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Fully Resolved Simulations of Complex Multiphase Flows

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Modeling and Simulations in Fluids
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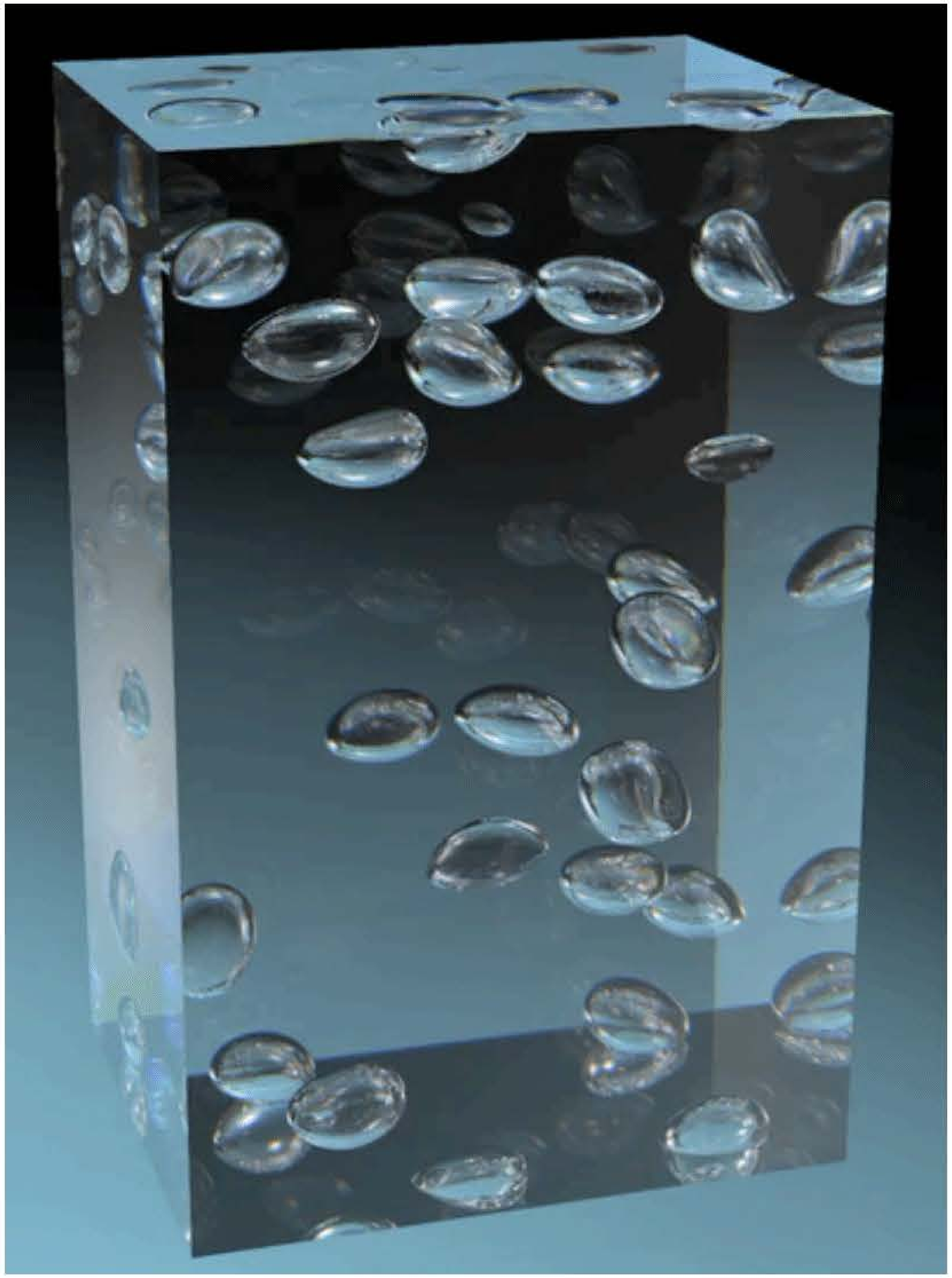
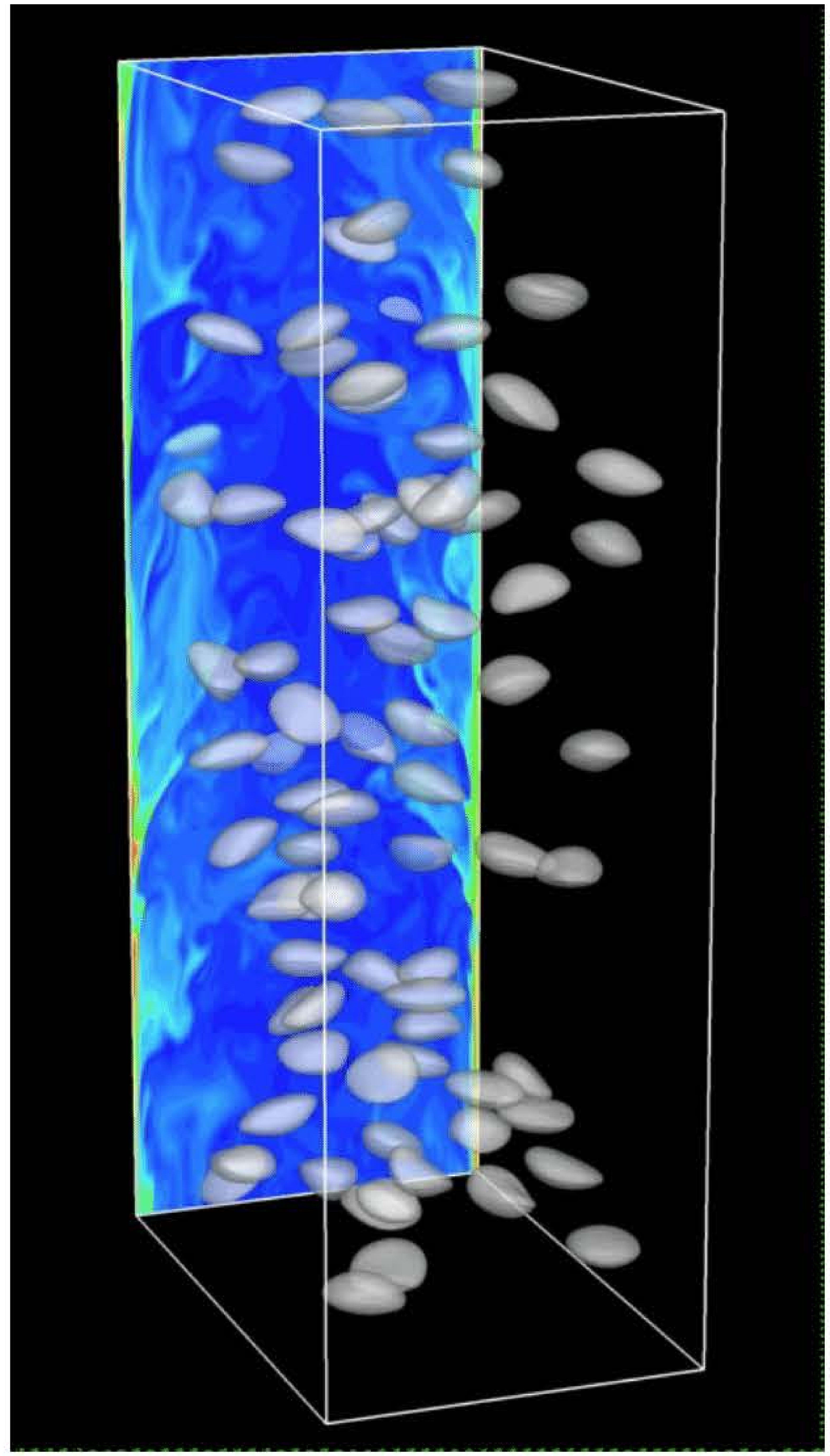
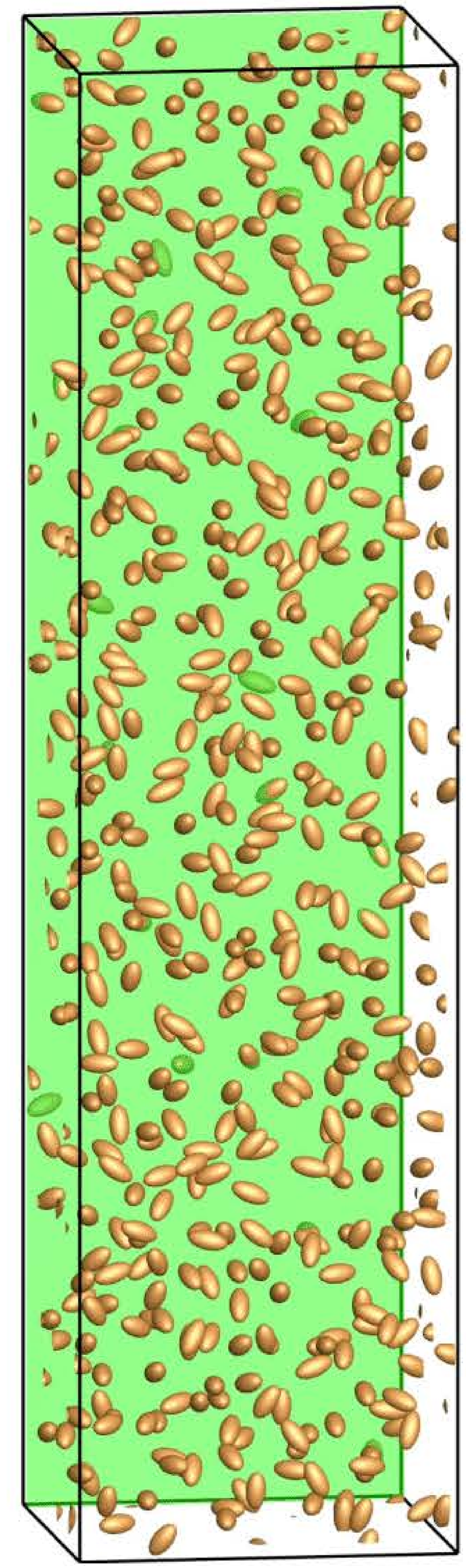
Fully Resolved Simulations of Disperse Multiphase Flows







We have come a long way and simulations of disperse multiphase flows are now relatively routine

Where We Are

While continuing refinement of the methods, making them more accurate and more robust are important pursuits, the progress made so far is opening up new possibilities.

Two important questions are:

- How do we use the abundance of information that is already available most effectively to generate models for closure terms in RANS and LES computations of industrial systems?
- How do we extend current capabilities to more complex multi-phase, multi-physics and multi-scale systems in the most effective way?

Froth Flotation—Single Bubble

Outline

- Numerical Approach
- Three Phase Flows
- Coarsening and Modeling

Numerical Approach

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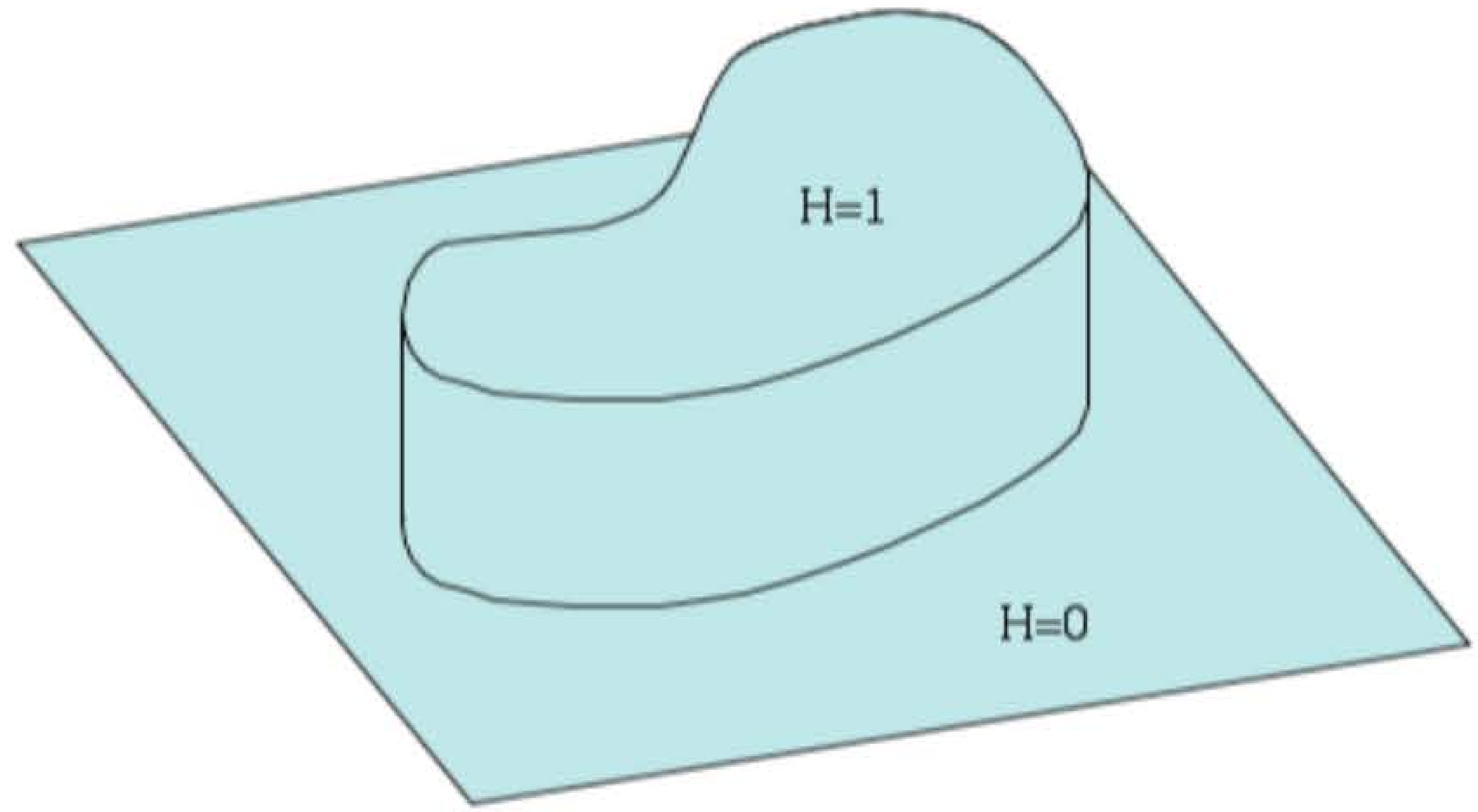
One-fluid (or one-field) approach:

Introduce a numerical marker function approximating H. The advection is governed by:

$$\frac{\partial H}{\partial t} + \mathbf{u} \cdot \nabla H = 0$$

Integrating this equation in time, for a discontinuous initial data, is one of the hard problems in computational fluid dynamics!

The marker function allows us to set the material properties and solve the Navier-Stokes equation



For solid particles the surface tension term is replaced by a force that keeps the deformation inside the solid zero and a collision force

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p + \nabla \cdot \mu(\nabla \mathbf{u} + \nabla^T \mathbf{u}) + \rho \mathbf{g} + \underline{\sigma \kappa \mathbf{n}_f \delta(n)}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \frac{D\rho}{Dt} = 0; \quad \frac{D\mu}{Dt} = 0$$

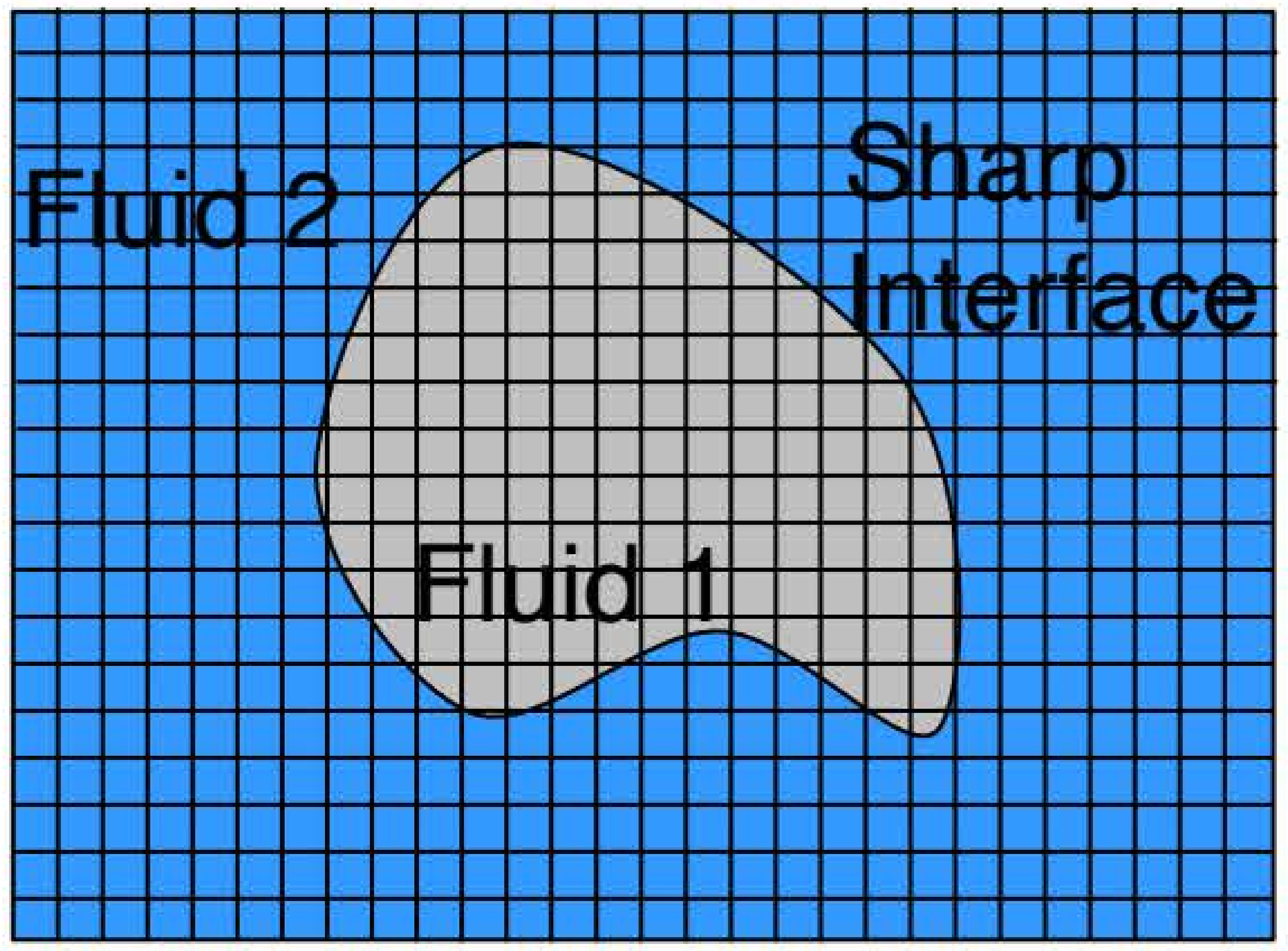
Singular interface term

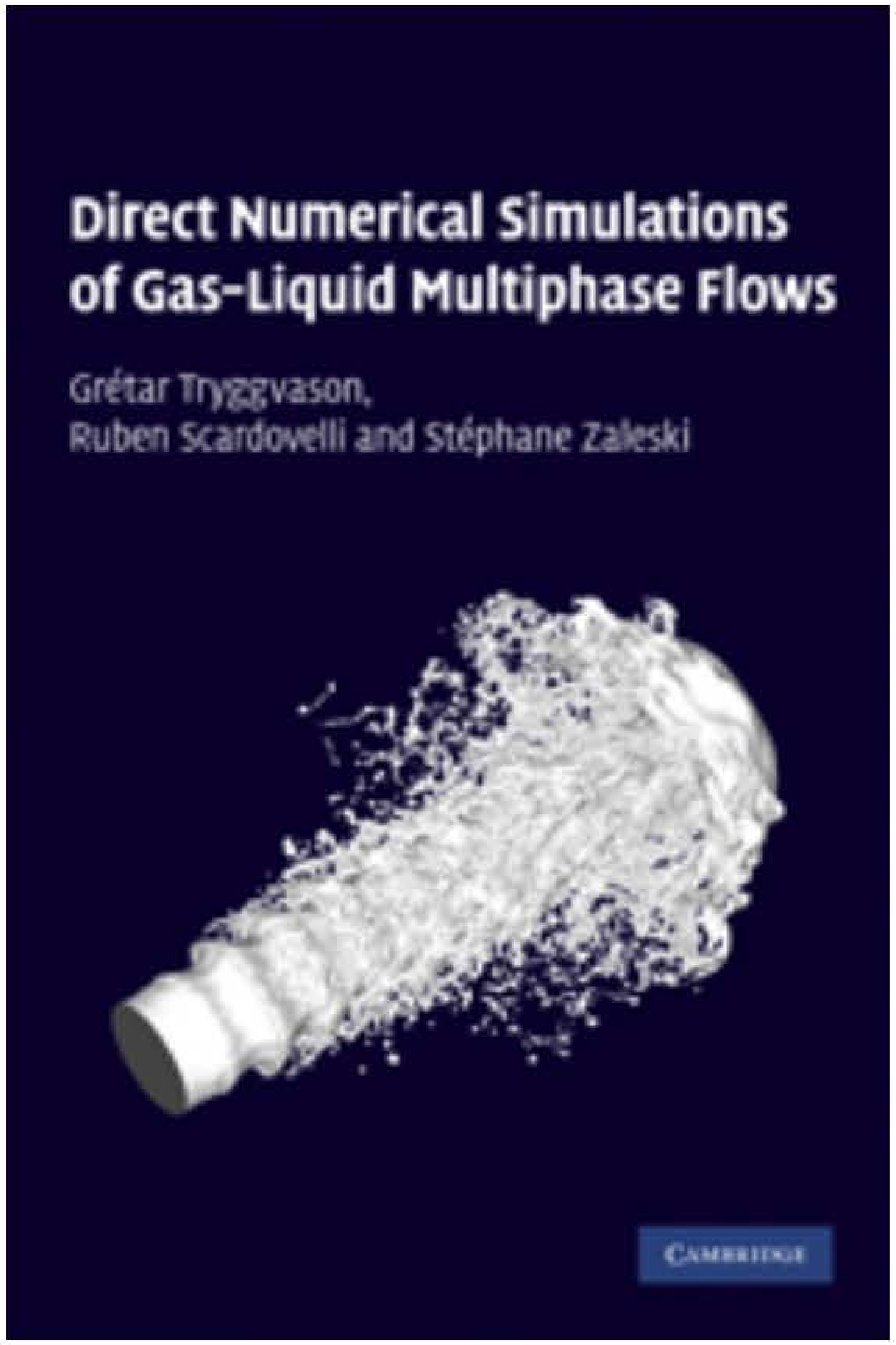
One-fluid (or one-field) approach:

One set of equations for the whole flow field. Different fluids/phases have different properties and are identified by an index/marker function. Interfacial effects added as delta functions

- One fluid formulation for multi fluid flows, where a single set of equations are solved for the whole flow field
- A single stationary grid is used for the whole domain to discretize the governing equations
- Finite Volume Method for the Navier-Stokes Equations
- A method to advect the index function identifying the different fluids or phases. This can be done in different ways, such as by VOF, LS or Front Tracking.

This approach forms the basis of a large number of methods and has been widely implemented and tested





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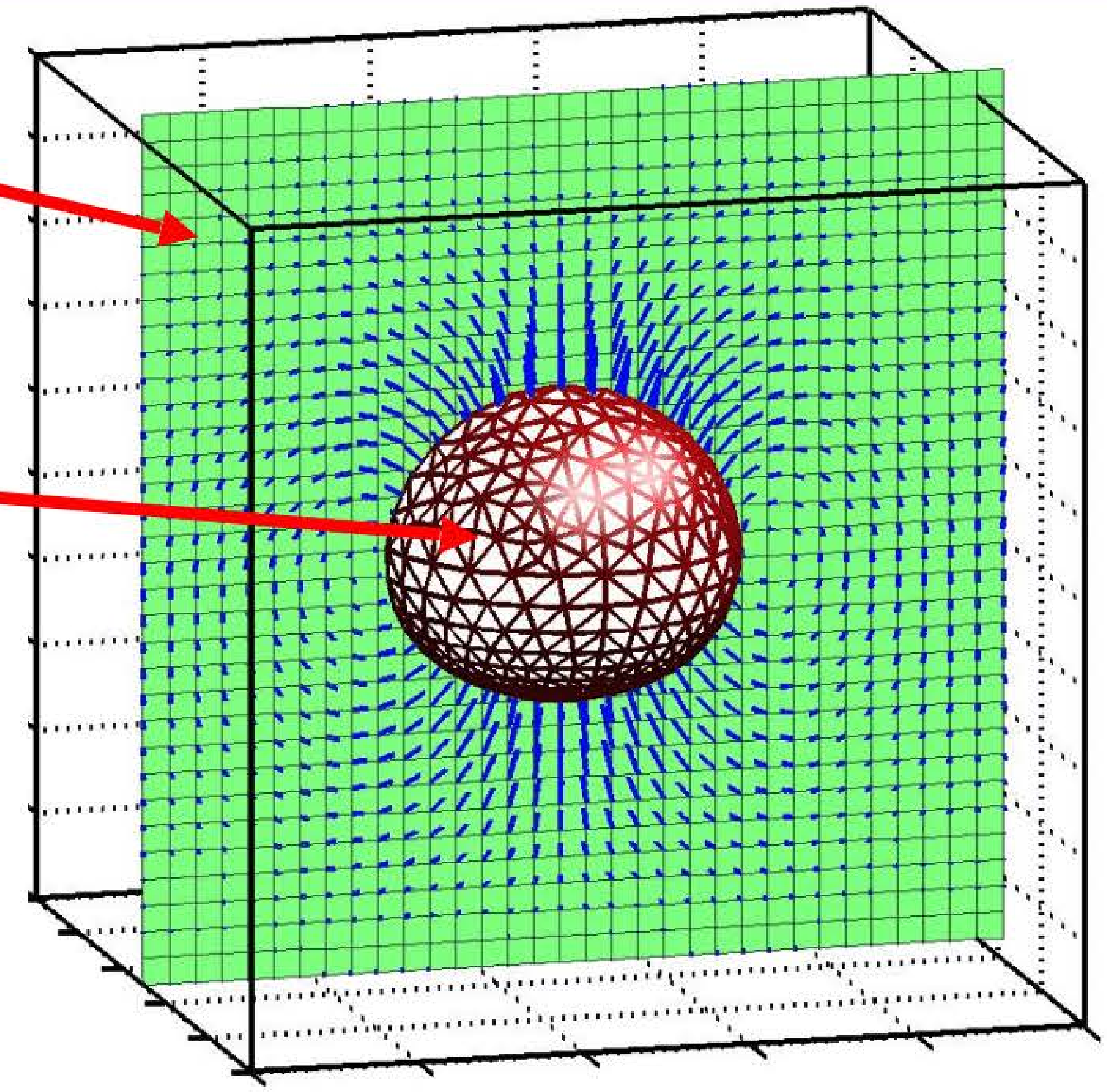
Front Tracking

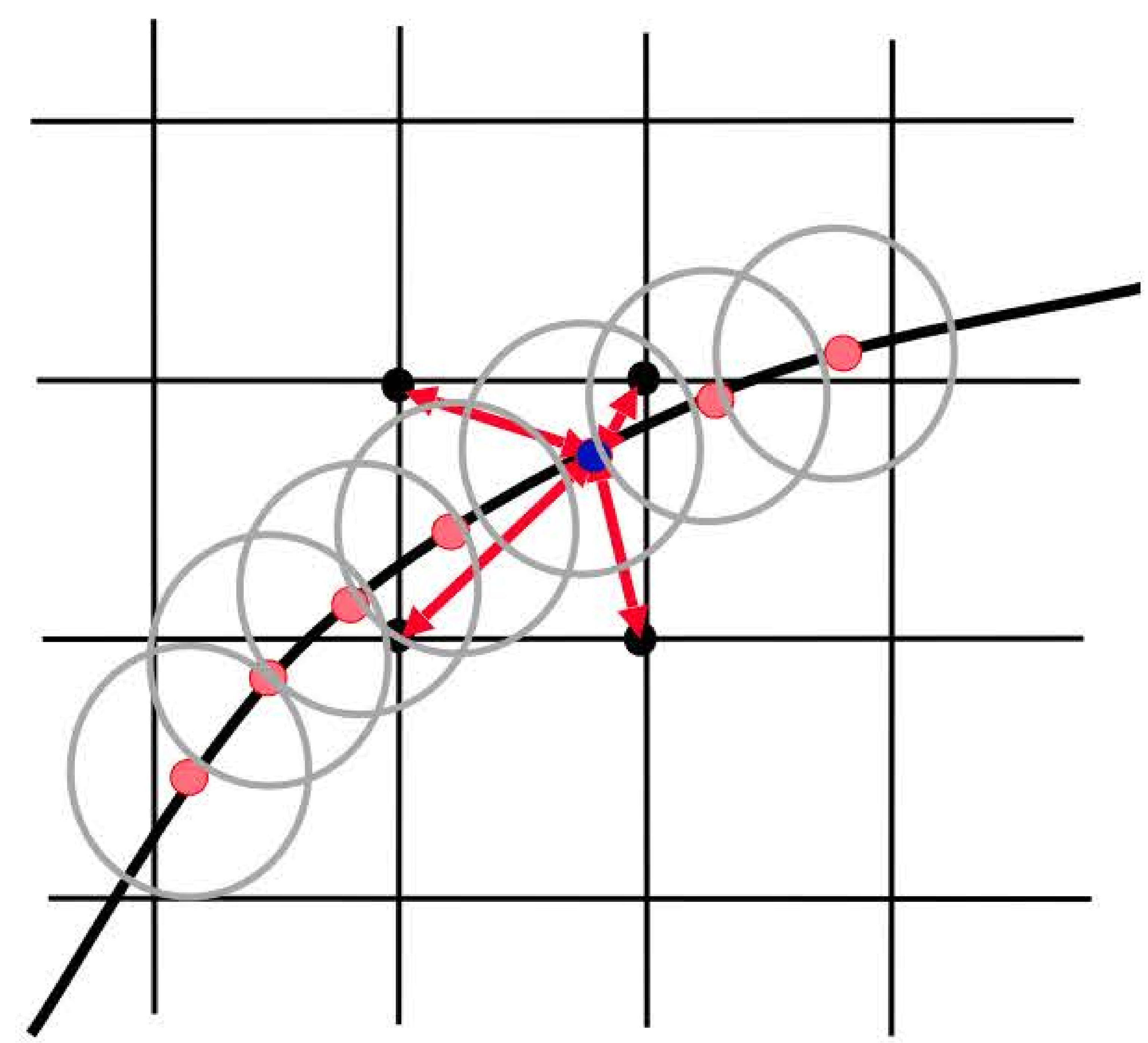


Fixed grid used for the solution of the Navier-Stokes equations

Tracked front to advect the fluid interface and find surface tension

The front is used to update the index function and compute the surface tension

The Navier-Stokes equations are solved on a regular structured staggered grid, using an explicit second order projection method for the time integration.



Information must be passed between the two grids

The front provides accurate solution and the flexibility to include interface physics in a relatively straightforward way

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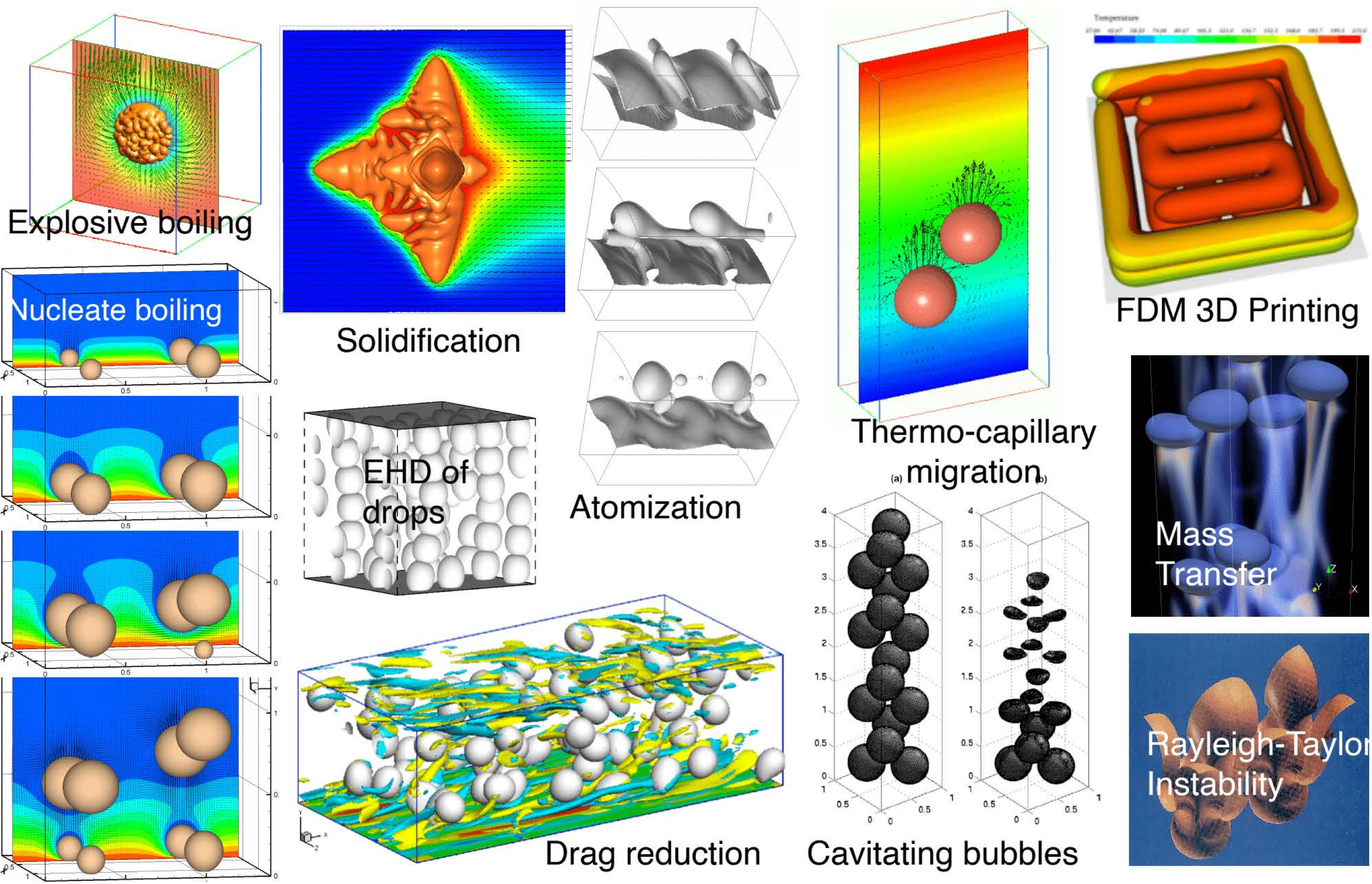
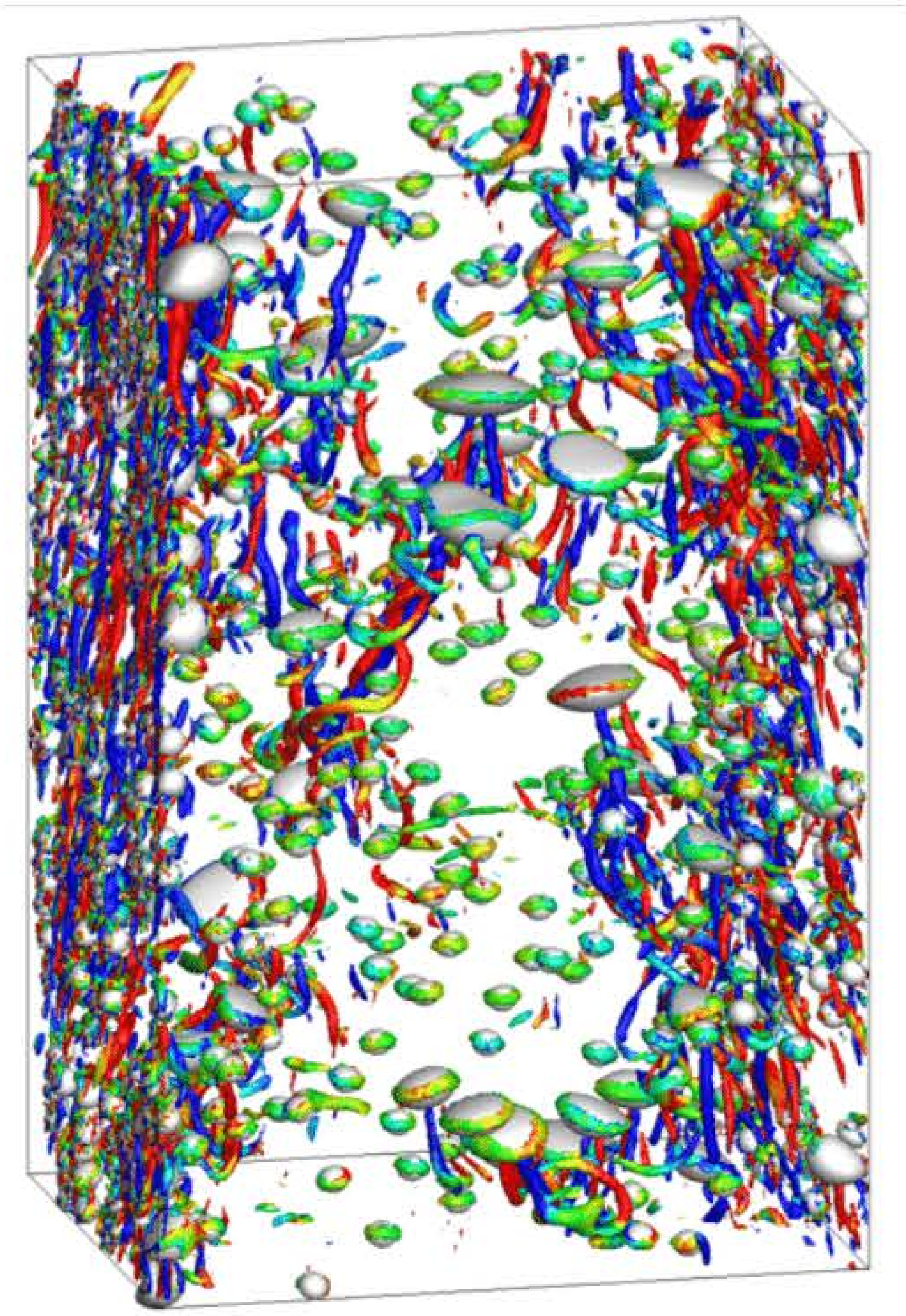
Examples



A Few Bubble Papers



Hundreds of bubbles of different sizes in turbulent channel flow.
G. Tryggvason, M. Ma & J. Lu. DNS–Assisted Modeling of Bubbly Flows in Vertical Channels, Nuclear Science and Engineering, 184:3 (2016), 312-320

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- E.A. Ervin and G. Tryggvason. “The Rise of Bubbles in a Vertical Shear Flow.” ASME J. Fluid Engineering 119 (1997), 443-449.
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- A. Esmaeeli and G. Tryggvason. “A DNS study of the buoyant rise of bubbles at O(100) Reynolds numbers.” Physics of Fluids 17, 093303 2005 (19 pages)
- J. Lu, S. Biswas, and G. Tryggvason. “A DNS study of laminar bubbly flows in a vertical channel.” Int’l J. Multiphase Flow 32 (2006), 643-660.
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- J. Lu and G. Tryggvason. “Effect of Bubble Size in Turbulent Bubbly Downflow in a Vertical Channel.” Chemical Engineering Science. 62 (2007), 3008-3018.
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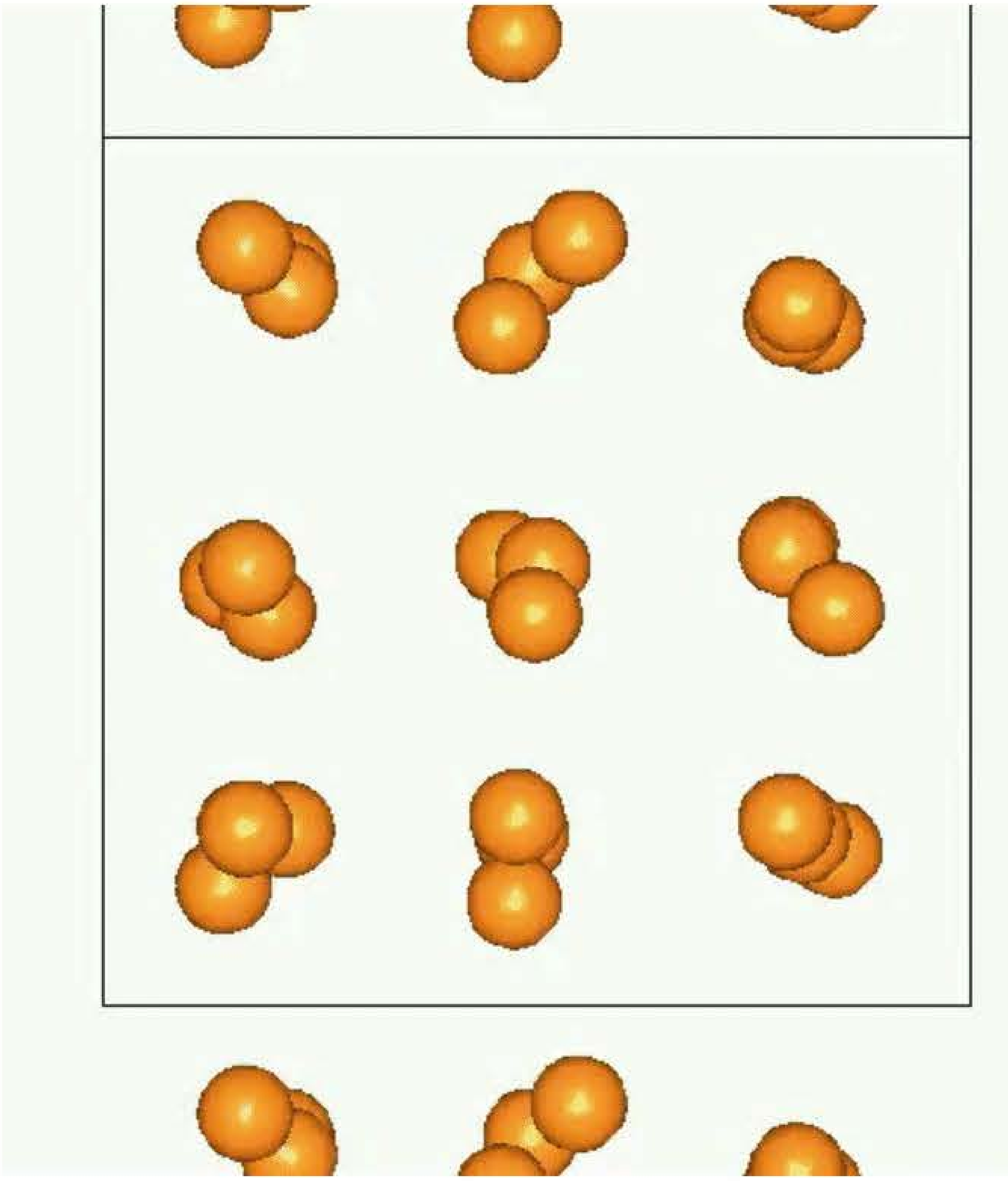
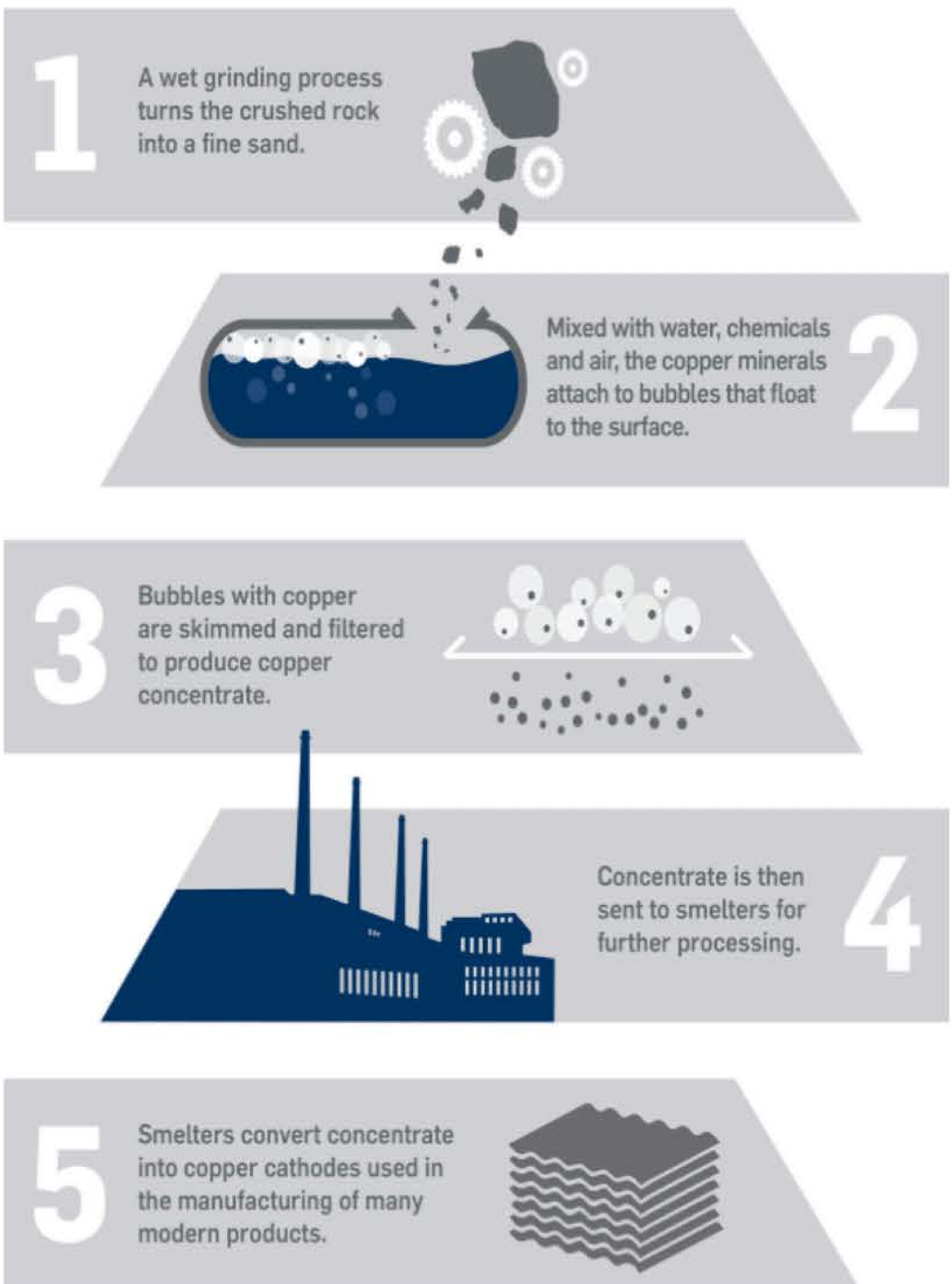


Deformable bubbles rising in fully periodic domains.
B. Bunner and G. Tryggvason. “Effect of Bubble Deformation on the Stability and Properties of Bubbly Flows.” J. Fluid Mech. 495 (2003), 77-118.

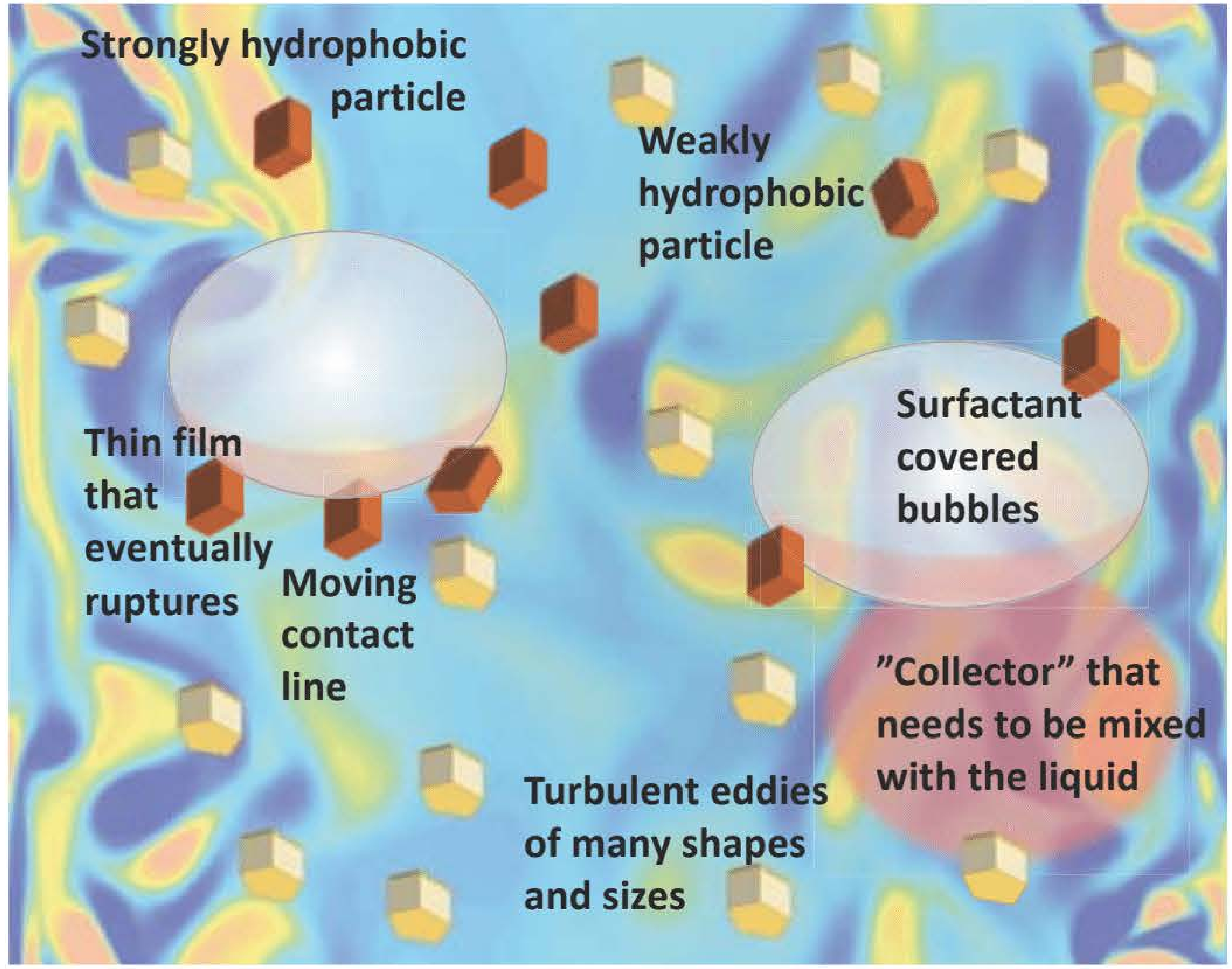
Three Phase Gas-Liquid-Solid Flows

Mineral Processing

What is froth flotation?



https://resolutioncopper.com/mining-method/



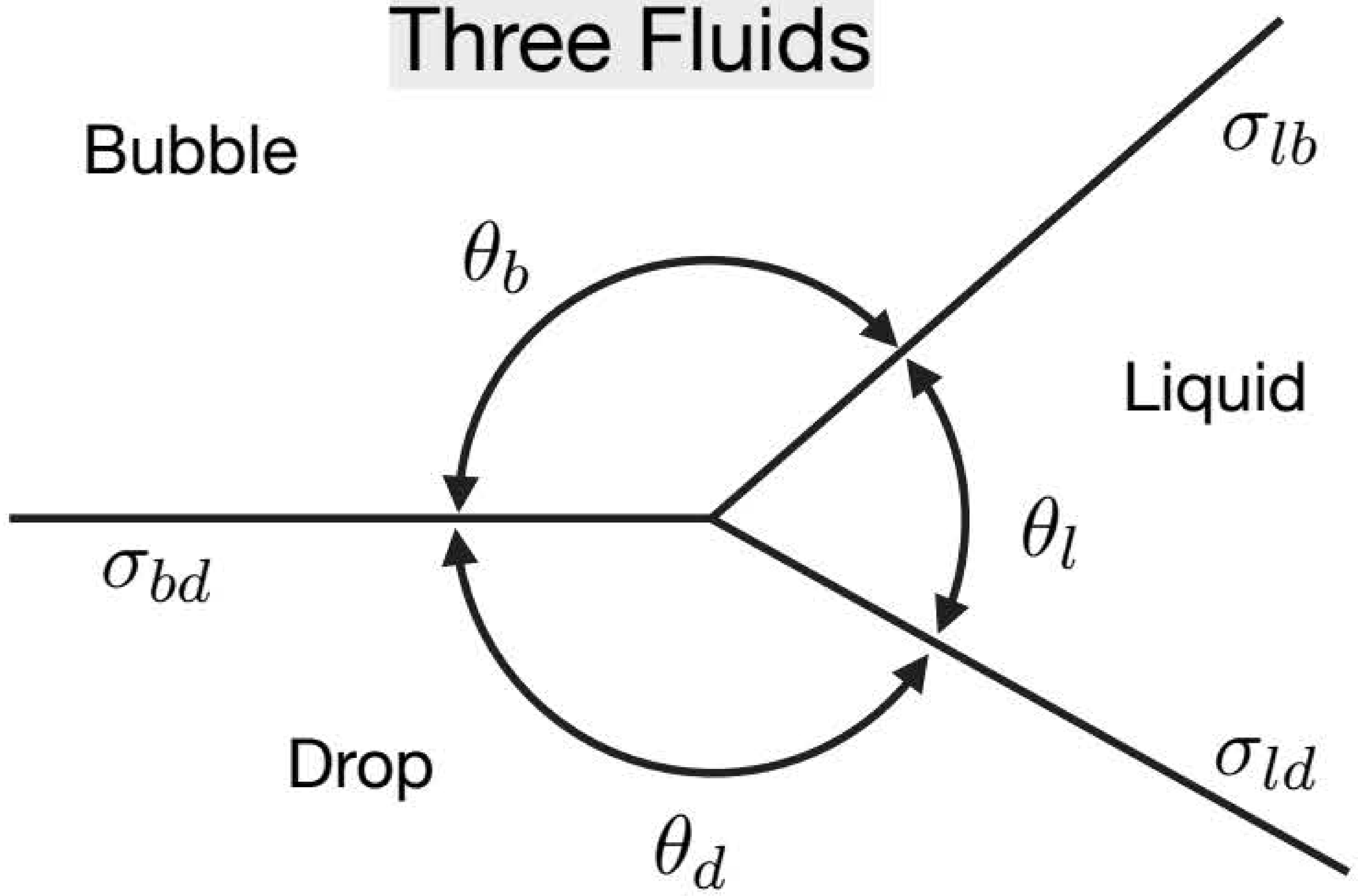
Froth flotation to select hydrophobic particles in mineral processing and plastic recycling. A variety of chemicals is usually added to make some particles hydrophobic and others not

Mineral Processing

Small copper mine
Minera San Pedro S.A. Tiltil, Chile
Capacity: 300 tonnes of ore
Yield: up to 3%
Visited January 22, 2020

Contact Angles

Three Fluids



The horizontal and vertical forces are

$$f_h = \sigma_{bd} + \sigma_{lb}\cos\theta_b + \sigma_{ld}\cos\theta_d$$
$$f_v = \sigma_{lb}\sin\theta_b - \sigma_{ld}\sin\theta_d$$

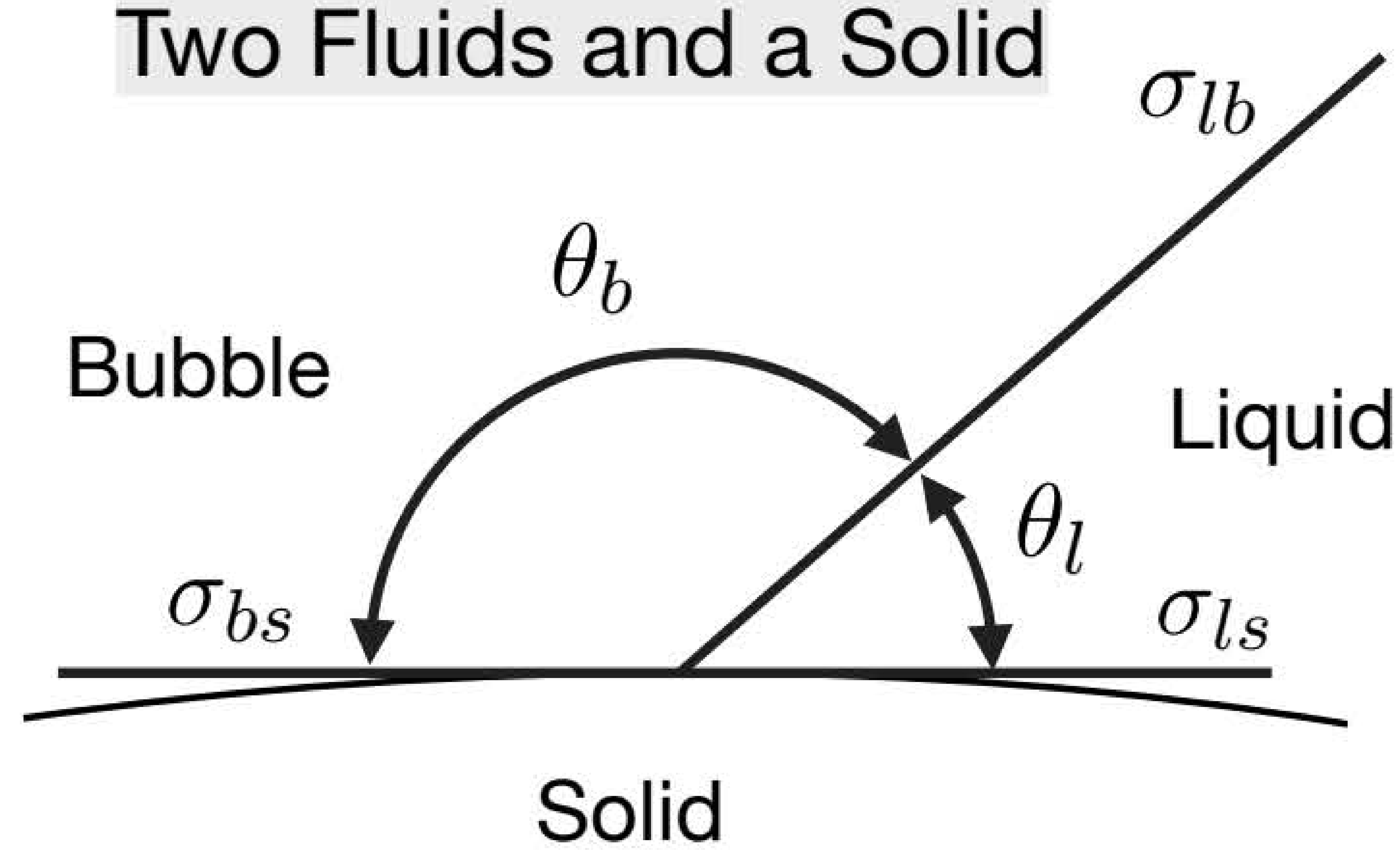
At steady state the forces balance

$$f_h = f_v = 0$$

So we can solve for the angles

$$\cos\theta_l = \frac{1}{2}\left(\frac{\sigma_{bd}}{\sigma_{ld}}\frac{\sigma_{bd}}{\sigma_{lb}} - \frac{\sigma_{ld}}{\sigma_{lb}} - \frac{\sigma_{lb}}{\sigma_{ld}}\right)$$

Two Fluids and a Solid



The tangent and normal forces are

$$f_t = \sigma_{ls} - \sigma_{bs} + \sigma\cos\theta$$
$$f_n = \sigma\sin\theta$$

At steady state

$$\sigma_{ls} - \sigma_{bs} = -\sigma\cos\theta_o$$

Thus

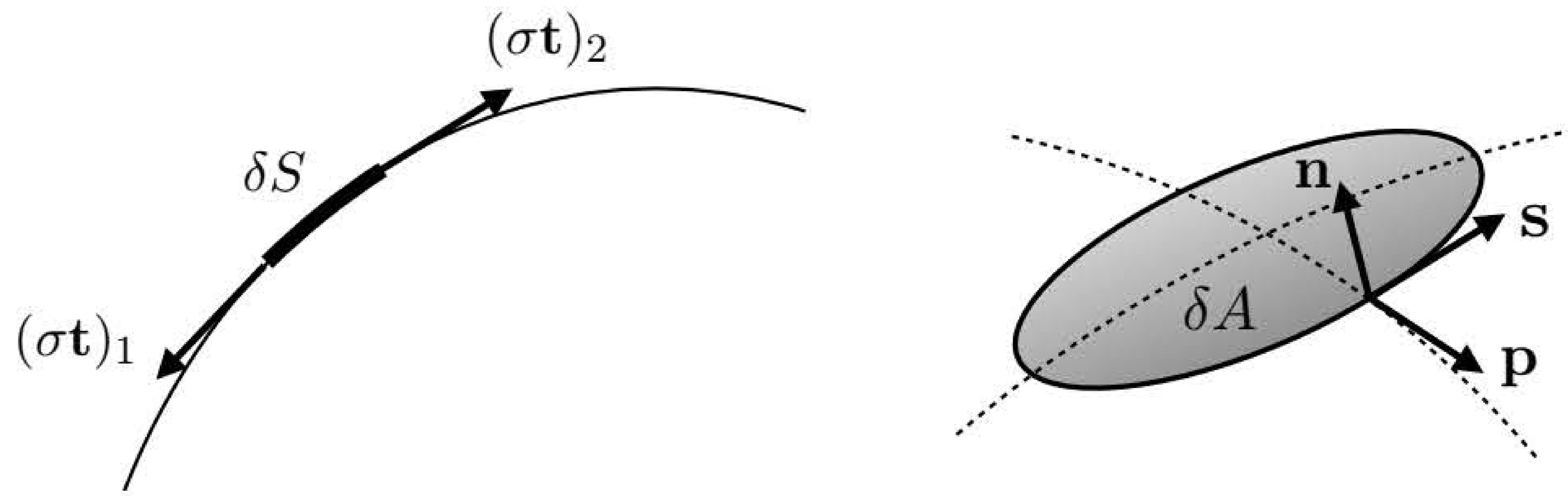
$$f_t = \sigma(\cos\theta - \cos\theta_o)$$

To move the contact point we need to allow slip

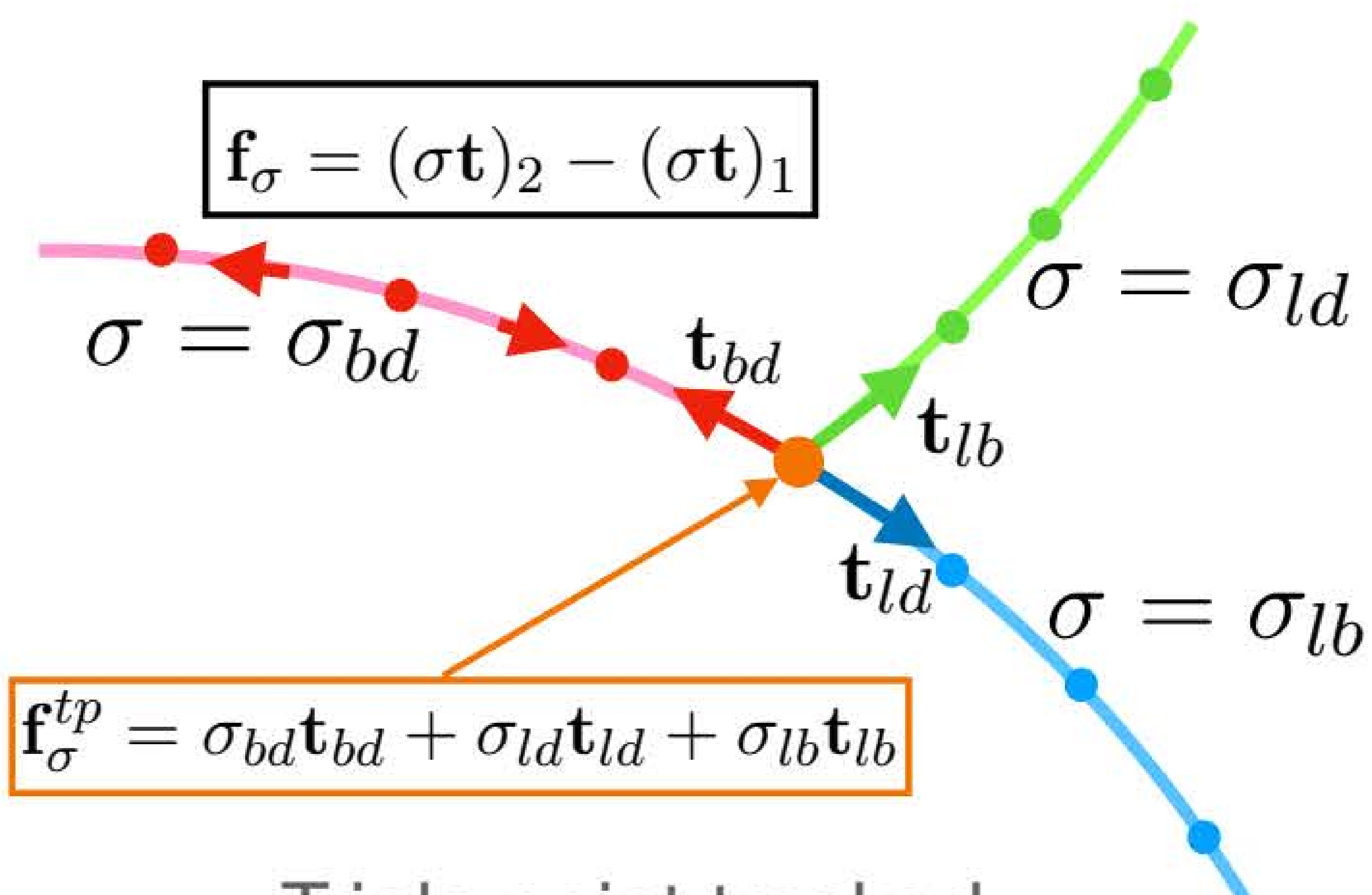
Three Fluid Flow—Two Approaches

We allow for variable surface tension and compute the force on a small surface element by

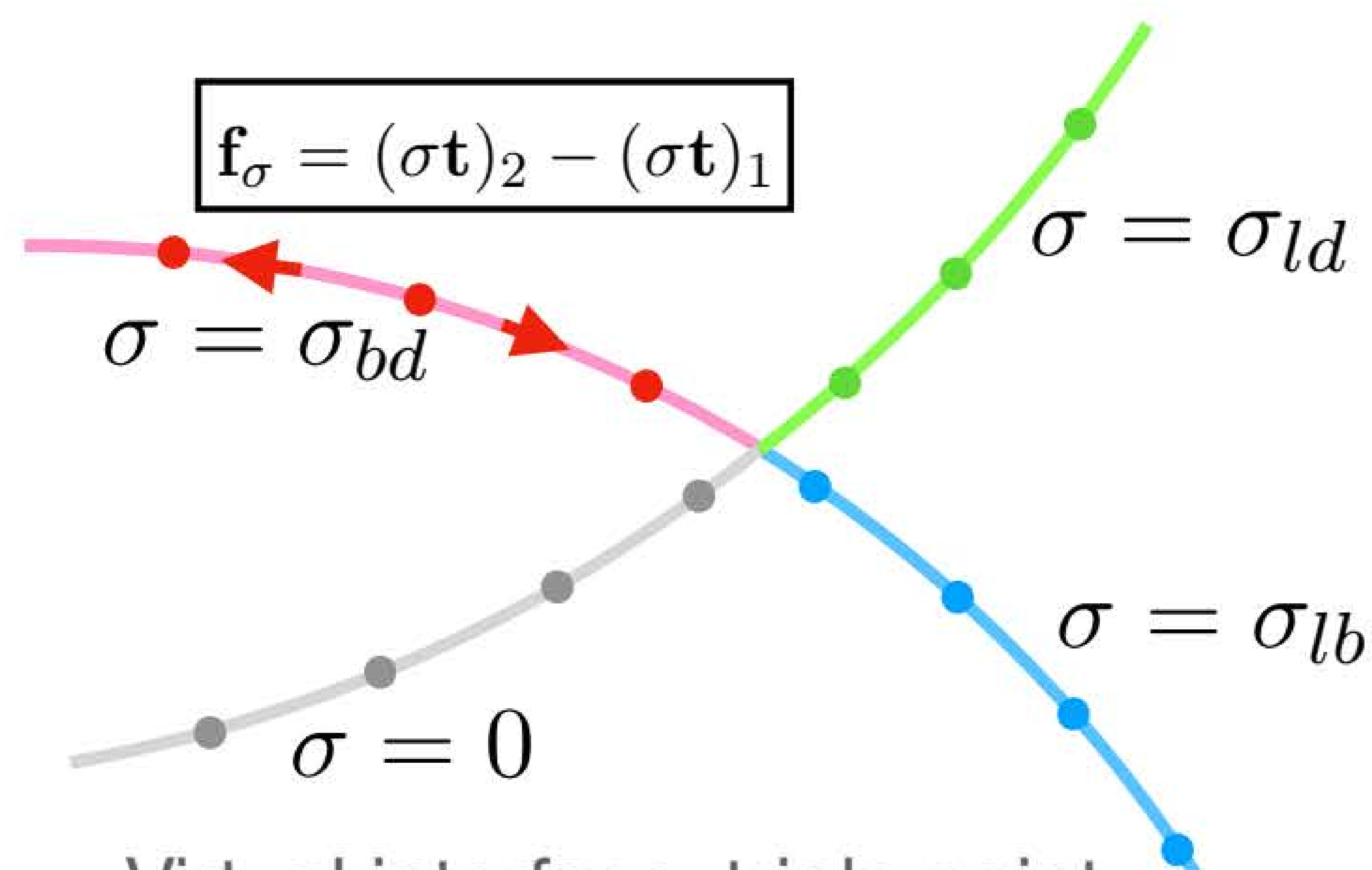
$$\mathbf{f}_\sigma = \oint \sigma \mathbf{s} \times \mathbf{n} ds$$



We can handle the contact point (line) in two different ways: We can explicitly track it, or we can extend one of the interfaces into the other fluid but set the surface tension equal to zero. For the three fluid case nothing else needs to be done, simplifying implementation considerably



Triple point tracked separately



Virtual interface, triple point not tracked separately

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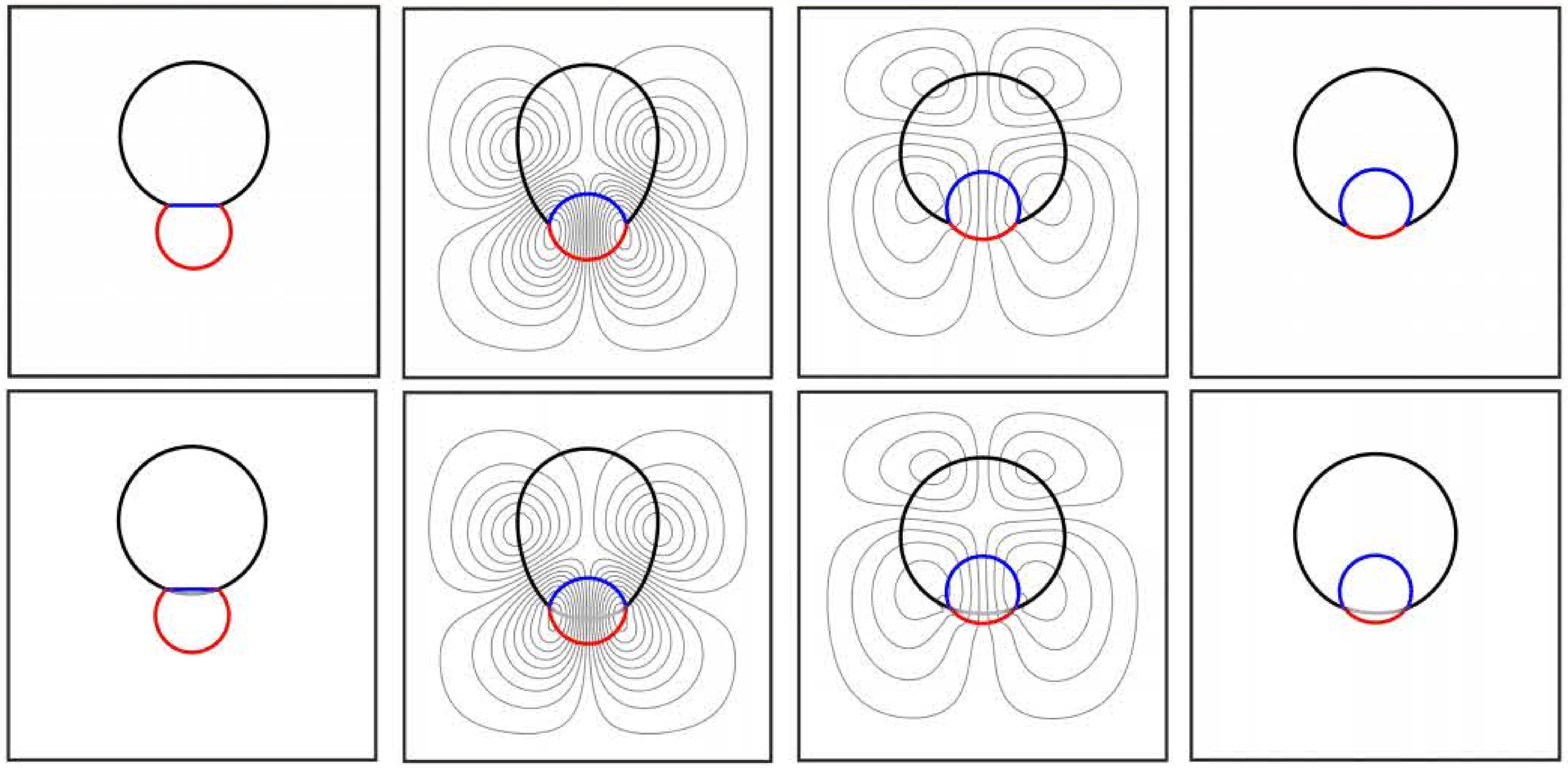
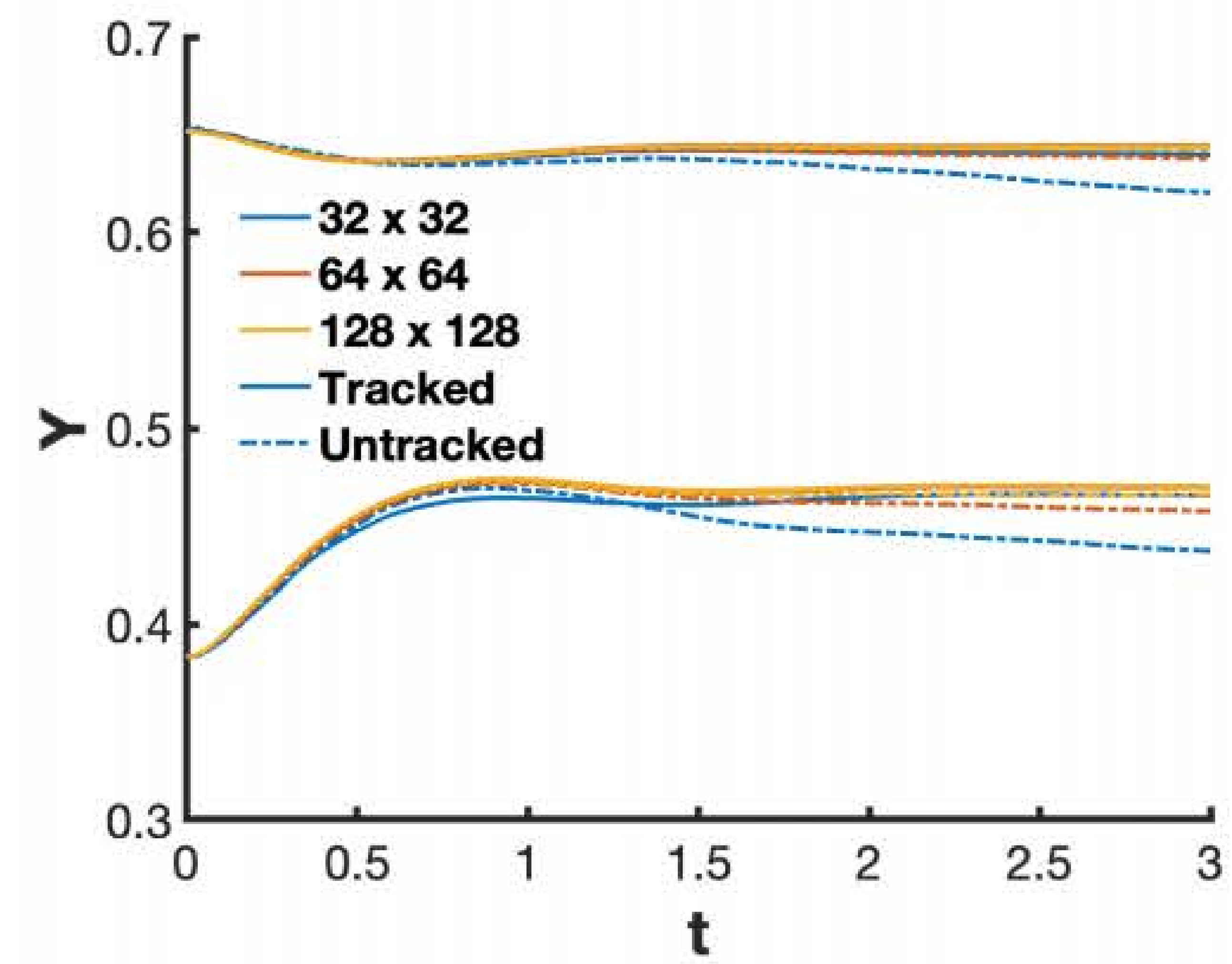
Three Fluid Flows

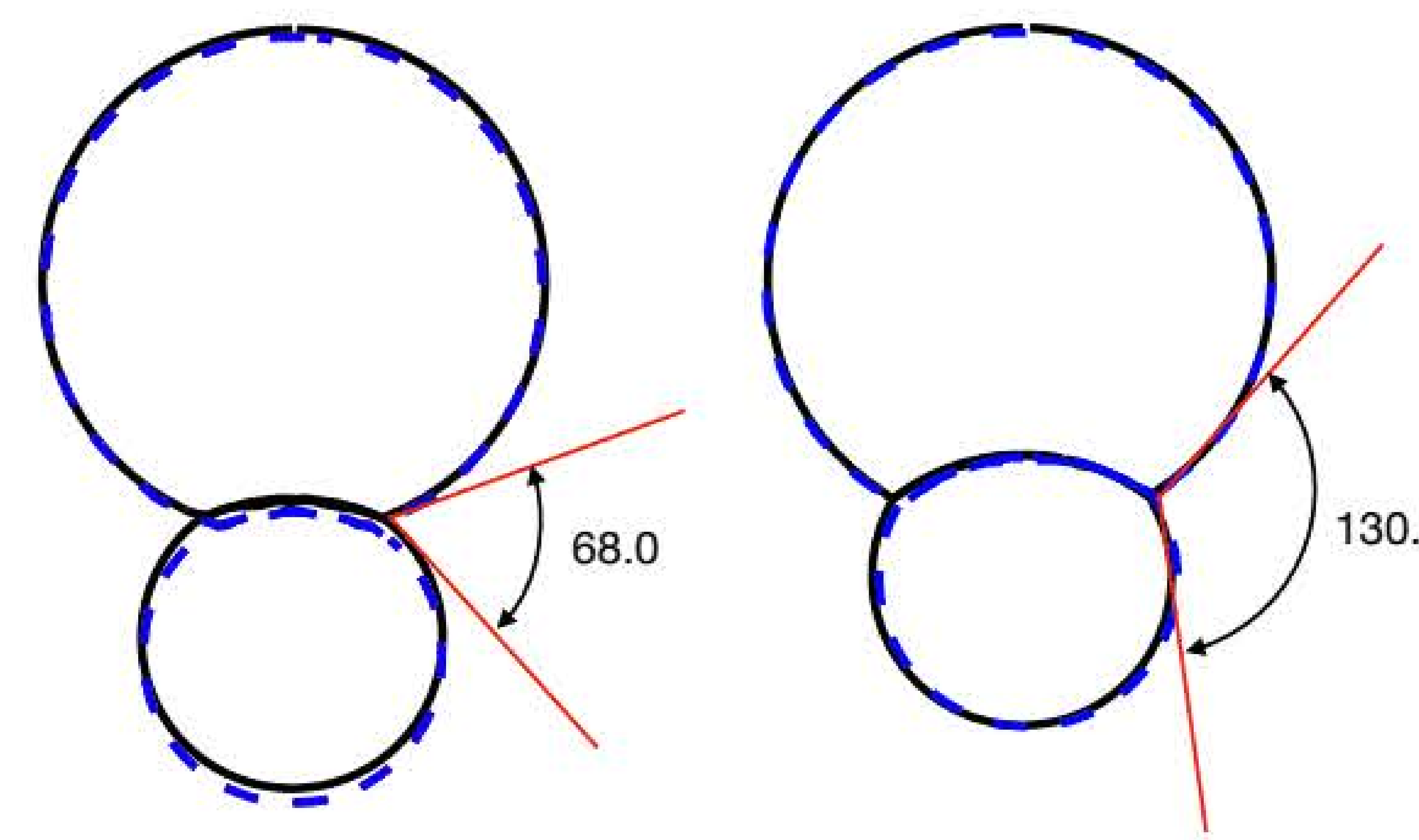


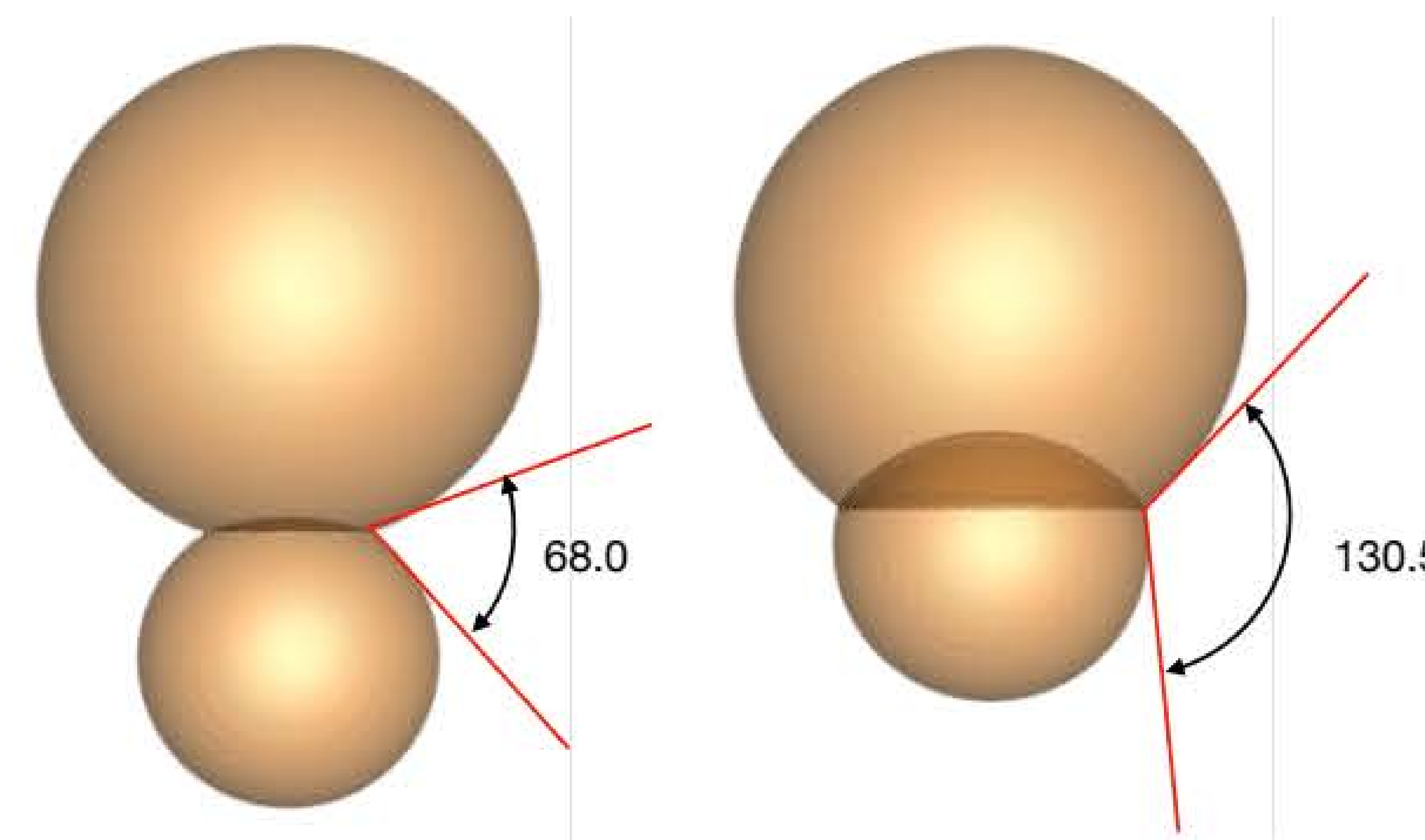
The transient evolution for two-dimensional flow. The triple point is explicitly tracked in the top row, but not in the bottom row. Times are 0.0, 0.2, 0.6, 2.0.

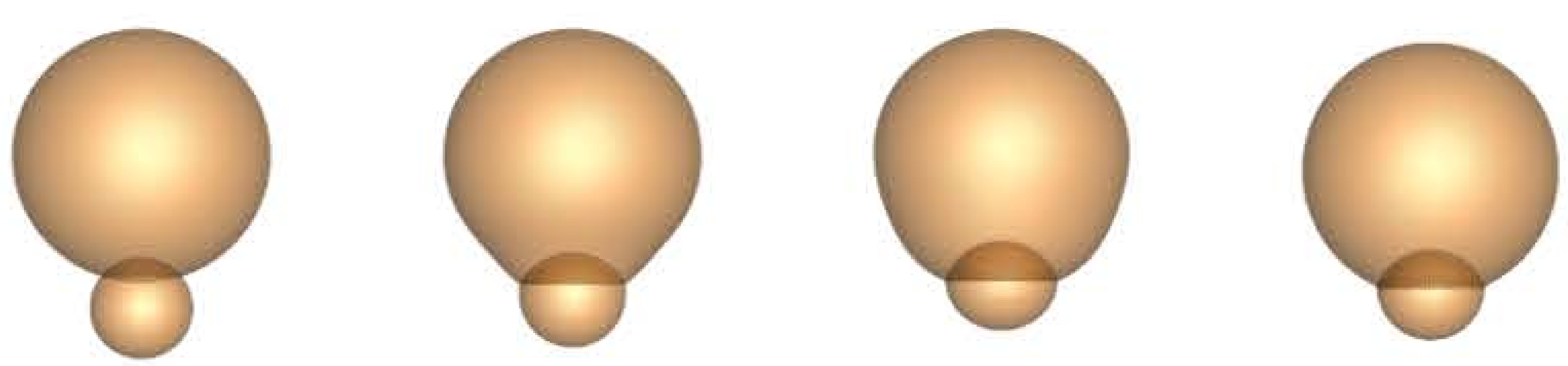


The motion of the centroid of the bubble and drop versus time for three different resolutions.

Both approaches give the same results but the untracked one using a virtual interface is much easier to implement, particularly for three-dimensional flow







The transient evolution of a fully three-dimensional flow, computed using the untracked approach. Times are 0.0, 0.2, 0.6, 2.0

The steady state for two resolutions and two different contact angles.

Left $\theta_l = 68^o$; Right $\theta_l = 130.5^o$

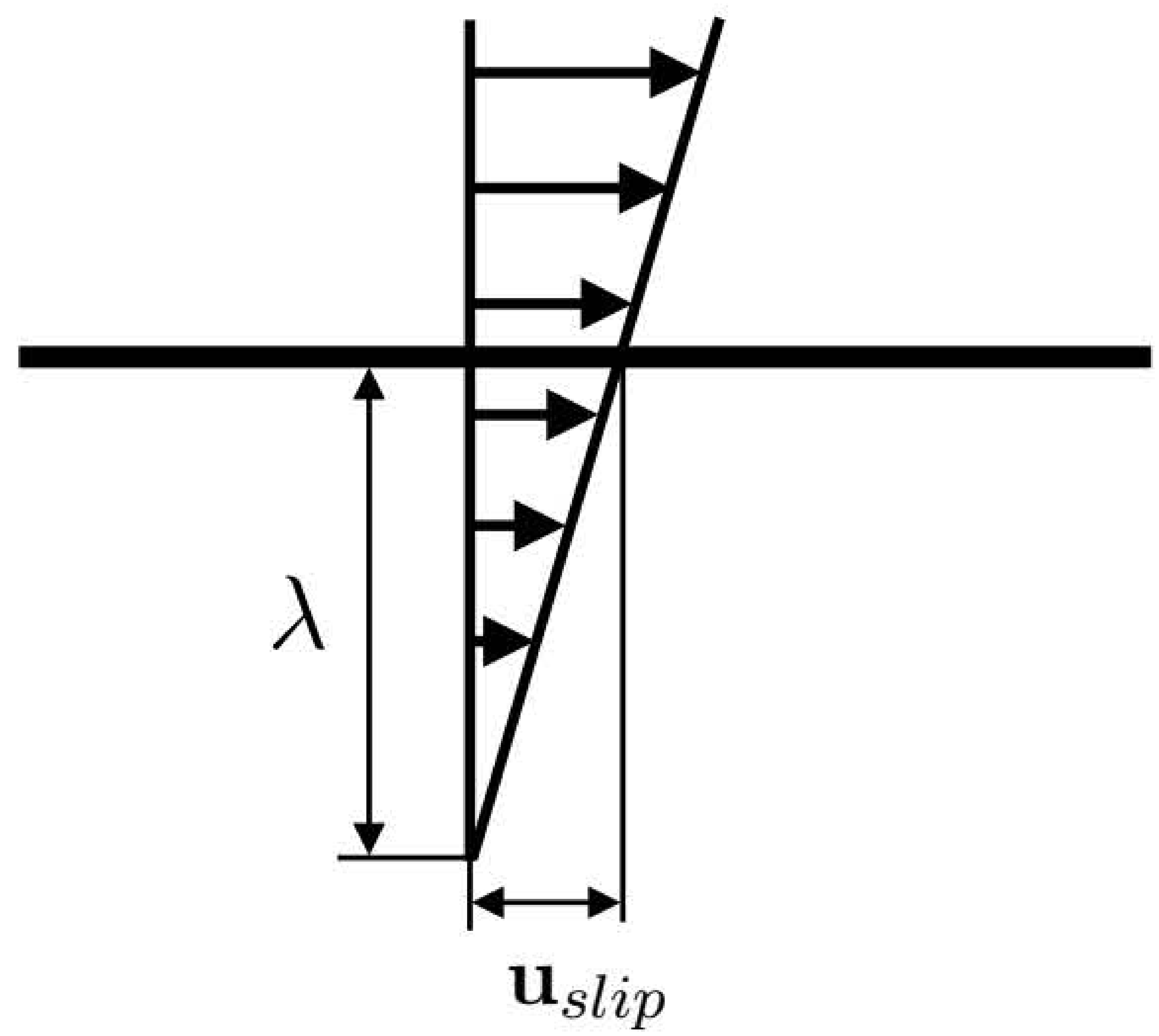
Froth Flotation—Solid Particles

For a moving contact line the unbalanced force along the interface results in slip velocity.

We assume that the slip velocity is proportional to the unbalanced force, assuming Generalized Navier Boundary Conditions (GNBC).

$$\beta u_{slip} = \tau_{visc} - \tau_Y \qquad \beta = \mu/\lambda$$

The slip length thus becomes a parameter determining how fast the solid particle is “engulfed” into the bubble.



$$\Delta u_{slip} = C_{slip} f_t$$

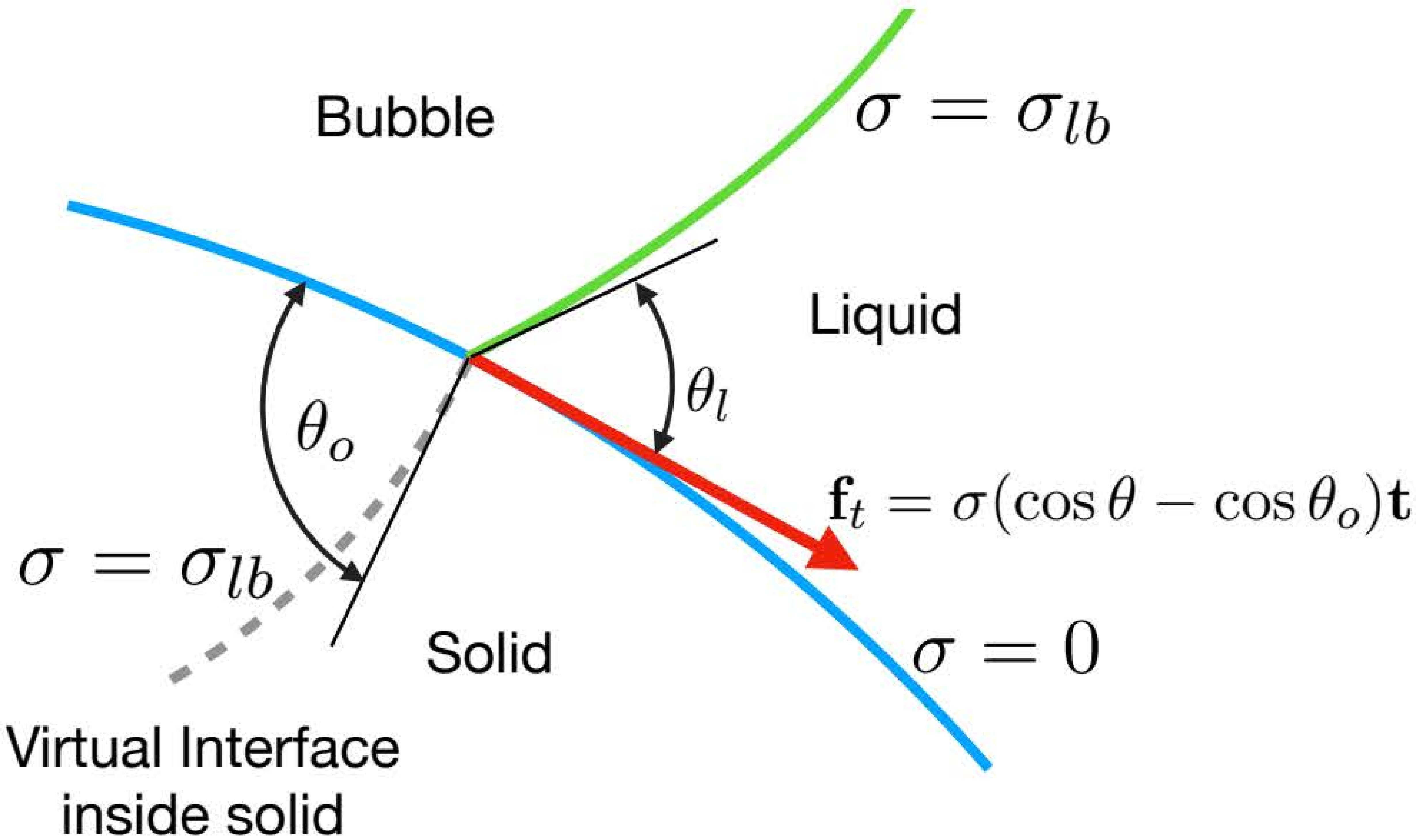
GNBC:

T. Qian, X.-P. Wang and P. Shen. Generalized Navier Boundary Condition for the Moving Contact Line. Comm. Math. Sci. Vol. 1, No. 2, pp. 333–341.

For a general review: Weiqing Ren, Dan Hu, and Weinan E. Continuum models for the contact line problem. Physics of Fluids 22, 102103 (2010);

Froth Flotation—Solid Particles

Numerical implementation using a "virtual interface" inside the solid



In principle, the force applied to the solid to keep it rigid should balance the "pull" from the interface. However, ensuring momentum conservation turned out to be challenging so we have extended the interface through the solid, which gives better conservation

The end point of the virtual interface (at the solid surface) is moved with the slip velocity, the first point is set at the correct angle and the location of other points inside the solid is set by minimizing

$$E = \int \left| \frac{\partial^2 \mathbf{x}}{\partial s^2} \right|^2 ds.$$

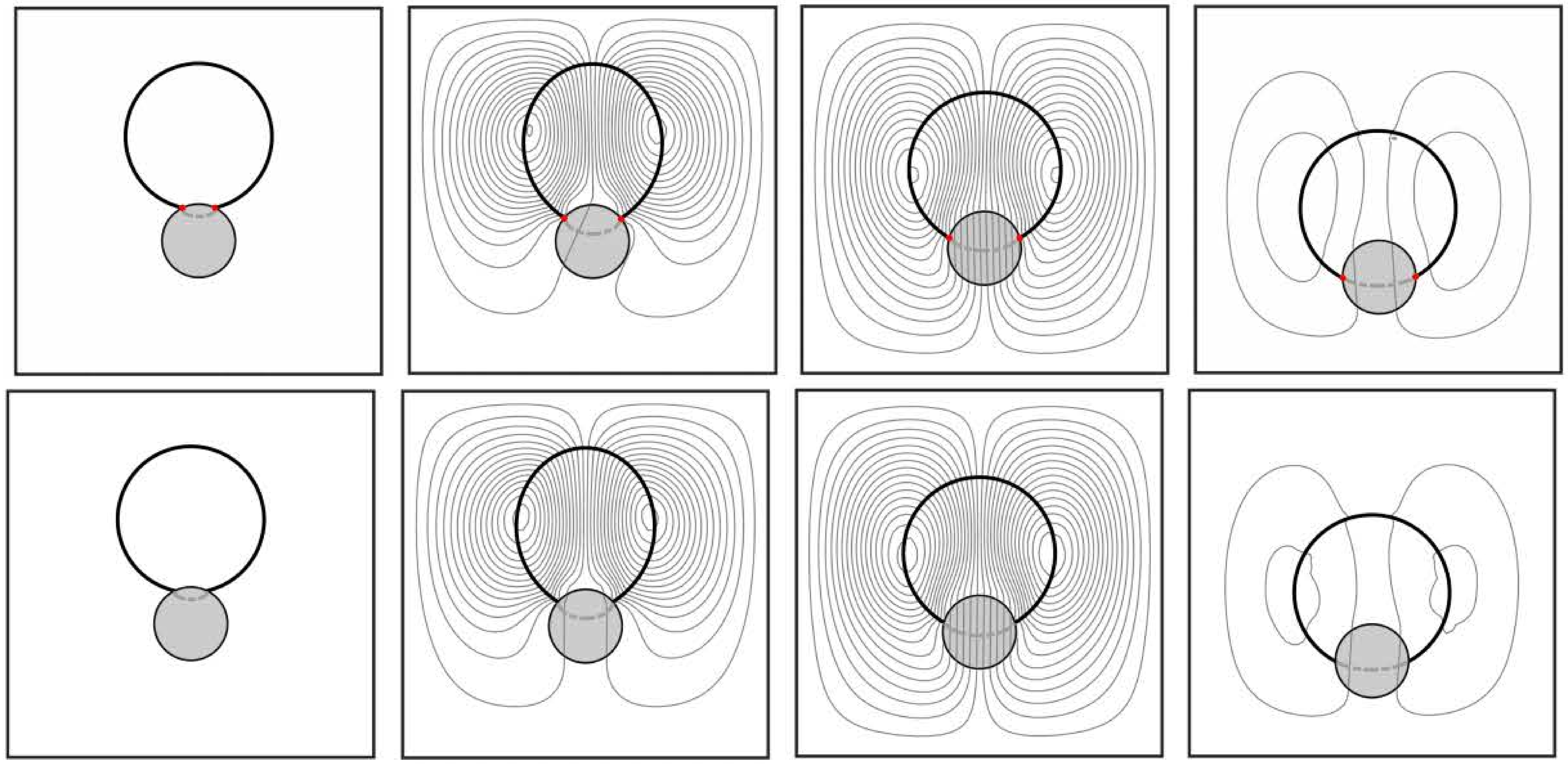
using iteration

$$\tilde{\mathbf{x}}_l = (\mathbf{x}_{l+1} + \mathbf{x}_l + \mathbf{x}_{l-1})/3$$
$$\tilde{\tilde{\mathbf{x}}}_l = (\tilde{\mathbf{x}}_{l+1} + \tilde{\mathbf{x}}_l + \tilde{\mathbf{x}}_{l-1})/3$$
$$\mathbf{x}_l = 2\,\tilde{\mathbf{x}}_l - \tilde{\tilde{\mathbf{x}}}_l$$

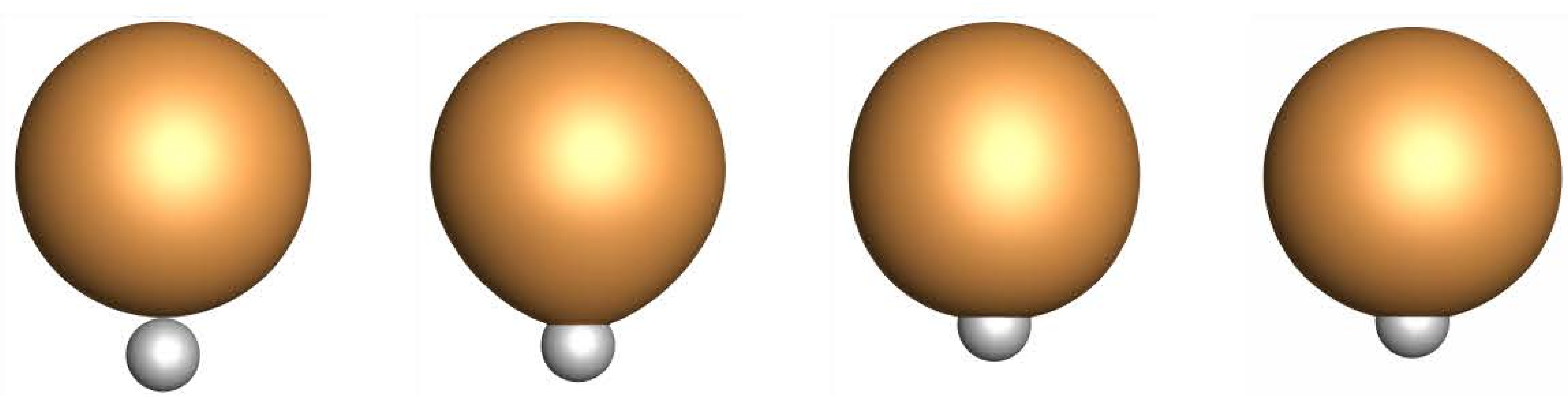
Following ideas originally presented by:

M. Fujita, O. Koike, and Y. Yamaguchi. Computation of capillary interactions among many particles at free surface. Applied Physics Express, 6:036501, 2013.

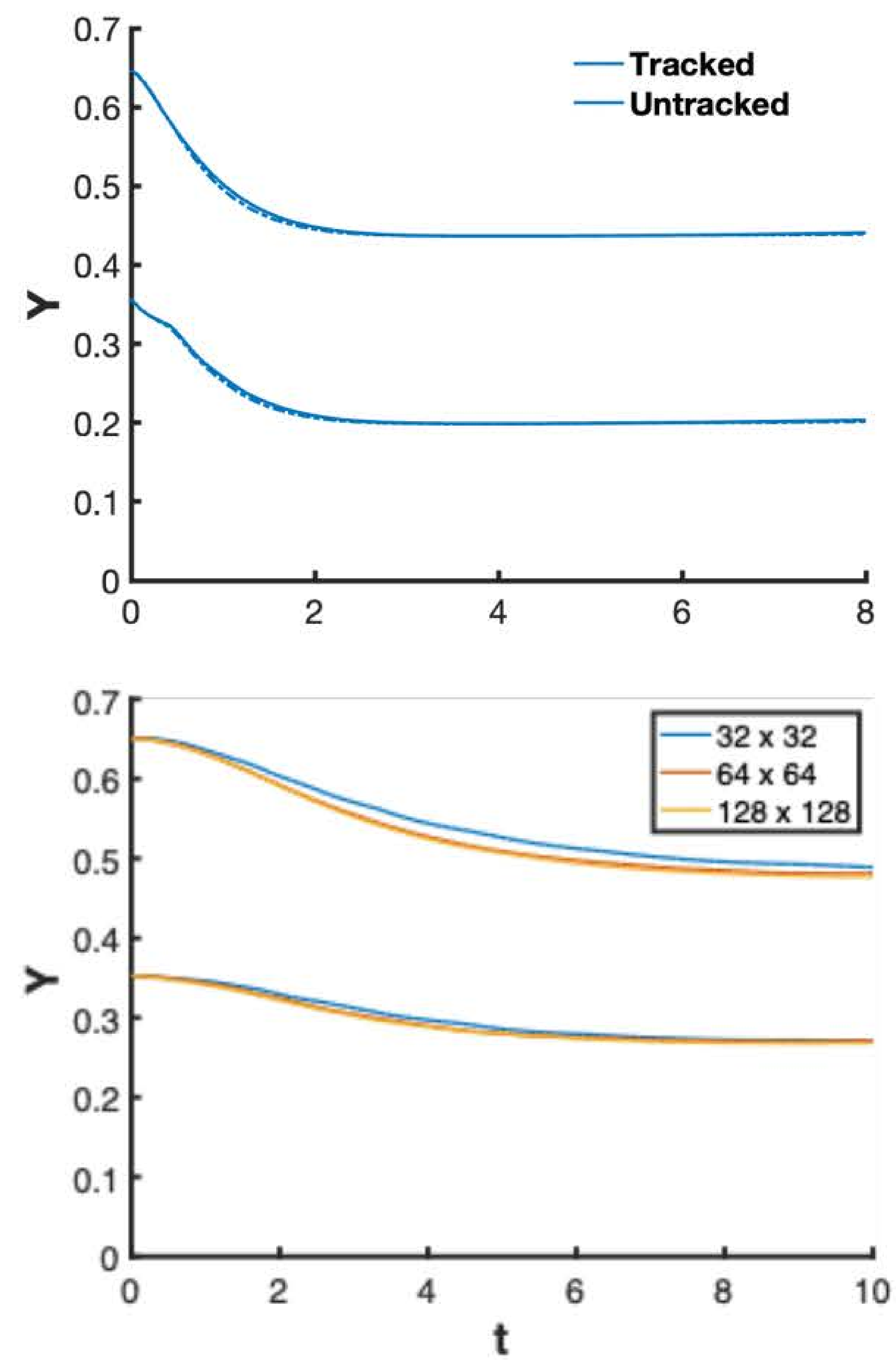
Froth Flotation—Solid Particles



Transient for a solid particle and a bubble computed using both the tracked and the untracked approach, at times 0, 0.5, 1.0 and 2.0. The domain is resolved by 64 × 64 grid.



Transient for a solid particle and a bubble for fully three-dimensional flow, computed using the tracked approach. Times are 0, 0.5, 1.0 and 2.0. The domain is resolved by 64 × 64 grid.



Convergence for solid particle. The domain is resolved by 32 × 32 grid in the left column and by 64 × 64 grid in the right column.

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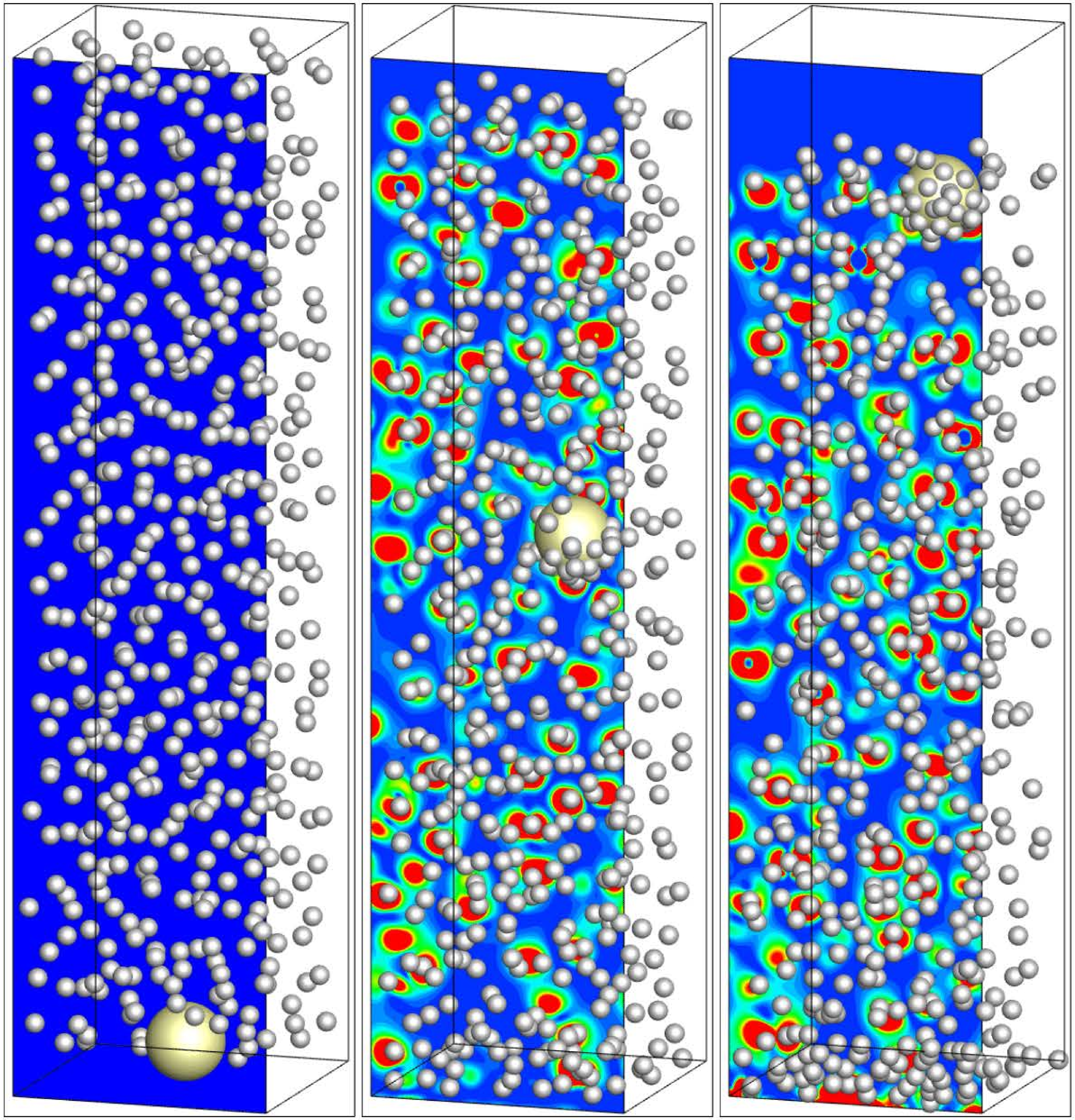
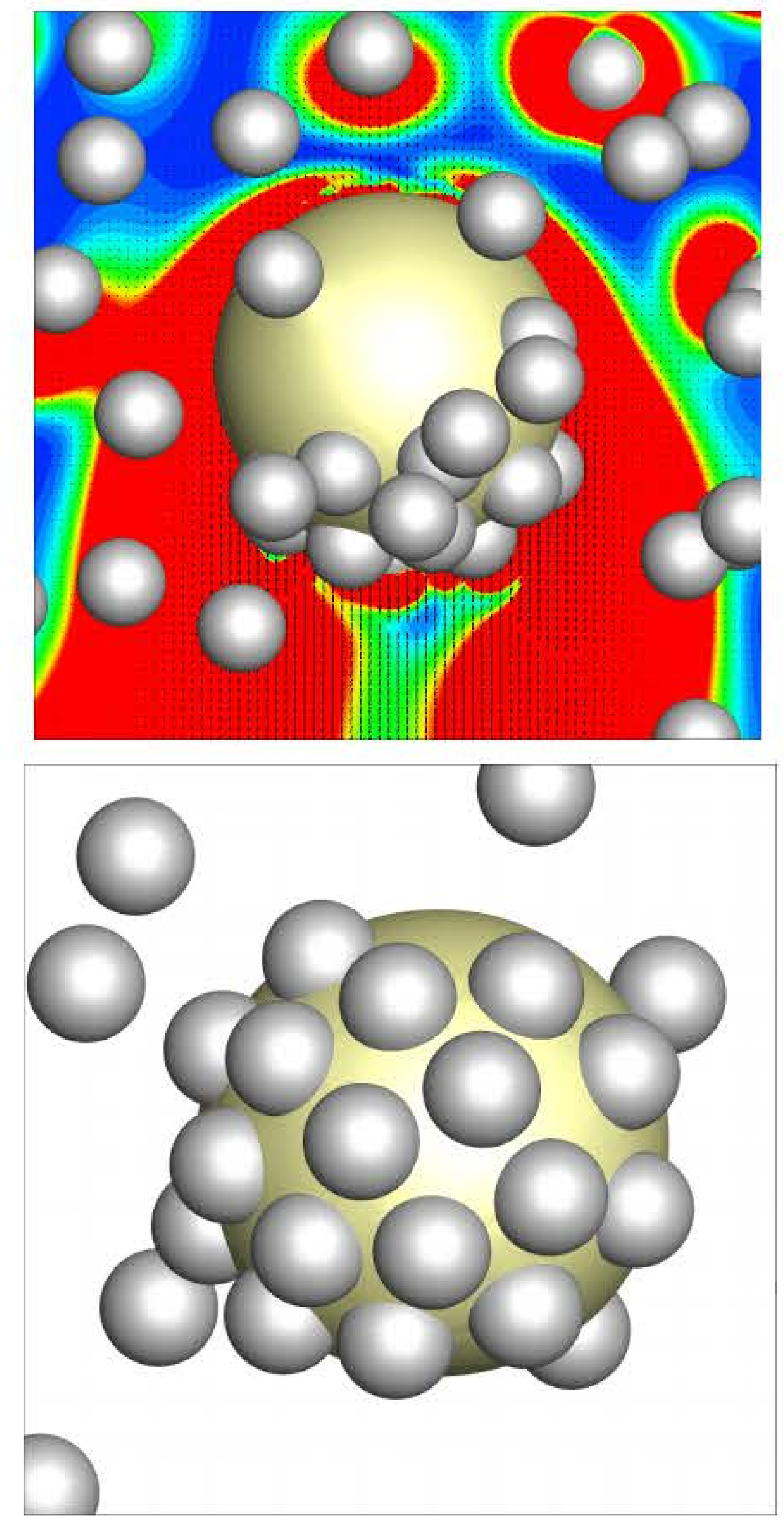
Froth Flotation—Solid Particles

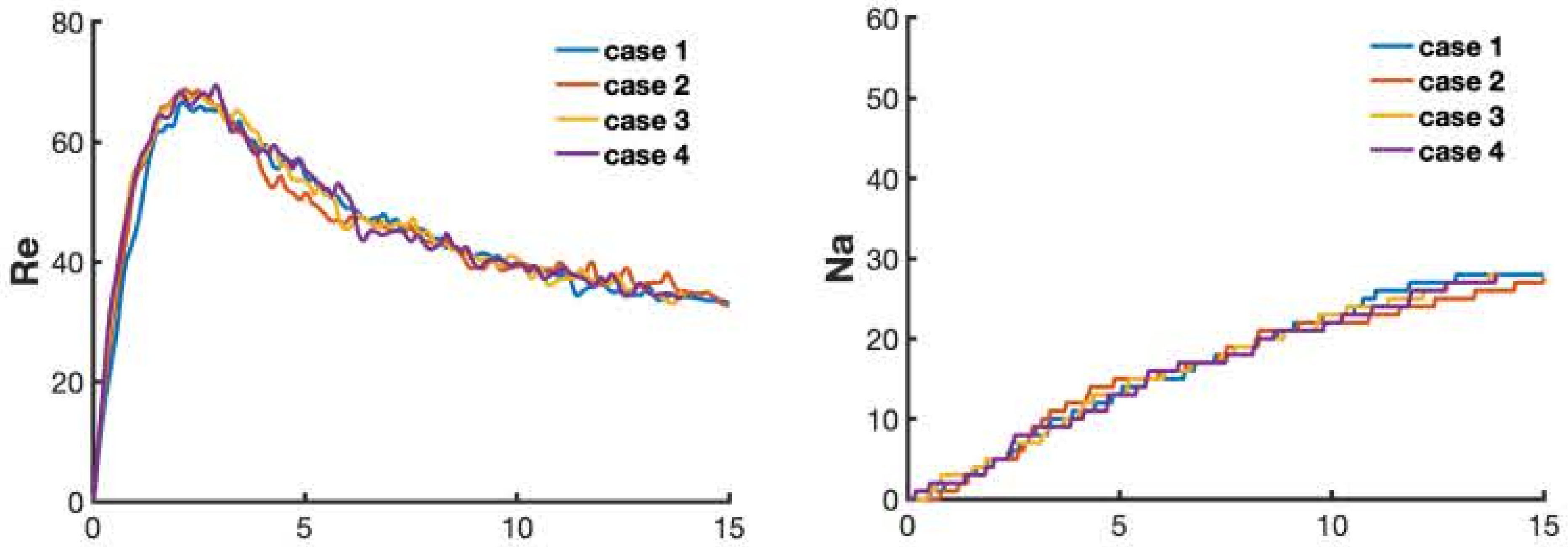


1 bubble (yellow) and 500 hydrophobic particles (grey) with Eo = 1, Ar = 3110.4, $\gamma = 4$ and $\theta_S = 100^\circ$ at time $\tau = [0, 7.5, 15]$. The enstrophy is shown in a plane at the back of the domain.

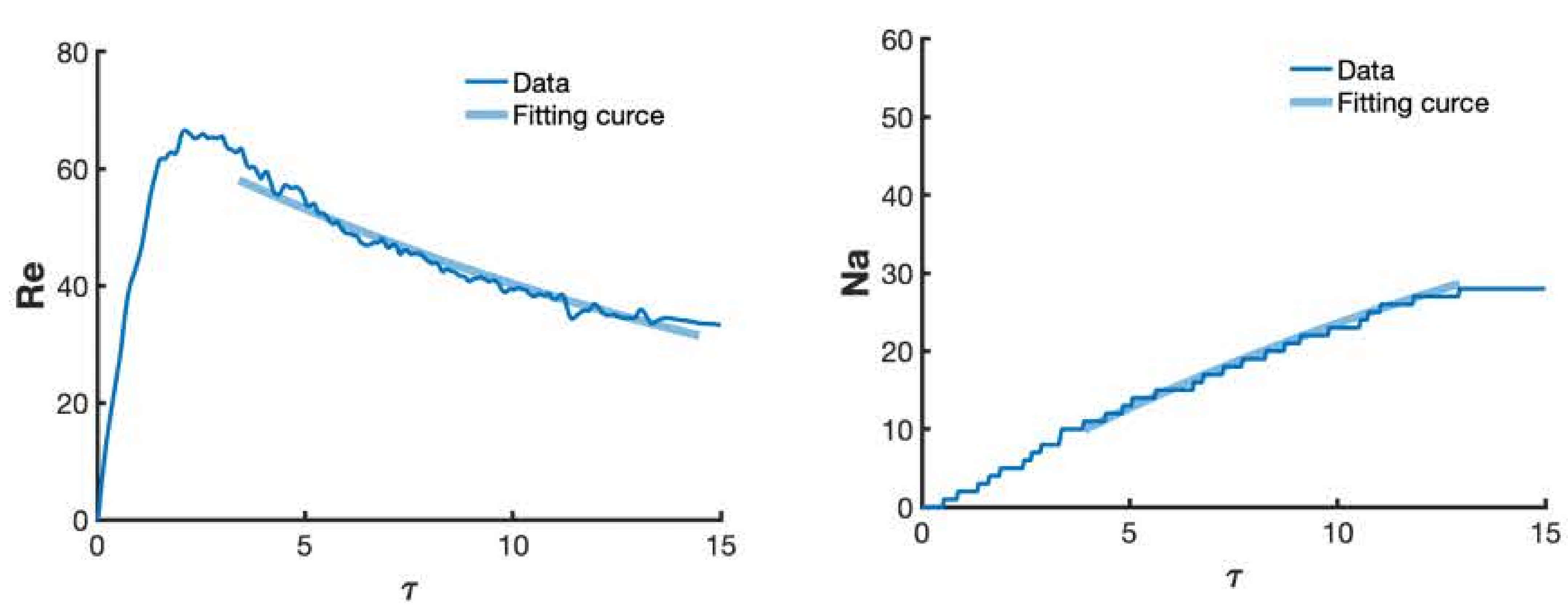


Details of figure 2 at $\tau = 7.5$. (a) Side view with velocity vector and enstrophy in the back plane. (b) Bottom view.

Froth Flotation—Single Bubble



(a) The rise velocity of bubble and solid particles for Eo = 1, Ar = 3110.4, γ = 4 and θ_S = 100°, and (b) Number of particles attached to the bubble (N_a) versus time for the different initial distribution of particles.



The fitting model for (a) the relative velocity of bubble and solid phases and (b) the number of particles attached to the bubble (N_a) for Eo = 1.

Use the simple model to fit the data

$$N_a(\tau) = \frac{1}{r} + \left(N_0 - \frac{1}{r}\right)\text{Exp}\left[-\frac{2C_a}{k}\left(\frac{D_b}{D_s}\right)^3 \alpha r\sqrt{Ar}(\tau - \tau_0)\right]$$

$$Re(\tau) = -\frac{4}{3k}Ar\left(N_0 - \frac{1}{r}\right)\text{Exp}\left[-\frac{2C_a}{k}\left(\frac{D_b}{D_s}\right)^3 \alpha r\sqrt{Ar}(\tau - \tau_0)\right]$$

Where N_o is the number of attached particles at time τ_o.

Define

$$C_\tau = \left[-\frac{2C_a}{k}\left(\frac{D_b}{D_s}\right)^3 \alpha r\sqrt{Ar}(\tau - \tau_0)\right]$$

$$r = \frac{\Delta\rho_s V_s}{\Delta\rho_b V_b}$$

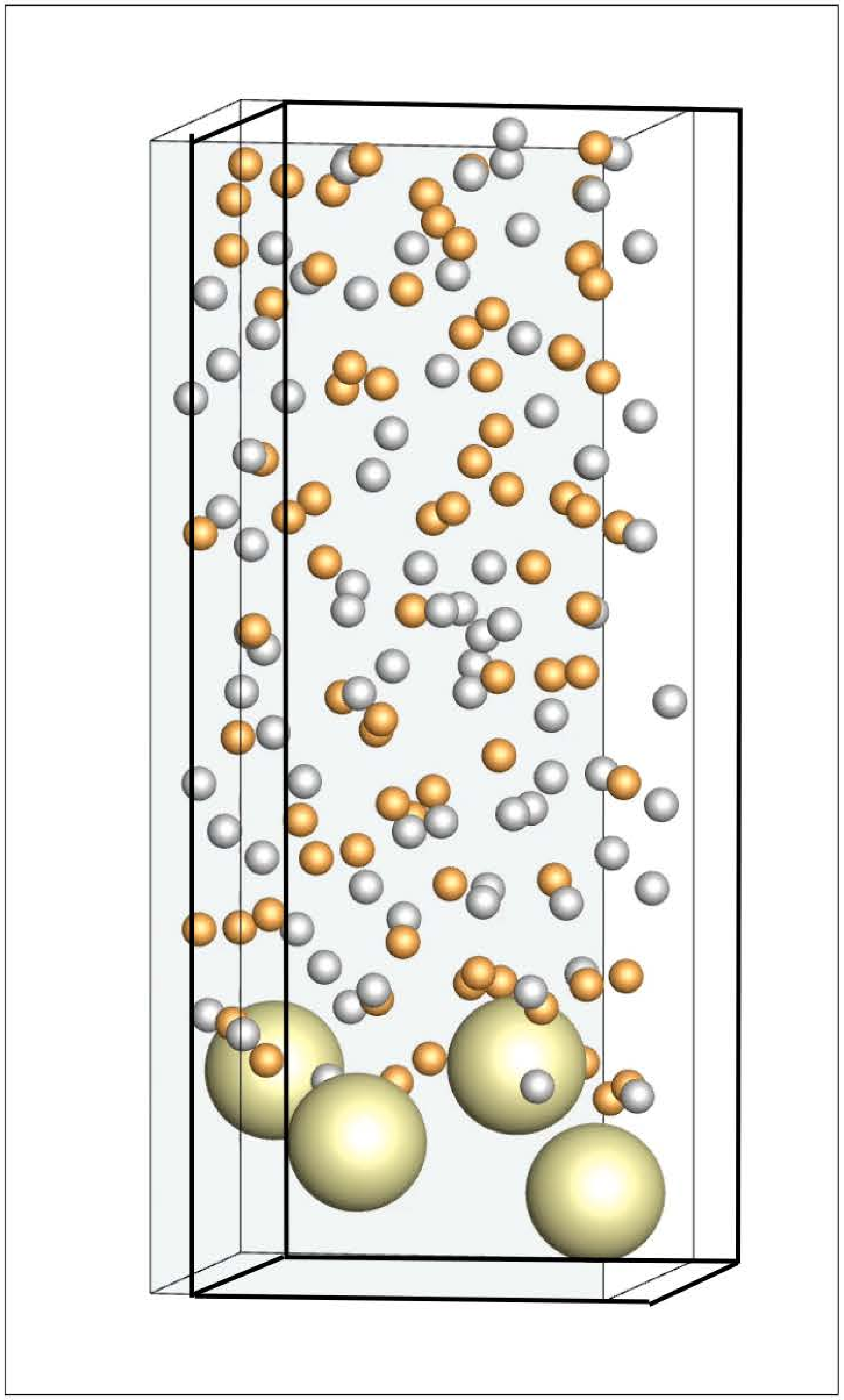
$$C_u = -\frac{4}{3k}Ar\left(N_0 - \frac{1}{r}\right) \qquad C_N = \left(N_0 - \frac{1}{r}\right)$$

Fit

$$\log(Re) = C\tau + C_u \qquad \log\left(N_a - \frac{1}{r}\right) = C\tau + C_N$$

Solve for C_a and k

Froth Flotation—Many Bubbles



Domain Size $(L_x \times L_z \times L_y)$	$3 \times 3 \times 8$
Resolution $(N_x \times N_z \times N_y)$	$192 \times 192 \times 512$
Gravity (g)	-0.1
Number of bubble(N_b)	12
Viscosity (μ_l/μ_b)	$0.0025/0.00025$
Density $(\rho_l/\rho_b/\rho_s)$	$1.0/0.1/2$
Diameter (D_b/D_s)	$0.6/0.15$
Static contact angle (θ_s)	$100°$
Contact point slip velocity (u_{slip})	$[0.1, 0.2]$

Eötvös number (Eo)	$[1, 3]$
volume fraction (α)	$[2.7\%, 5.4\%]$

σ	0.0648	0.0324	0.0162	0.0081
Eo	0.5	1.0	2.0	4.0
M	1.29×10^{-8}	1.03×10^{-7}	8.27×10^{-7}	6.62×10^{-6}

	Eo	α_1 (Hydrophobic)	$\alpha_2(Hydrophilic)$
Case 1	1	2.7%	0%
Case 2	3	2.7%	0%
Case 3	3	5.4%	0%
Case 4	3	2.7%	2.7%

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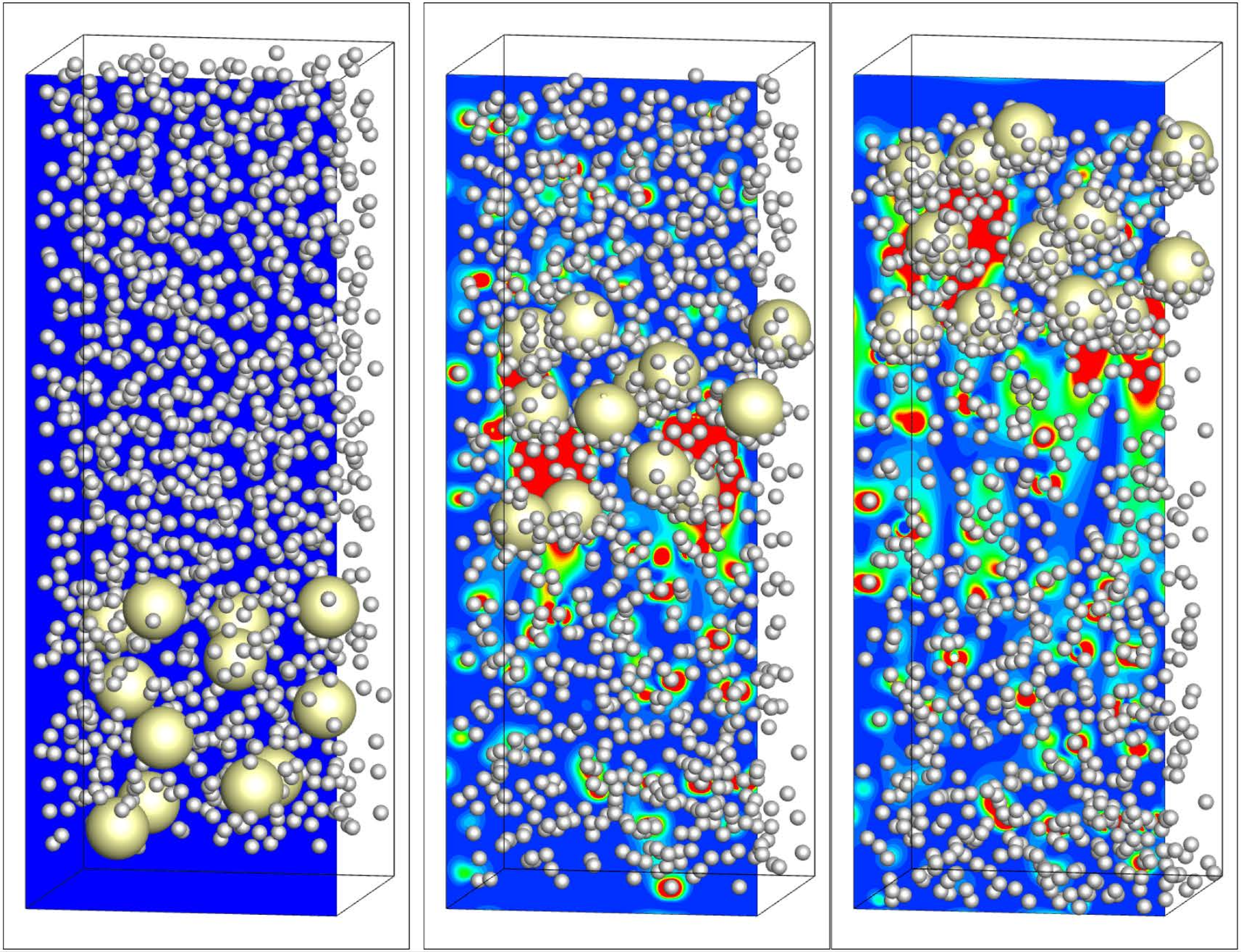
Froth Flotation—Many Bubbles



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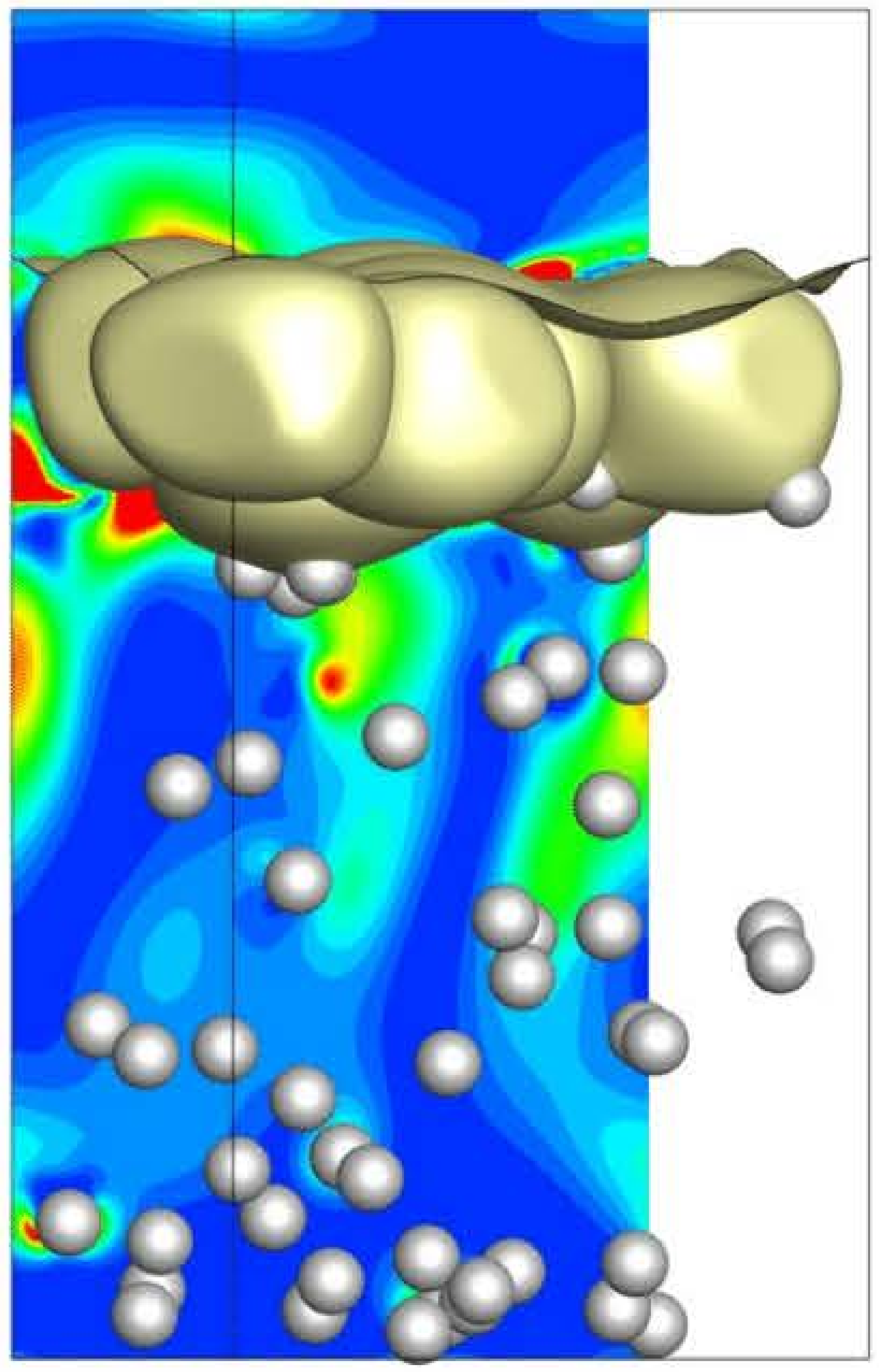
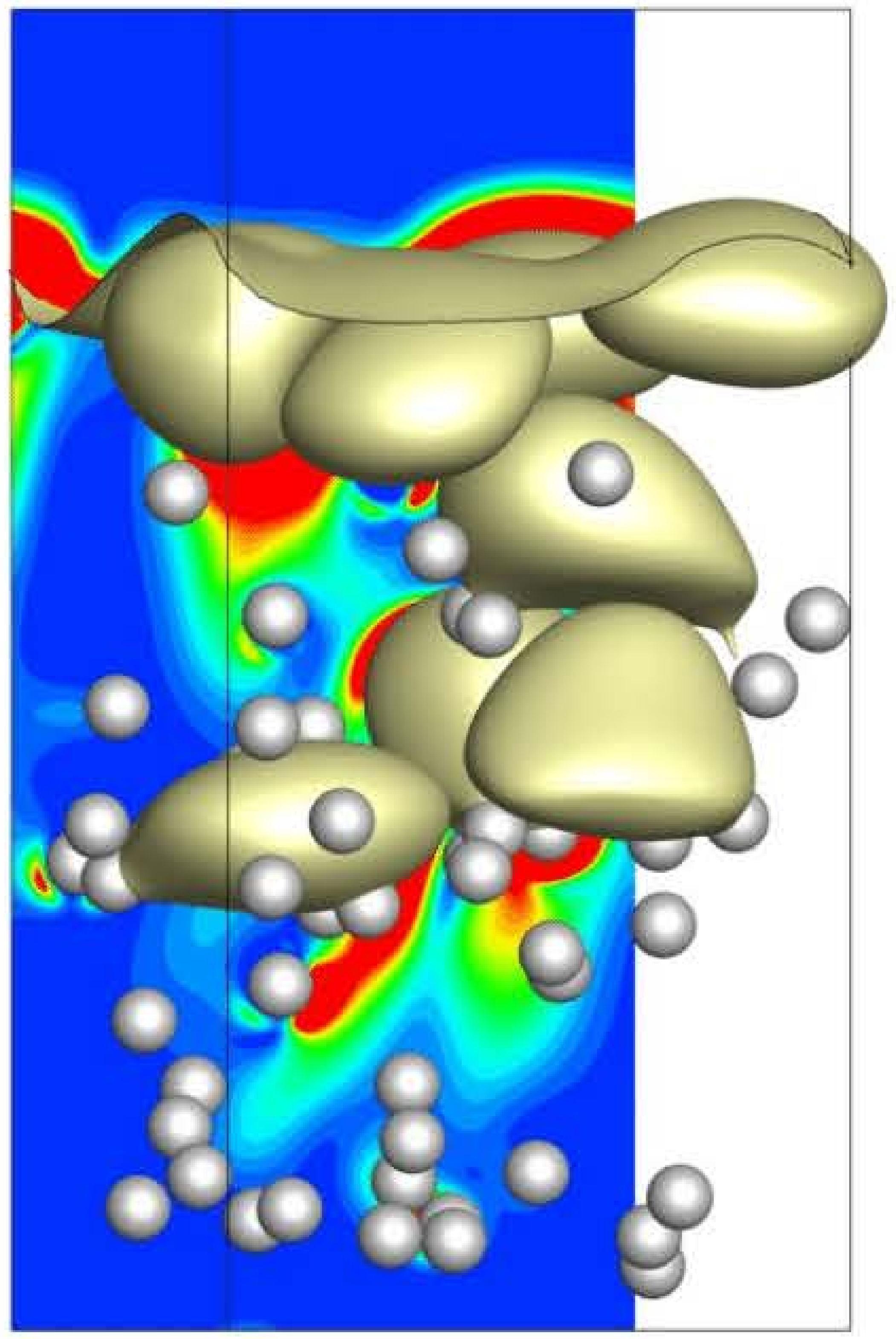
Froth Flotation



Froth flotation is a complex process with complex chemistry and hydrodynamics, where bubbles and particles of different sizes and shapes interact and mix in turbulent flow with surfactants and frothers.

However: Exactly how differences in wettability translate into selectivity is still essentially unknown.

Accurate modeling of selection by flotation require capturing many processes taking place on a large range of length and time scales, requiring multiscale approaches that capture different physical processes in different ways



Froth flotation is a problem of enormous and growing economic significance. First of all, in mineral processing its significance will grow as it becomes necessary to mine deposits of lower quality and environmental concerns demand more efficiency, thus requiring better insight and predictability. Secondly, the use of flotation in recycling of plastic is likely to grow significantly in the near future, demanding understanding and predictive capabilities in a different operational range from mineral processing.

Interface
Retaining
Coarsening

Coarse Grained Models for Multiphase Flows

JOHNS HOPKINS
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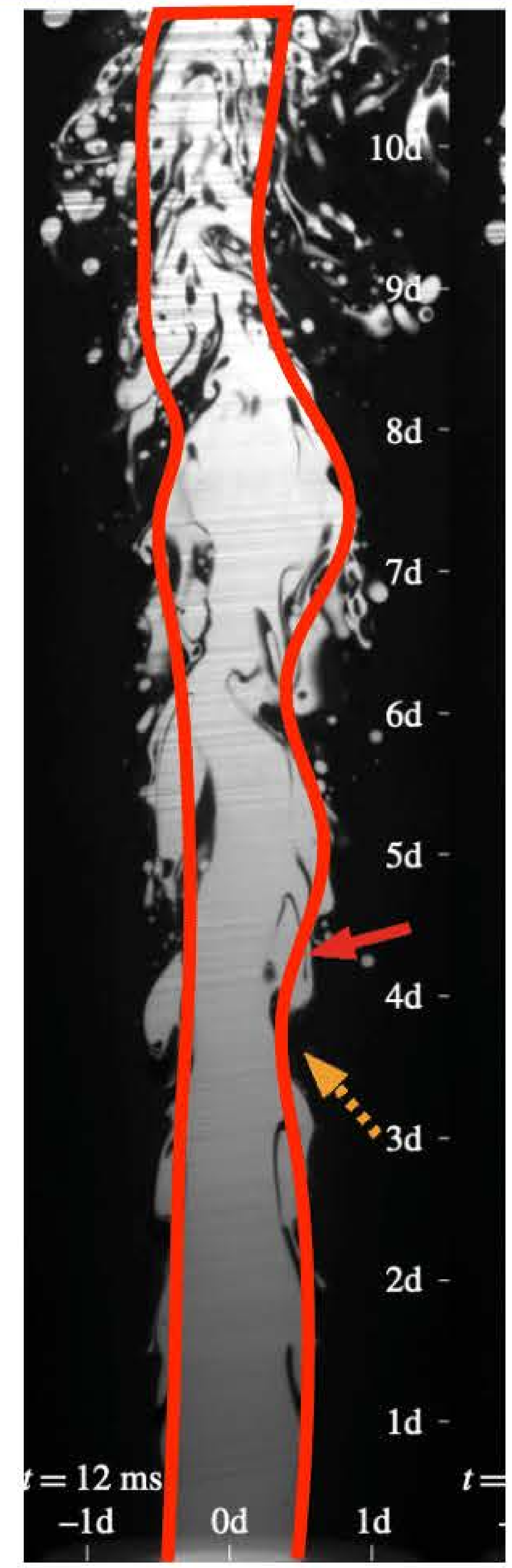
For multiphase flows where sharp moving phase boundaries separate different fluids or phases, the dynamics of the interface often determines the behavior of the flow.

In a coarse, or reduced order model, it may therefore be important to retain a sharp interface for the resolved scales. Somewhat like modeling of disperse flows often retain bubbles or drops as point particles.

Here we seek one way to coarsen DNS results in a formal way

A formal coarsening process allows :

- Validation by comparison with filtered fully resolved solutions
- May help with determine the structure of the coarse equations



An example where the interface retaining assumption may be “iffy,” or require an additional interface—the cloud cavitation examples show by other presenters are other examples.

Xue, X., & Katz, J. (2019). Formation of compound droplets during fragmentation of turbulent buoyant oil jet in water. *Journal of Fluid Mechanics, 878*, 98-112. doi:10.1017/jfm.2019.645

Coarsening by Diffusion

Filtering and diffusion are closely linked. The solution of the time dependent constant coefficient diffusion equation in 2D unbounded domain

$$\frac{\partial g(t,\mathbf{x})}{\partial t} = D\nabla^2 g(t,\mathbf{x})$$ is given by $$g(\mathbf{x},\tau) = \frac{1}{4\pi D\tau}\int_{Area} e^{-\frac{||\mathbf{x}-\mathbf{x}'||^2}{4D\tau}} g_o(\mathbf{x}')da'.$$

If we take $4D\tau = \Delta^2/6.$ filtering and diffusion are interchangeable. Same in 3D

We prefer to work with the diffusion equations, since we can generalize the coarsening by modifying it and making the diffusion coefficient variable, such as by preventing diffusion or making it directionally dependent, and work close to boundaries

$$\tilde{D}(\boldsymbol{x},\tau) = D \text{ modified by setting } D(\boldsymbol{x}_f) = 0;$$

$$\frac{\partial \alpha'}{\partial \tau} = \nabla \cdot \tilde{D}\nabla\chi;$$

Identify the different phases by and index function

$$\chi(\boldsymbol{x}) = \begin{cases} 0 \text{ in fluid } 0 \\ 1 \text{ in fluid } 1. \end{cases}$$

Evolve the index field in pseudo time by

$$\frac{\partial \chi}{\partial \tau} = \nabla^2\chi$$

Interface velocity is determined from

$$\frac{D\chi}{D\tau} = \frac{\partial \chi}{\partial \tau} + \boldsymbol{u}\cdot\nabla\chi = 0.$$ and $$\frac{d\boldsymbol{x}_I}{d\tau} = \boldsymbol{u}_I$$

Interface Retaining Coarsening of Multiphase Flows

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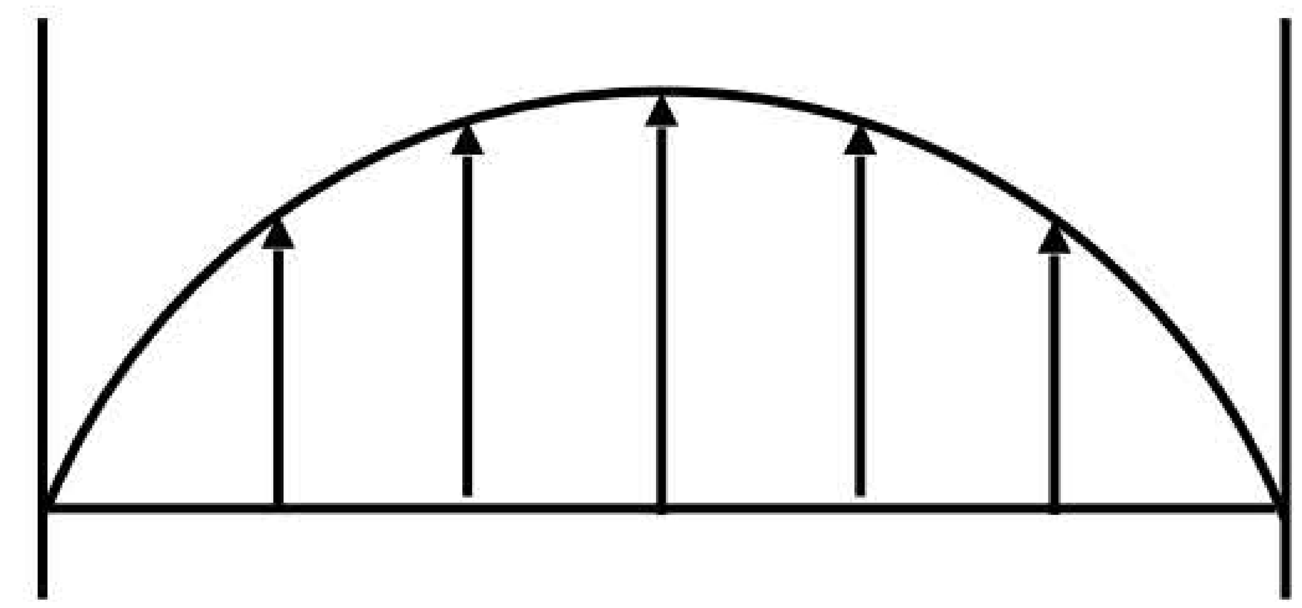
Can we derive the overall form the equations, even only for very simple situations?

Consider a flow in a vertical channel

$$\frac{\partial \rho u}{\partial t} = \frac{\partial}{\partial x}\mu\frac{\partial u}{\partial x} - \frac{\partial p}{\partial y} - \rho g; \quad u(0) = u(H) = 0;$$



We are interested in flow with an interface, but we start with a single phase flow and as simple model as possible

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + B;$$

Smooth the velocity

$$\frac{\partial \tilde{u}}{\partial \tau} = D\frac{\partial^2 \tilde{u}}{\partial x^2}$$

Write the governing equation as

$$L = \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} - B - \frac{\partial G}{\partial x} = 0$$

where

$$G(x) = \tau(0)\delta(x) + \tau(H)\delta(x - H)$$

Diffusing the operator

$$\frac{\partial \tilde{L}}{\partial \tau} = D\frac{\partial^2 \tilde{L}}{\partial x^2}$$

gives

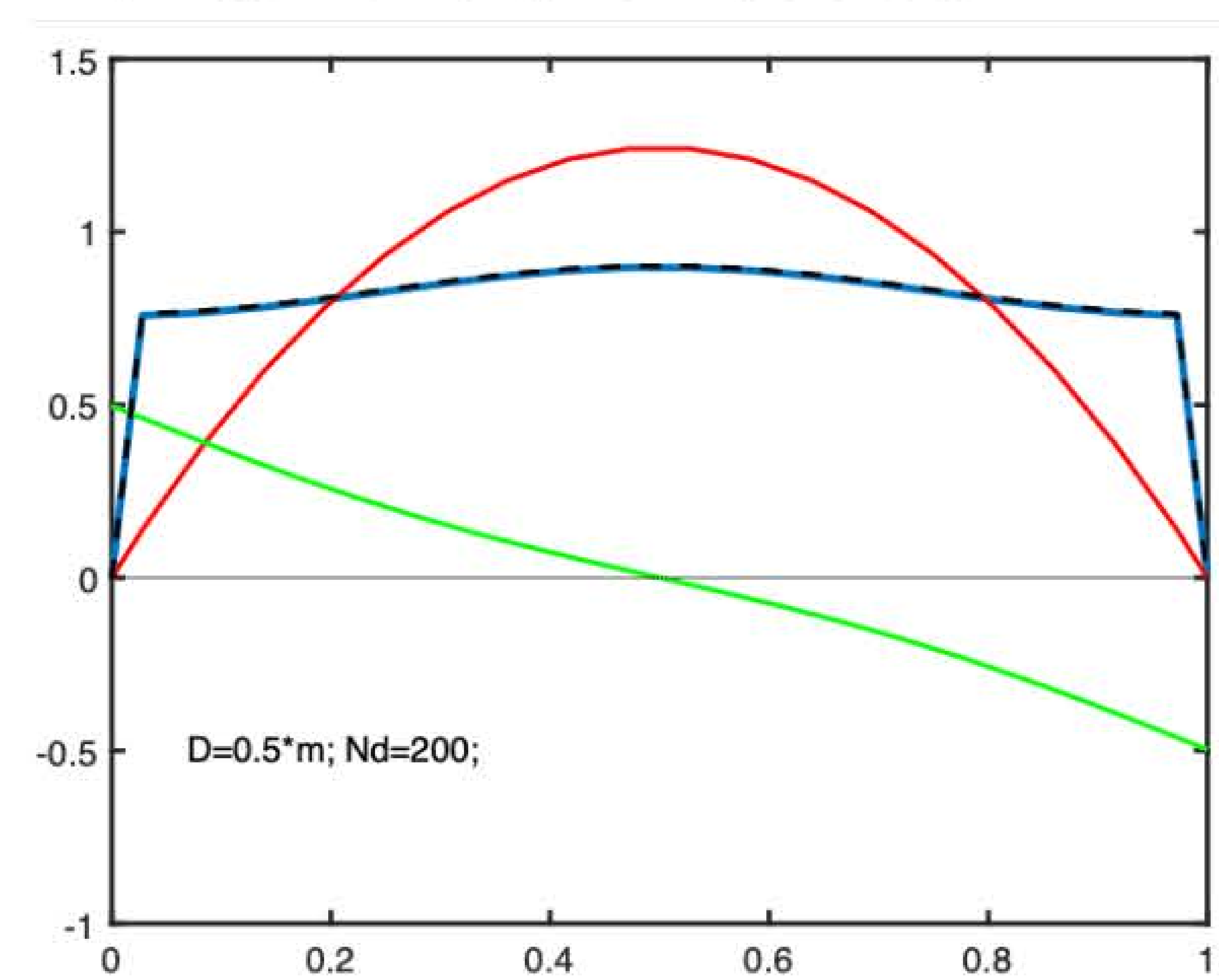
$$\frac{\partial \tilde{u}}{\partial t} = \frac{\partial}{\partial x}\nu\left(\frac{\partial \tilde{u}}{\partial x}\right) + B + \frac{\partial \tilde{G}}{\partial x}$$

$$\frac{\partial \tilde{G}}{\partial \tau} = D\frac{\partial^2 \tilde{G}}{\partial x^2}$$

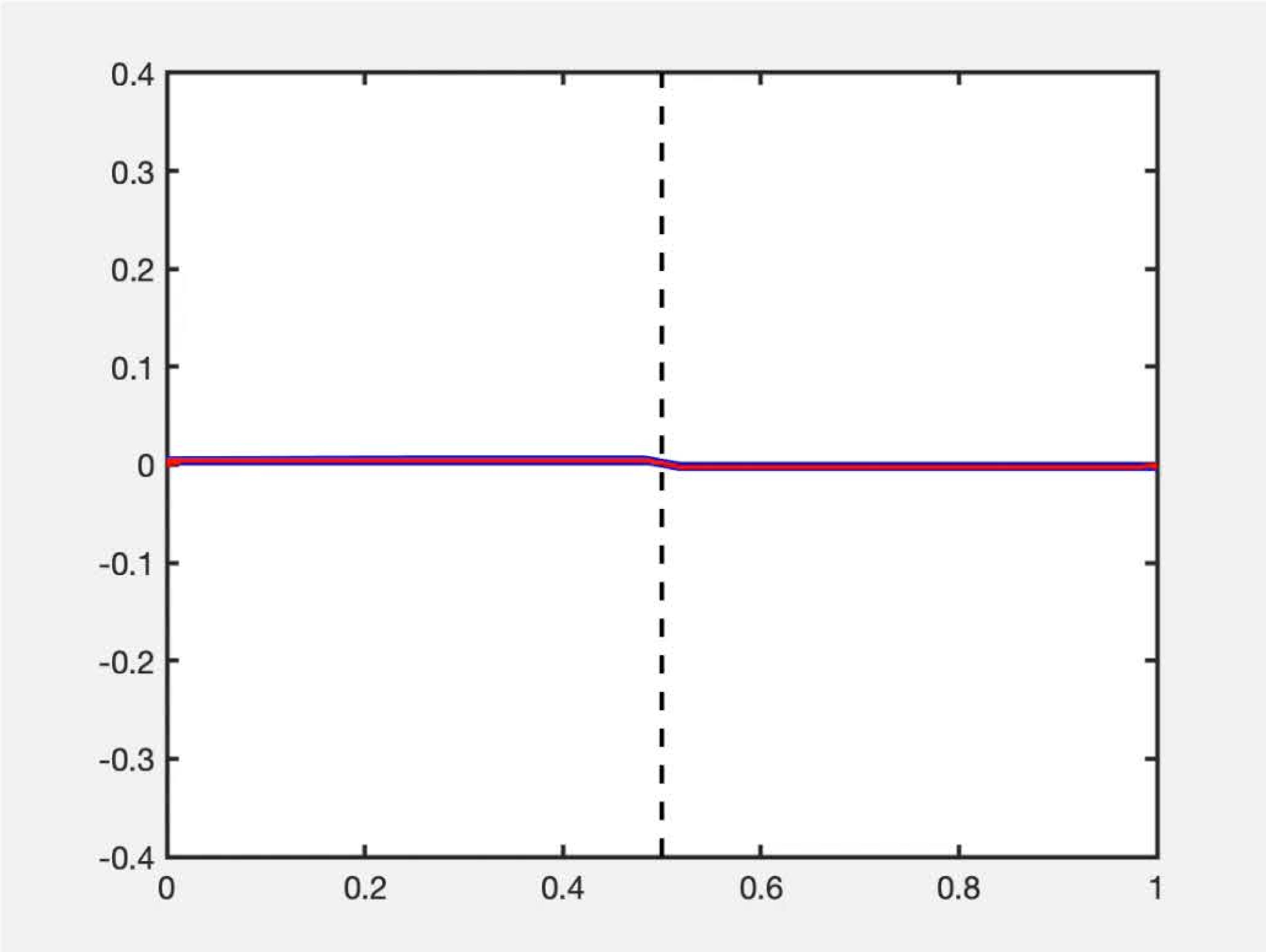
where

$$\tilde{G}(\tau = 0) = G(t) = \tau(t, 0)\delta(x) + \tau(t, H)\delta(x - H)$$

Comparing the smoothed velocity and the evolved coarse velocity, using the exact shear stresses



Interface Retaining Coarsening of Multiphase Flows



The same approach works for two fluid layers

$$\frac{\partial \tilde{u}}{\partial t} = \frac{1}{\rho}\left(\frac{\partial}{\partial x}\mu\left(\frac{\partial \tilde{u}}{\partial x}\right) + (\rho - \rho_{av})g - \beta + \tilde{S}\right)$$

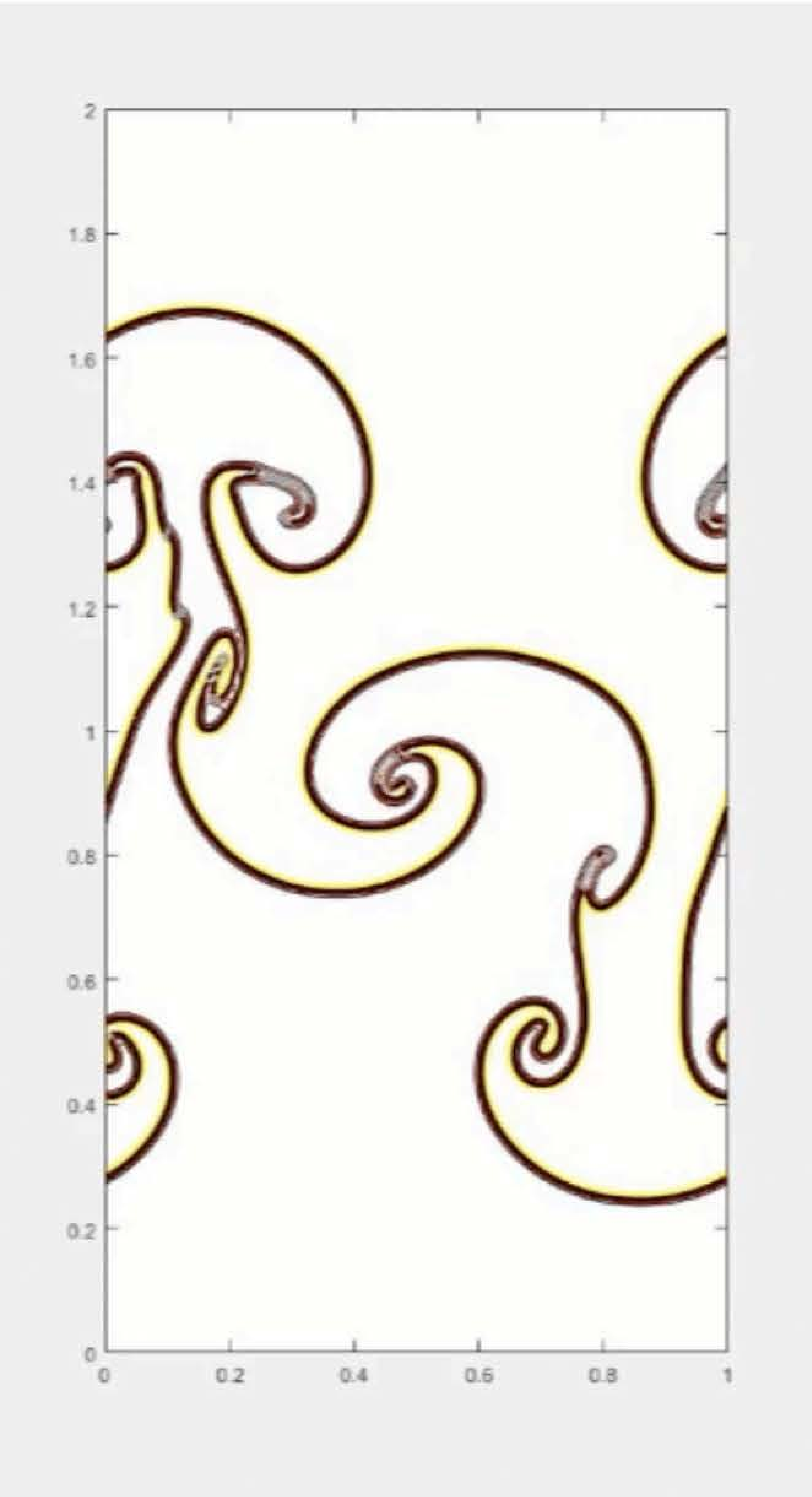
$$\frac{\partial \tilde{S}}{\partial \tau} = D\frac{\partial^2 \tilde{S}}{\partial x^2} \qquad S = \frac{\partial G}{\partial x}$$

$$\tilde{G}(\tau = 0) = G(t) = \tau(t,0)\delta(x) + \tau(t,x_I)\delta(x - x_I) + \tau(t,H)\delta(x - H)$$

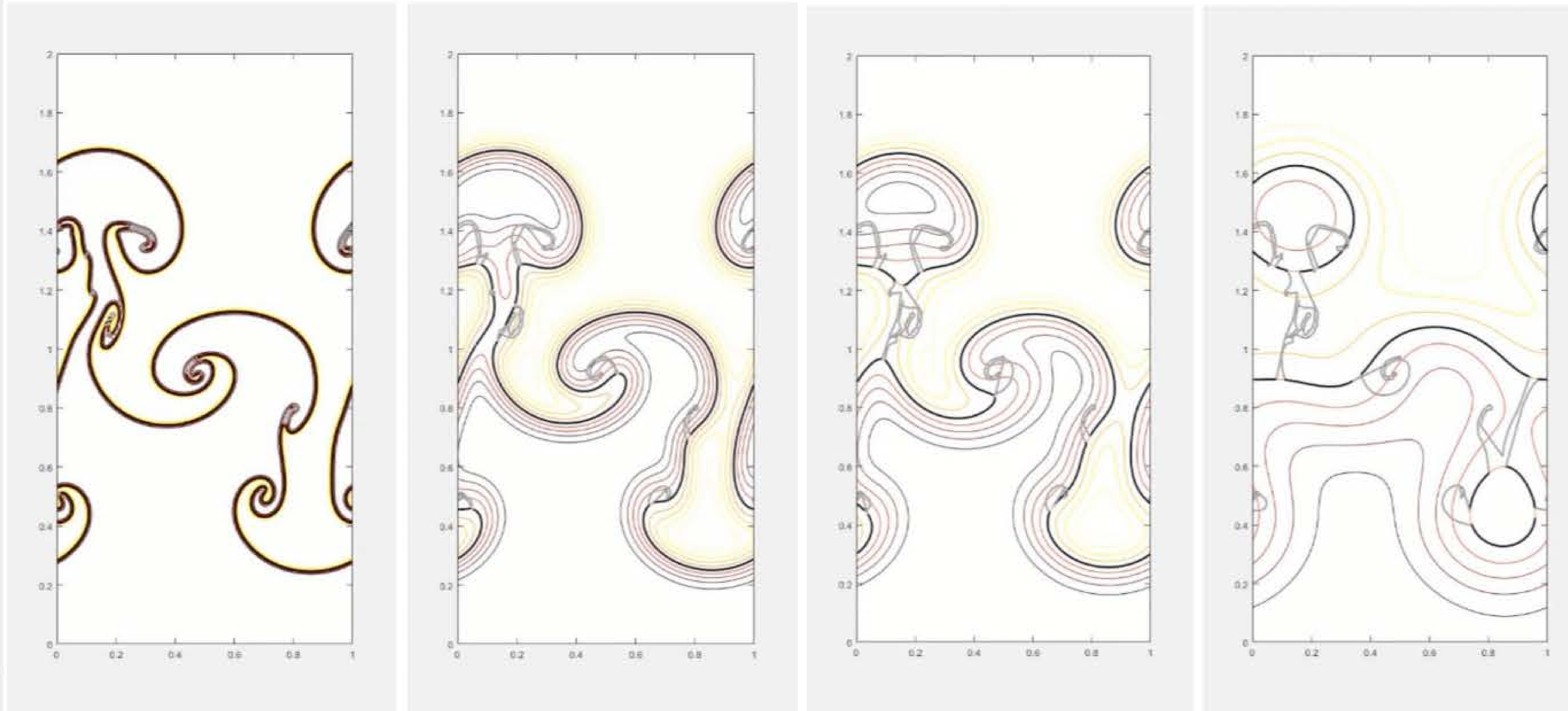
The very simple model suggests that:

- We can derive equations for the coarse flow that give the same results as the smoothed exact solution
- Shear stresses (momentum fluxes) at walls and interfaces need be replaced by sources and must be found separately
- Interfacial and wall stresses (or their derivatives) must be diffused in pseudo-time at each time step. Thus, the “non-localization” of information is a formal part of the model
- We may need to diffuse the diffusion coefficient to bring it smoothly to zero at the interface to get a “monotonic” profile

Coarsening the Interface

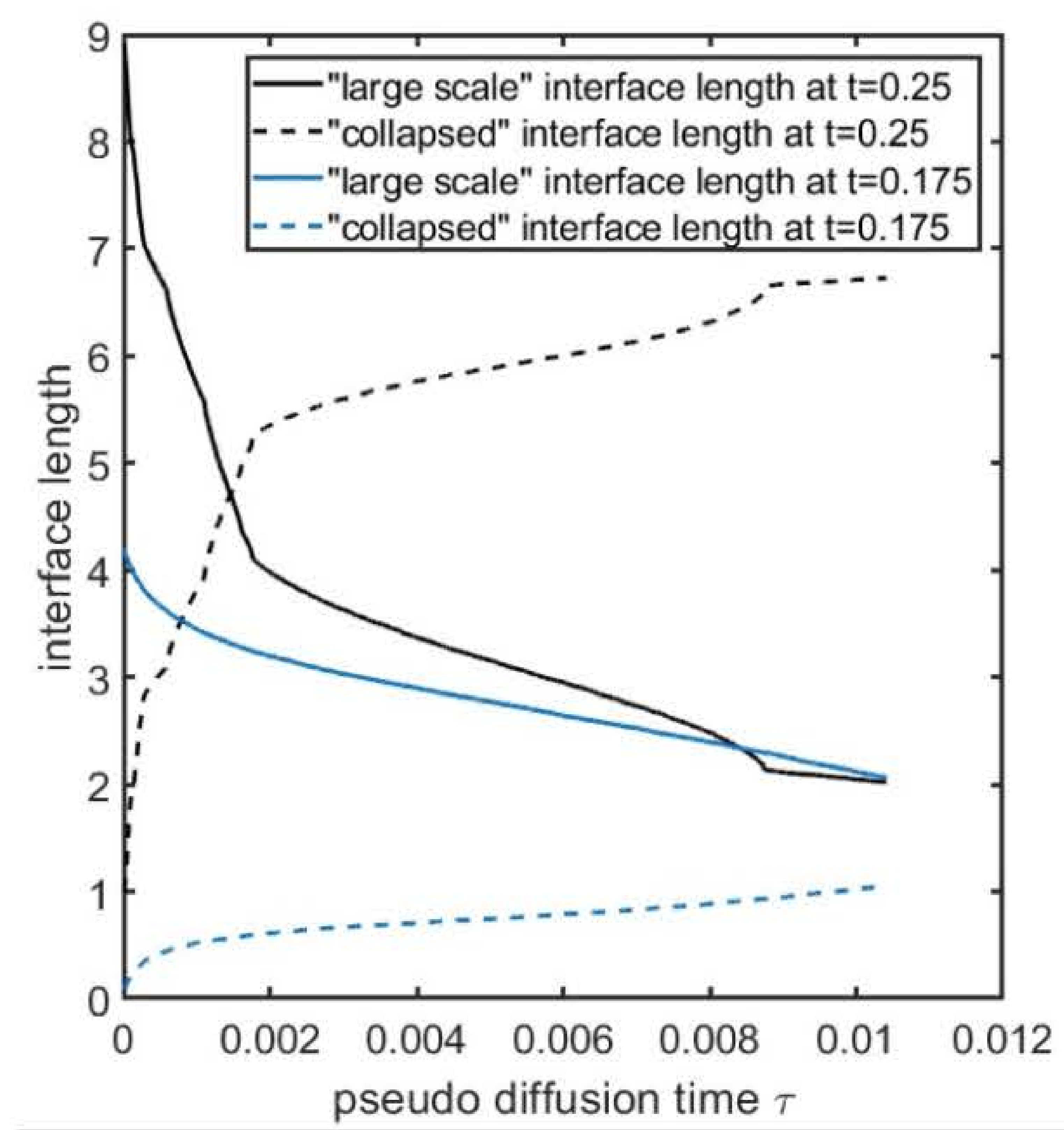


Evolution in pseudo-time



The index function is diffused in pseudo time and the total time determines the filter “size.”

The interface is simplified by “straitening” and by parts that “collapse.”



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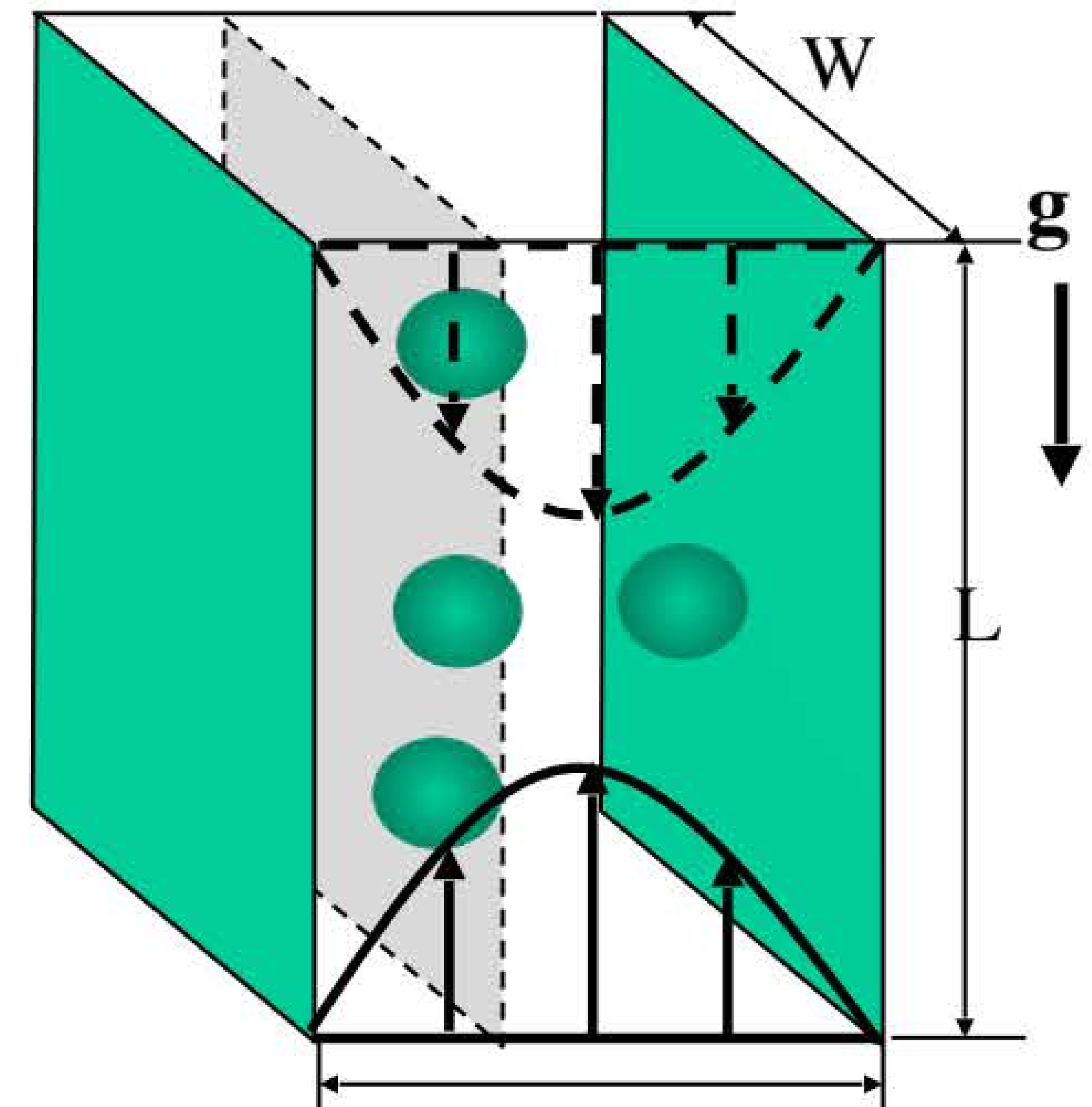
Closure for a simple system by Machine Learning

M. Ma, J. Lu, and G. Tryggvason. “Using Statistical Learning to Close Two-Fluid Multiphase Flow Equations for a Simple Bubbly System.” Physics of Fluids, 27 (2015) 092101.

M. Ma, J. Lu, and G. Tryggvason. “Using statistical learning to close two-fluid multiphase flow equations for bubbly flows in vertical channels.” International Journal of Multiphase Flows, 85 (2016) 336–347

Closure Terms by Machine Learning

A simple description of the average flow in a vertical channel can be derived by integrating the vertical momentum equation and assuming that the density and viscosity of the gas is zero



$$\alpha_i = \frac{1}{A_{zy}} \int \chi_i da \qquad < v >= \frac{1}{\alpha_i A_{zy}} \int \chi v da$$

Horizontal flux of bubbles

$$\frac{\partial \alpha_b}{\partial t} + \frac{\partial}{\partial x} F_b = 0$$

$$F_i = \frac{1}{\alpha A_{zy}} \int \chi_i u_i da$$

Plus a surface tension term for non-spherical bubbles

Averaged vertical momentum of the liquid:

$$\frac{\partial}{\partial t}\alpha < v > + \frac{\partial}{\partial x}\alpha < u >< v >= -\frac{1}{\rho_l}\frac{dp_o}{dy} - g_y\alpha + \nu_l \frac{\partial}{\partial x}\left(\alpha \frac{\partial < v >}{\partial x}\right) - \frac{\partial}{\partial x}\alpha < u'v' >$$

Find the closure terms (red circles) using neural networks

$$F_b = f\left(\alpha, \frac{\partial \alpha}{\partial x}, \frac{\partial < v >}{\partial x}\right); \qquad < u'v' >= g\left(\alpha, \frac{\partial \alpha}{\partial x}, \frac{\partial < v >}{\partial x}\right);$$

Assuming spherical bubbles. For deformable bubbles we have an additional closure term

M. Ma, J. Lu, and G. Tryggvason. "Using Statistical Learning to Close Two-Fluid Multiphase Flow Equations for a Simple Bubbly System." Physics of Fluids, 27 (2015) 092101.

M. Ma, J. Lu, and G. Tryggvason. "Using statistical learning to close two-fluid multiphase flow equations for bubbly flows in vertical channels." International Journal of Multiphase Flows, 85 (2016) 336–347

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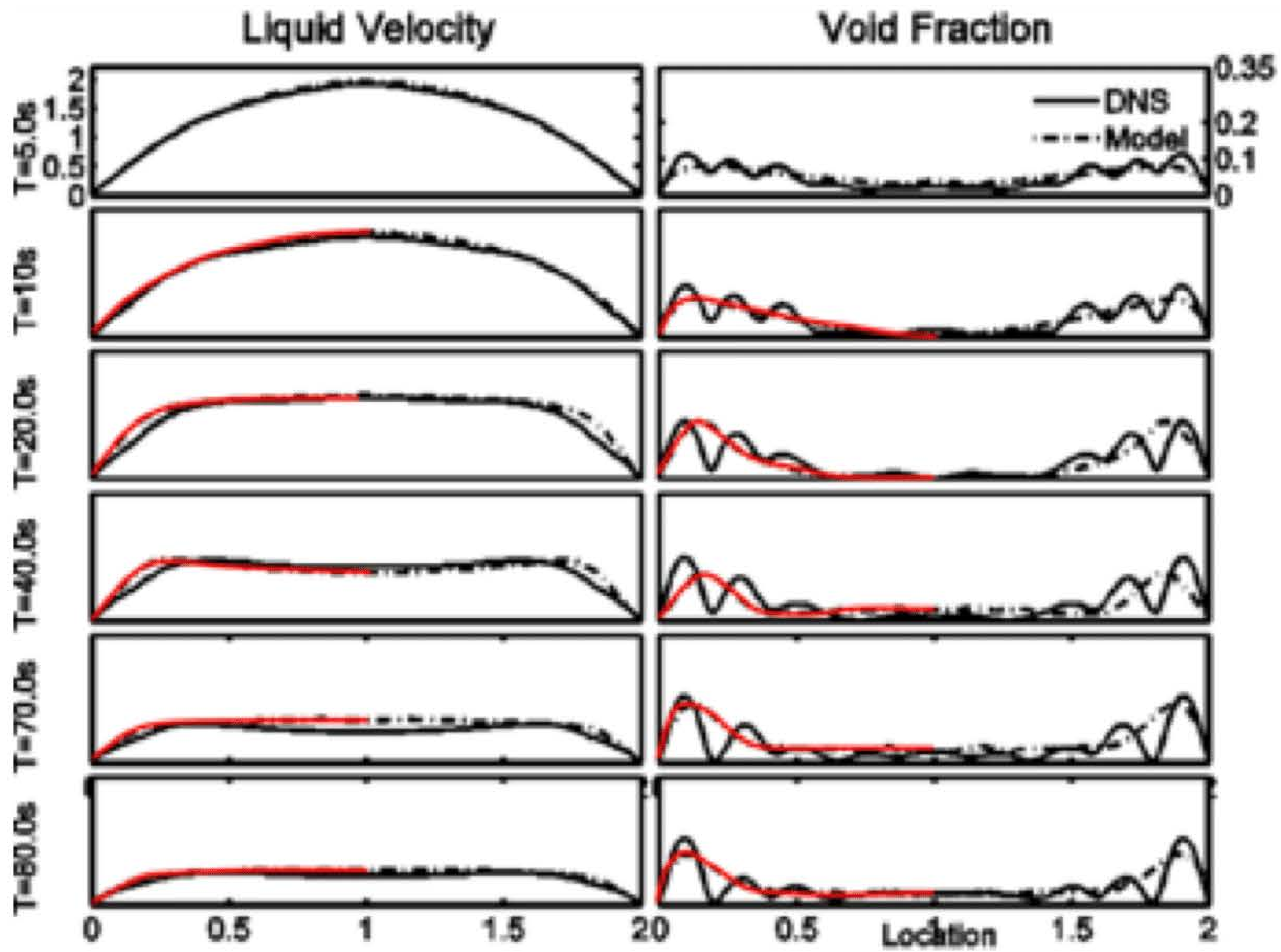
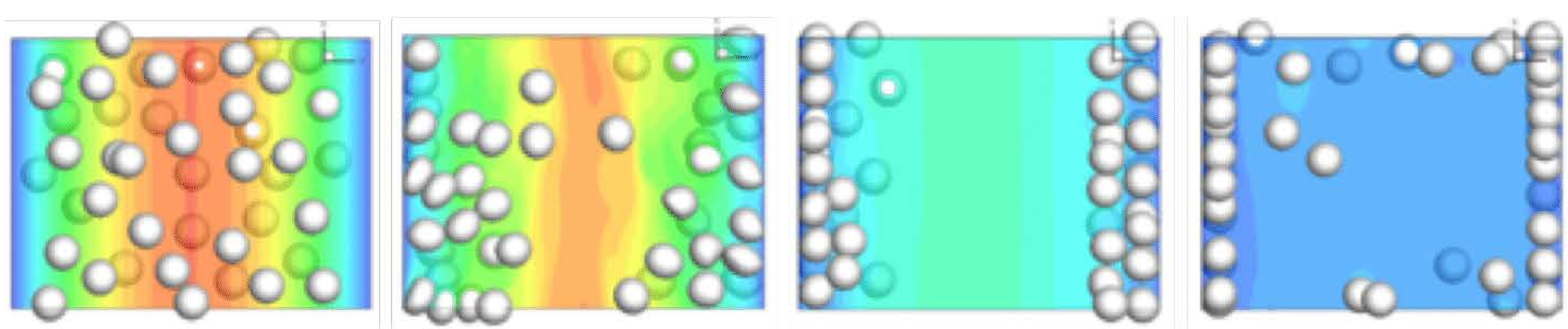
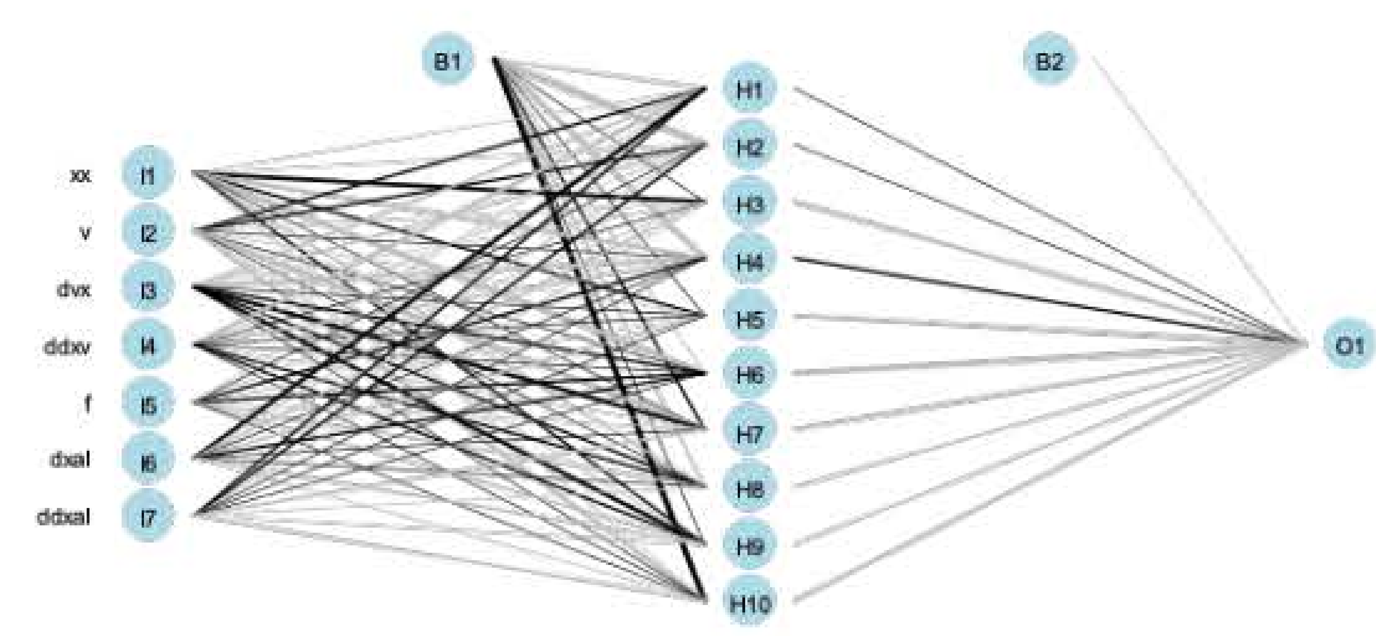
Closure Terms by Machine Learning

The transient motion of bubbles in a vertical channel flow. Averaged DNS results (solid line) and Model predictions (dashed/red line) using the ANN closure terms at several different times. Similar results are found for other initial condition, and downflow is also accurately predicted using closures "learned" in upflow



Time →



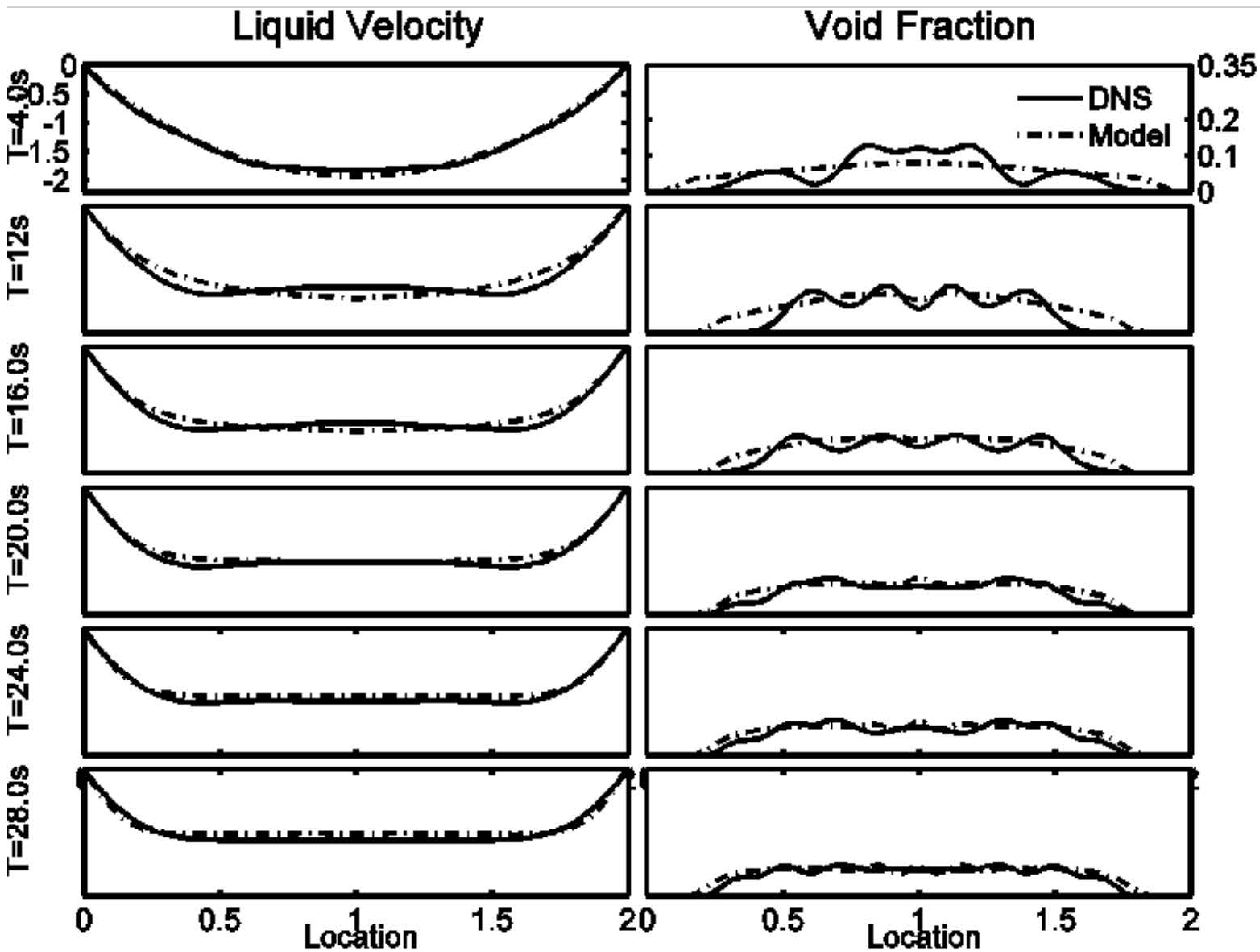


Closure Terms by Machine Learning

The important question is: How general are the closure terms?

The figure shows the closure relations derived from the upflow cases applied to downflow.

Similar results for different initial conditions.



On
Closures for Coarse Models Retaining the Interface

Evolving the Coarse Field

The goal is to separate the flow into large scale flow which are evolved deterministically and small scale flow which is modeled.

As the coarsening is reduced, we should recover the solution to the original continuum equations.

Away from an interface we should be able to use standard models that ignore the interface, both for the two (multi) phase mixture and the turbulent flow

Simplifying the interface is relatively straight forward but what about the mass and momentum?

We have at least two options:

- We can mix the fluid “left behind” and evolve the mixtures using two-fluid models.

- We can “push” the phases with the interface, keeping them separate.

The first leads to Euler-Euler like models and the second to Euler-Lagrange like models

Trajectory Modeling: Finding Closure Terms from Coarse Data

Equations for the evolution of coarse grained flows are usually derived from equations for the fully resolved flow by adding closure terms to account for the effect of unresolved scales, the coarse field is generated by explicit filtering, and the closure terms constructed by comparing with the filtered fully resolved solution.

An alternate approach is to find the closure terms directly from the evolution of the coarse field by asking how the traditional fluid equations need to be modified to ensure that the coarse field evolves correctly.

	Structure/Function Modeling	Trajectory Modeling
Represent the flow by a truncated series of modes (analytical basis functions, POD, DMD, ……). Reduced Order Models	Review of closure models for ROM: S. E. Ahmed, S. Pawar, O. San, A. Rasheed, T. Iliescu, and B. R. Noack. On closures for reduced order models—a spectrum of first-principle to machine-learned avenues. Phys. Fluids, 33:091301, 2021.	
Simplify the field by averaging or filtering (RANS, LES, ….). Coarse Models	Most turbulence work. Focus on *a priori* tests Multiphase flows: Ma et al, 2015, 2016	Chen et al (2D turbulence) Current work on multiphase flow
	Compute closure terms from fully resolved solutions and develop models to match those	Modify the governing equations so that the coarse field evolves ``correctly”

Trajectory modeling/regression for single phase flow

We assume we have a coarse or filtered flow field $(\tilde{\mathbf{u}}_c(\mathbf{x}, t), \tilde{p}_c(\mathbf{x}, t))$

To find equations for the evolution of the coarse field, we assume that the flow is governed by the standard conservation equations augmented by a closure terms that accounts for the effects of the unresolved scales.

$$\frac{\partial \tilde{\mathbf{u}}_c}{\partial t} + \nabla \tilde{\mathbf{u}}_c \tilde{\mathbf{u}}_c = -\nabla \tilde{p}_c + \tilde{\mathbf{T}}$$

Since we know the complete coarse field, we can solve for the closure term

$$\tilde{\mathbf{T}} = \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \nabla \tilde{\mathbf{u}} \tilde{\mathbf{u}} + \nabla \tilde{p}$$

For single phase flow these can be written as the divergence of fluxes, but for more complex flow it can also contain sources/sinks

$$\tilde{\mathbf{T}} = \nabla \cdot \tilde{\mathbf{F}}$$

For "mild" coarsening, it is likely that we can write

$\mathbf{T}$ or $\mathbf{F}$=f(local state of the coarse flow)

For aggressive coarsening, however, it is likely that the closure terms depend on the history of the flow so we need to evolve $\mathbf{T}$ or $\mathbf{F}$

$$\frac{\partial \tilde{\mathbf{F}}}{\partial t} + \tilde{\mathbf{u}}_c \cdot \nabla \tilde{\mathbf{F}} = \tilde{\mathbf{G}}$$

Once we have found $\mathbf{F}$, we can solve for $\mathbf{G}$, which then needs to be related to the local flow state

Trajectory modeling/regression for single phase flow

Simple Example—2D Turbulence

Assume the flow is governed by

$$\frac{\partial \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\tilde{\mathbf{u}}\tilde{\mathbf{u}}) = -\frac{1}{\rho}\nabla \tilde{p} + \nu \nabla^2 \tilde{\mathbf{u}} + \mathcal{F}$$

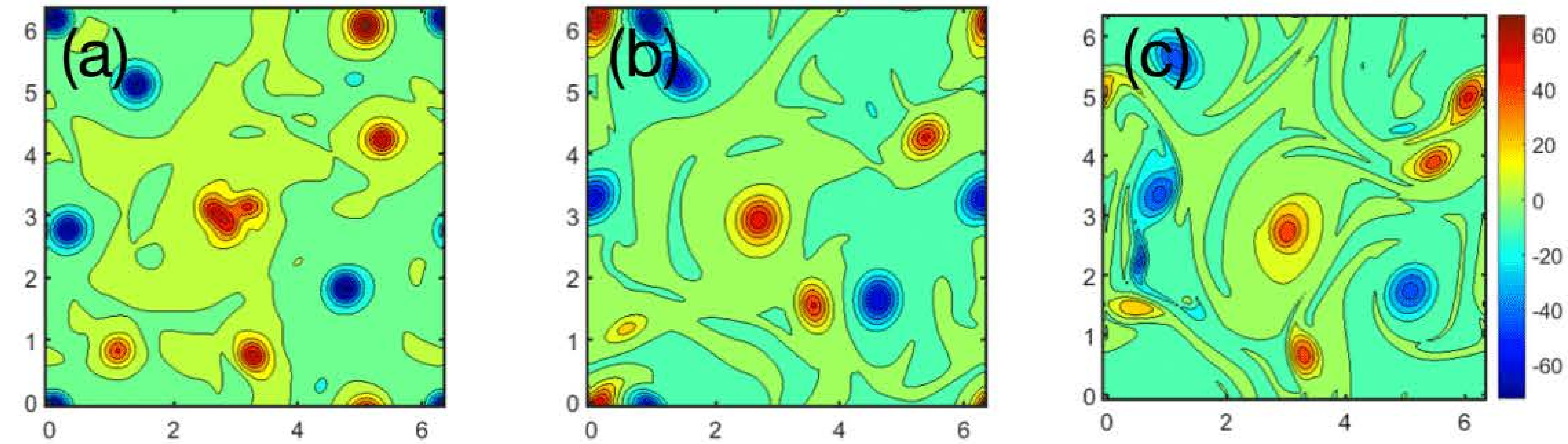
Filter a DNS solution and find

$$\mathcal{F} = \frac{\partial \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\tilde{\mathbf{u}}\tilde{\mathbf{u}}) + \frac{1}{\rho}\nabla \tilde{p} - \nu \nabla^2 \tilde{\mathbf{u}}$$

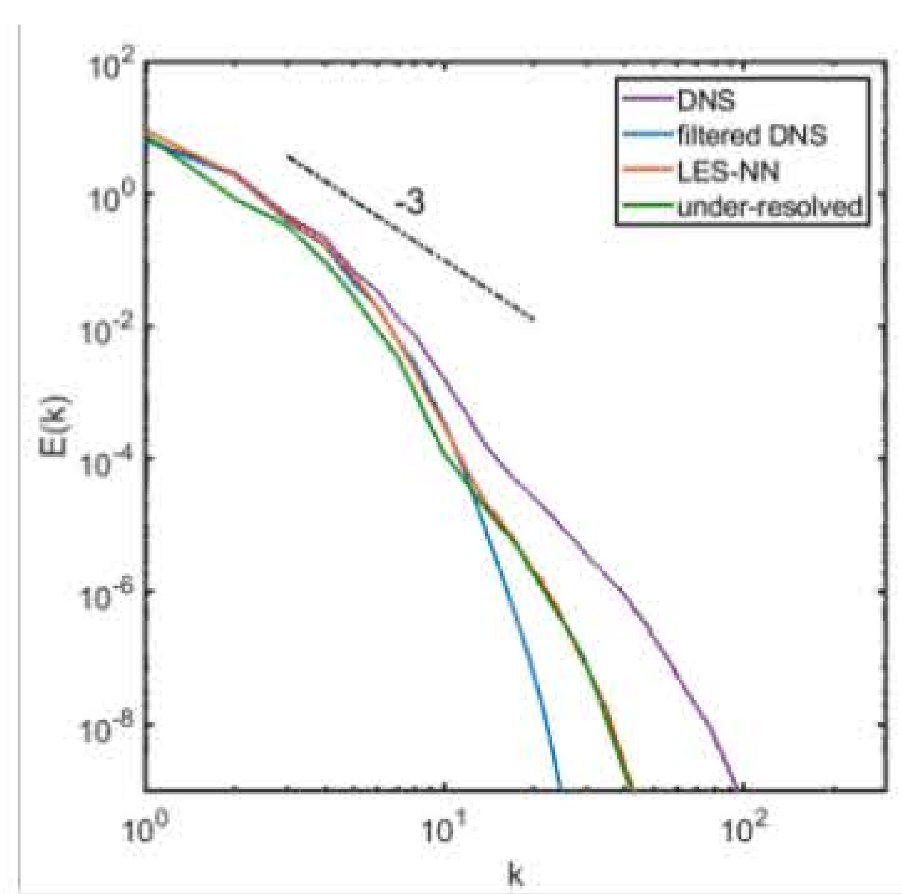
Use Neural Networks to find

$$\mathcal{F}_x = \mathcal{M}\left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial v}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial x \partial y}, \frac{\partial^2 u}{\partial y^2}, \frac{\partial^2 v}{\partial x^2}\right)$$

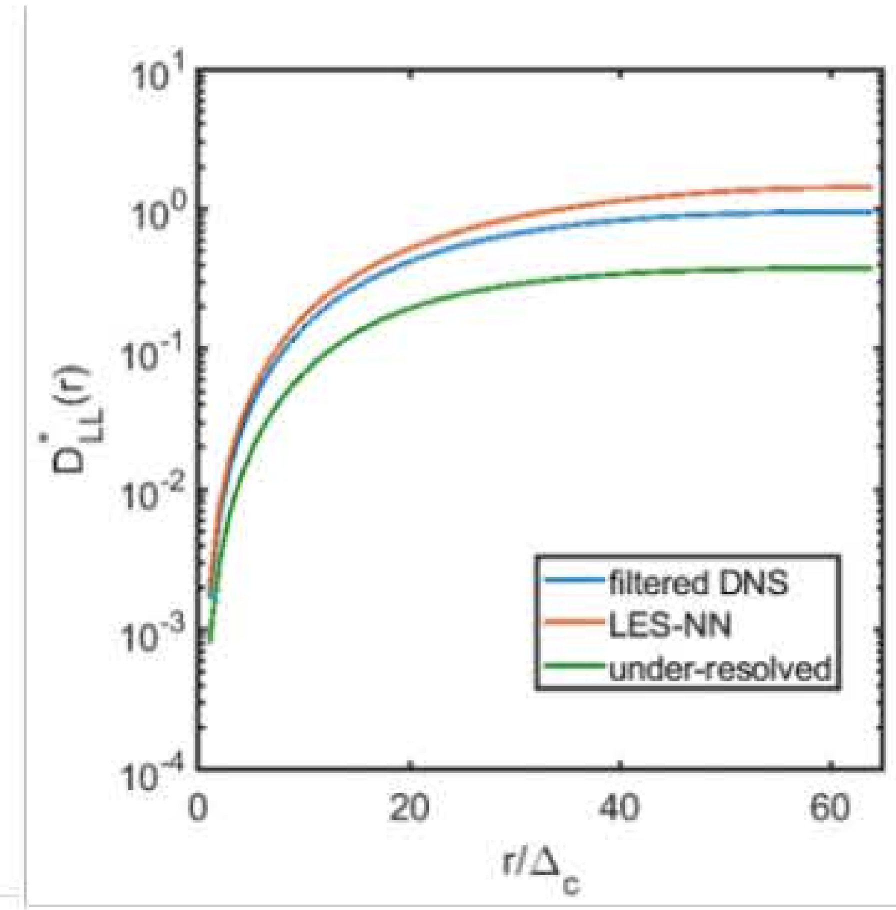
For short time the trajectory is nearly the same, but at longer time we compare the statistical state



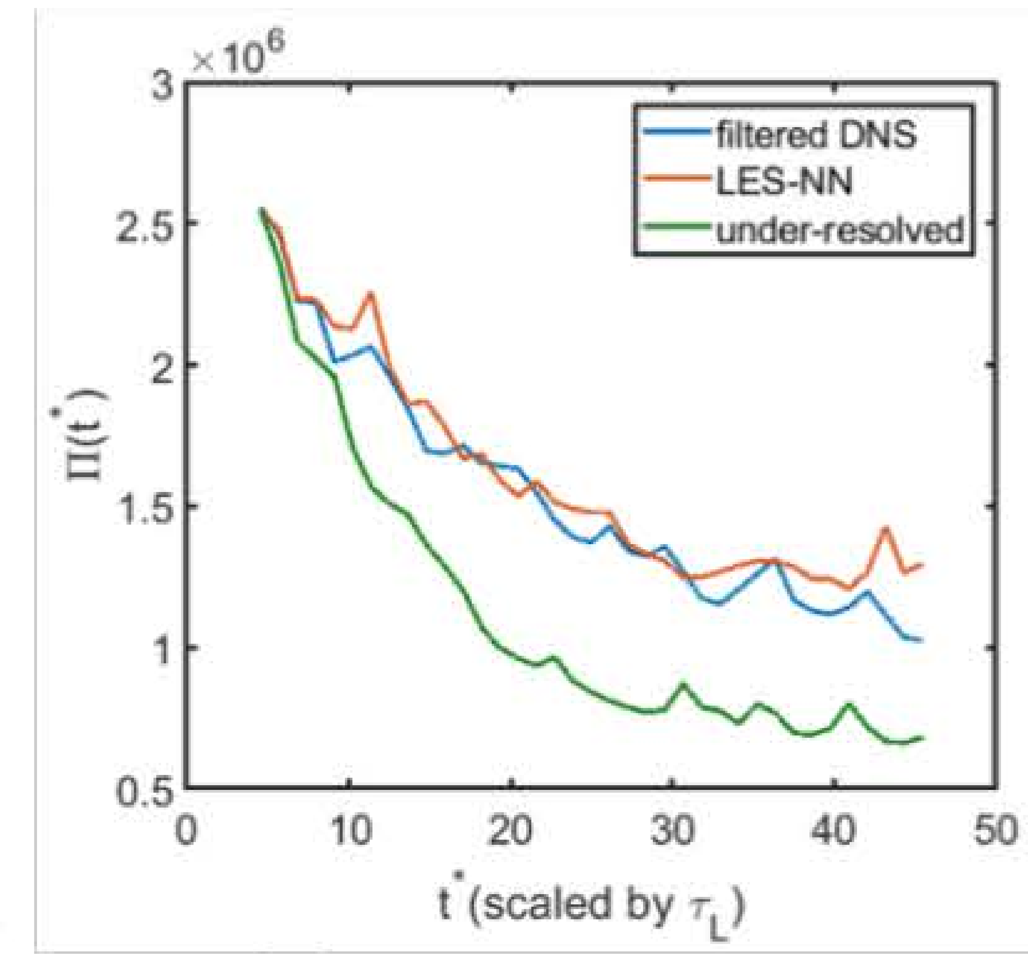
Vorticity at time 10 for (a) Filtered DNS; (b) NN model; (c) Under-resolved "DNS"



Energy spectrum



Structure Function



Enstropy versus time

X. Chen, J. Lu and G. Tryggvason. Finding Closure Terms Directly from Coarse Data for 2D Turbulent Flow. Fluids 2022, 7, 154.

Not surprisingly, doing the closure this way works, at least for this simple case

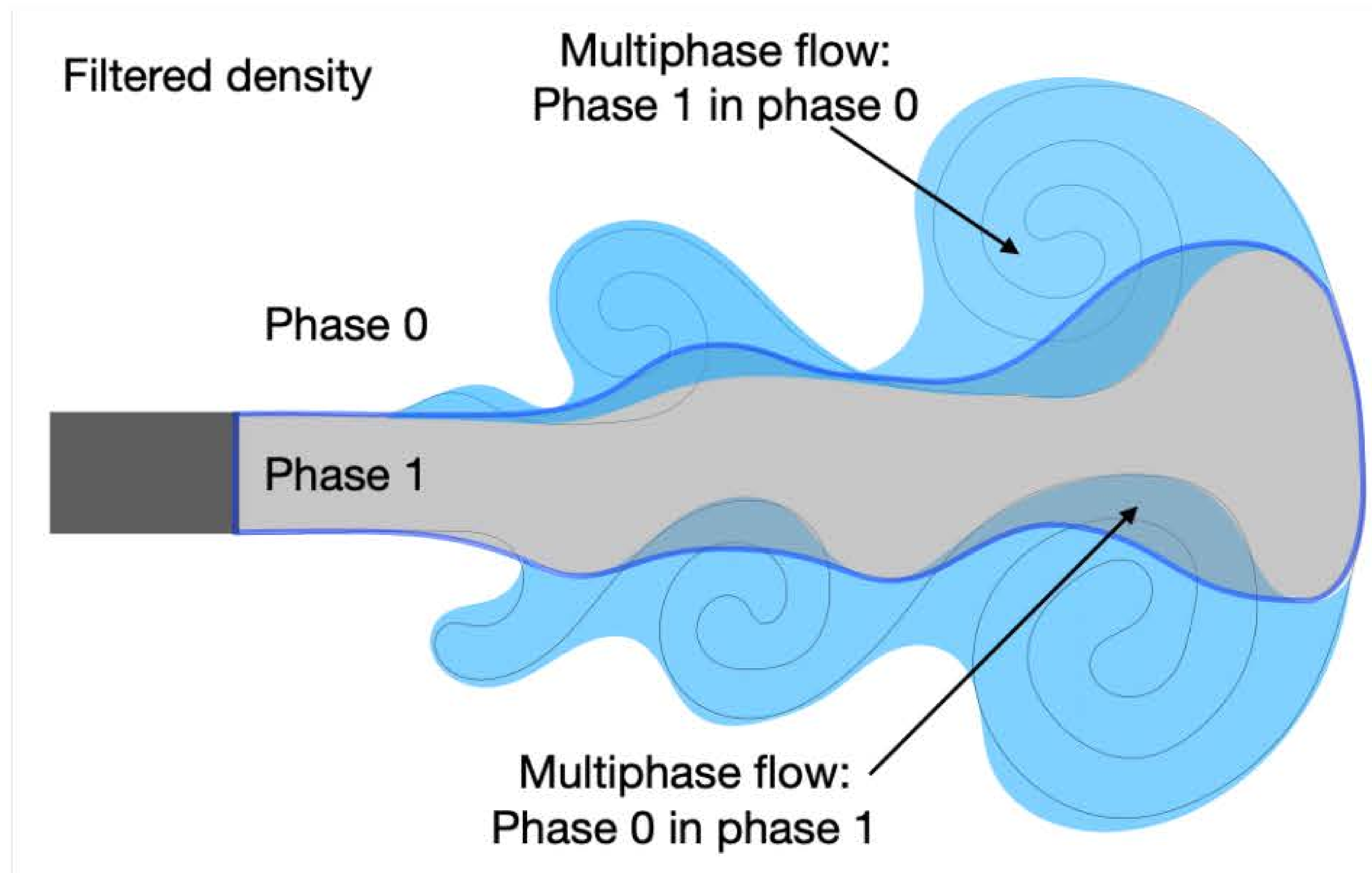
Mixing the Phases

Interface Retaining Coarsening of Multiphase Flows

Mixing the phases:

As the interface moves, one phase is “left behind” in the other phase and is treated as small scale flow that needs to be modeled. Thus, generally we expect a two phase mixture of small scales on both side of the coarse interface

Xianyang Chen, Jiacai Lu and Gretar Tryggvason. Interface Retaining Coarsening of Multiphase Flows. Phys. Fluids 33, 073316 (2021)



Generating the Small Scale Index Function by Mixing

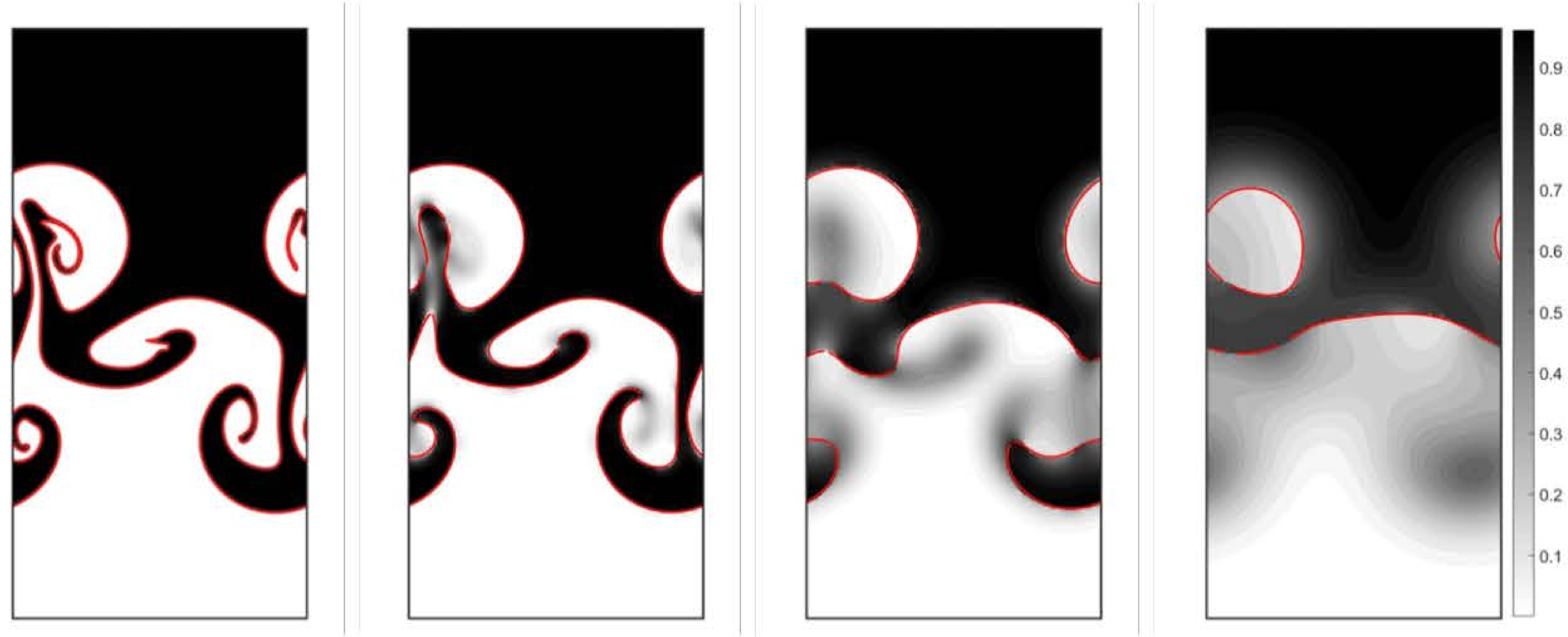
After the smoothing the different phases are identified by the filtered, or diffused, index function

$$\tilde{\chi}(\boldsymbol{x}) = \begin{cases} 0 \text{ in fluid } 0 \\ 1 \text{ in fluid } 1 \end{cases}$$

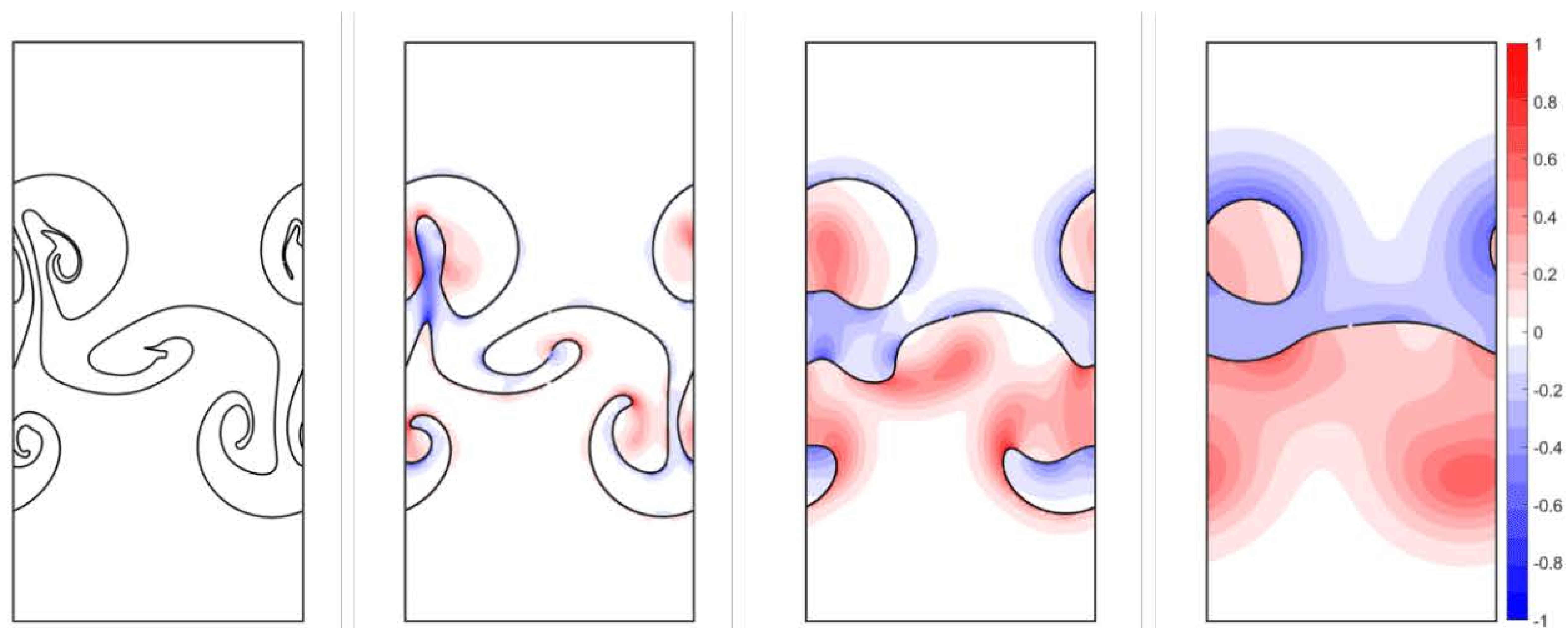
Moving the interface results in one phase that has been "left behind." Diffusing the index function again, but preventing diffusion across the interface, mixes this phase with the other phase. This gives the volume fraction α

Often we prefer to work with the perturbation volume fraction, which is the deviation from the filtered index function

$$\alpha' = \alpha - \tilde{\chi}$$



The evolution of the volume fraction α in pseudo time



The evolution of the perturbation volume fraction α' in pseudo time

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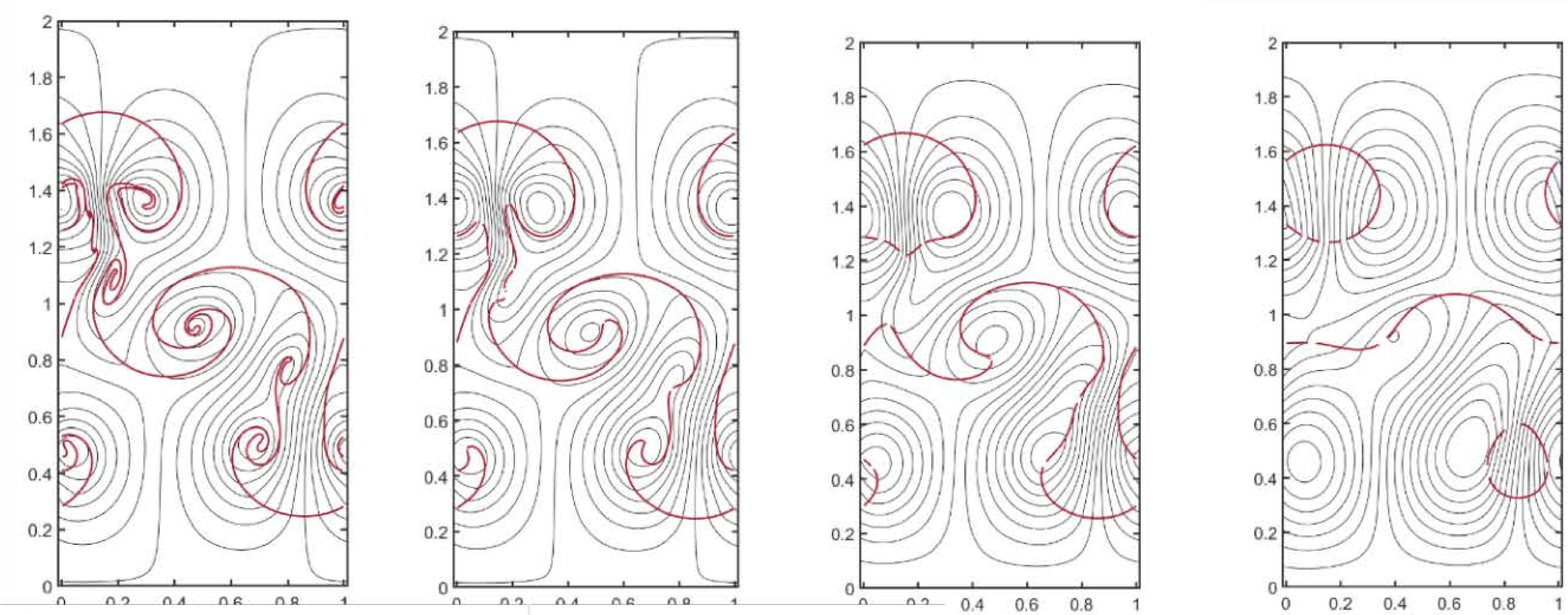
Coarsening the Momentum Field

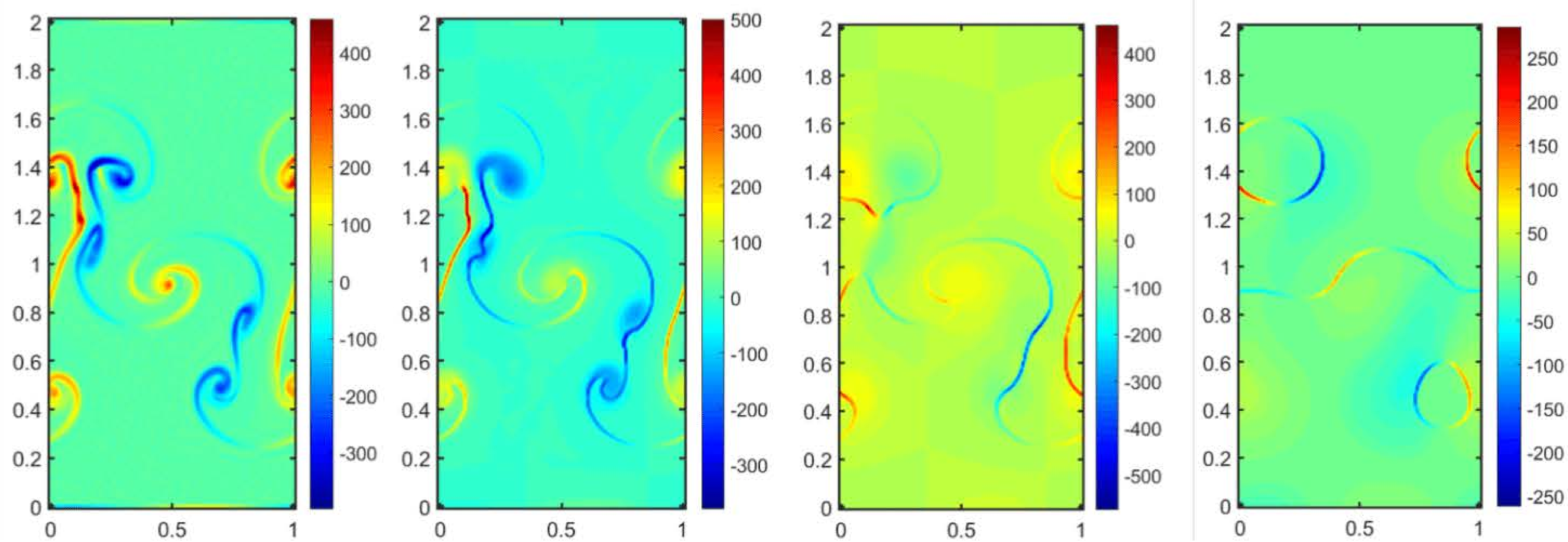
Diffusing the momentum separately on either side of the interface generally does not preserve incompressibility, so we evolve it in pseudo time using a pressure like term to keep the divergence of the volumetric velocity equal to zero.

$$\frac{\partial(\widetilde{\rho \boldsymbol{u}})}{\partial \tau} = -\nabla \tilde{p} + \nabla \cdot \tilde{D} \nabla (\widetilde{\rho \boldsymbol{u}})$$

$$\nabla \cdot \tilde{\boldsymbol{u}} = 0$$

The evolution of the streamfunction in a stationary frame of reference in pseudo time





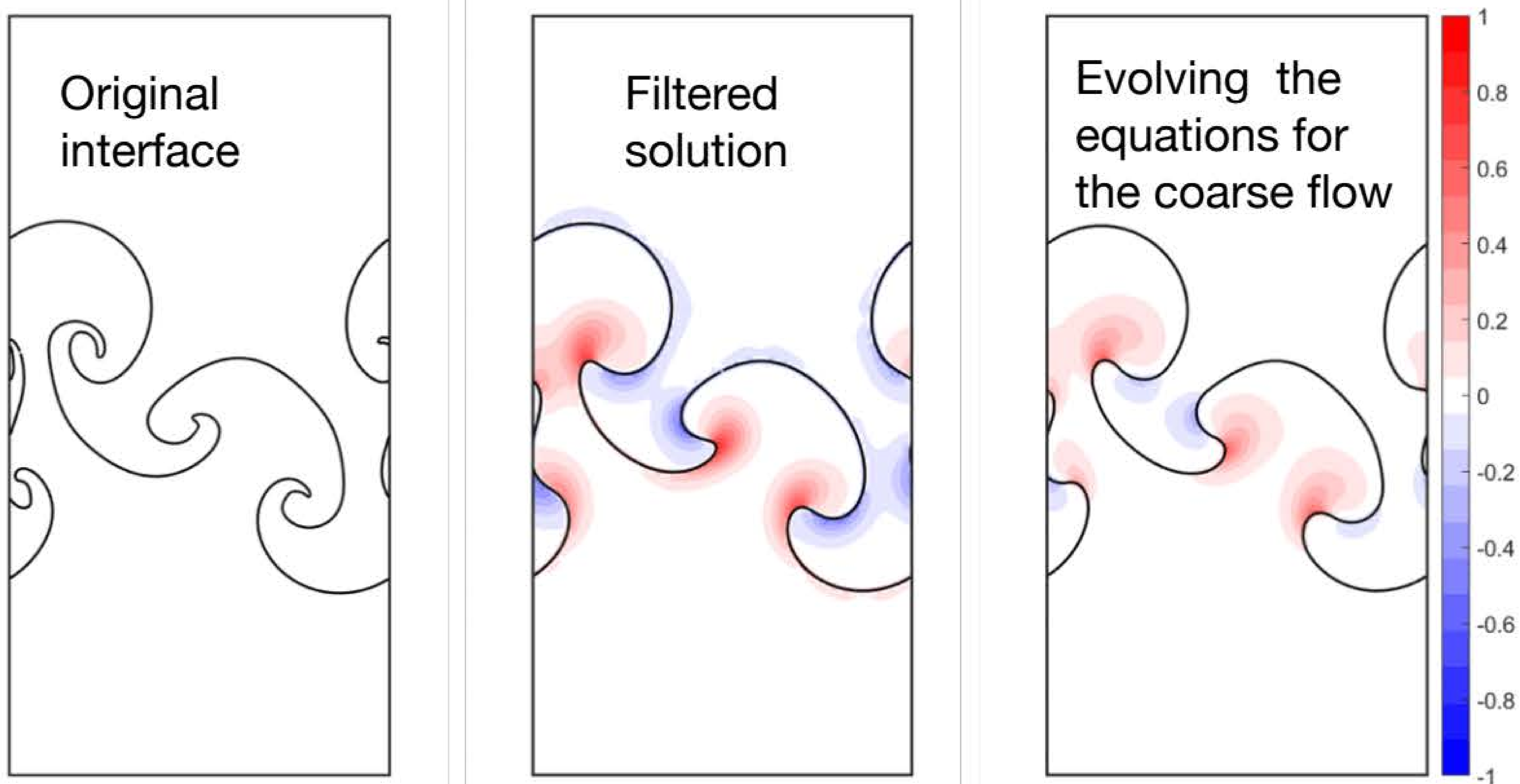
The evolution of the vorticity in in pseudo time

Johns Hopkins Whiting School of Engineering

Evolving the Coarse Field

The solution of the model equations

As a start we are using a very simple homogeneous mixture model where we need models for the interface velocity, dispersion of the small scales and stresses due to the small scales



$$d\boldsymbol{x}_I/dt = \boldsymbol{u}_f - \Delta u_I \boldsymbol{n}$$

$$\frac{\partial \alpha'}{\partial t} + \boldsymbol{u}\cdot\nabla\alpha' = \nabla\cdot D_e \nabla\alpha' + S_I$$

$S_I = [\chi](\boldsymbol{u}_f - \boldsymbol{u}_I)\cdot\boldsymbol{n} = [\chi]\Delta u_I$ interface source

$\tilde{\rho} = (\alpha' + \tilde{\chi})\rho_1 + (1-\alpha' - \tilde{\chi})\rho_o$ density

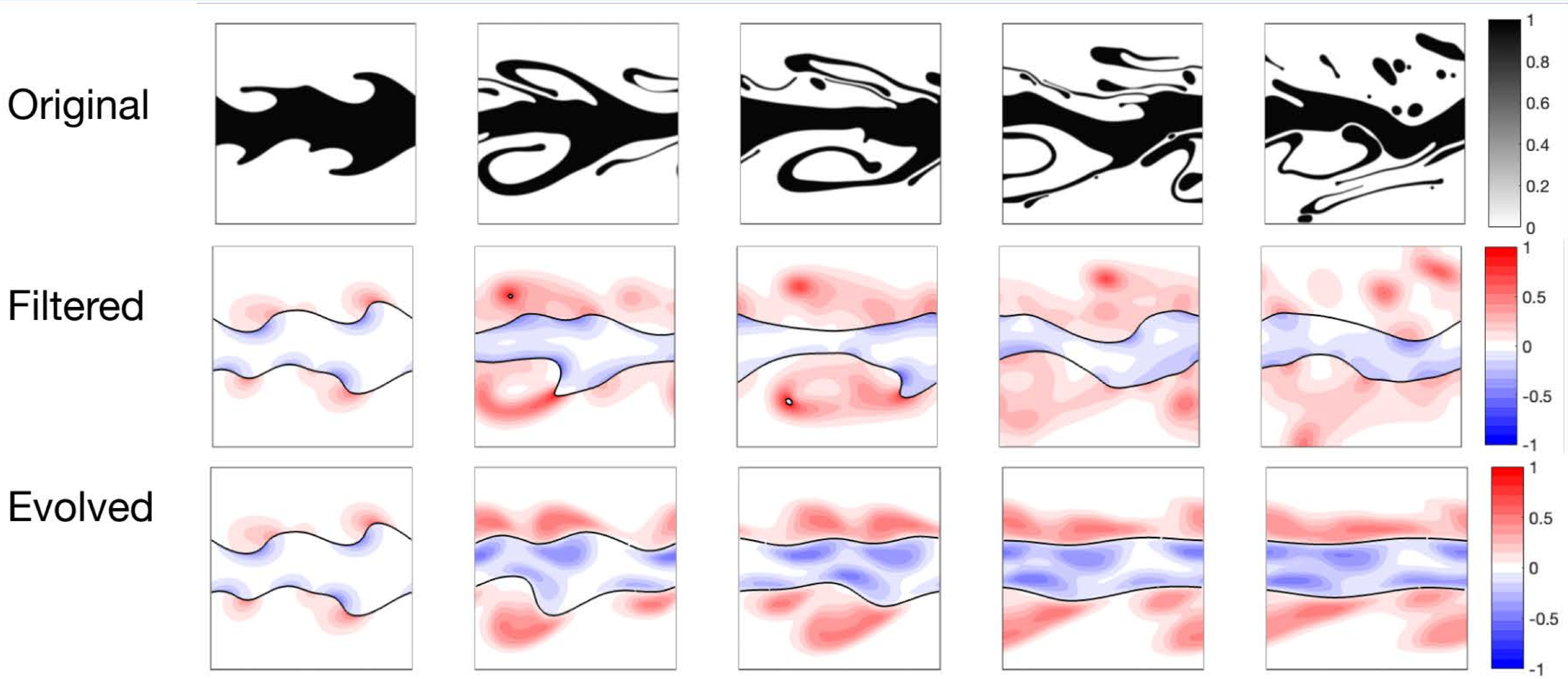
$\frac{\partial(\tilde{\rho}\tilde{\boldsymbol{u}})}{\partial t} + \nabla\cdot(\tilde{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}) = -\nabla\tilde{p} + \tilde{\rho}\boldsymbol{g} + \nabla\cdot\boldsymbol{\tau}_e$ momentum

$\boldsymbol{\tau}_e = \mu_e(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)$ effective stress

Here we have simply picked "plausible" values for the interface velocity and the mixture diffusivity

The simplest version requires the jump in the interface velocity; the effective viscosity and the effective diffusivity

Interface Retaining Coarsening of Multiphase Flows



Preliminary results using a very simple mixture model.

$$\frac{\partial(\tilde{\rho}\tilde{\boldsymbol{u}})}{\partial t} + \nabla\cdot(\tilde{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}}) = -\nabla\tilde{p} + \tilde{\rho}\boldsymbol{g} + \nabla\cdot\boldsymbol{\tau}_e$$

$$\boldsymbol{\tau}_e = \mu_e(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T).$$

$$d\boldsymbol{x}_I/dt = \boldsymbol{u}_f - \Delta u_I\boldsymbol{n}$$

$$\frac{\partial\alpha'}{\partial t} + \boldsymbol{u}\cdot\nabla\alpha' = \nabla\cdot D_e\nabla\alpha' + S_I$$

$$S_I = [\chi](\boldsymbol{u}_f - \boldsymbol{u}_I)\cdot\boldsymbol{n} = [\chi]\Delta u_I$$

$$\tilde{\rho} = (\alpha - \alpha')\rho_1 + (1 - \alpha - \alpha')\rho_o.$$

$$\Delta u_I = f(\kappa, \partial\boldsymbol{u}_f/\partial s, \partial^2\boldsymbol{u}_f/\partial s^2, \ldots\ldots\ldots, \Delta)$$

Jump in normal velocity found with the aid of machine learning–but fluid viscosity and mass diffusivity taken as constant here

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Separating the Phases

Interface Retaining Coarsening of Multiphase Flows

Instead of mixing momentum of one phase with the momentum the other as the interface moves, we can "pull" the momentum behind the interface.

For cases where one phase "collapses," as in the point particle approximation, the result is one phase filling the domain and the momentum of the other phase being carried by a point particle.

Consider flow in a vertical channel again. The momentum equation is:

$$\frac{\partial \rho u}{\partial t} = \frac{\partial}{\partial x}\mu\frac{\partial u}{\partial x} - B - \rho g$$

The boundary conditions as source terms are

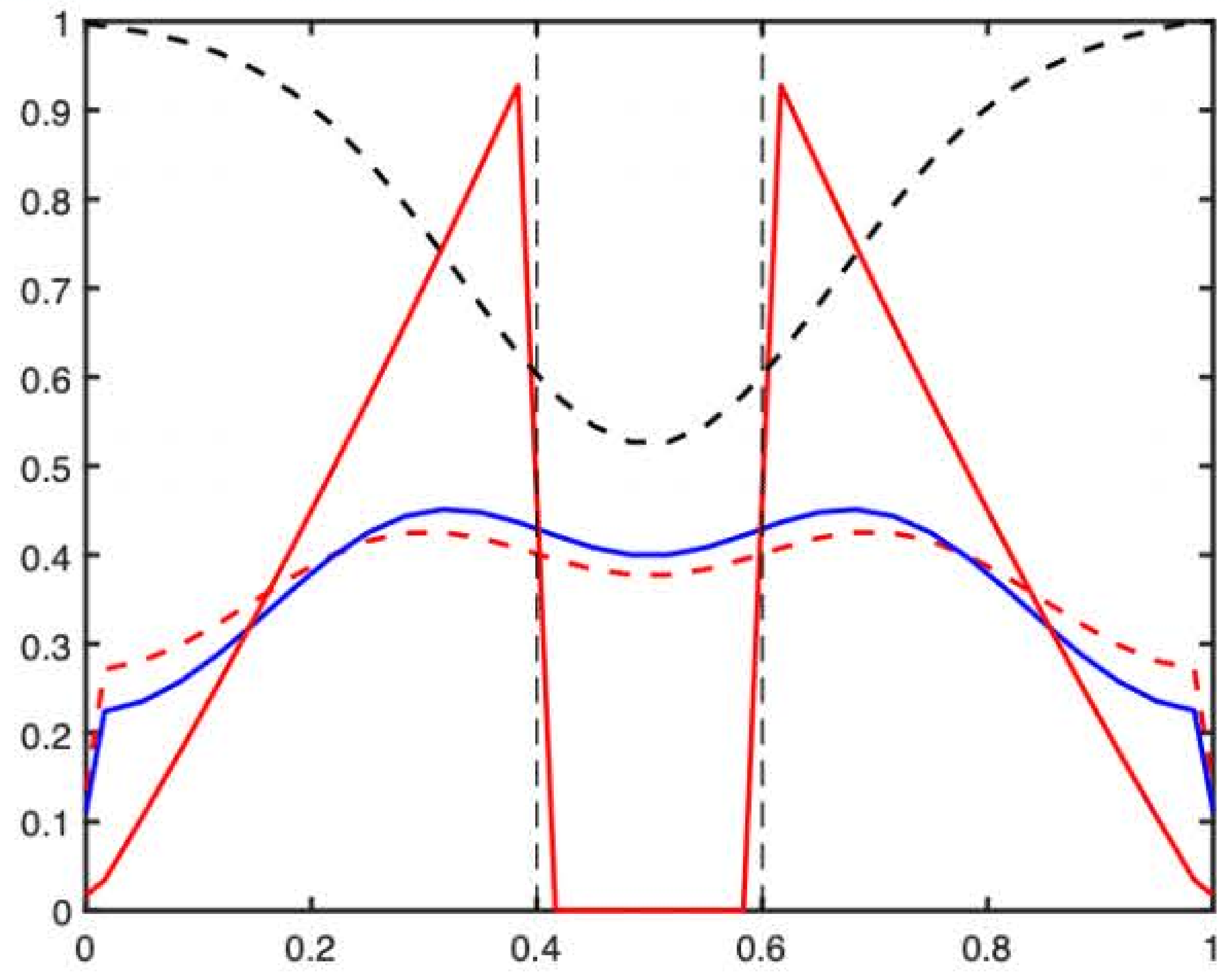
$$S(t) = \tau_w(t,0)\delta(x) + \tau_r(t,x_r)\delta(x-x_r) + \tau_l(t,x_l)\delta(x-x_l) + \tau_w(t,H)\delta(x-H)$$

The smoothed momentum equation is

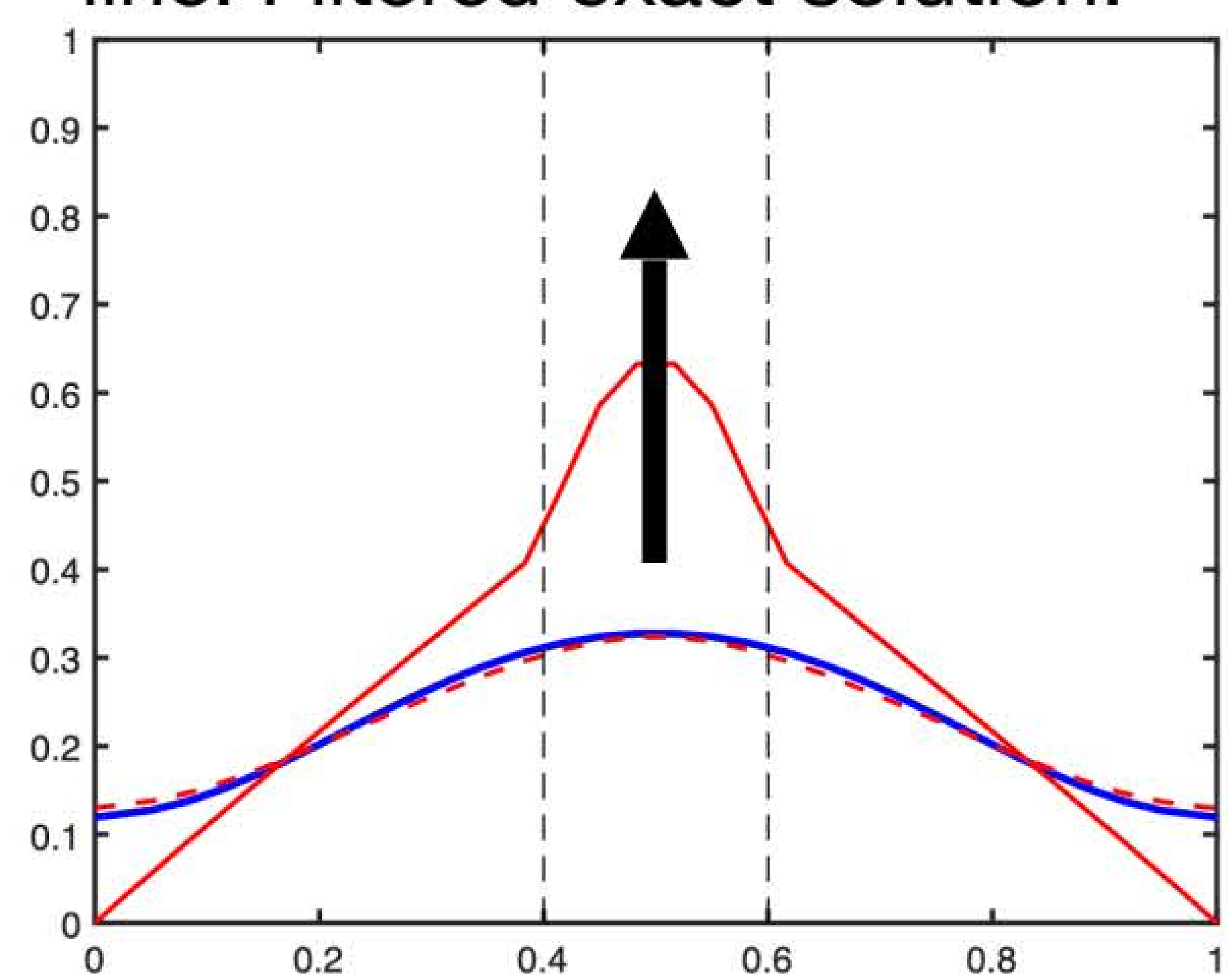
$$\frac{\partial \widetilde{\rho u}}{\partial t} = \mu_o\frac{\partial^2 \tilde{u}}{\partial x^2} - \Big(B + \rho_o g\Big)\tilde{\chi} + \tilde{S}$$

Where

$\tilde{u} = \widetilde{\rho u}/\tilde{\rho}$ and $\tilde{\rho} = \rho_o\tilde{\chi}$



The momentum of the outer fluid. Red: Exact Solution; Blue: Coarse solution; Red dashed line: Filtered exact solution.



The velocity

Evolving the Coarse Field

For the full flow field we solve

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p + \rho \mathbf{g} + \nabla \cdot \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \mathbf{f}_\sigma \quad \text{and} \quad \nabla \cdot \mathbf{u} = 0.$$

$$\frac{\partial \chi}{\partial t} + \mathbf{u} \cdot \nabla \chi = 0$$

Then we smooth the solution in the liquid, assuming the bubbles have "shrunk" to a point.

$$\frac{\partial \chi_f}{\partial \tau} = \nabla^2 \chi_f \qquad \frac{\partial \mathbf{m}_f}{\partial \tau} = \nabla \phi + \nabla^2 \mathbf{m}_f \qquad \rho_f = \rho_l \chi_f \qquad \mathbf{u}_f = \frac{\mathbf{m}_f}{\rho_f}$$

$$\mathbf{m}(\tau = 0) = \rho_l \mathbf{u}_l \chi_l$$

The coarse solution is then advanced in time

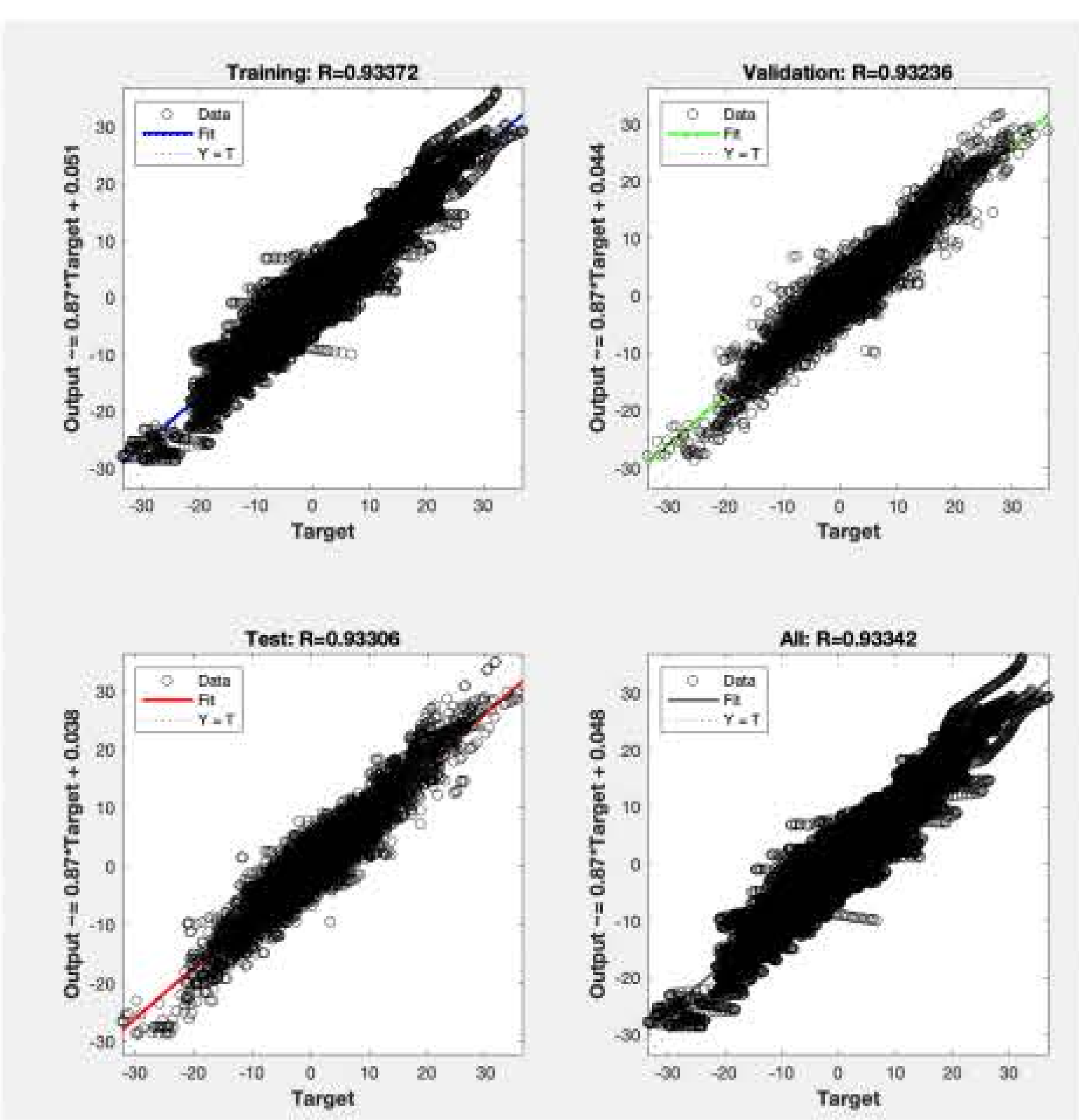
$$\frac{\partial \rho_c \mathbf{u}_c}{\partial t} + \nabla \cdot \rho \mathbf{u}_c \mathbf{u}_c + \nabla p_c - \rho_c \mathbf{g} + \mu_f \nabla^2 \mathbf{u}_c + \mathbf{F}_c \qquad \mathbf{F}_c^p = \rho_b \mathbf{g} + \frac{\mathbf{u}_f^p - \mathbf{u}_c^p}{\Delta t}$$

$$\mathbf{F}_c(x,y) = A \sum_p \mathbf{F}_c^p e^{-\frac{||\mathbf{x}-\mathbf{x}_p||^2}{B}} \qquad \tilde{\chi}_p(x,y) = A \sum_p e^{-\frac{||\mathbf{x}-\mathbf{x}_p||^2}{B}} \qquad \rho_c = \rho_f(1 - \tilde{\chi}_p)$$

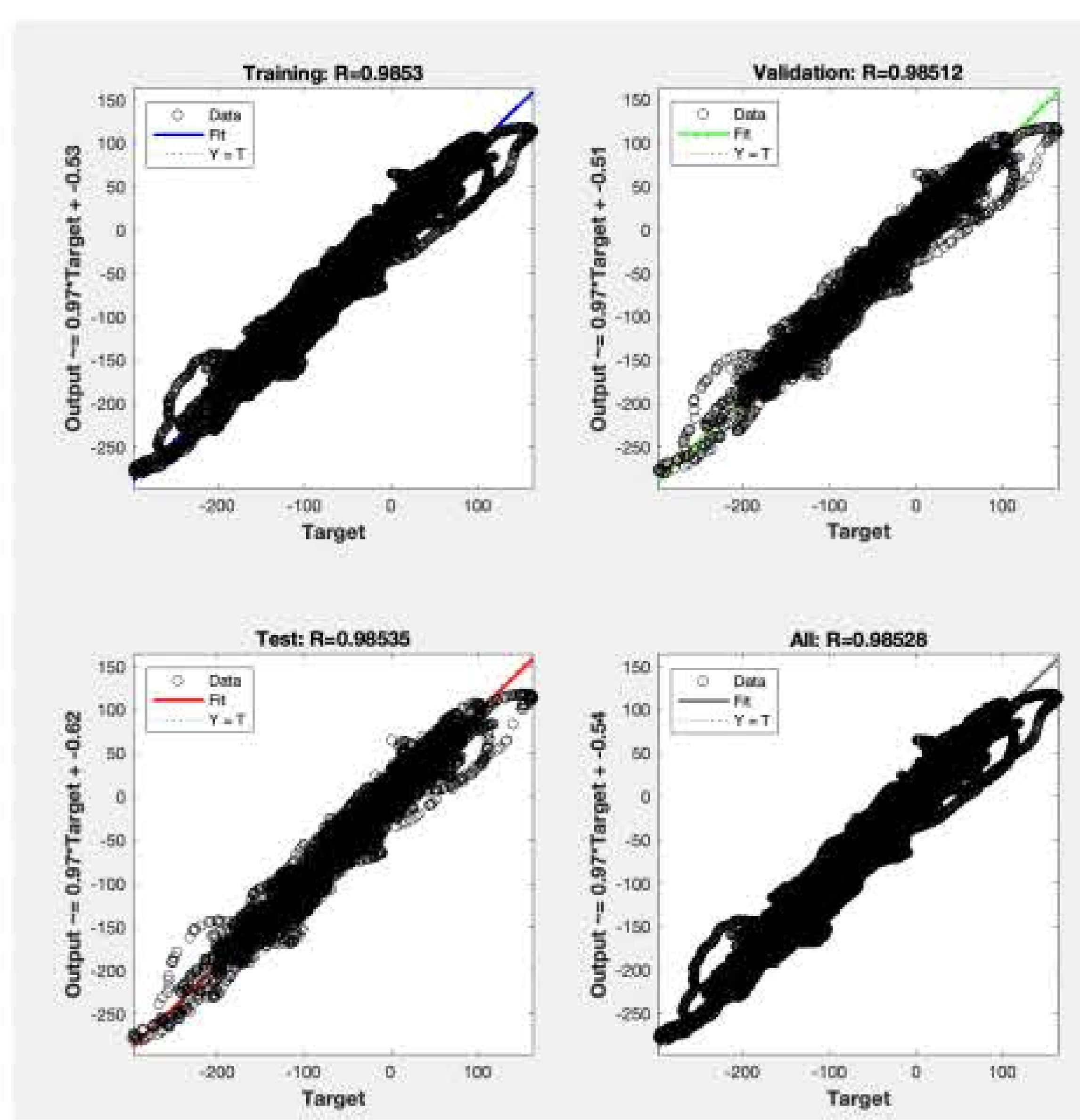
Evolving the Coarse Field

Since the force from the particle on the fluid is only approximate, we rerun the coarse point particle model, using the slip velocity and the force from the particles and record the conditions at the particle center to generate a database to be used to find expressions for the force and the slip velocity from conditions at the particle location.

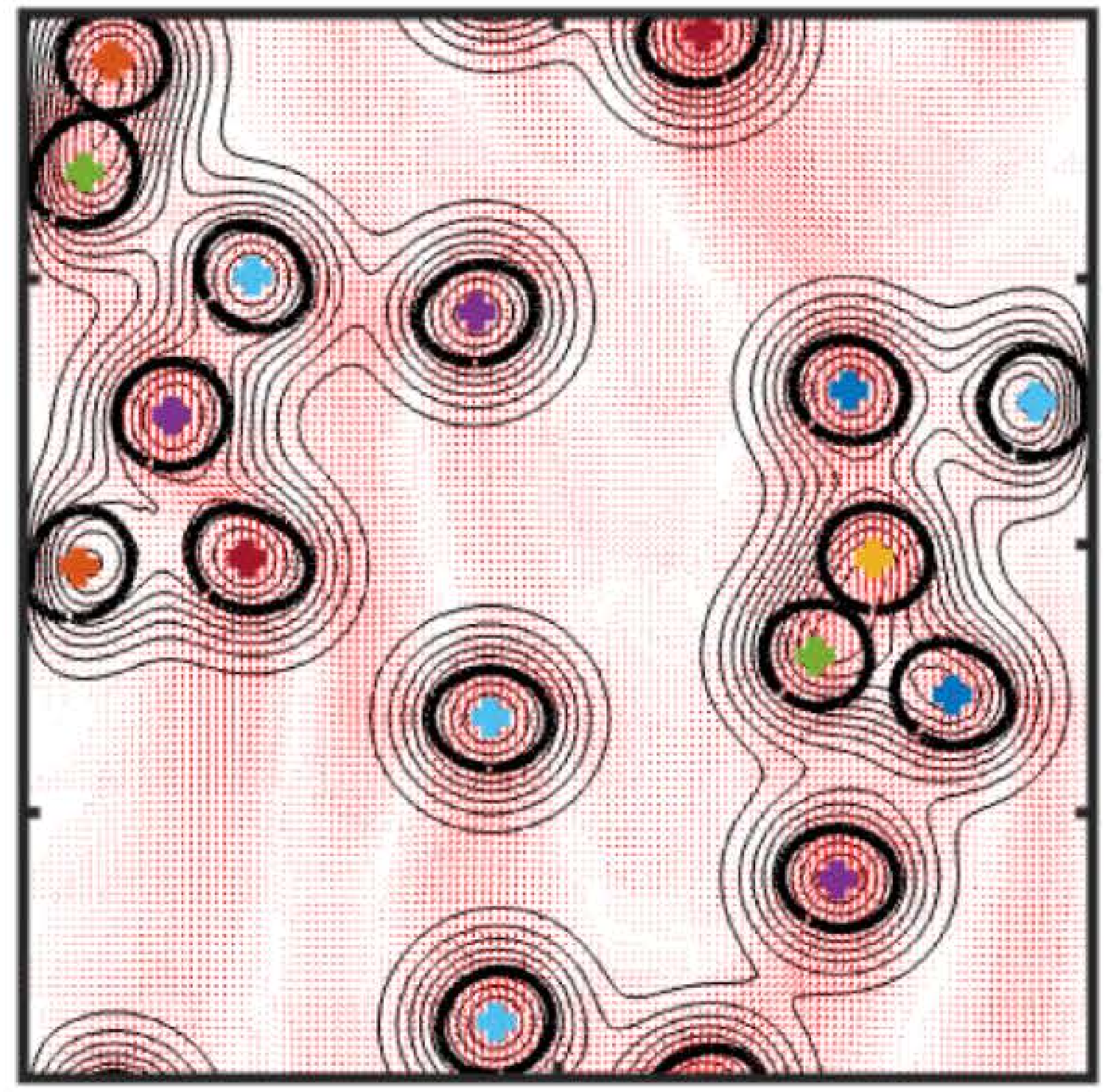
We have done a few preliminary tests using machine learning but this work is not complete. The correlation is generally reasonable but the current data is too sparse.

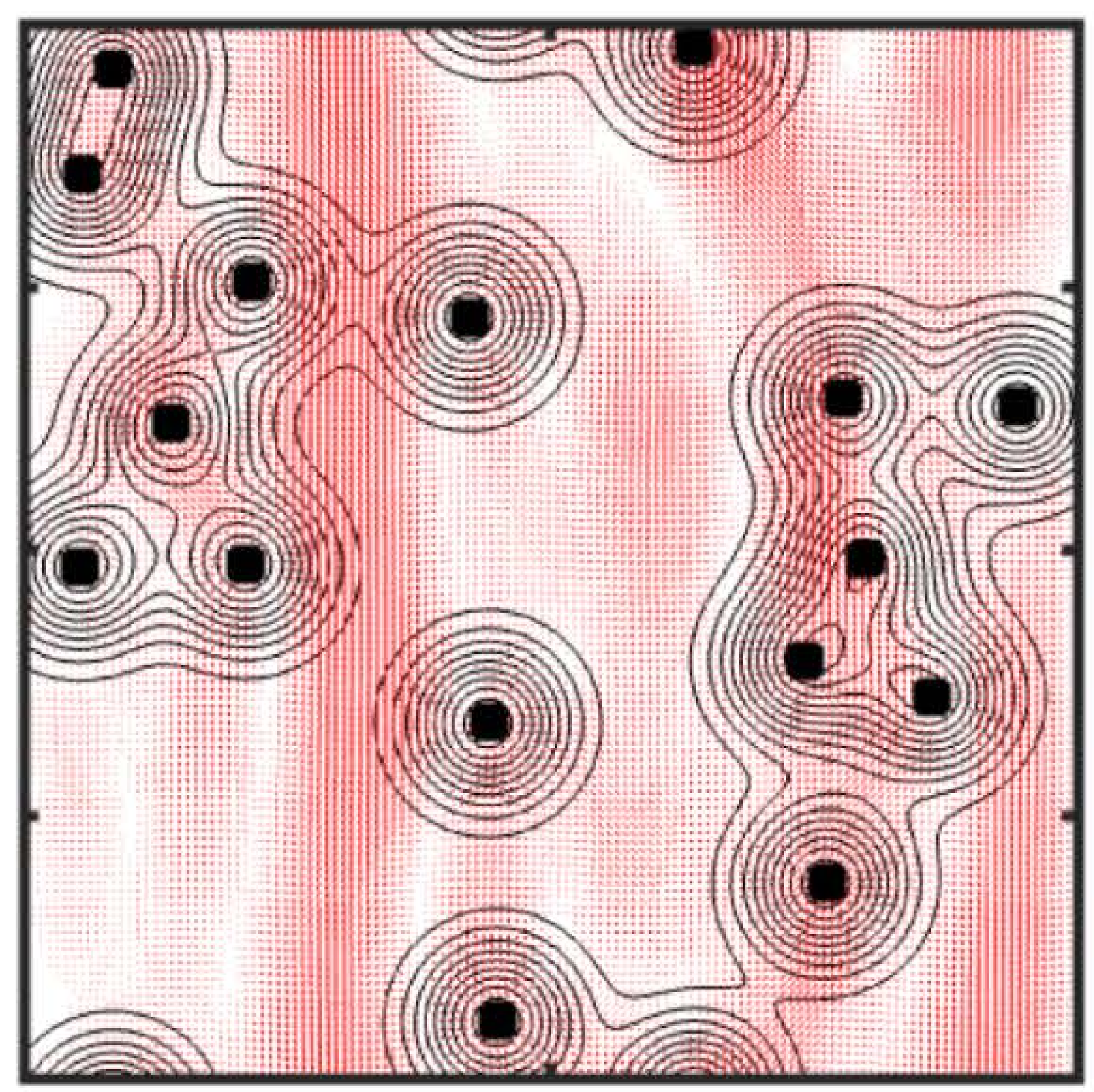


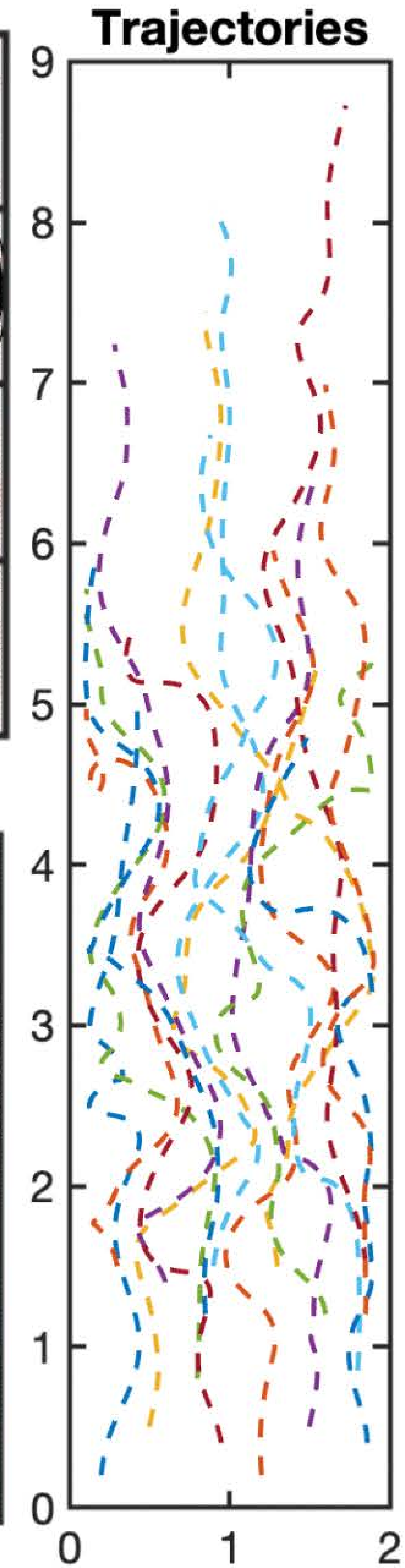
Acceleration



Force







Coarse Grained Models for Multiphase Flows

The key aspects of the modeling are:

Coarsening: Small scales are filtered. Not decomposed into modes.

Interface retaining: The interface is simplified but stays sharp.

Trajectory modeling: The conservation equations are augmented to ensure that the coarse flow evolves correctly. Not structure or function modeling, so a priori tests are irrelevant.

Scale aware: The level of coarsening is explicitly accounted for going from fully resolve results on one end and fully averaged steady results at the other.

Additional Thoughts on Trajectory Modeling

Trajectory Modeling

Trajectory modeling requires only the coarse flow. When the coarse flow comes from filtered fully resolved simulations we must resolve all smaller scales, severely limiting the scale range we can obtain.

In experiments, we just need to measure the flow at the coarse scale. Smaller scales are taken care of by the physics. Thus, the range of scales below the observed scale can be arbitrarily large.

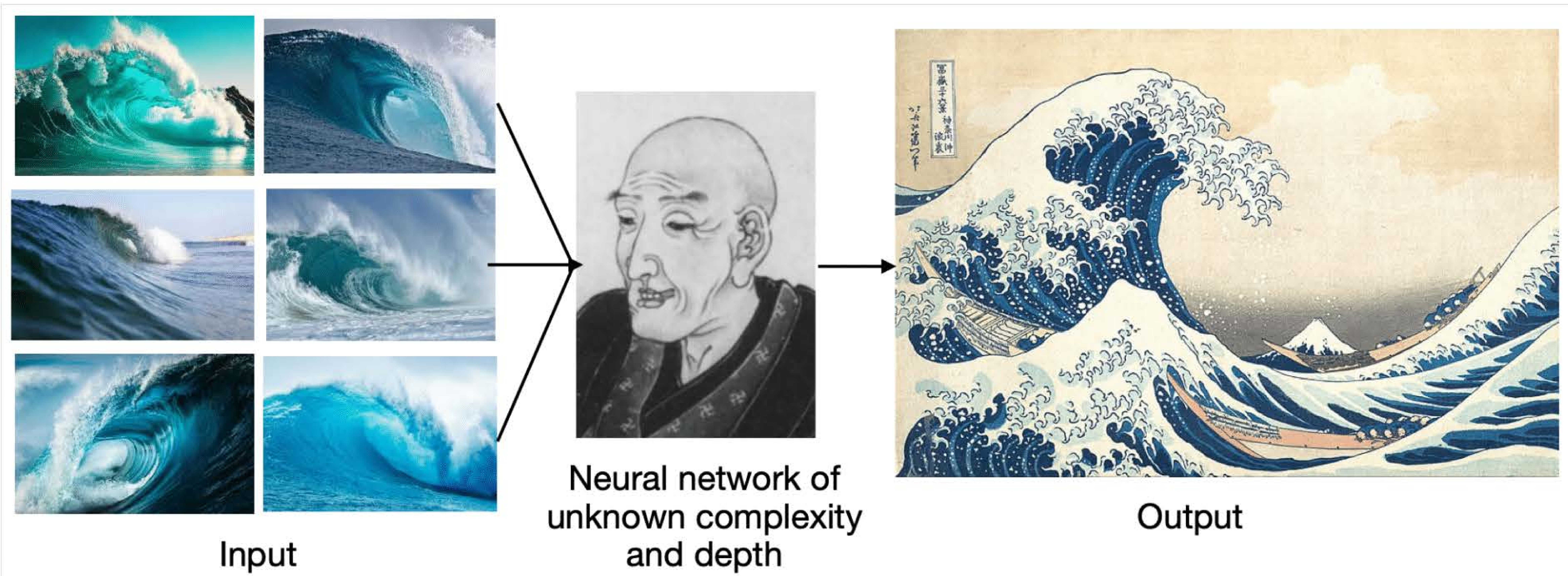
In many applications we don't fully know small scale physical processes, but as long as they are repeatable we don't need to, as long as we are in the appropriate parameter range.

The amount of experimental data may still be limited, but progress in reconstructing the flow (such as PINNs) should allow us to get both the full (but coarse) velocity field and the closure terms, as correction to the standard NS equations

Experimentally based, scale aware, trajectory, modeling for single phase flow seems relatively straight forward, but the need for some knowledge of what the model looks adds complications for multiphase flows

Trajectory Modeling

Predictions based on models derived from observations/ measurements at the scale that we wish to predict are likely to play a key role as we seek to build digital twins of everything. Predicting based on observations is, of course, exactly what humans do!



Artist Katsushika Hokusai presumably generated his masterpiece by observing real waves, not starting with solutions of the Euler or Navier-Stokes equations. (Pictures from Wikipedia and the web.)