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Multiscale Considerations in DNS Studies of Multiphase Flows

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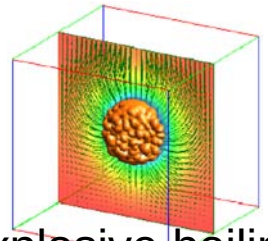
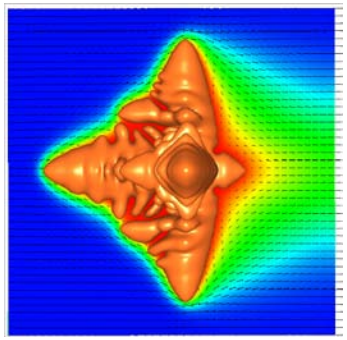
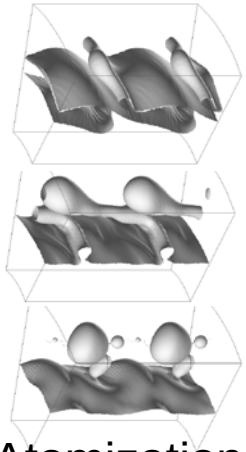
DNS of Multiphase Flows
Examples



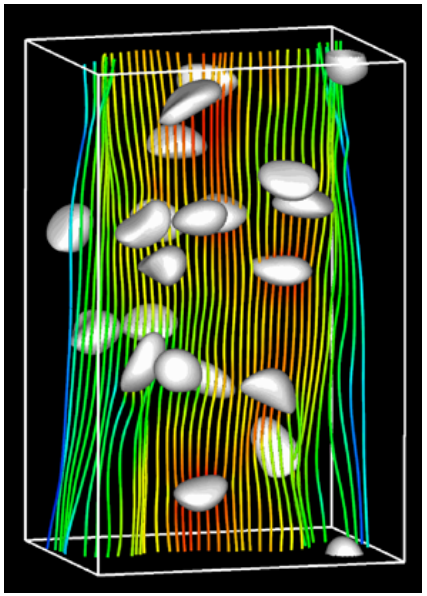
Explosive boiling



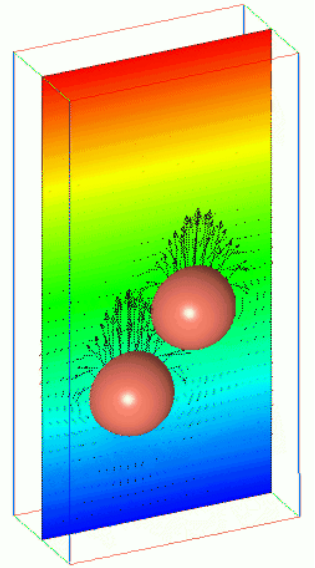
Solidification



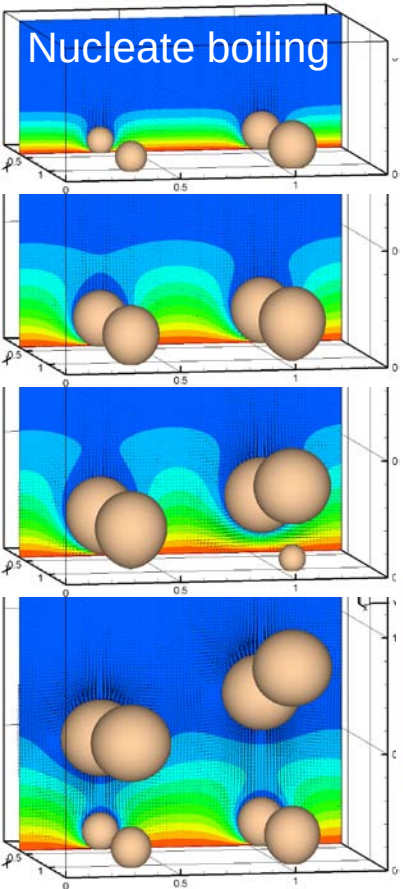
Atomization

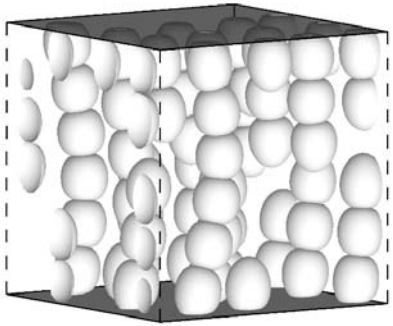


Bubbles in channels

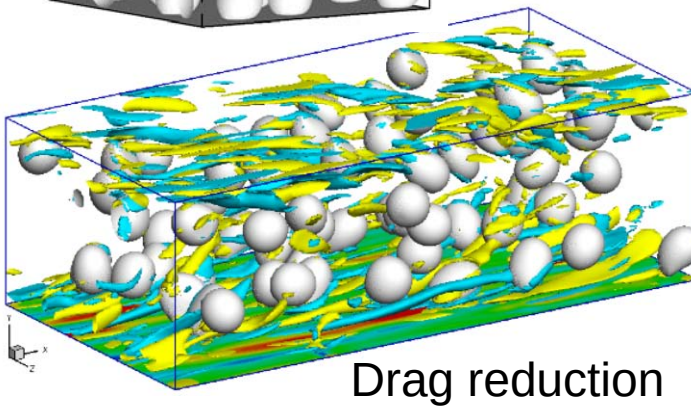


Thermo-capillary migration

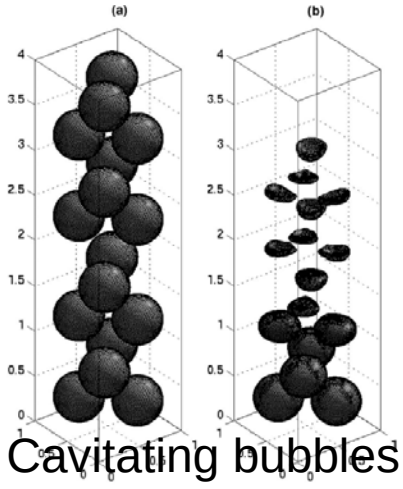




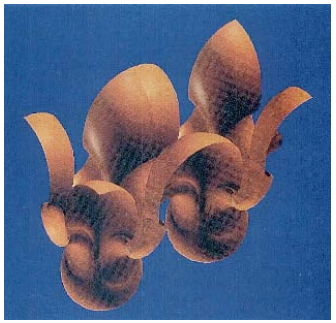
EHD of drops



Drag reduction



Cavitating bubbles



Rayleigh-Taylor Instability

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DNS of Multiphase Flows
Multiscale Issues

Contents:

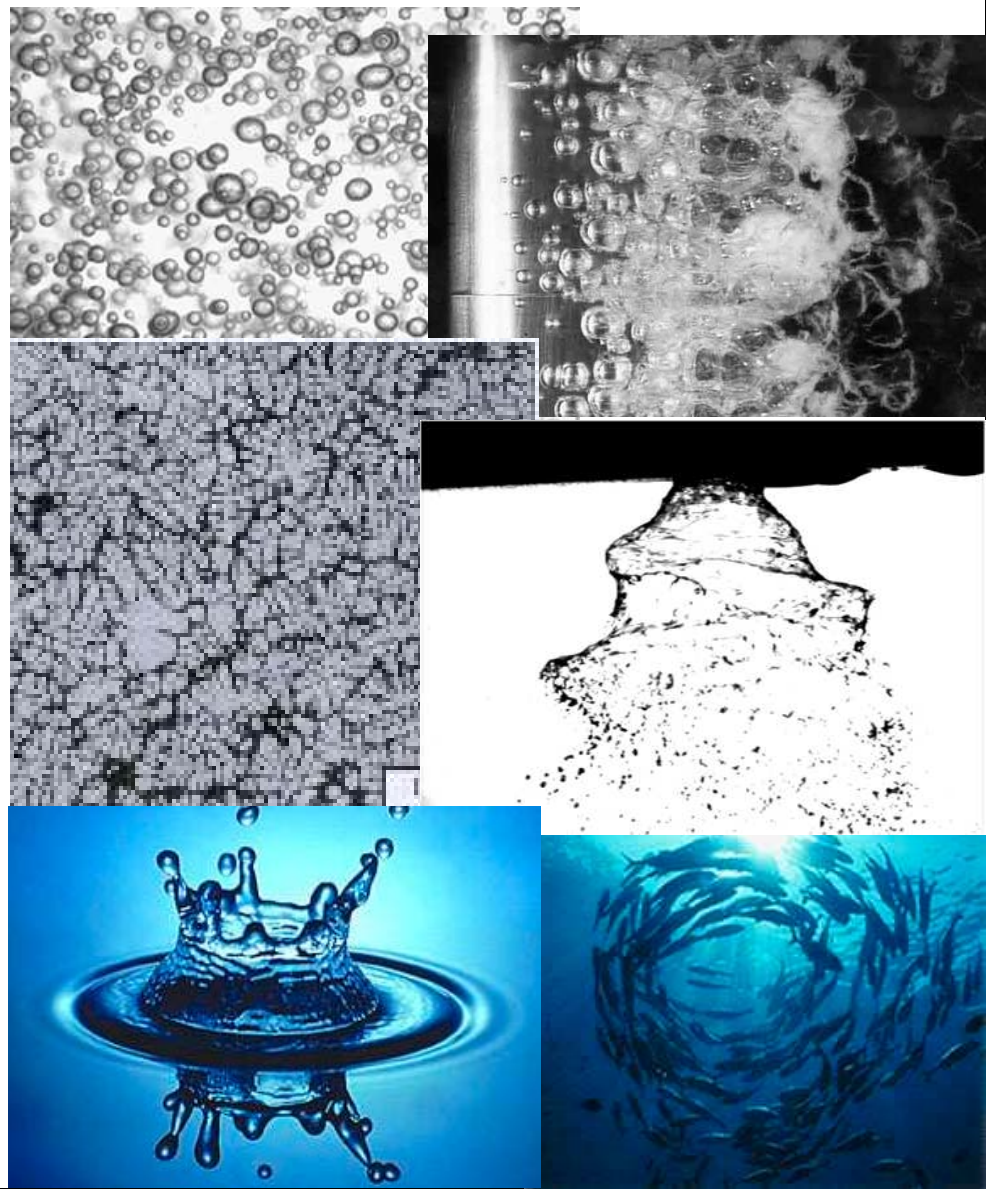
I: Bubbles in turbulent channels flows

II: Multiscale descriptions of small scale phenomena

III: Boiling

Direct Numerical Simulations:

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

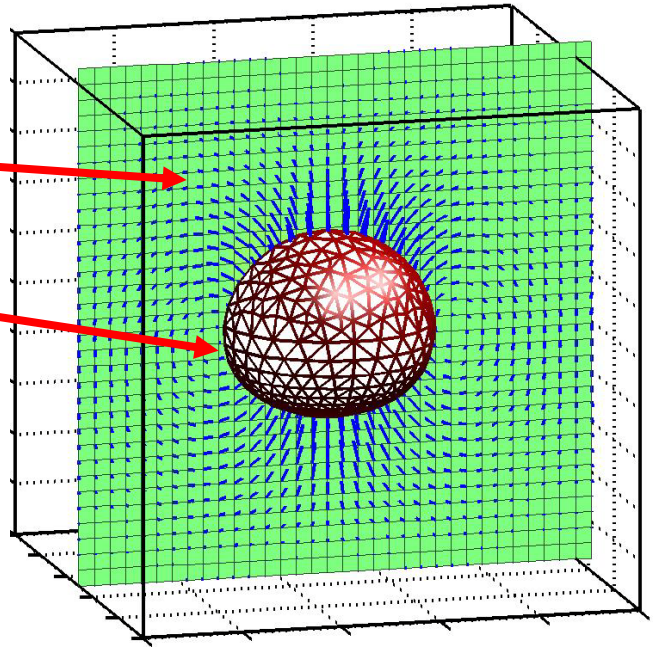


Front Tracking

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



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

Singular interface term

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

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DNS of Multiphase Flows
Multiscale Issues

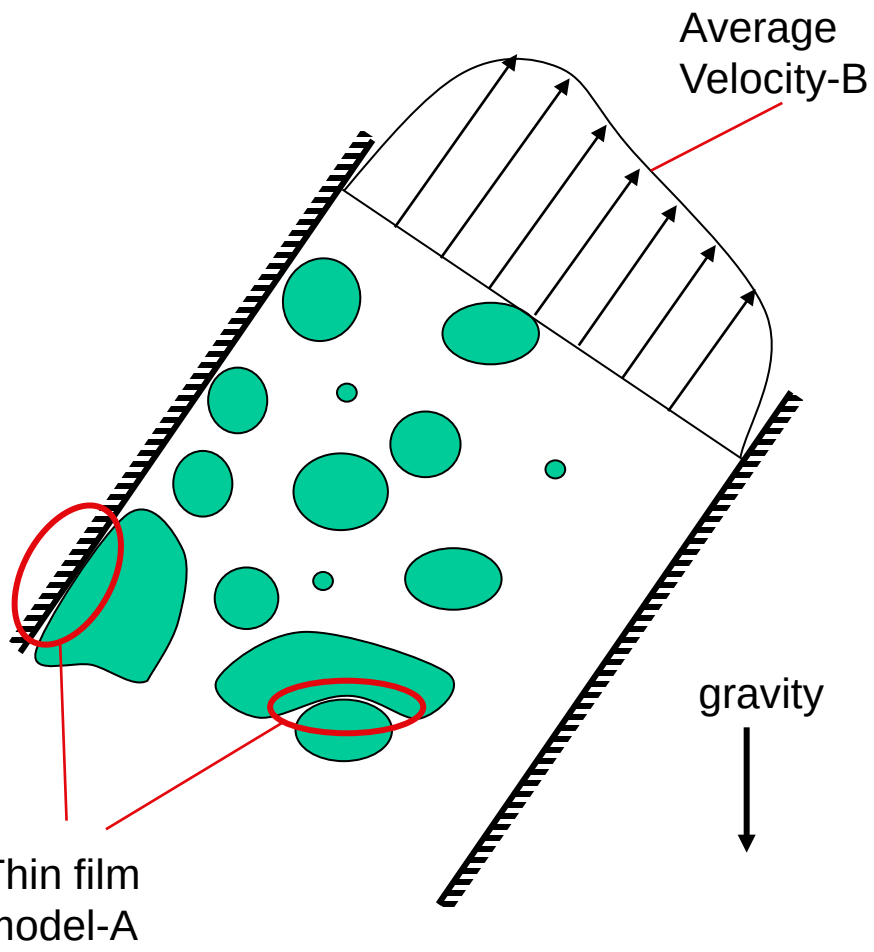
Some communities have defined two types of multi-scale problems.

Type A Problems: Dealing with Isolated Defects

Type B Problems: Constitutive Modeling Based on the Microscopic Models

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

Buoyant bubbles in an inclined channel flow



Bubbly Flows

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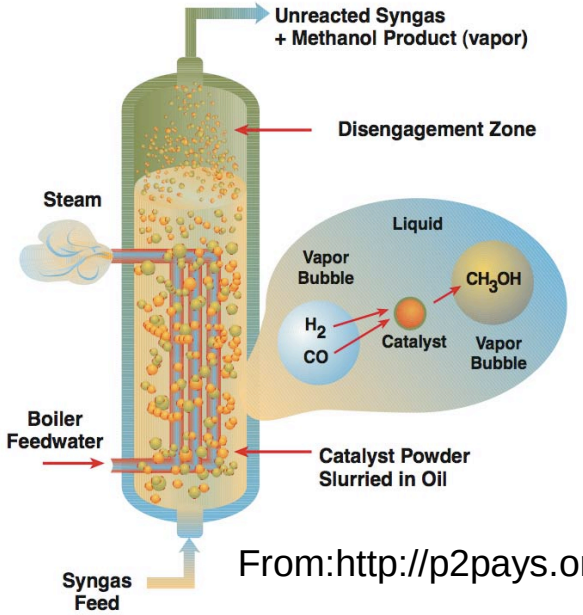
DNS of Multiphase Flows
Why Multiphase Flows are Important!



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

Liquid Phase Methanol (LPMEOH™) Process

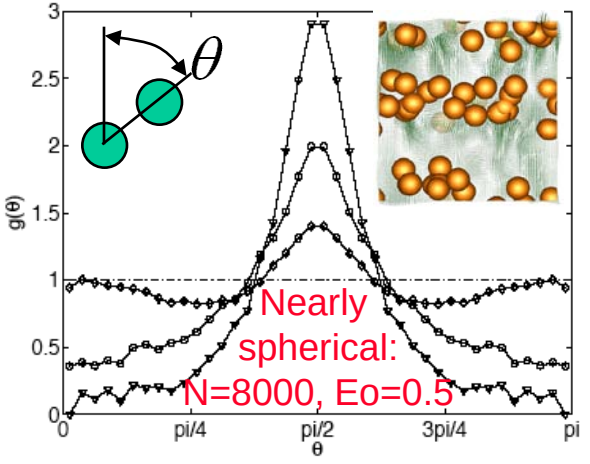
Examples of Applications of Bubble Columns

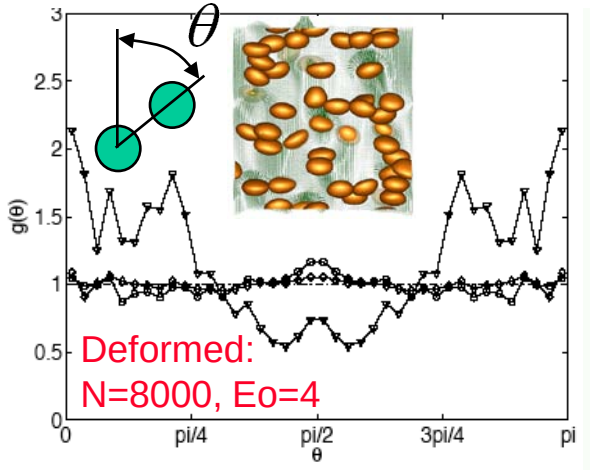
Process	Methods and/or Reactants
Acetone	Oxidation of cumene
Acetic acid	Oxidation of acetaldehyde
	Oxidation of sec-butanol
	Carbonylation of methanol
Acetic anhydride	Oxidation of acetaldehyde
Acetaldehyde	Partial oxidation of ethylene
Acetophenone	Oxidation of ethylbenzene
Barium chloride	Barium sulfide 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

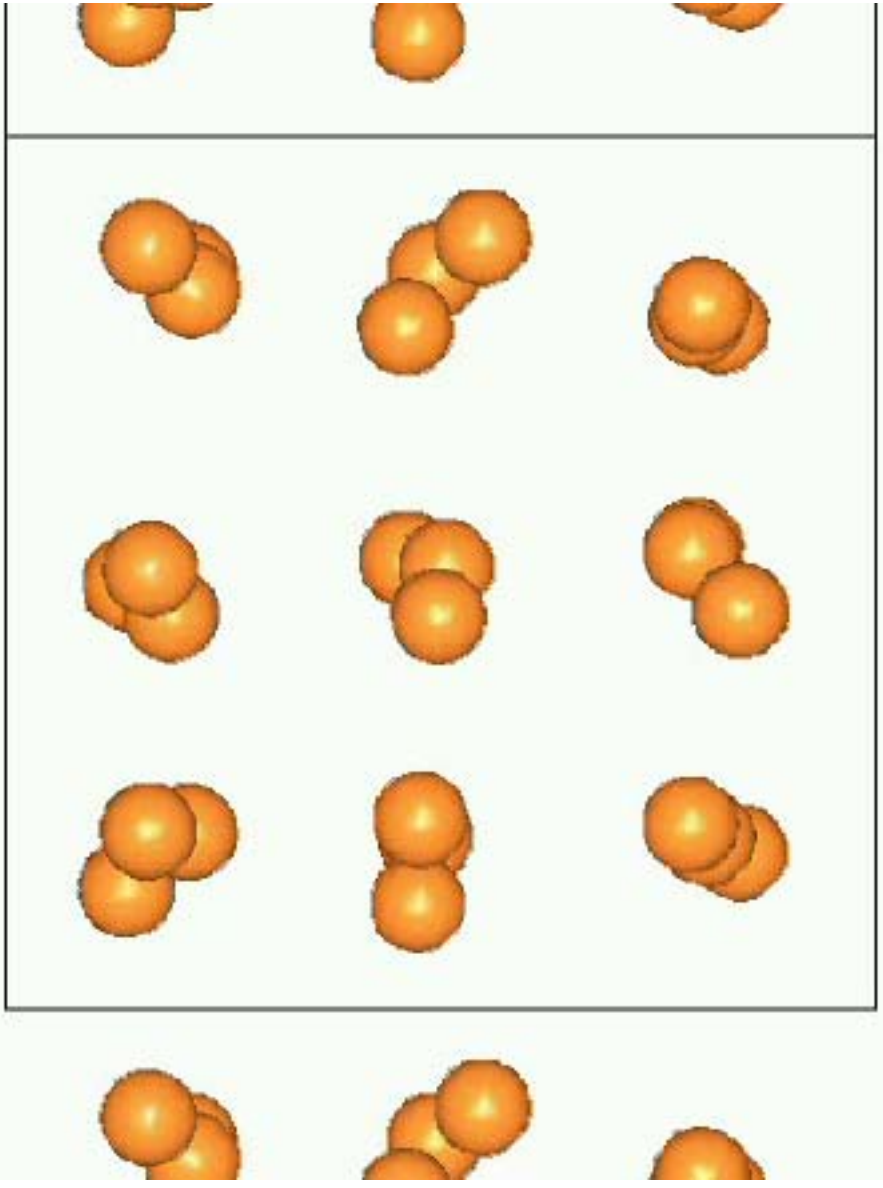
DNS of Multiphase Flows
Applications of DNS to bubbly flows

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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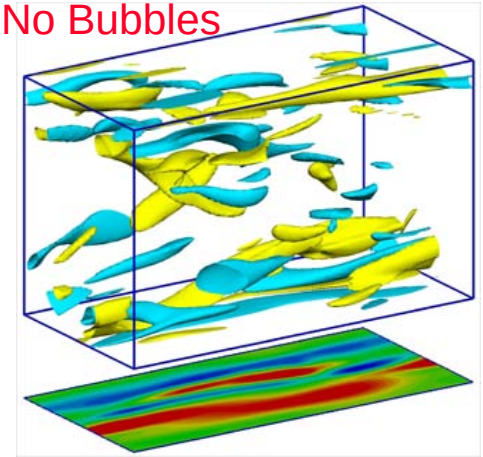
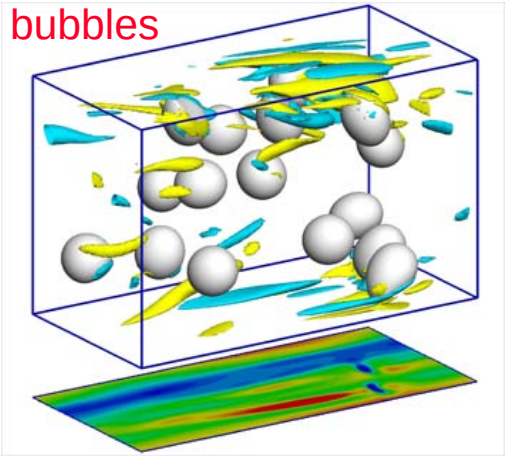
DNS of Multiphase Flows
Bubble Induced Drag Reduction

No Bubbles

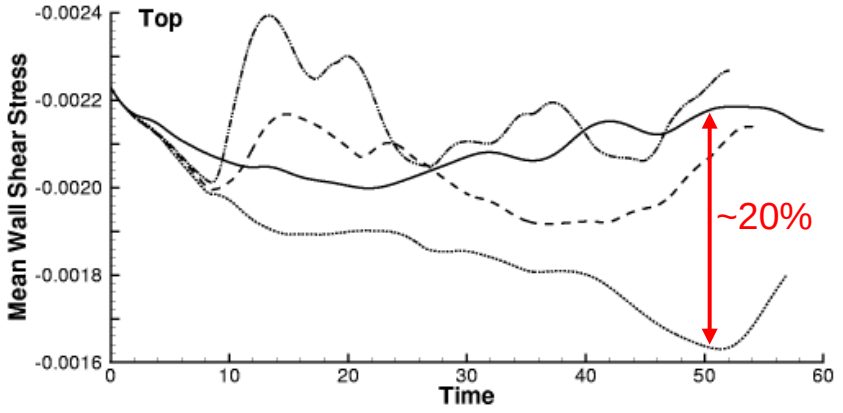


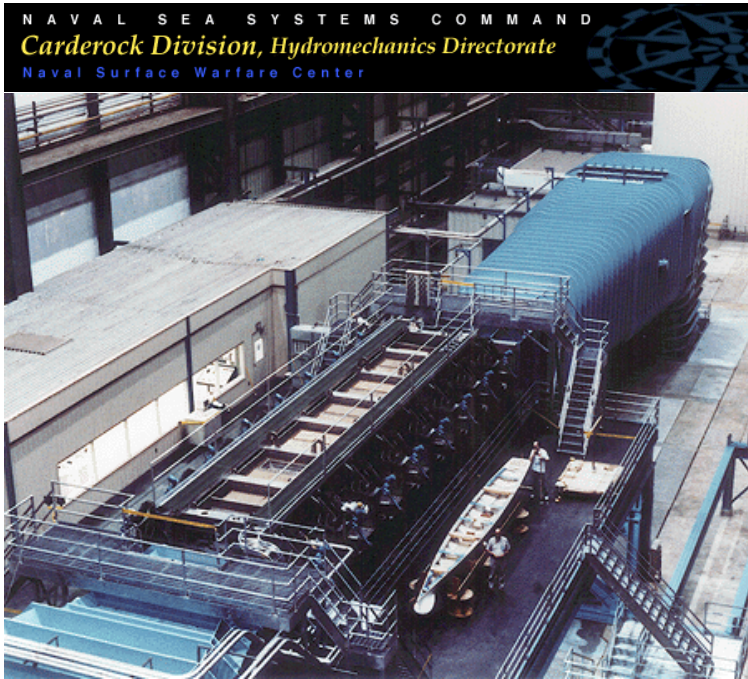
Slightly deformable bubbles



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.





Bubbly Turbulent Flows in Vertical Channels

With
Jiacai Lu & Sadegh Dabiri

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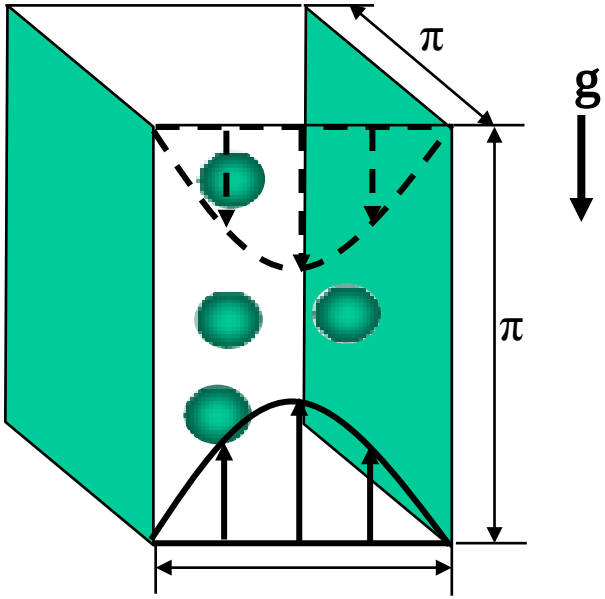
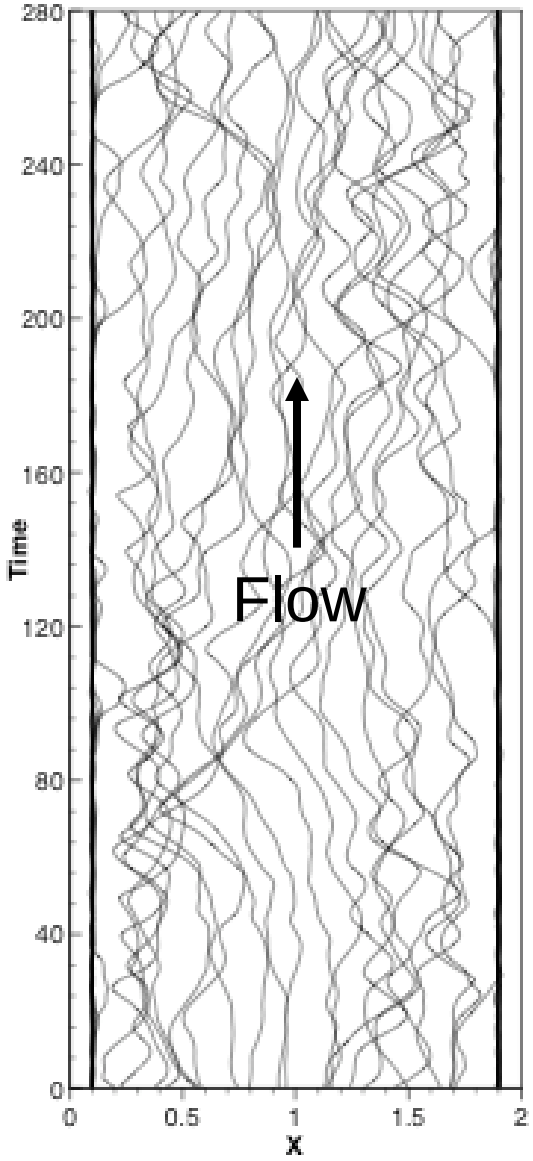
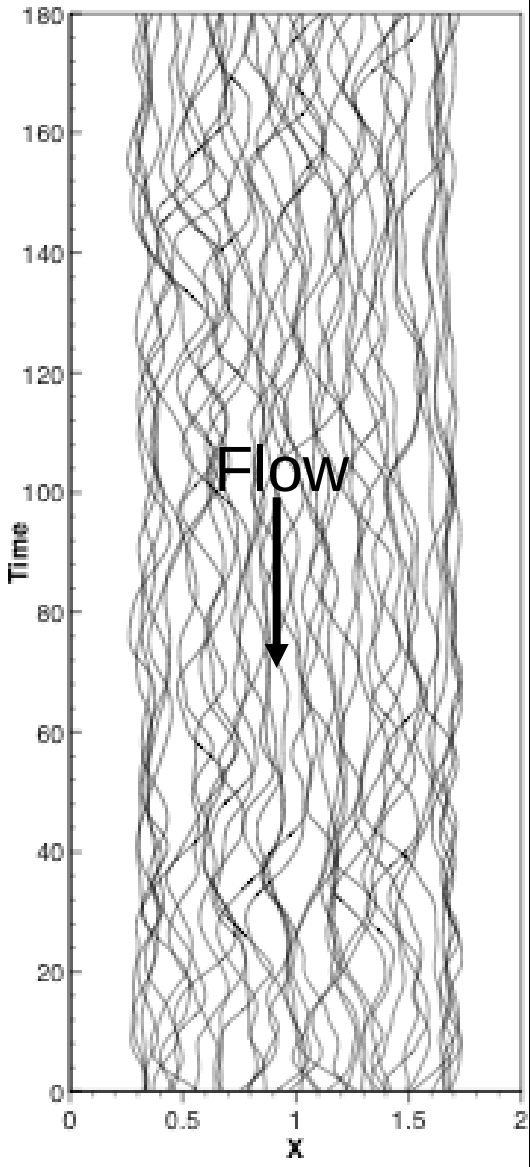
DNS of Multiphase Flows

The path of bubbles. The cross-channel coordinate versus time for the upflow (left) and the downflow (right) at approximately steady state.







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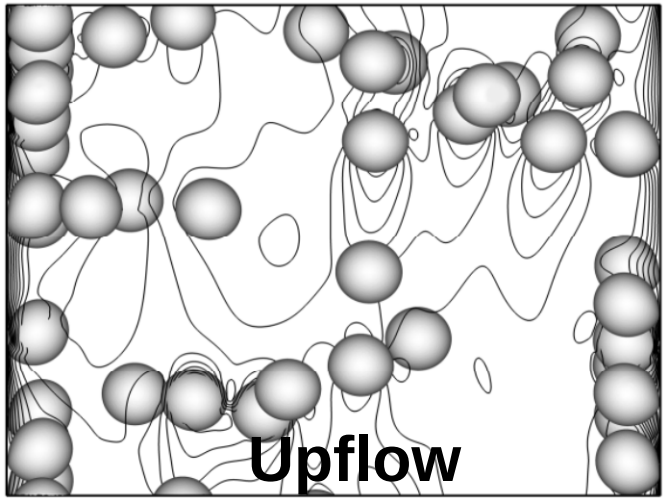
DNS of Multiphase Flows
Spherical Bubbles in Vertical Channels

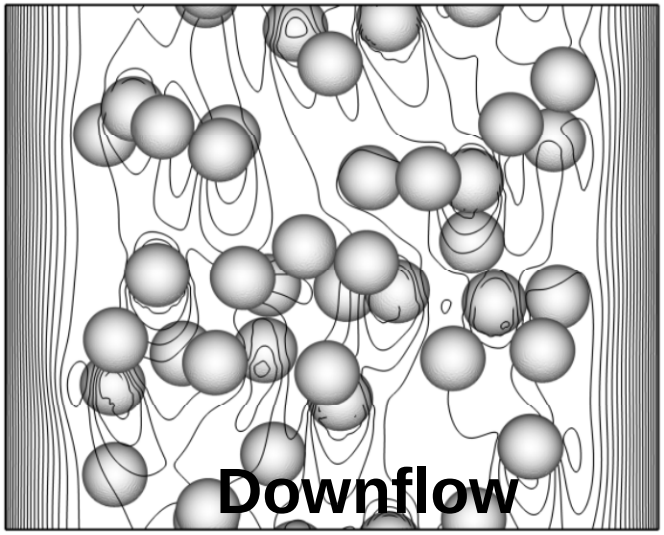
For nearly spherical bubbles in laminar and weakly turbulent flows the flow consists of a homogeneous core where the mixture is in hydrostatic equilibrium and a wall-layer.

For upflow the wall-layer is bubble rich and the total flow rate depends strongly on the deformability of the bubbles.

For downflow the wall-layer has no bubbles and the velocity profile is easily found for both laminar and turbulent flow. For downflow the exact size of the bubbles plays only a minor role, as long as they remain nearly spherical.

For upflow deformable bubbles stay away from walls, completely changing the flow structure





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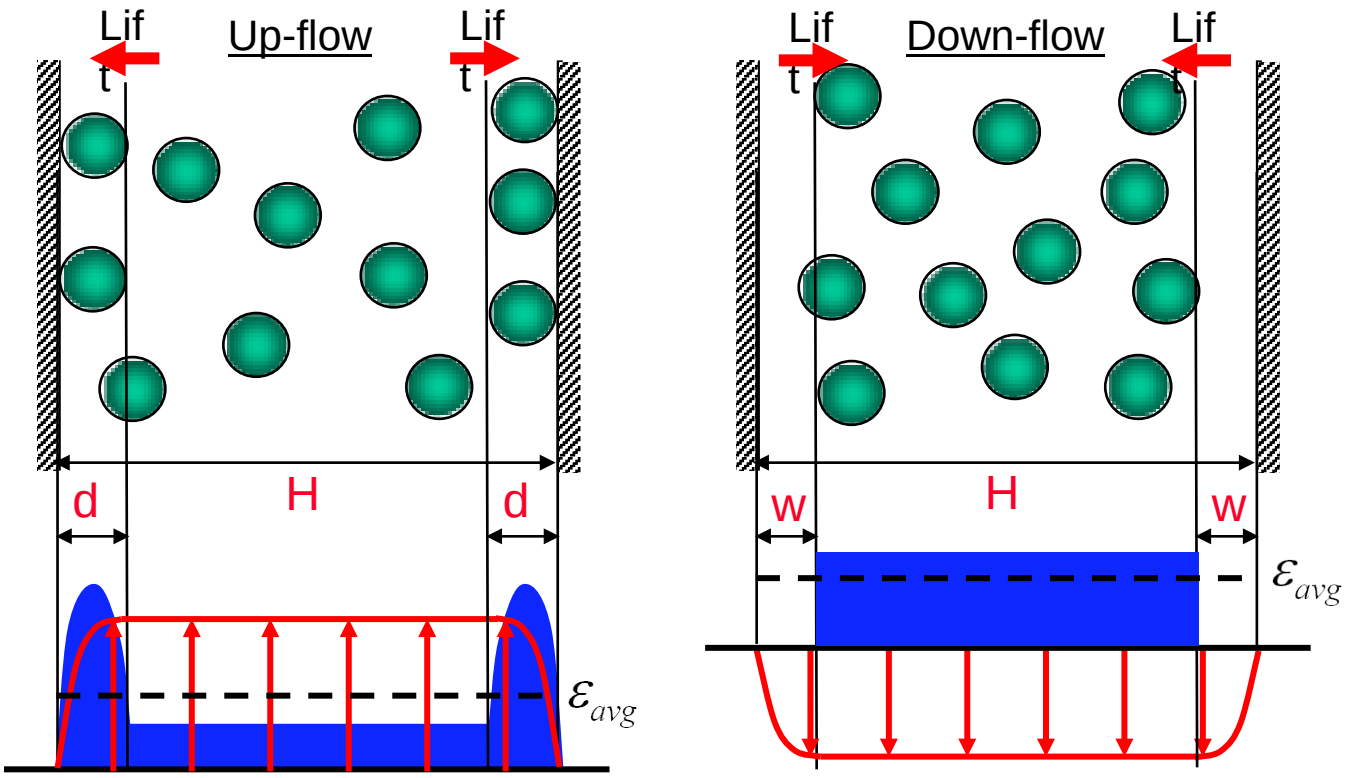
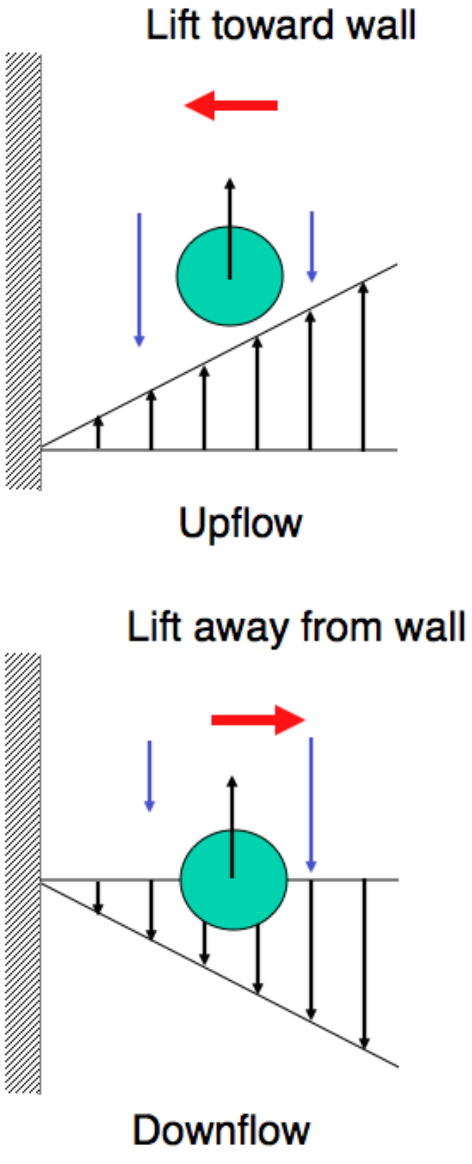
DNS of Multiphase Flows
Bubbles in Vertical Channels

Simple two-fluid model for the flow of nearly spherical bubbles in a vertical channel. Lift drives bubbles toward wall in upflow but away from the wall in downflow.





$$\beta = \frac{dp}{dy} + \rho_{avg} g \qquad \beta = -\Delta\rho g\left(\varepsilon_{avg} - \varepsilon_c\right) \quad \Rightarrow \quad \varepsilon_c = \varepsilon_{avg} + \frac{\beta}{\Delta\rho g}$$

DNS of Multiphase Flows
Bubbles in Laminar Channel Flows

Force balance at steady state:

$$\frac{d\tau}{dx} - \beta - \Delta\rho g\left(\varepsilon_{avg} - \varepsilon(x)\right) = 0 \qquad \beta = \frac{dp}{dy} + \rho_{avg} g$$

In the center of the channel there is no shear, therefore

$$\beta = -\Delta\rho g\left(\varepsilon_{avg} - \varepsilon_c\right) \quad \Rightarrow \quad \varepsilon_c = \varepsilon_{avg} + \frac{\beta}{\Delta\rho g}$$

upflow: $\beta < 0 \quad \Rightarrow \quad \varepsilon_c < \varepsilon_{avg}$

downflow: $\beta > 0 \quad \Rightarrow \quad \varepsilon_c > \varepsilon_{avg}$

Downflow: The wall layer is void of bubbles. To find its thickness, use the fact that the total bubble volume is conserved:

$$\varepsilon_{avg} H = \varepsilon_c\left(H - 2w\right) \Rightarrow w = \frac{H}{2}\left(\varepsilon_c - \varepsilon_{avg}\right) \Rightarrow w = \frac{-\beta H}{2\Delta\rho g}$$

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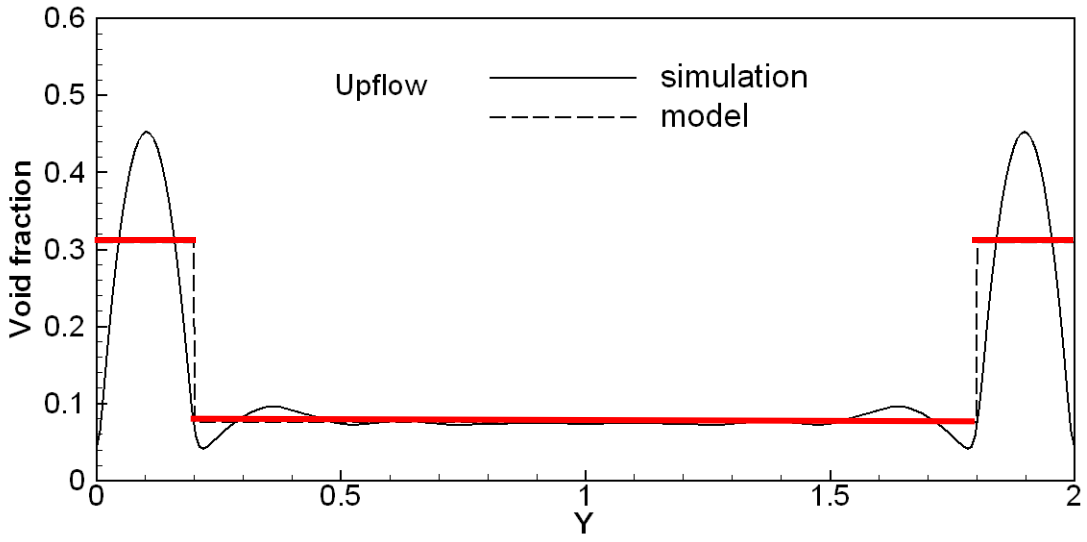
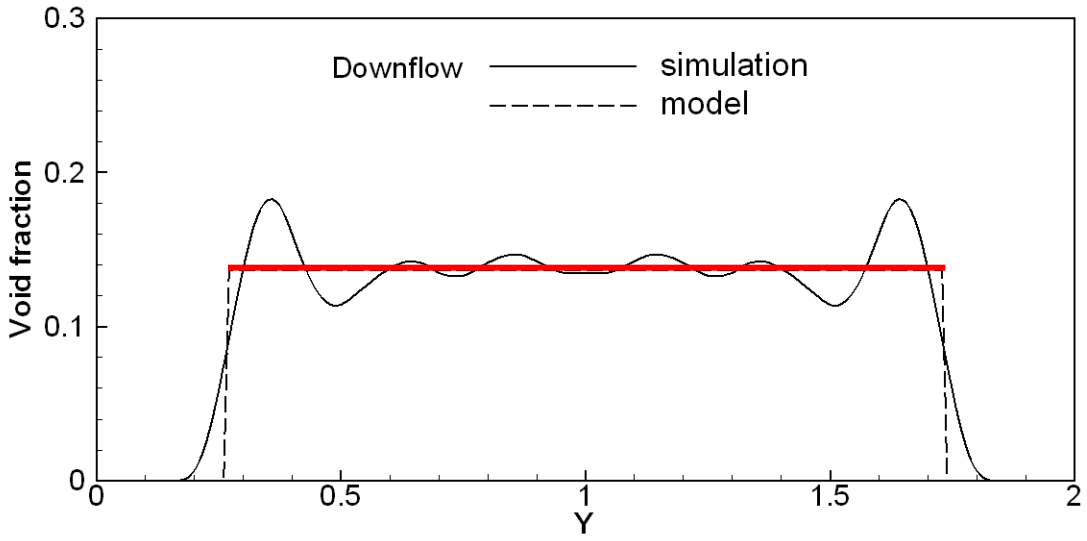
DNS of Multiphase Flows
Bubbles in Laminar Channel Flows

The average void fraction profile across the channel for the upflow (top) and the downflow (bottom). The solid lines denote the results from the simulations and the dashed lines are the analytical results.





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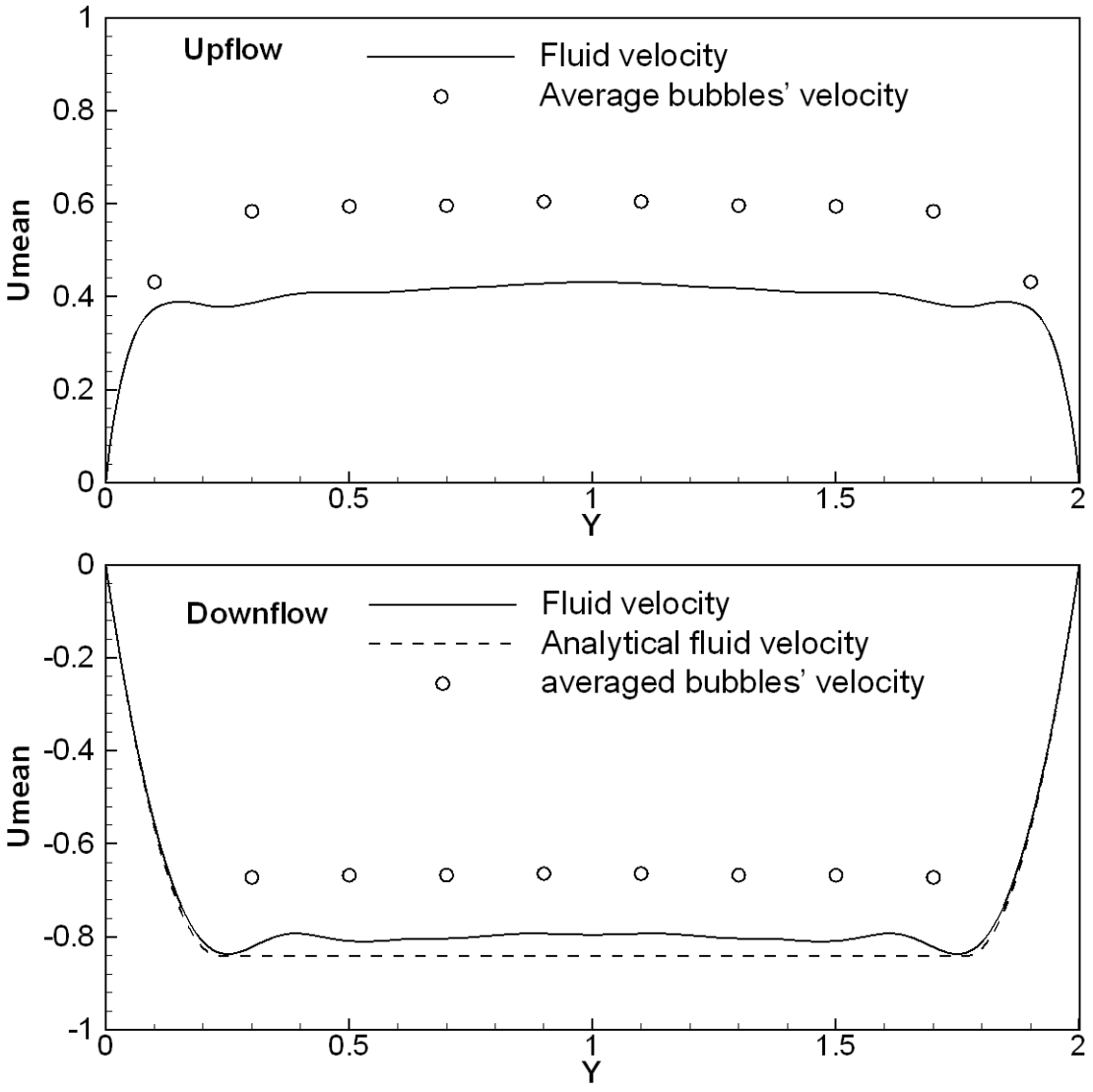
DNS of Multiphase Flows
Bubbles in Laminar Channel Flows

The average vertical liquid velocity profile across the channel for the upflow (top) and the downflow (bottom). The solid lines are the simulated results, averaged over 80 time units. The dashed line is the analytical results for the downflow. The circles represent the average bubble velocities in 10 equal sized bins across the channel.



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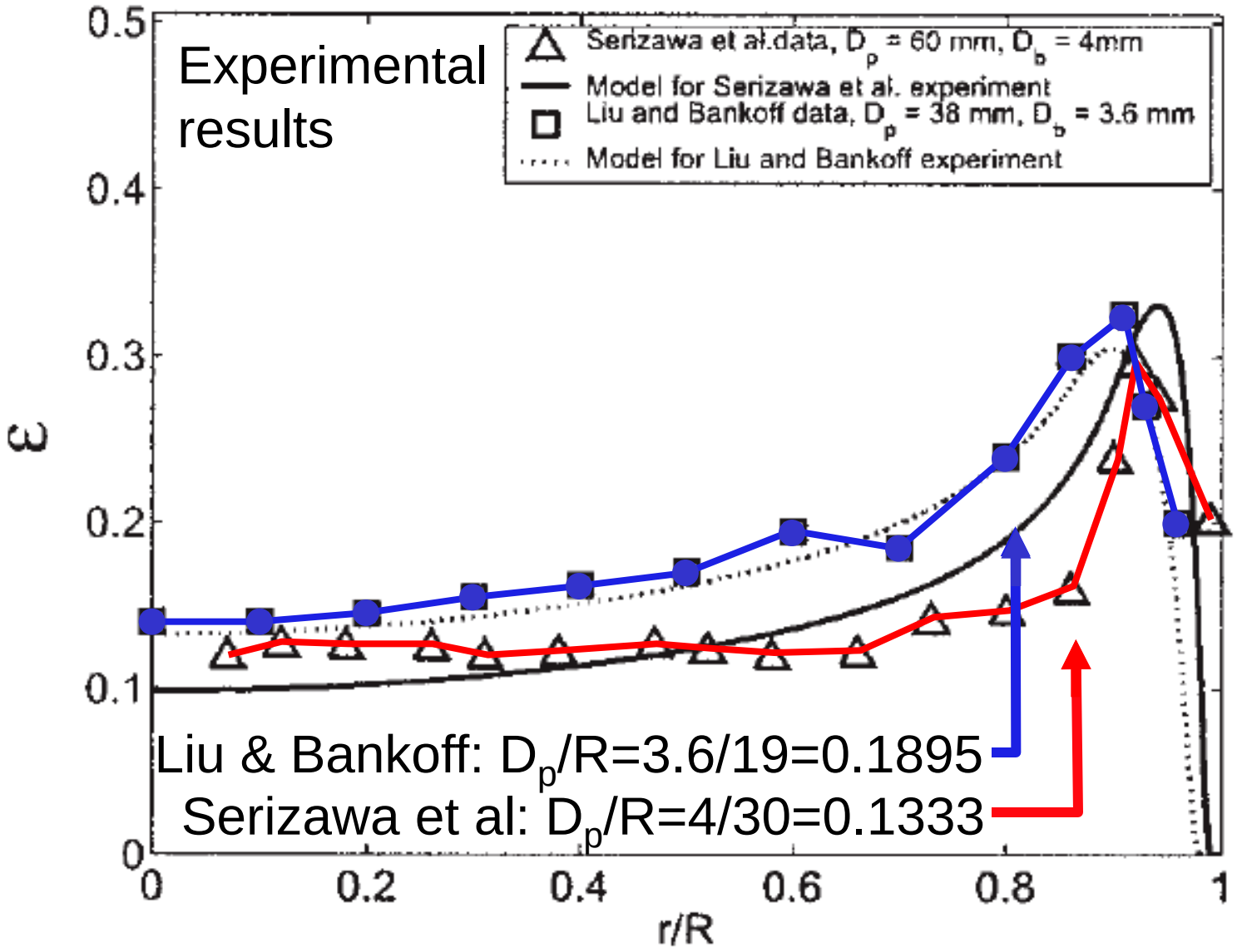
DNS of Multiphase Flows
Bubbles in Laminar Channel Flows



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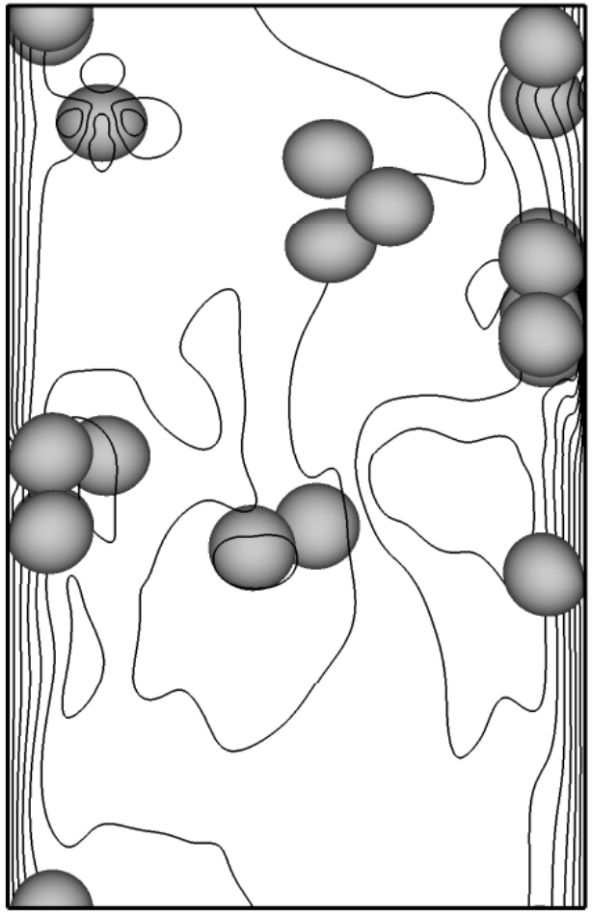
DNS of Multiphase Flows

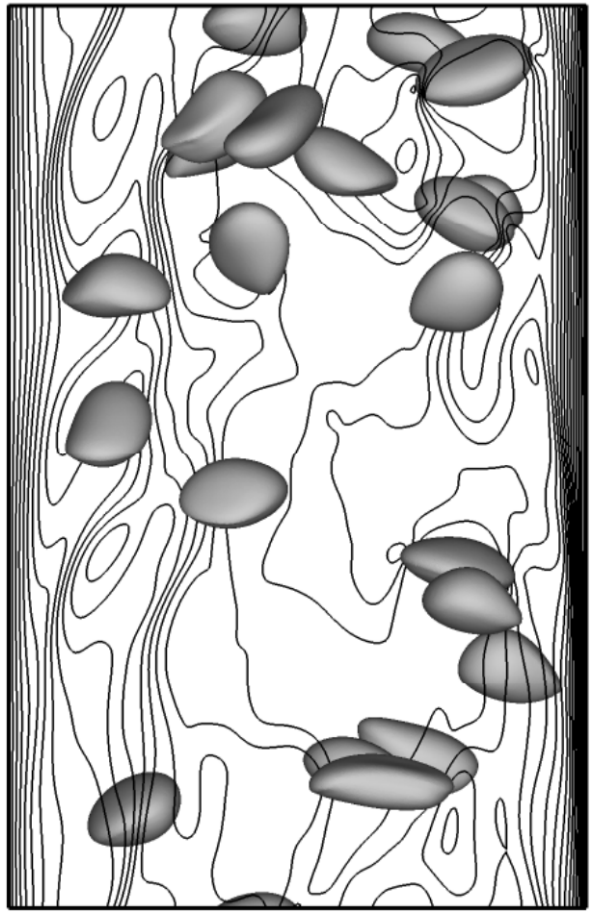
Turbulent Upflow: Effect of Deformability

The bubbles and iso-contours of the instantaneous vertical velocity in a plane through the middle of the channel for the upflow of nearly spherical (left) and much more deformable (right) bubbles at one time when the flow is approximately at steady state.



$M=1.54 \times 10^{-10}$

Eo=0.45



$M=1.54 \times 10^{-7}$

Eo=4.5

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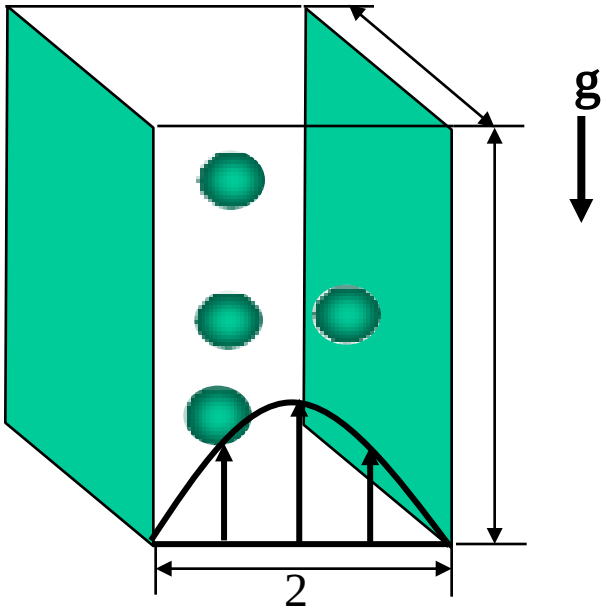
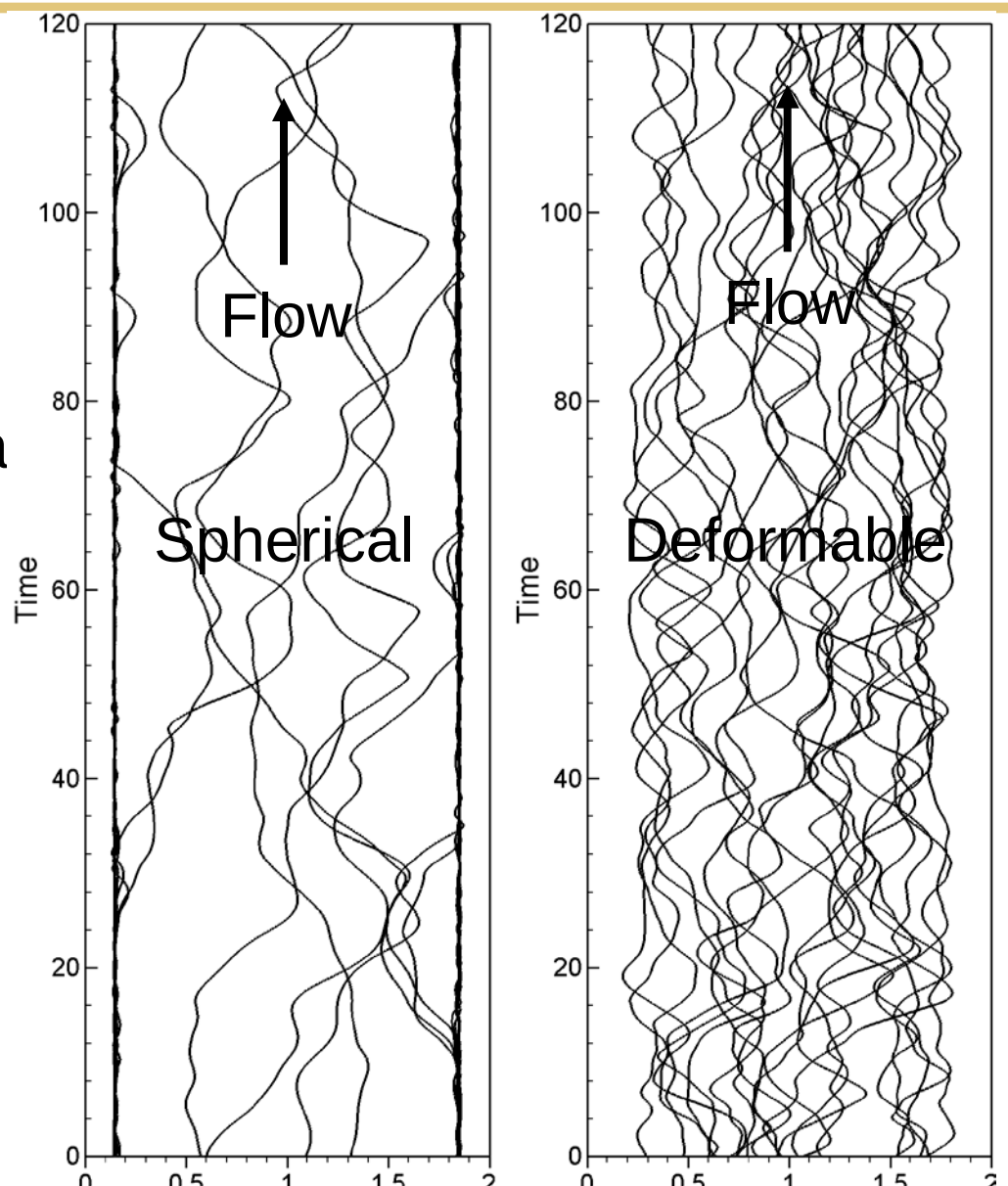
DNS of Multiphase Flows

Turbulent Upflow: Effect of Deformability

The path of bubbles in turbulent vertical channel flows. The cross-channel coordinate versus time for the spherical (left) and the deformable (right) bubbles a approximately steady state.





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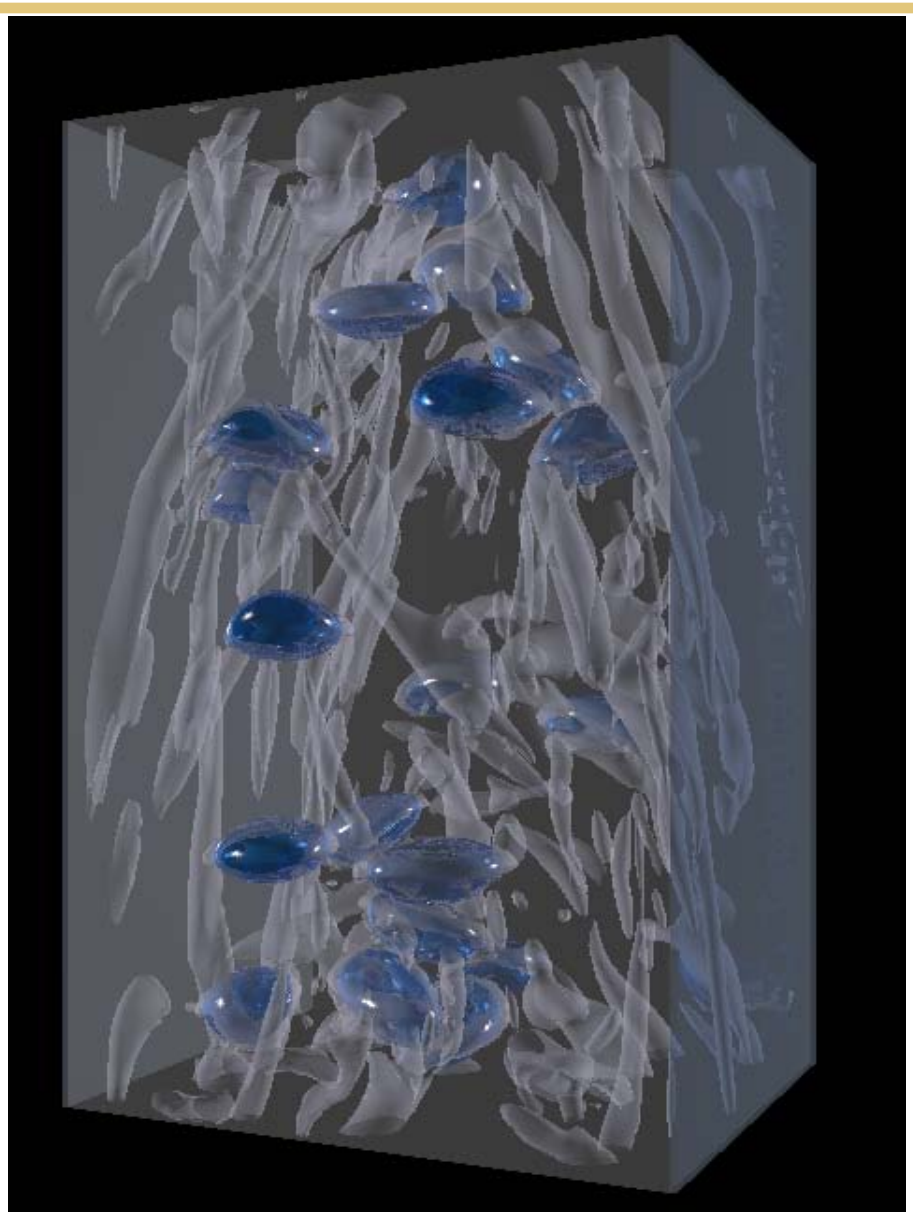
DNS of Multiphase Flows
Bubbles in Vertical Channels



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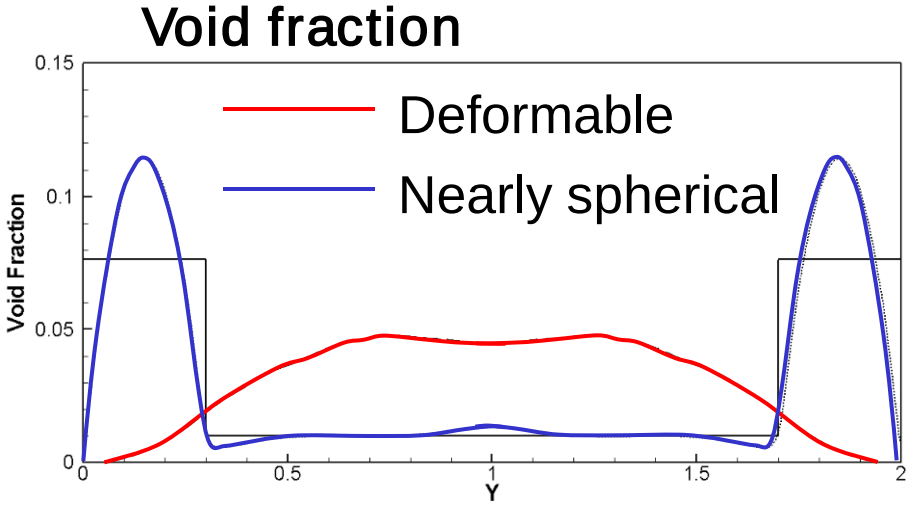
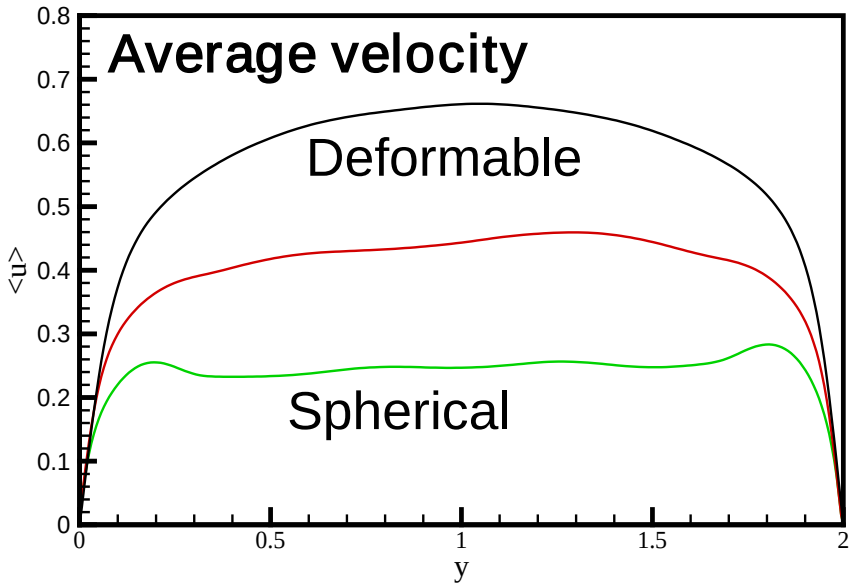
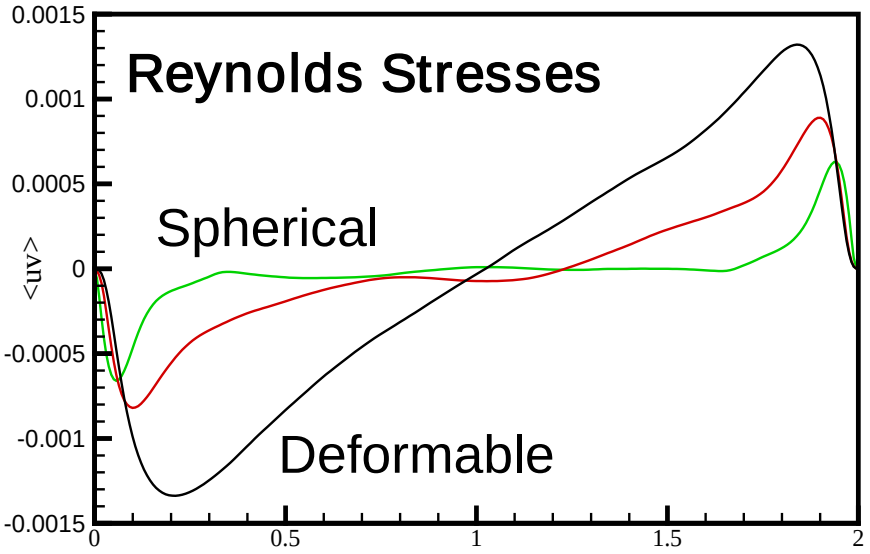
DNS of Multiphase Flows

Turbulent Upflow: Effect of Deformability



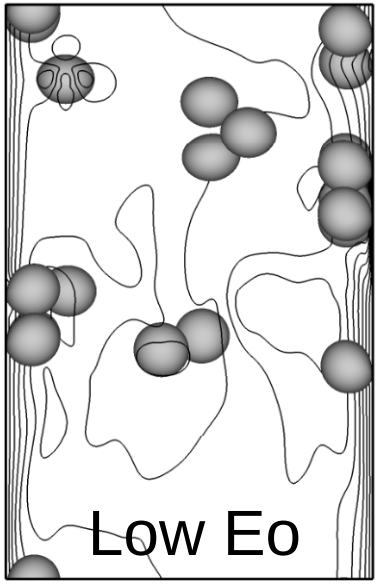


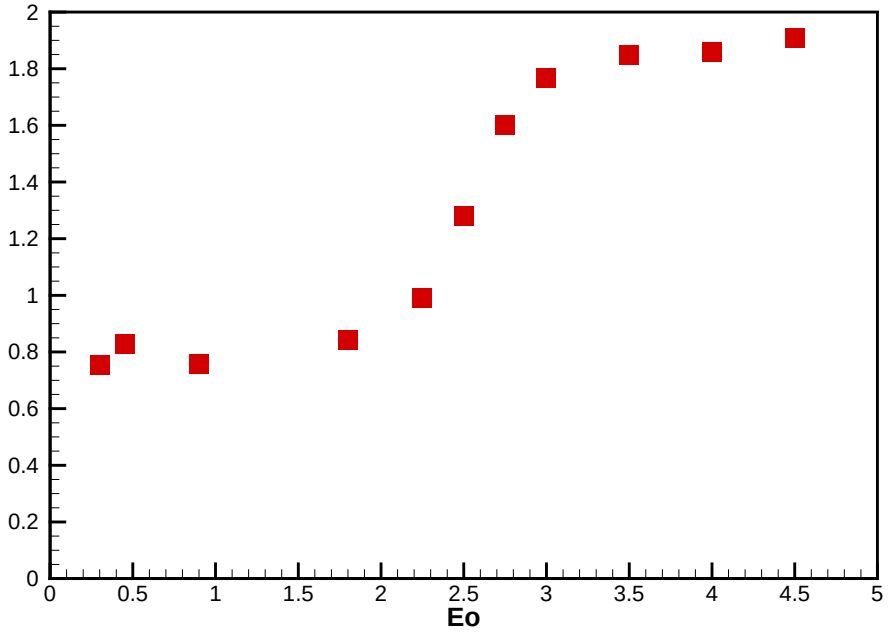
The void fraction has major influence of the flow behavior. The void fraction is plotted above and the velocity profiles and the Reynolds stresses to the right. For deformable bubbles, the flow is similar to turbulent flow without bubbles (using rescaled pressure gradient to account for the weight of the mixture).

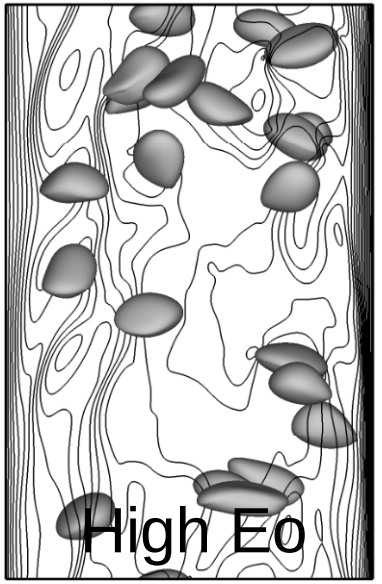


DNS of Multiphase Flows
Bubbles in Turbulent Channel Flows

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. The transition takes place around Eo = 2.5-3.0.

Why Higher Reynolds Numbers and Polydisperse flow?

Strong velocity fluctuations may disrupt the wall layer and “kick” bubbles into the core

If the bubbles are small compared to the wall layer, we may have bubbles that are pushed away, at the wall, but to the wall, further away, resulting in a high bubble concentration away from the walls

The wall layer is likely to exhibit complex structure with clusters of bubbles separated by bubble free regions

The core flow may exhibit large scale flow structures, including meandering and recirculating flows

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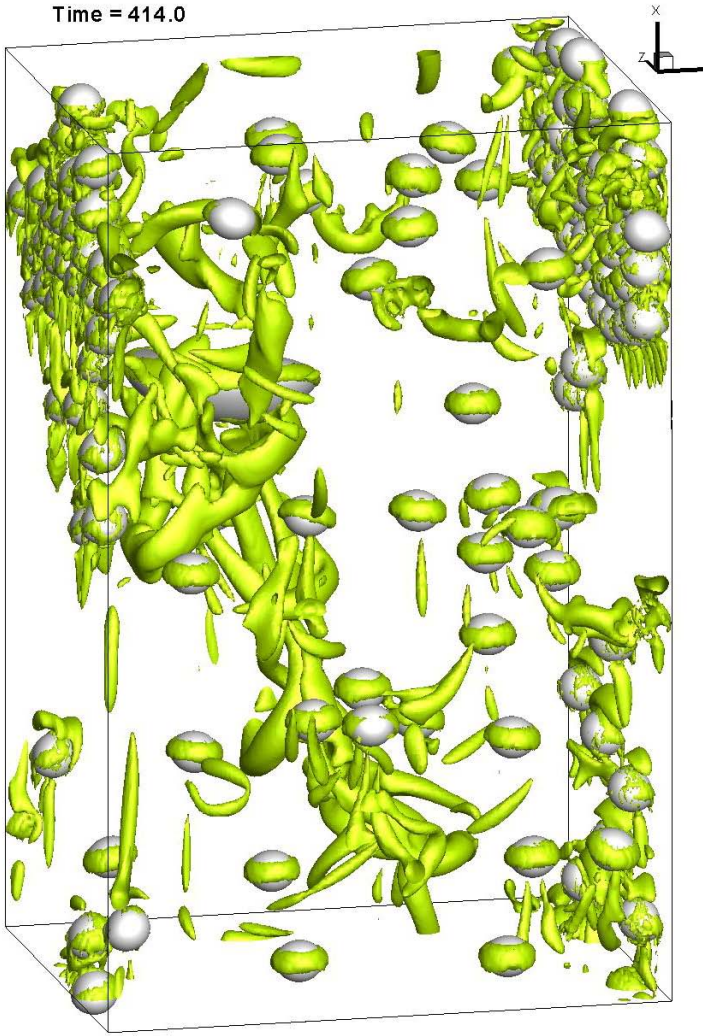
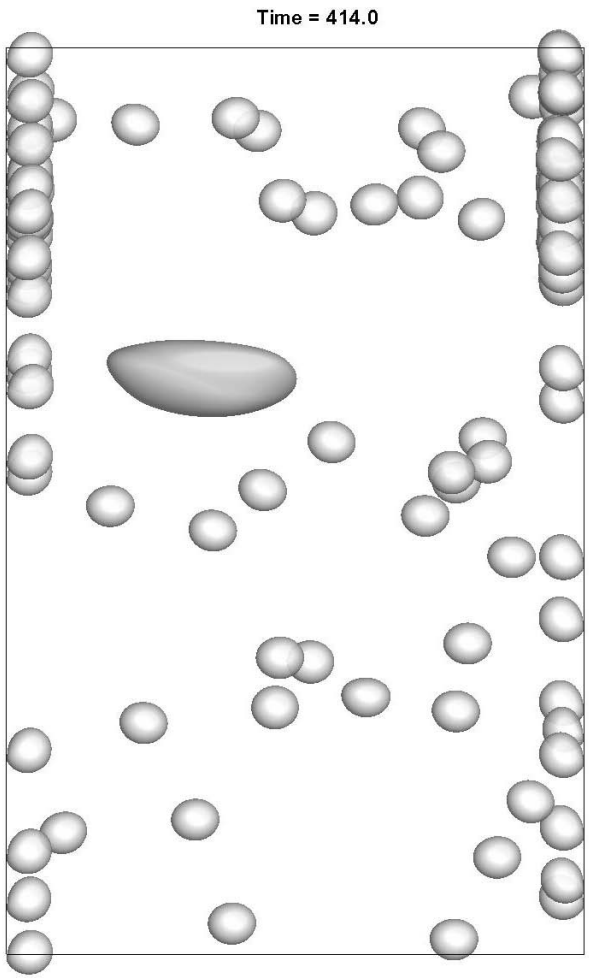
DNS of Multiphase Flows
Bubbles in Vertical Channels

Turbulent Upflow:
Different bubble sizes

512 x 384 x 256 grids, 192 cores)
Re+ = 250; void faction = 3%

The figures are from a current study of the effect of a large number of bubbles of different sizes in turbulent upflow. Some of the small bubbles hug the wall but the large one stays in the center region. If the bubbles coalesced, the flow rate would eventually increase





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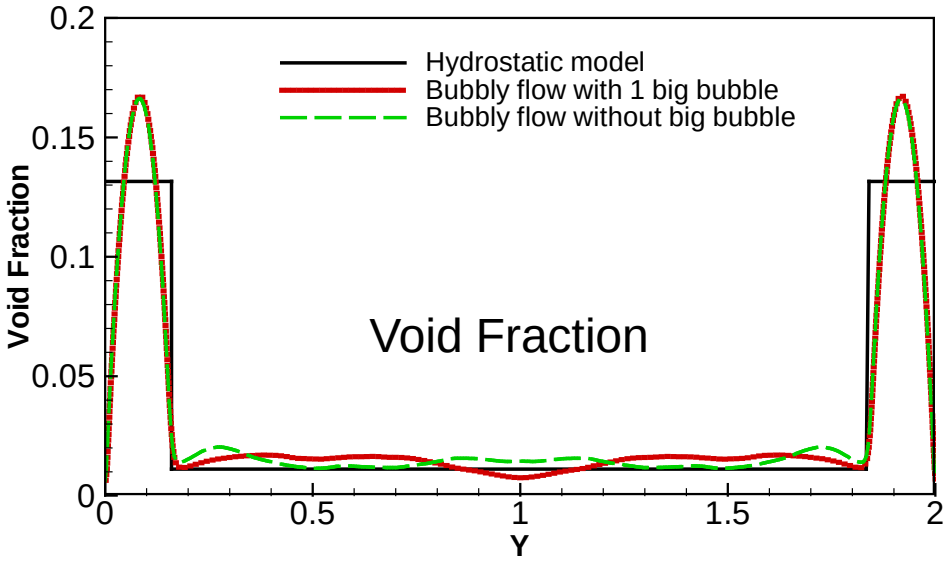
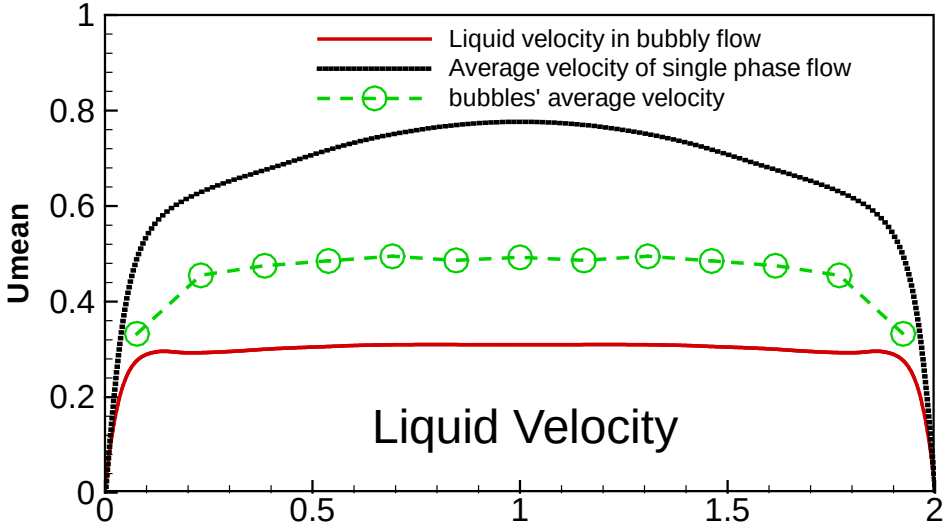
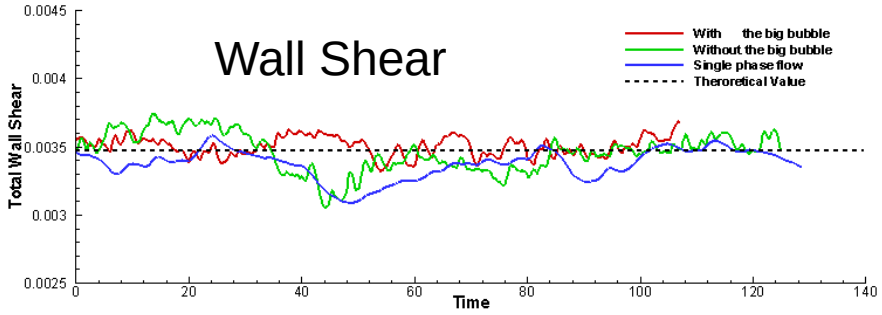
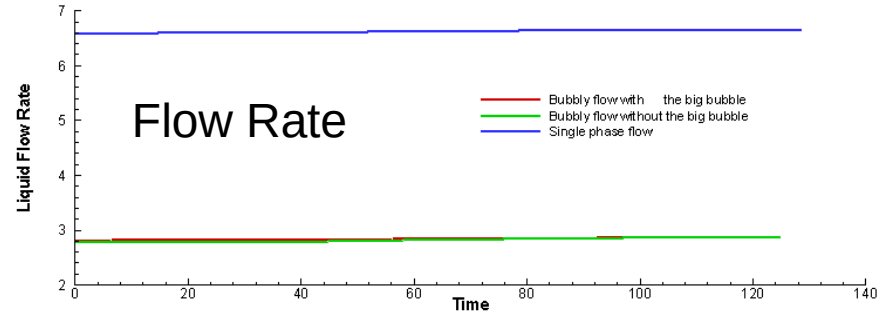
DNS of Multiphase Flows
Bubbles in Vertical Channels

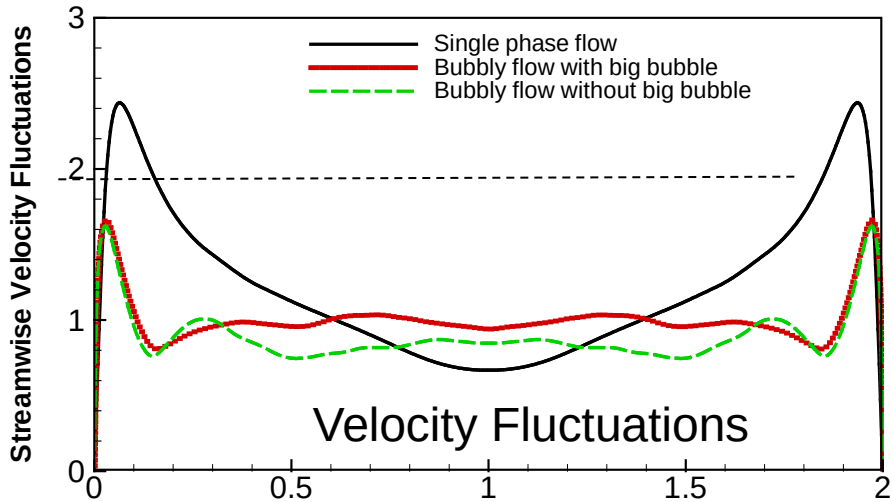
Turbulent Upflow: Different bubble sizes











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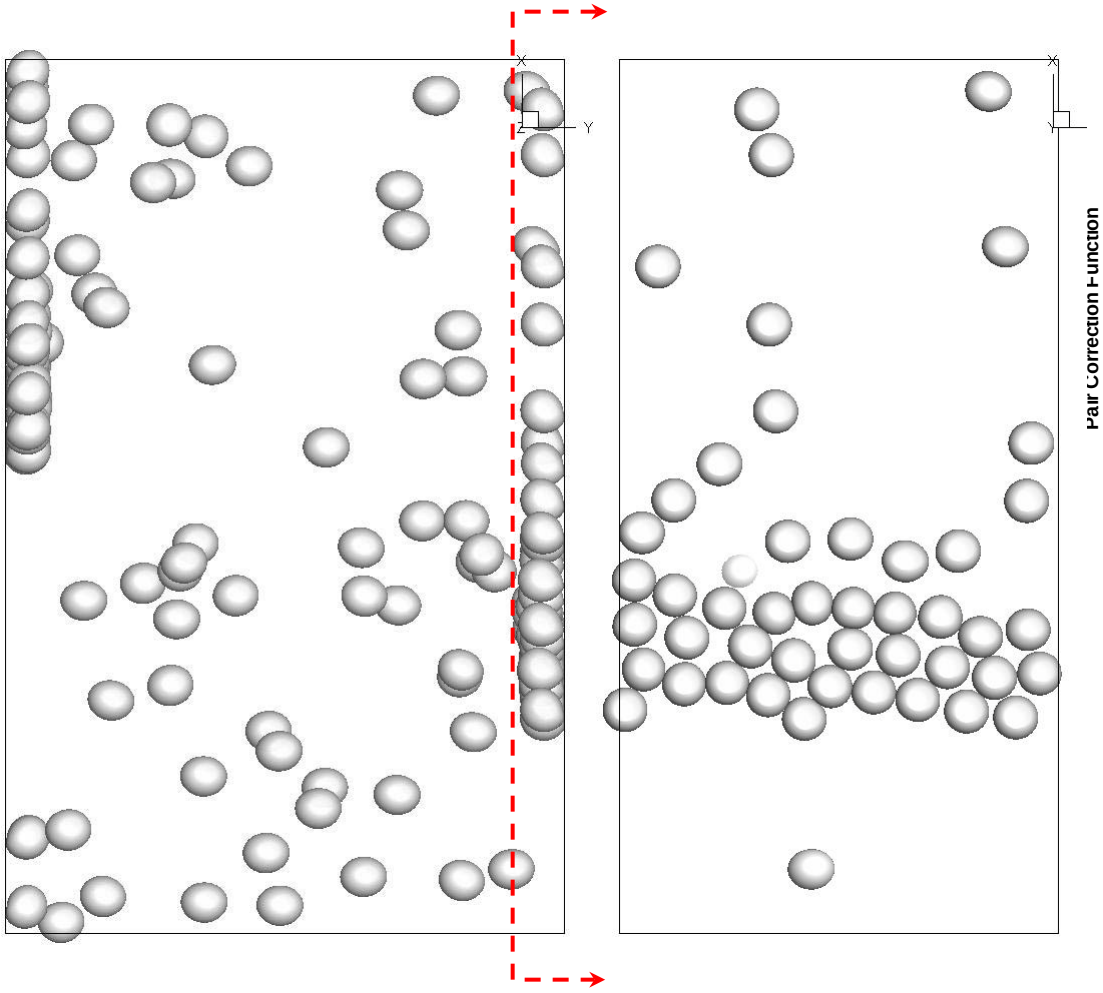
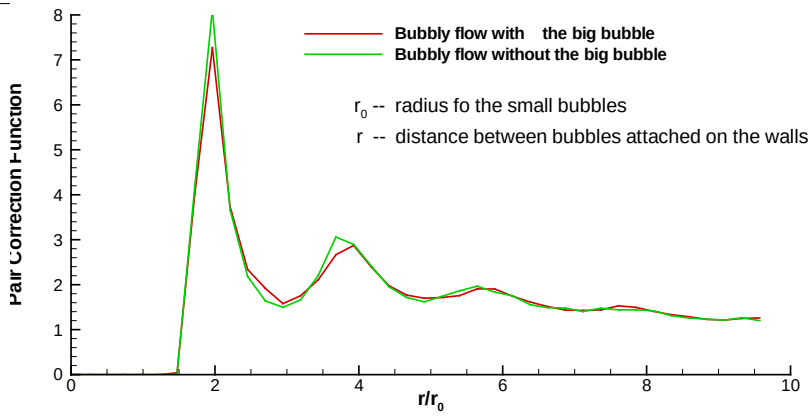
DNS of Multiphase Flows
Bubbles in Vertical Channels



Pair Distribution Function



For large domains the bubbles in the wall-layer can form structures that seem to be more or less independent of the bulk flow

Capturing small-scale processes

Embedded Analytical Descriptions

With
Bahman Aboulhasanzadeh and Siju Thomas

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DNS of Multiphase Flows
Multiscale Issues

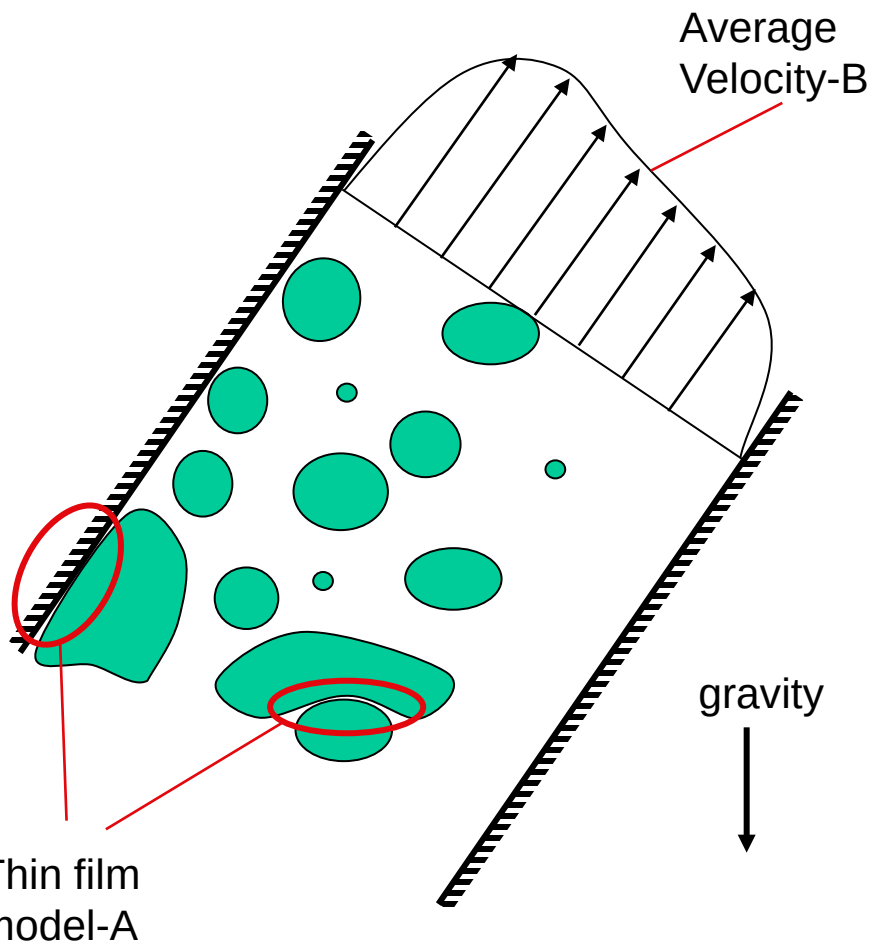
Some communities have defined two types of multi-scale problems.

Type A Problems: Dealing with Isolated Defects

Type B Problems: Constitutive Modeling Based on the Microscopic Models

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

Buoyant bubbles in an inclined channel flow



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DNS of Multiphase Flows
Multiscale Issues

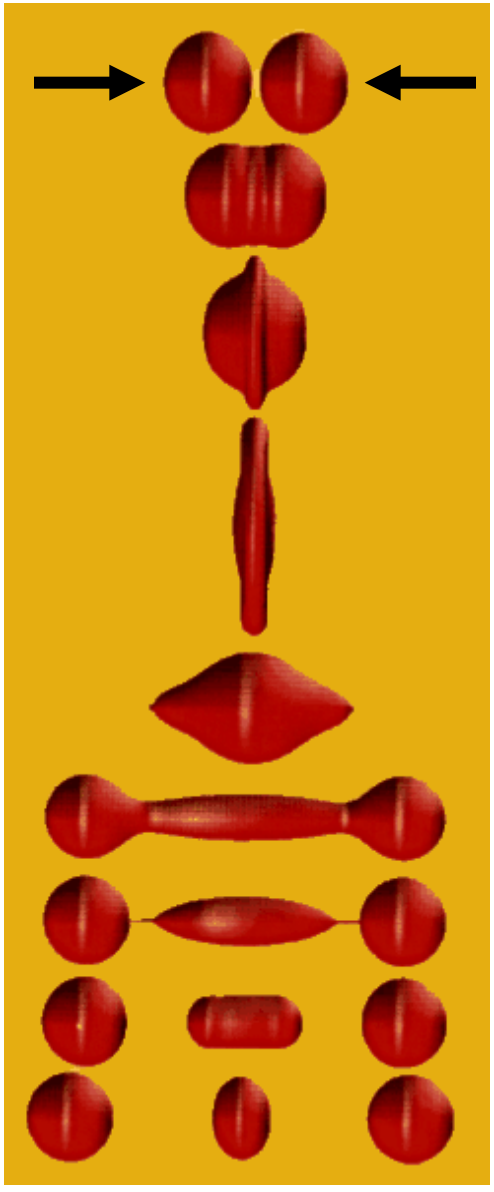
Capturing isolated small-scale motion in simulations where the focus is on the larger scales can be done in many ways, such as be various grid refinement techniques (unstructured grids, AMR for Cartesian grids, wavelets, etc.) or reduced order models

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



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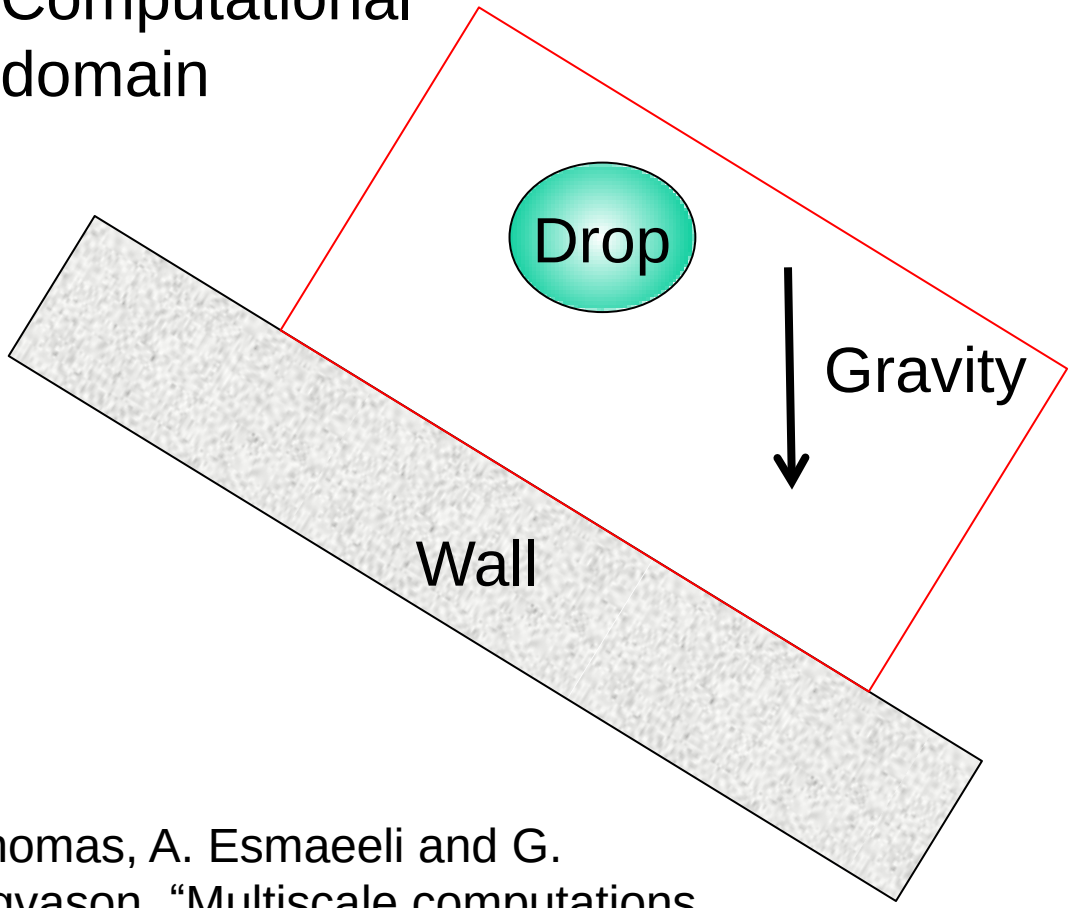
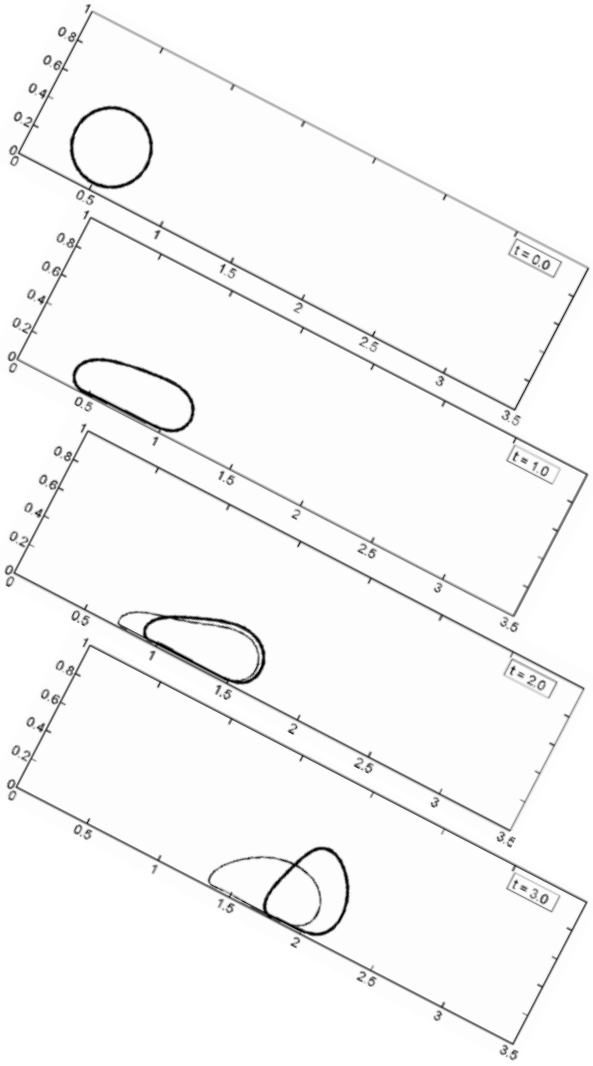
DNS of Multiphase Flows
Thin films near walls

Computational domain





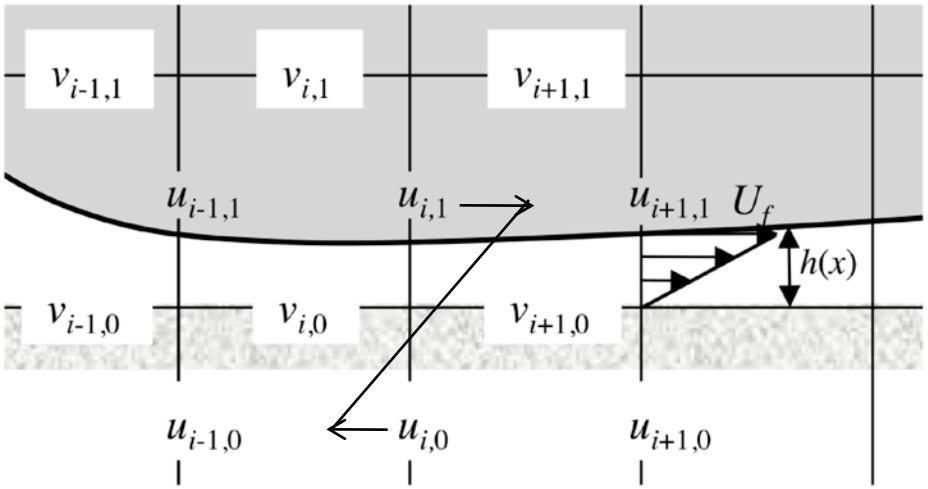
S. Thomas, A. Esmaeeli and G. Tryggvason. “Multiscale computations of thin films in multiphase flows.” *Int1 J. Multiphase Flow* 36 (2010), 71-77.

DNS of Multiphase Flows
Thin films near walls

Film model—linear velocity profile

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

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



Wall shear and ghost velocity:

$$\tau_f=\mu_o\frac{U_f}{h} \quad \rightarrow \quad u_{i,0}=u_{i,1}-\frac{\tau_f \Delta y}{\mu_d}$$

1. Identify whether a grid points at a wall belong to a film or not.

2. For film wall-points, given h and U_f, find the wall-shear and set the ghost velocities. For points outside the film, use the no-slip boundary condition.

3. Solve the Navier-Stokes equations for the velocity and pressure at the next time step, using the ghost velocities set above.

4. Integrate the thin film equations, using the pressure at the wall as computed by solving the Navier-Stokes equations (step 3).

5. Go back to (1)

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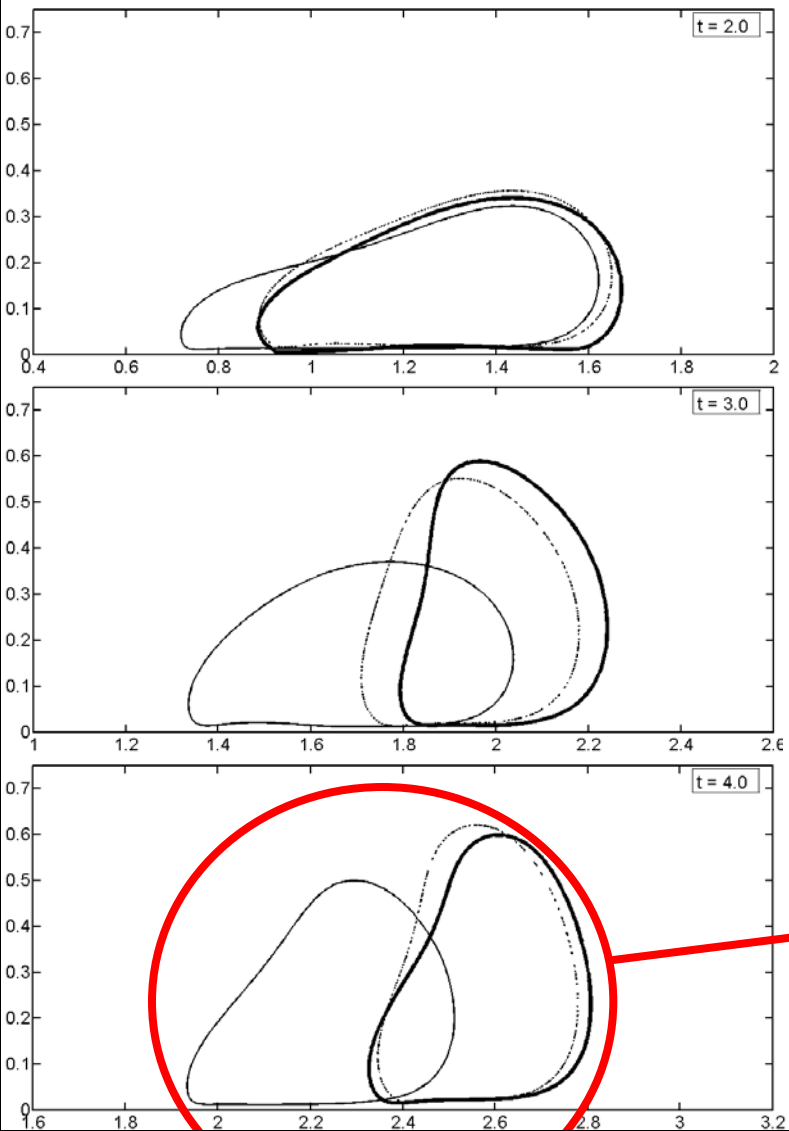
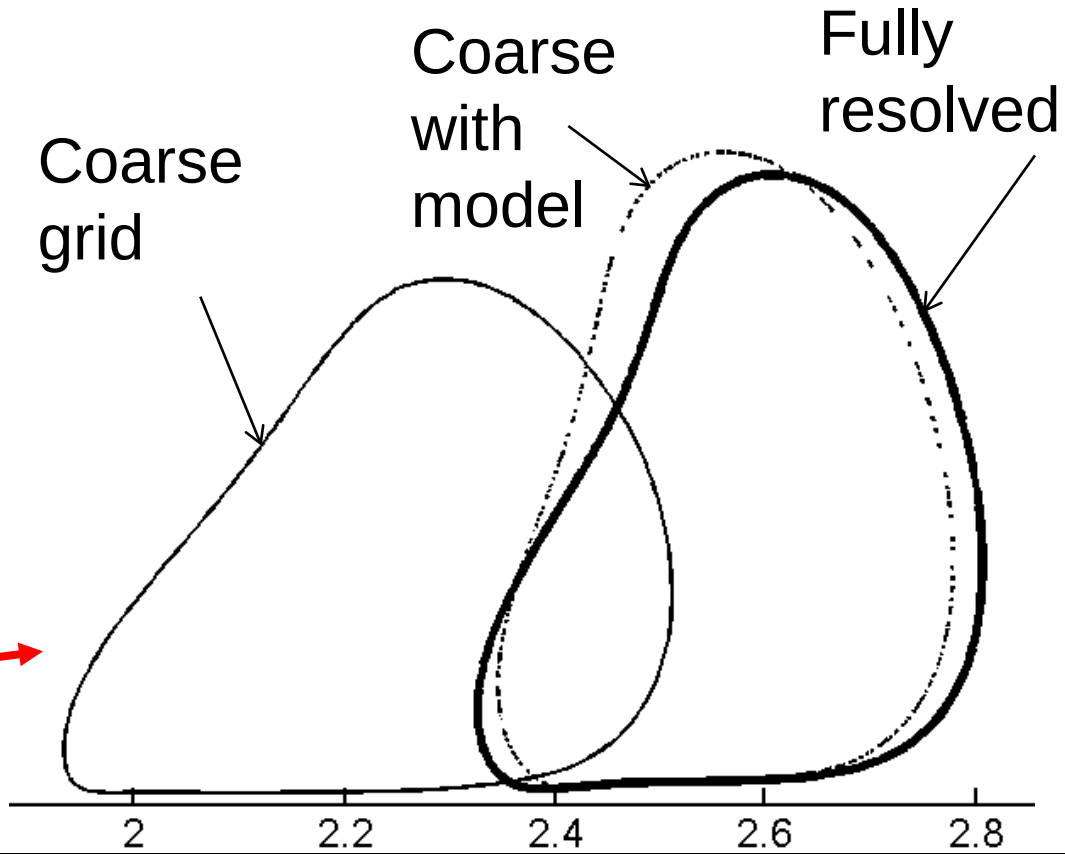
DNS of Multiphase Flows
Thin films near walls



Drop motion on a sloping wall. Impact of fully resolving the film between the drop and the wall



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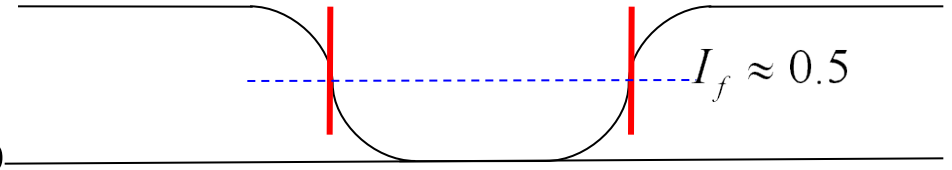
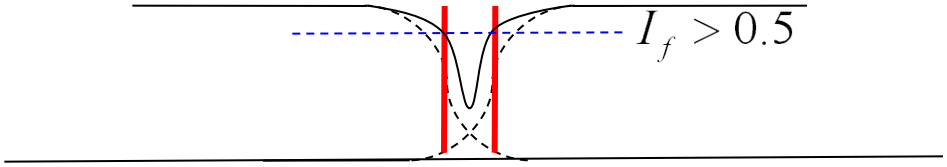
DNS of Multiphase Flows
Thin Films Anywhere

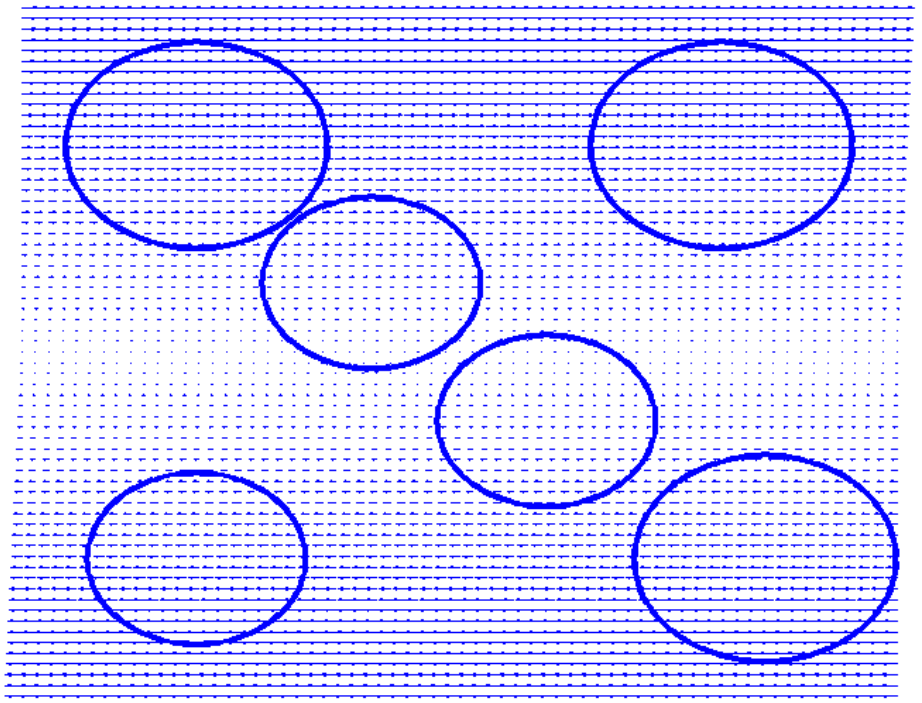
To capture thin films located between two drops anywhere in the computational domain, we first need to locate thin films

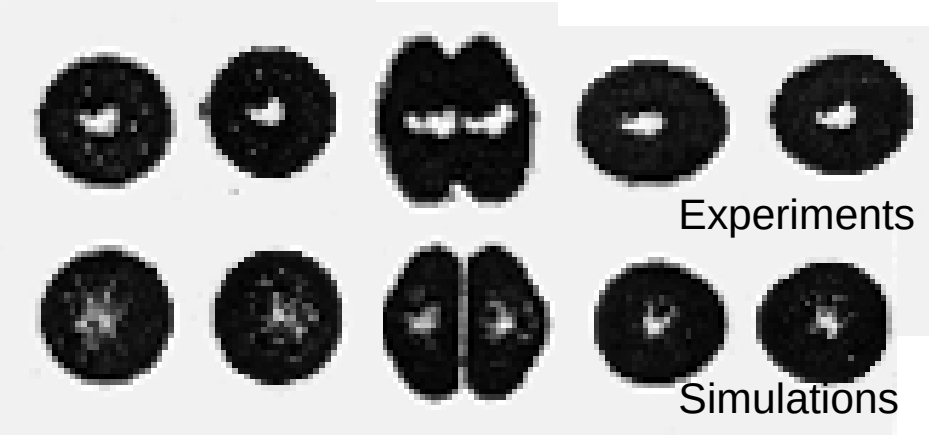
The indicator field, at the front location, is 0.5 for an isolated interface but when two interfaces are close together the value is higher or lower.

Describing the film: To be done!









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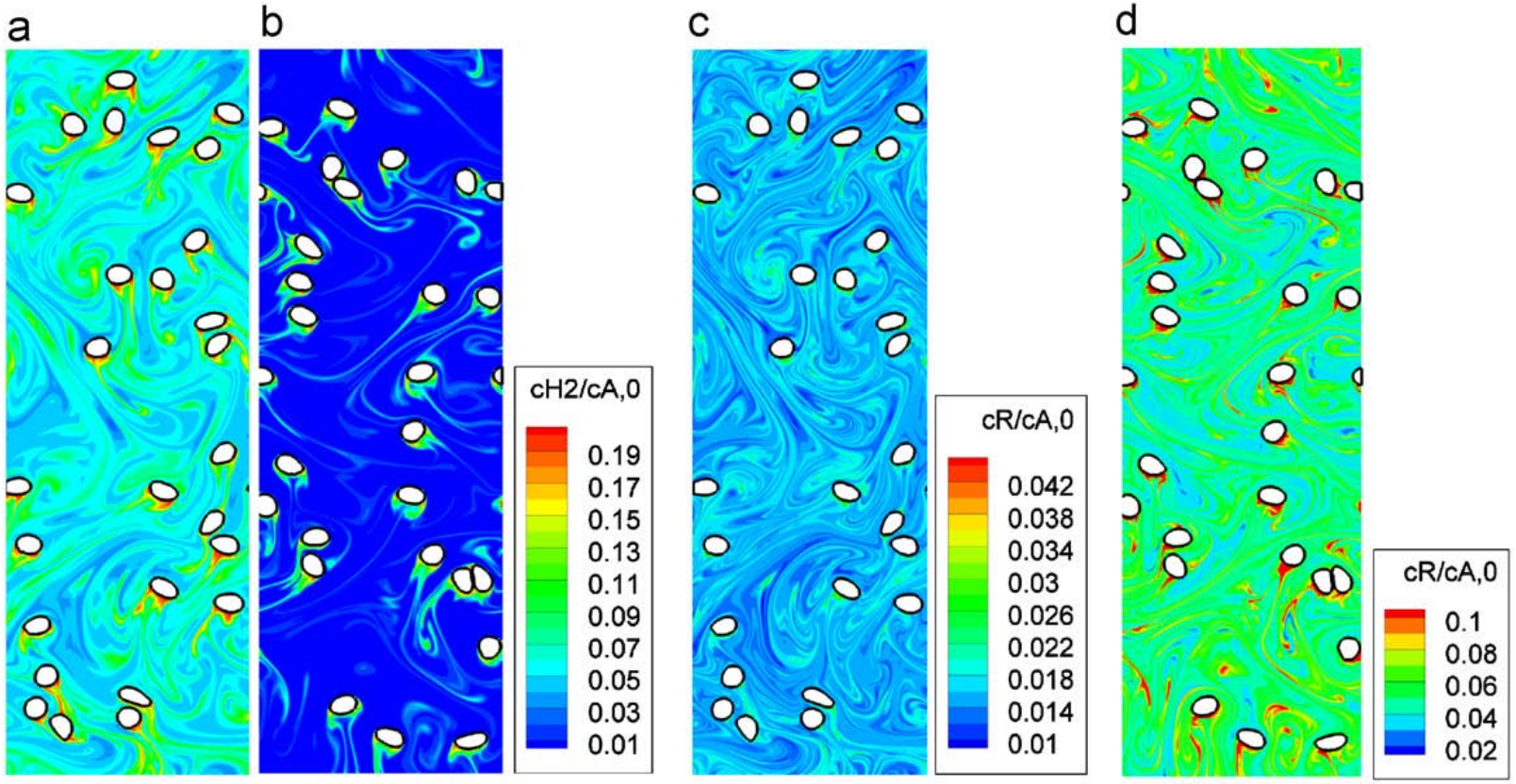
DNS of Multiphase Flows
Mass Transfer in Gas-Liquid Systems



Results from simulations of the of the catalytic hydrogenation of nitroarenes. The hydrogen (frames a and b) and hydroxylamine (frames c and d) concentration profiles are shown for one time for two simulations. In frames a and c the reaction rates are relatively slow, compared with the mass transfer, but in frames b and d the reaction is relatively fast. From Radl et al.

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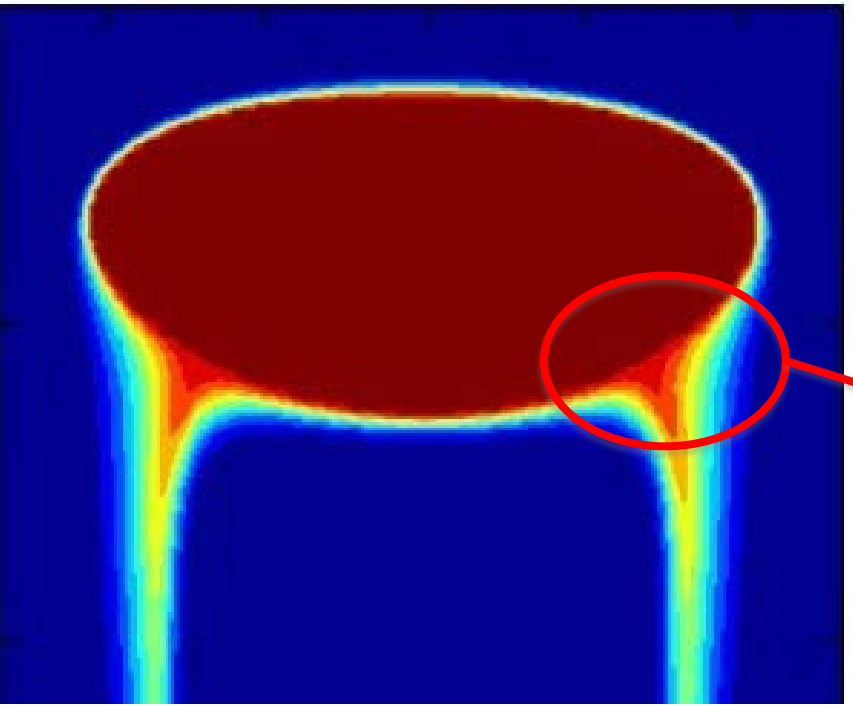
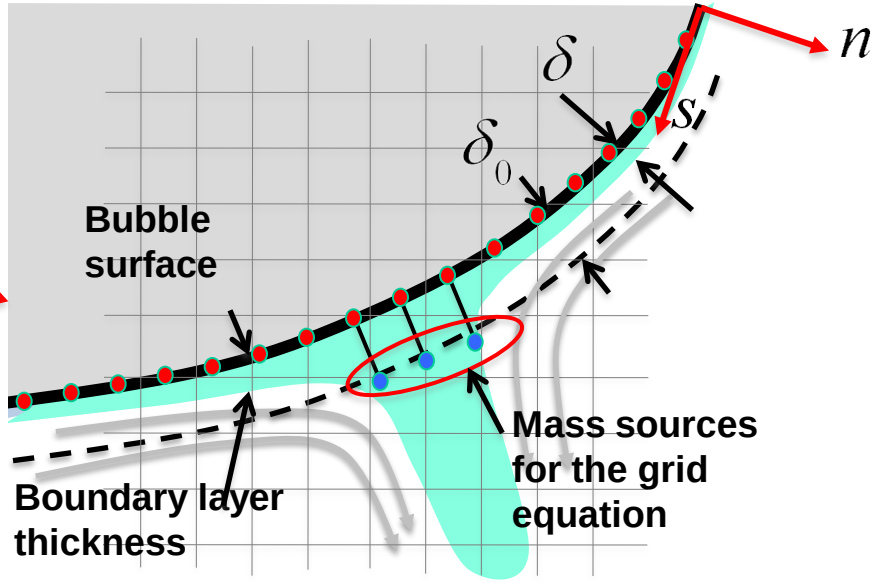
DNS of Multiphase Flows
Mass Transfer in Gas-Liquid Systems



Capturing the mass boundary layer



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

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

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

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

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

DNS of Multiphase Flows
Mass Transfer in Gas-Liquid Systems

Assume a two parameter profile

$$f(n)=\begin{cases} f_0\left(1-(1-a)\left(\frac{n}{\Delta}\right)-a\left(\frac{n}{\Delta}\right)^2\right); & n\le\Delta \\ 0; & n>\Delta \end{cases}.$$

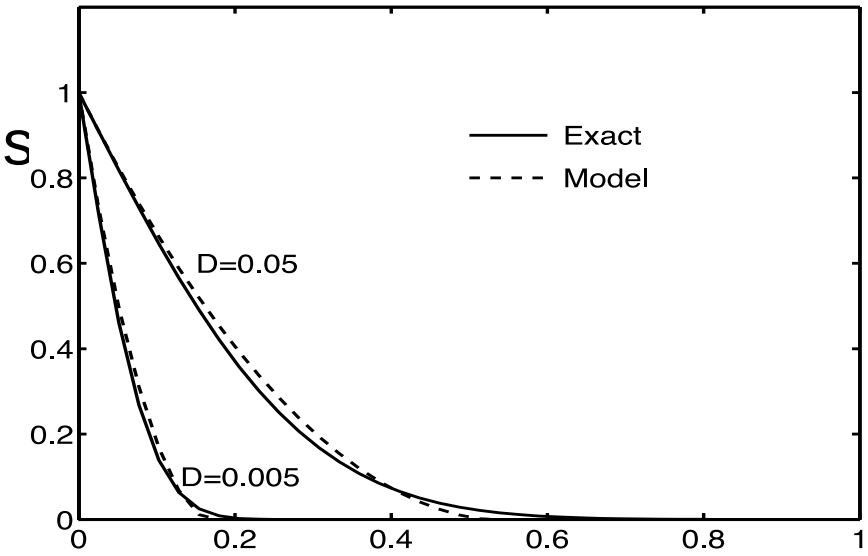
The moments are:

$$M_0=f_0\Delta\left(\frac{4-a}{6}\right);\quad M_1=f_0\Delta^2\left(\frac{3-a}{12}\right)$$

Substituting into the evolution equations for the moments gives

$$\frac{d\Delta^2}{dt}=-2\sigma\Delta^2+D\frac{12a}{4-a}$$

$$\frac{da}{dt}=\frac{12D}{\Delta^2}\left(\frac{4a-4-a^2}{4-a}\right).$$



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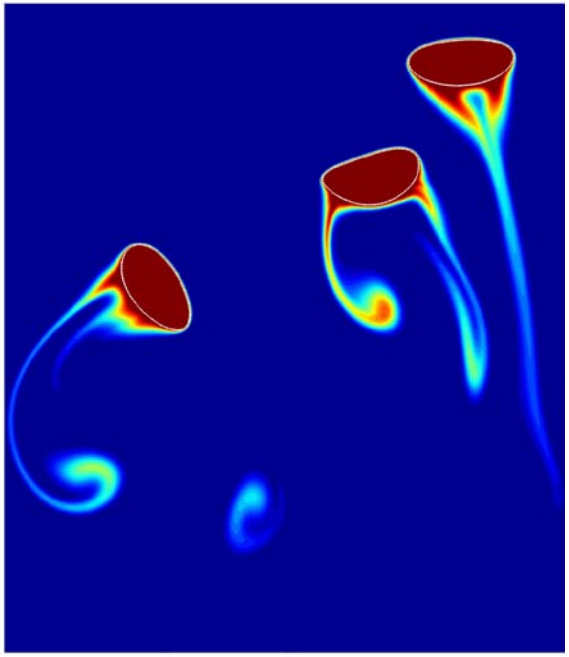
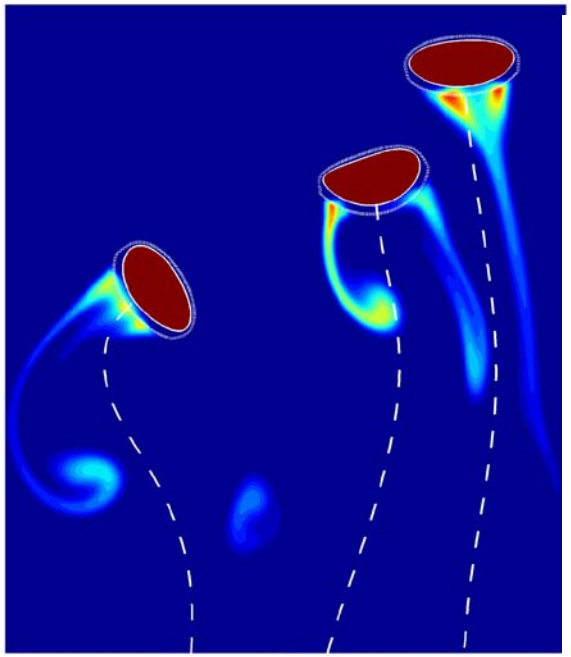
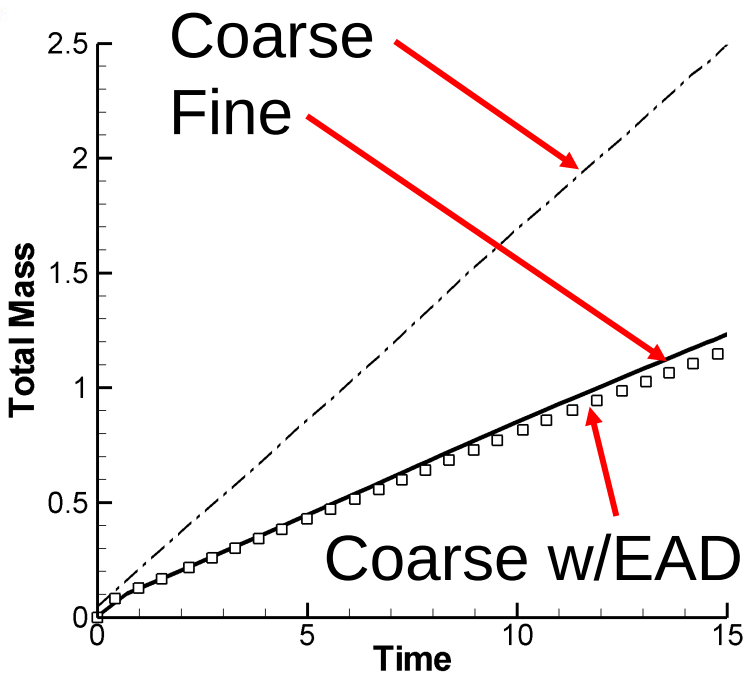
DNS of Multiphase Flows
Mass Transfer in Gas-Liquid Systems







Full Using Model

Re = 60, Sc = 15

Using one moment and a one-parameter profile

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

$$f(n) = \begin{cases} f_0\left(1 - 2\left(\frac{n}{\delta}\right) + \left(\frac{n}{\delta}\right)^2\right); & n \le \delta_0 \\ 0; & n > \delta \end{cases}$$

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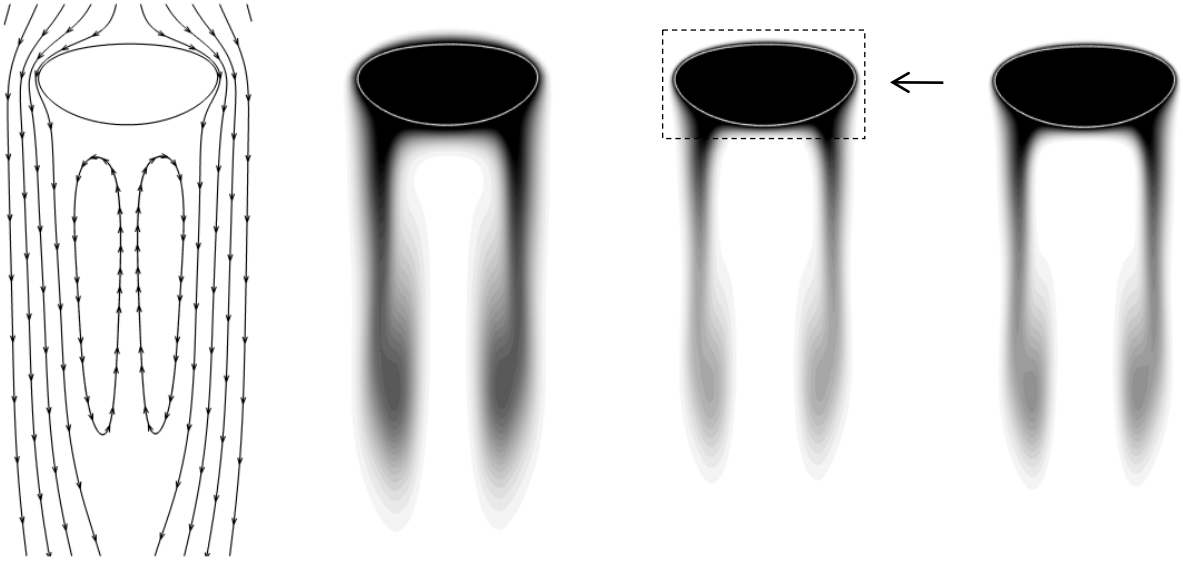
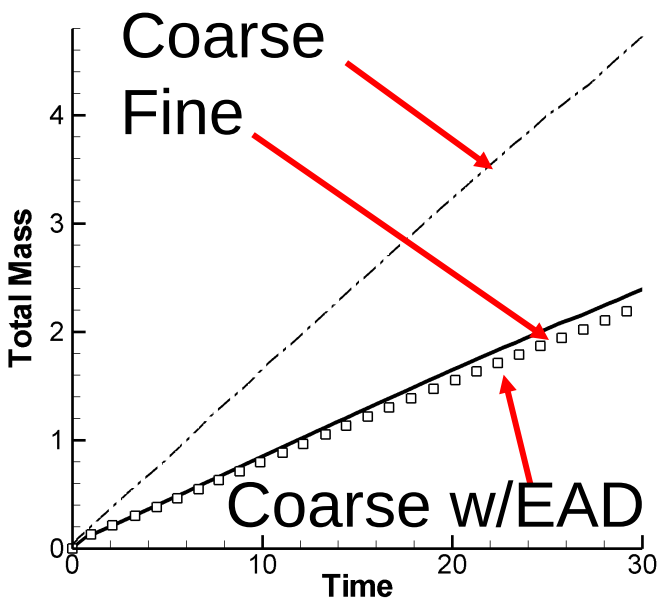
DNS of Multiphase Flows

Capturing the mass boundary layer





Re = 60, Sc = 15

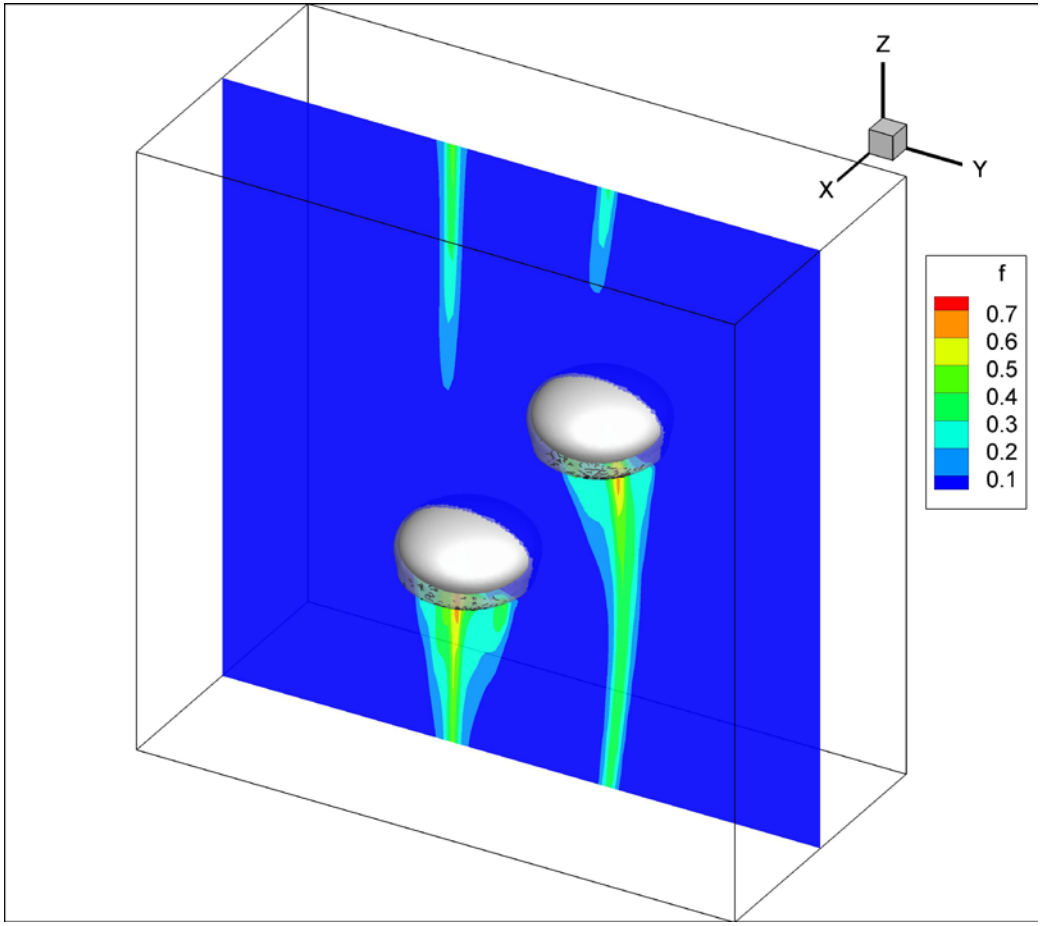
Using one moment and a one-parameter profile

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

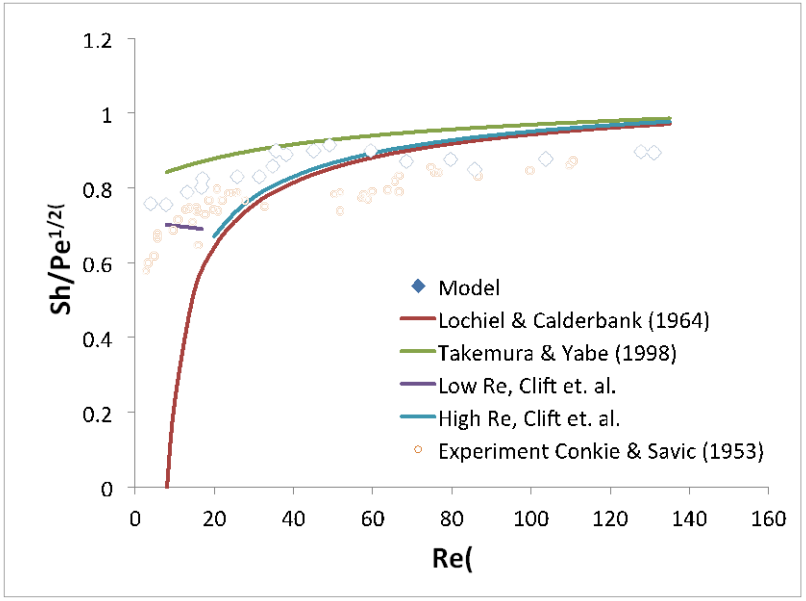
$$f(n) = \begin{cases} f_0\left(1 - 2\left(\frac{n}{\delta}\right) + \left(\frac{n}{\delta}\right)^2\right); & n \le \delta_0 \\ 0; & n > \delta \end{cases}$$

DNS of Multiphase Flows

Preliminary results for 3D flows.



One frame of a simulation of two bubbles in a periodic domain.



The mass transfer versus Re, along with the predictions of experimental correlations

Simulations of Boiling Flows

DNS of Multiphase Flows
Governing Equations

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

$$\frac{\partial cT}{\partial t}+\mathbf{u}\cdot\nabla cT=\nabla\cdot k\nabla T+\int\dot{q}\delta(\mathbf{x}-\mathbf{x}_{f})dA$$ Energy equation

$$\dot{q}=k_{1}\frac{\partial T}{\partial n}\Big)_{1}-k_{2}\frac{\partial T}{\partial n}\Big)_{2}$$ Heat source

$$T_{l}=T_{v}=T_{sat}(p_{sys})$$ Thermodynamic

$$\nabla\cdot\mathbf{u}=\frac{1}{L}\left(\frac{1}{\rho_{v}}-\frac{1}{\rho_{f}}\right)\int\dot{q}\delta(\mathbf{x}-\mathbf{x}_{f})dA$$ Mass conservation

$$V_{n}=\frac{1}{2}\left(u_{l}+u_{v}\right)-\frac{\dot{q}}{L}\left(\frac{1}{\rho_{v}}+\frac{1}{\rho_{f}}\right)$$

$$\frac{dx_{f}}{dt}=V_{n}\mathbf{n}+\mathbf{u}$$

} Velocity of bdry

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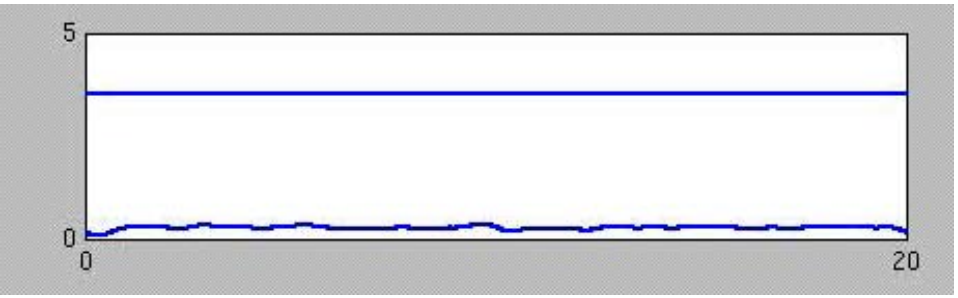
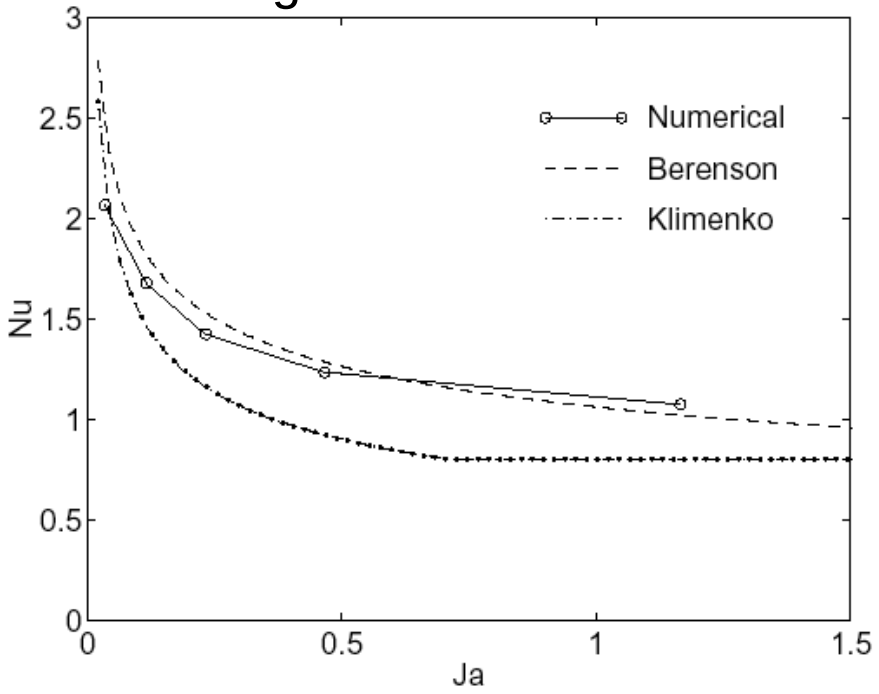
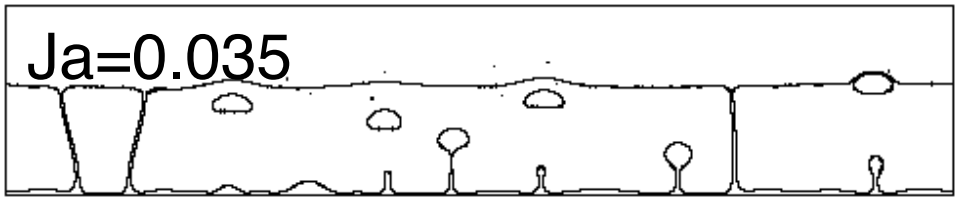
DNS of Multiphase Flows

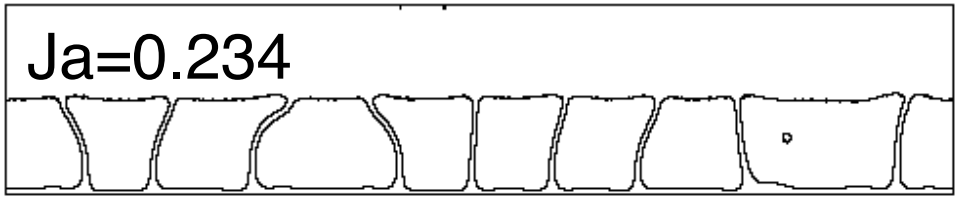
Boiling Flows

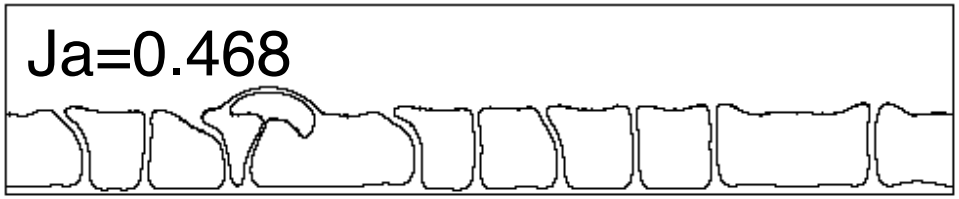


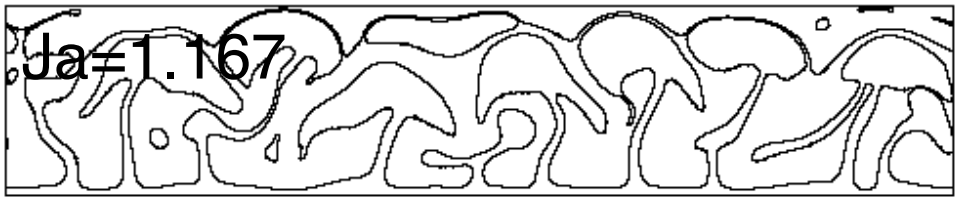
The effect of Jacob number (wall superheat) on Nu for near critical film boiling





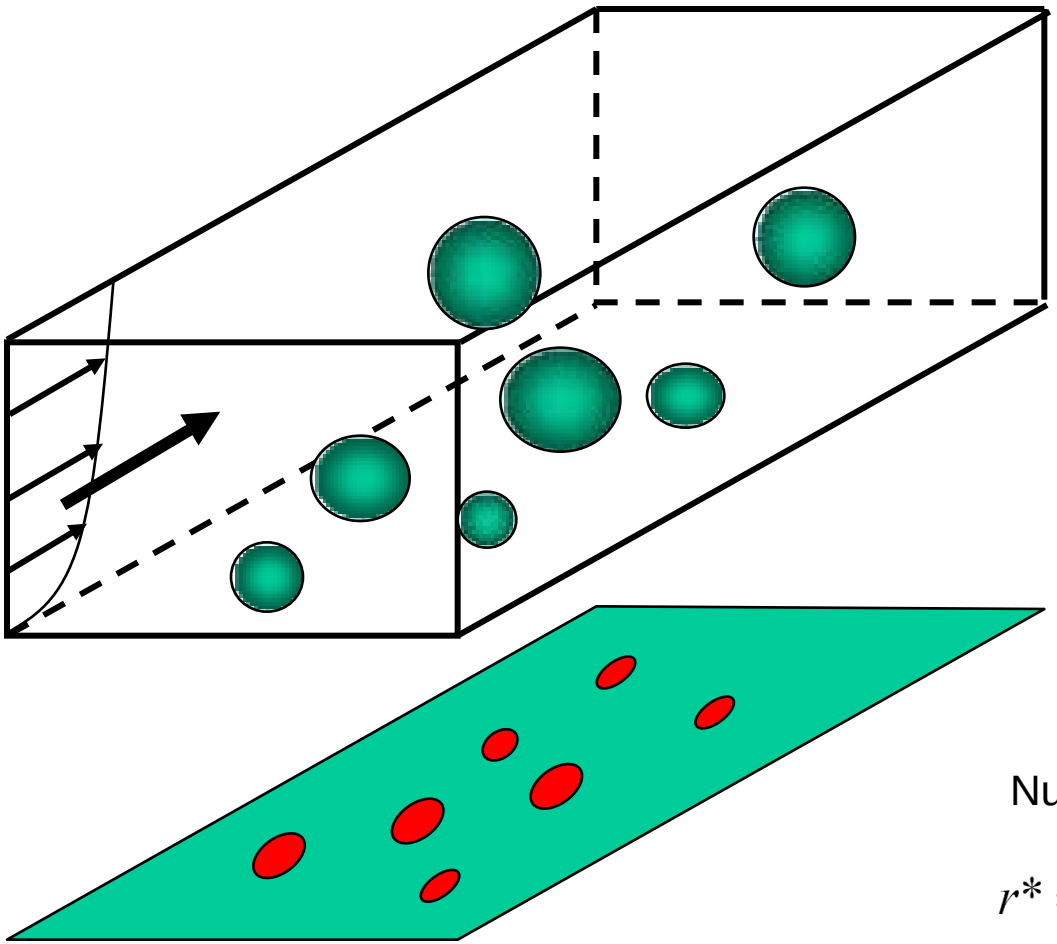






Nucleate Boiling

Nucleate Flow Boiling



Assumption : Surface nucleation characteristics determined by size distribution of potentially active sites

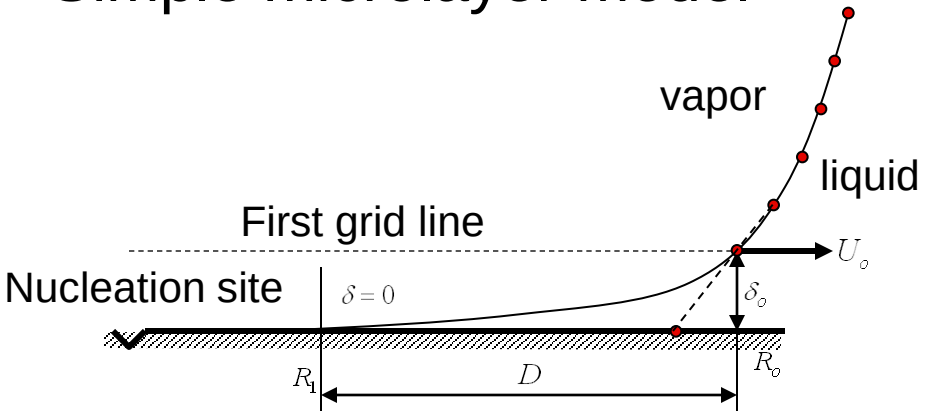
- Random spatial site distribution
- Random conical cavity size (mouth radius, r) distribution
- Assume vapor embryo radius = r
- Assume near wall liquid film is stationary

Nucleation site is active if $r_{min} > r^*$

$$r^* = \frac{2\sigma T_{sat} \upsilon_{lv}}{h_{lv}\left[T_l - T_{sat}\right]}$$

Carey (1992)

Simple microlayer model



Evaporation of the film

$$\dot{q} = k\frac{T_w - T_f}{\delta} = k\frac{\Delta T}{\delta}$$ Heat transfer

$$\frac{d\delta}{dt} = -\frac{\dot{q}}{\rho_f L} = -\frac{k\Delta T}{\delta \rho_f L} = -\frac{\beta}{\delta}$$ Evaporation

$$\delta = \sqrt{\delta_o^2 - 2\beta t}$$ Integrate to find thickness

$$t_e = \delta_o^2 / 2\beta$$

$$D = U_o t_e = \frac{U_o \delta_o^2}{2\beta}$$ Find length of film

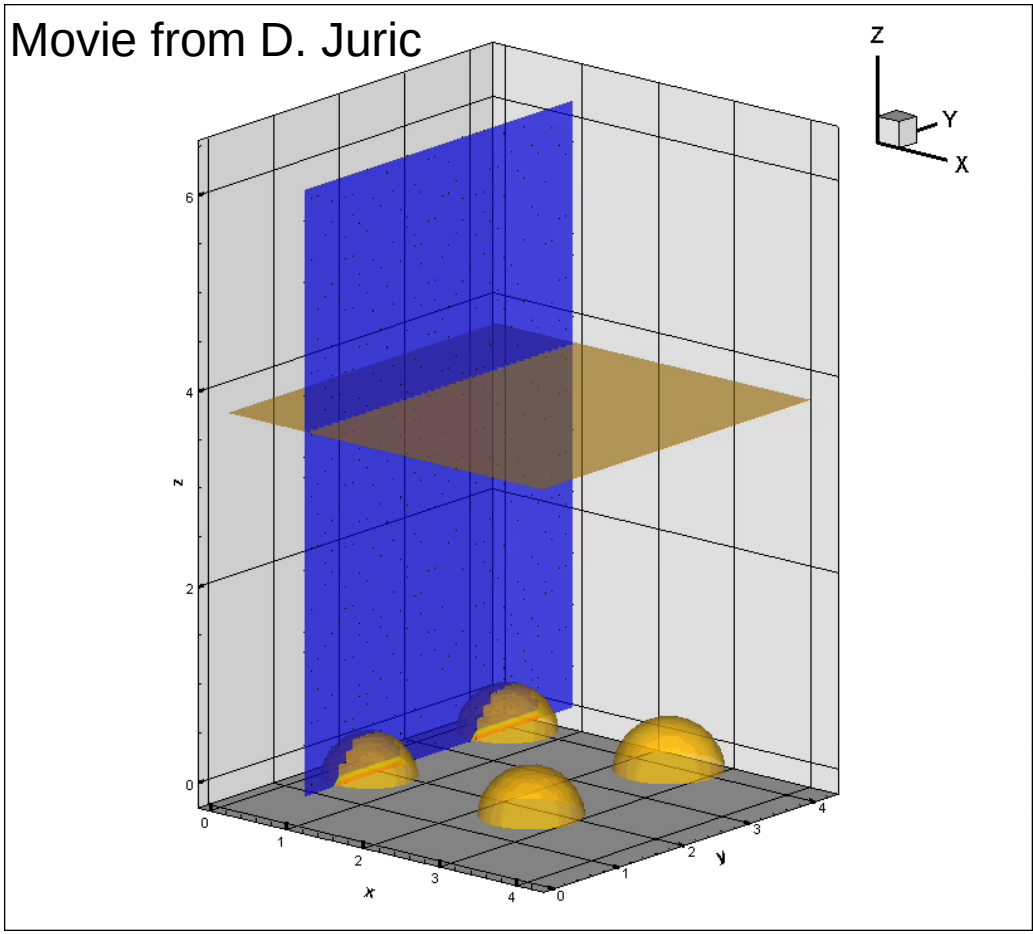
Total heat transfer to the microlayer

$$\dot{Q} = \int_0^D \dot{q}\, dx = \int_0^D \frac{k\Delta T}{\sqrt{\delta_o^2 - (2\beta/U_o)x}}\, dx = \frac{k\Delta T}{\delta_o}\int_0^D \frac{1}{\sqrt{1 - (2\beta/\delta_o^2 U_o)x}}\, dx \rightarrow \dot{Q} = \delta_o U_o L \rho_f$$

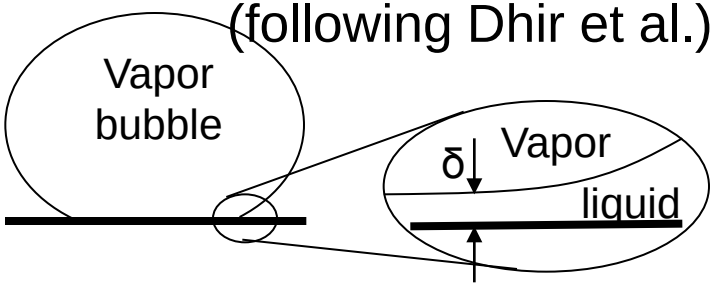
Volume expansion $\dot{V} = \frac{\dot{Q}}{L}\left(\frac{1}{\rho_v} - \frac{1}{\rho_f}\right)$ Applied near the apparent contact

DNS of Multiphase Flows
Nucleate Boiling

Simulation of the generation of bubbles in a shallow pool. In addition to solving the energy equation, the latent heat and the volume expansion at the phase boundary must be included. Most simulations so far have been for film boiling. The nucleation of a vapor bubble and the evaporation in the microlayer must be addressed by multiscale modeling.



Microlayer modeling (following Dhir et al.)



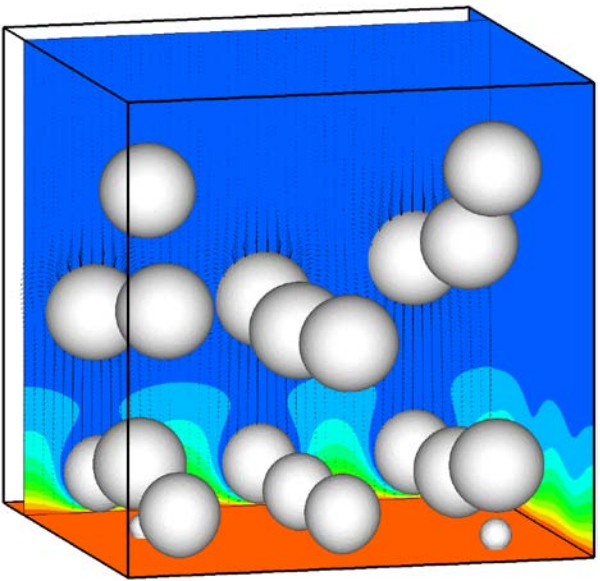
Water at 1atm, Tsat=373.15K; liquid/vapor density ratio=1605; viscosity ratio=23; thermal conductivity ratio=27; specific heat ratio=1; domain size: 10.5x10.5x15.75 mm; Wall superheat: 18K 40x40x60 grid resolution

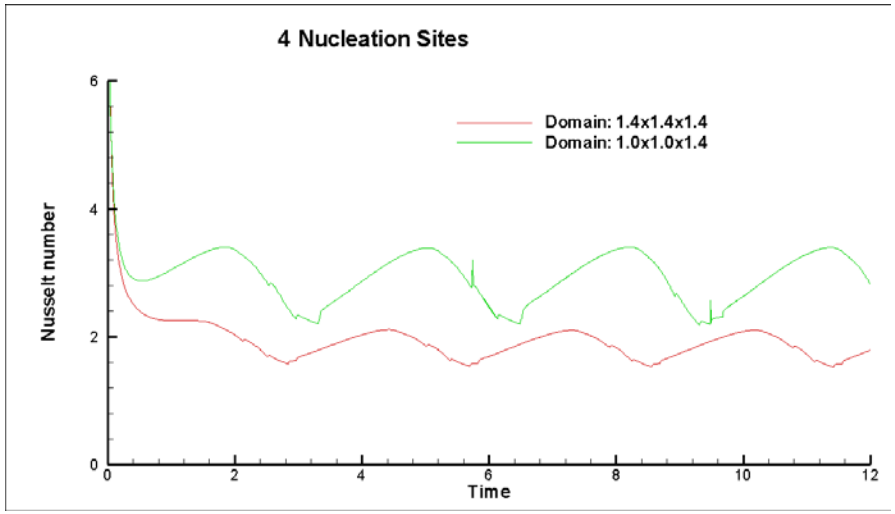
DNS of Multiphase Flows
Nucleate Boiling

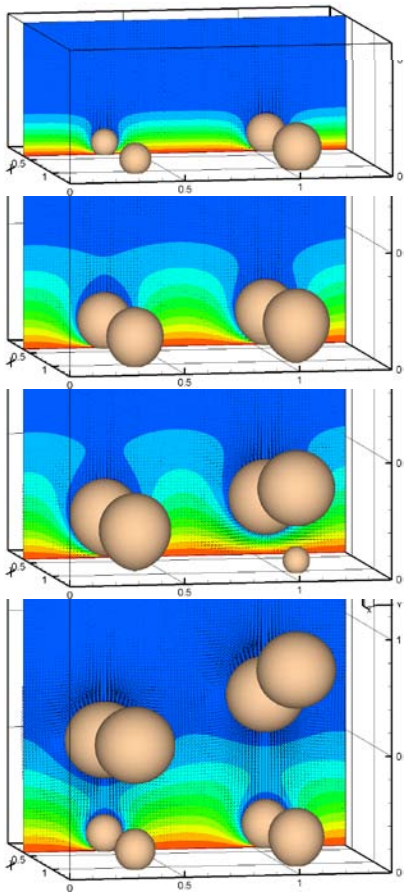
There appears to be no significant technical obstacles for conducting large scale simulations of nucleate flow boiling—however, some development works still needs to be done!

Such simulations should allow us to

- Assess the accuracy of the assumptions made in the modeling of the microlayer
- Use the simulations to make predictions about boiling under conditions where experiments are difficult or do not yield the necessary data.







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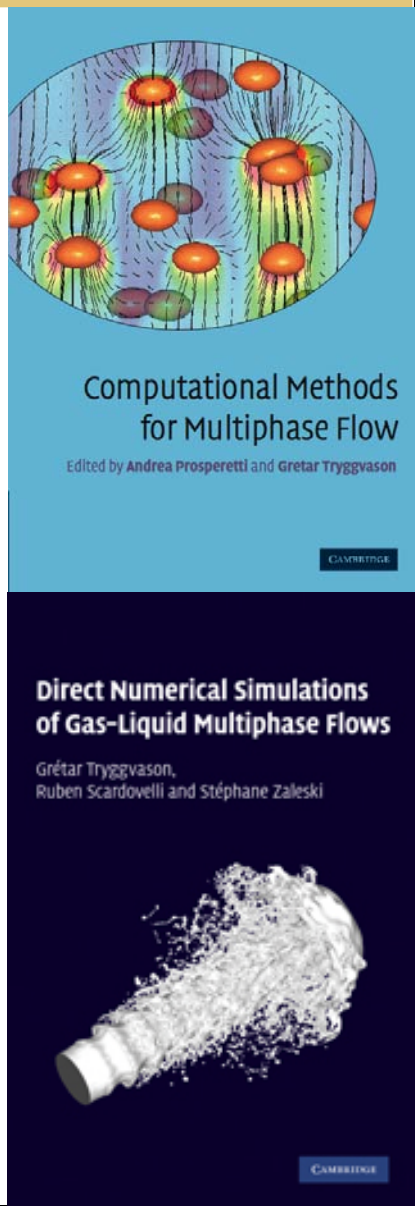
DNS of Multiphase Flows
Now What?

DNS of bubbly flows in turbulent channels have been developed to the point that they should be able 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.



The End!