

# Direct Numerical Simulations of Multiphase Flows-1

## Introduction

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### DNS of Multiphase Flows

Software is needed for a variety of purposes.

In addition to large scale “somewhat” general purpose codes that represent close to the state-of-the-art and often can be used as “black-boxes,” there are needs for simple codes that are easily understood and modified.

Those needs include:

- Codes for educating students and showing them how numerical algorithms can be implemented
- Codes that can easily be modified to test new numerical ideas or extensions to new problems

The key need is for new investigators to get up-to-speed quickly so they can start addressing cutting-edge problems

Here, a relatively simple method to simulate the unsteady two-dimensional flow of two immiscible fluids, separated by a sharp interface is introduced.

### DNS of Multiphase Flows

## Multiphase Flows

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Multiphase flows are everywhere:

Rain, air/ocean interactions, combustion of liquid fuels, boiling in power plants, refrigeration, blood,

Research into multiphase flows usually driven by “big” needs

Early Steam Generation  
Nuclear Power  
Space Exploration  
Oil Extraction  
Chemical Processes

Many new processes depend on multiphase flows, such as cooling of electronics, additive manufacturing, carbon sequestration, etc.

### DNS of Multiphase Flows

Multiphase flows are usually defined as two or more distinct phases or components flowing together. Examples include air bubbles and oil drops in water, vapor bubbles in liquids and fuel vapor and drops in sprays.

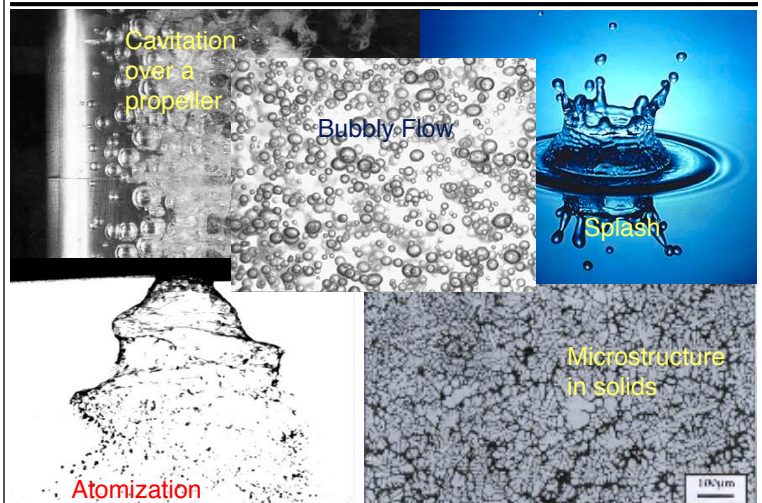
Generally we do not refer to mixtures of two or more chemical species as multiphase flows. Those include air, which is a mixture of several gases (such as oxygen, nitrogen, carbon-dioxide, and others) and water containing dissolved sugar or gases

Here we will not consider miscible fluids, although often, particularly for short times, their evolution is very well described by standard approaches to describing multiphase flow.

Multiphase flows can be classified in a variety of ways, such as gas-liquid, gas-solid and three-phase flows. In many applications liquid-liquid flows are important.

The difference between gas-liquid and liquid-liquid is simply the ratio of their properties so we will only distinguish between fluid-fluid and fluid-solid systems.

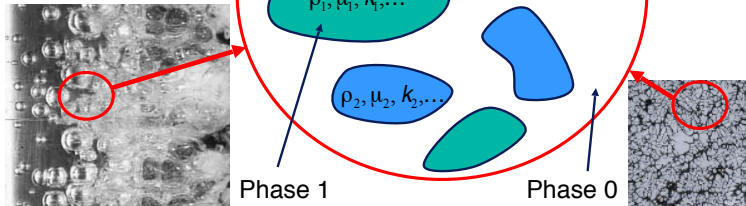
### DNS of Multiphase Flows



## DNS of Multiphase Flows

### Evolving Heterogeneous Continuum Systems

Systems composed of different phases and materials, separated by a sharp interface whose location changes with time



## DNS of Multiphase Flows

# Direct Numerical Simulations of Multiphase Flows

## DNS of Multiphase Flows

For many multiphase systems the governing equations are reasonably well known so if we could solve them accurately enough, we expect to replicate the behavior of the physical system.

Many multiphase systems evolve in complex ways with a wide range of spatial and temporal scales. For industrial size system the range of scales require excessive resolution that makes numerical simulations impractical or impossible on current computers.

In many cases we can, however, study smaller systems with a more limited range of scales and use those to infer the behavior of larger systems

## DNS of Multiphase Flows

### Direct Numerical Simulations (DNS):

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

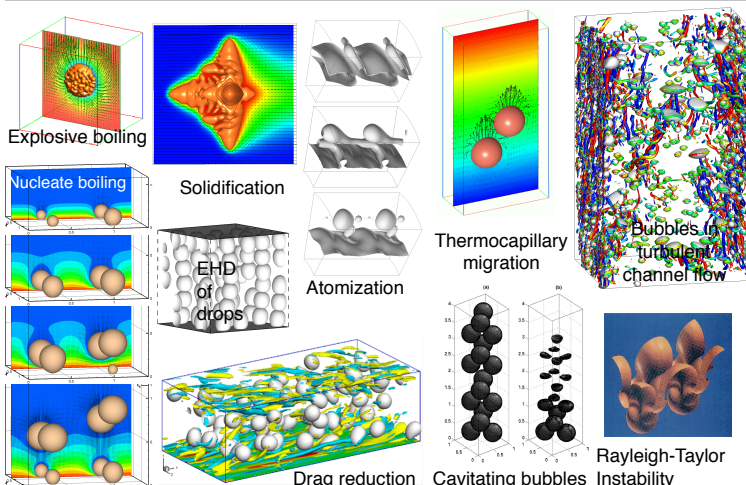
DNS provide us with full details of the flow in both space and time and allow us to compute any derived quantity

DNS allow us to turn the various physical processes on and off at will to determine their effect

DNS allow us to precisely define the initial conditions for each case and determine their effects

The purpose of DNS is not just to reproduce experiments!

## DNS of Multiphase Flows



## DNS of Multiphase Flows

The code developed here introduces the basic methodology used for DNS of multiphase flows, but is not really suitable for "real" DNS

It is designed and implemented for two-dimensional flows only and no parallelization is used

It is, however, suitable for fully resolved simulations of simple problems

For DNS we need more advanced codes for three-dimensional flows, designed to run efficiently on massively parallel computers

## What Are We Looking For?

### For bubbly flows:

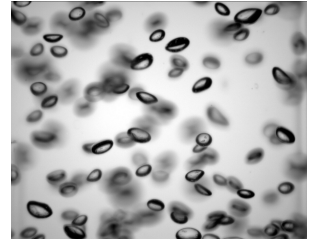
How does the void fraction and the bubble size and shape affect their average rise velocity

How do the bubbles disperse as they rise

Do the bubbles form microstructures as they rise and how do such structures affect rise velocity and dispersion

Does the bubbles size distribution change as the bubbles rise due to coalescence, breakup or size dependent migration

How do bubbles interact with wall and boundaries



### For atomization of liquid jets:

What are the resulting drop sizes and their distribution, and velocities, and how does these quantities depend on the initial nozzle shape and flow conditions



How long does it take for the jet to break up and how does it depend on the initial nozzle shape and flow conditions

What are the basic mechanisms that control the initial breakup and the drop formation and how do they depend on turbulence in the jet and the air flow

DNS allows us to compute directly the average evolution and properties of the mixture, including slip velocity, most probable configuration, change of composition, effective conductivity, etc. Quantities of interest range from simple volume averages to more sophisticated measures of the phase distribution. Often we are interested in phasic averages, where we average over the different fluids separately.

$$\text{Indicator function } \chi_i(\mathbf{x}) = \begin{cases} 1 & \text{in fluid } i \\ 0 & \text{otherwise} \end{cases}$$

Volume fraction of phase  $i$       Phasic average of  $f_i$

$$\alpha_i = \frac{1}{Vol} \int_V \chi_i(\mathbf{x}, t) dv \quad \langle f_i \rangle = \frac{1}{\alpha_i Vol} \int_V \chi_i(\mathbf{x}, t) f_i(\mathbf{x}, t) dv$$

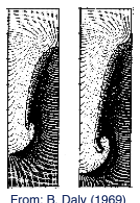
Many other quantities to characterize the flow, such as structure functions, turbulent quantities, etc.

## A Few Historical Notes

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



From: B. Daly (1969)

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

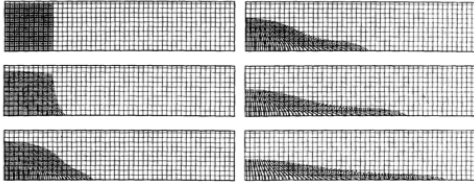
## DNS of Multiphase Flows

### The MAC Method for incompressible flows

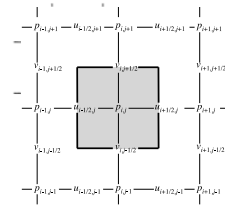
Primitive variables (velocity and pressure) on a staggered grid

The velocity is updated using splitting where we first ignore pressure and then solve a pressure equation with the divergence of the predicted velocity as a source term

Marker particles used to track the different fluids



The dam breaking problem simulated by the MAC method, assuming a free surface. From F. H. Harlow and J. E. Welch. Numerical calculation of time-dependent viscous incompressible flow of fluid with a free surface. Phys. Fluid, 8: 2182–2189, 1965.



## DNS of Multiphase Flows

## Outline

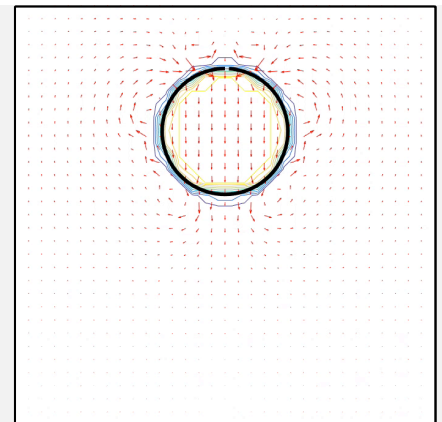
## DNS of Multiphase Flows

- The flow solver is an explicit projection finite-volume method, third order in time and second order in space, and the interface motion is computed using a front-tracking method, where connected marker point that move with the flow identify the interface.
- The method is described in detail and a numerical code is developed, using a step-by-step approach where we start with a simple but not very accurate code and gradually make it more complete and more accurate.
- The code is written in Matlab, but the information presented here should allow an implementation in any other programming language.
- Here we assume two-dimensional flows, but most of the discussion carries over to fully three-dimensional flows in a straightforward way. This is, in particular, true for the flow solver.

## DNS of Multiphase Flows

In these lectures we develop a code to follow the time evolution of a two-dimensional two-fluid immiscible system, tracking the interface with connected marker particles.

We will develop the code in the context of a falling drop, bouncing of a wall.



A falling drop, using a 32 by 32 grid.

## DNS of Multiphase Flows

Lecture 1: Introduction (this lecture)

Lecture 2: One fluid formulation

Lecture 3: Flow solver

Lecture 4: Advecting the marker function

Lecture 5: Front tracking

Lecture 6: Completing the code

Lecture 7: Results and Tests

Lecture 8: Additional considerations

## DNS of Multiphase Flows

Several review articles and books treat the material presented here in more detail. Those include:

A. Prosperetti and G. Tryggvason (editors). Computational Methods for Multiphase Flows. Cambridge 2007

G. Tryggvason, R. Scardovelli and S. Zaleski. Direct Numerical Simulations of Gas-Liquid Multiphase Flow. Cambridge 2011

The first gives a broad introduction to numerical simulations but the second is more focused on the topic covered here.

