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DFG SPP 1740

Numerical simulation techniques for the efficient and accurate treatment of local fluidic transport processes together with chemical reactions

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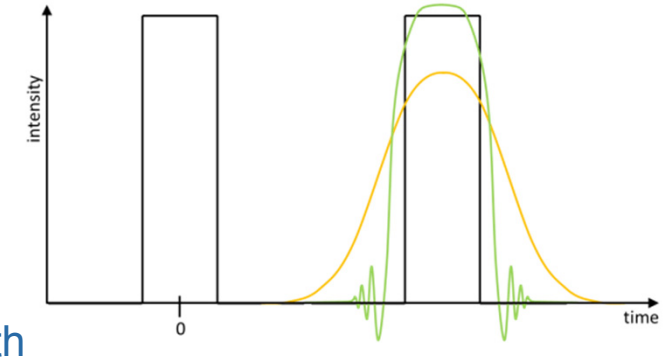
Scientific goals

Extend the up-to-now developed and validated methodology and realize the corresponding software implementation in the CFD package FEATFLOW.
The main numerical ingredients to be combined/extended are the following:

- high-resolution Algebraic Flux Correction (AFC) stabilization schemes to suppress numerical diffusion and to prevent nonphysical oscillations
- locally adaptive Grid Deformation (GD) techniques applied on (general) unstructured meshes with the aim to obtain high-resolution computational meshes satisfying additional requirements on the relative orientation with respect to local velocity fields in order to further decrease the extent of numerical diffusion
- time-scale independent reaction modules for the treatment of mutually coupled fast chemical reactions supplemented with appropriate models to reflect the extent of segregation of the individual species
- High-order Level Set techniques for accurate tracking of fluid interfaces

High-resolution AFC stabilization

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{v}c) - \alpha \Delta c = f(c) \qquad \text{with} \quad \alpha \longrightarrow 0$$

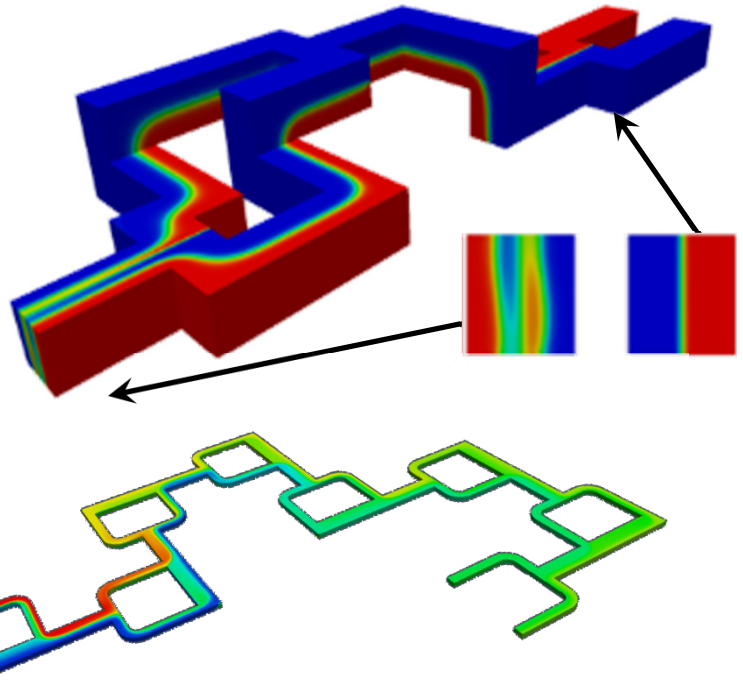


Standard discretizations face shortcomings for non-smooth solutions

- Low order methods lead to smearing
- High order methods introduce unphysical oscillations (potentially leading to simulation blowup)

<u>Remedy:</u> Algebraic Flux Correction method

- Local extremum diminishing (+)
- Positivity preserving (+)
- Transforms the linear problem to a non-linear one (-)
- Robust and highly accurate (+)



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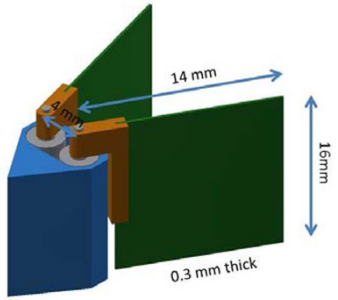
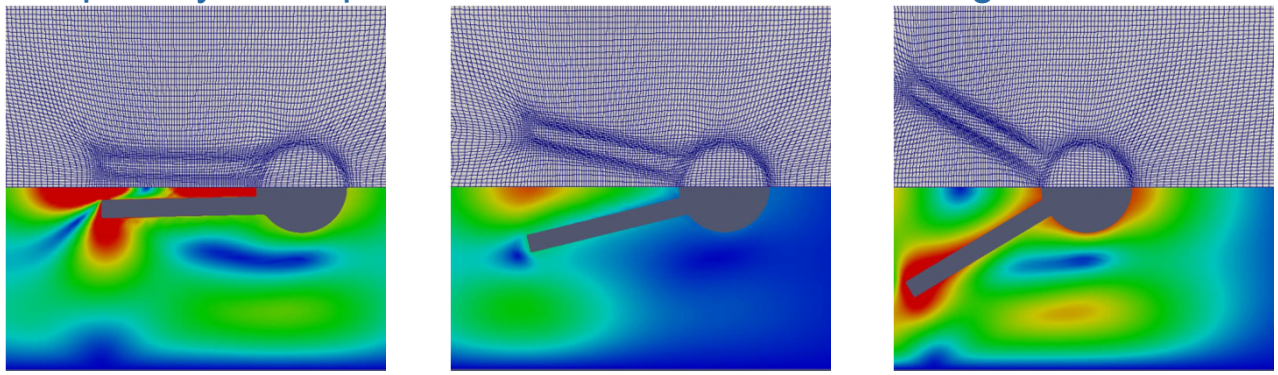
PDE-free mesh deformation method

- Construction of (dynamic) monitor function (distance to interface, curvature, concentration gradients, vorticity)
- Anisotropic Laplace smoothening (fast)
- Arbitrary Lagrangian-Eulerian Method (ALE) for non-stationary problems
- Handling geometrically complex/dynamic problems in the framework moving interfaces

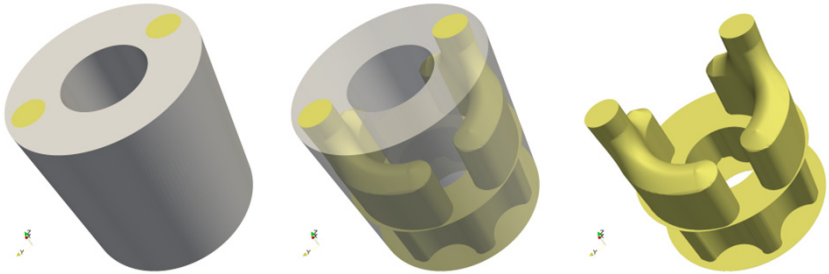
Microfishes

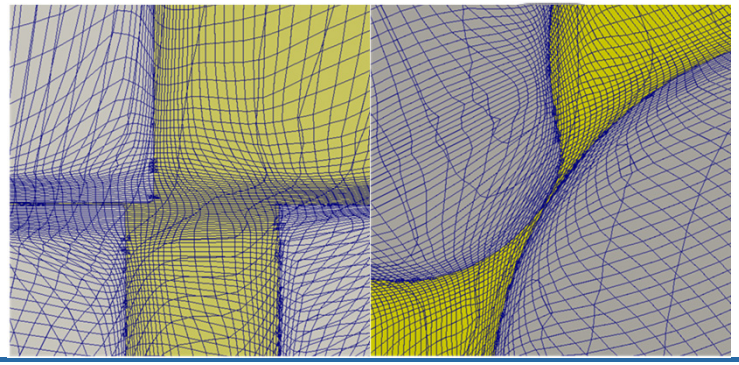




Scientific cooperation with: Prof. Fischer @ MPI IS Stuttgart, Published in: Nature Communications, 2014.

Micro gear pumps





Industrial cooperation with: Roche @ Switzerland, 2015.

Numerical simulation of chemical reactions

Possible difficulties

- Extreme resolution requirements of the ch. species
- Extremely different time-scales (ch. r. vs transport)
- Micromixing – subgrid mixing models (ch.r. rate limiter)

Remedies:

→ AFC + GD

→ Operator splitting

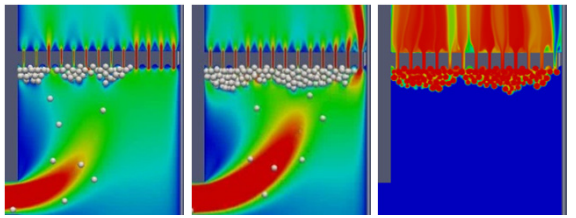
→ MEMM (Fox et al.)

PDE in spatial dimension Δt ODE in chem. species dimension $M\left(\frac{\Delta t}{M}\right)$

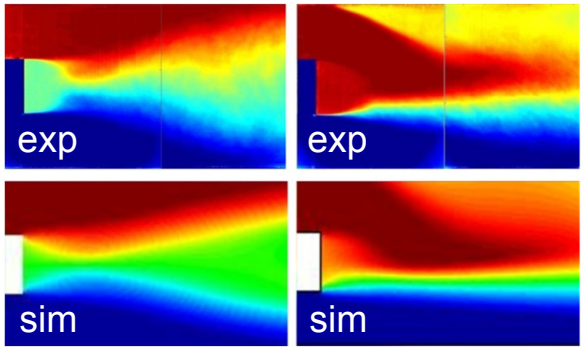
$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{v} c_i) - \alpha \Delta c_i = s(c_{j=1,2,\dots N}) \quad i = 1,2,\dots N$$

RHS terms:
Reaction mechanism/constant specific!

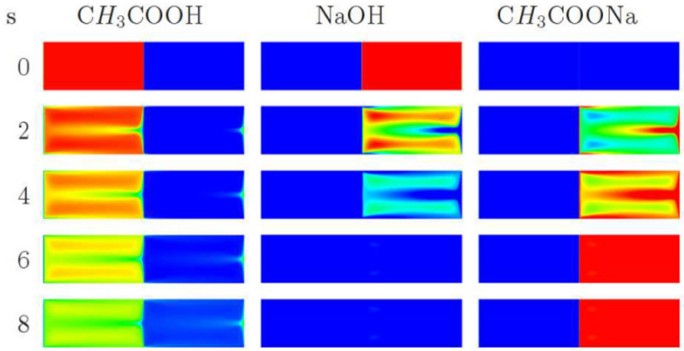
Laminar catalythic reactions (Münster)



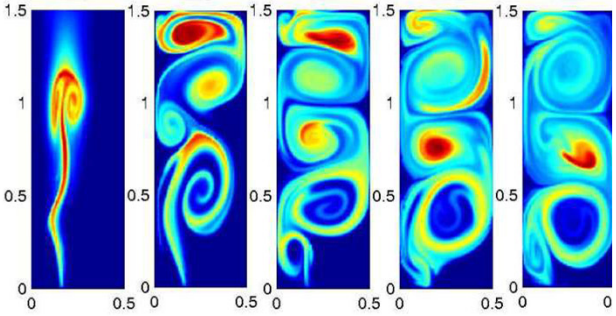
Turbulent singlephase flows (Mierka)



Laminar multiphase flows (Kashid)



Turbulent multiphase flows (Kuzmin)



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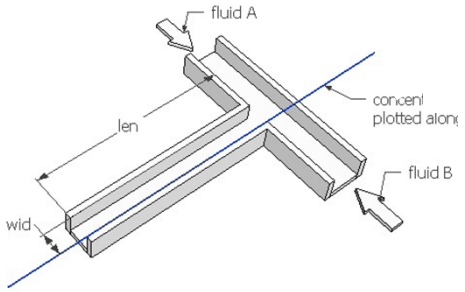
Simulation of chemical reactions (preliminary work within the SPP 1740)

$A + B \xrightarrow{k\to\infty} P$ $\quad \partial_t\phi + u\cdot\nabla\phi = \nabla\cdot(d\nabla\phi)$ with $\phi = c_A\text{-}c_B$ Toor and Chiang

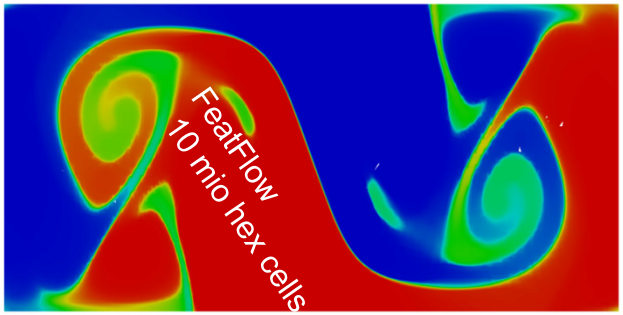


Adopted simulation technique:
Simultaneous use of two meshes /discretizations:

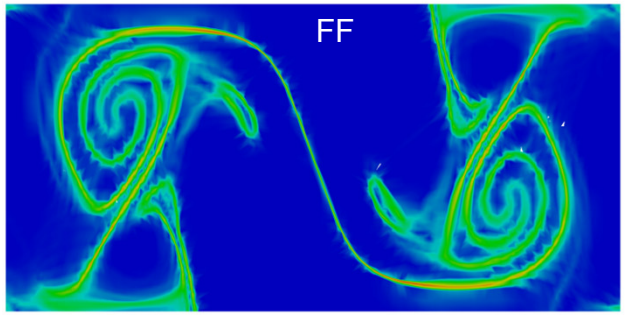
- equidistant , structured, low resolution for velocity
- deformed, structured, high resolution for passive/active scalar

Efficient and robust interpolation from mesh to mesh in parallel framework

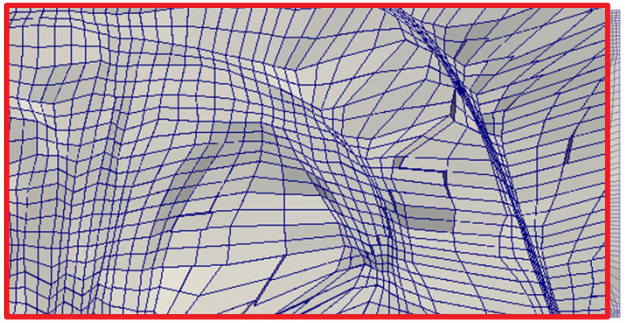
Transported scalar field ϕ



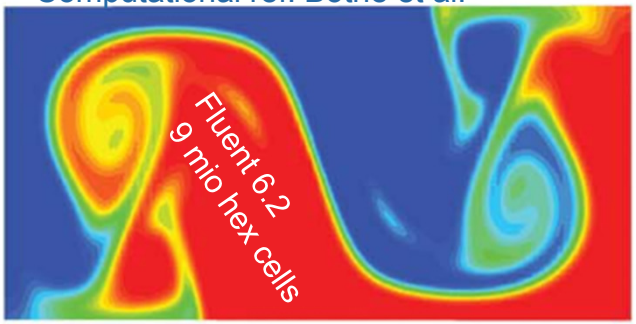
Monitor function

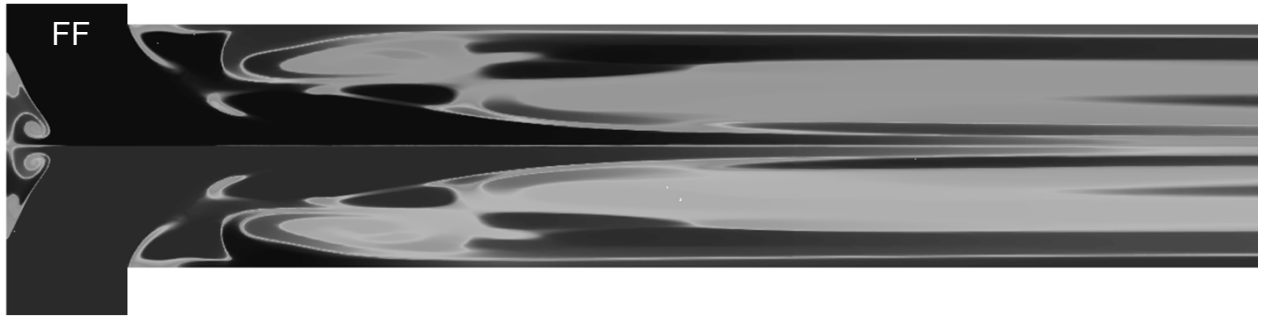


Computational mesh

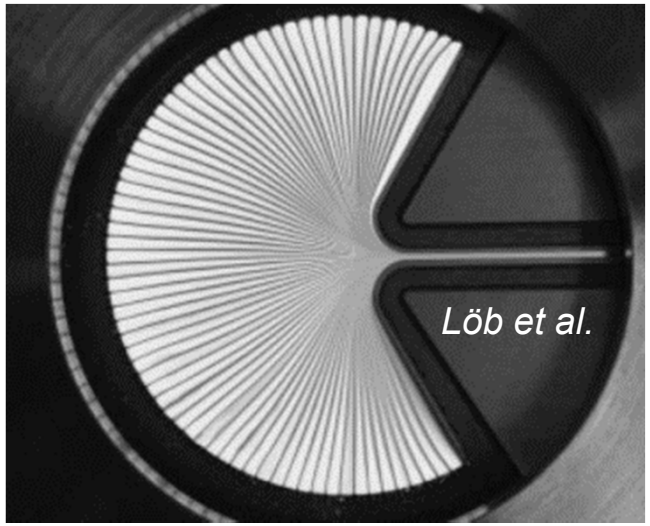


Computational ref. Bothe et al.





Simulation of the super-focus mixer (SFM)



Geometry of the final SFM with visualization of the reactants

Intantaneous reaction scheme:

$A + B \xrightarrow{k\to\infty} P$

Geometrical simplification:
Application of a twofold symmetry

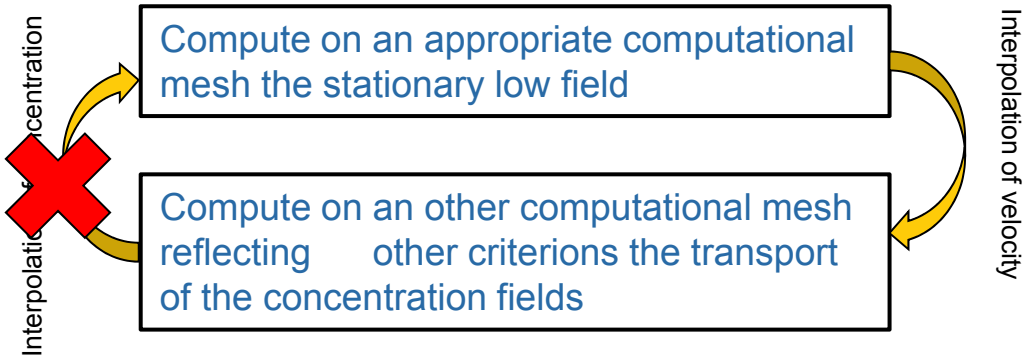
Expected maximum Re number range for flowrates

$\dot{V} = 100\ mL/h$	Re~ 50
$\dot{V} = 250\ mL/h$	Re~125
$\dot{V} = 500\ mL/h$	Re~250

… at the outflow

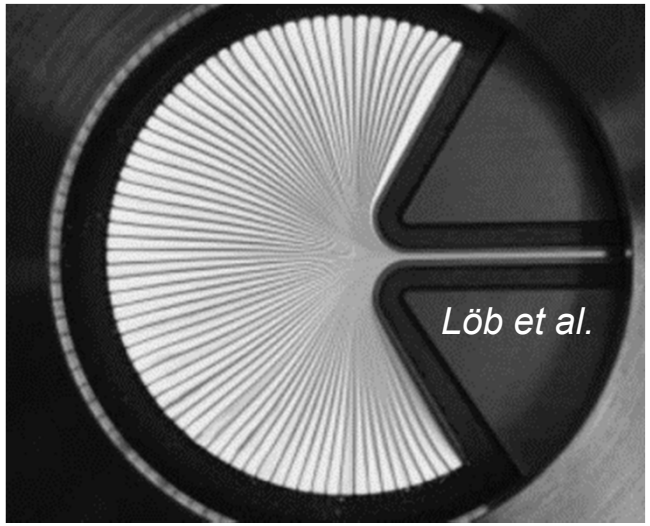
For stationary inflow conditions
stationary velocity fields are to be expected!

This fact defines the computational strategy:



…. if there is only a negligible back-coupling (dilute solutions)

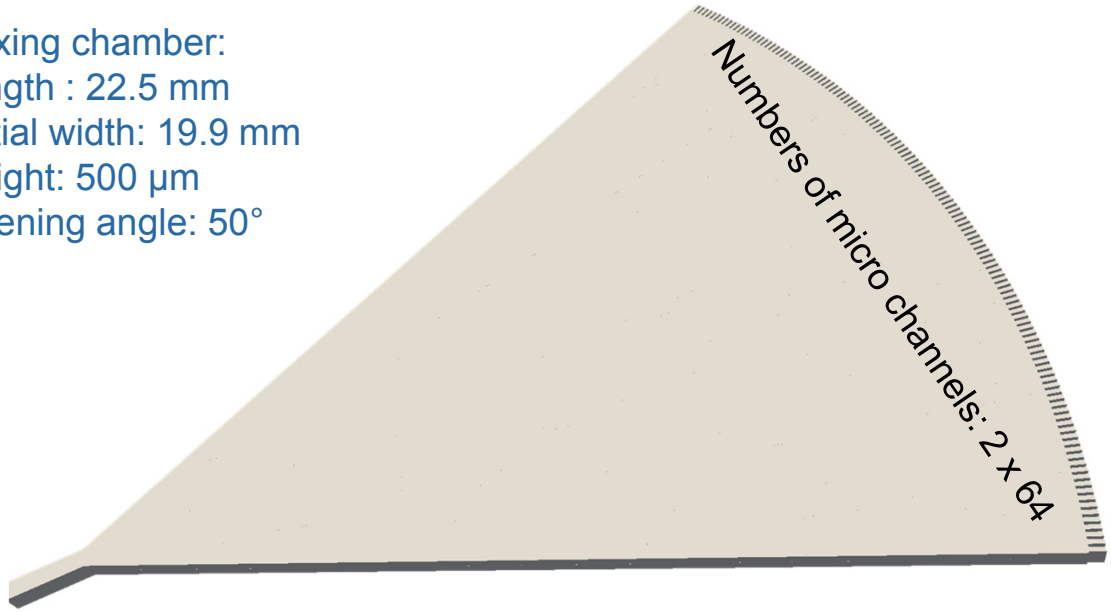
Simulation of the super-focus mixer (SFM)



Geometry of the final SFM with visualization of the reactants

Intermediate SFM geometry and operation conditions

Mixing chamber:
length : 22.5 mm
initial width: 19.9 mm
height: 500 µm
opening angle: 50°



Intantaneous reaction scheme:

$$A + B \xrightarrow{k\to\infty} P$$

Investigated flowrates:
100 mL/h
250 mL/h
500 mL/h

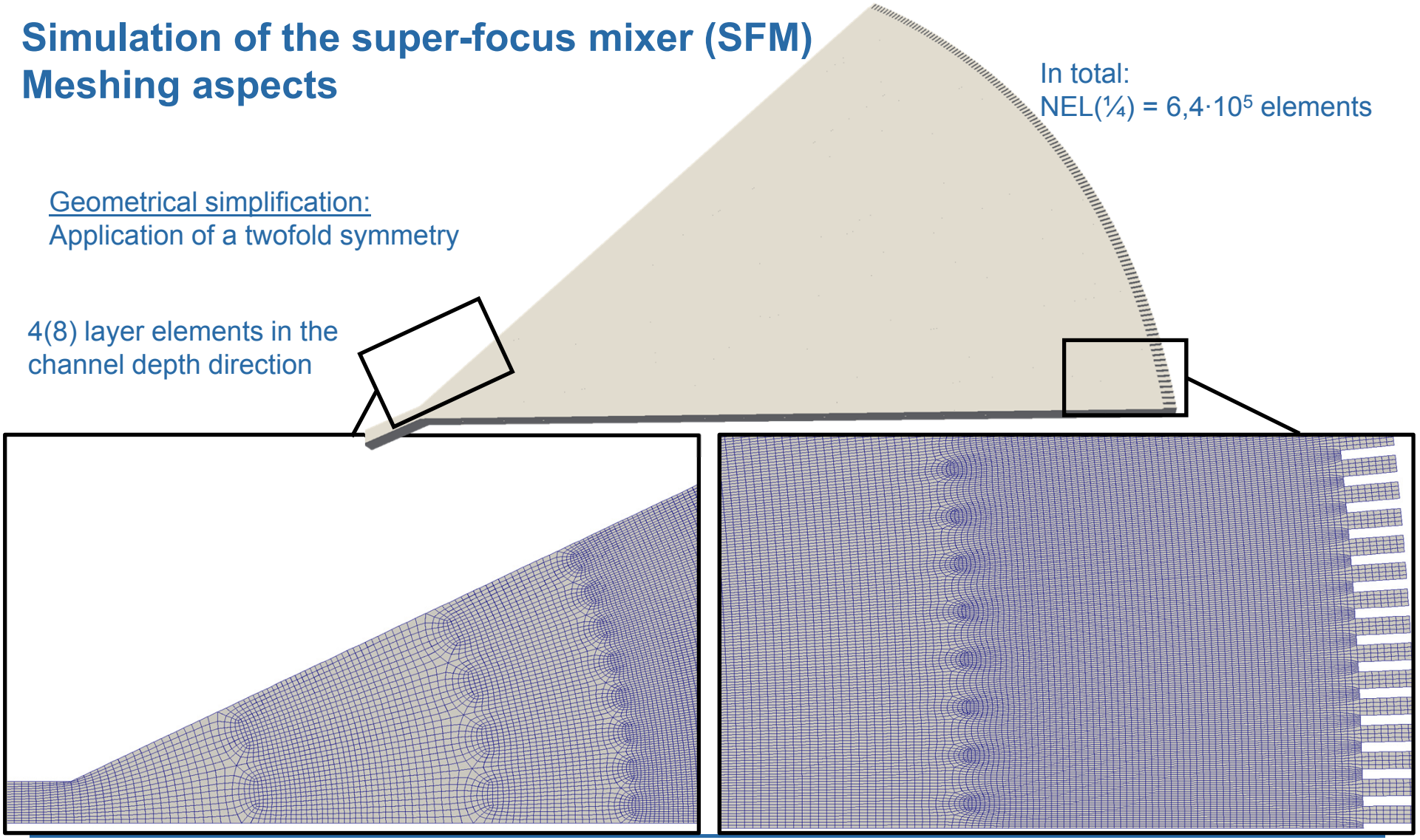
$$D_{A,B} = 3.0 \cdot 10^{-10} m^2/s$$

Simulation of the super-focus mixer (SFM)
Meshing aspects

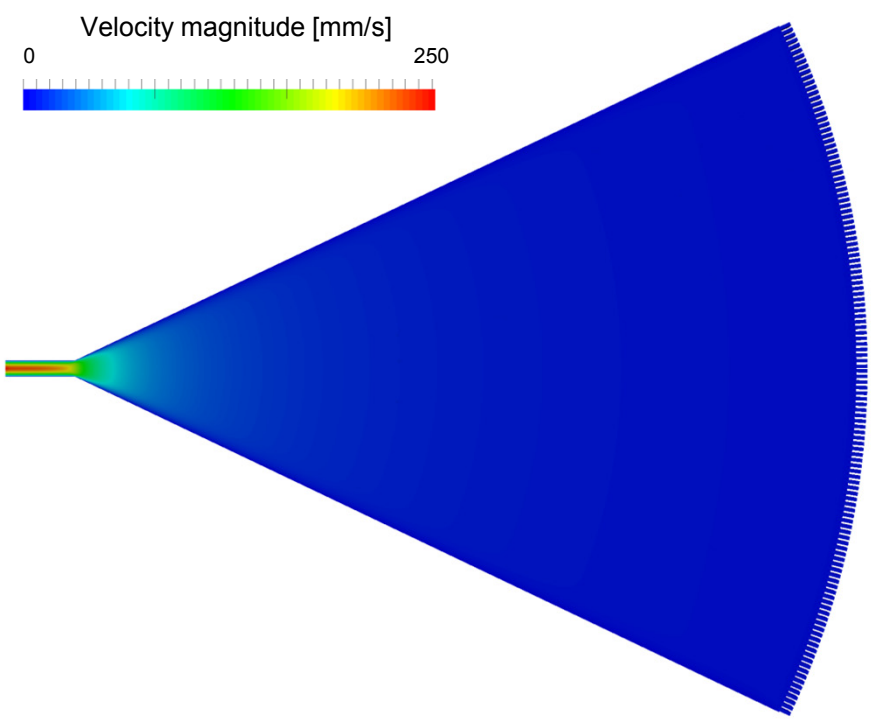
In total:
NEL(¼) = $6{,}4 \cdot 10^5$ elements

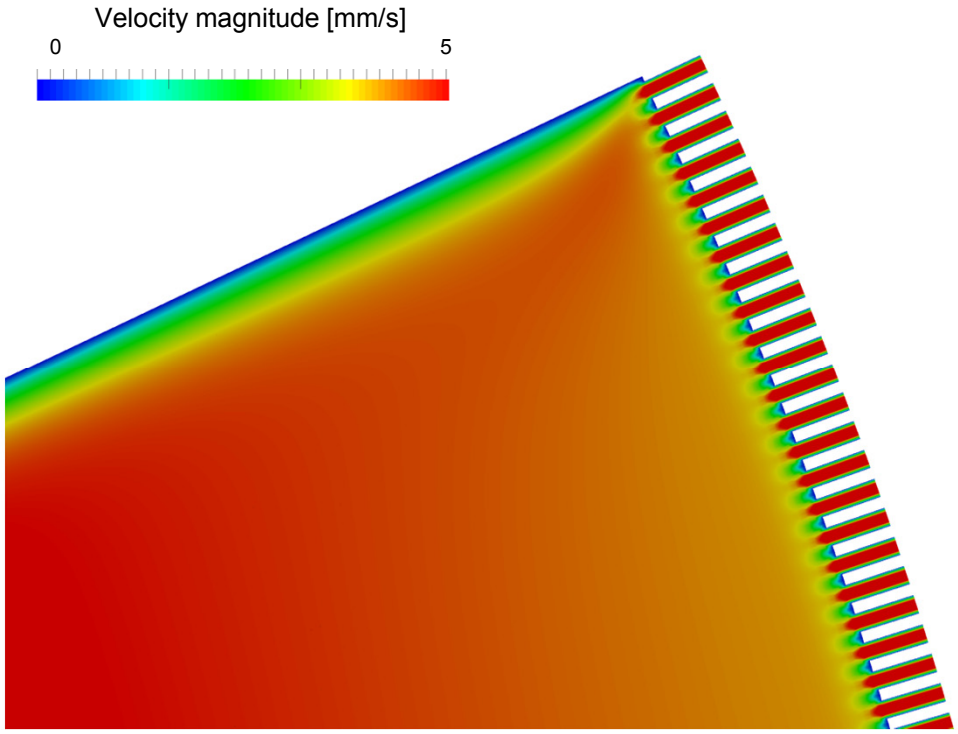
Geometrical simplification:
Application of a twofold symmetry

4(8) layer elements in the channel depth direction



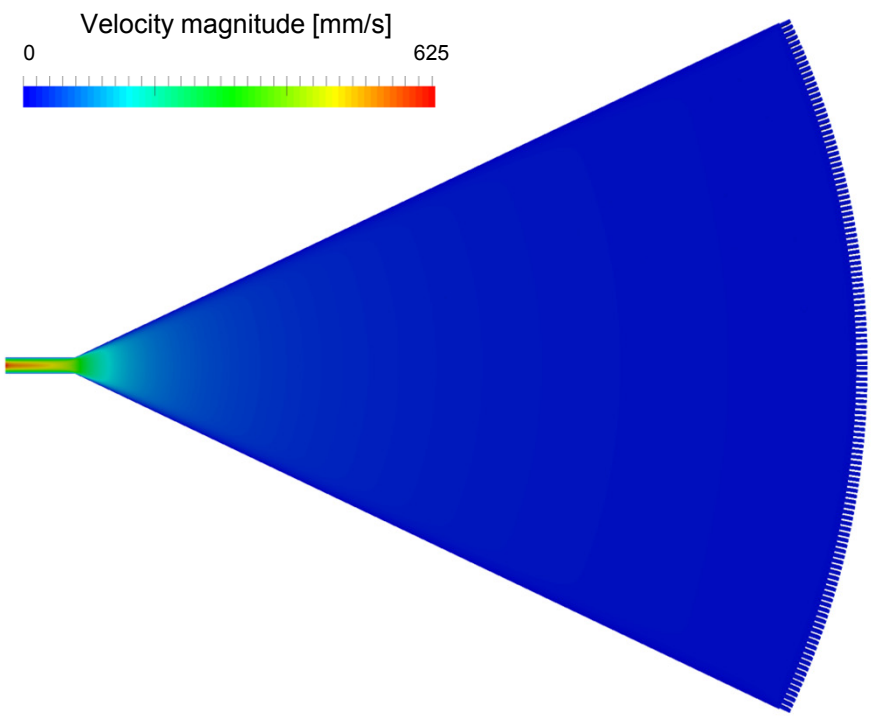
Computationally obtained flowfield in the Superfocus mixer

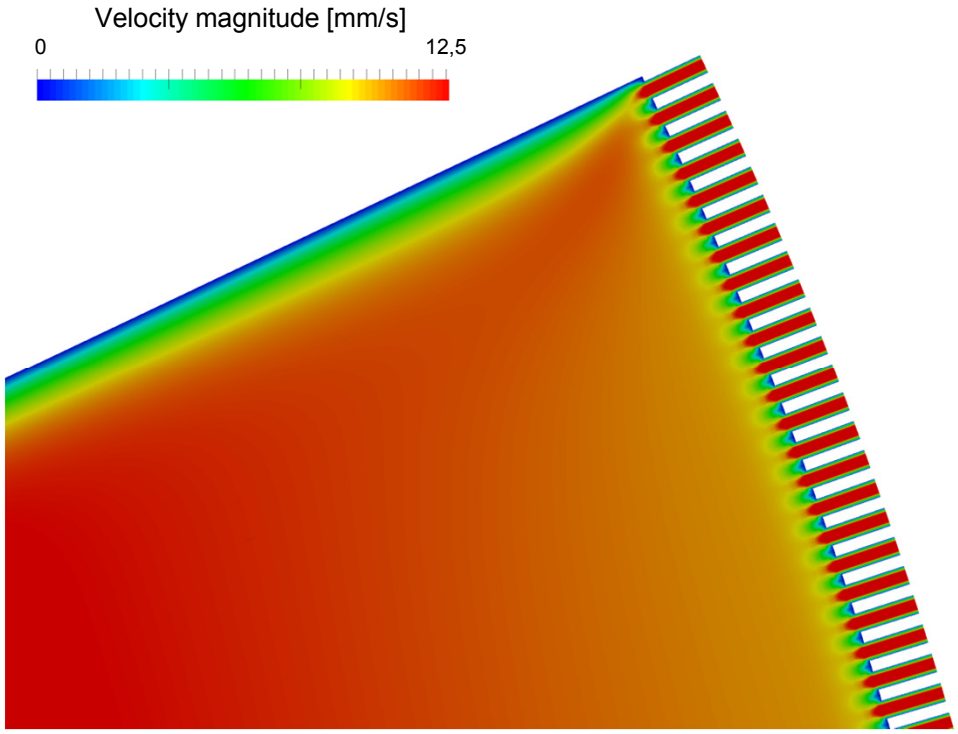




Flowrate: $\dot{V} = 100\, mL/h$

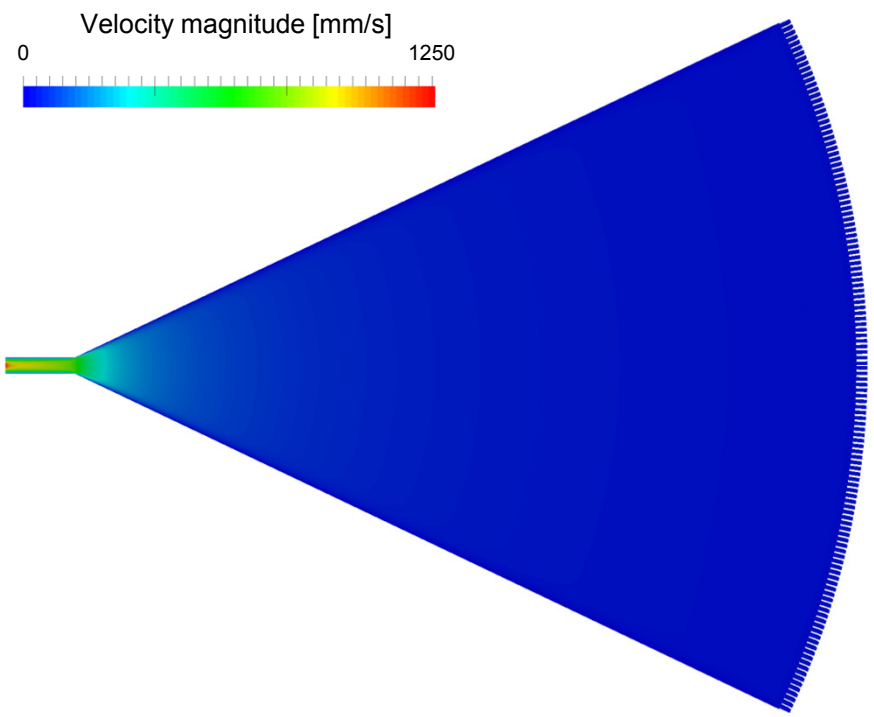
Computationally obtained flowfield in the Superfocus mixer

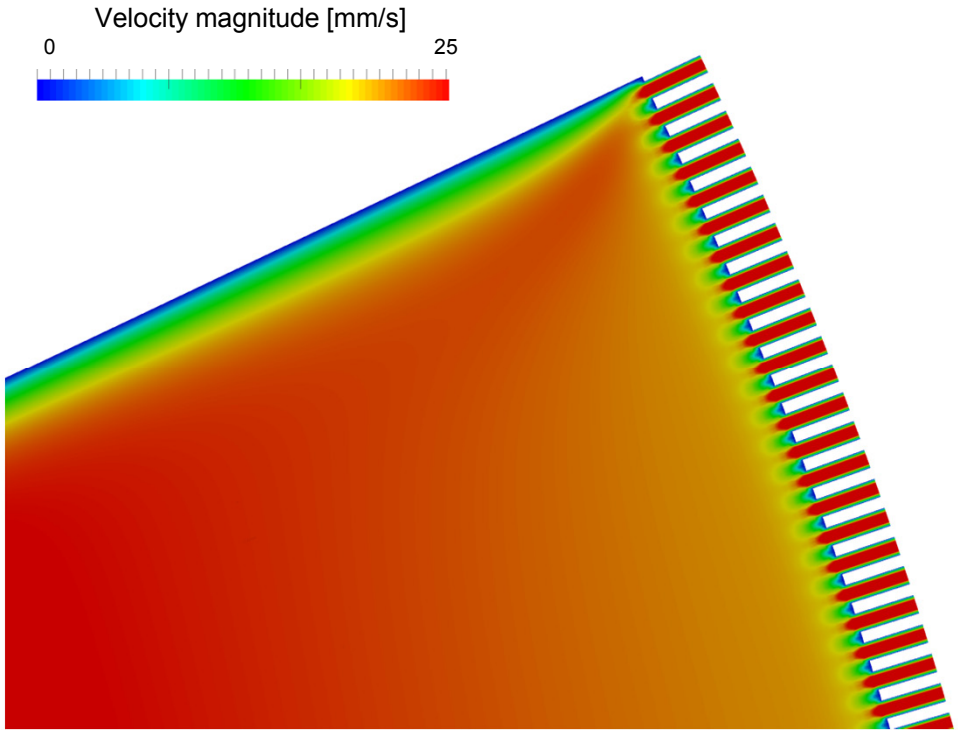




Flowrate: $\dot{V} = 250\, mL/h$

Computationally obtained flowfield in the Superfocus mixer





Flowrate: $\dot{V} = 500\, mL/h$

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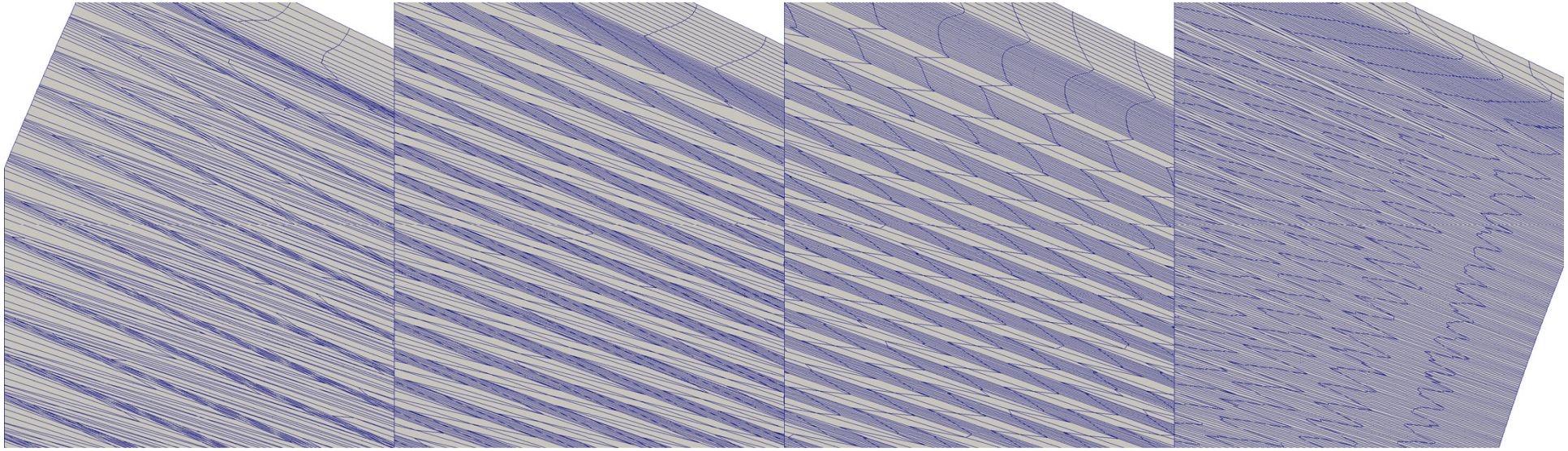
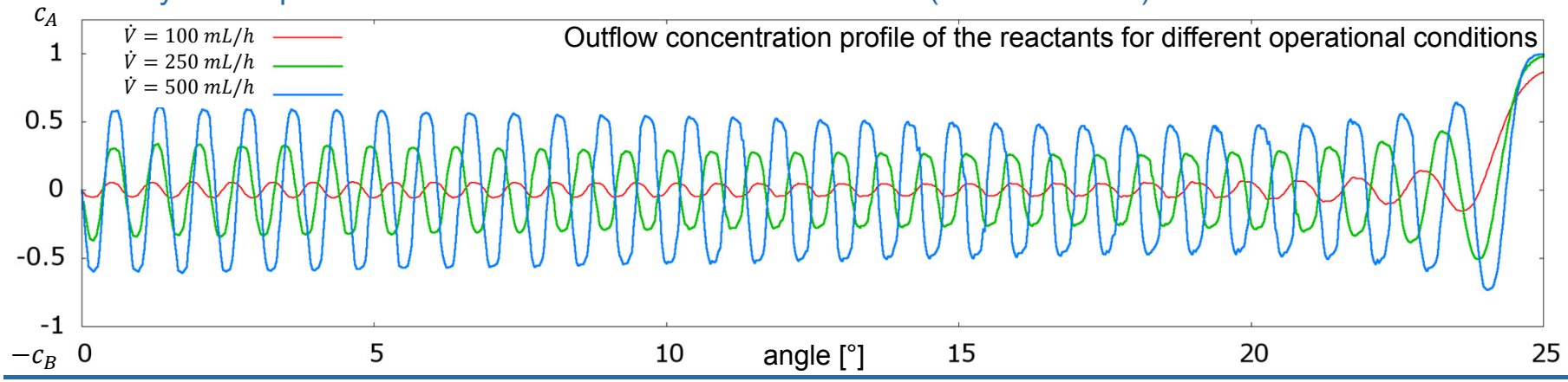
Exploiting the two-fold symmetry only the ¼ of the domain needs to be meshed.
Two consecutive mesh resolutions are used NEL(¼) = 1,25·10^6 (M_1) and 10 ·10^6 (M_2) elements.



Velocity is interpolated in an L2 sense from the unstructured (non-deformed) mesh to the deformed mesh.



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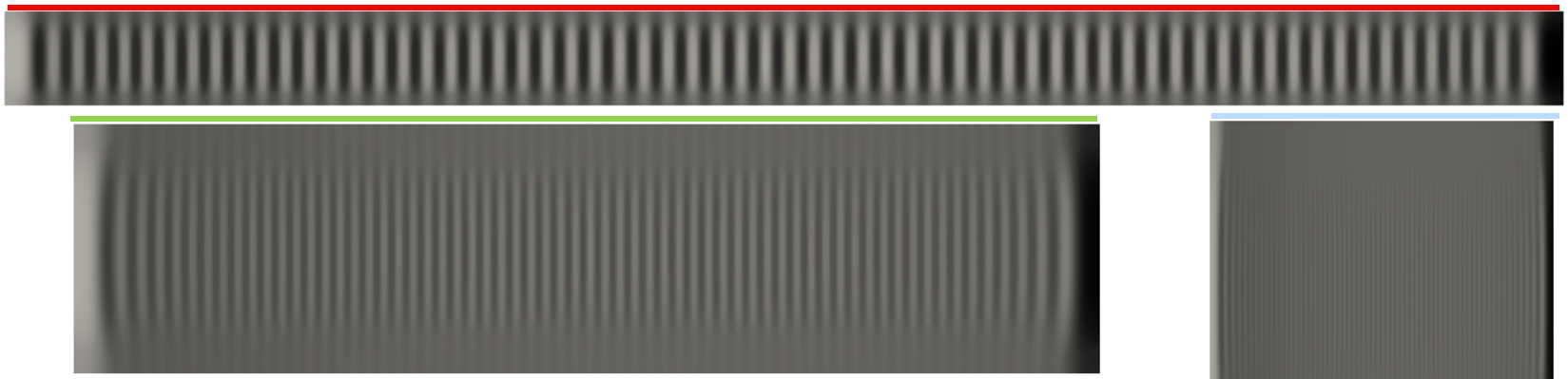
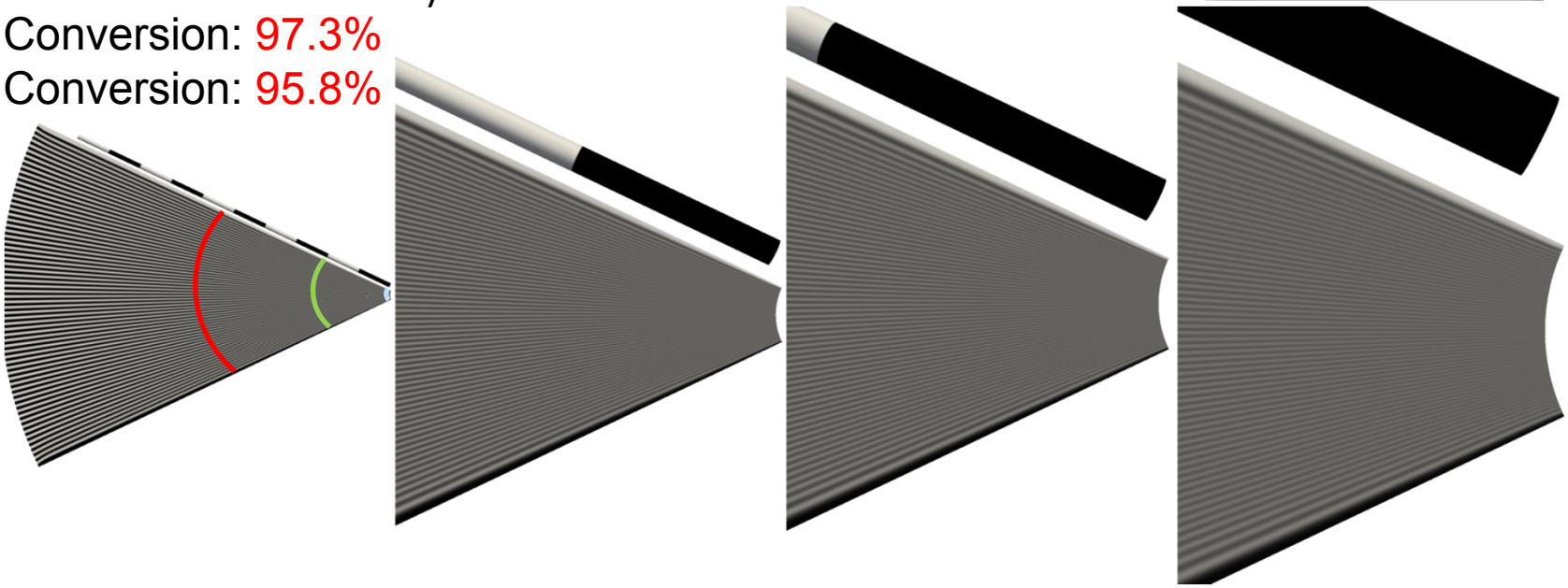


Flowrate: $\dot{V} = 100mL/h$

M_1 Conversion: 97.3%

M_2 Conversion: 95.8%



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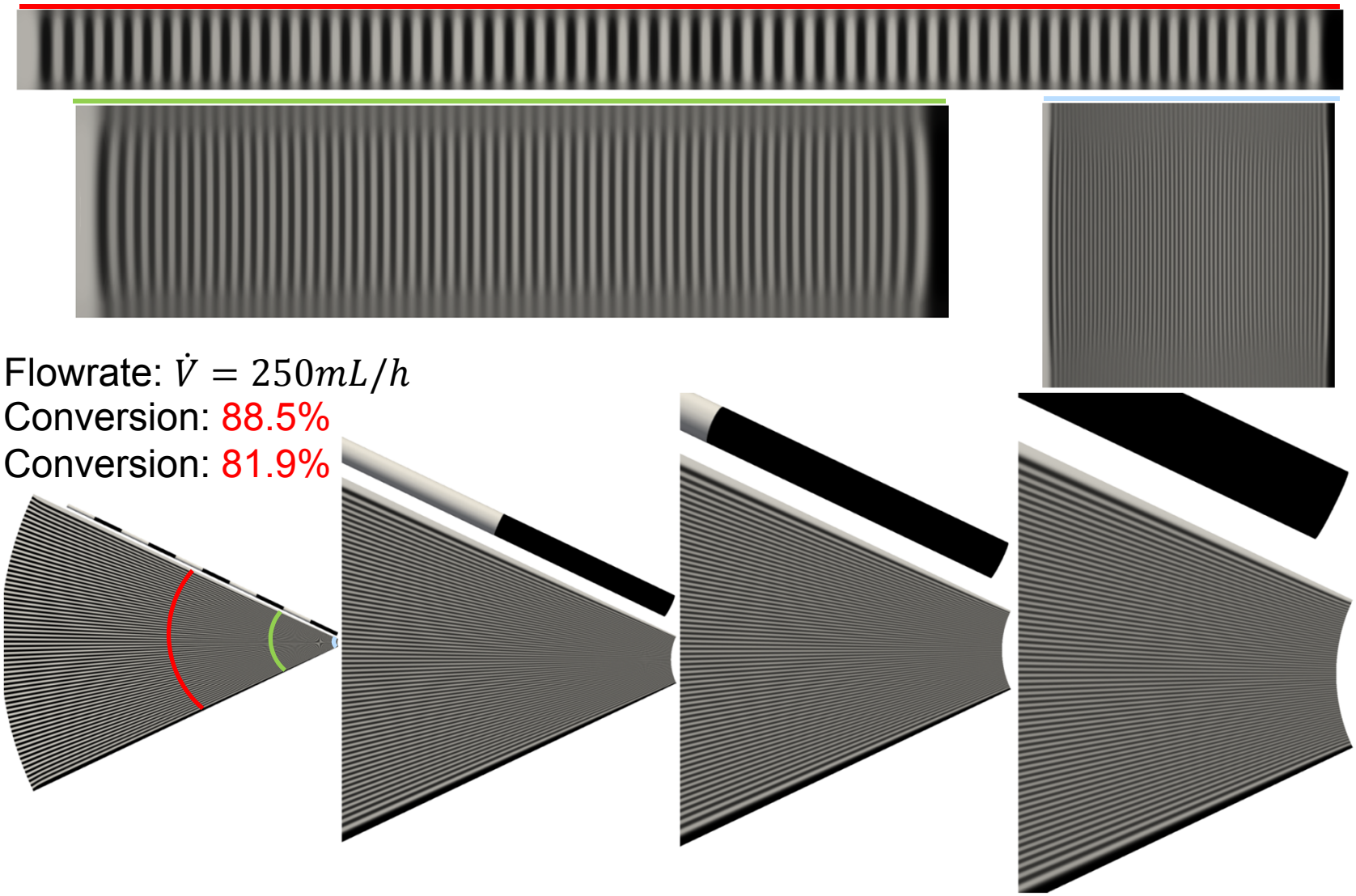

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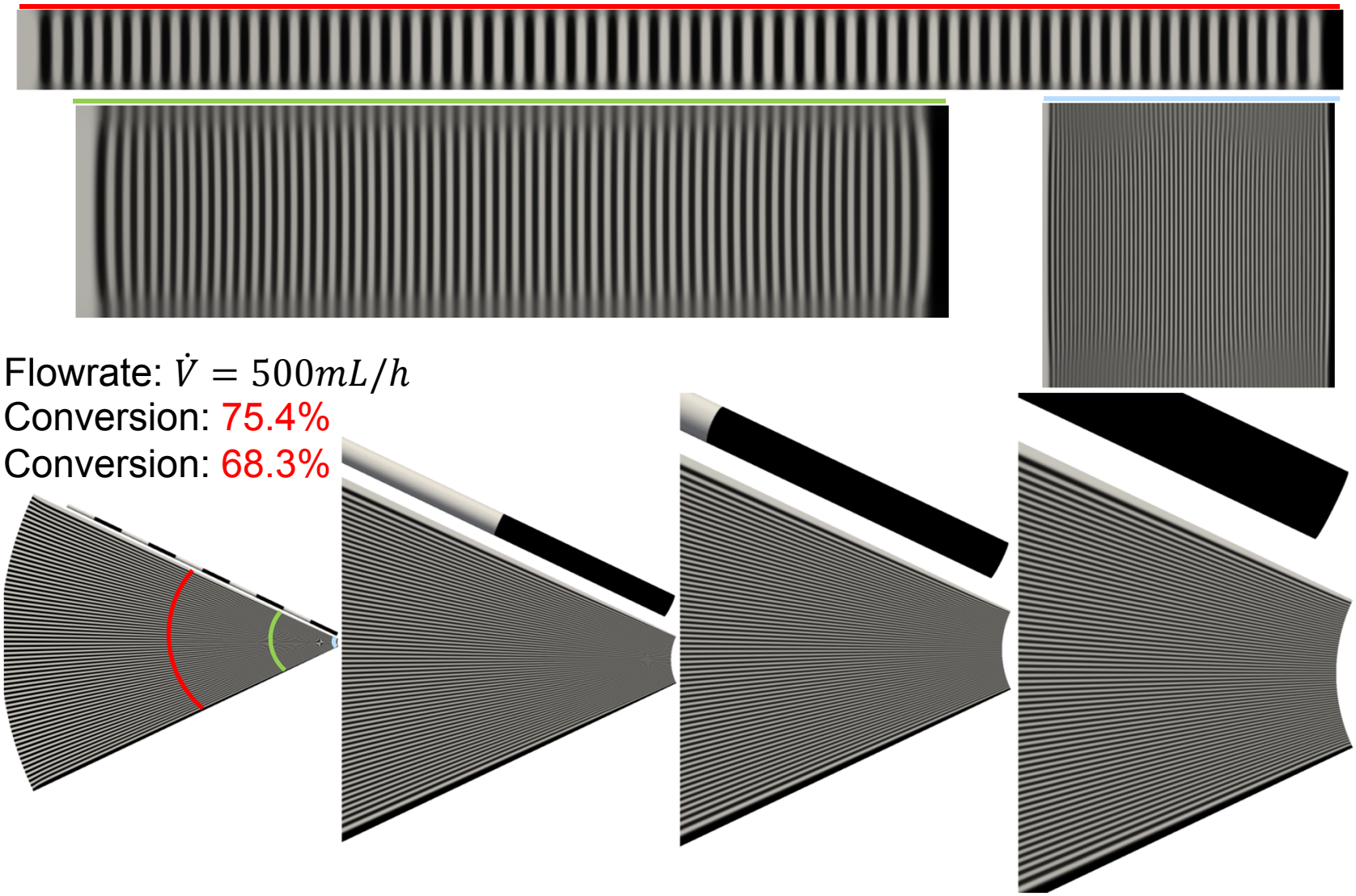

Next tasks:

Superfofus mixer

Modeling:
- Quantification of the product distribution
- Extension to general reaction schemes (consecutive competitive reaction networks)
- Comparison with experimental data

Numerics:
- Convergence estimation for simplified geometries in relation to flowrates (Re numbers)

Taylor flow

- Cooperation and joining the SPP 1506 Benchmark initiative (Pure flow)
- Combination of the Level Set techniques with transport of species + mass transport
- Taking part and support the “upgraded” benchmark initiative

What do we need … ?

Results of experimental observations serving as reference for validation purposes
- Integral and spatial (+temporal) measured data obtained for gradually increased (geometrical, reaction) complexity
- Local reaction mechanisms/constants under well defined operation conditions
- Practical suggestions for the design of a joint benchmark initiative supported with exp./sim. results

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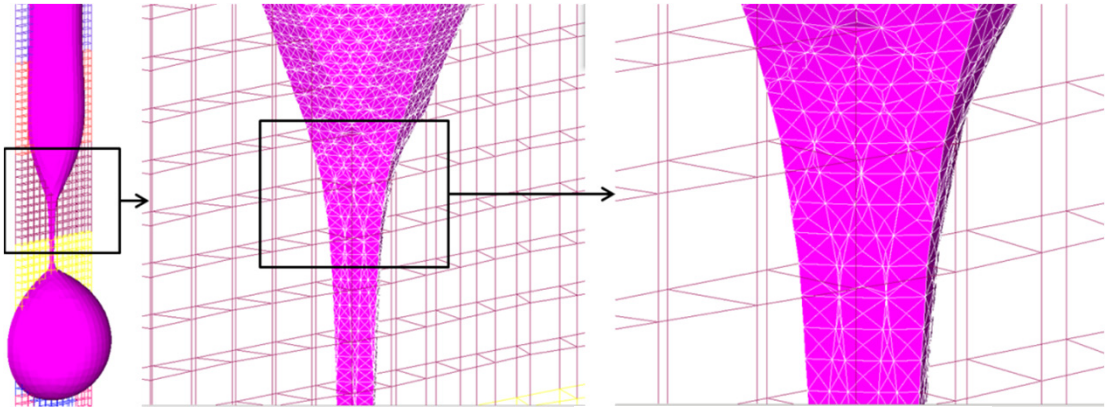
Level Set based Interface tracking

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

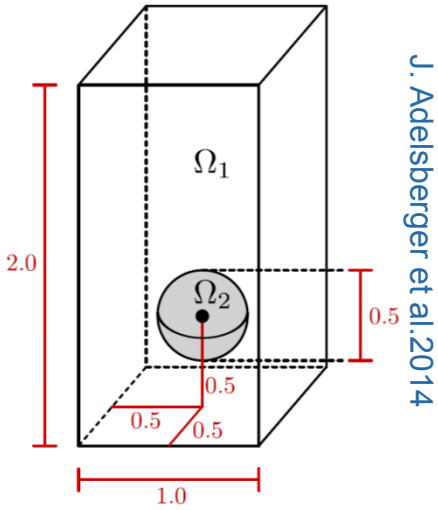
- High order discretization
- Surface reconstruction in terms of surface triangulation
- Recursive subdivision of interface intersected elements (downward direction)
- Hierarchical storage of triangulated subsets (upward direction)
- Reinitialization in terms of L_2 projection of the distance distribution



3D Rising Bubble benchmark initiative:

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

	μ_l	μ_g	ρ_l	ρ_g	σ_{12}	g_z
Case 1	10	1	1000	100	24,5	-0,98
Case 2	10	0,1	1000	1	1,96	-0,98



J. Adelsberger et al.2014

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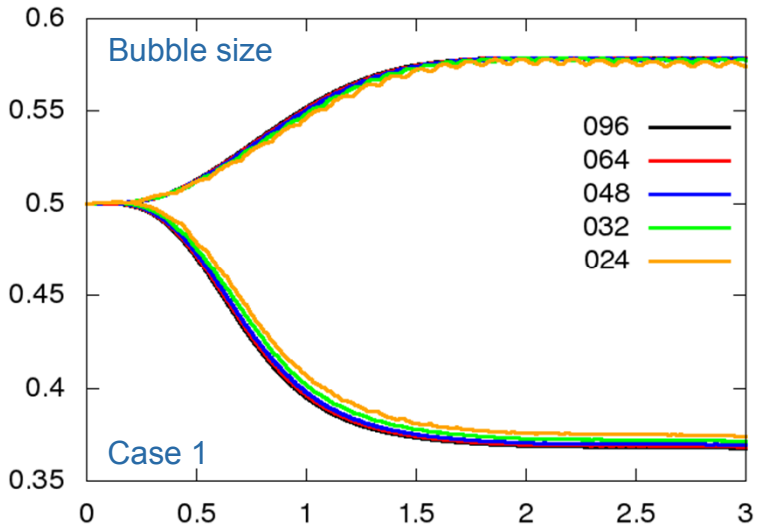
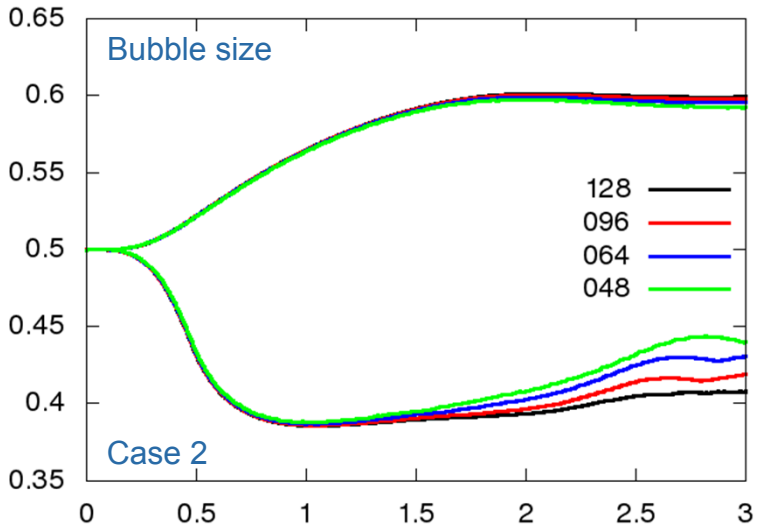
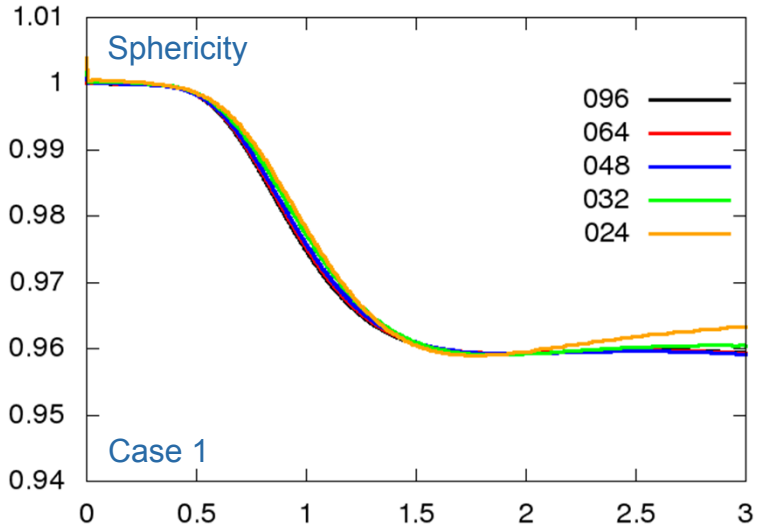
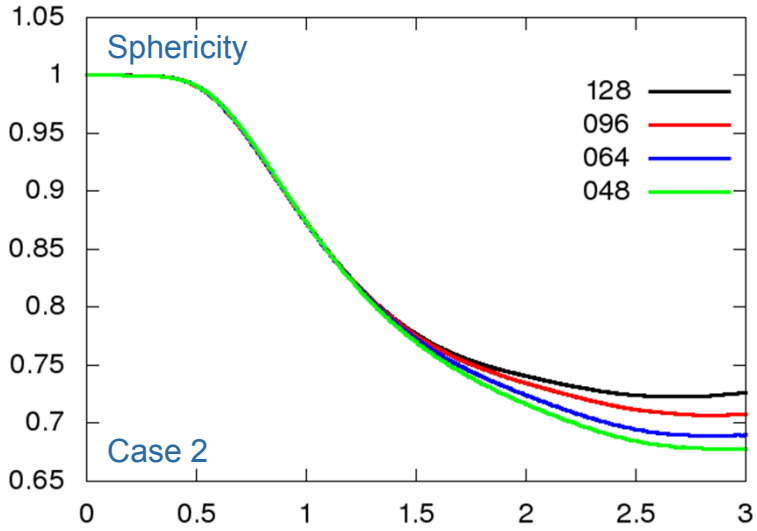
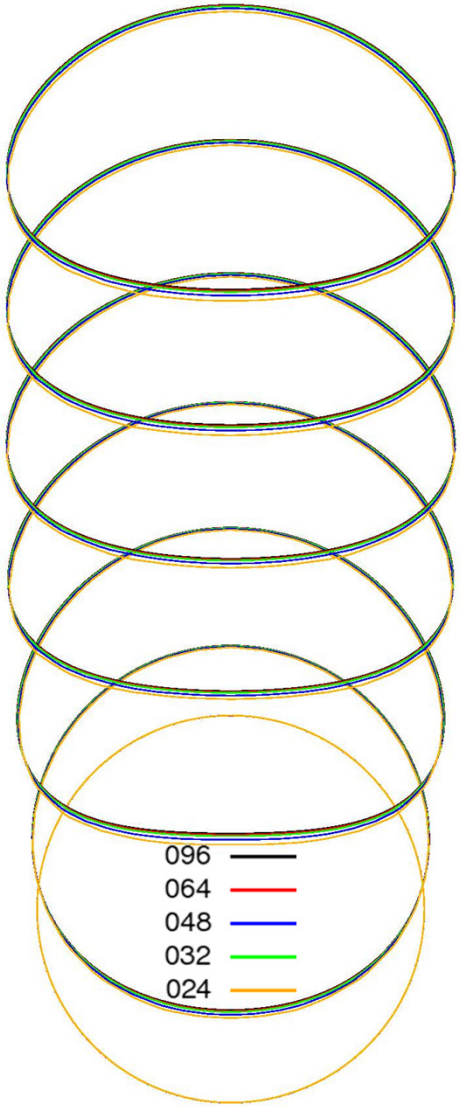


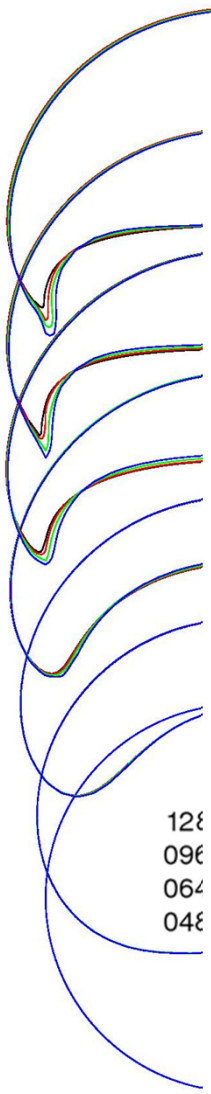


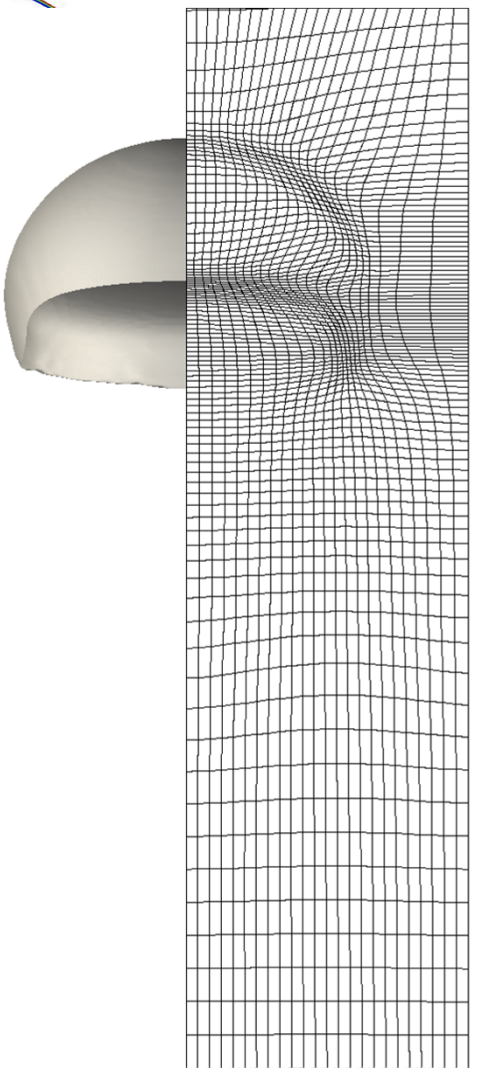




Future perspectives of MD







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Chair of Applied Mathematics and Numerics, LS III

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