Fully resolved numerical simulations of complex multiphase flows

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Thermal & Fluids Analysis Workshop
TFAWS 2019
August 26-30, 2019
NASA Langley Research Center
Hampton, VA

Outline

For many multiphase flow problems, direct numerical simulations of large systems have become routine

- Introduction
- Numerical Approach
- Multiscale issues: Coarse models from detailed results
- Multiscale issues: Dealing with isolated small scale features
- Conclusion

Why DNS?

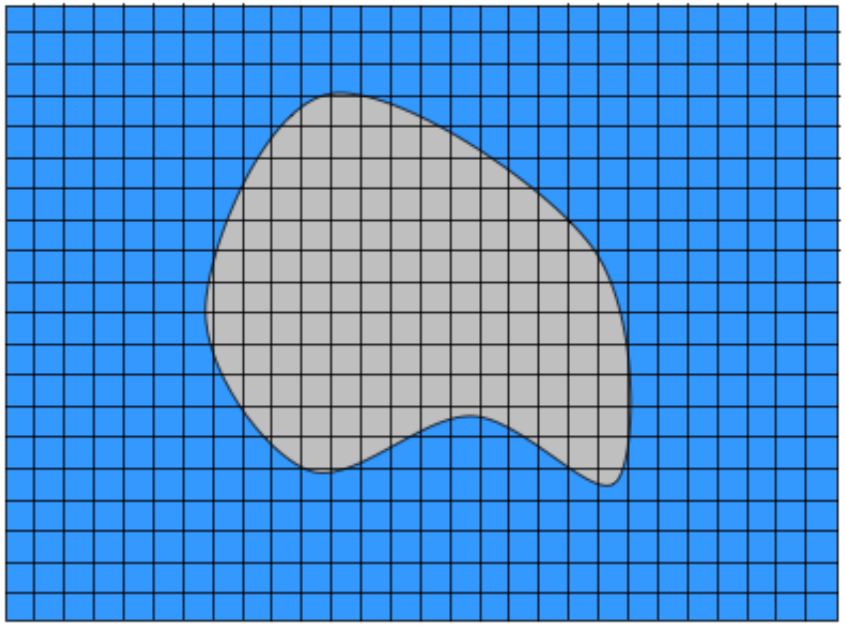
Why fully resolved numerical simulations?

- Sometimes you just want to know. Shear breakup of drops, bubble induced drag reduction, dependency of lift on bubble formation, void fraction distribution in bubbly channels, etc
- As the “ground truth” for reduced order models. Two-fluid models need closure terms that must be modeled and then validated by comparison with a more fundamental solution
- To sort out the physics. The mathematical models describing complex processes may not be fully known. Simulations produce predictions that can be compared to experimental results to check the accuracy of models for surfactants, for example.

Numerics

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
- A single stationary grid is used for the whole domain to discretize the governing equations

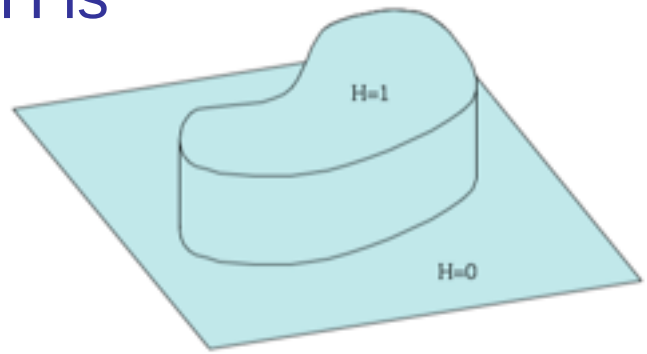


Many different methods have been proposed to advect the marker field

Numerics

The advection of the marker function H 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

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

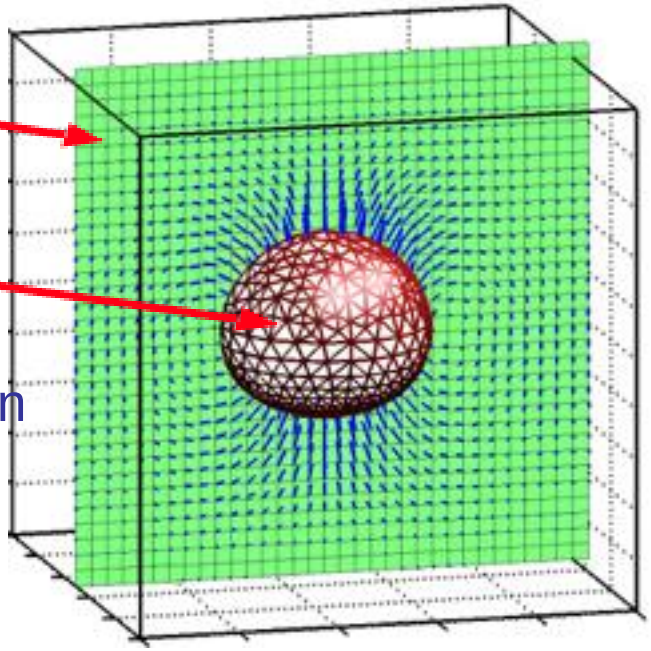
$$\nabla \cdot \mathbf{u} = 0 \qquad \frac{D\rho}{Dt} = 0; \quad \frac{D\mu}{Dt} = 0$$

Front Tracking

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

Tracked front to advect the fluid interface and find surface tension

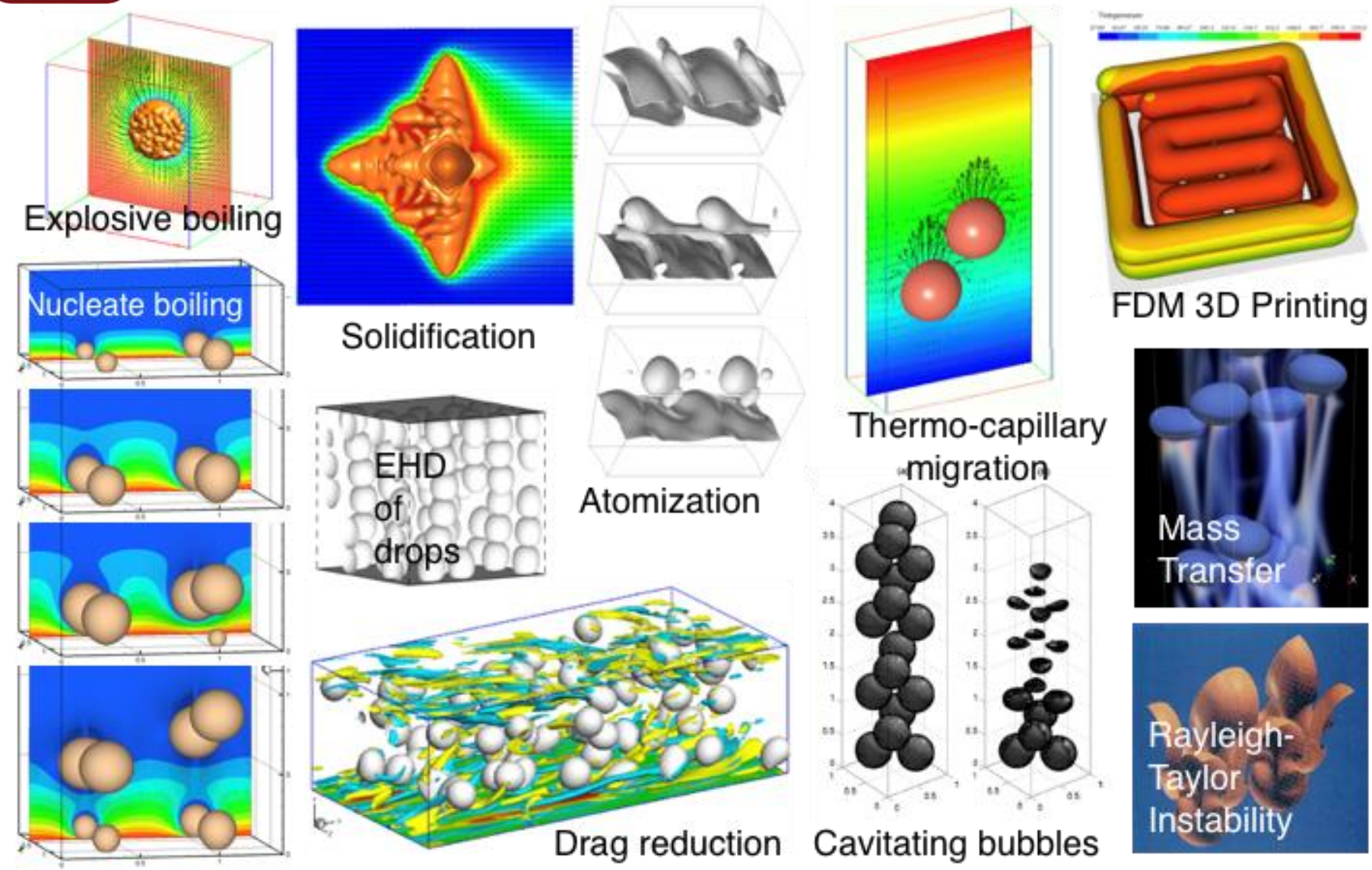
The front is used to set the marker function and compute the surface tension



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

The method has been used to simulate many problems and extensively tested and validated

Front Tracking—Examples



Numerics

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:

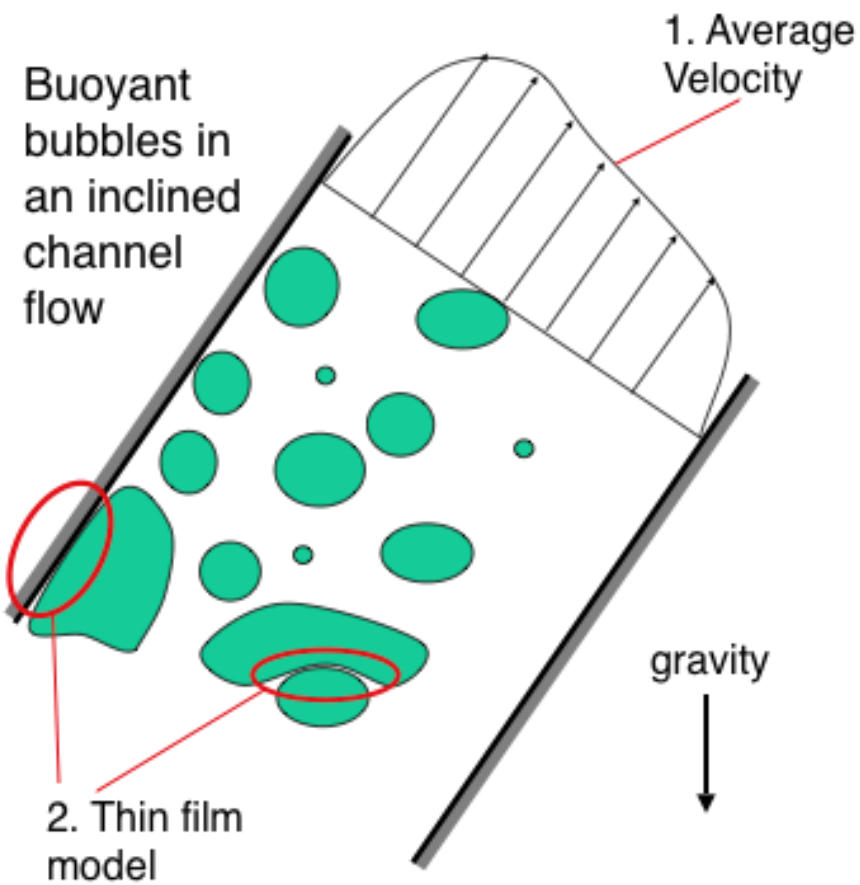
- How do we use the abundance of information that is already available most effectively to generate models for closure terms in RANS and LES computations of industrial systems?
- How do we model complex multi-physics and multi-scale systems in the most effective way?

Multiscale Issues

We have two basic types of multi-scale problems.

1: Constitutive Modeling Based on the Microscopic Models or Models for the Large-Scale Motions

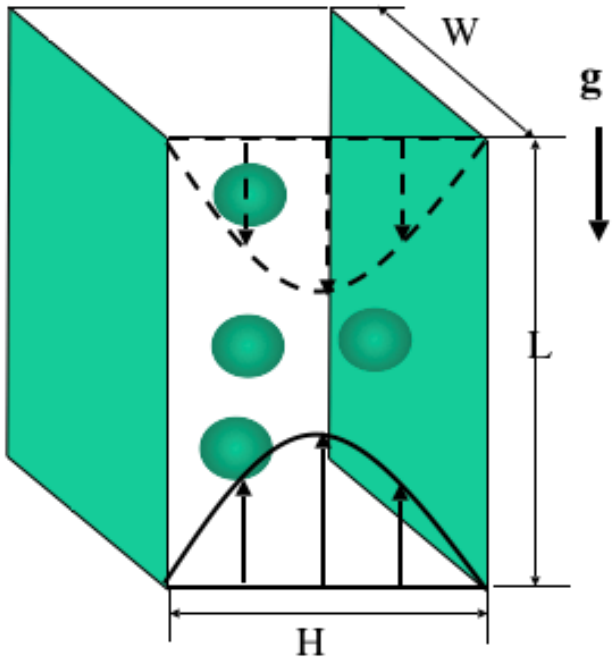
2: Dealing with Isolated Defects or Small-Scale Features



Reference: W. E and B. Enquist, The heterogeneous multiscale methods, Comm. Math. Sci. 1(2003), 87—133.

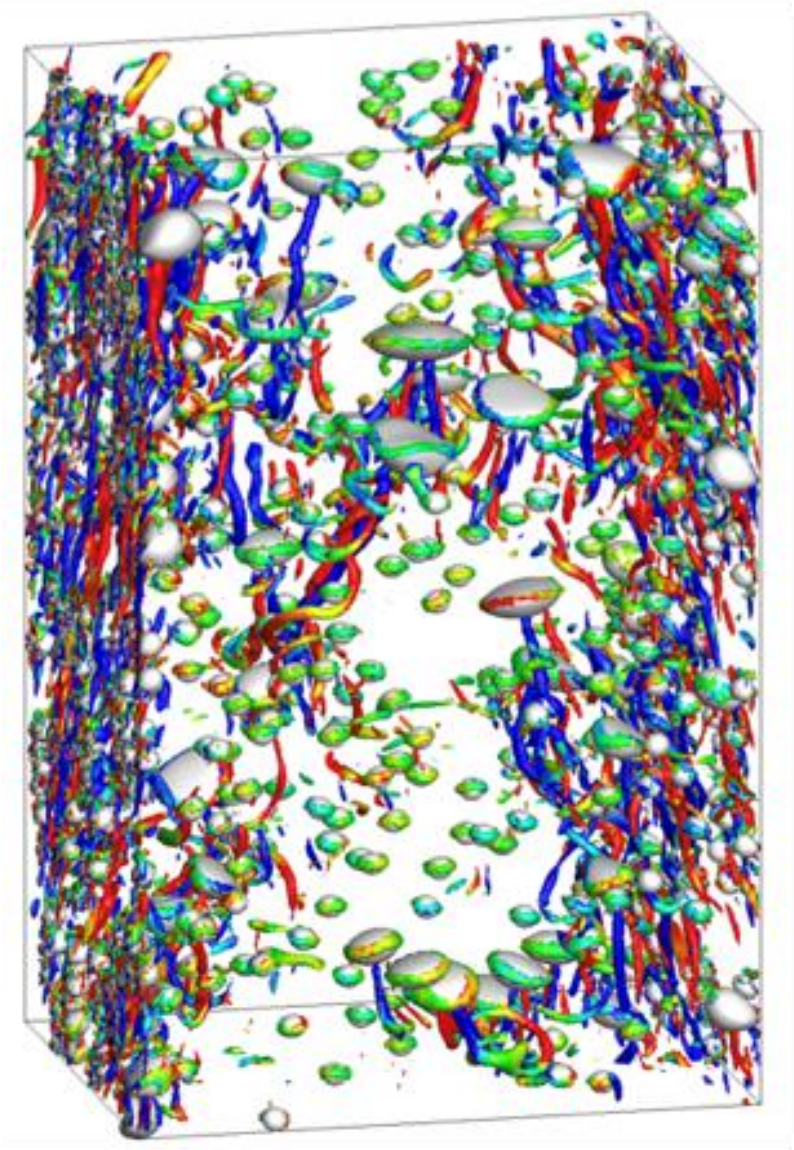
Bubbly Flow

Most of the discussions here are in the context of buoyant bubbly flows in a vertical channels or periodic domains



Bubbly Flow

Multiscale: Behavior of the large scale flow



Bubbly Flows

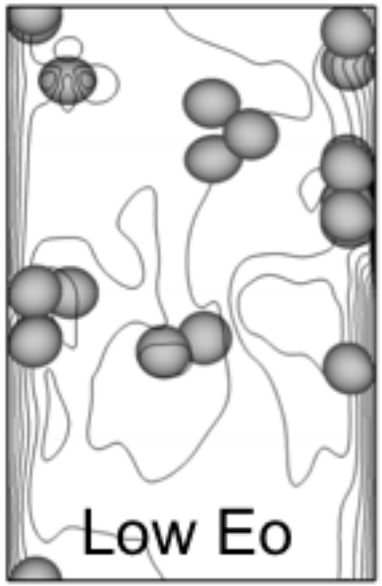
For disperse flows, where bubbles neither coalesce or breakup, simulations have provided significant new insight:

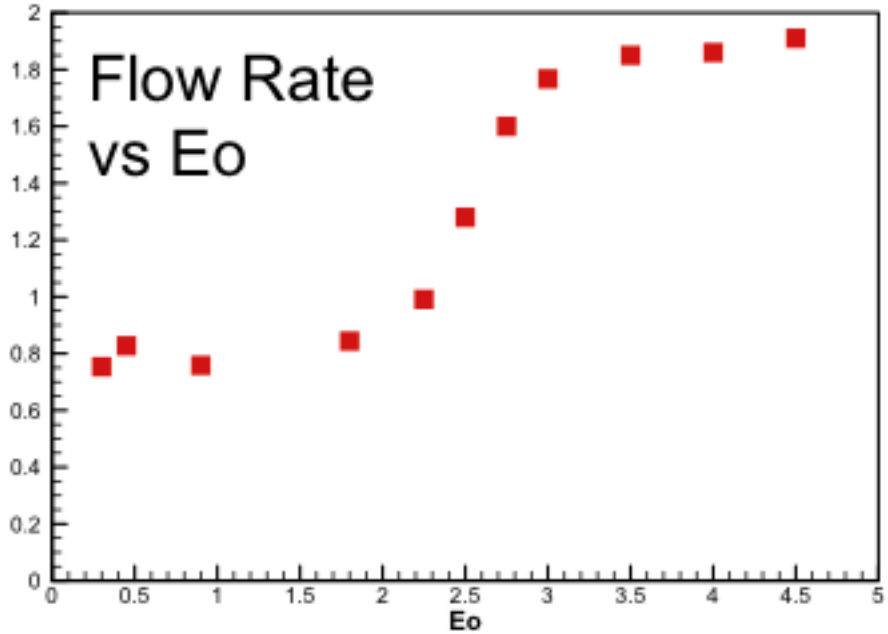
- Effect of bubble deformability and flow direction
- How the void distribution and the flow rate depends on the bubble deformability
- Effect of surfactants on the void distribution and the flow rate
- Effect on heat and mass transfer in bubbly flows

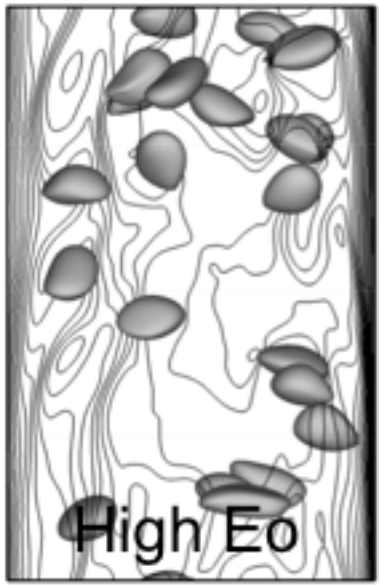
Results of DNS are also being used to improve models for the large scale flows, although this is in an early stage

Bubbly Flows

Turbulent Upflow: Effect of Bubble Deformability on Flow Rate







Nearly spherical bubbles hug the wall and greatly increase the wall friction, resulting in a lower flow rate. Deformable bubbles, on the other hand, stay in the middle and have relatively little impact on the flow rate. For the parameters used here, the transition takes place around Eo = 2.5-3.0.

Bubbly Flows

Use of Machine Learning to extract relationships from large datasets

$$\frac{\partial \alpha_l}{\partial t} + \frac{\partial F_l}{\partial x} = 0$$

Resolved average variables

Averaging the DNS results over planes parallel to the walls,

F_g	$<u'v'>$	f_σ	α_g	$\frac{\partial \alpha_g}{\partial x}$	$\frac{\partial <v>_l}{\partial x}$	d_w	k_t	ε_t	a	a_{ij}
	Data obtained by averaging the DNS results									

Not include here

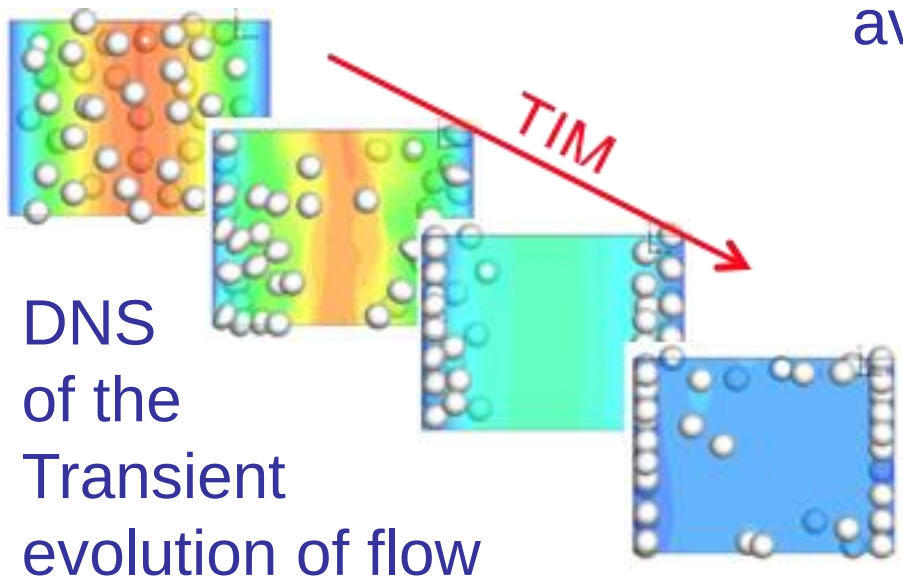
Using Neural Networks, we fit the data, resulting in:

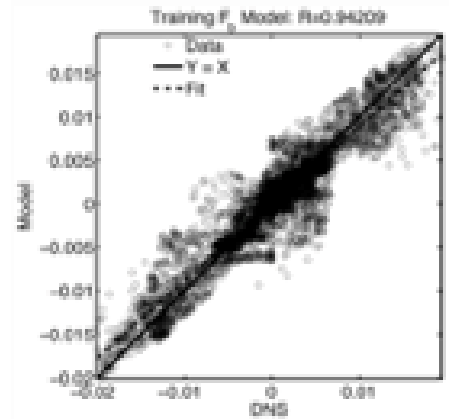
$$F_b = f_1(\mathbf{x}); \quad <u'v'> = f_2(\mathbf{x}); \quad F_\sigma = f_3(\mathbf{x}); \quad \mathbf{x} = \left(\alpha, \frac{\partial \alpha}{\partial x}, \frac{\partial <v>}{\partial x}, d_w\right)$$

These relationships are used when solving the average equations for the void fraction and the vertical liquid velocity

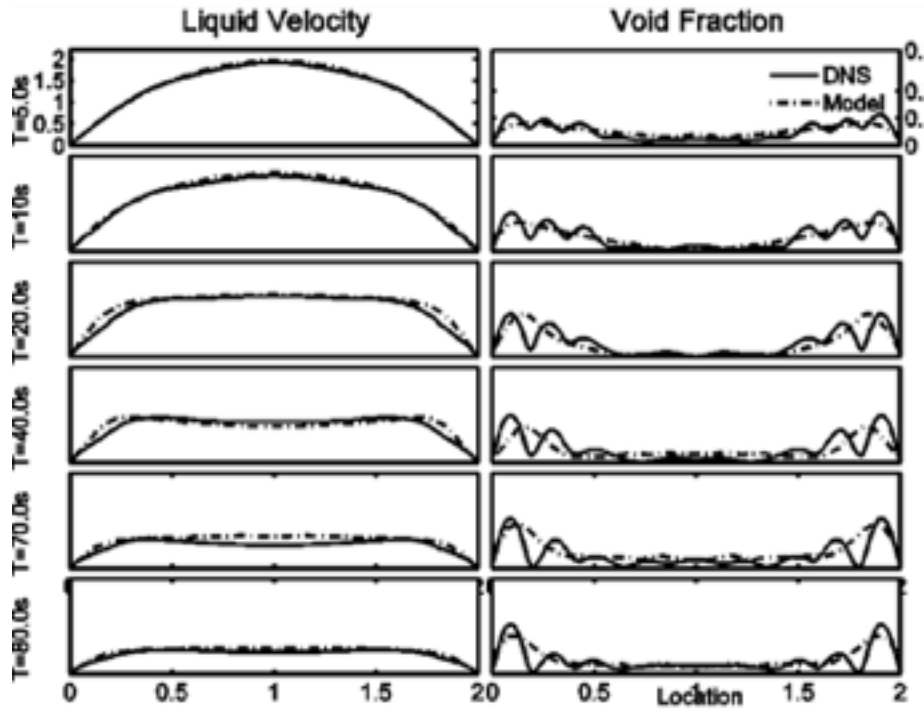
Bubbly Flows

The use of machine learning to find closure relationships for a simple averaged model

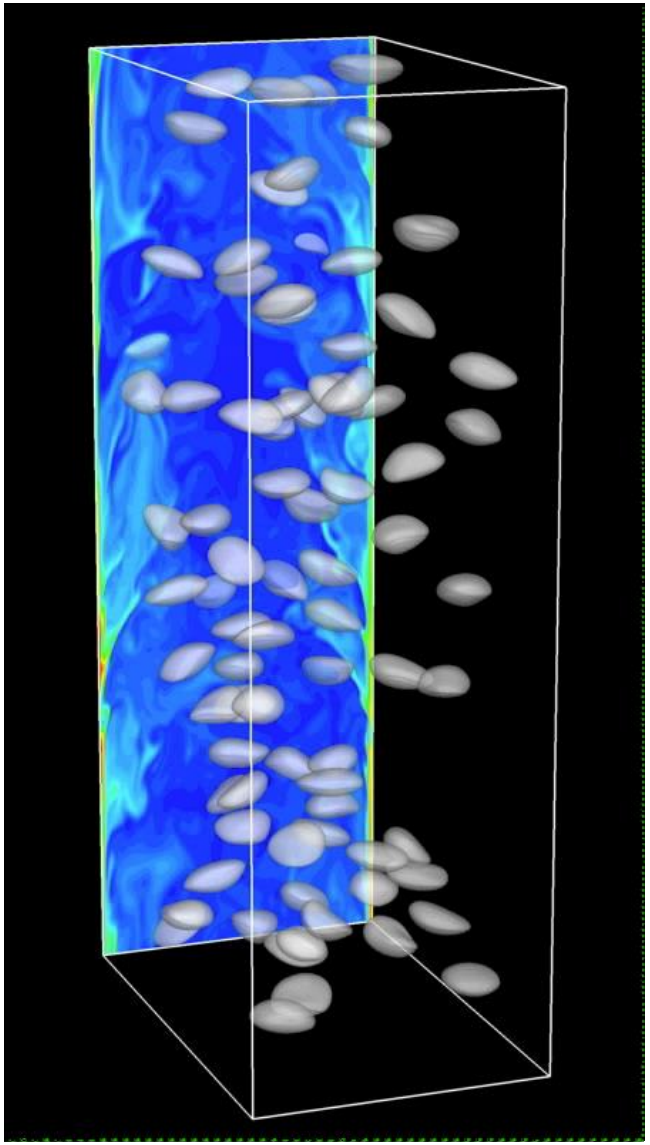




DNS of the Transient evolution of flow with a uniform distribution of bubbles that remain nearly spherical are used to proved closure for a model of the average flow



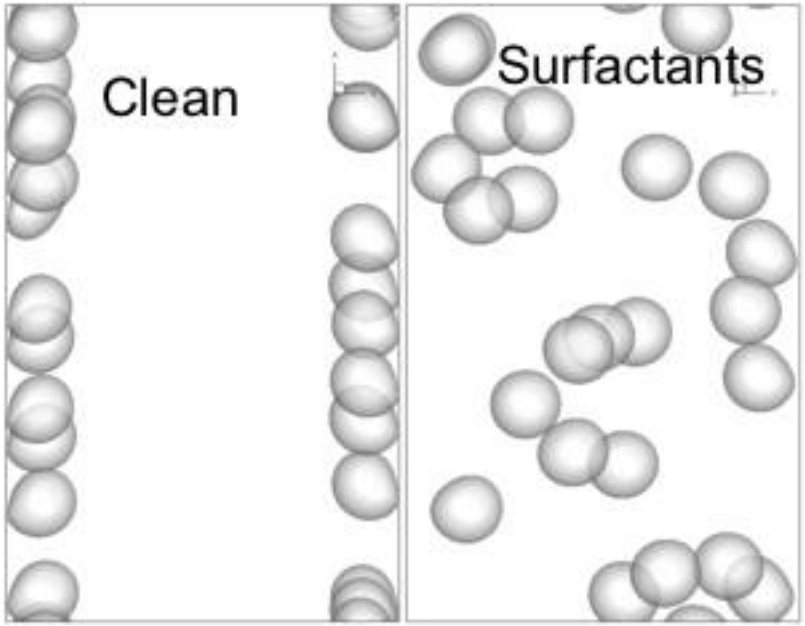
Bubbly Flow



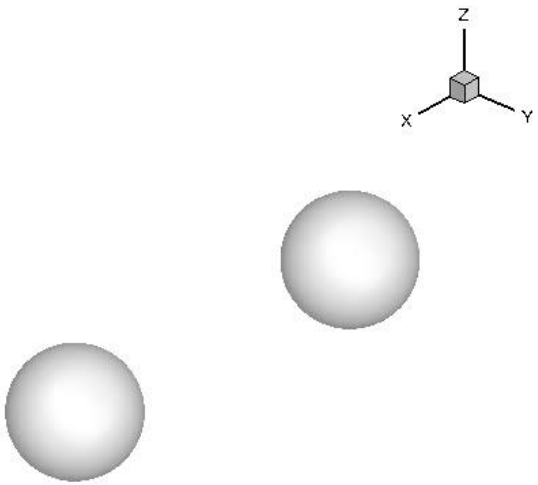
S. Dabiri and G. Tryggvason. Heat transfer in turbulent bubbly flow in vertical channels. Chemical Engineering Science. 122 (2015), 106-113.

Some efforts have been made to extend DNS to flows where additional physical processed are important

J. Lu, M. Muradoglu and G. Tryggvason. "Effect of Insoluble Surfactant on Turbulent Bubbly Flows in Vertical Channels." International Journal of Multiphase Flow. 95 (2017), 135-143.



Complex Flows



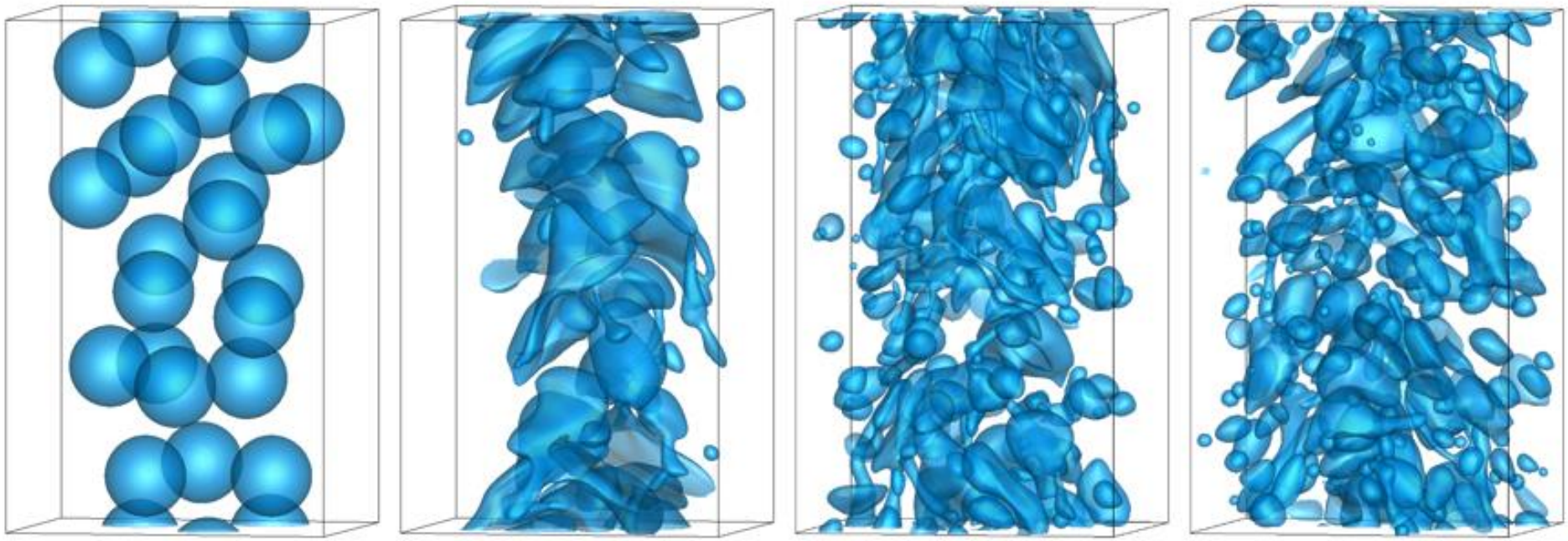
Except for low void fraction gas-liquid flows, distinct bubbles are the exception rather than the rule and in most flow the interface is not only complex, but keep undergoing breakup and coalescence

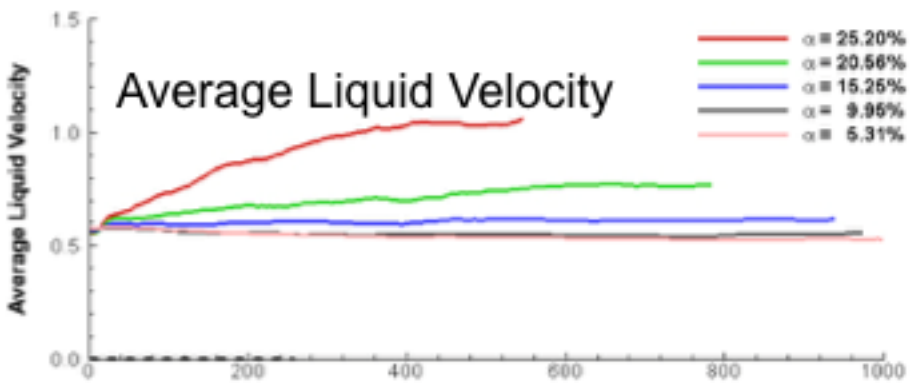
Topology changes in two-phase flows take place in two ways:

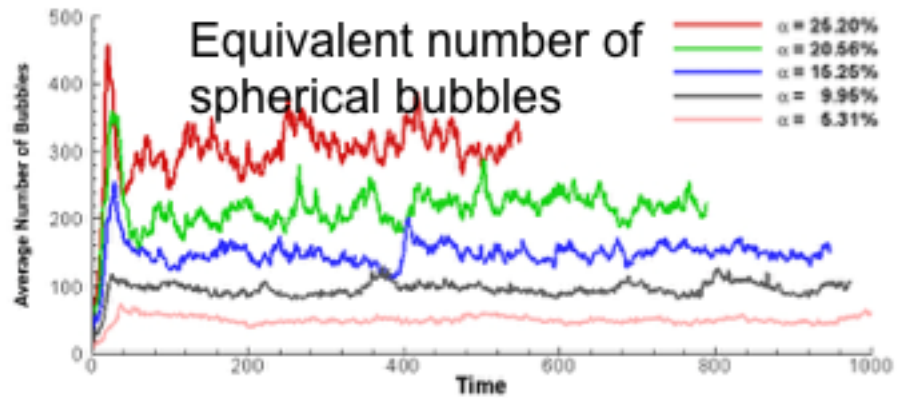
- Breakup usually takes up when thin threads break into a string of small drops or bubbles
- Coalescence usually takes place when a thin film becomes unstable and breaks

When the interface is tracked explicitly, we can control when coalescence takes place

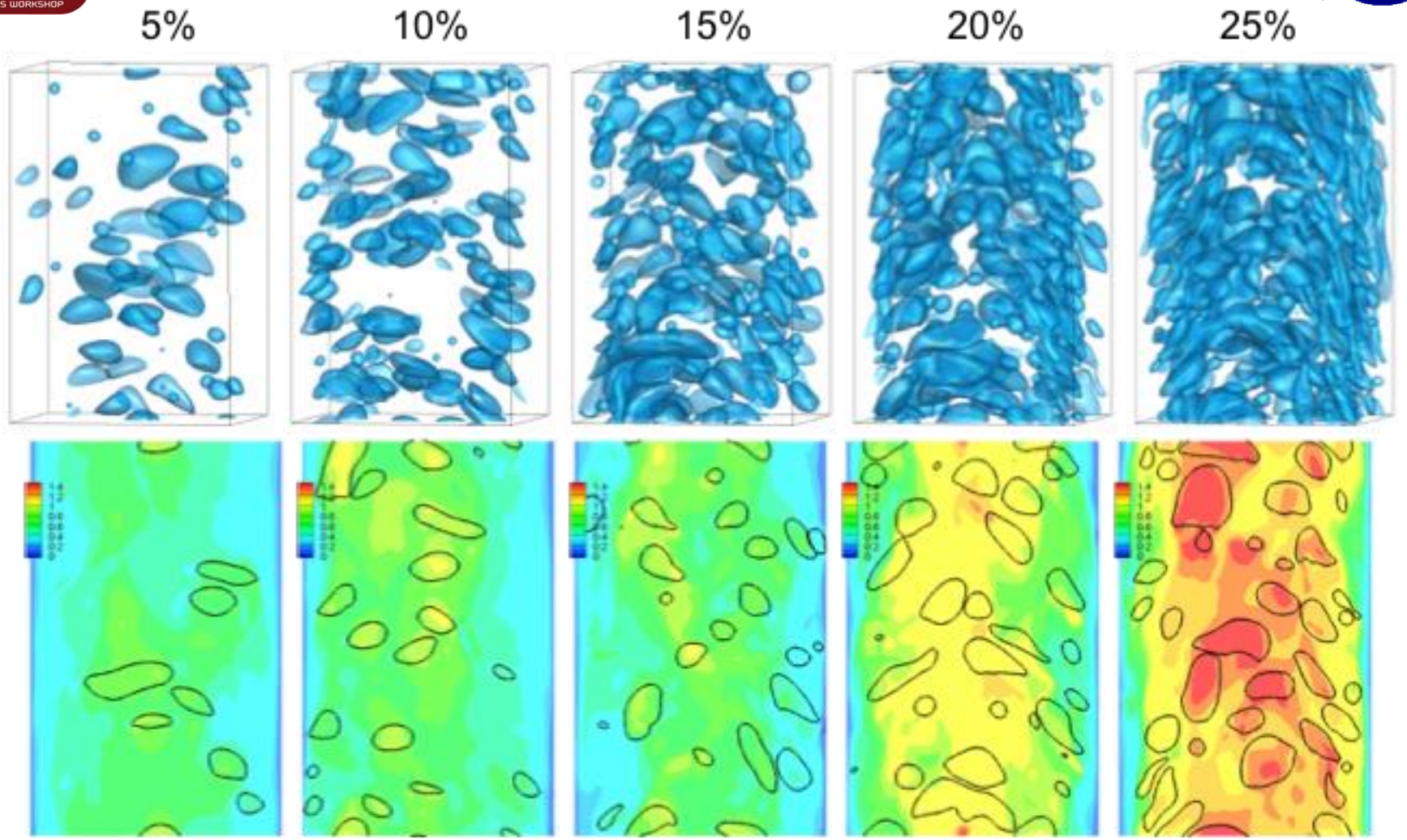
Complex Flows





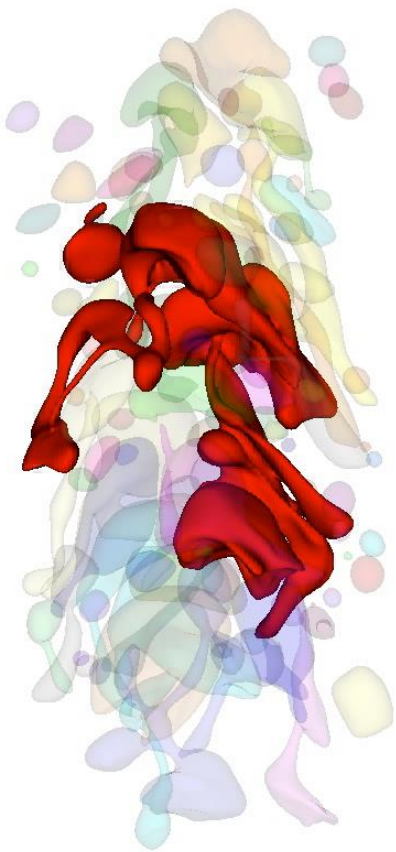


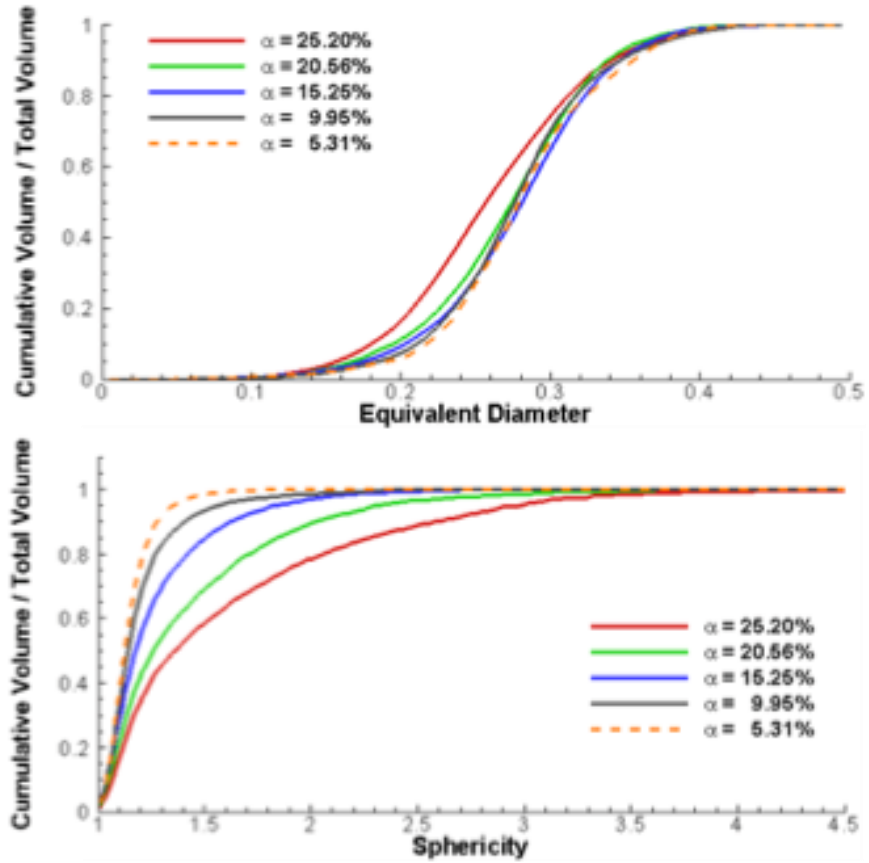
Complex Flows



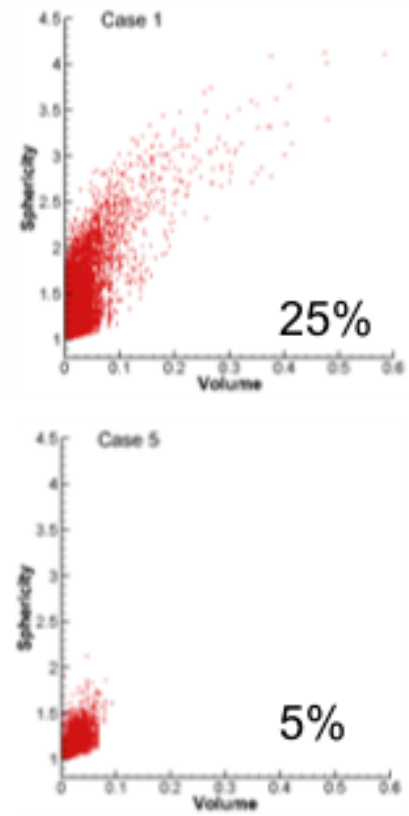
The fluid interface at late times for all five cases in the top row and contours of the vertical velocity in a plane through the middle of the domain in the bottom row.

Complex Flows





The normalized cumulative volume (top) and the sphericity (bottom) versus equivalent diameter



The sphericity versus volume

The size and shape of blobs of the light fluid at late times

Multiscale Issues

Multiscale: Capturing small-scale features using Embedded Analytical Descriptions

Small-scales, much smaller than the “dominant” scale can arise spontaneously due to collisions and breakup of fluid masses, or due to the presence of physics occurring on different spatial and temporal scales. Examples include:

- Mass transfer in high Schmidt number liquids
- Collision of drops with solid walls

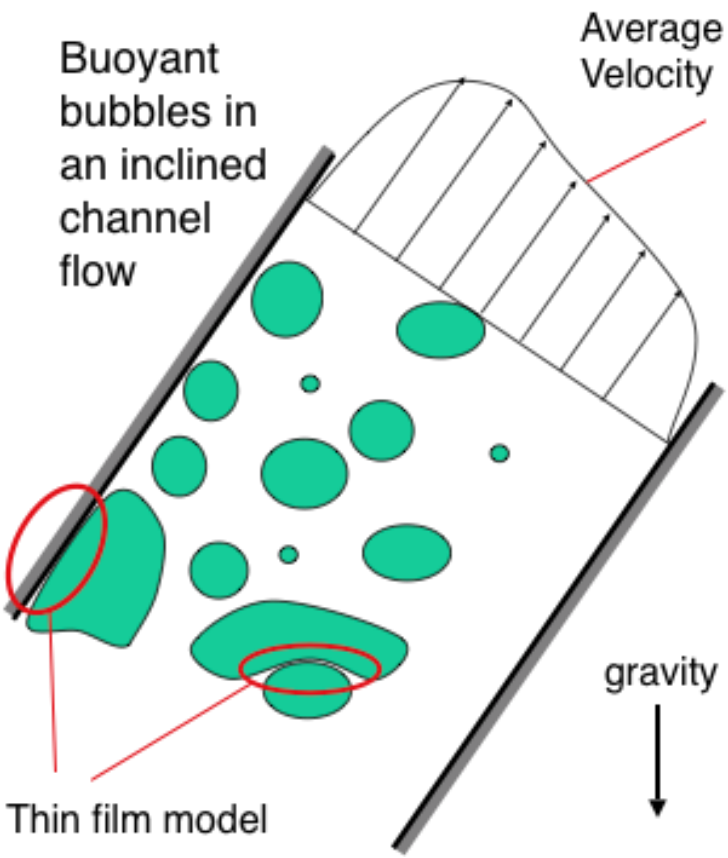
Multiscale Issues

Capturing isolated small-scale motion in simulations where the focus is on the larger scales can be done in many ways, such as be various grid refinement techniques (unstructured grids, AMR for Cartesian grids, wavelets, etc.) or reduced order models

However:

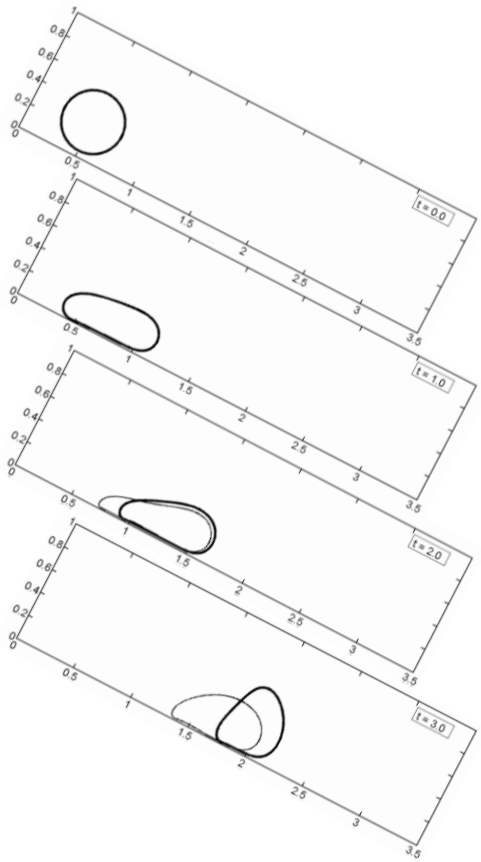
- At small scales, the effect of surface tension is strong so interface geometries are simple
- At small scales the effect of viscosity is strong so the flow is simple

Those are exactly the situation that can be—and have been—handled analytically



Capturing Thin Films

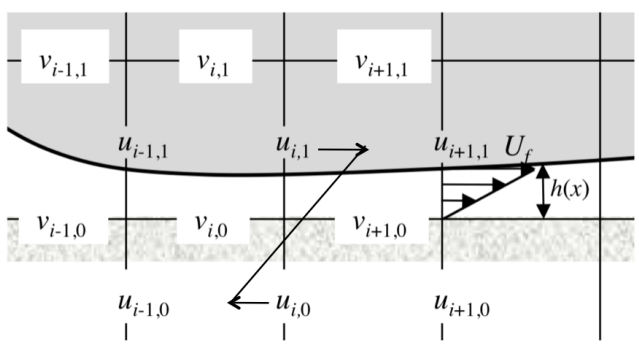
Drop motion on a sloping wall. Impact of resolving the film between the drop and the wall. The film becomes very thin but determines the slide velocity of the drop



Film model—linear velocity profile

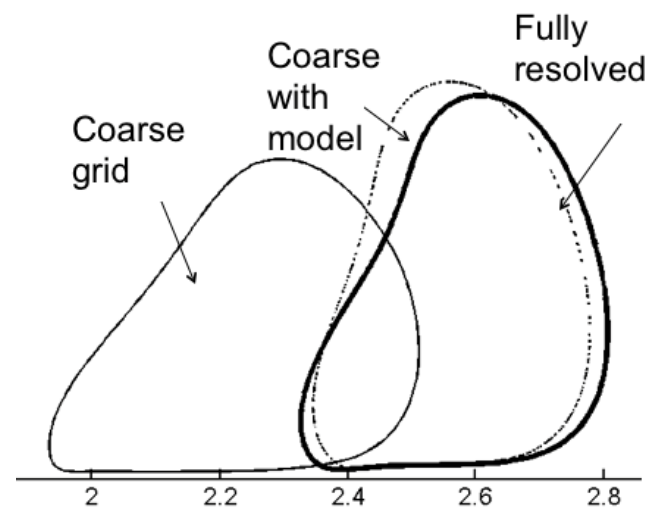
$$\frac{\partial h}{\partial t} + \frac{1}{2}\frac{\partial}{\partial x}(hU_f) = 0;$$

$$\frac{\partial}{\partial t}(hU_f) + \frac{2}{3}\frac{\partial}{\partial x}(hU_f^2) = -\frac{2h}{\rho_o}\left(\frac{dp}{dx}\right)_f,$$



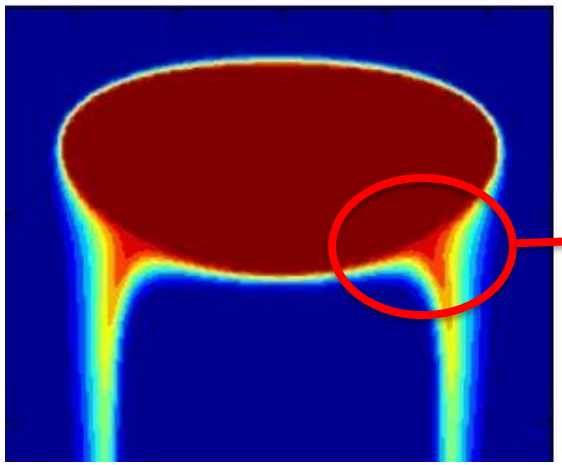
Wall shear and ghost velocity:

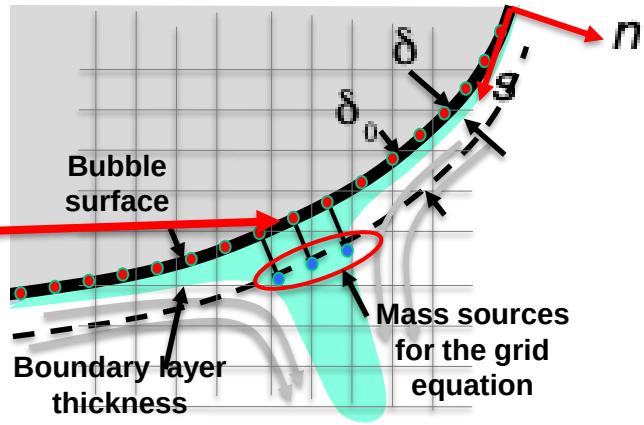
$$\tau_f = \mu_o \frac{\partial u}{\partial y} = \mu_o \frac{U_f}{h} \Rightarrow u_{i,0} = u_{i,1} - \frac{\tau_f \Delta y}{\mu_d}$$

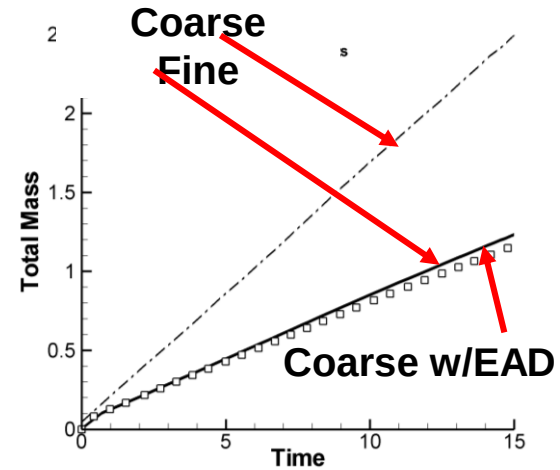


S. Thomas, A. Esmaeeli and G. Tryggvason. "Multiscale computations of thin films in multiphase flows." Int'l J. Multiphase Flow 36 (2010), 71-77.

Capturing the mass boundary layer



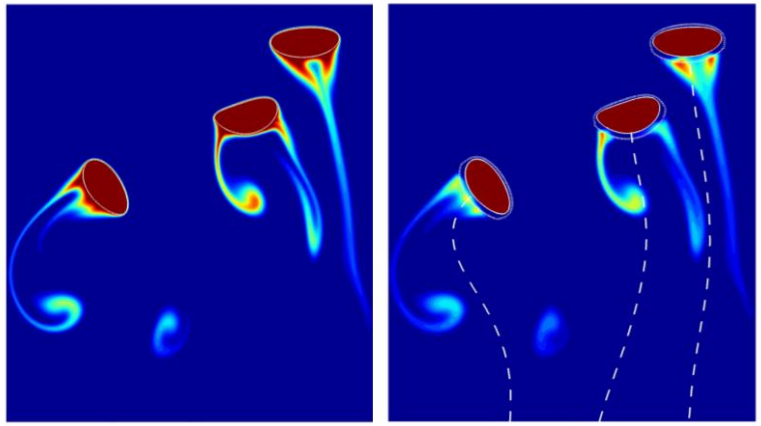




$$\frac{\partial f}{\partial t} = \sigma n \frac{\partial f}{\partial n} + D \frac{\partial^2 f}{\partial n^2}.$$

$$M_0 = \int_0^{\delta_0} f \, dn.$$

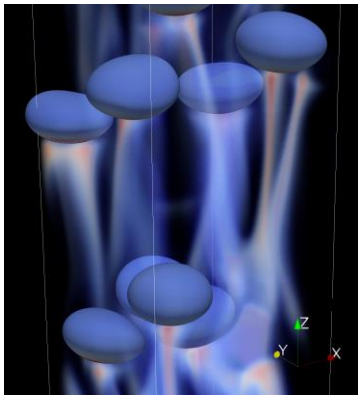
$$\frac{dM_0}{dt} = -\sigma M_0 + \sigma f_{\delta_0} \delta_0 - D\left(\left.\frac{\partial f}{\partial n}\right|_0 - \left.\frac{\partial f}{\partial n}\right|_{\delta_0}\right)$$



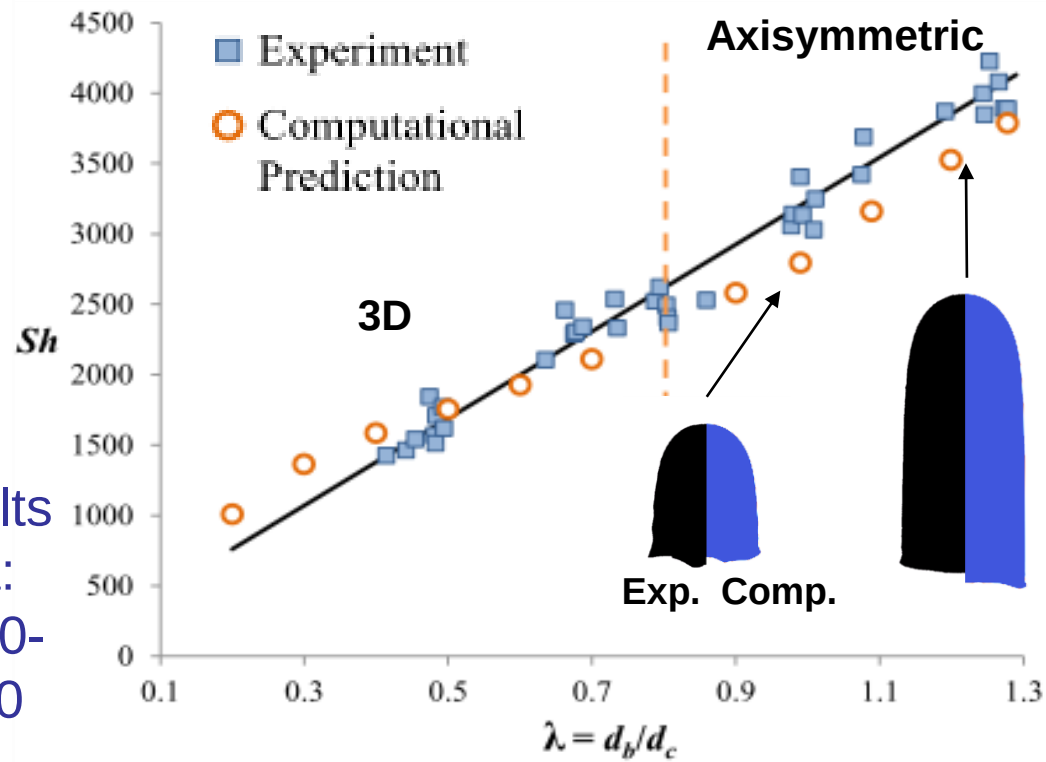
B. Aboulhasanzadeh, S. Thomas, M. Taeibi-Rahni, and G. Tryggvason. Chemical Engineering Science 75 (2012) 456–467.

Comparison between simulations on a very fine grid and a coarser one with the model

Capturing the mass boundary layer



Comparison with experimental results from A. Tomiyama: Eo = 24.7, Mo = 10-7.78 and Sc= 8260



The use of an analytical embedded description for the mass transfer should allow us to examine how it depends on the collective motion of many bubbles and the effect of void fraction and bubble deformability, for high Sc gas/liquid systems

Conclusions

- DNS of bubbly flows in turbulent channels have been developed to the point that they can now be used to help produce new models for “industrial” simulations.
- DNS data is putting new demands on the modeling of complex multiphase flows. Currently, such modeling relies of fairly basic ideas, first put forward many years ago. DNS should make much more comprehensive models possible:
- DNS needs to be extended to handle flows with more complex topology and those undergoing flow regime transitions
- Complex isothermal flows and flows with phase change and other additional physics, such as mass transfer, need multiscale modeling that must be developed further and put on a rigorous theoretical basis.
- One of the biggest obstacle for more rapid increase in the use of DNS is the high “entry barrier” for new investigators. Many “things” to learn! See: http://www.multiphaseflowdns.com