Moving Interface Problems: Methods & Applications Tutorial Lecture IV

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Moving Interface Problems and Applications in Fluid Dynamics
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Outline

Flows with phase change
- Solidification
- Boiling

Electrohydrodynamics

Flows with topology changes
- Regime changes in bubbly flows
- Atomization and sprays

Outlook

Phase Change

The phase change between liquid and solid or between liquid and vapor is the critical step in the processing of most material as well as in energy generation. Computations will make it possible to predict the small scale evolution of systems undergoing phase change from first principles.

To simulate such flows, it is necessary to solve the energy equation for the temperature distribution and to account for the change of phase at the phase boundary.

In addition to solving the energy equation and including the phase change, we must

- Account for volume expansion at the interface for boiling

- Accommodate a zero velocity field in the solid, for the solidification problem.

In reality there is a slight volume change for the solidification as well, but this can usually be neglected.

Formation of Microstructure during Solidification

Early papers on dendritic growth in the presence of flow:

Two-dimensional systems
- Tonhardt and Amberg (1998)
- Beckermann, et al (1999)
- Juric (1998),
- Shin and Juric (2000)
- Al-Rawhai and Tryggvason (2001)

Three-dimensional system:
- Danzig et al (2001)
- Al-Rawhai and Tryggvason (2002)

Pure material

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

$$T_f = T_m \left(1 + \frac{\kappa}{L} + \cdots\right)$$

$$q = L V_n$$

$$\frac{dx_f}{dt} = V_n \mathbf{n}$$

- D. Juric and G. Tryggvason, "A Front Tracking Method for Dentritic Solidification." J. Comput. Phys. 123, 127-148, (1996).
- N. Al-Rawahi and G. Tryggvason. Computations of the growth of dendrites in the presence of flow. Part I-Two-dimensional Flow. *J. Comput. Phys.* 180, 471–496 (2002)
- N. Al-Rawahi and G. Tryggvason. “Numerical simulation of dendritic solidification with convection: Three-dimensional flow.” *Journal of Computational Physics.* 194 (2004) 677–696

Moving Interface Problems—Complex Flows
Solidification

Alloy

In addition to the energy equation, we must solve a species concentration equation

$$(C, D) = \begin{cases} (c_1 / k, kD_1) & \textit{in the solid} \\ (c_2, D_2) & \textit{in the liquid} \end{cases}$$

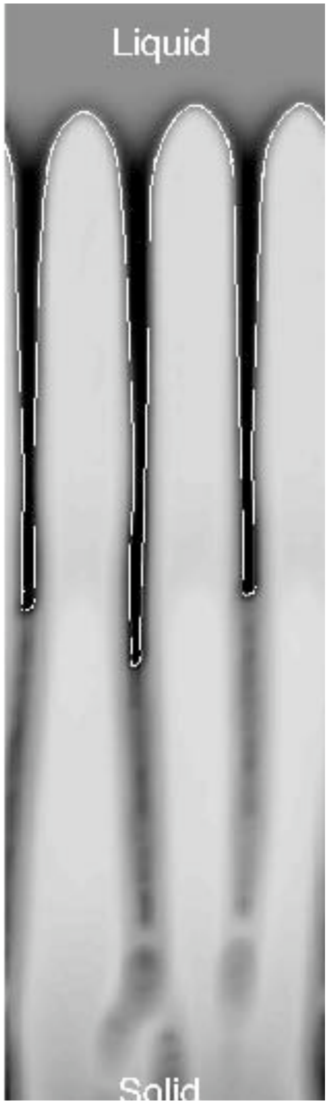
$$k = c_1 / c_2$$

$$\frac{\partial C}{\partial t} = \nabla \cdot D \nabla T + \int s \delta(\mathbf{x} - \mathbf{x}_f) dA$$

$$s = C(1-k)V_n$$

m: slope
of liquidus line

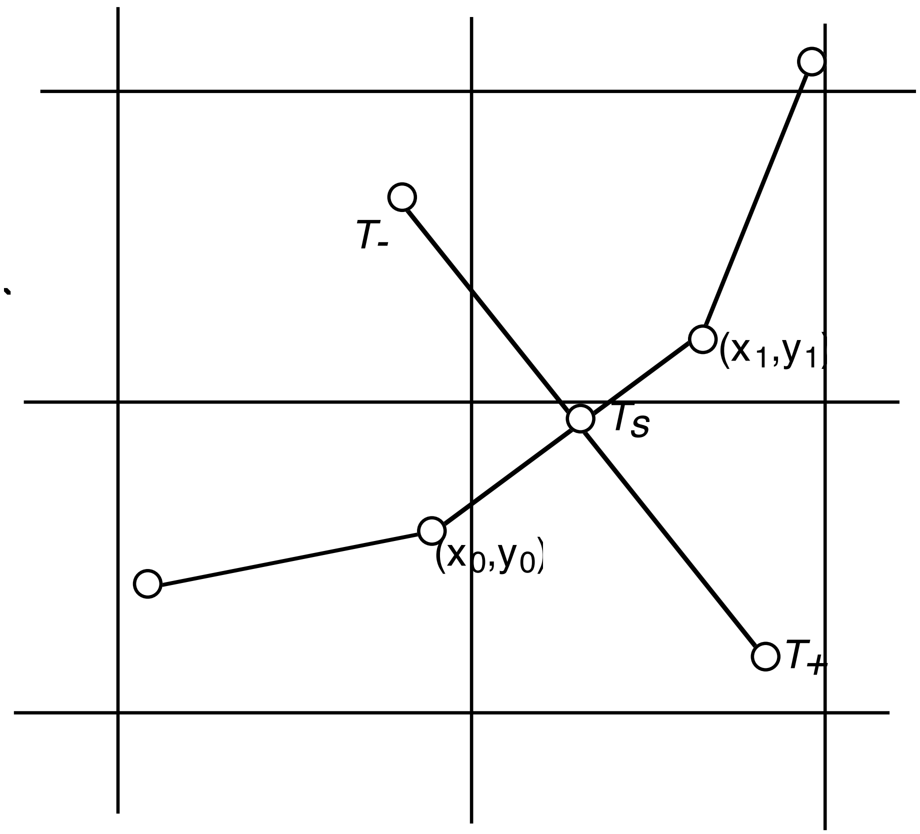
$$T_f = T_m \left(1 + \frac{\kappa}{L} - Cm\right)$$



Compute the heat source at the interface

$$\dot{q} = k\left.\frac{\partial T}{\partial n}\right)_l - k\left.\frac{\partial T}{\partial n}\right)_s$$

Originally we found the heat source iteratively such that the interface temperature matched the target value. Currently we use "normal probes," following Udaykumar et al.



Including the solid:

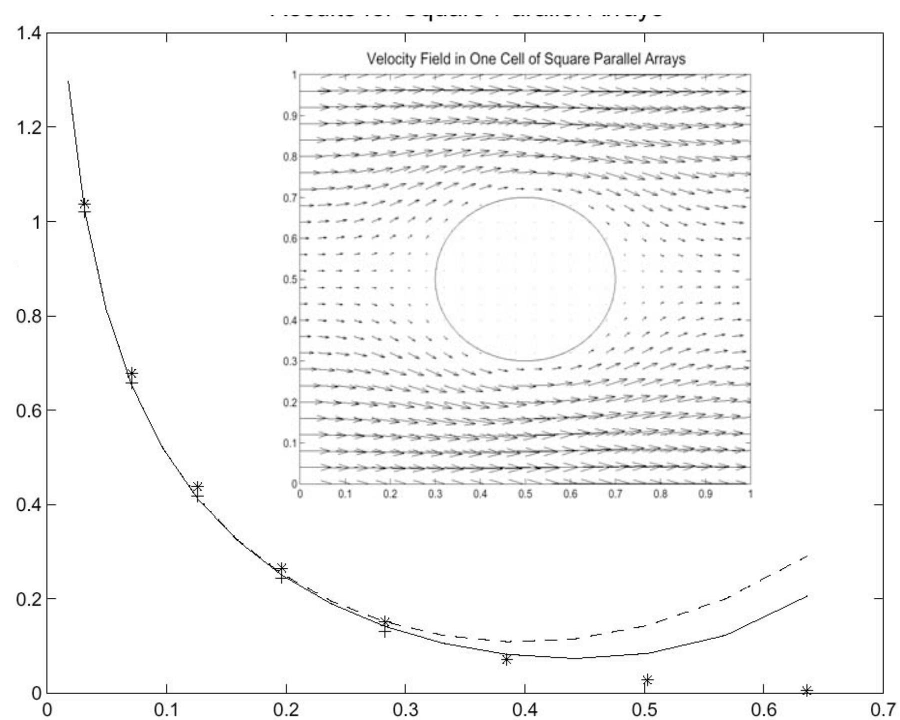
Simplified Procedure

$$\mathbf{u}^* = \mathbf{u}^n + \Delta t \mathbf{A}(\mathbf{u}^n)$$

$$\mathbf{u}^{**} = \mathbf{u}^* - \Delta t \nabla P$$

$$\mathbf{u}^{n+1} = \phi \mathbf{u}^{**}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0$$



Enforcing incompressibility

~0

$$\nabla \cdot \mathbf{u}^{n+1} = \nabla \cdot \phi \mathbf{u}^{**} = \phi \nabla \cdot \mathbf{u}^{**} + \mathbf{u}^{**} \cdot \nabla \phi = 0$$

$$\nabla \cdot \mathbf{u}^{**} = 0$$

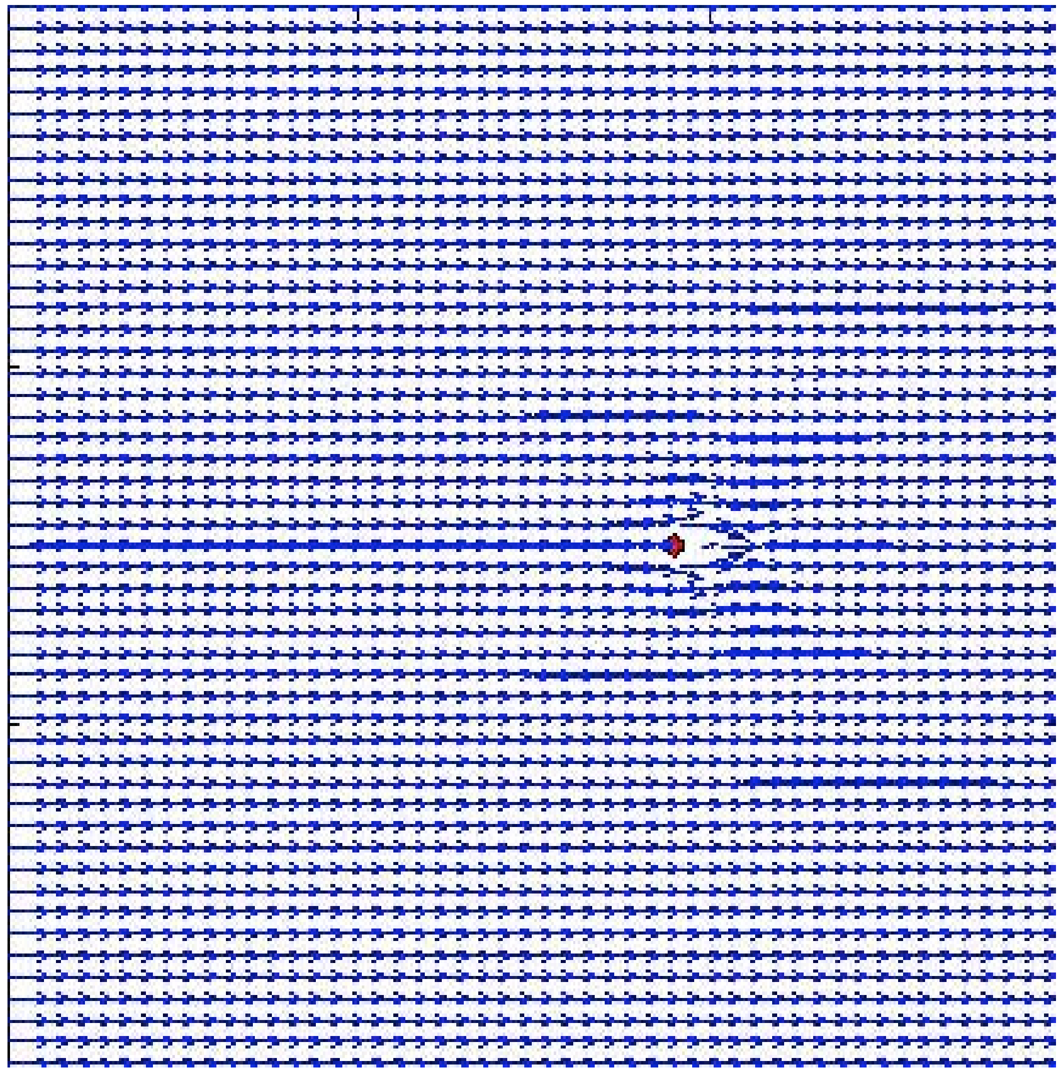
Dendrite growing in a uniform flow

401 by 401grid

Anisotropy=0.4

$$St = \frac{c(T_\infty - T_m)}{L} = -0.3$$

$$Re = \frac{\rho U Z}{\mu} = 600$$



Moving Interface Problems—Complex Flows Solidification

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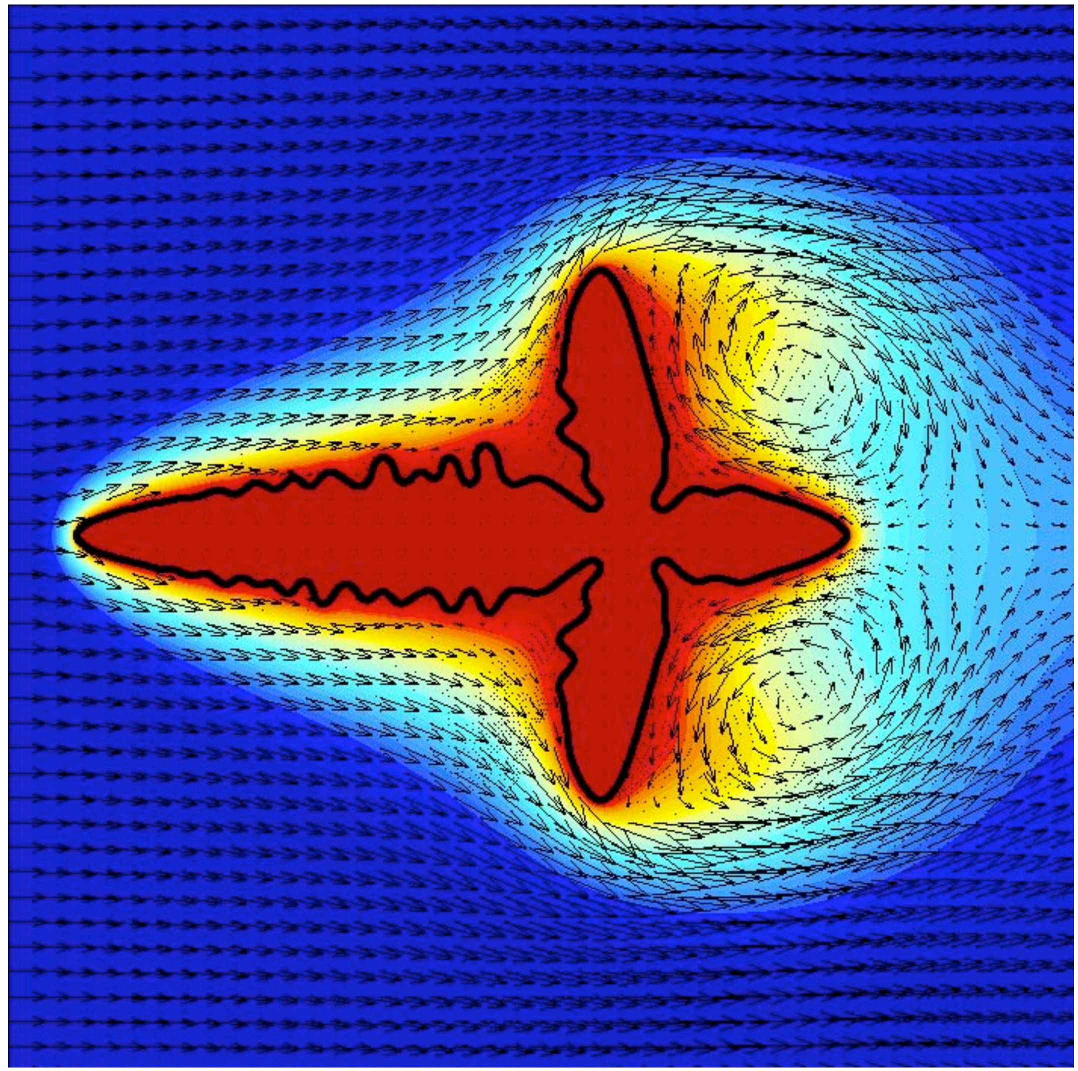

Moving Interface Problems—Complex Flows
Solidification

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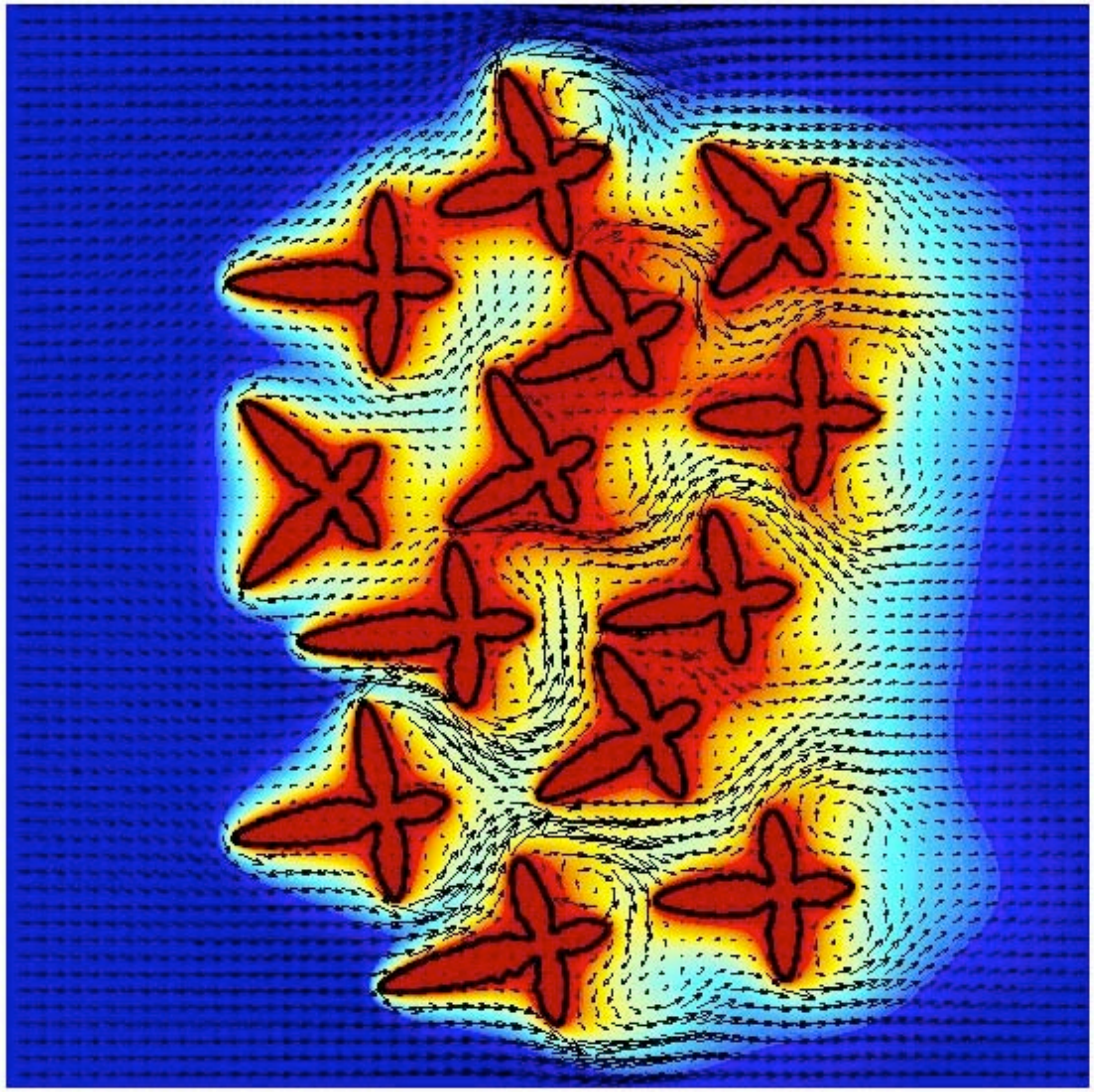
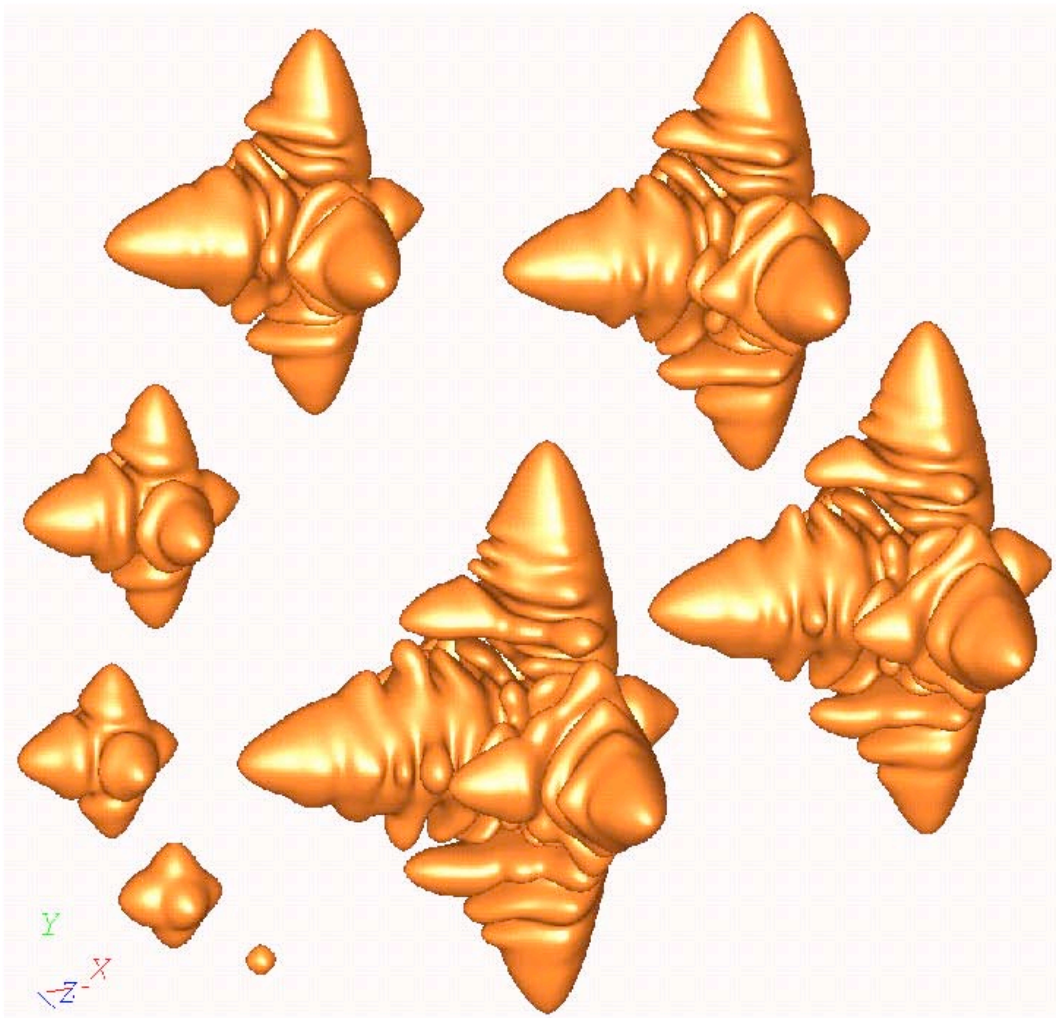
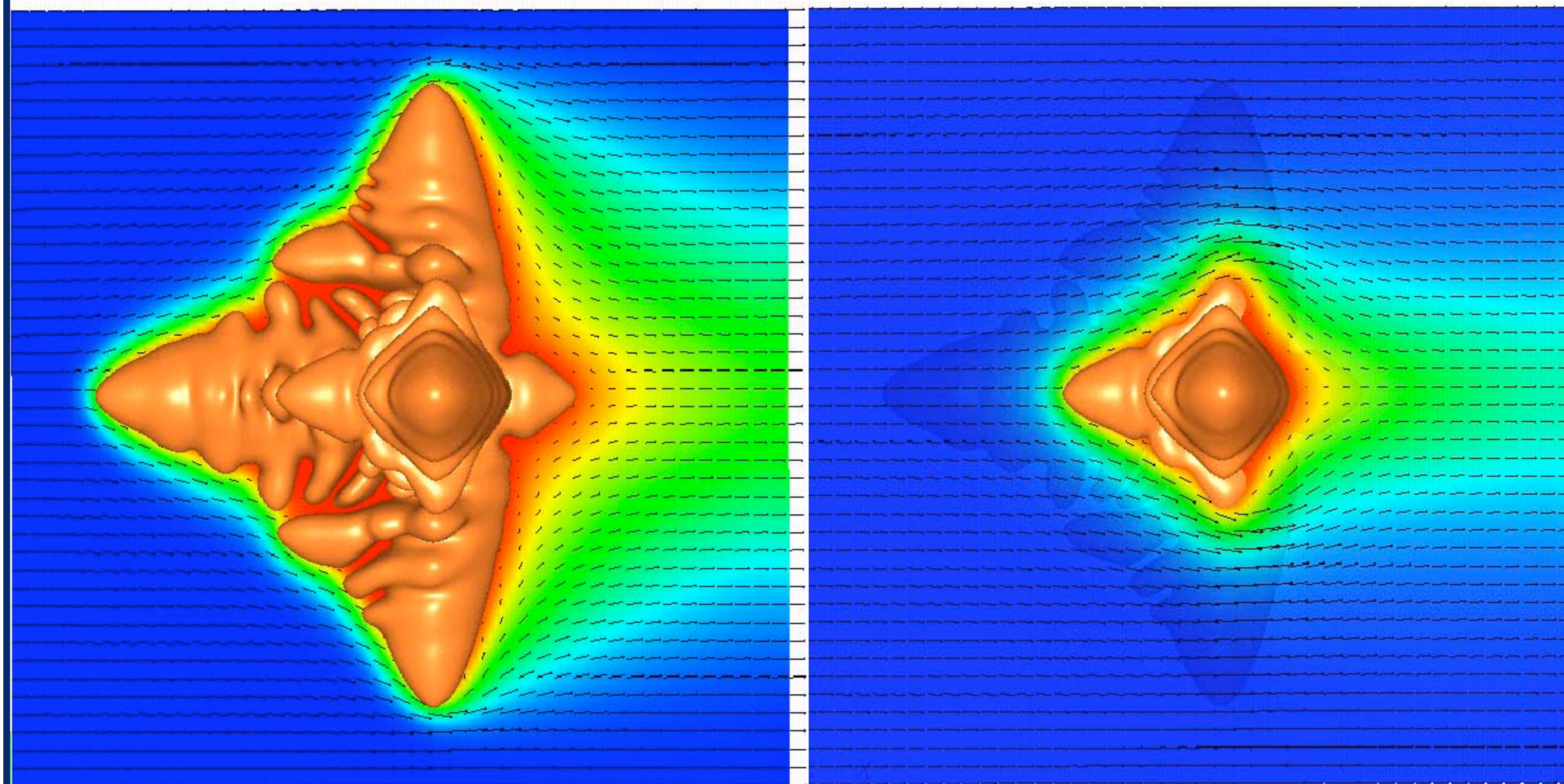


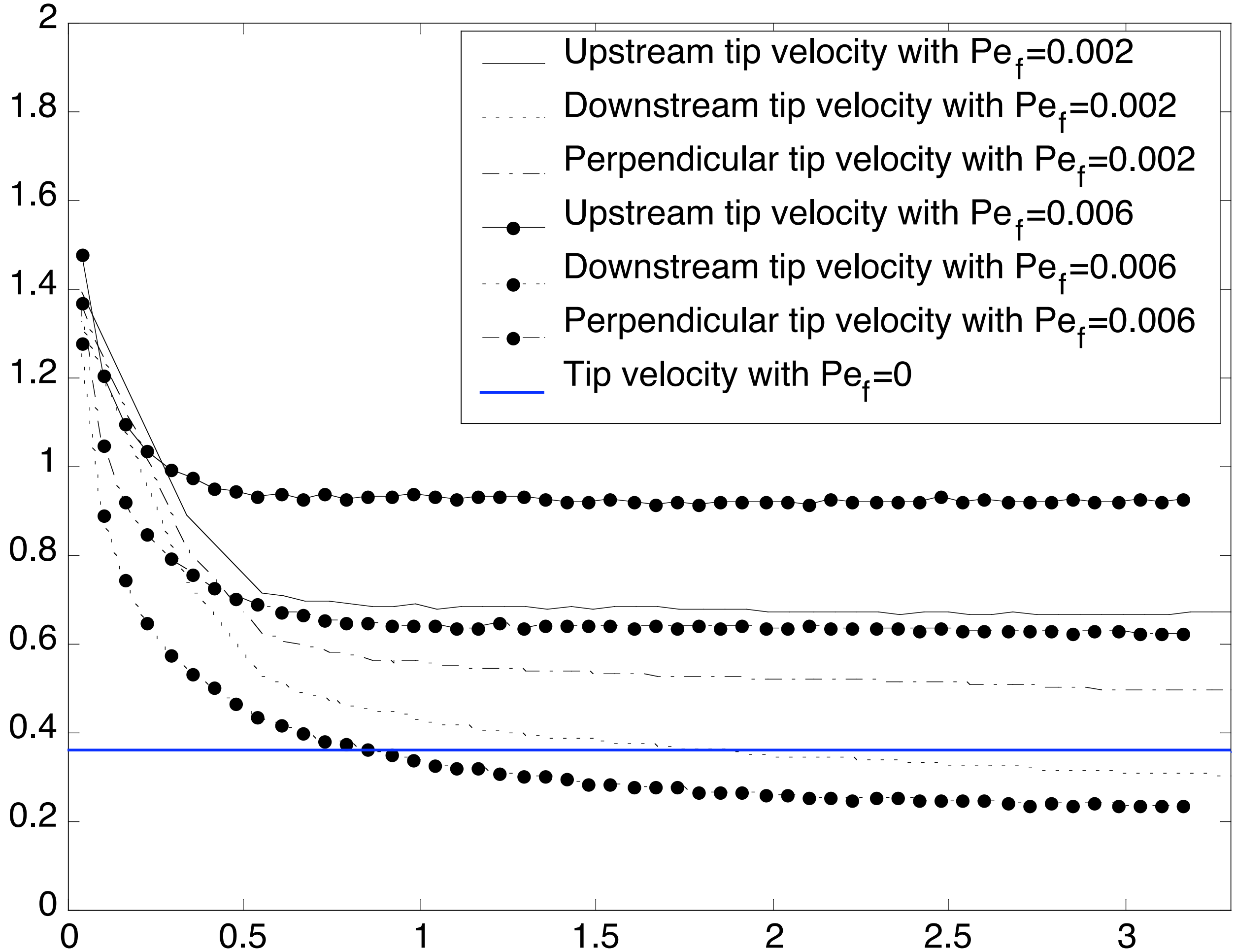
Moving Interface Problems—Complex Flows
Solidification



Moving Interface Problems—Complex Flows
Solidification



Moving Interface Problems—Complex Flows
Solidification

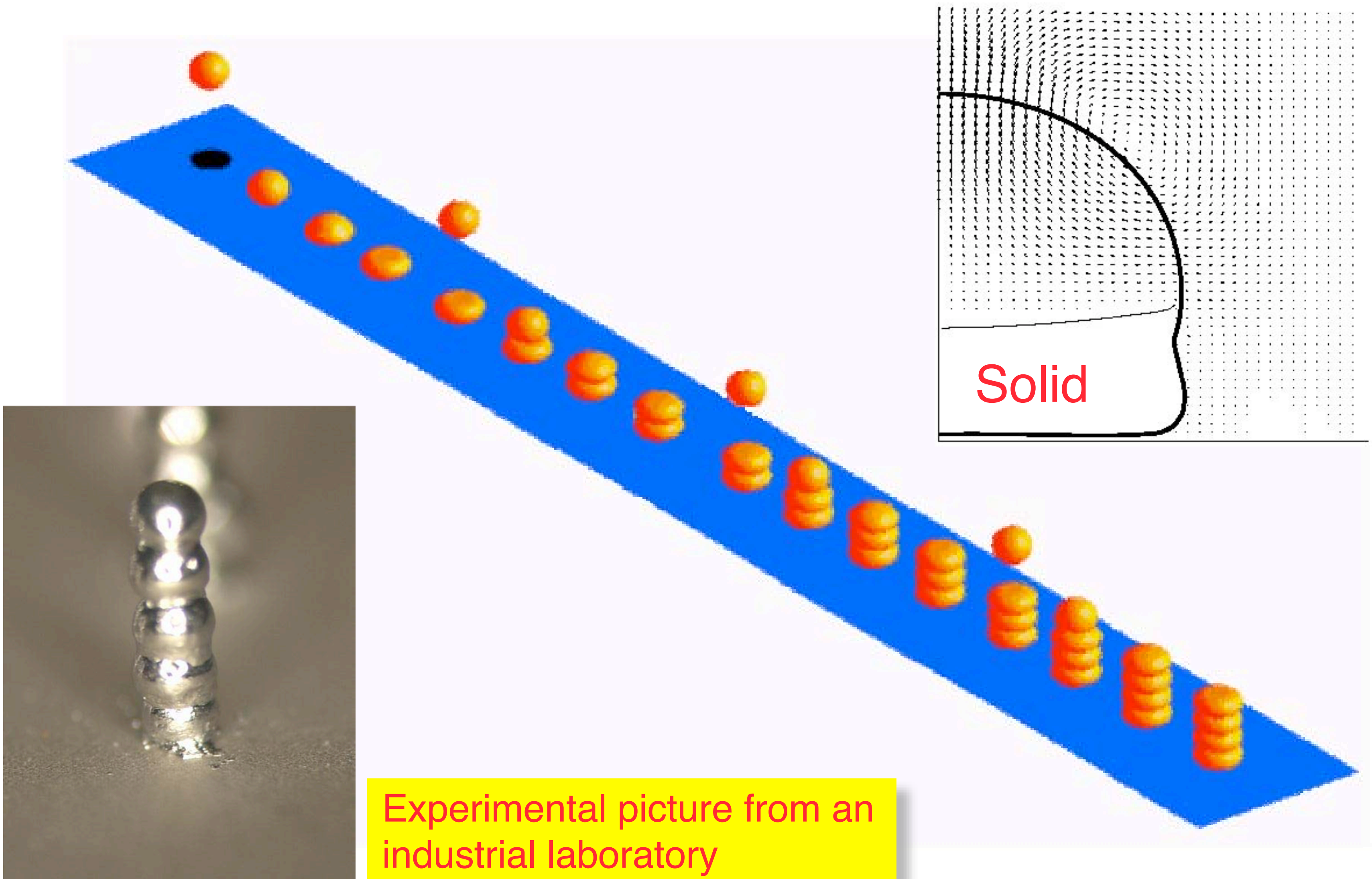


Velocity of the tip of the arms

Key challenges include:

- The extension of the numerical methods to alloys
- Inclusion of more complex interfacial effects
- The use of simulations to predict microstructure of fully solidified materials and the bulk properties of the material
- More complex processes, such as solidification of stirred melts

Moving Interface Problems—Complex Flows
Droplet Impingement and Solidification



Experimental picture from an industrial laboratory

Simulations of Boiling Flows

Early papers on boiling

Juric and Tryggvason (1998)
Son and Dhir (1998)
Son, Ramanujapu, and Dhir (2002)
Welch and Wilson (2000)
Song and Juric (2002)
Esmaeeli and Tryggvason (2002)
Kunugi et al., (2001,2002)

Moving Interface Problems—Complex Flows
Boiling Flows

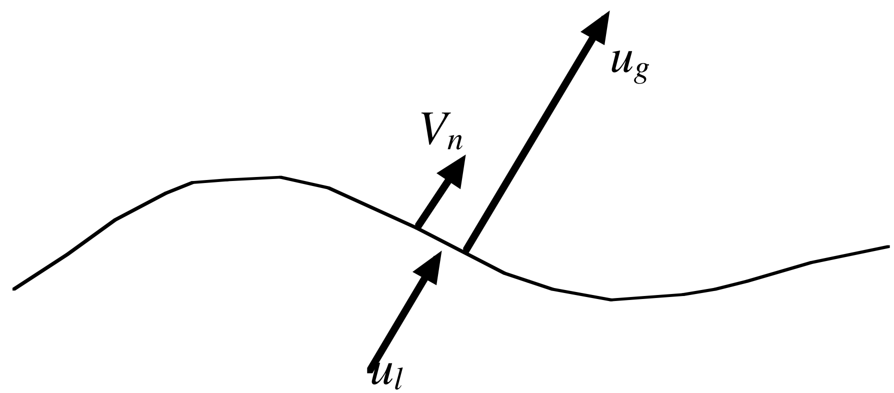
Energy equation	$\frac{\partial cT}{\partial t} + \nabla \cdot \bar{u}T = \nabla \cdot k\nabla T + \int q\delta(\mathbf{x} - \mathbf{x}_f)dA$
Thermodynamic	T_f : Modified Clausius-Clapeyron eq.
Heat source	$q = L(\mathbf{V} - \bar{u}) \cdot \mathbf{n}$
Velocity of bdry	$\frac{dx_f}{dt} = V_n\mathbf{n} + \mathbf{u}$
Mass conservation	$\nabla \cdot \bar{u} = \frac{1}{\rho}\frac{D\rho}{Dt}$

D. Juric and G. Tryggvason. Computations of Boiling Flows. Int'l. J. Multiphase Flow. 24 (1998), 387-410.

A. Esmaeeli and G. Tryggvason. Computations of Explosive Boiling in Microgravity. *J. Scient. Comput*. 19 (2003), 163-182

Computing the volume source

$$\dot{m} = \rho_l(u_l - V_n) = \rho_v(u_v - V_n)$$



Volume expansion:

$$u_v - u_l = \dot{m}\left(\frac{1}{\rho_v} - \frac{1}{\rho_l}\right)$$

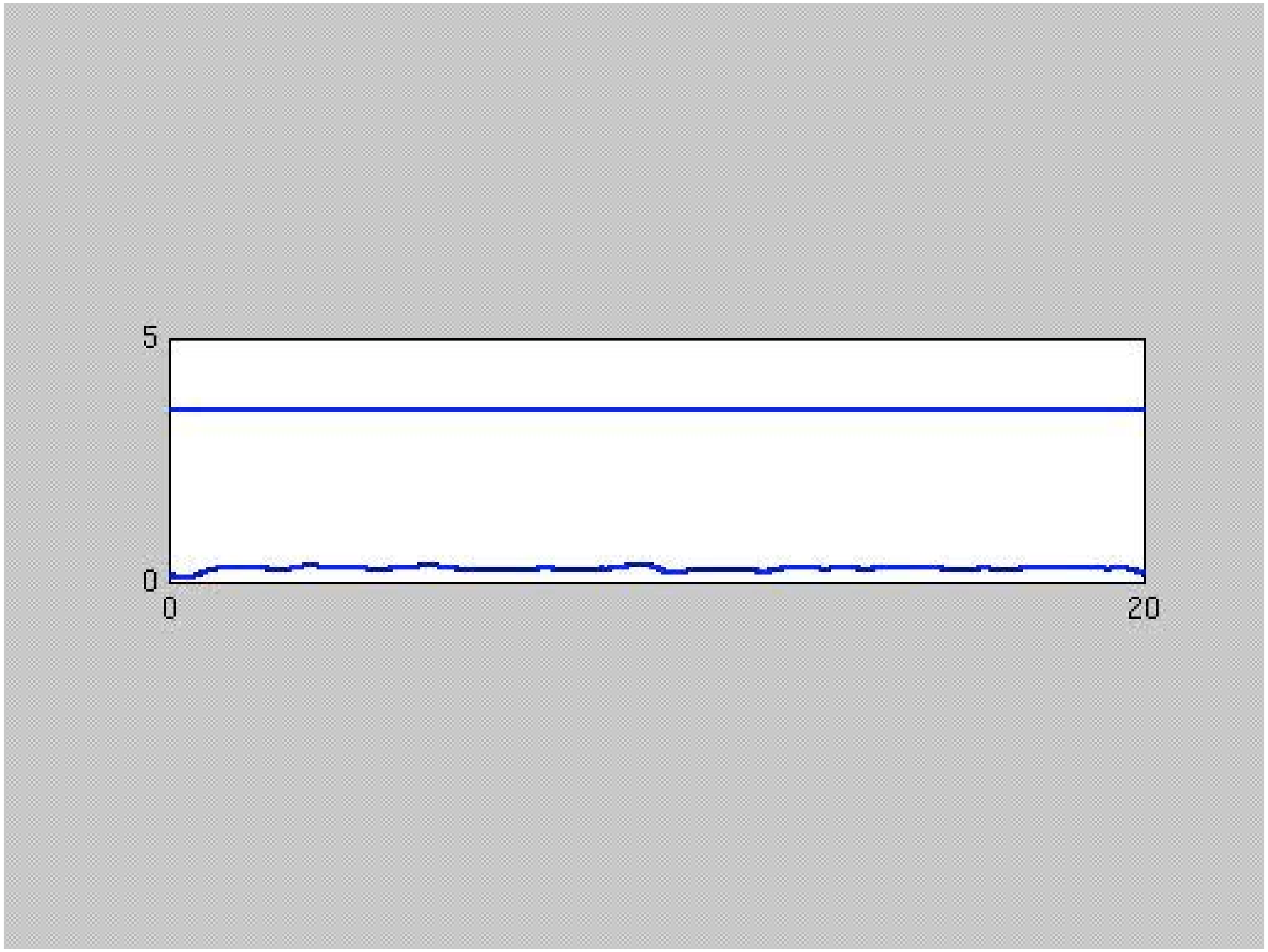
Normal velocity

$$V_n = \frac{1}{2}(u_v + u_l) - \frac{\dot{m}}{2}\left(\frac{1}{\rho_v} + \frac{1}{\rho_l}\right)$$

Source term

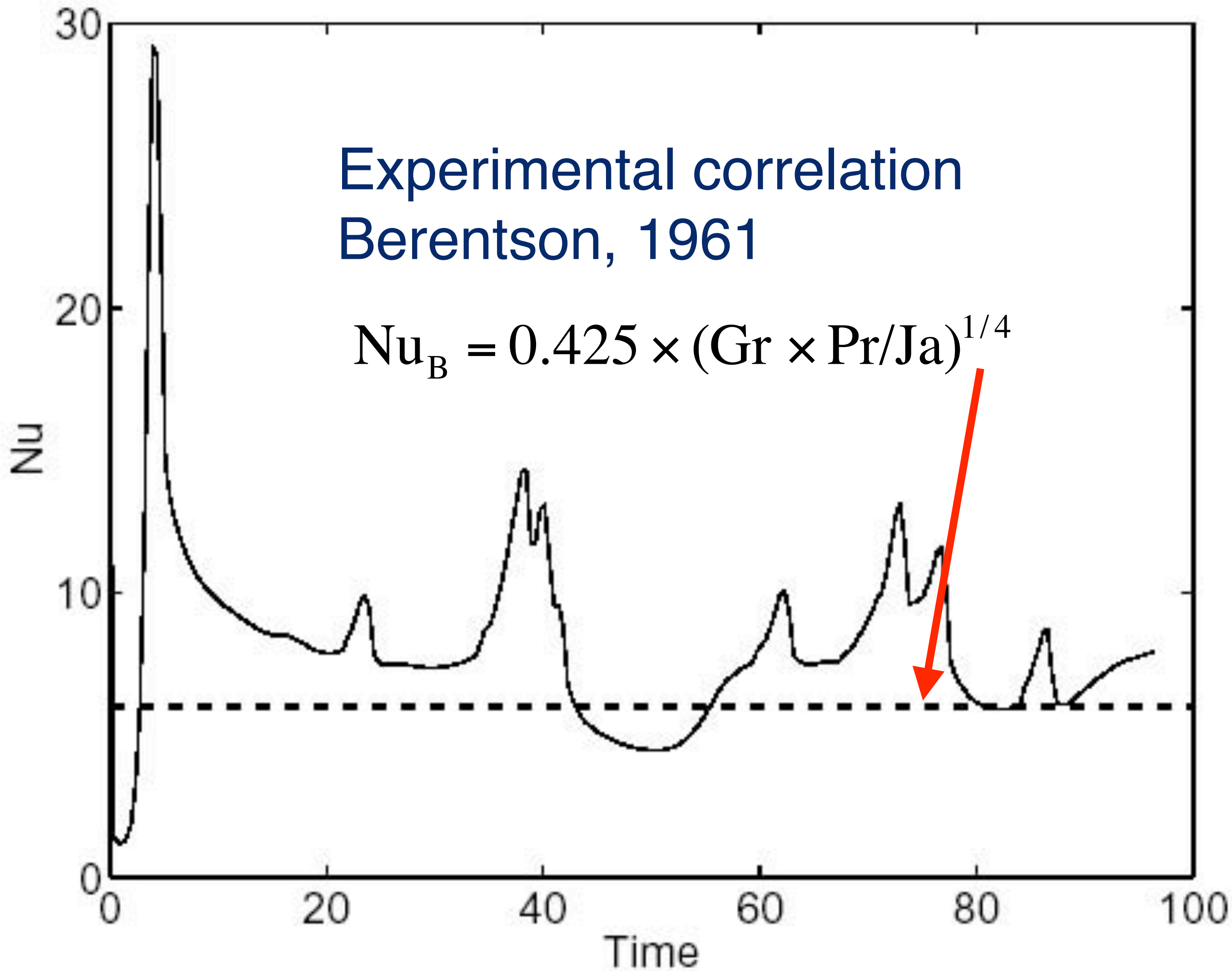
$$\nabla \cdot \mathbf{u} = \frac{\dot{q}}{L}\left(\frac{1}{\rho_v} - \frac{1}{\rho_l}\right)\int \delta(\mathbf{x} - \mathbf{x}_f)\,ds$$

Moving Interface Problems—Complex Flows
Boiling Flows



Moving Interface Problems—Complex Flows
Boiling Flows

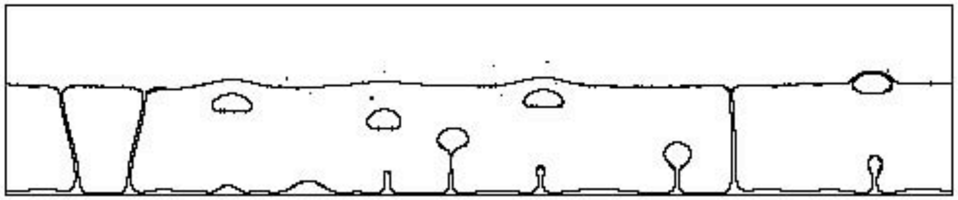
Nusselt number versus time



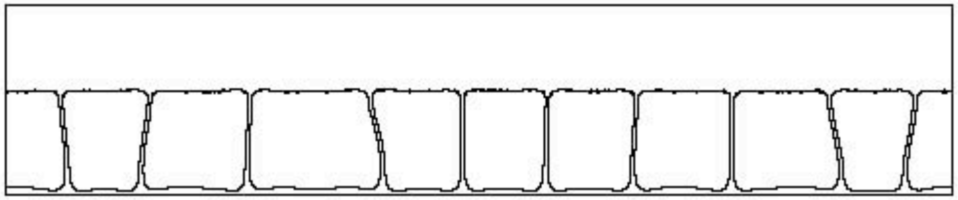
Moving Interface Problems—Complex Flows
Boiling Flows

The effect of the Jacobi number on the boiling for near critical film boiling

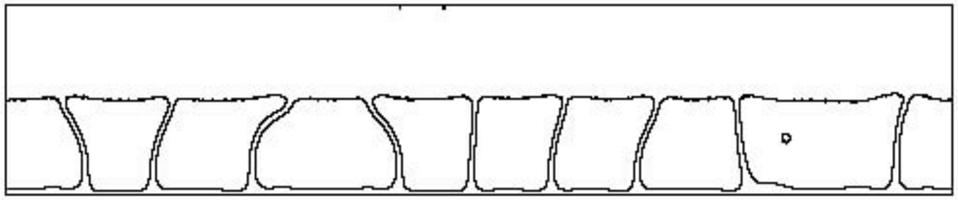
Ja=0.035



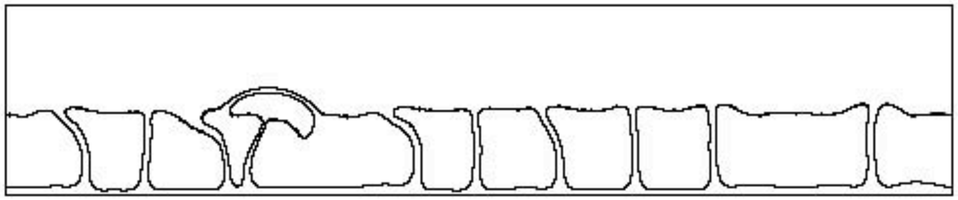
Ja=0.117



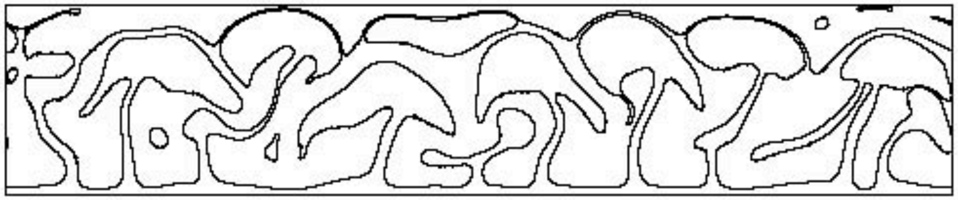
Ja=0.234



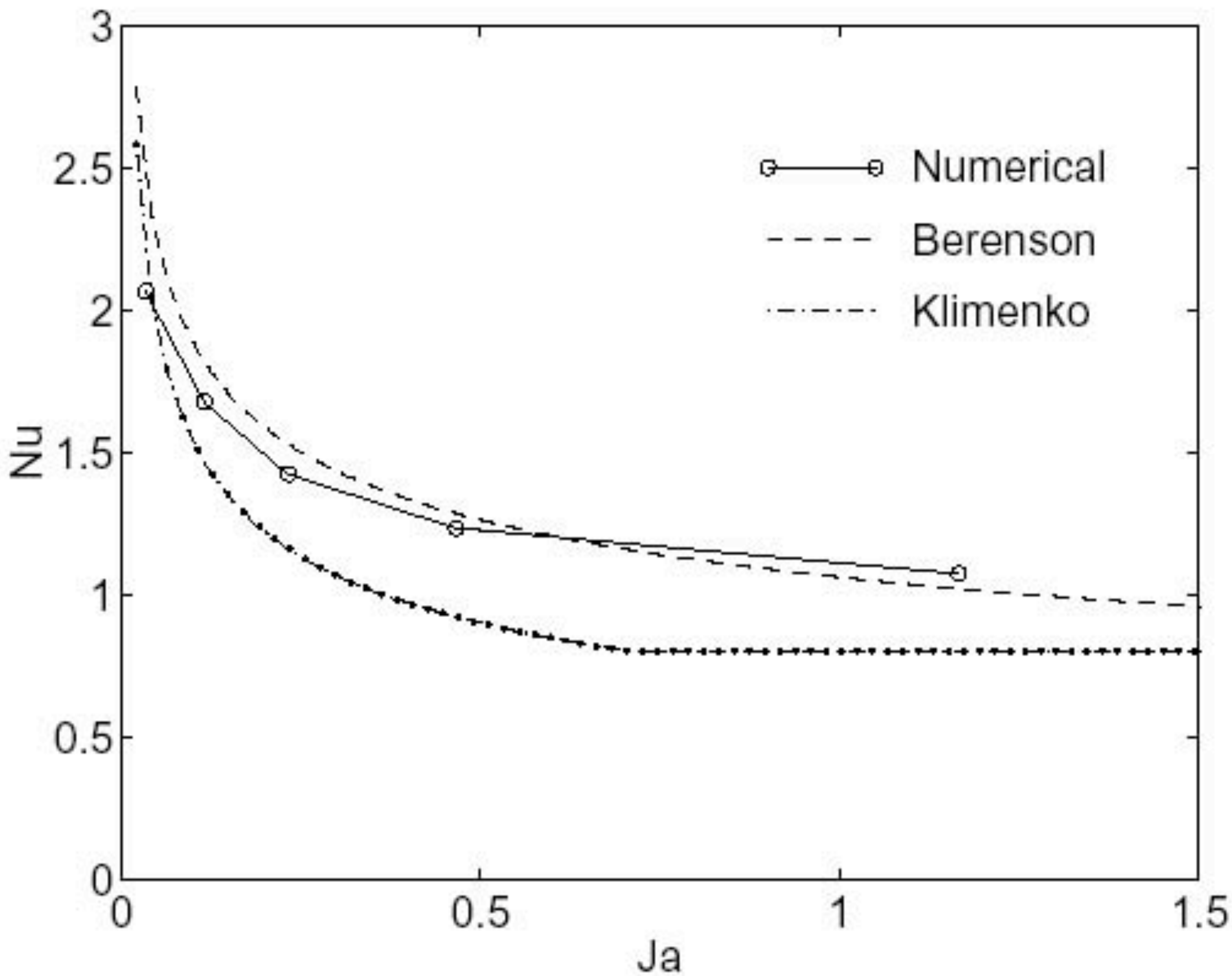
Ja=0.468



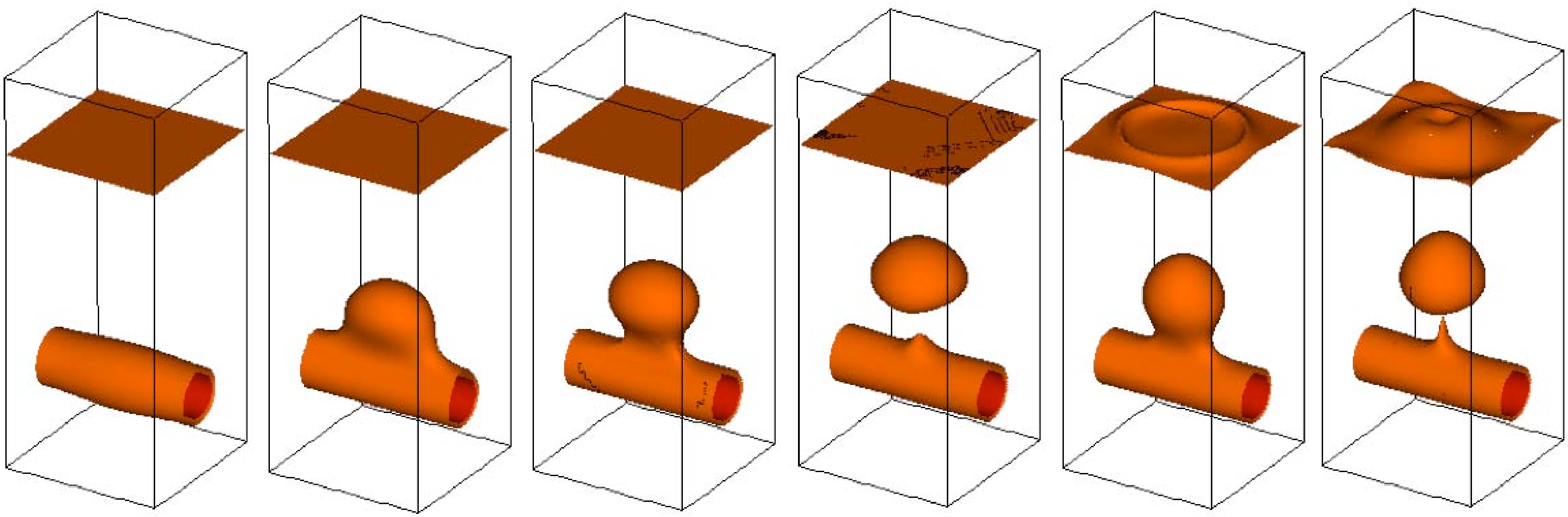
Ja=1.167



Moving Interface Problems—Complex Flows
Boiling Flows

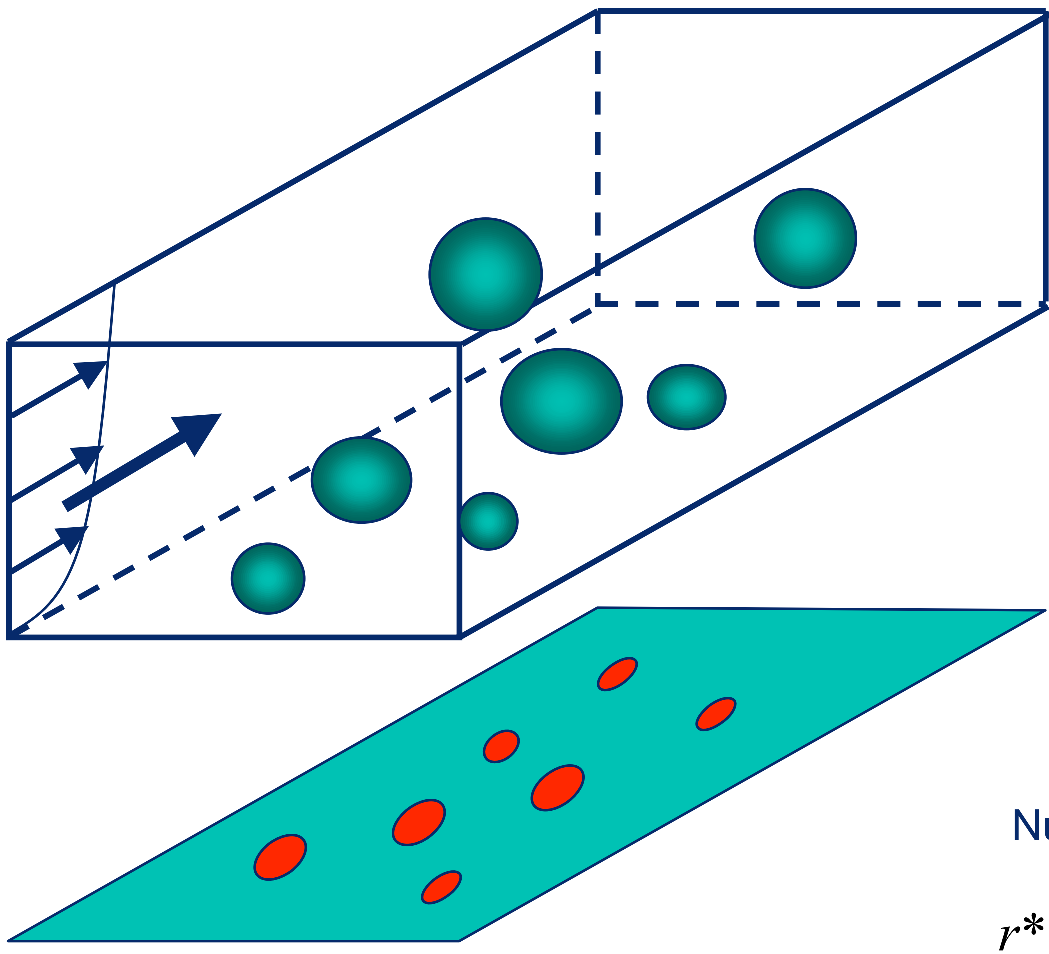


Film boiling from an embedded solid object. A hot solid cylinder is represented by an indicator function on a rectangular structured grid. As the vapor region around the cylinder grows, bubbles periodically break off and rise to the free surface



Time →

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)

Moving Interface Problems—Complex Flows
Boiling Flows

Heat Conduction across Liquid Film

$$\dot{q} = \frac{k_l\left(T_{wall} - T_{int}\right)}{\delta}$$

Modified Clausius-Clapeyron equation

$$\dot{q} = 2(M/2\pi \bar{R} T_v)^{1/2}\frac{\rho_v h_{lv}^2}{T_v}$$

$$\left[T_{int} - T_v + (P_l - P_v)T_v/\rho_l h_{lv}\right]$$

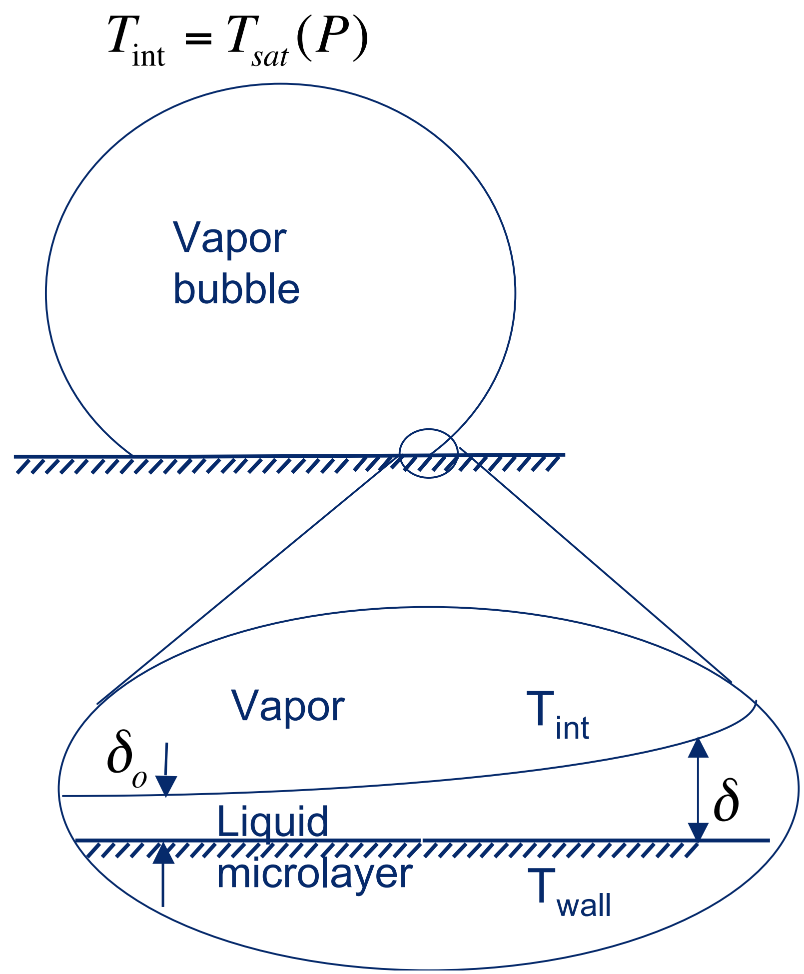
Modified Laplace-Young equation

$$p_l - p_v = -\sigma\kappa - \frac{A}{\delta^3} + \frac{\dot{q}}{\rho_v h_{lv}^2}$$

Combine to find: $\dot{q} = \dot{q}(\delta)$

Model of: Son, Dhir, Ramanujapu (1999)

Microlayer Modeling



Moving Interface Problems—Complex Flows
Boiling Flows

Rise of a Steam Bubble in Saturated Water

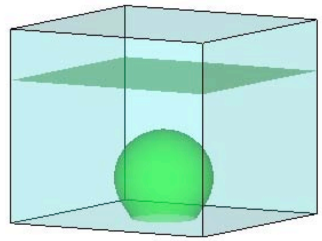
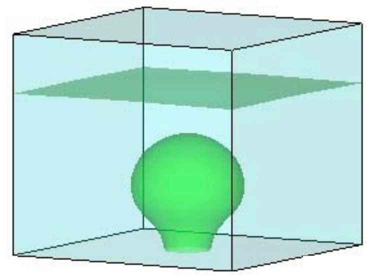
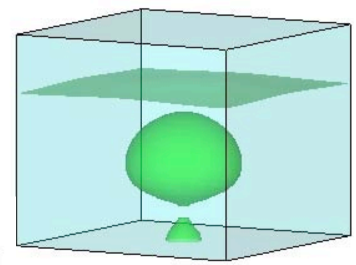
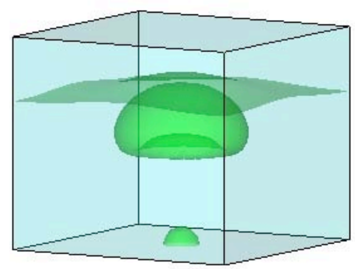
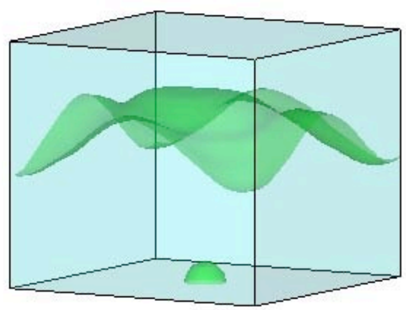
From Damir Juric

- $15mm^3$ horizontally periodic box
- Initial bubble radius 2.5 mm
- Cavity radius 1 mm

- Liquid/Vapor:

density ratio = 1605
viscosity ratio = 23
thermal conductivity ratio = 27
specific heat ratio = 1

- Wall superheat = 5K

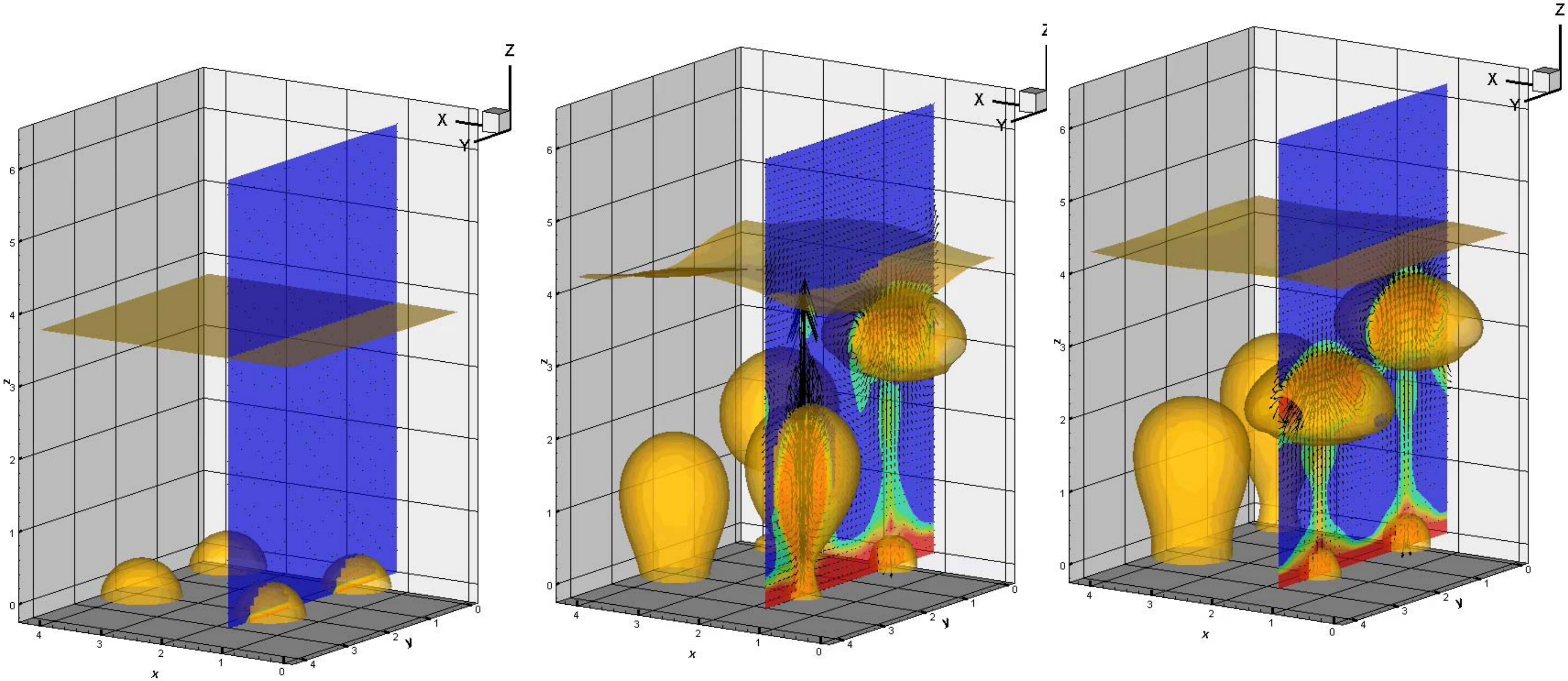






•Front Tracking with Level Contour Reconstruction

•Staggered grid MAC/Projection solution of two-phase incompressible Navier-Stokes Equations

•2nd order ENO advection
•Wall refined grid
•BiCGSTAB solution of pressure Poisson equation

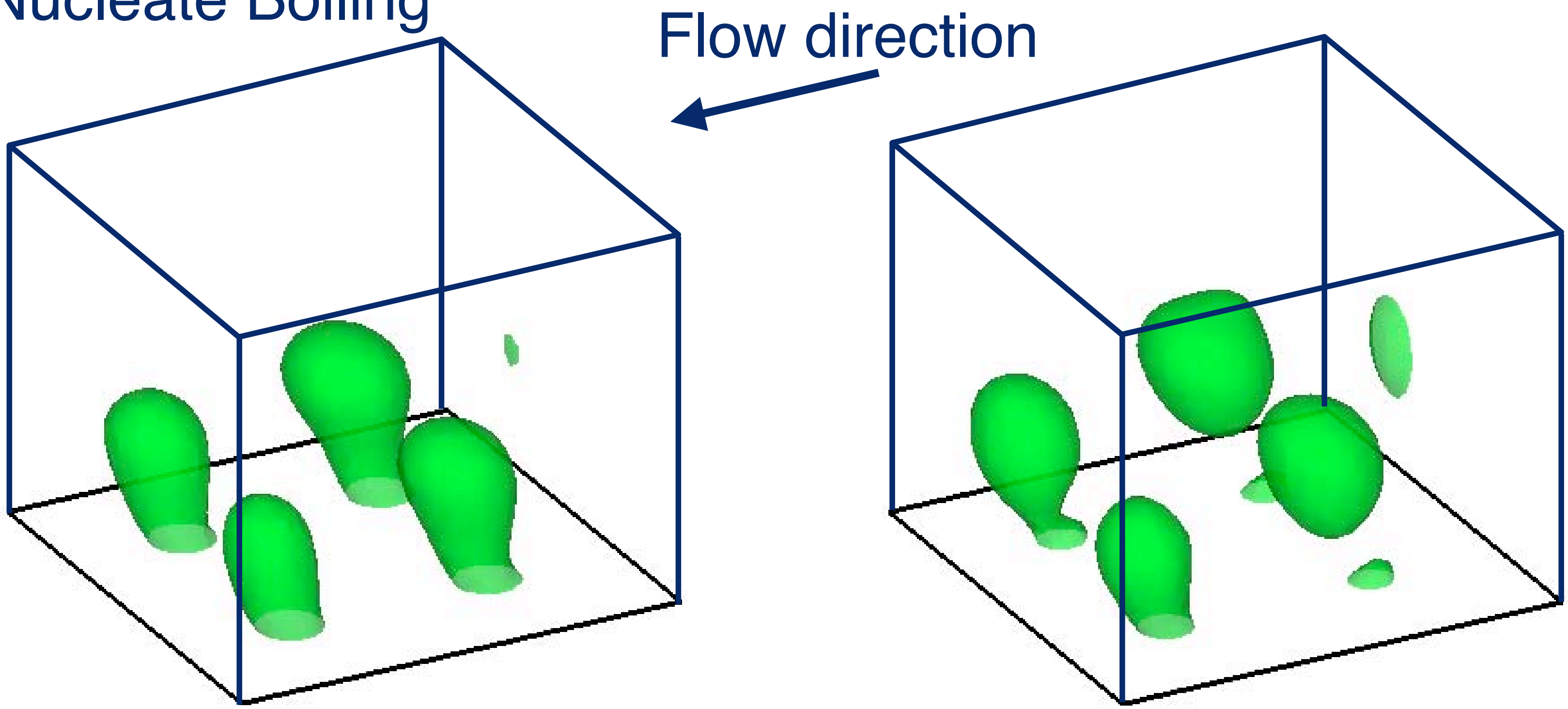
Moving Interface Problems—Complex Flows



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

Moving Interface Problems—Complex Flows
Boiling Flows

Nucleate Boiling



• Liquid/Vapor:
density ratio = 1605
viscosity ratio = 23
thermal conductivity ratio = 27
specific heat ratio = 1
• Wall superheat = 5K

• 15mm^3 horizontally periodic box
• Initial bubble radius 2.5 mm
• Cavity radius 1 mm

•2nd order ENO advection
•Wall refined grid
•BiCGSTAB solution of pressure Poisson equation

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.

Electrohydrodynamics of Droplet Suspensions

Electrostatic fields are known to have strong influence on multiphase flows:

- Breakup of jets and drops
- Phase distribution in suspensions

Here, we examine the effect of electrostatic fields on a suspension of drops in channel flows by direct numerical simulations.

For fluids with small but finite conductivity, Taylor and Melcher (1969) proposed the “leaky dielectric” model. This model allows both normal and tangential electrostatic forces on a two fluid interface.

The fluid flow

Momentum (conservative form, variable density and viscosity)

$$\frac{\partial \rho \bar{u}}{\partial t} + \nabla \cdot \rho \bar{u}\,\bar{u} = -\nabla p + \bar{f}$$

Electric force

$$+ \nabla \cdot \mu\left(\nabla \bar{u} + \nabla^T \bar{u}\right) + \int_F \sigma \kappa\, \bar{n}\, \delta\left(\bar{x} - \bar{x}_f\right) da$$

Surface tension

Mass conservation (incompressible flows)

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

Moving Interface Problems—Complex Flows
Electrohydrodynamics

The electric field is obtained from the equation for the conservation of current:

$$\cancelto{0}{\frac{Dq}{Dt}} = \nabla \cdot \sigma\mathbf{E}$$

neglecting also convection of charge

the charge accumulation is found by:

$$q = \nabla \cdot \varepsilon\mathbf{E}$$

The force on the fluid is then found by:

$$\mathbf{f} = q\mathbf{E} - \tfrac{1}{2}(\mathbf{E}\cdot\mathbf{E})\nabla\varepsilon$$

Boundary between prolate and oblate drops

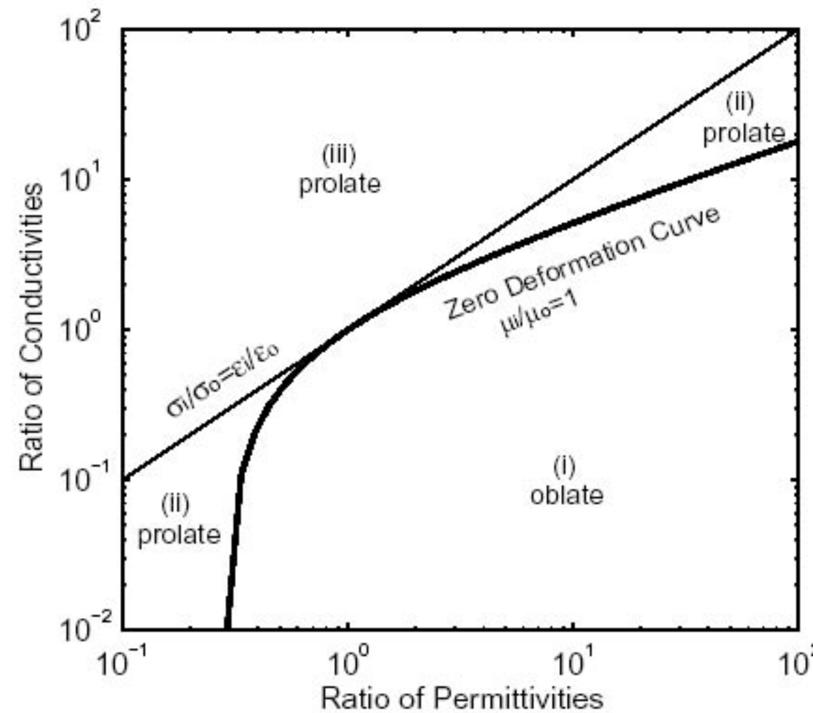
$$\Phi_{3D} = \frac{\varepsilon_o}{\varepsilon_i}\left(\left(\frac{\sigma_i}{\sigma_o}\right)^2 + 1\right) - 2 + \frac{3}{5}\left(\frac{\sigma_i}{\sigma_o}\frac{\varepsilon_o}{\varepsilon_i} - 1\right)\left(\frac{2\left(\frac{\mu_o}{\mu_i} + 3\right)}{\frac{\mu_o}{\mu_i} + 1}\right)$$

Taylor (1966)

$$\Phi_{2D} = \left(\frac{\sigma_i}{\sigma_o}\right)^2 + \frac{\sigma_i}{\sigma_o} + 1 - 3\frac{\varepsilon_i}{\varepsilon_o}$$

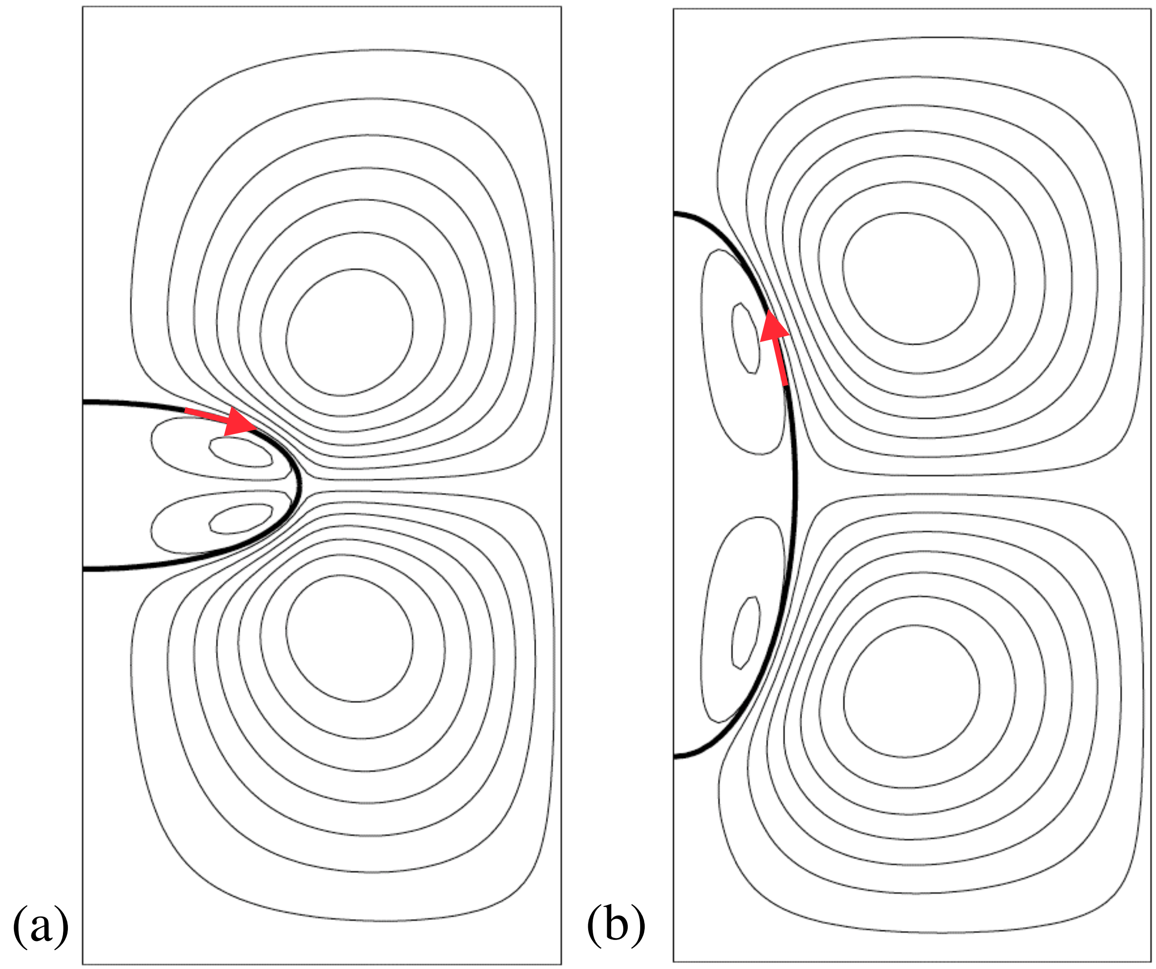
Rhodes et al. (1988)

$$\Phi = \begin{cases} > 1 & \text{Prolate} \\ = 0 & \text{Spherical} \\ < 1 & \text{Oblate} \end{cases}$$

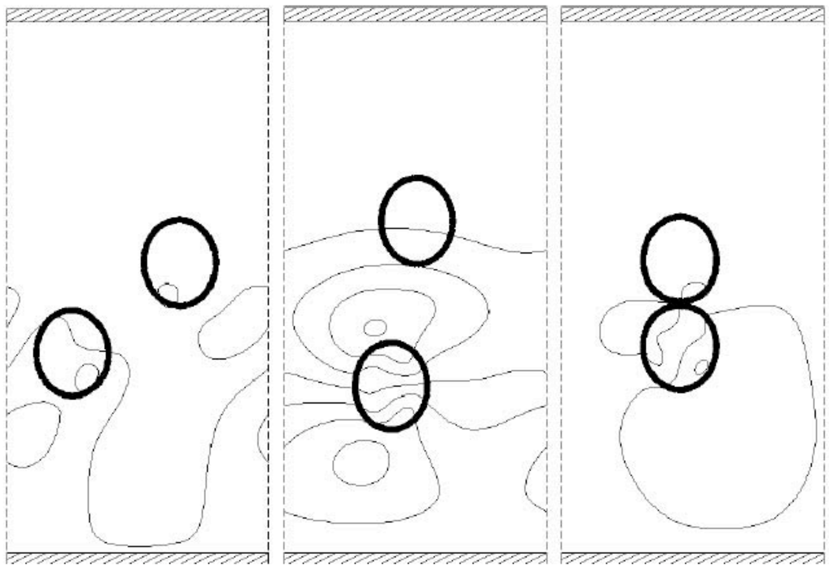


Deformation of a Single Drop

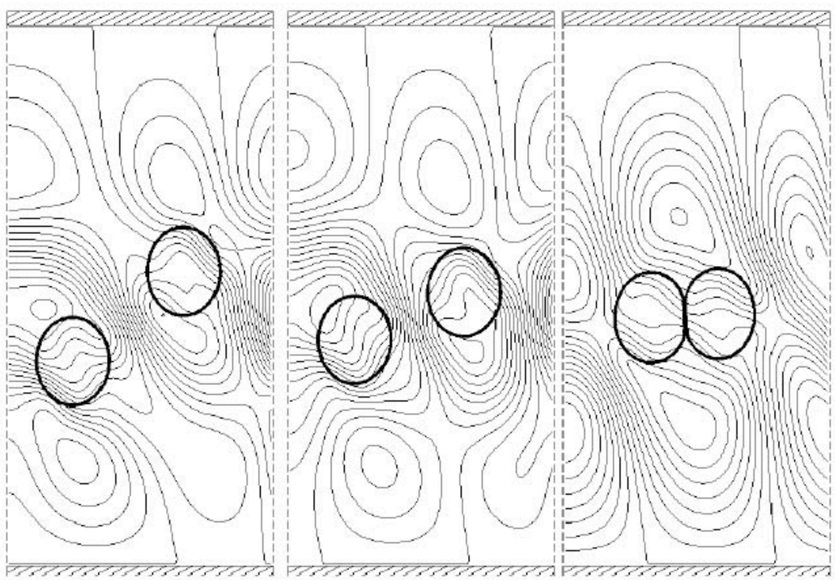
Electrostatic deformation of axisymmetric drops. The steady state obtained after following the transient motion of an initially spherical drop. For the oblate drop in (a) the ratio of the dielectric constant of the drop to the dielectric constant of the suspending fluid is much larger than the conductivity ratio, but for the prolate drop in (b) both ratios are comparable



Moving Interface Problems—Complex Flows
Electrohydrodynamics



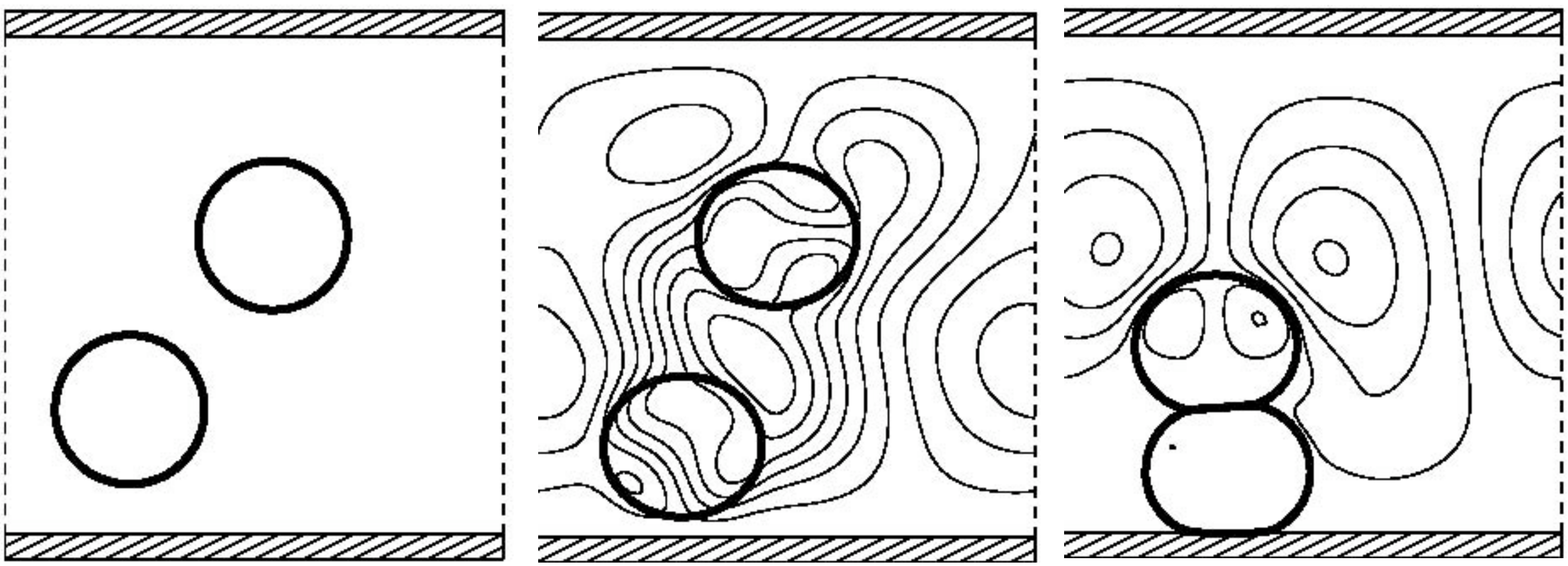
Drop distribution and streamlines for the interaction between two prolate drops. $S^{-1} = 0.01$, R=0.1; initial distance between the drops centroids r_0=3.5 times the radius



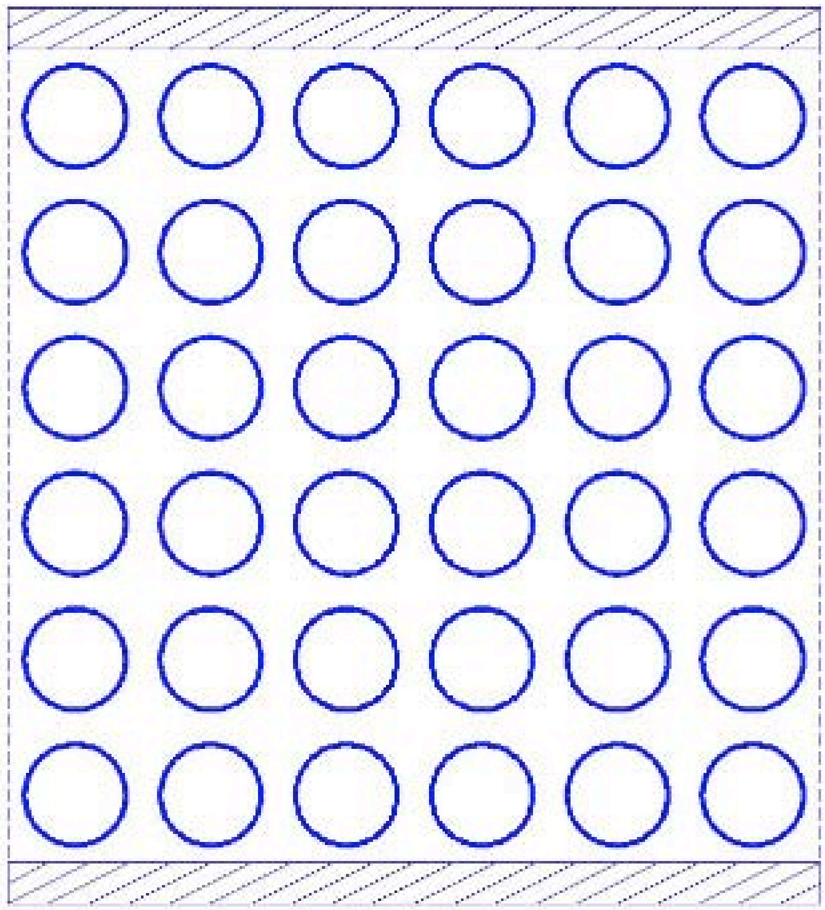
Drop distribution and streamlines for the interaction between two prolate drops. $S^{-1} = 0.01$, R=1.0; initial distance between the drops centroids r_0=3.5 times the radius

$$R = \frac{\sigma_i}{\sigma_o}; \quad S^{-1} = \frac{\varepsilon_i}{\varepsilon_o};$$

Interaction of Two Drops



The motion of two oblate drops in a quiescent flow. The drops align with the electric field and attract each other. The drops are also attracted to the wall

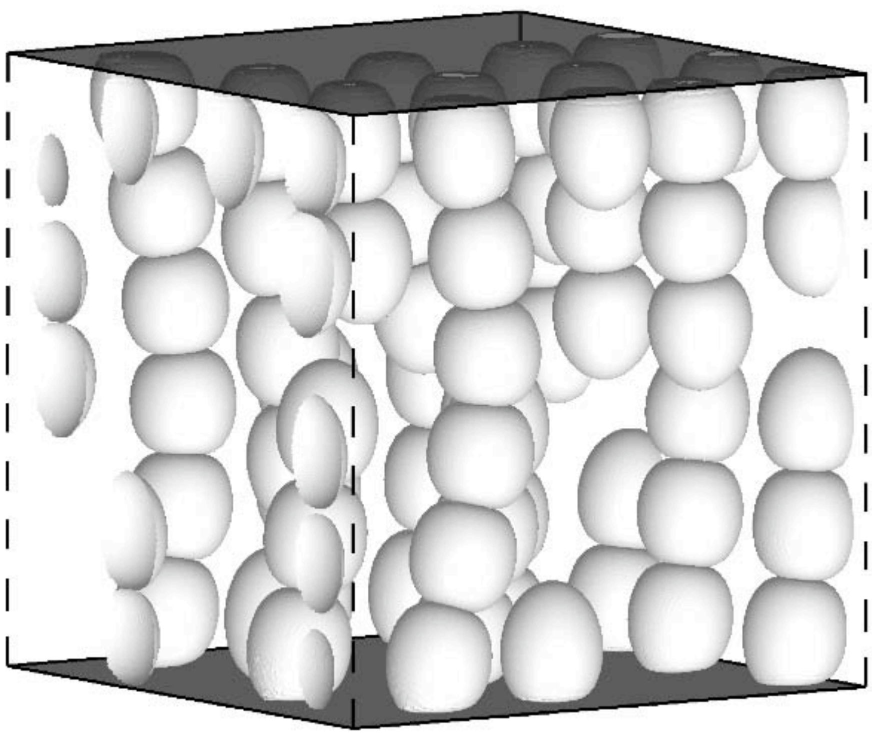


Moving Interface Problems—Complex Flows
Electrohydrodynamics

$\sigma_i/\sigma_o = 0.005 \quad \mathrm{Re} = 20$

$\varepsilon_i/\varepsilon_o = 0.01 \quad We = 0.0625$

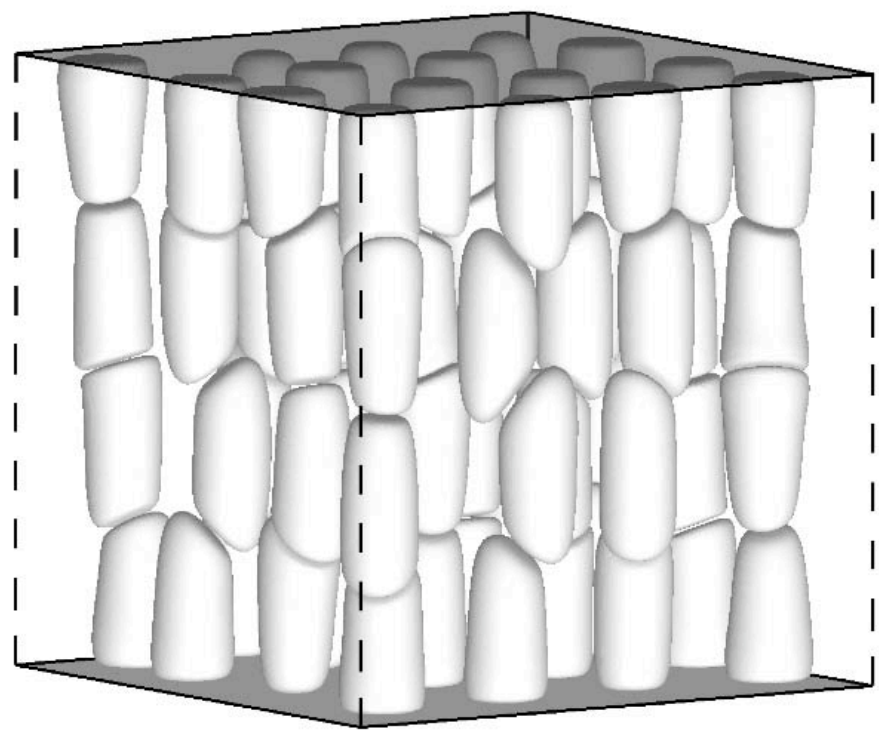
$\alpha = 20\% \quad E^* = 0.0182$



$\sigma_i/\sigma_o = 0.01 \quad \mathrm{Re} = 20$

$\varepsilon_i/\varepsilon_o = 0.1 \quad We = 0.0625$

$\alpha = 20\% \quad E^* = 0.04$



The interaction of many drops in channels, with and without flow has been examined.

Oblate drops always fibrate as the electrohydro-dynamically induced fluid motion works with the electric interactions to line up the drops

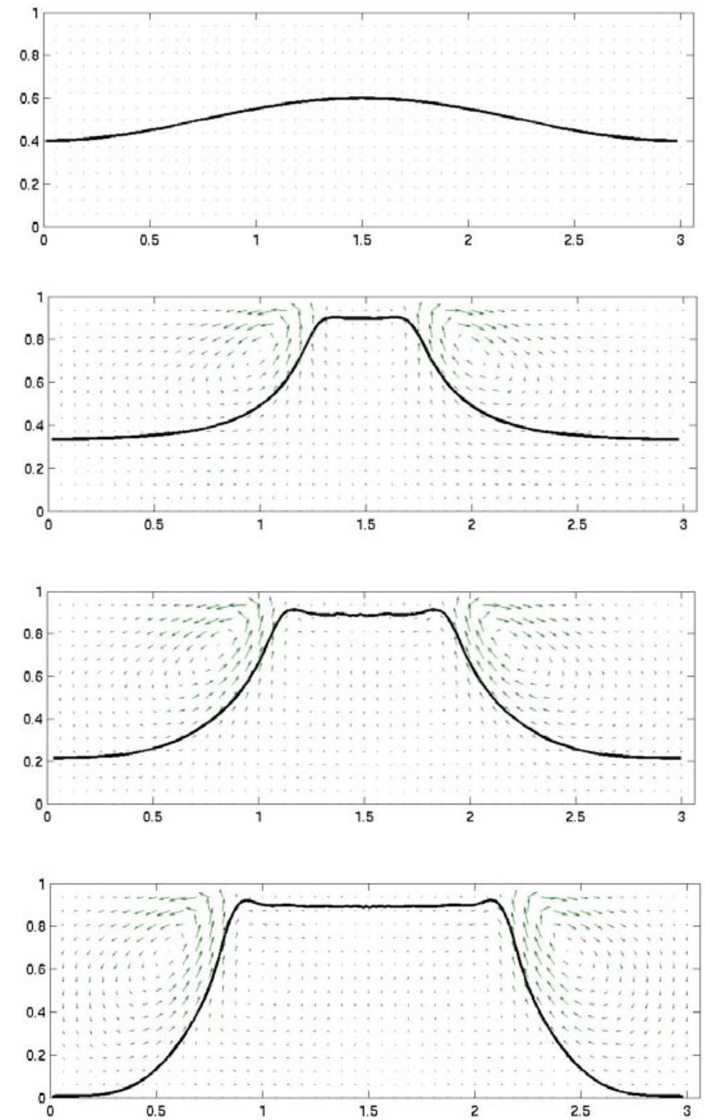
Fluid shear breaks up the fibers, depositing them on the walls for intermediate flow rate and keeping them in suspension for high enough flow rates

Prolate drops exhibit more complex interaction and form additional structures

Moving Interface Problems—Complex Flows
Electrohydrodynamics

The instability of a thin film:

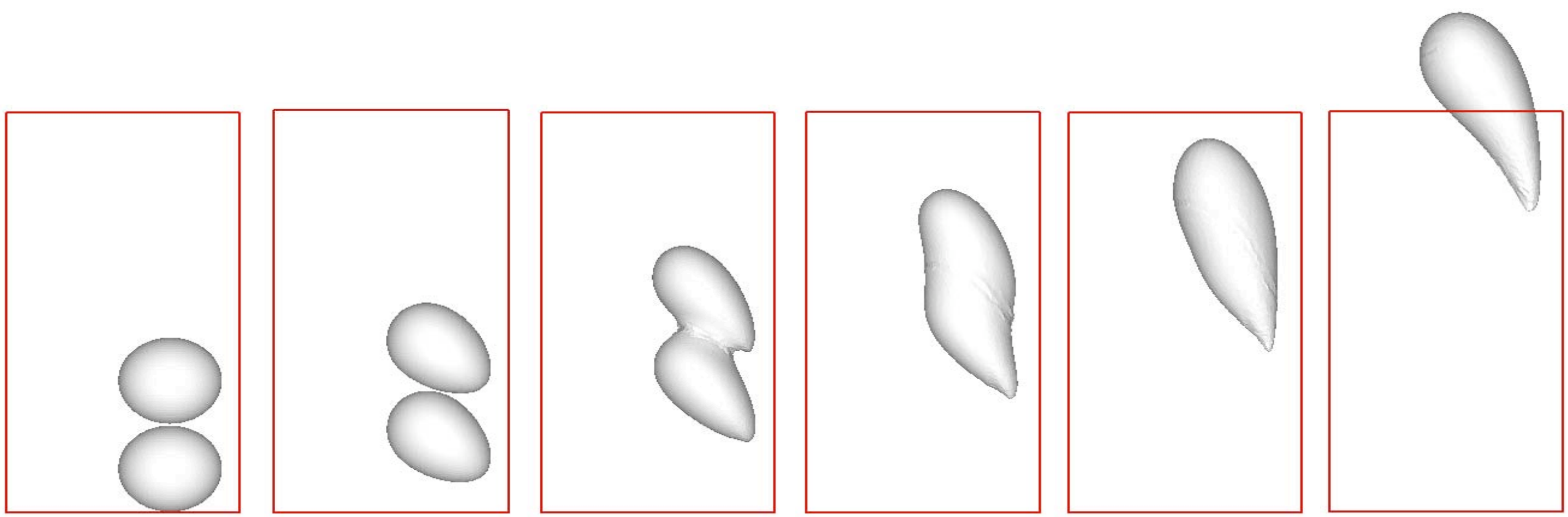
The interface and the velocity field at time zero and three subsequent times for S=1 and R=100.



Coalescence induced flow regime transitions

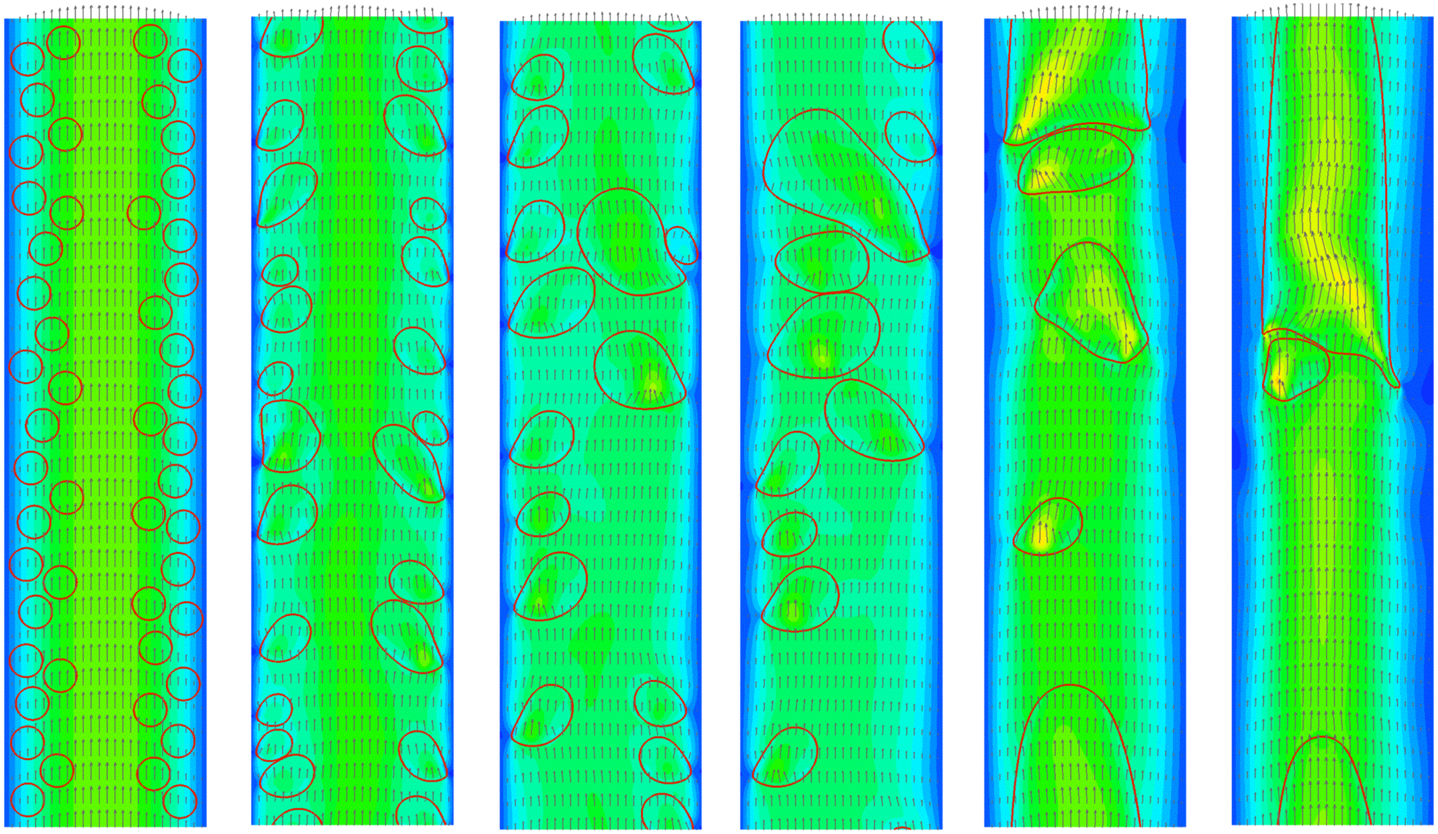
Moving Interface Problems—Complex Flows
Coalescence

High bubble concentration at the walls is likely to lead to bubble collisions and coalescence. The collision of small and nearly spherical bubbles-which hug the wall-to form large deformable bubbles—that are repelled by the wall—is likely to be one of the major mechanism responsible for changing the void fraction distribution from “wall-peak” to a maximum in the core. The figure shows a simulation of the collision of two nearly spherical bubbles and the evolution of the resulting large bubble.

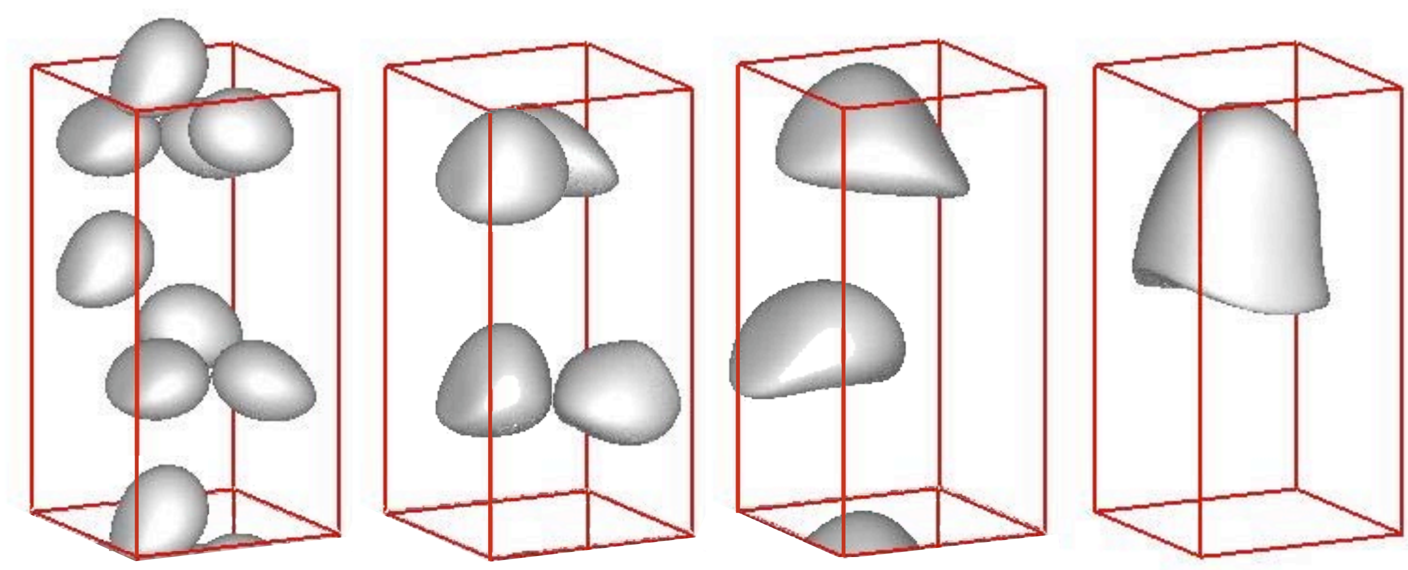


Moving Interface Problems—Complex Flows
Flow regime changes

Coalescence induced flow regime transitions in a laminar bubbly channel flow: The figure shows a preliminary two-dimensional simulation of the transition from a wall peaked distribution of many bubbles to a single large slug in the channels center.



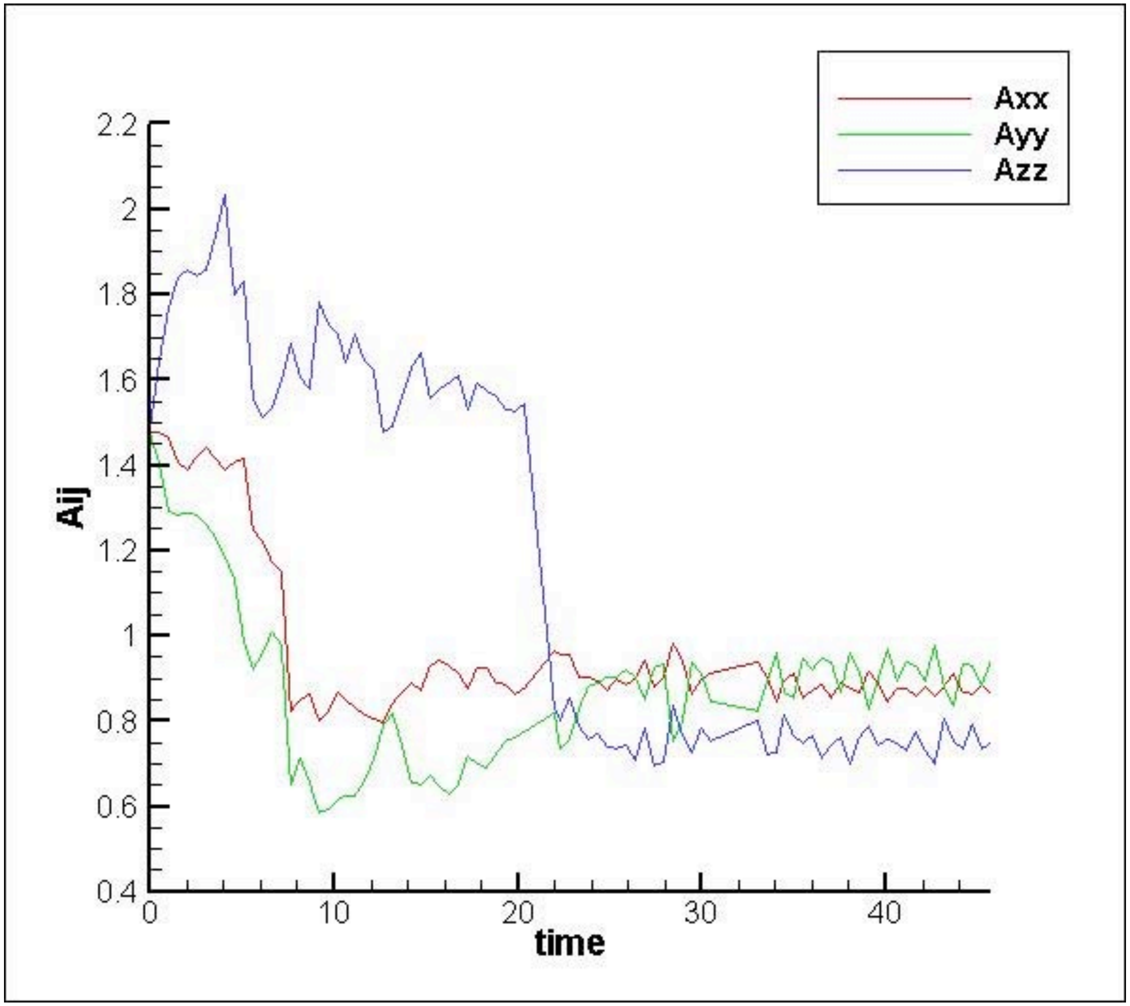
A simulation of a coalescence induced regime transition in a small three-dimensional system



Time →

The components of the interface area tensor versus time

$$\frac{1}{Vol}\int_S \boldsymbol{nn}\,da$$



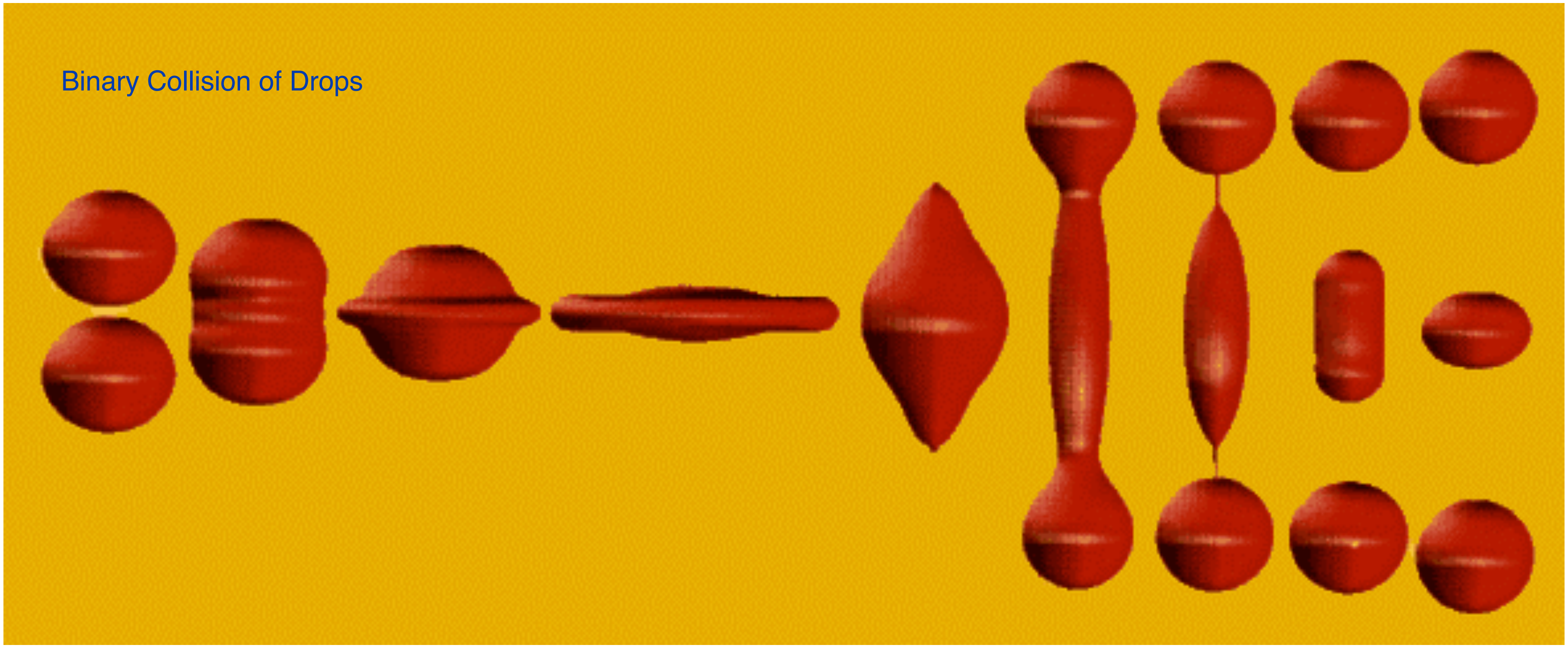
Atomization and droplet breakup

In general, the interface separating two fluids will undergo topology changes where two regions of one fluid coalesce, or one region breaks in two. Of those, the coalescence problem appears to be the harder one.

In their simples implementation, explicit tracking method never allow coalescence and method based on a marker function always coalesce two interfaces that are close.

In reality, films between two fluid interfaces take a finite time to drain and rupture only when the thickness is sufficiently small so the film is unstable to non-continuum attractive forces. In general this draining can not be resolved and must be modeled.

Moving Interface Problems—Complex Flows



References:

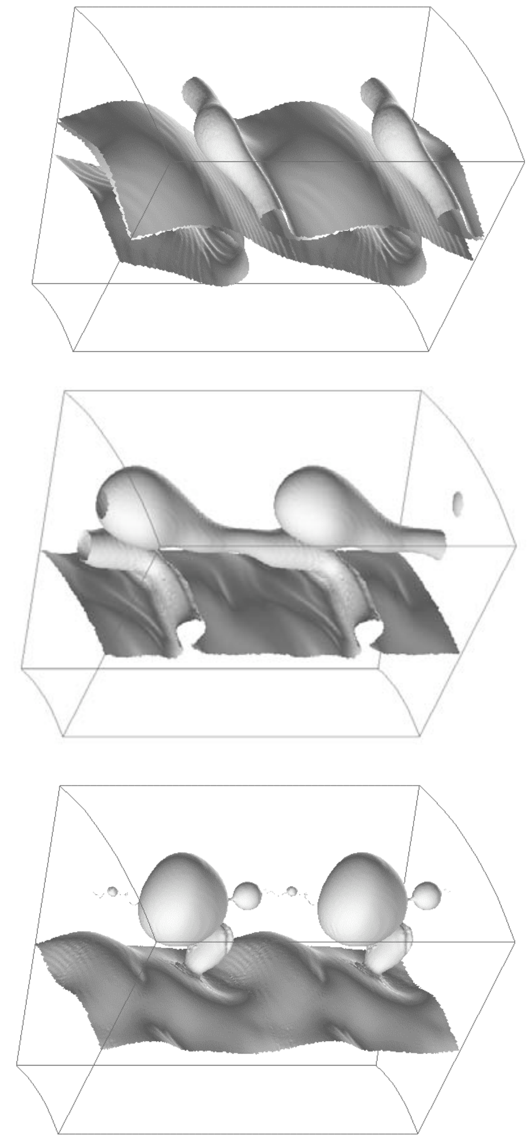
M.R.H. Nobari, Y.-J. Jan and G. Tryggvason. "Head-on Collision of Drops--A Numerical Investigation."Phys. of Fluids 8, 29-42 (1996).

M.R.H. Nobari, and G. Tryggvason, "Numerical Simulations of Three-Dimensional Drop Collisions."AIAA Journal 34 (1996), 750-755.

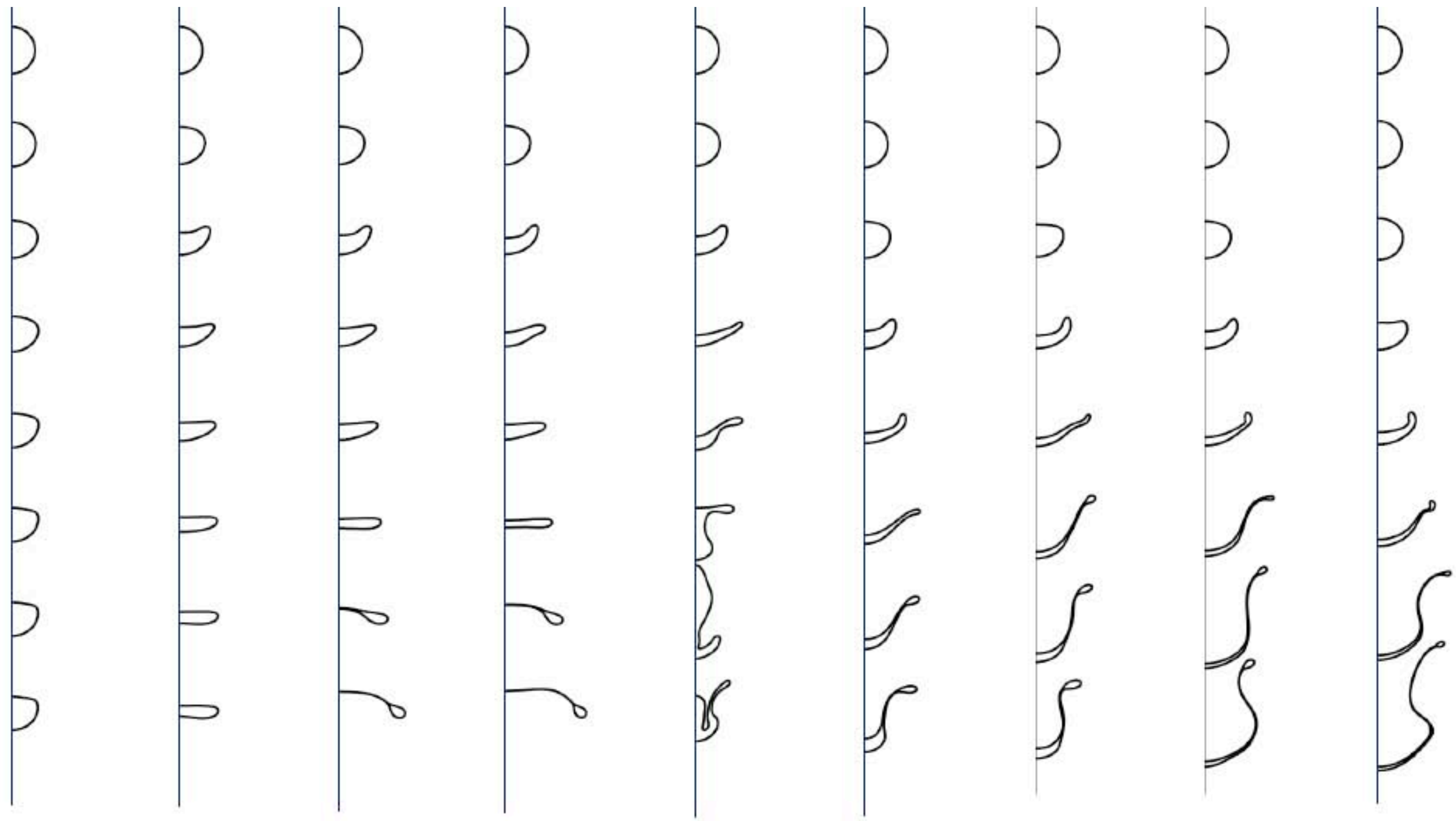
J. Qian, G. Tryggvason, and C.K. Law. An Experimental and Computational Study of Bouncing and Deforming Droplet Collision. Submitted to Phys. Fluids

Moving Interface Problems—Complex Flows
Primary breakup of jets

Three frames from a simulation of the three-dimensional breakup of a jet. The initial two-dimensional fold becomes unstable and generates fingers that eventually break into drops. Here, Re=1000, We=5, and the density ratio is 10. The simulation is done using 72 by 48 by 38 unevenly spaced grid points in the radial, axial, and azimuthal direction, respectively.

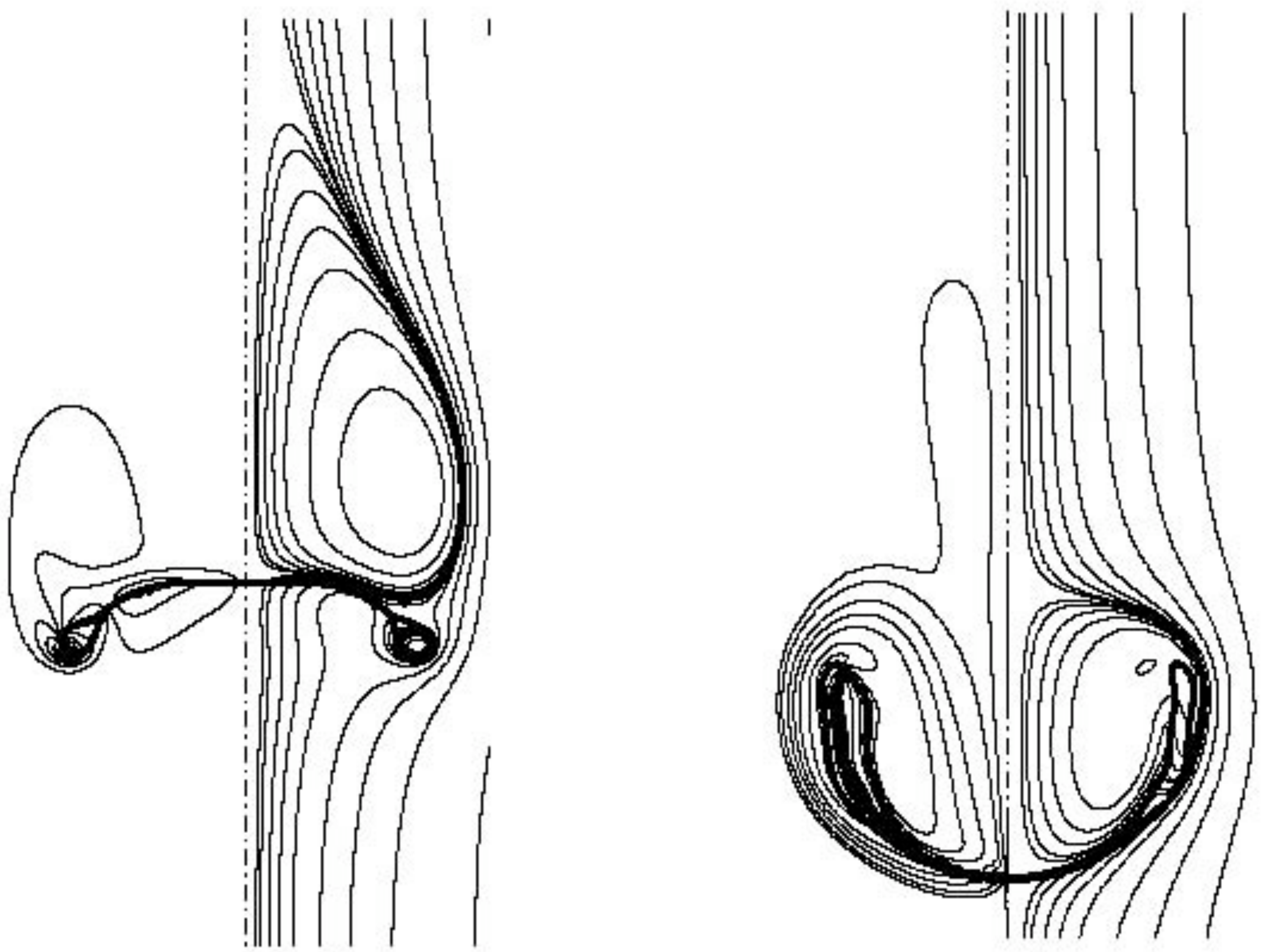


Moving Interface Problems—Complex Flows
Secondary breakup of drops



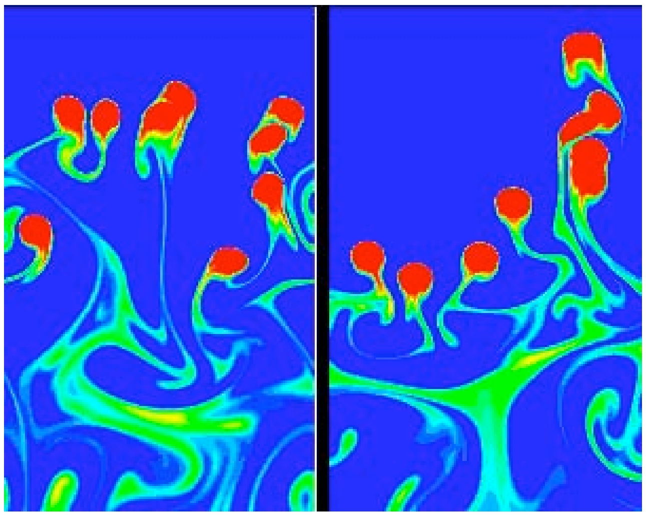
(a) $Eo = 12$ (b) $Eo = 24$ (c) $Eo = 28.8$ (d) $Eo = 36$ (e) $Eo = 48$ (f) $Eo = 60$ (g) $Eo = 72$ (h) $Eo = 96$ (i) $Eo = 144$

Moving Interface Problems—Complex Flows
Secondary breakup of drops

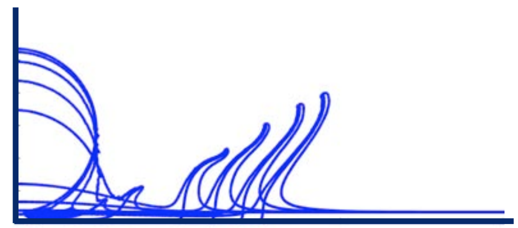


Moving Interface Problems—Complex Flows
DNS of Multiphase Systems

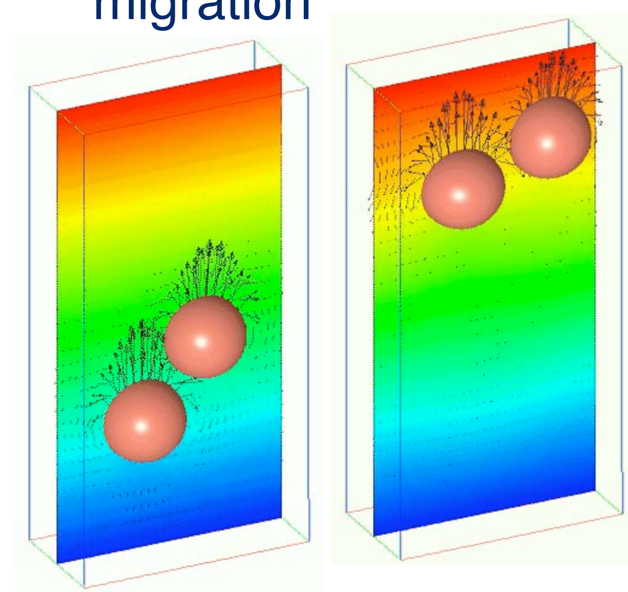
Mass transfer & chemical reactions



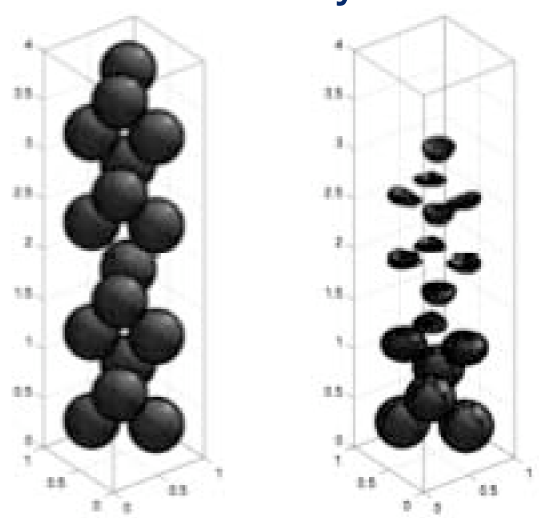
Splatting drops



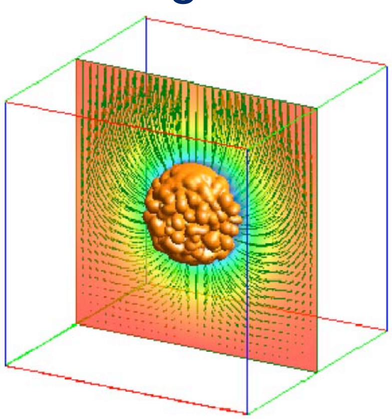
Thermocapillary migration



Shocks in bubbly flows



Explosive Boiling



Summary

- Multifluid simulations of relatively simple systems are well under control and can be used to understand such systems.
- Large scale three-dimensional simulations are emerging. The challenge is to use the results to produce engineering/scientific knowledge.
- Methods for multiphase flows are in their infancy.

System size:
<1980: Mostly two-dimensional systems
1980: early three-dimensional studies
1990: less than 100^3 grid points
2006 > 1000^3 grid points + new computational techniques