Direct Numerical Simulations of Multiphase Flows. Now What?

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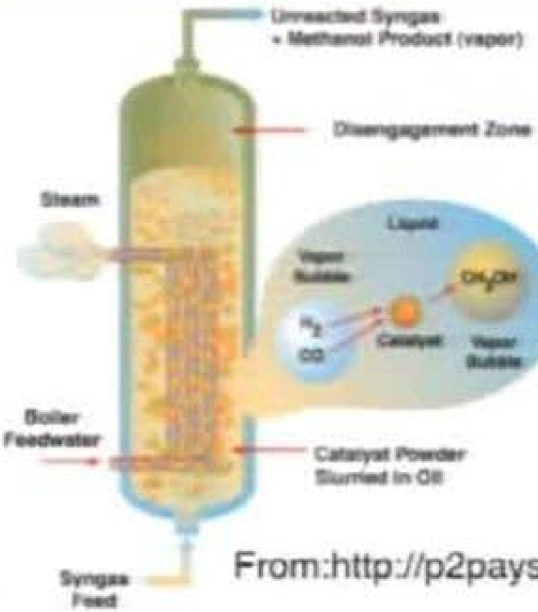
Modeling and Computing Complex Flows

Why Multiphase Flows are Important!



Liquid Phase Methanol (LPMEOH™) Process

From:http://p2pays.org/ref/16/15865.pdf

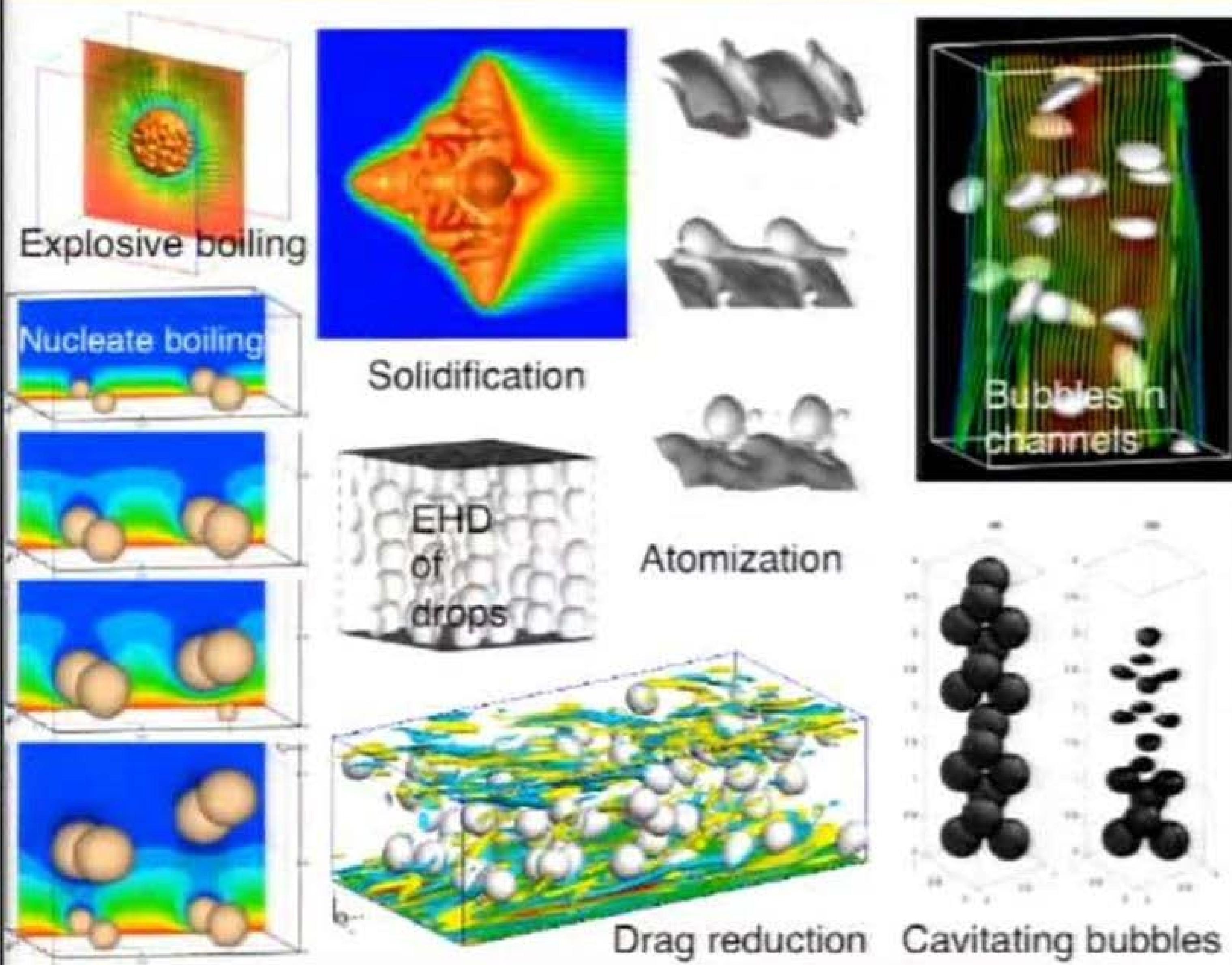
Synthetic fuel production, Mossgas, Mossel Bay, SA
From: http://www.fischer-tropsch.org

Examples of Applications of Bubble Columns

Process	Methods and/or Reactants
Acetone	Oxidation of cumene
Acetic acid	Oxidation of acetaldehyde
	Oxidation of sec-butanol
	Carbonylation of methanol
Acetic anhydride	Oxidation of acetaldehyde
Acetaldehyde	Partial oxidation of ethylene
Acetophenone	Oxidation of ethylbenzene
Barium chloride	Barium sulfide and chlorine
Benzoic acid	Oxidation of toluene
Bleaching powder	Aqueous calcium oxide and chlorine
Bromine	Aqueous sodium bromide and chlorine
Butene	Absorption in aqueous solutions of sulfuric acid
Carbon Dioxide	Absorption in ammoniated brine
Carbone tetrachloride	Carbon disulphide and chlorine
Copper oxychloride	Oxidation of cuprous chloride
Cumene	Oxidation of phenol
Cupric chloride	Copper and cupric acid or hydrochloric acid
Dichlorination	Oxychlorination of ethylene
Ethyl benzene	Benzene and ethylene
Hexachlorobenzene	Benzene and chlorine
Hydrogen peroxide	Oxidation of hydroquinone
Isobutylene	Absorption in aqueous solutions of sulfuric acid
Phtalic acid	Oxidation of xylene
Phenol	Oxidation of cumene
Potassium bicarbonate	Aqueous potassium carbonate
Sodium bicarbonate	Aqueous sodium carbonate
Sodium metabisulphides	Carbon dioxide, aqueous sodium carbonate, and sulfur dioxide
Thiuram disulphides	Dithiocarbamates, chlorine, and air
Vinyl acetate	Oxidation of ethylene in acetic acid solutions
Water	Wet oxidation of waste water

After: S. Furusaki, L.-S. Fan, J. Garside. **The Expanding World of Chemical Engineering** (2nd ed), Taylor & Francis 2001

Modeling and Computing Complex Flows
DNS Examples



Direct Numerical Simulations:

Fully resolved and verified simulation of a validated system of equations that include non-trivial length and time scales

CFD of Multiphase Flows—one slide history

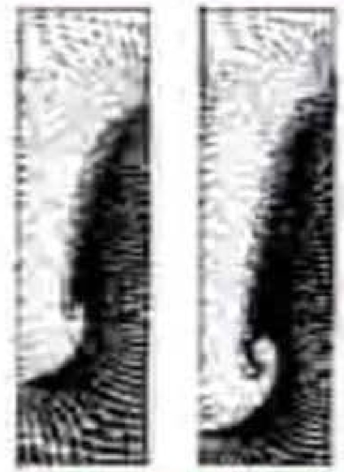
BC: Birkhoff and boundary integral methods for the Rayleigh-Taylor Instability

65' Harlow and colleagues at Los Alamos: The MAC method

75' Boundary integral methods for Stokes flow and potential flow

85' Alternative approaches (body fitted, unstructured, etc.)

95' Beginning of DNS of multiphase flow. Return of the "one-fluid" approach and development of other techniques



Simulation of cavitation using 13 trillion grid points to resolve the collapse of 15,000 bubbles, using 1.6 million cores of Sequoia, reaching 55% of its nominal peak performance

2013 ACM Gordon Bell Award

11 PFLOP/s Simulations of Cloud Cavitation Collapse
SC '13 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis, Article No. 3
Diego Rossinelli, Babak Hejazialhosseini, Panagiotis Hadjidoukas, Costas Bekas, Alessandro Curioni, Adam Bertsch, Scott Futral, Steffen J. Schmidt, Nikolaus A. Adams and Petros Koumoutsakos

Modeling and Computing Complex Flows
Governing Equations

In many cases, incompressible isothermal problems with immiscible flows describe the flows of interest. In this case, the equations are

Conservation of Momentum

$$\rho\frac{\partial \boldsymbol{u}}{\partial t}+\rho\nabla\cdot\boldsymbol{u}\boldsymbol{u}=-\nabla p+\boldsymbol{f}+\nabla\cdot\mu\left(\nabla\boldsymbol{u}+\nabla^T\boldsymbol{u}\right)+\int_F\sigma\kappa\mathbf{n}\delta\left(\boldsymbol{x}-\boldsymbol{x}_f\right)da$$

Singular interface term

Conservation of Mass

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

Incompressible flow

Equation of State:

$$\frac{D\rho}{Dt}=0;\quad \frac{D\mu}{Dt}=0$$

Constant properties

Oscillating drop: pressure

The conservation equations can be solved by relatively standard methods. In most cases regular structured fixed grid are used

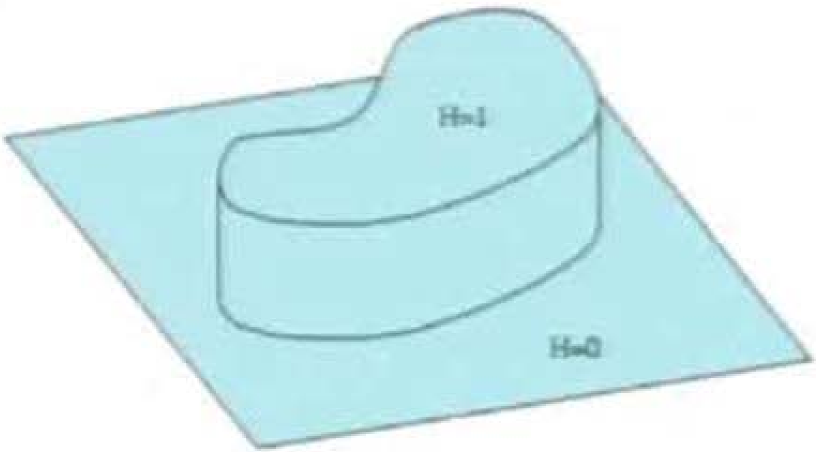
The main challenge is how to advect the marker function

Advecting the Marker Function

The conservation equations for mass, momentum and and energy can be solved by standard techniques. The main challenge is the advection of the marker function

$$H = \begin{cases} 1 & \text{in fluid 1} \\ 0 & \text{Otherwise} \end{cases}$$

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

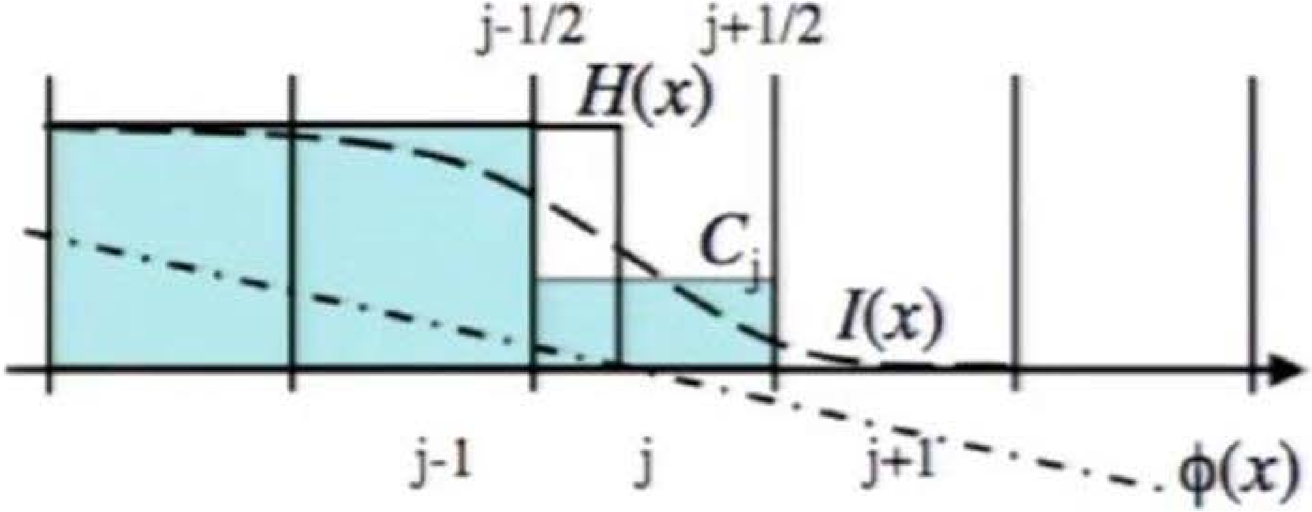


Other challenges include

- computing surface tension,
- handling large density and viscosity differences, and
- topology changes.

Updating H—in spite of its apparent simplicity—is one of the hard problems in CFD!

The sharp marker function H can be approximated in several different ways for computational purposes.



Marker Points | Marker Function

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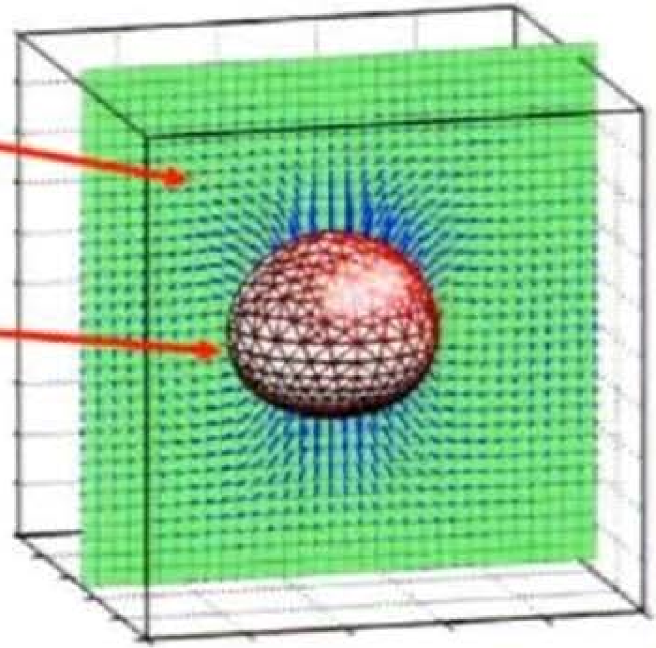
Modeling and Computing Complex Flows
Advecting the Marker Function

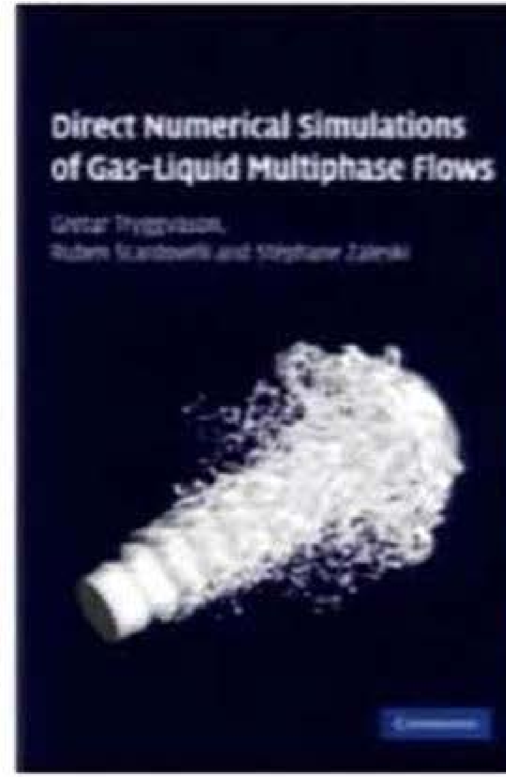
Front Tracking

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

Tracked front to advect the fluid interface and find surface tension

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





$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \nabla \cdot \boldsymbol{u}\boldsymbol{u} = -\nabla p + \boldsymbol{f} + \nabla \cdot \mu\left(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u}\right) + \underbrace{\int_F \sigma \kappa \mathbf{n} \delta\left(\boldsymbol{x} - \boldsymbol{x}_f\right) da}$$

Singular interface term

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

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Bubbles in Vertical Channels

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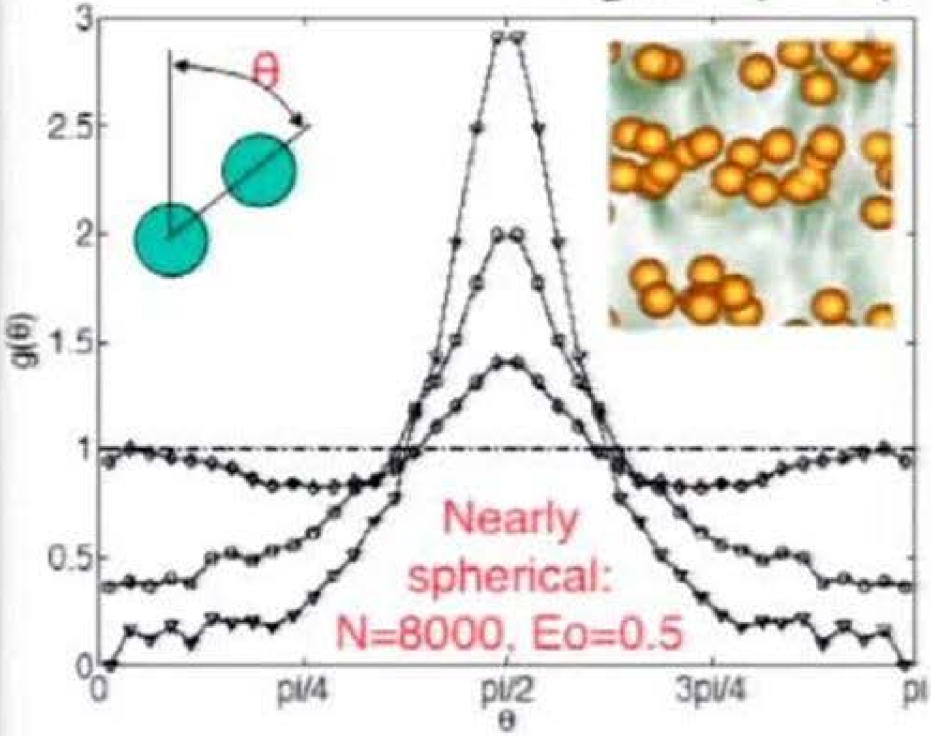
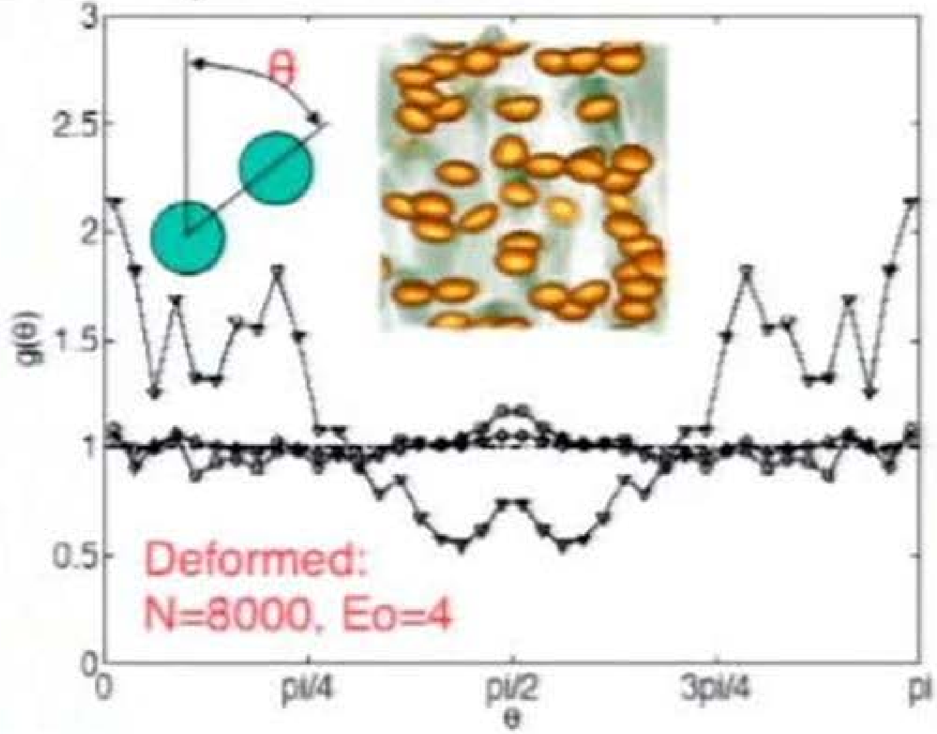
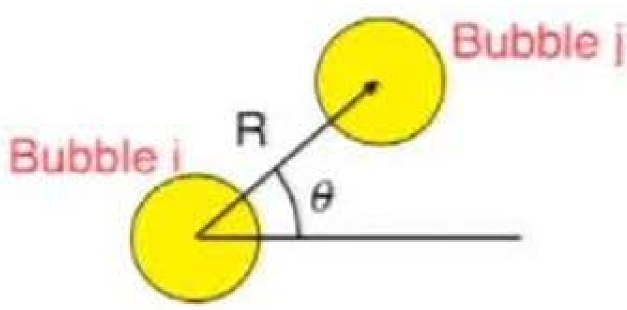
Modeling and Computing Complex Flows

High Reynolds Number Bubbles

Angular pair probability distribution







$$G(\bar{r}) = \frac{V}{N(N-1)} \left\langle \sum_{i} \sum_{j \neq i} \delta(\bar{r} - \bar{r}_{ij}) \right\rangle$$

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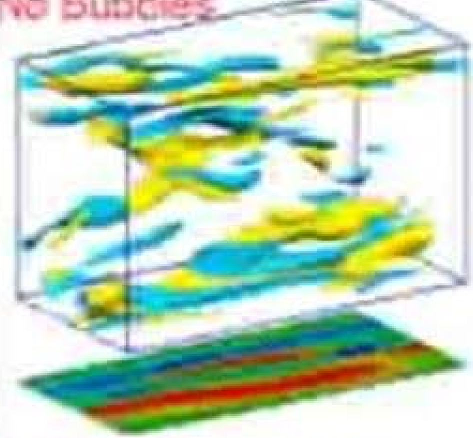
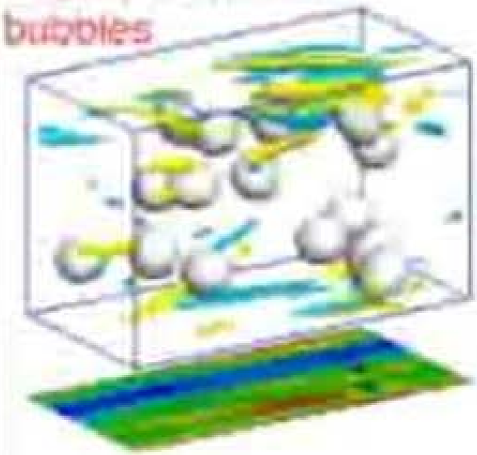
Modeling and Computing Complex Flows

Bubble Induced Drag Reduction

No Bubbles

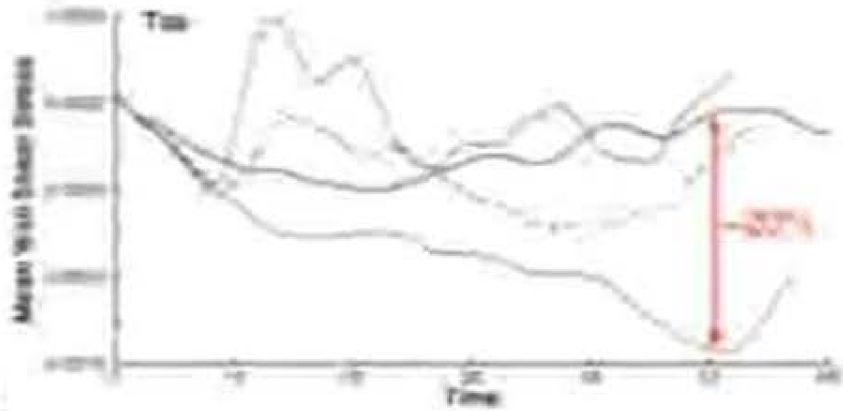


Slightly deformable bubbles



Experiment:
$d^+=120$; $We=0.686$
Simulations:
$d^+=54$; $We=0.203$-0.405

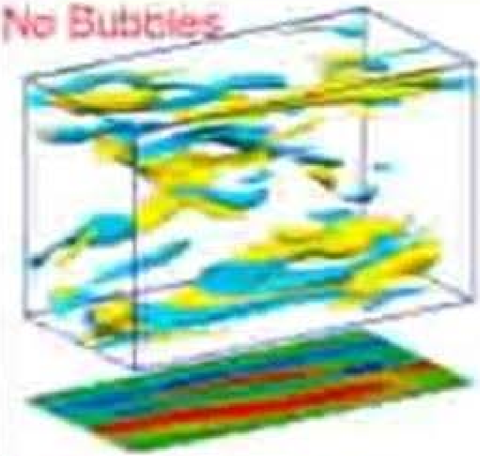
DNS of bubbles injected near the wall in a a turbulent channel flow show that the deformability of the bubbles plays a major role. Bubbles with a deformability comparable to what is seen experimentally (S. L. Ceccio, taken in the LCC) can lead to drag significant drag reduction, but only for a short time. The simulations clarified the turbulent modification and showed that less deformable bubbles can lead to an increase in the wall drag.



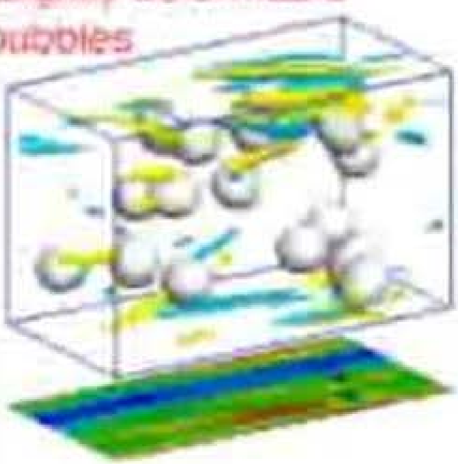
Modeling and Computing Complex Flows

Bubble Induced Drag Reduction

No Bubbles



Slightly deformable bubbles



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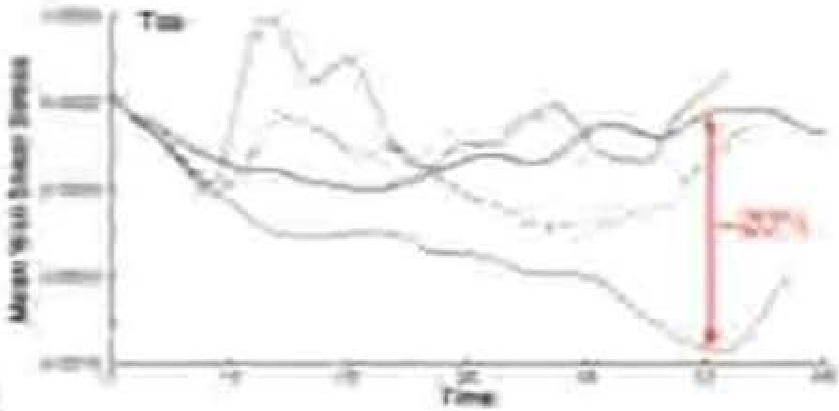

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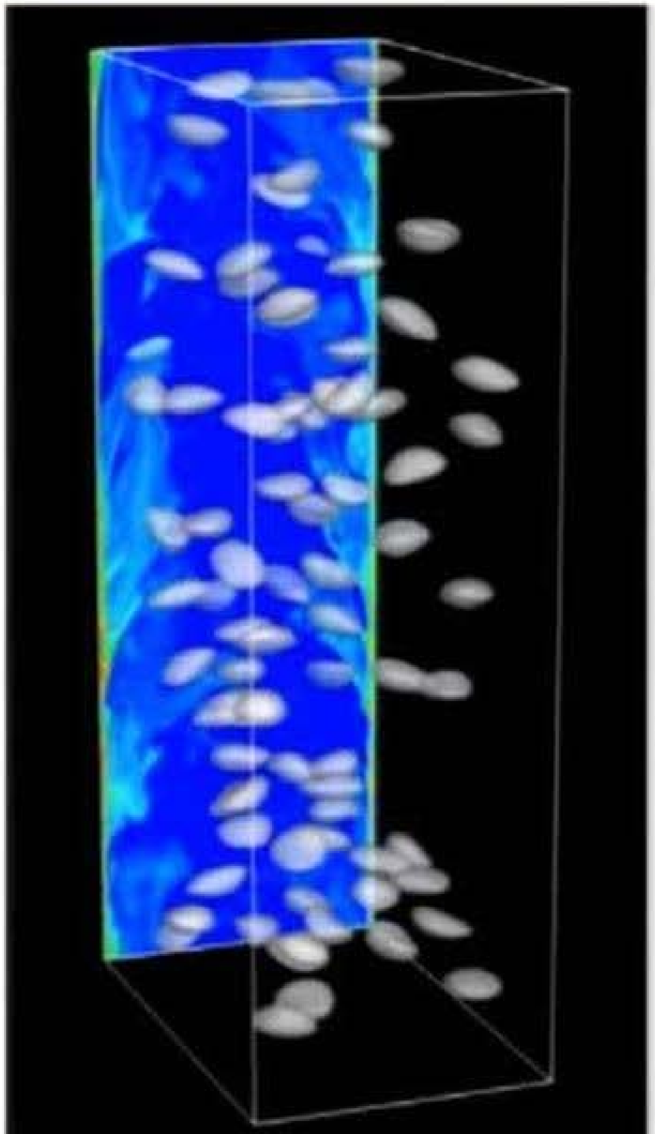
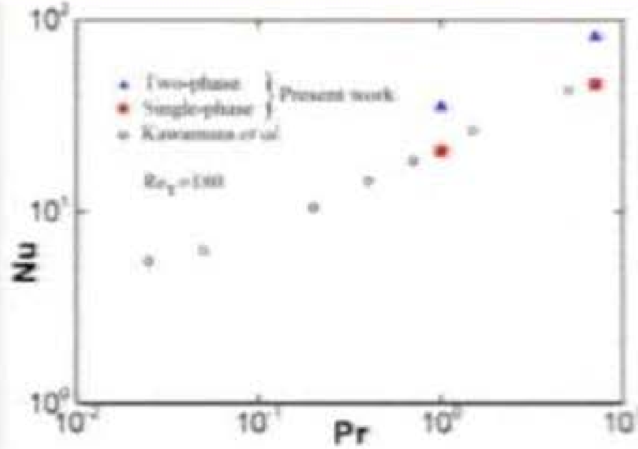
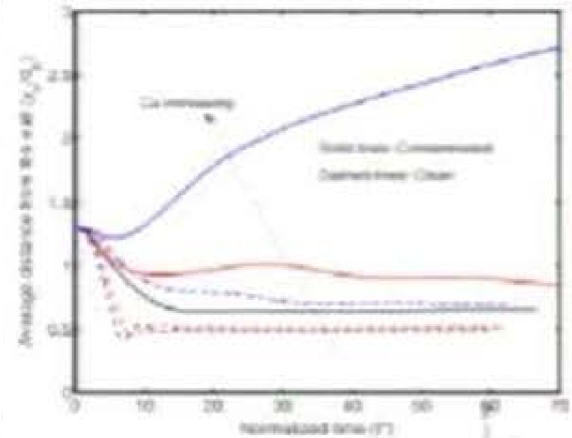
Modeling and Computing Complex Flows Heat/Mass Transfer & Surfactants

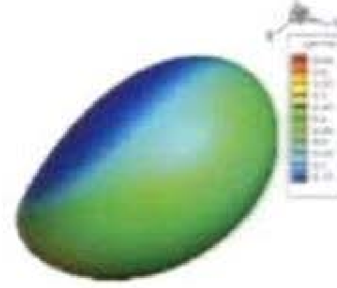


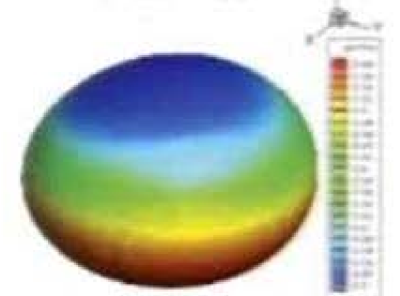


M. Muradoglu and G. Tryggvason. Simulations of Soluble Surfactants in 3D Multiphase Flow. *Journal of Computational Physics*. 274 (2014), 737-757.

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







Mining DNS Data for Closure Relations

With
Ming Ma & Jiacai Lu

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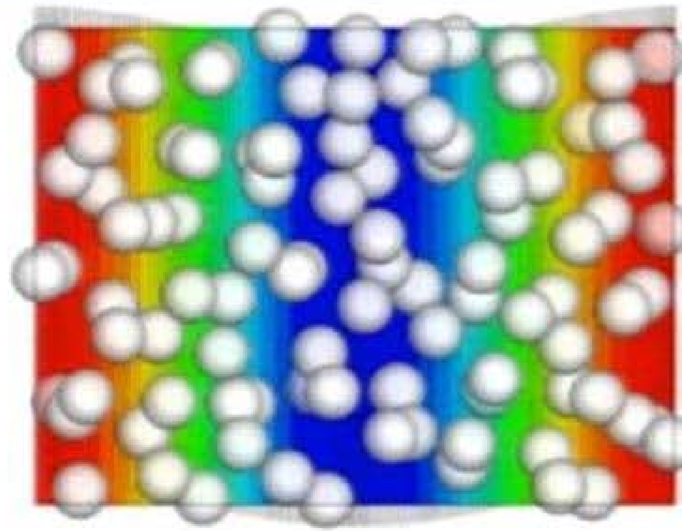
Modeling and Computing Complex Flows
Finding Closure Terms by Data Mining

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



Void fraction and phase averaged velocity

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

Horizontal flux of bubbles

$$\frac{\partial \alpha_i}{\partial t} + \frac{\partial F_i}{\partial x} = 0 \qquad F_i = \frac{1}{\alpha A_{zy}} \int \chi_i u_i da$$

Obviously:

$$F_b = \alpha_b < u_b >$$

Averaged vertical momentum of the liquid:

$$\frac{\partial}{\partial t} \alpha_l < v_l > + \frac{\partial}{\partial x} \alpha_l < v_l >< u_l >=$$

$$-\frac{1}{\rho_l}\frac{dp}{dy} - \frac{1}{\rho_l}\alpha_l \rho_l g + -\frac{1}{\rho_l}\frac{\partial}{\partial x}\left(\alpha_l \mu_l \frac{\partial v_l}{\partial x}\right) - \frac{\partial}{\partial x}\left(\alpha_l < uv >_l\right)$$

Plus surface tension term

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Modeling and Computing Complex Flows
Finding Closure Terms by Data Mining

"Closure" variables needed for models of the average flow

Resolved average variables

Quantities summarizing the state of the unresolved flow

F_g	$<u'v'>$	α_g	$\frac{\partial \alpha_g}{\partial x}$	$\frac{\partial <v>_l}{\partial x}$	d_w	k_t	ε_t	A	

DNS data provides any quantity that we care to record or collect at any point in the flow, or as averages over any time or spatial region that we select. "Mining" the data allows us to correlate any variable with any others and quantify the accuracy of the fit.

We have used several data mining techniques to find the fit, including regression and neural networks

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

$$f(\mathbf{x}) = b_0 + \sum_{i=1}^{n} b_i h_i(\mathbf{x}); \quad h_i(\mathbf{x}) = s\left(a_{0i} + \sum_{i=1}^{n} x_i a_{i,j}\right); \quad s(u) = \frac{2}{1+e^{-2u}} - 1$$

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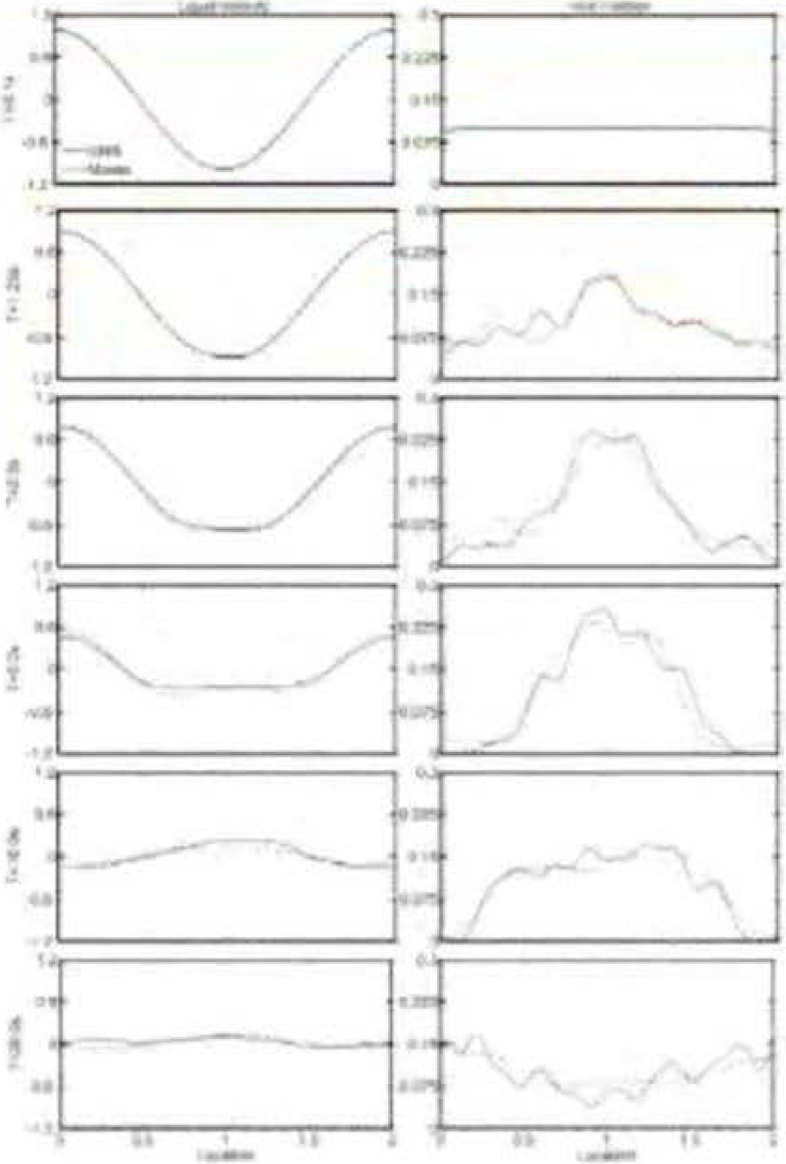
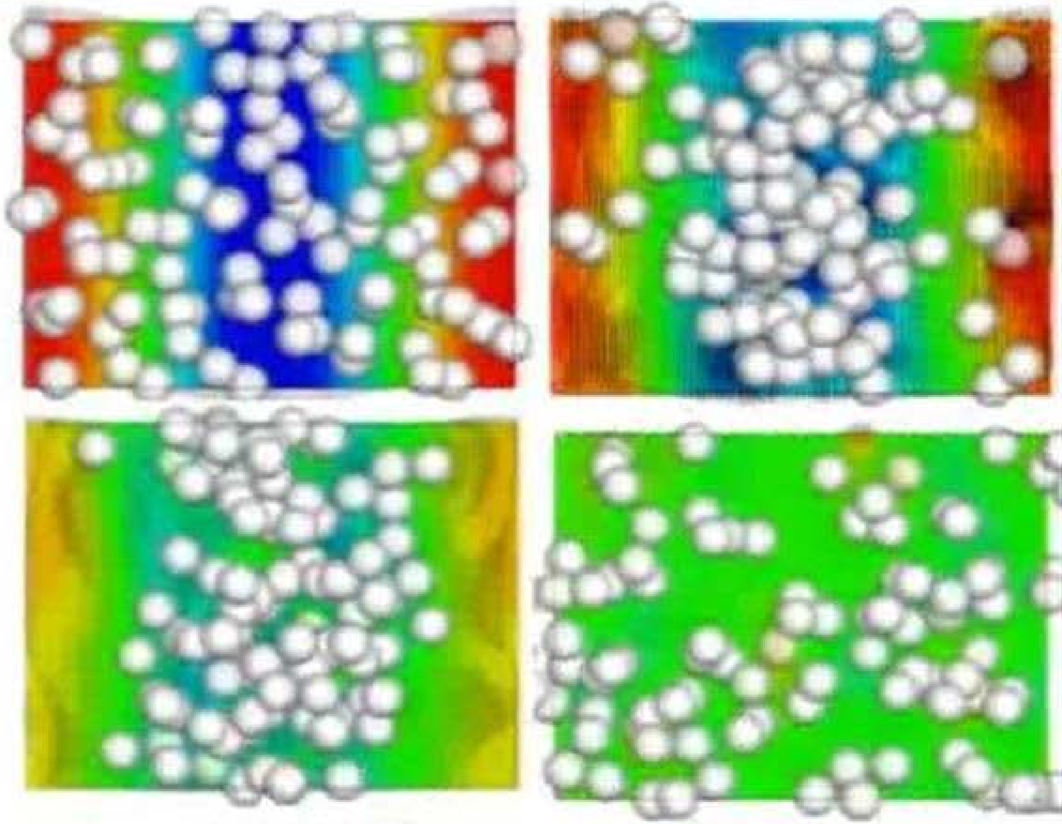
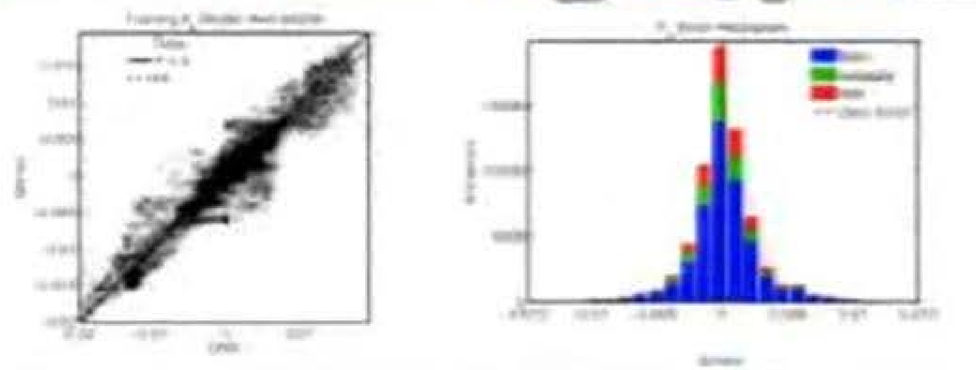
Modeling and Computing Complex Flows
Finding Closure Terms by Data Mining







Capturing small-scale processes using Embedded Analytical Descriptions

With
Bahman Aboulhasanzadeh and Siju Thomas

Modeling and Computing Complex Flows
Embedded Analytical Descriptions

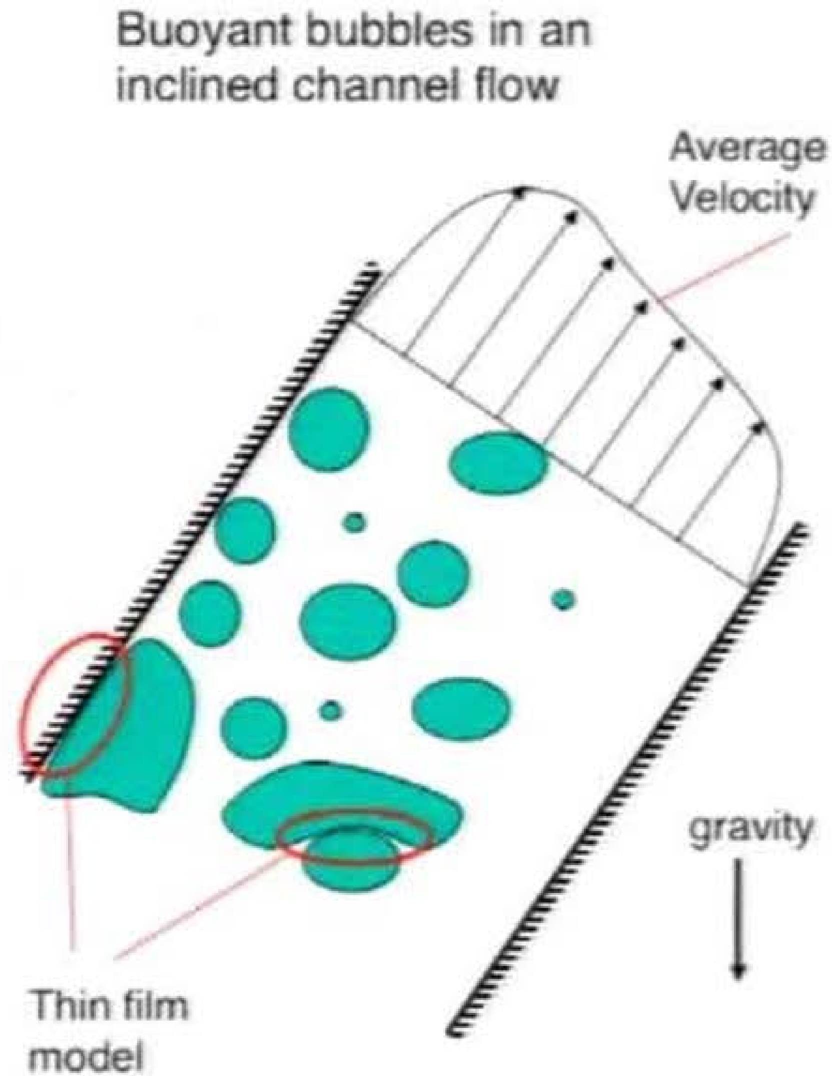
Capturing isolated small-scale motion in simulations where the focus is on the larger scales can be done in many ways, such as be various grid refinement techniques (unstructured grids, AMR for Cartesian grids, wavelets, etc.) or reduced order models

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



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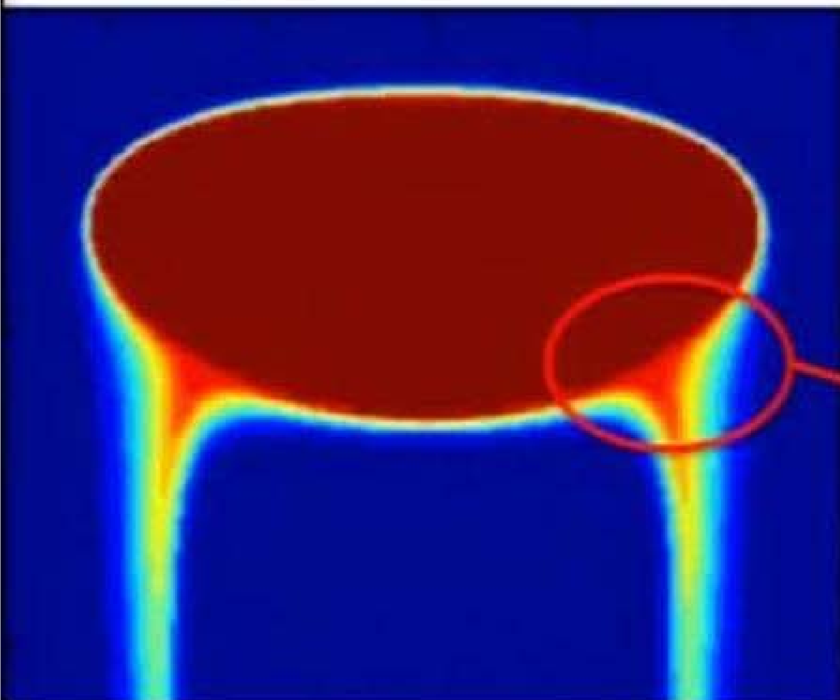
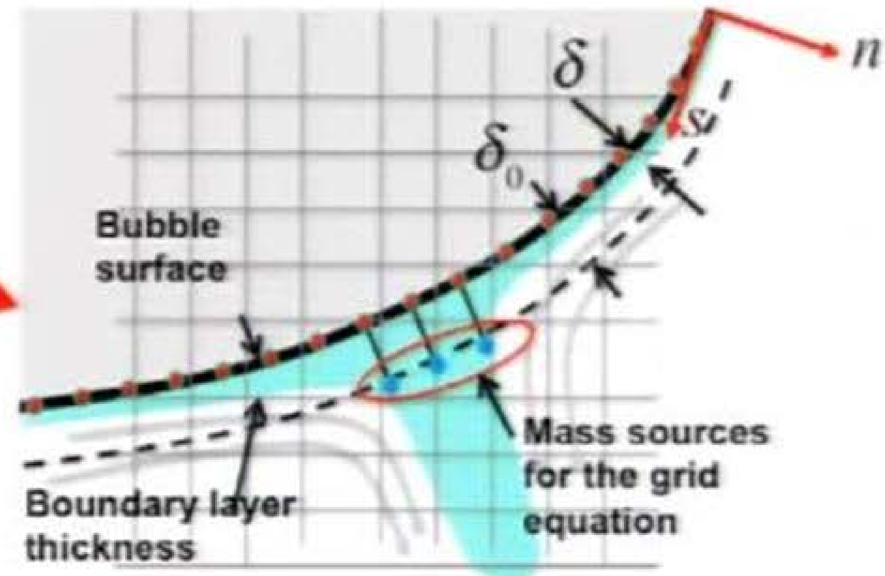
Modeling and Computing Complex Flows
Mass Transfer in Gas-Liquid Systems



Capturing the mass boundary layer



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

$$M_0 = \int_0^\infty f \, dn$$

$$M_1 = \int_0^\infty n f \, dn$$

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

$$\frac{dM_1}{dt} = -\sigma\left(2M_1 - \delta_o^2 f_\delta\right) + D\left(f_o - f_\delta\right)$$

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

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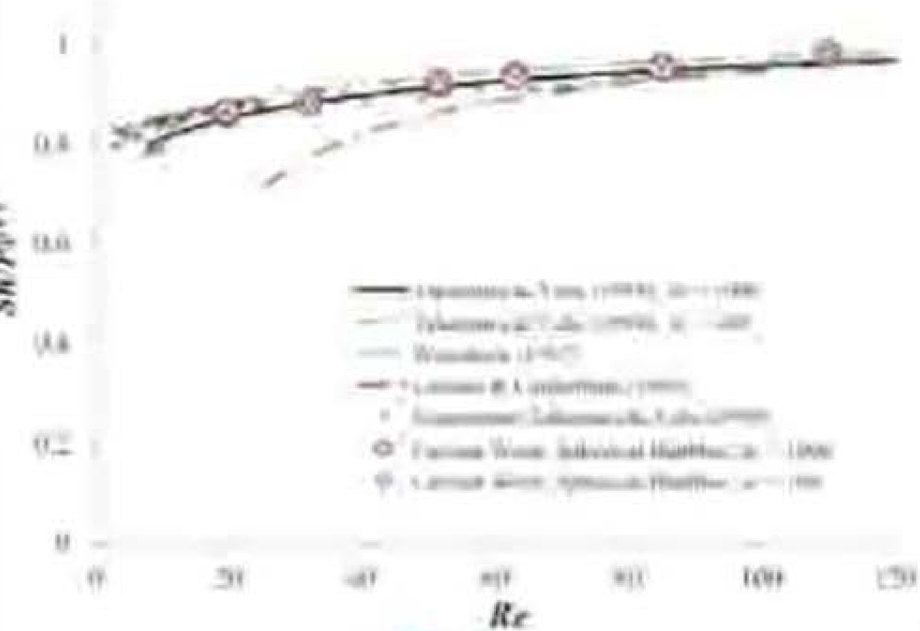
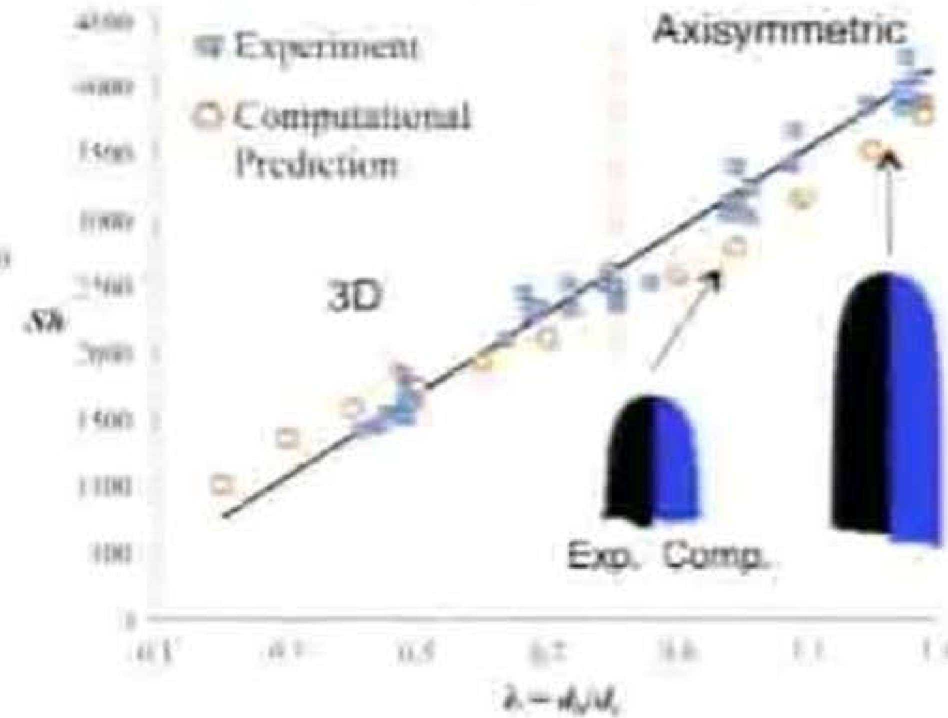
Modeling and Computing Complex Flows
Mass Transfer in Gas-Liquid Systems



The mass transfer versus Re, for a single bubble in a large domain, along with the predictions of experimental correlations

Comparison with experimental results from A. Tomiyama:
Eo = 24.7
Mo = $10^{-7.78}$ and
Sc= 8260



B. Abouhasanzadeh, S. Hosoda, A. Tomiyama, G. Tryggvason. *Chemical Engineering Science*, 101 (2013), 165-174.

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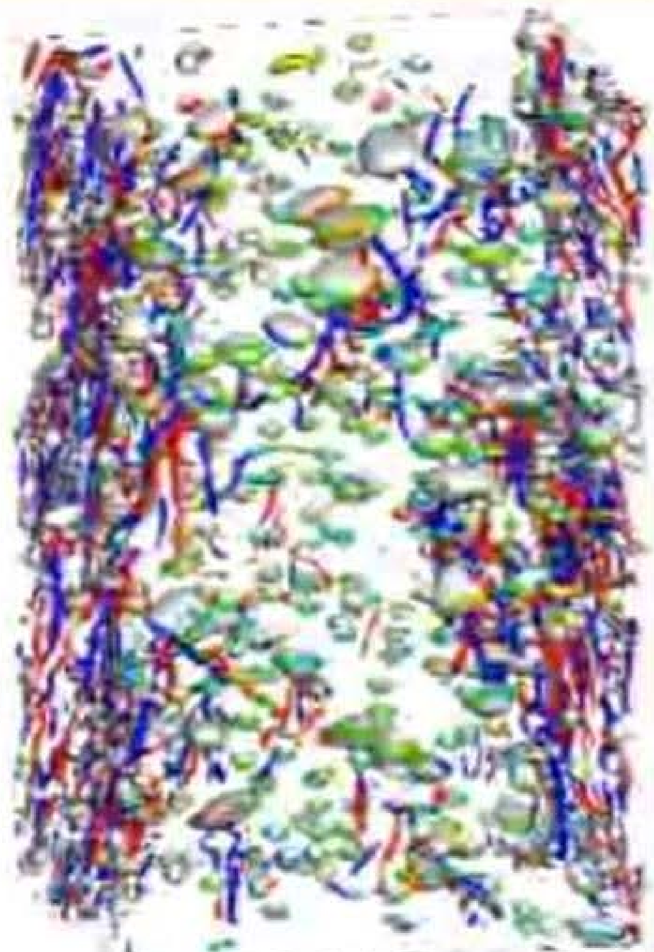
Modeling and Computing Complex Flows Now What?

DNS of several flows have been developed to the point that they should be able to help produce new models for "industrial" simulations. The availability of the data is putting new demands on the modeling of complex multiphase flows.

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. Need "almost" DNS

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!



500 bubbles of different sizes in channel flow with $Re^{+}=500$
$1024 \times 768 \times 512$ grid points
2048 processors on the Titan