Coalescence and transport of bubbles and drops

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Outline

Subject:
a new method for curvature estimation with superior accuracy at low resolutions

- Formulation
- Benchmarks
  - curvature of a sphere
  - translating droplet
- Applications
  - bubble coalescence
  - turbulent flows with bubbles

Formulation

Model

Two-component incompressible flow

- Navier-Stokes equations

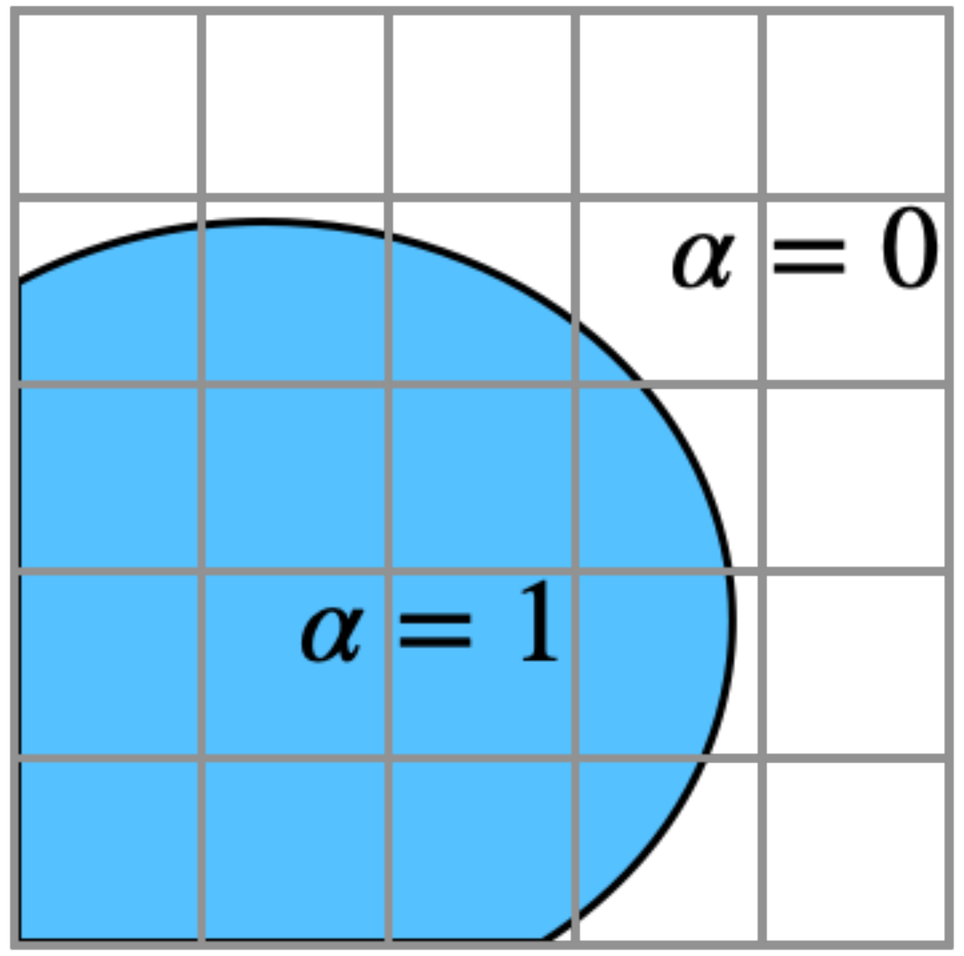
$$\nabla \cdot \mathbf{v} = 0$$

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

- Advection of volume fraction

$$\frac{\partial \alpha}{\partial t} + (\mathbf{v} \cdot \nabla)\alpha = 0$$

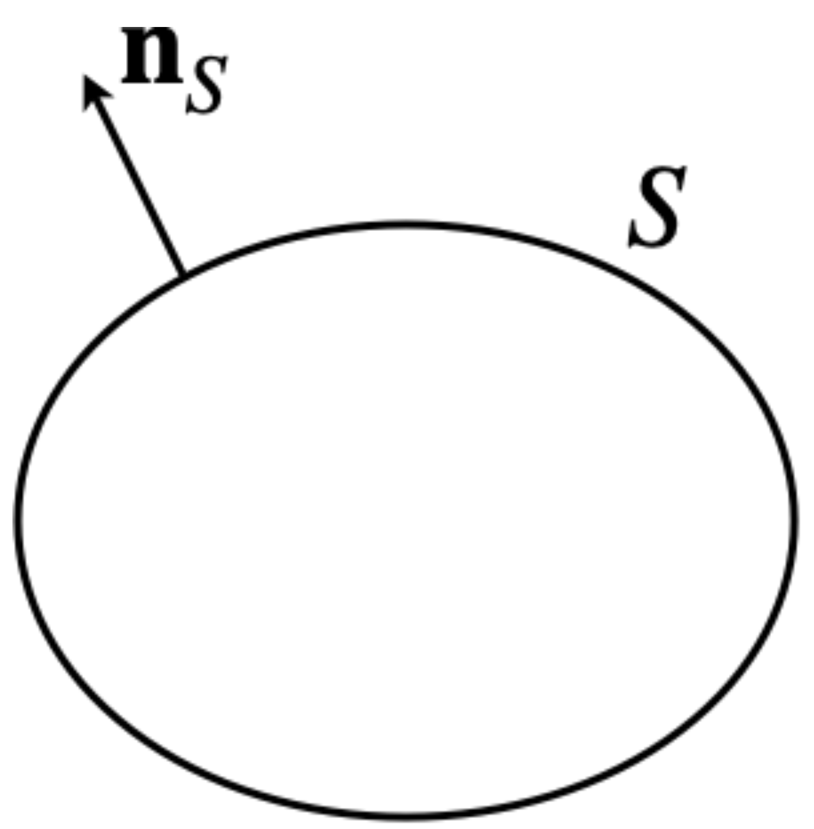
$$\rho = (1-\alpha)\rho_1 + \alpha\rho_2$$
$$\mu = (1-\alpha)\mu_1 + \alpha\mu_2$$



- Discretization
  - Finite Volume on a uniform grid
  - SIMPLE for pressure coupling
  - VOF advection [Aulisa 2007]
- Implementation
  - Hypre for linear solvers [Falgout 2002]
  - Cubism for parallelization [Wermelinger 2018]

Surface tension

- Calculation of surface tension $\mathbf{f}_\sigma = \sigma\,\kappa\,\mathbf{n}_S\,\delta_S$
  relies on interface curvature $\kappa = \nabla_S \cdot \mathbf{n}_S$



- Existing methods show poor accuracy at low resolution
  - volume fraction [Brackbill 1992]
  - level-set [Sussman 1998]
  - height functions [Cummins 2005]
  - generalized height functions:
    parabolic fit to reconstructed interface [Popinet 2009]

VOF reconstruction

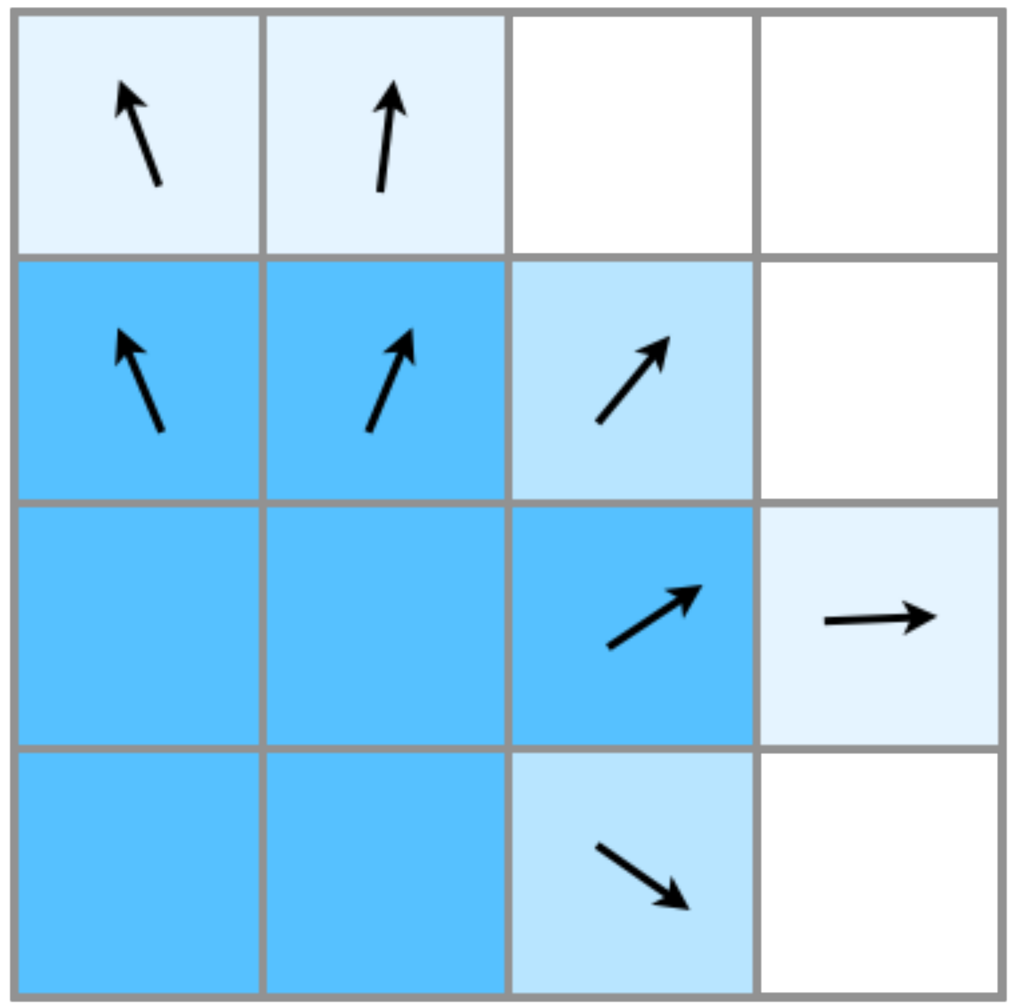
Piecewise-linear interface from volume fraction

Line segments in 2D and polygons in 3D

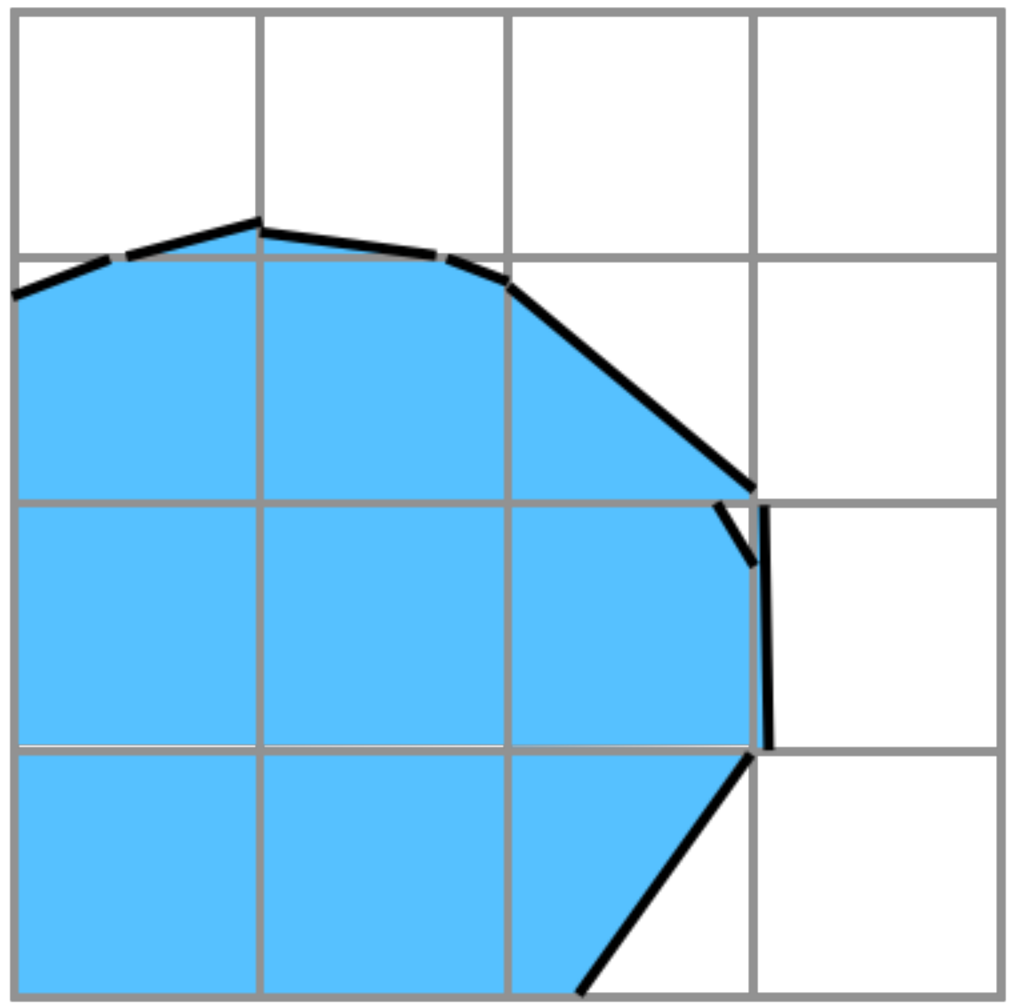
- Volume fraction field

0.1	0.1	0	0
0.9	0.9	0.5	0
1	1	0.9	0.1
1	1	0.6	0

- Normals as gradients



- Lines cutting cells
  at given volume fraction



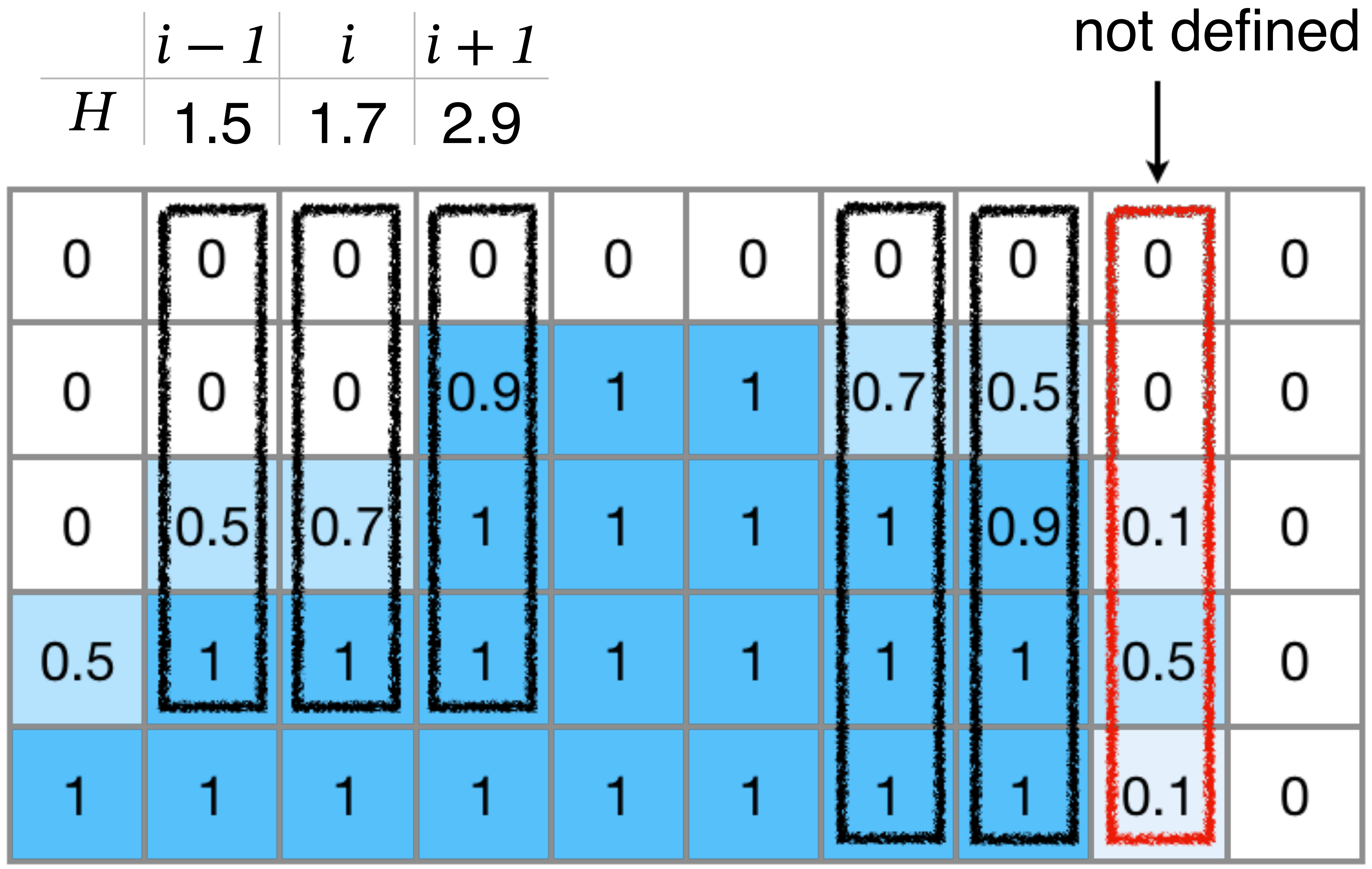
Height functions

Generalized height function method [Popinet 2009] for curvature estimation implemented in Basilisk `[basilisk.fr]`

- Height function
    - sum of volume fraction over column
    - defined if the column connects 0 and 1
- Curvature computed using
    - finite differences of height function (if 3 points available)
    - parabola fitted to interface centroids (if fewer points)
- Used for comparison

$$\kappa \approx \frac{1}{h} \frac{H_{i-1} - 2H_i + H_{i+1}}{\left(1 + \left(\frac{H_{i+1} - H_{i-1}}{2}\right)^2\right)^{1.5}}$$

	$i-1$	i	$i+1$
H	1.5	1.7	2.9

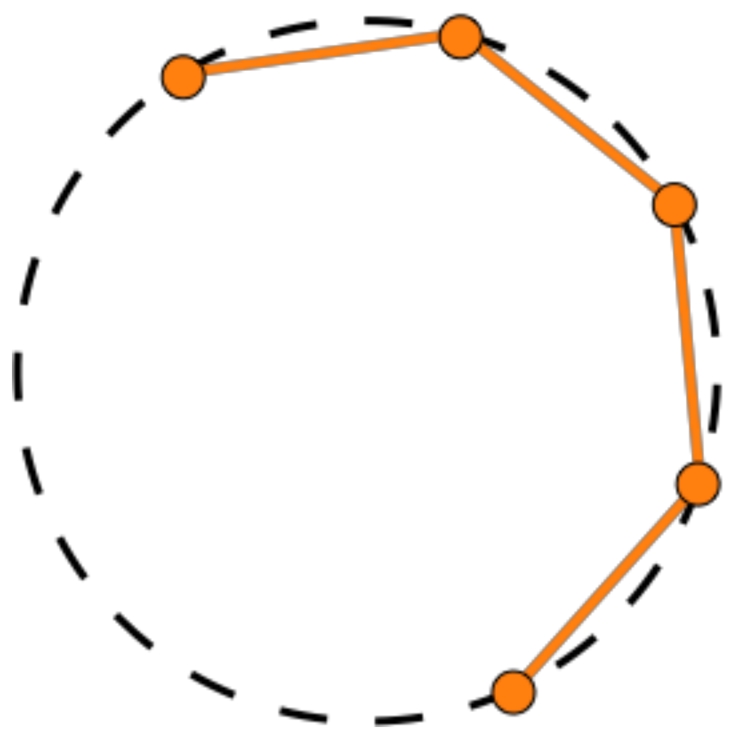


Proposed method

Curvature from positions of constrained particles attracted to the interface

1. Interface

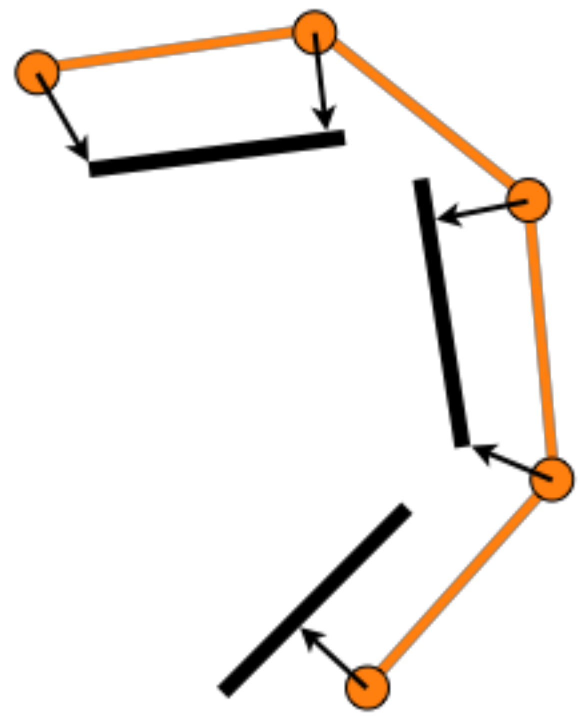
- line segments (e.g. from VOF reconstruction)



2. Constrained particles

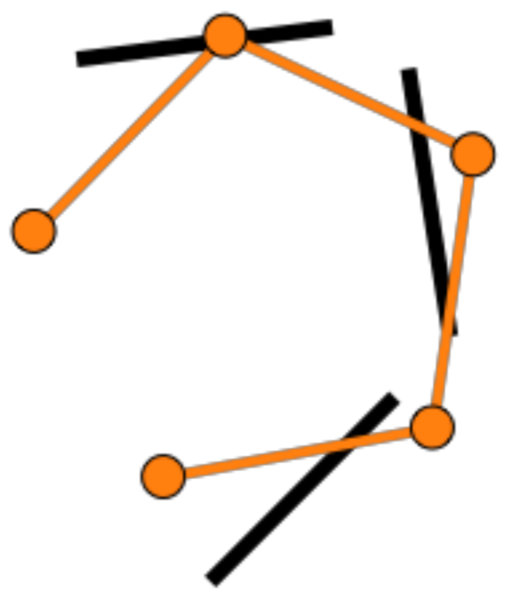
- fixed distance
- uniform angle

⇒ particles belong to a circle



3. Forces

- attraction to nearest point on the interface



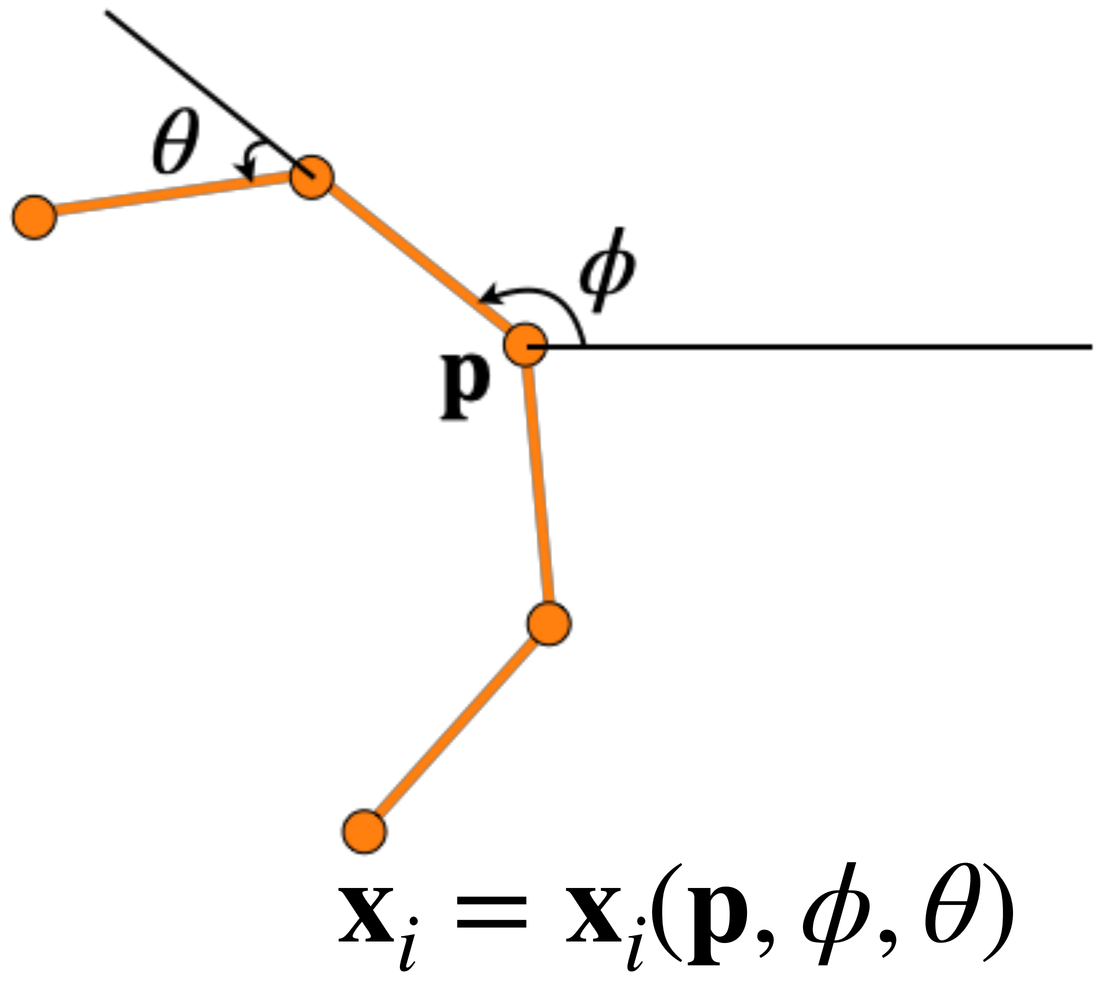
4. Equilibrium positions

- provide the estimate of curvature

Proposed method

Evolution of particles in terms of parameters satisfying the constraints

- Constraints leave 4 scalar parameters
  - position of central particle $\mathbf{p} = (x_c, y_c)$
  - orientation angle ϕ
  - bending angle θ



- Attraction forces $\mathbf{f}_i$ from $\mathbf{x}_i$ to nearest point on the interface
- Each step applies corrections

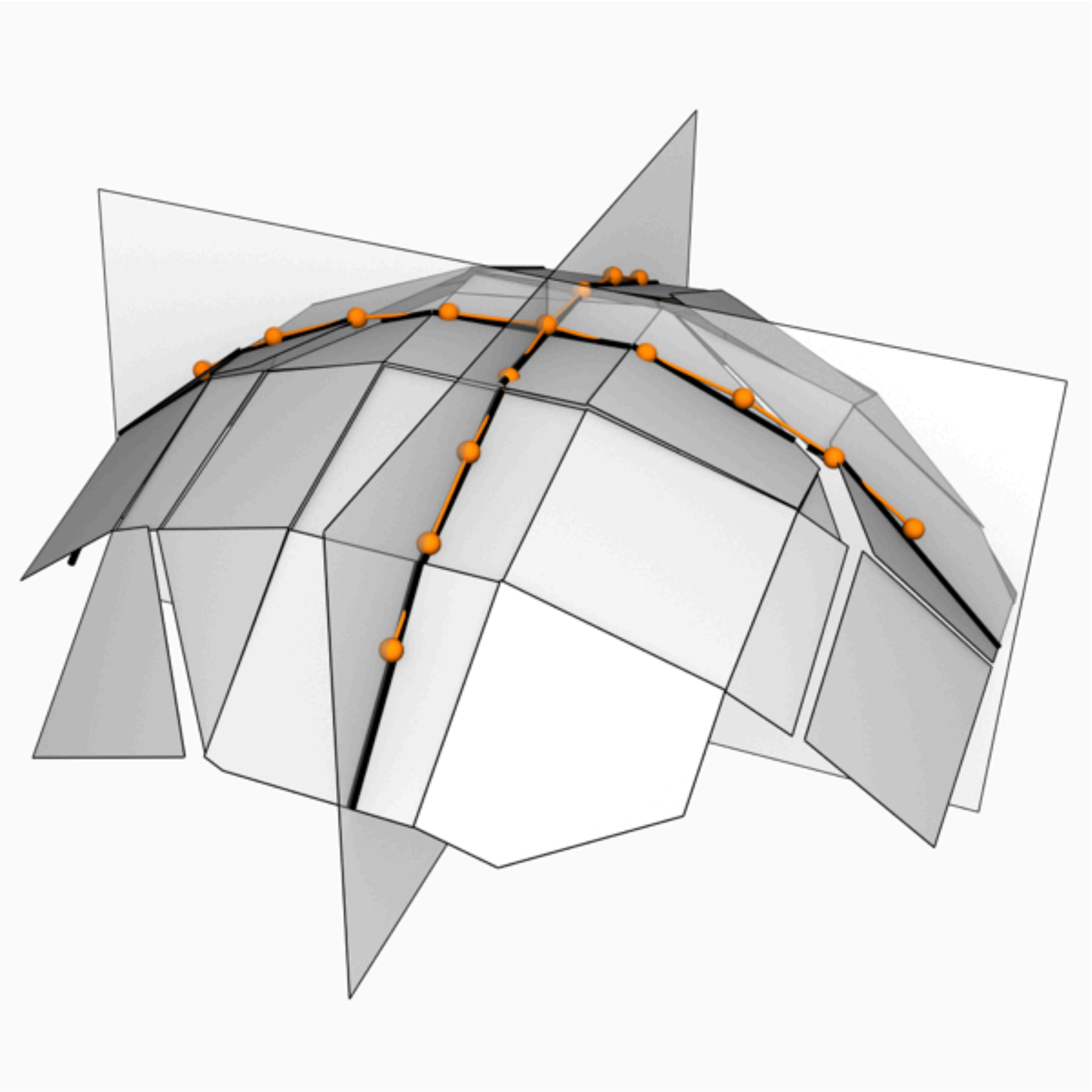
$$\Delta\phi = \sum_i \mathbf{f}_i \cdot \frac{\partial \mathbf{x}_i}{\partial \phi} \Big/ \sum_i \frac{\partial \mathbf{x}_i}{\partial \phi} \cdot \frac{\partial \mathbf{x}_i}{\partial \phi}$$

(similar for $\mathbf{p}$ and θ)

Proposed method

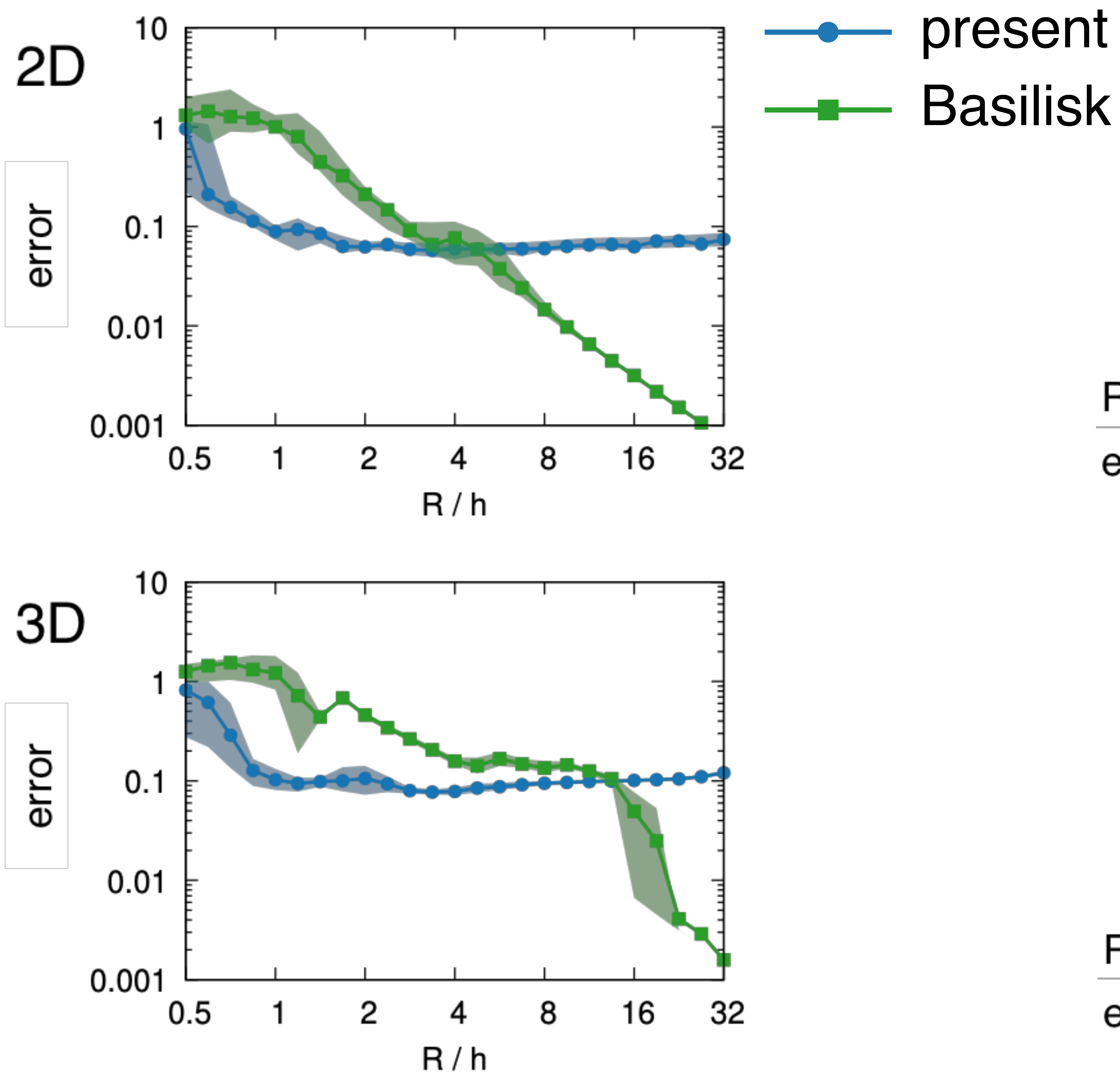
Mean curvature in 3D

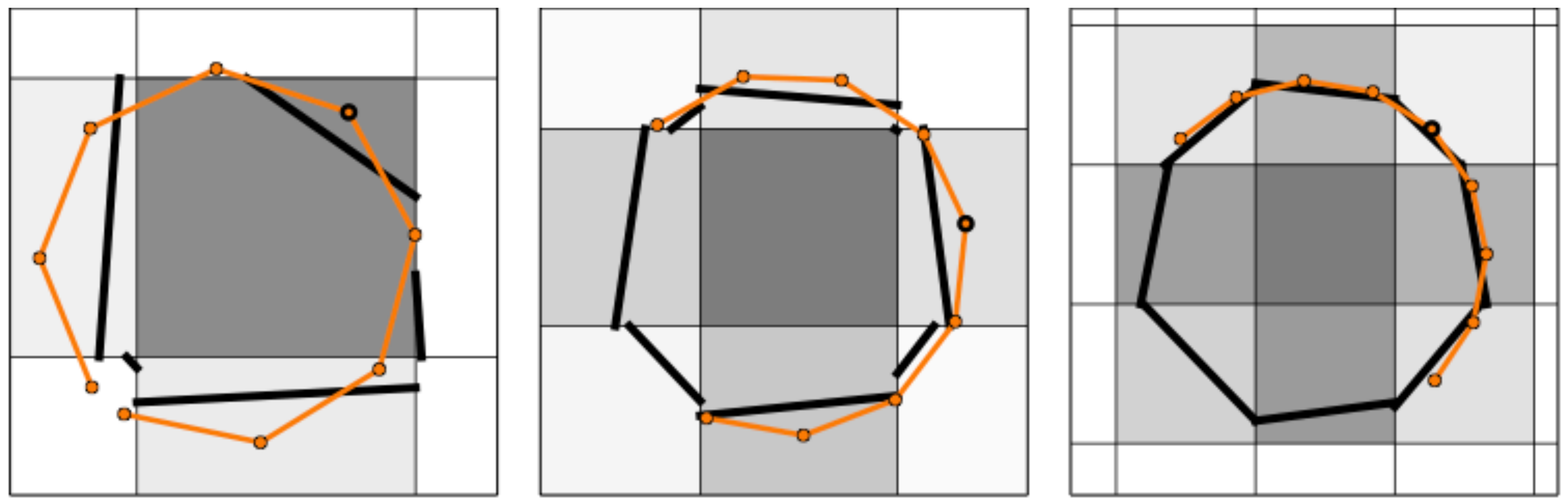
- Interface consists of polygons
- Plane section consists of line segments
  ⇒ problem reduced to 2D
- Mean curvature is arithmetic mean over plane sections



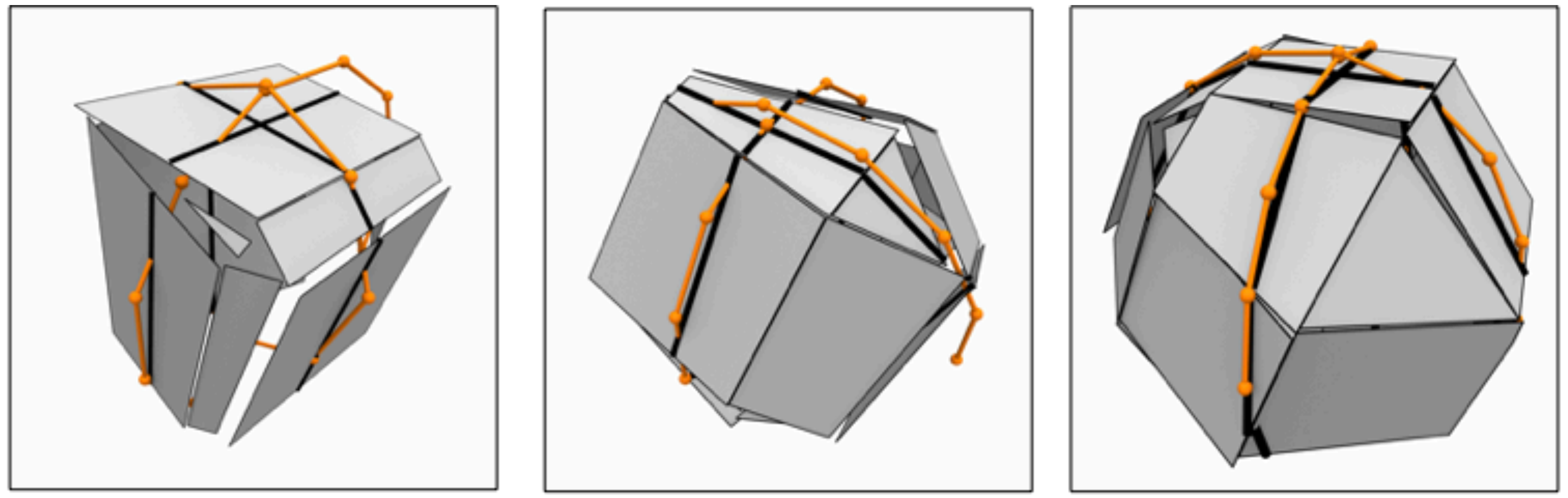
Benchmarks

Curvature of a sphere





R / h:	0.59	0.84	1.19
error:	0.17	0.10	0.07



R / h:	0.59	0.84	1.19
error:	0.42	0.08	0.09

Translating droplet

- Uniform initial velocity $\mathbf{u}_0$
- Flow driven by surface tension

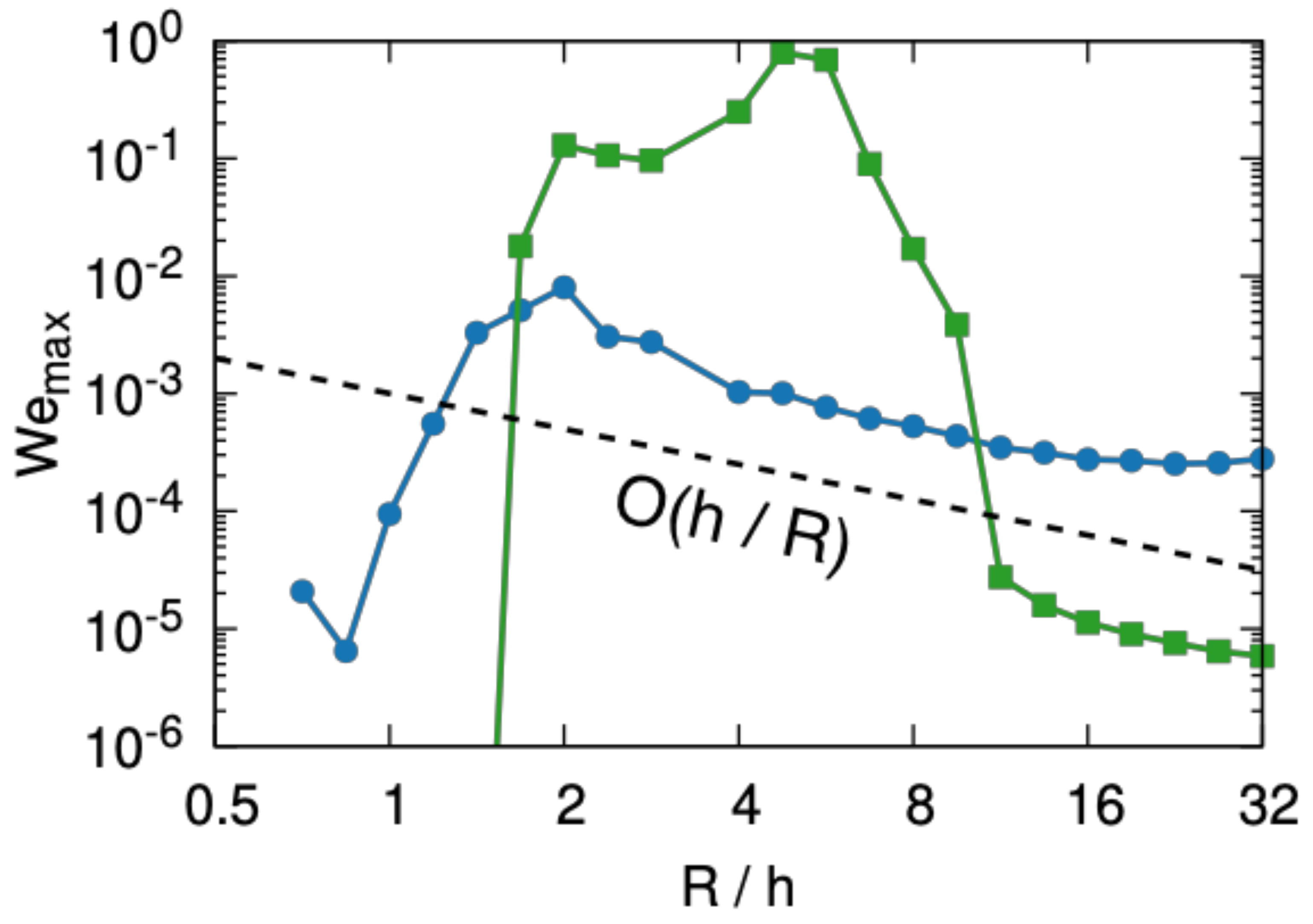
$$\mathrm{We}_0 = \frac{2\rho R\,|\mathbf{u}_0|^2}{\sigma} = 0.1$$

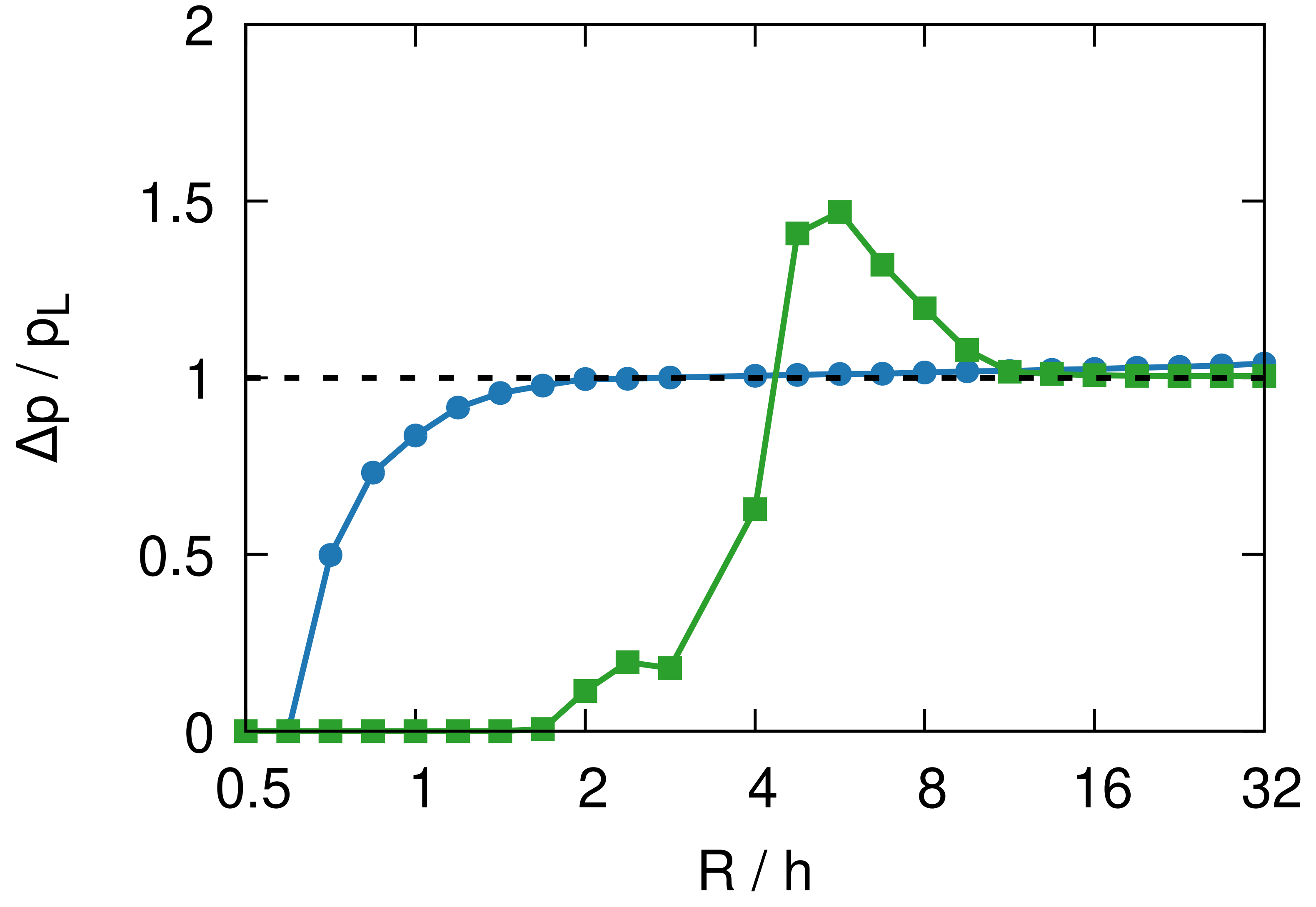
- Magnitude of the spurious flow

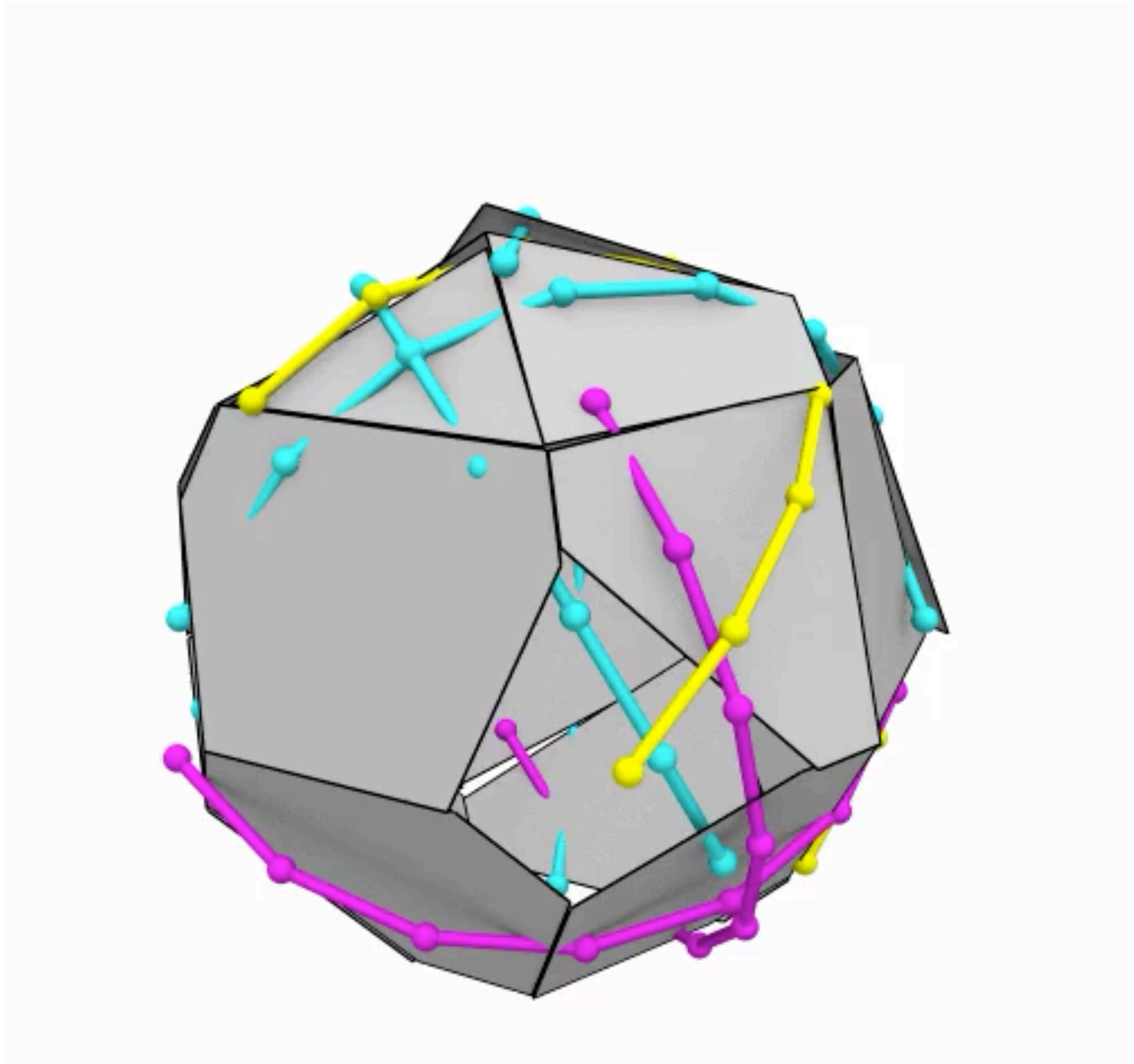
$$\mathrm{We}_{\max} = \frac{2\rho R}{\sigma}\max|\mathbf{u} - \mathbf{u}_0|^2$$

- Pressure jump

$$\Delta p = \max p - \min p$$





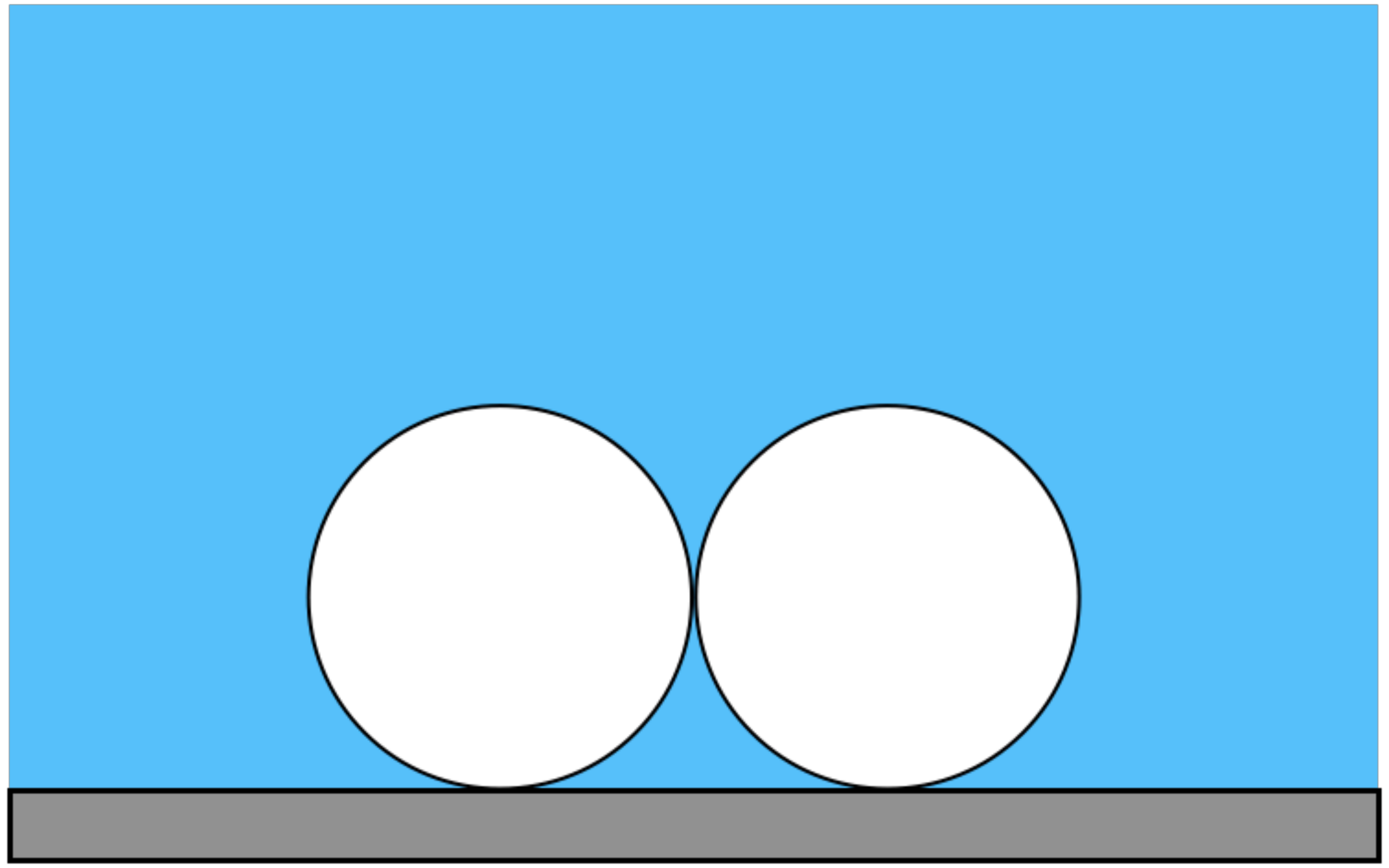


R / h = 1.19

Applications

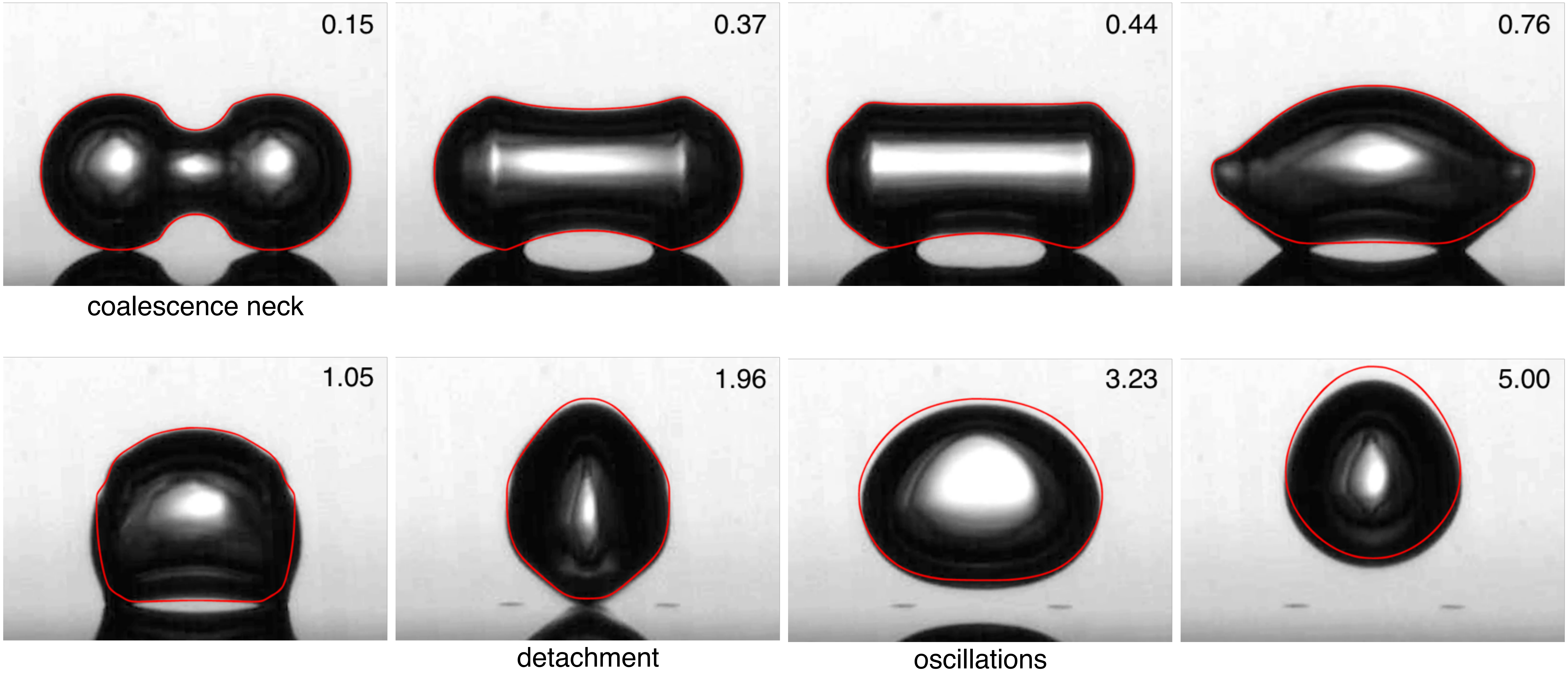
Coalescence of bubbles

- Experiment on near-wall coalescence
- Bubbles grow due to diffusion of dissolved gas
- Simulations reproduce the experiment

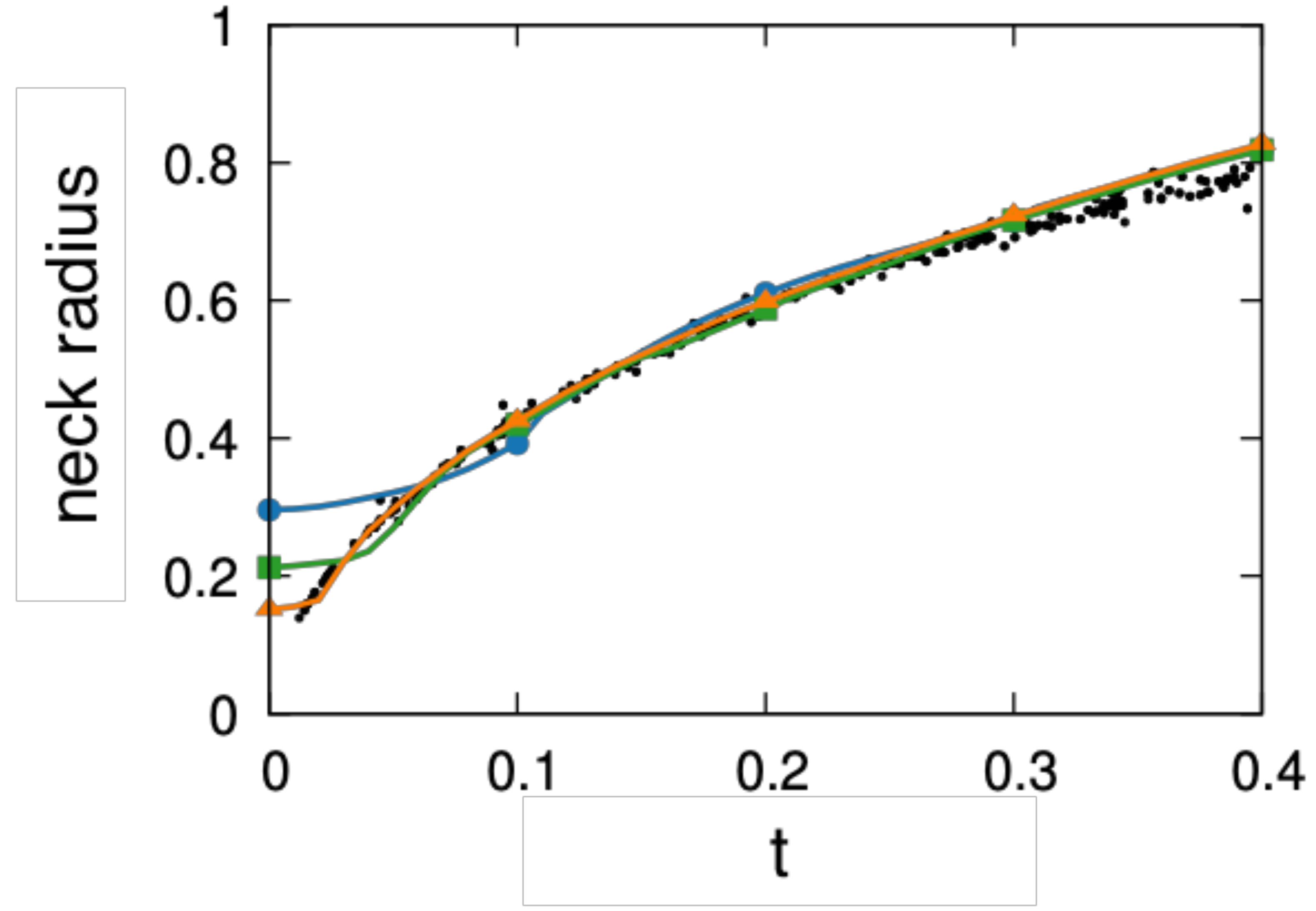


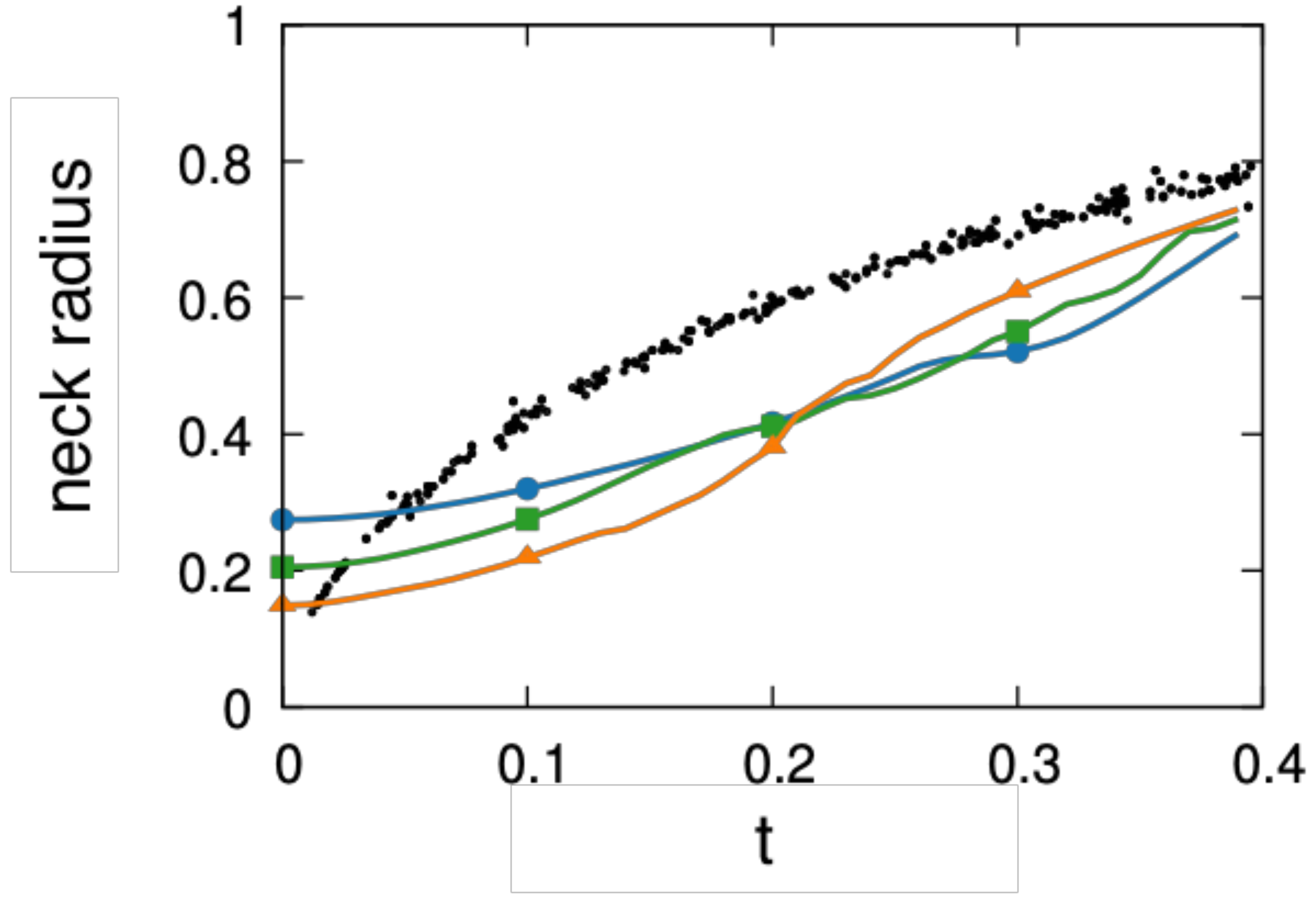
Soto ÁM, Maddalena T, Fraters A, Van Der Meer D, Lohse D.
Coalescence of diffusively growing gas bubbles.
Journal of fluid mechanics. 2018

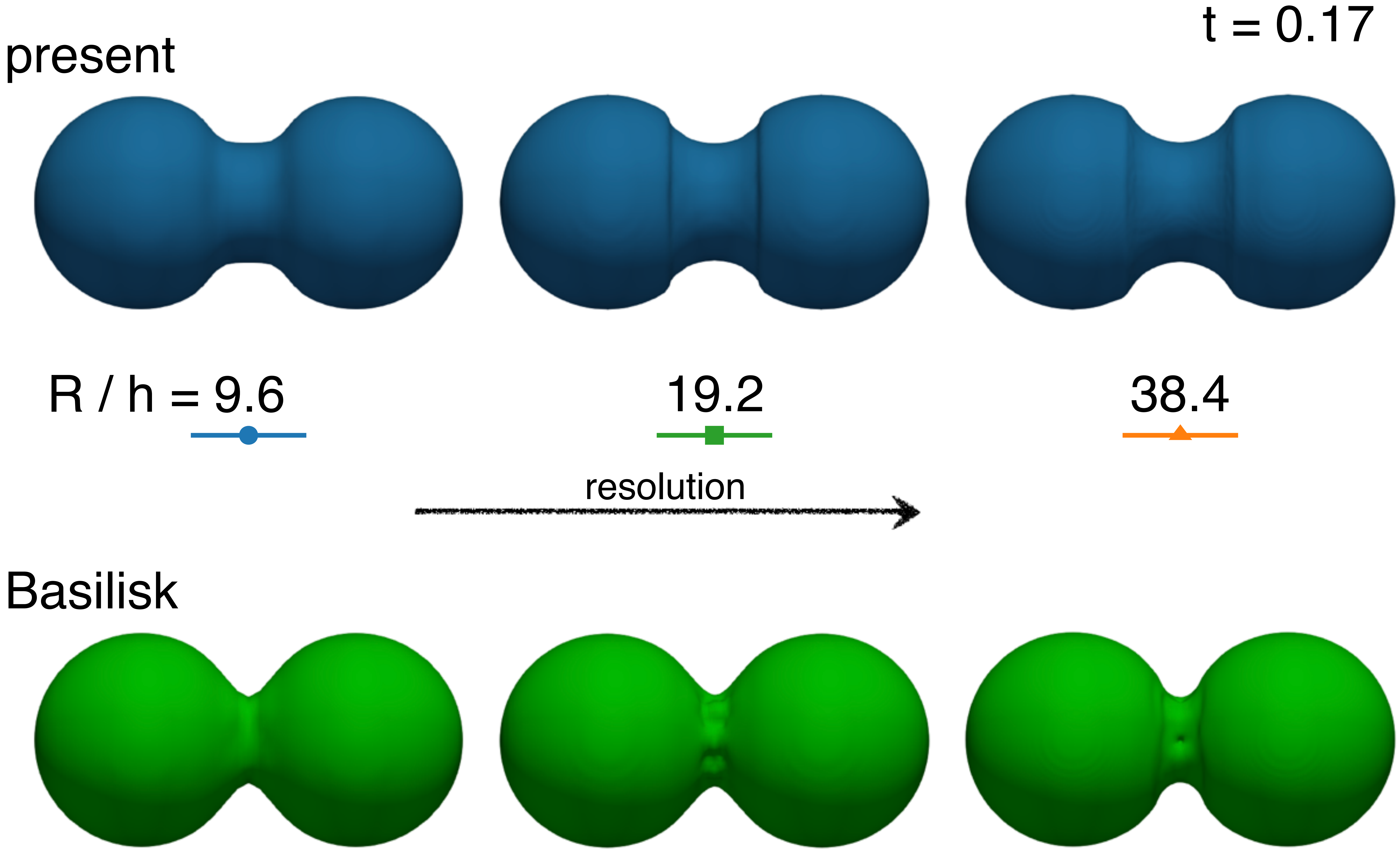
Coalescence of bubbles



Coalescence of bubbles







Taylor-Green vortex with bubbles

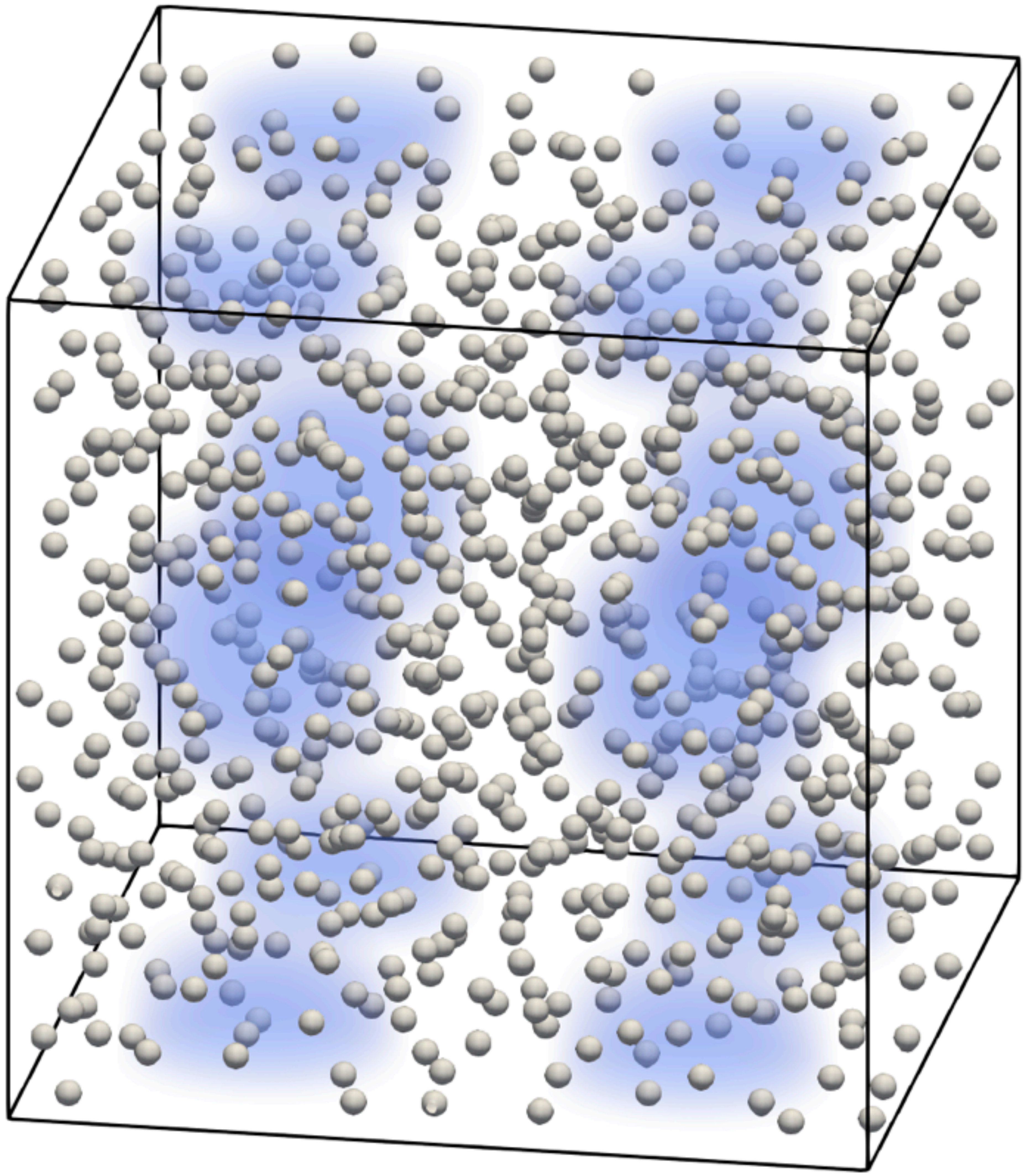
- Periodic domain $[0,\, 2\pi]^3$
- Initial velocity

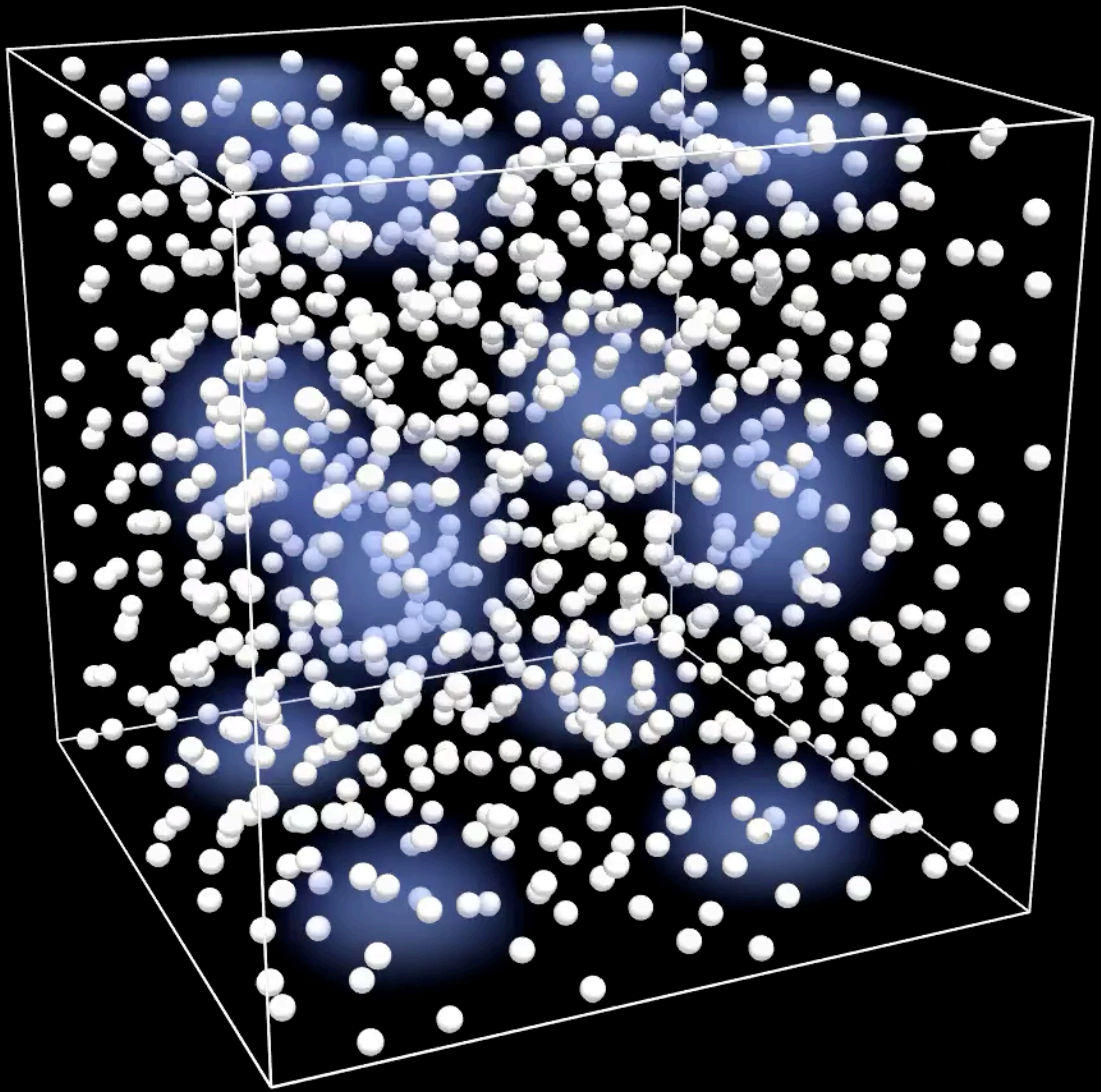
$$v_x = \sin x \ \cos y \ \cos z$$

$$v_y = -\cos x \ \sin y \ \cos z$$

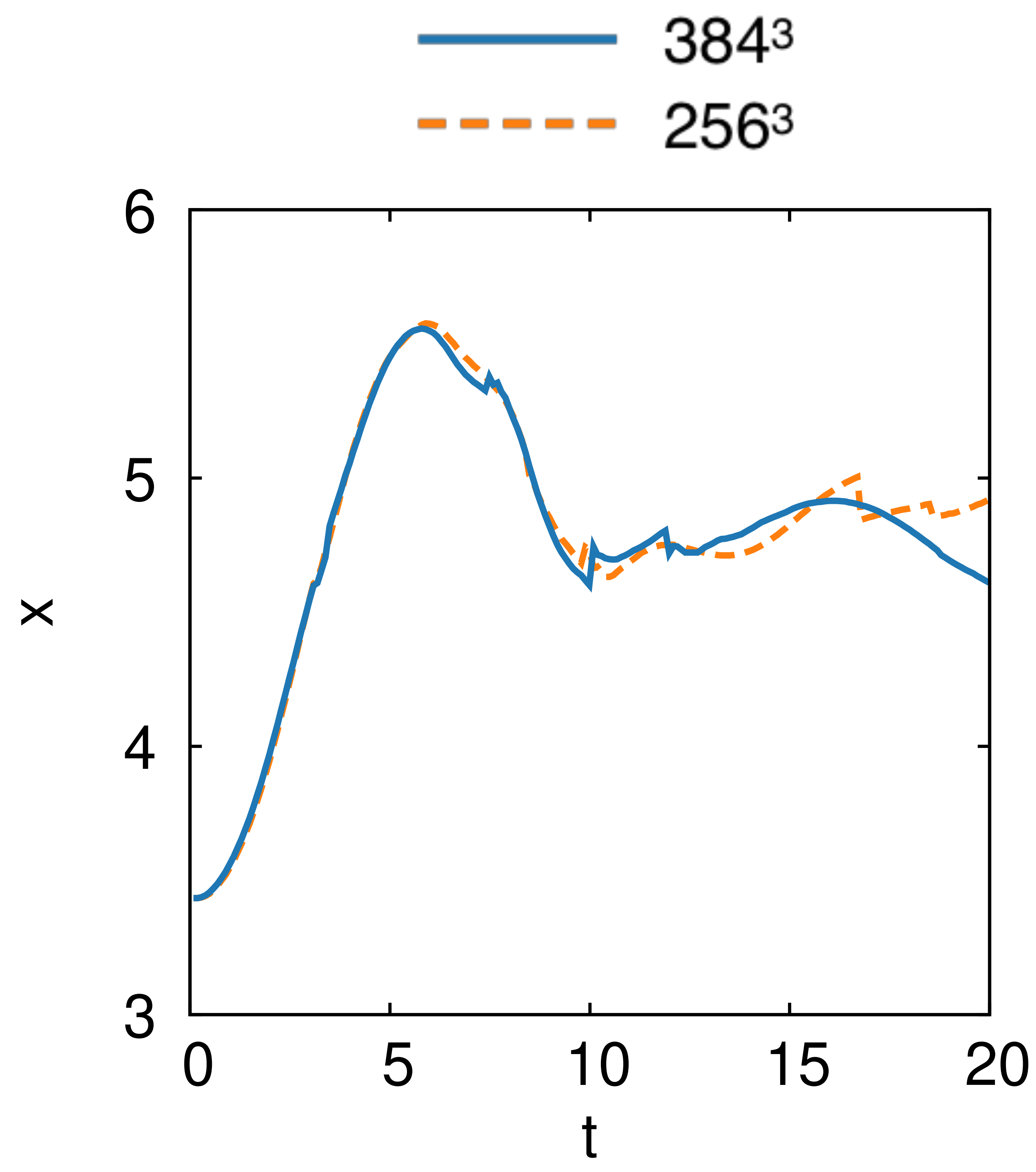
$$v_z = 0$$

- 890 bubbles, volume fraction 1.4%
- $\mathrm{Re} = \dfrac{\rho}{\mu} = 1600 \qquad \mathrm{We} = \dfrac{2\rho R}{\sigma} = 2$
- Mesh 256^3 or 384^3

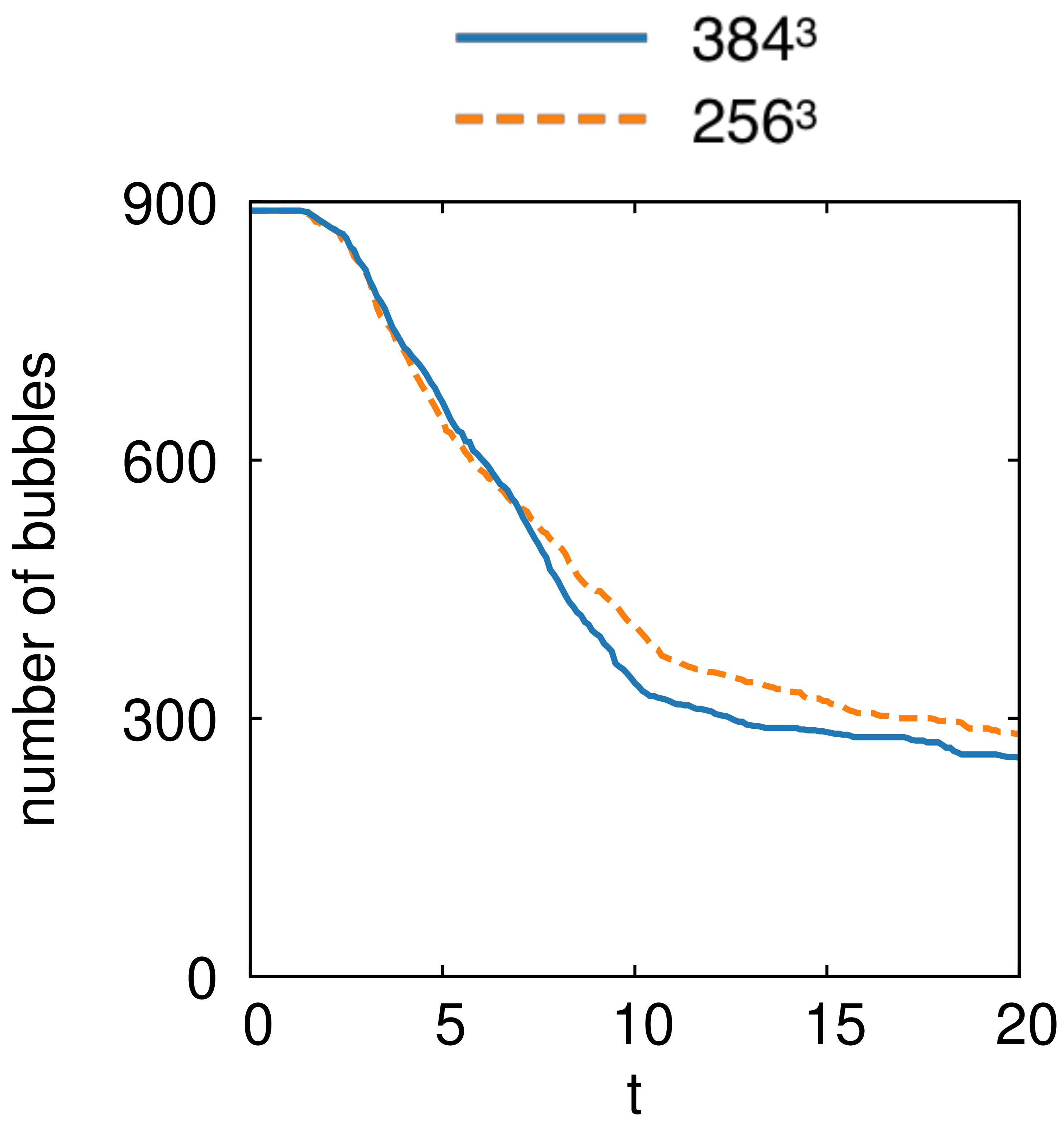




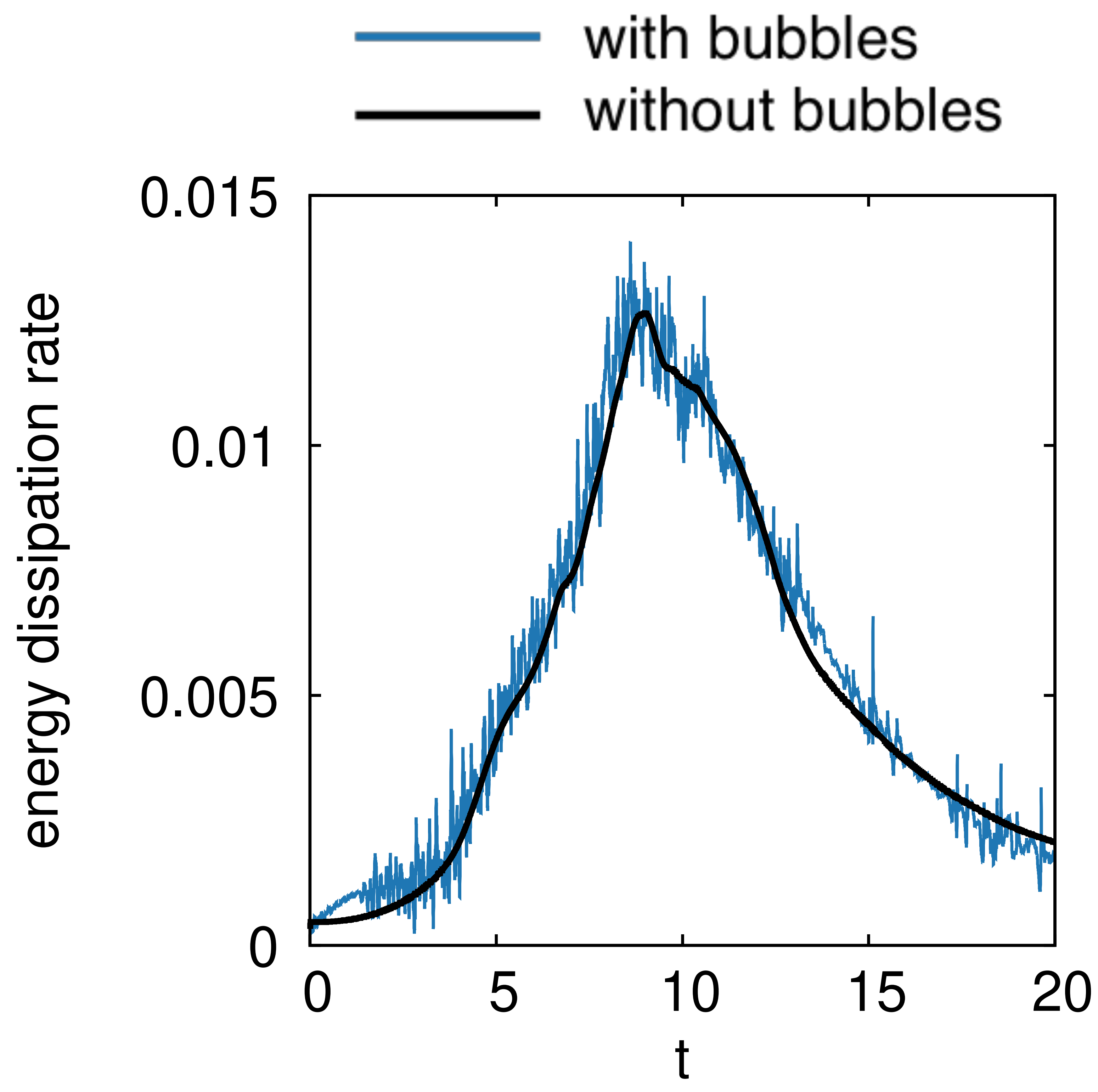
Taylor-Green vortex with bubbles



trajectory of one bubble,
no change on finer mesh



number of bubbles reduces
with time due to coalescence



coalescence causes
fluctuations of dissipation rate

Summary

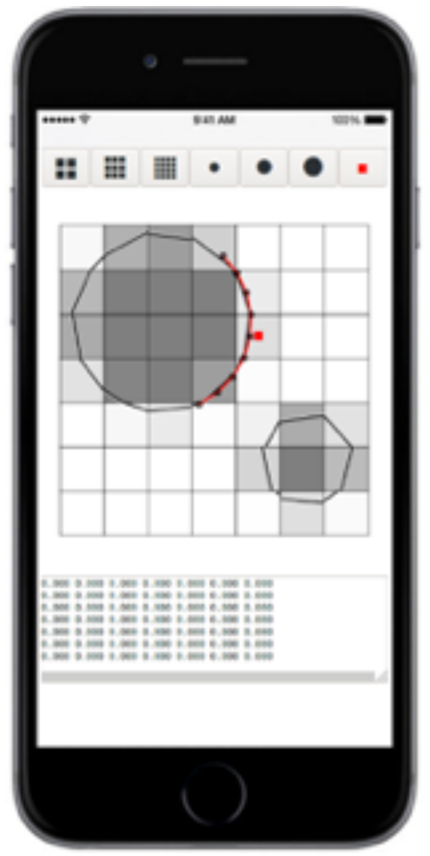
The proposed method:

- more accurate at low resolutions than standard techniques (curvature error below 0.1 even with one cell per radius)
- straightforward to implement
- naturally describes contact angles of 0° and 180°

Outlook:

- hybrid method using height functions at high resolution

Thank you!



web demonstration

`tinyurl.com/demogrid`

References

1. P. Karnakov, S. Litvinov, and P. Koumoutsakos, “Connected particles for curvature estimation applied to flows with surface tension” (in preparation)

2. P. Karnakov, F. Wermelinger, M. Chatzimanolakis, S. Litvinov, and P. Koumoutsakos, “A High Performance Computing Framework for Multiphase, Turbulent Flows on Structured Grids" in *Proceedings of the platform for advanced scientific computing – PASC ’19*, 2019. (accepted)

3. S. M. H. Hashemi, P. Karnakov, P. Hadikhani, E. Chinello, S. Litvinov, C. Moser, P. Koumoutsakos, and D. Psaltis, “A versatile and membrane-less electrochemical reactor for the electrolysis of water and brine," *Energy & environmental science*, 2019.

Contact angle