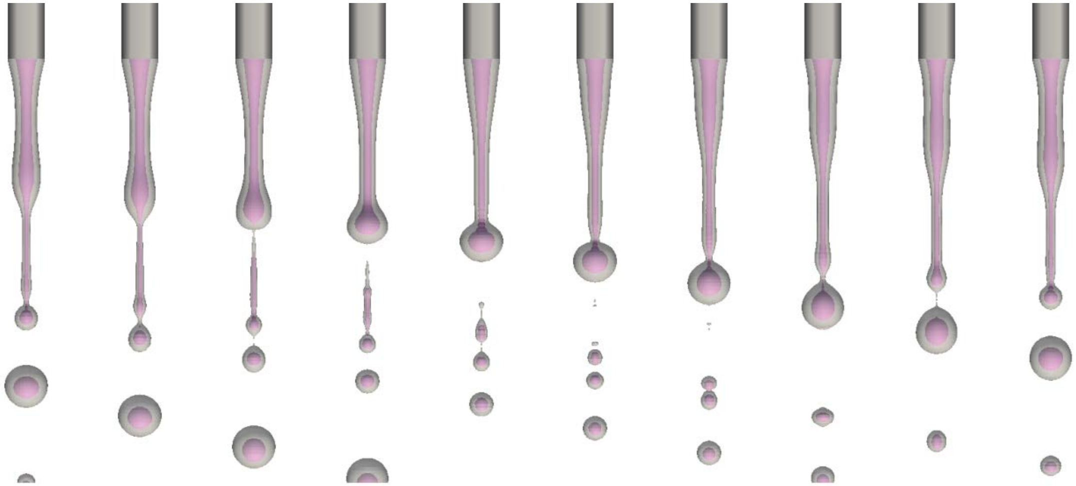
$$\sigma_{12} : \sigma_{23} = 1 : 1$$

$$\dot{V}_2 : \dot{V}_3 = 1 : 3.5$$

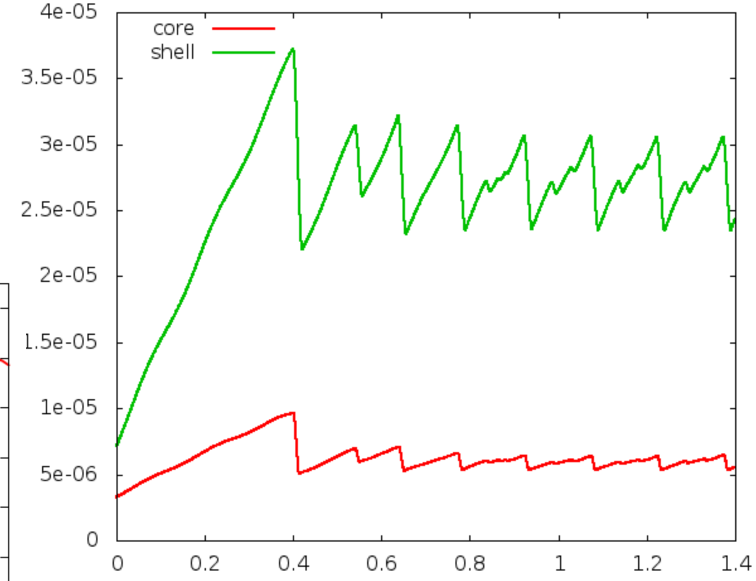
Modulation characteristic function



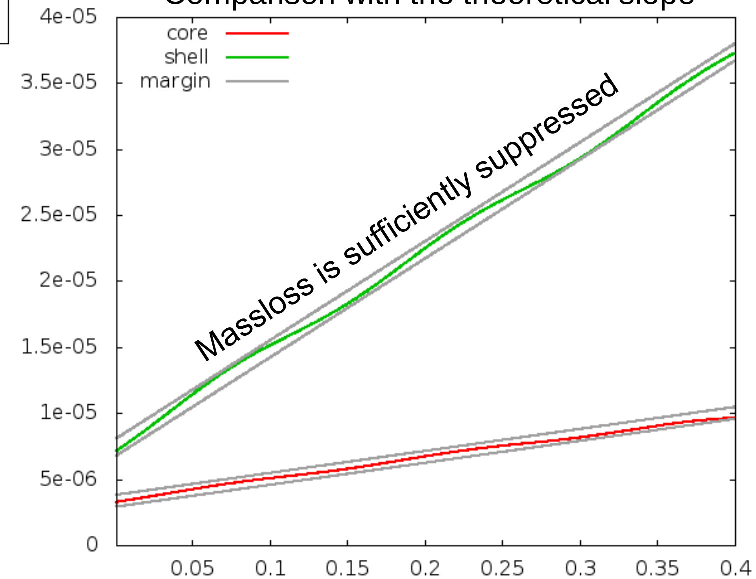
Periodical sequence of droplet generation



Core/shell volume evolution in time

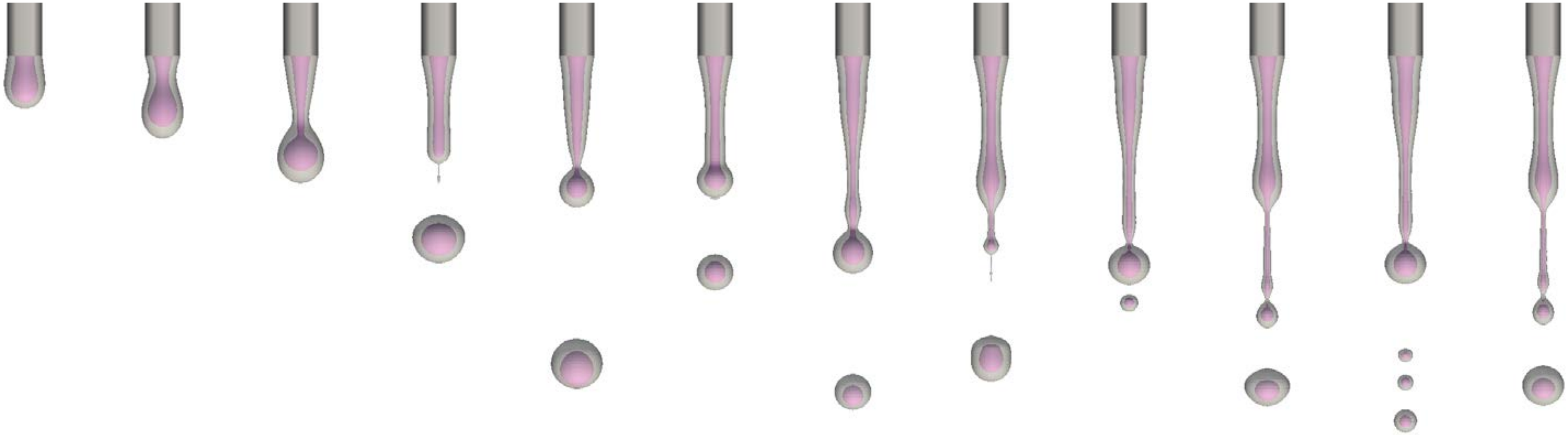


Comparison with the theoretical slope

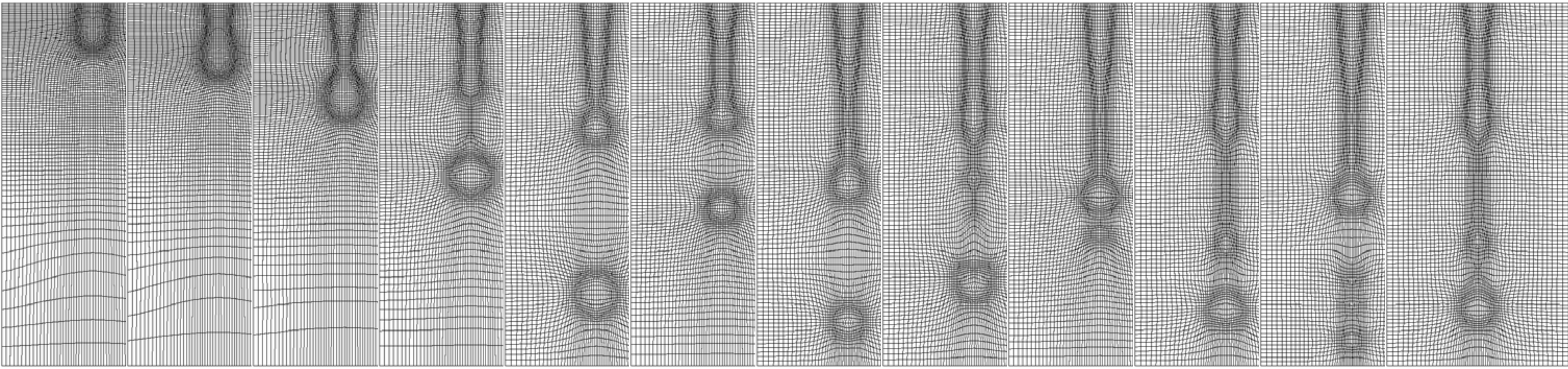


Encapsulation via modulation

Reference case Newtonian inner/outer liquid

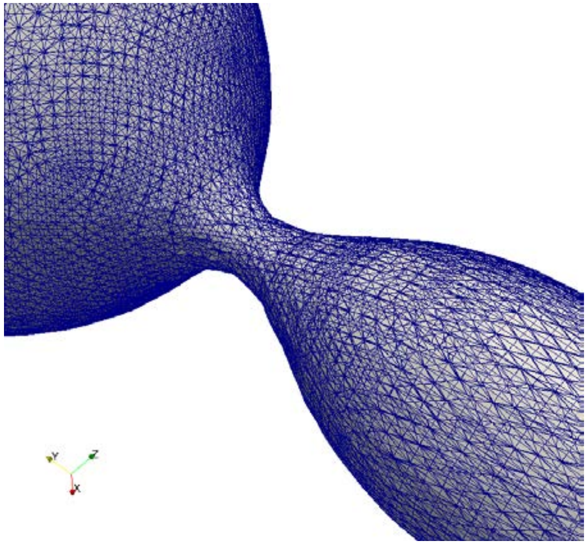


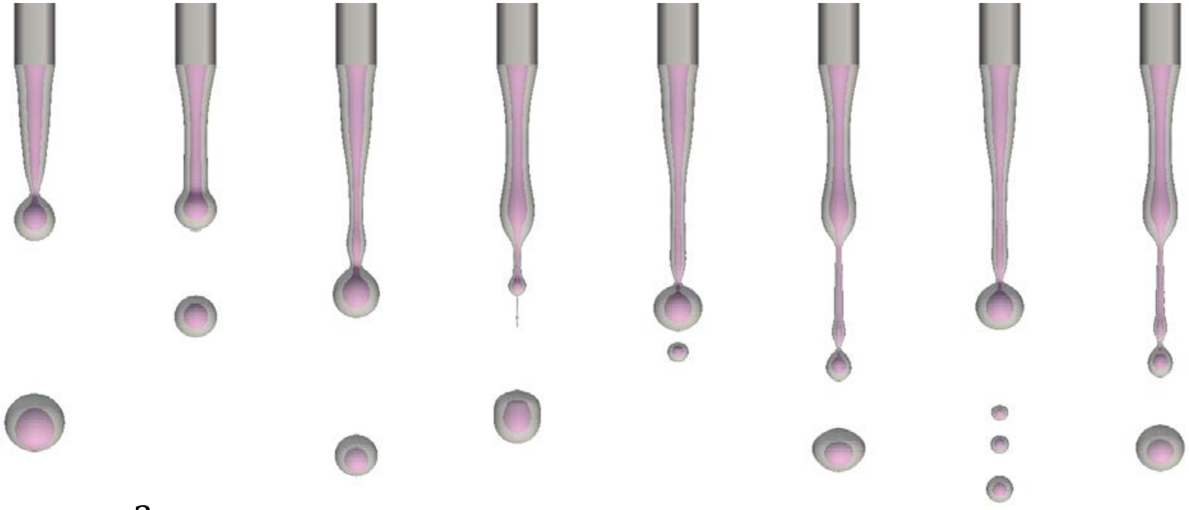
Triangulation oriented mesh deformation



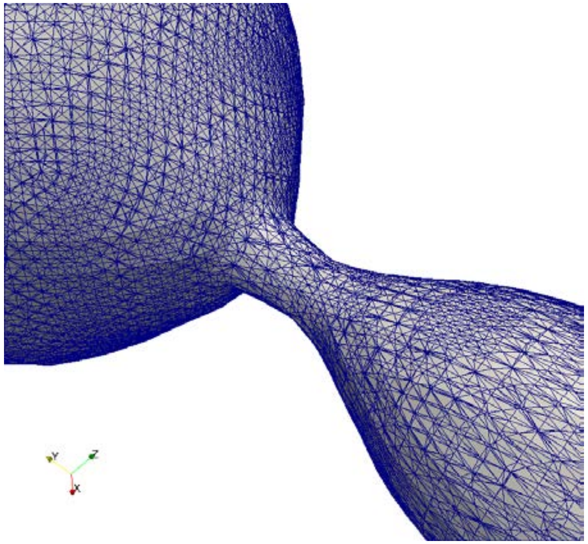
Encapsulation via modulation

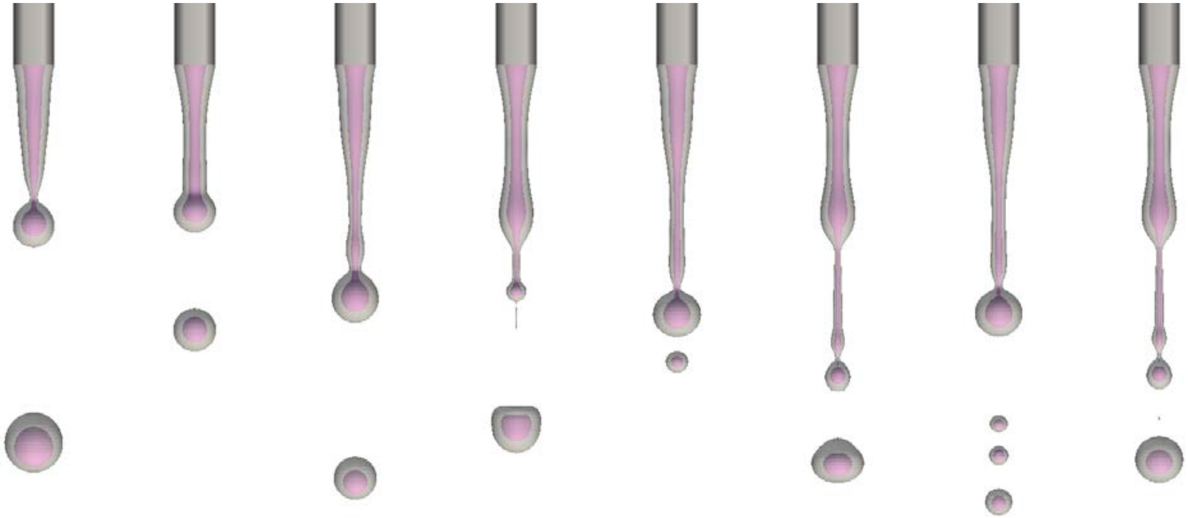
Influence of the mesh resolution → mesh convergence





~30% less surface resolution in a 1.5^3 larger domain





Encapsulation via modulation

Non-Newtonian shell / Newtonian core material

<u>Viscosity model:</u>

Shear thinning power law:

$$\mu = \mu_0(\varepsilon + \dot{\gamma})^{n-1}$$

where

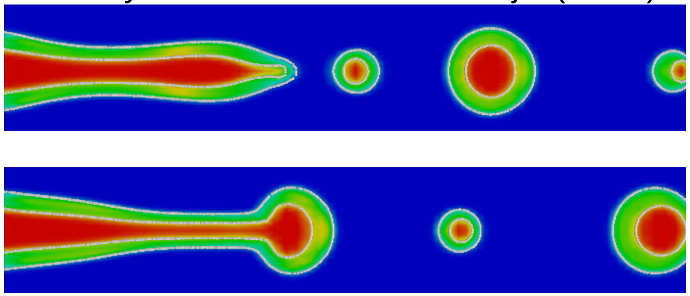
$$\dot{\gamma} = \|D(u)\| = \left\|\frac{1}{2}[\nabla u + (\nabla u)^T]\right\|$$

$$\varepsilon = 10^{-4}$$

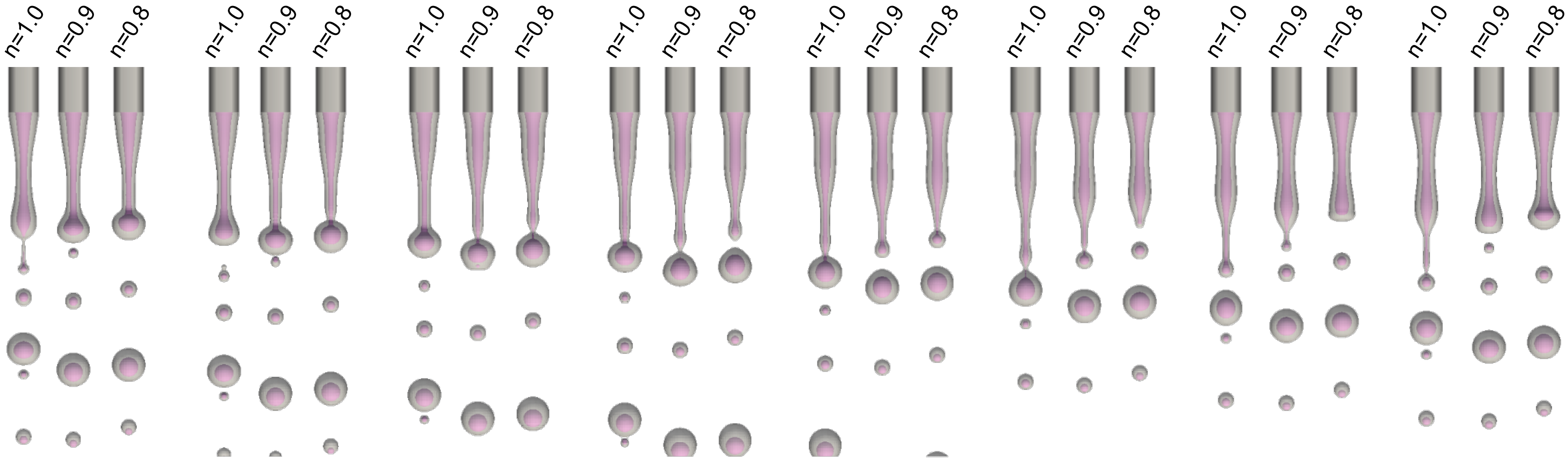
<u>Solver adjustments</u>

- Fixed point iteration for the nonlinearity
- Defect evaluation with the deformation tensor
- Preconditioned with shear dependent diff. operator

Viscosity distribution in the laminar jet (n=0.8)



Increasing shear thinning effects leading to suppressed satellite droplet formation



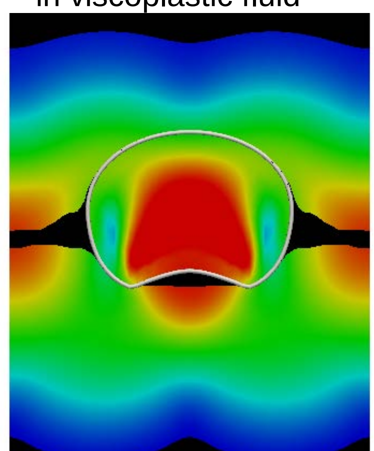
Conclusions

- ALE based grid deformation guarantees a **speedup** equivalent to one resolution level (that corresponds to 8 times better performance compared to a static mesh simulation with a comparable resolution)
- High order discretization together with the developed reinitialization procedure guarantees excellent mass conservation and convergence properties
- The simulation tool has been validated in a sequence of stages of development
- The developed production code is configured for realistic encapsulation processes

Outlook

Encapsulation in the framework of fluids obeying more specific rheological models:
 - Viscoelastic fluids (single phase with LCR is already implemented)
 - Viscoplastic fluids (cooperation with Prof. Frigaard @ Vancouver)

Gas bubble encapsulation in viscoplastic fluid



Thank You for Your attention