Moving Interface Problems: Methods & Applications
Tutorial Lecture I

Grétar Tryggvason
Worcester Polytechnic Institute

Moving Interface Problems and Applications in Fluid Dynamics
Singapore National University, 2007
Lecture 1: Basic equations, numerical solutions of the Navier-Stokes equations. Advection of a marker function

Lecture 2: Front tracking for two-fluid problems


Lecture 4: Computing complex flows, including electrohydrodynamics, solidification and boiling
Lecture 1:

Motivation

The One Fluid Formulation

Solving the Navier-Stokes Equations

Methods for the advection of a marker function
- Volume of Fluid (VOF)
- Level Sets
- Others methods
Motivation: Direct Numerical Simulations for Studies of the Dynamics of Heterogeneous Continuum Systems
Moving Interface Problems—Fundamentals

Motivation and Goals

- Cavitation
- Microstructure
- Bubbly Flow
- Atomization
- Splash
- School of fish
Dynamics of Heterogeneous Continuum Systems

- Systems composed of different phases and materials, separated by a sharp interface whose location changes with time
- The physics is well described by continuum theories
- The systems are sufficiently large so that simulations resolving the smallest and the largest scales are impractical
- There are good reasons to believe that the behavior of the smallest scales is—in some sense—universal
- The goal is to use fully resolved numerical simulations of the small scale behavior to help understand how the large and the small scale motion are coupled and to develop “closure” models
Evolving Heterogeneous Continuum Systems

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

\[ x_f(s,t) \]

\( \rho, \mu, k, \ldots \)

Phase 0

\( \chi_1 = 0 \)

Phase 1

\( \chi_1 = 1 \)

Motivation and Goals

\( \rho_0, \mu_0, k_0, \ldots \)

\( \rho_1, \mu_1, k_1, \ldots \)

\( \rho_2, \mu_2, k_2, \ldots \)
Moving Interface Problems—Fundamentals

Motivation and Goals

The goal is to simulate accurately the smallest continuum scales for multiphase systems that are sufficiently large so that meaningful averages can be obtained and the results used to help generate insight and closure models for engineering tools.

Example: The “two-fluid model”

\[
\frac{\partial}{\partial t} \varepsilon_p \rho_p + \nabla \cdot (\varepsilon_p \rho_p \mathbf{u}_p) = \dot{m}_p
\]

\[
\frac{\partial}{\partial t} \left( \varepsilon_p \rho_p \mathbf{u}_p \right) + \nabla \cdot \left( \varepsilon_p \rho_p \mathbf{u}_p \mathbf{u}_p \right) = -\varepsilon_p \nabla p_p
\]

\[
+ \nabla \cdot \left( \varepsilon_p \mathbf{u}_p \mathbf{D}_p \right) + \varepsilon_p \rho_p \mathbf{g} + \nabla \cdot \left( \varepsilon_p \rho_p \langle \mathbf{uu} \rangle \right) + \mathbf{F}_{\text{int}}
\]

Equations for the average motion of each constituent

Reynolds stresses

interfacial forces
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:

Volume fraction of phase $i$

$$\varepsilon_i = \frac{1}{Vol} \int_v \chi_i(x, t) dv$$

Volume average of $f_i$

$$\langle f_i \rangle = \frac{1}{\varepsilon_i Vol} \int_v \chi_i(x, t) f_i(x, t) dv$$

Characterization of the mixture

$$\frac{1}{Vol} \int_s nn da \quad \frac{1}{Vol} \int_s nnnn da$$

Structure functions, turbulent quantities, etc.
Moving Interface Problems—Fundamentals
Motivation and Goals

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
Governing Equations
Conservation of mass
\[ \frac{\partial}{\partial t} \int_V \rho \, dv = -\oint_S \rho \mathbf{u} \cdot \mathbf{n} \, ds \]

Conservation of momentum
\[ \frac{\partial}{\partial t} \int_V \rho \mathbf{u} \, dv + \oint_S \rho \mathbf{u} (\mathbf{u} \cdot \mathbf{n}) \, ds = \int_V \rho f \, dv + \oint_S \mathbf{n} \mathbf{T} \, ds \]

Stress Tensor
\[ \mathbf{T} = (-p + \lambda \nabla \cdot \mathbf{u}) \mathbf{I} + 2\mu \mathbf{D} \]

Deformation Tensor
\[ \mathbf{D} = \frac{1}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \]
\[ D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]
The differential form:

**Conservative Form**

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0
\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot \rho uu = \rho f + \nabla \cdot T
\]

**Convective Form**

\[
\frac{D \rho}{Dt} + \rho \nabla \cdot u = 0
\]

\[
\rho \frac{Du}{Dt} = \rho f + \nabla \cdot T
\]

Using:

\[
\nabla \cdot (\rho u) = u \cdot \nabla \rho + \rho \nabla \cdot u
\]

\[
\frac{D()}{Dt} = \frac{\partial()}{\partial t} + u \cdot \nabla()
\]
Incompressible flows:

\[
\frac{D\rho}{Dt} = 0
\]

\[
\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0 \quad \rightarrow \quad \nabla \cdot \mathbf{u} = 0
\]

Navier-Stokes equations (conservation of momentum)

\[
\frac{\partial}{\partial t} \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{uu}) = -\nabla p + \rho \mathbf{f}_b + \nabla \cdot \mu \left( \nabla \mathbf{u} + \nabla^T \mathbf{u} \right)
\]

The advection terms can also be written as:

\[
\frac{\partial}{\partial t} \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{uu}) = \rho \left( \frac{\partial}{\partial t} \mathbf{u} + \nabla \cdot \mathbf{uu} \right) = \rho \left( \frac{\partial}{\partial t} \mathbf{u} + \mathbf{u} \nabla \mathbf{u} \right)
\]
The two-dimensional Navier-Stokes Equations in component form

\[
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \mu \left( \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \mu \left( \frac{\partial u}{\partial x} \right) + f_x
\]

\[
\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial y} \mu \left( \frac{\partial v}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial x} \mu \left( \frac{\partial v}{\partial y} \right) + f_y
\]

Incompressibility

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]
Sharply stratified flows

The conservation equations for mass and momentum apply to any flow situation, including flows of multiple immiscible fluids. Each fluid generally has properties that are different from the other constituents and the location of each fluid must therefore be tracked. We usually also have additional physics that must be accounted for at the interface, such as surface tension.

The “regular” conservation equations can be extended to handle these situations by using generalized functions
Identify each fluid by a marker function \( H \)

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

The marker moves with the fluid and is updated by integrating the following advection equation in time

\[
\frac{\partial H}{\partial t} + u \cdot \nabla H = 0
\]

Updating \( H \)—in spite of its apparent simplicity—is one of the hard problems in CFD!
In addition to advect the marker function accurately, we must often account for physics unique to the interface. The most common example is surface tension.
A surface can be defined by:

\[ x(u,v) = (x(u,v), y(u,v), z(u,v)) \]

Define

\[ x_u = \frac{\partial x}{\partial u}; \quad x_v = \frac{\partial x}{\partial v} \]

The normal is given by:

\[ n = \frac{x_u \times x_v}{|x_u \times x_v|} \]

It can be shown that:

\[ k = -\nabla \cdot n \]

\[ kn = \lim_{\delta A \to 0} \int m \, ds \]
\[ H(x, y, t) = \int_{A(t)} \delta(x - x')\delta(y - y')\,da' \]

\[ \nabla H = \int_{A} \nabla'[\delta(x - x')\delta(y - y')]\,da' \]
\[ = -\int_{A} \nabla'[\delta(x - x')\delta(y - y')]\,da' \]
\[ = -\int_{S} \delta(x - x')\delta(y - y')n\,ds' \]
\[ = -\int_{S} \delta(s)\delta(n)\,ds' \]
\[ = -\delta(n)n \]

Using:
\[ \delta(x - x')\delta(y - y') = \delta(s)\delta(n) \]
Conservation of Momentum

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot \mathbf{uu} = -\nabla p + \mathbf{f} + \nabla \cdot \mu \left( \nabla \mathbf{u} + \nabla^T \mathbf{u} \right) + \sigma \kappa \mathbf{n} \delta(n)
\]

Conservation of Mass

\[\nabla \cdot \mathbf{u} = 0\]

Incompressible flow

Equation of State:

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

Oscillating drop: pressure

The conservation equations are solved on a regular fixed grid and the front is tracked by connected marker points.
The “one-fluid” formulation implicitly contains the proper interface jump conditions. Integrating each term across a small control volume centered at the interface:

$$\int_{\delta V} \rho \frac{Du}{Dt} dv = -\int_{\delta V} \nabla p dv + \int_{\delta V} f dv + \int_{\delta V} \nabla \cdot \mu (\nabla u + \nabla^T u) dv + \int_{\delta V} \kappa \sigma n \delta(n) dv$$

Jump Condition:

$$[-p + \mu (\nabla u + \nabla^T u)]n = -\kappa \sigma n$$
We can also show that the “one-fluid” formulation contains the equations written separately for each fluid and the jump conditions:

Write:

\[ u = H_1 u_1 + H_2 u_2 \]
\[ P = H_1 p_1 + H_2 p_2 \]
\[ \rho = H_1 \rho_1 + H_2 \rho_2 \]

Substitute into the momentum equation

\[ H_1 (\ldots) + H_2 (\ldots) + \delta(x_f)(\ldots) = 0 \]

\( = 0 \quad = 0 \quad = 0 \)

Momentum equation in phase 1
Momentum equation in phase 2
Interface conditions
As the interface evolves, the topology of the interface can change. Topology changes come in two types:

A thin thread can pinch. This usually happens when an interface breaks up.

A thin film ruptures. This usually happens when two fluid masses coalesce.
Numerical Solutions
Solution Strategy

For the solutions of the Navier-Stokes equations we must decide:

• How the velocity field is integrated in time
• How the advection and the viscous terms are discretized
• How the pressure equation is solved
• How the boundary conditions are implemented

In addition, we must decide:

• How the marker function is advected in time
• How the surface tension is computed
Moving Interface Problems—Fundamentals

Work with the finite volume approximation

\[
\frac{\partial}{\partial t} \int \rho u \, dv + \oint \rho u (u \cdot n) \, ds = \\
\int \rho f \, dv + \oint \mu (\nabla u + \nabla^T u) \, ds + \int_V \sigma \kappa n \delta(n) \, dv
\]

Discretize each term

\[
u = \frac{1}{V} \int_V u \, dv
\]

\[
A_c = \frac{1}{V} \int_V \nabla \cdot (uu) \, dV = \frac{1}{V} \oint_s u (u \cdot n) \, ds
\]

\[
D_c = \frac{1}{V} \int_V \nabla \cdot \mu (\nabla_h u + \nabla^T_h u) \, dV = \frac{1}{V} \oint_s \mu (\nabla_h u + \nabla^T_h u) \, ds
\]
Evolution of the velocity—first order explicit in time:

$$\frac{\mathbf{u}_{i,j}^{n+1} - \mathbf{u}_{i,j}^{n}}{\Delta t} = -\mathbf{A}_{i,j}^{n} - \frac{1}{\rho^{n}} (\nabla_h p + \mathbf{D}_{i,j}^{n} + \mathbf{f}_{\sigma}^{n}) + \mathbf{f}_{b}^{n}$$

Constraint on velocity

$$\nabla_h \cdot \mathbf{u}_{i,j}^{n+1} = 0$$

No explicit equation for the pressure!
Moving Interface Problems—Fundamentals
Discretization in time

Split

\[ \frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = -A_{i,j}^n - \frac{1}{\rho^n} (\nabla_h p + D_{i,j}^n + f_{\sigma}^n) + f_b^n \]

into

\[ \frac{u_{i,j}^{tmp} - u_{i,j}^n}{\Delta t} = -A_{i,j}^n + f_b^n + \frac{1}{\rho^n} (D_{i,j}^n + f_{\sigma}^n) \]

and

\[ \frac{u_{i,j}^{n+1} - u_{i,j}^{tmp}}{\Delta t} = - \frac{1}{\rho^n} \nabla_h p_{i,j} \]

by introducing the temporary velocity \( u^{tmp} \)

Projection Method
To derive an equation for the pressure we take the divergence of

$$u_{i,j}^{n+1} = u_{i,j}^{tmp} - \Delta t \frac{\nabla_h p_{i,j}}{\rho_n}$$

and use the mass conservation equation

$$\nabla_h \cdot u_{i,j}^{n+1} = 0$$

The result is

$$\nabla_h \cdot u_{i,j}^{n+1} = \nabla_h \cdot u_{i,j}^{tmp} - \Delta t \nabla_h \left( \frac{1}{\rho_n} \nabla_h p_{i,j} \right)$$

$$\nabla_h \left( \frac{1}{\rho_n} \nabla_h p_{i,j} \right) = \frac{1}{\Delta t} \nabla_h \cdot u_{i,j}^{tmp}$$
1. Find a temporary velocity using the advection and the diffusion terms only:

\[ u_{i,j}^{tmp} = u_{i,j}^n + \Delta t \left( -A_{i,j}^n + f_b^n + \frac{1}{\rho^n} \left( D_{i,j}^n + f^o_n \right) \right) \]

2. Find the pressure needed to make the velocity field incompressible

\[ \nabla_h \cdot \left( \frac{1}{\rho^n} \nabla_h p_{i,j} \right) = \frac{1}{\Delta t} \nabla_h \cdot u_{i,j}^{tmp} \]

3. Correct the velocity by adding the pressure gradient:

\[ u_{i,j}^{n+1} = u_{i,j}^{tmp} - \frac{\Delta t}{\rho^n} \nabla_h p_{i,j} \]

4. Update the marker function to find new density and viscosity
Forward in time, centered in space:

$$\Delta t_{\text{adv}} \leq \frac{2\nu}{U^2} \quad \& \quad \Delta t_{\text{diff}} \leq \frac{1}{4} \frac{h^2}{\nu}$$

Define \( \tau = \frac{L}{U} \)

Therefore the nondimensional time step is:

$$\Delta t' = \frac{\Delta t}{\tau} \leq \frac{2\nu U}{U^2 L} = \frac{2}{\text{Re}}$$

and

$$\Delta t' = \frac{\Delta t}{\tau} \leq \frac{1}{4} \frac{h^2 U}{\nu L} = \frac{1}{4} \left( \frac{h}{L} \right)^2 \text{Re}$$

And \( \Delta t \rightarrow 0 \) for \( \text{Re} \rightarrow 0 \) and \( \text{Re} \rightarrow \infty \)

Advanced Solvers: use implicit methods for diffusion term in the limit of low Re and stable advection schemes for high Re.
Notice that when we apply the mass conservation equation to a control volume centered at \( i,j \), we naturally pick up the velocities at the edges of the control volume. Nothing has been said so far about how the velocities at the edges are found. They could be interpolated from values at the cell center, or found directly using control volumes centered around the velocity at the edges. The second approach leads to STAGGERED GRIDS.
Define Cell-Averages:

\[
\begin{align*}
    u &= \frac{1}{V} \iiint_{V_u} u \, dv \\
    v &= \frac{1}{V} \iiint_{V_v} v \, dv \\
    P &= \frac{1}{V} \iiint_{V_p} p \, dv
\end{align*}
\]
Moving Interface Problems—Fundamentals

**Predictor Step**

\[
\begin{align*}
\mathbf{u}^\text{tmp}_{i+1/2, j} &= \mathbf{u}^n_{i+1/2, j} + \Delta t \left\{ \left(-A_x\right)^n_{i+1/2, j} + \left(f_{bx}\right)^n_{i+1/2, j} + \frac{2}{\rho^n_{i+1, j} + \rho^n_{i, j}} \left( (D_x)^n_{i+1/2, j} + (f_{\alpha x})^n_{i+1/2, j} \right) \right\} \\
\mathbf{v}^\text{tmp}_{i, j+1/2} &= \mathbf{v}^n_{i, j+1/2} + \Delta t \left\{ \left(-A_y\right)^n_{i, j+1/2} + \left(f_{by}\right)^n_{i, j+1/2} + \frac{2}{\rho^n_{i, j+1} + \rho^n_{i, j}} \left( (D_y)^n_{i, j+1/2} + (f_{\alpha y})^n_{i, j+1/2} \right) \right\}
\end{align*}
\]

**Corrector Step**

\[
\begin{align*}
\mathbf{u}^{n+1}_{i+1/2, j} &= \mathbf{u}^\text{tmp}_{i+1/2, j} - \frac{2 \Delta t}{\rho^n_{i+1, j} + \rho^n_{i, j}} \frac{p_{i+1, j} - p_{i, j}}{\Delta x} \\
\mathbf{v}^{n+1}_{i, j+1/2} &= \mathbf{v}^\text{tmp}_{i, j+1/2} - \frac{2 \Delta t}{\rho^n_{i, j+1} + \rho^n_{i, j}} \frac{p_{i, j+1} - p_{i, j}}{\Delta y}
\end{align*}
\]

**Incompressibility**

\[
\frac{\mathbf{u}^\text{tmp}_{i+1/2, j} - \mathbf{u}^\text{tmp}_{i-1/2, j}}{\Delta x} + \frac{\mathbf{v}^\text{tmp}_{i, j+1/2} - \mathbf{v}^\text{tmp}_{i, j-1/2}}{\Delta y} = 0
\]
Advection term - x direction

\[(A_x^n)_{i+1/2,j} = \frac{(u_{i+1,j}^n)^2 - (u_{i,j}^n)^2}{\Delta x_{i+1/2}} + \frac{u_{i+1/2,j+1/2}^n v_{i+1/2,j+1/2}^n - u_{i+1/2,j-1/2}^n v_{i+1/2,j-1/2}^n}{\Delta y_j}\]

\[(A_x^n)_{i+1/2,j} = \frac{(0.5(u_{i+3/2,j}^n + u_{i+1/2,j}^n))^2 - (0.5(u_{i+1/2,j}^n + u_{i-1/2,j}^n))^2}{\Delta x_{i+1/2}} + \frac{0.25(u_{i+3/2,j}^n + u_{i+1/2,j}^n)(v_{i+3/2,j}^n + v_{i+1/2,j}^n) - 0.25(u_{i+3/2,j}^n + u_{i+1/2,j}^n)(v_{i+3/2,j}^n + v_{i+1/2,j}^n)}{\Delta y_j}\]

Diffusion term - x direction

\[(D_x^n)_{i+1/2,j} = \left\{ \frac{1}{\Delta x} \left( \frac{2}{\Delta x_{i+1/2}} \frac{\partial u}{\partial x}_{i+1,j} - 2 \frac{\partial u}{\partial x}_{i+1/2,j+1/2} \right) + \frac{1}{\Delta y} \left( \frac{2}{\Delta y_{i+1/2,j+1/2}} \frac{\partial u}{\partial y}_{i+1,j} + \frac{\partial u}{\partial x}_{i+1/2,j+1/2} \right) \right\}\]

\[(D_x^n)_{i+1/2,j} = \frac{1}{\Delta x_{i+1/2}} \left\{ \frac{2}{\Delta x_{i+1/2}} \left( u_{i+3/2,j}^n - u_{i+1/2,j}^n \right) + \frac{2}{\Delta x_{i+1/2}} \left( u_{i+1/2,j}^n - u_{i-1/2,j}^n \right) \right\} + \frac{1}{\Delta y_j} \left\{ \frac{2}{\Delta y_{j+1/2}} \left( v_{i+1,j+1/2}^n - v_{i+1,j}^n \right) - \frac{2}{\Delta y_{j+1/2}} \left( v_{i+1,j+1/2}^n - v_{i-1,j+1/2}^n \right) \right\} - \frac{1}{\Delta y_j} \left\{ \frac{2}{\Delta y_{j-1/2}} \left( v_{i+1,j-1/2}^n - v_{i-1,j-1/2}^n \right) - \frac{2}{\Delta y_{j-1/2}} \left( v_{i+1,j-1/2}^n - v_{i-1,j-1/2}^n \right) \right\}\]
The pressure equation is derived by substituting the expression for the correction velocities into the incompressibility equation, resulting in:

\[ \frac{1}{\Delta x^2} \left( \left( \frac{p_{i+1,j} - p_{i,j}}{\rho_{i+1,j}^n + \rho_{i,j}^n} \right) - \left( \frac{p_{i,j} - p_{i-1,j}}{\rho_{i,j}^n + \rho_{i-1,j}^n} \right) \right) + \]

\[ \frac{1}{\Delta y^2} \left( \left( \frac{p_{i,j+1} - p_{i,j}}{\rho_{i,j+1}^n + \rho_{i,j}^n} \right) - \left( \frac{p_{i,j} - p_{i,j-1}}{\rho_{i,j}^n + \rho_{i,j-1}^n} \right) \right) = \]

\[ \frac{1}{2\Delta t} \left( \frac{u_{i+1/2,j}^{\text{tmp}} - u_{i-1/2,j}^{\text{tmp}}}{\Delta x_i} + \frac{v_{i,j+1/2}^{\text{tmp}} - v_{i,j-1/2}^{\text{tmp}}}{\Delta y_j} \right) \]

The variable density leads to a non-separable elliptic equation.
Conservative form versus non-conservative form of the momentum equations
Essentially any advanced solution method for the Navier-Stokes equations can be used to integrate the “one-fluid” equations in time.

Example: Method of Kim and Moin (JCP 59 (1985), 8-23)

\[
\frac{u^{imp} - u^n}{\Delta t} = - \left( \frac{3}{2} A(u^n) - \frac{1}{2} A(u^{n-1}) \right) + \frac{1}{2\rho^n} \left( \nabla \cdot (D^n + D^{imp}) \right)
\]

\[
\frac{u^{n+1} - u^{imp}}{\Delta t} = - \frac{1}{\rho^n} \nabla \phi
\]

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

The first equation is implicit and must be solved by an iteration in the same way as the pressure equation.
Conservative vs non-conservative form of the Navier-Stokes equations

Consider inviscid, one-dimensional flow with no pressure gradient

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \]
\[ \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} = 0 \]

In the velocity is constant initially, \( u = u_0 \) it stays constant and any density profile is advected without change of shape.

Using centered differences for both the density and the momentum (ignoring that it is unstable), keeps the velocity constant

\[ \rho_j^{n+1} = \rho_j^n - \frac{u_0 \Delta t}{2h} \left( \rho_{j+1}^n - \rho_{j-1}^n \right) \]
\[ u_j^{n+1} = \frac{u_0}{\rho_j^{n+1}} \left[ \rho_j^n - \frac{u_0 \Delta t}{2h} \left( \rho_{j+1}^n - \rho_{j-1}^n \right) \right] \]

\( u_j^{n+1} = u_0 \)
If the density is advected in a different way (by upwind, say), then the same cancellation does not take place

\[
\rho_{j}^{n+1} = \rho_{j}^{n} - \frac{u_{o} \Delta t}{h} (\rho_{j}^{n} - \rho_{j-1}^{n}) \\
\rho_{j}^{n+1} = \frac{u_{0}}{\rho_{j}^{n+1}} \left[ \rho_{j}^{n} - \frac{u_{0} \Delta t}{2h} \left( \rho_{j+1}^{n} - \rho_{j-1}^{n} \right) \right]
\]

Using the non-conservative form of the momentum equation

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \quad \Rightarrow \quad u_{j}^{n+1} = \left[ u_{0} - \frac{u_{0} \Delta t}{2h} (u_{0} - u_{0}) \right] = u_{0}
\]

irrespective of how the density is advected.

Another way is to first advect the density using a method consistent with the momentum equation and then advect the density using a more sophisticated method.
Adveecting the marker function
Introduce a numerical marker function $f$, approximating $H$. The advection of $f$ is governed by:

\[
\frac{\partial f}{\partial t} + u \cdot \nabla f = 0
\]

Integrating this equation in time, for a discontinuous initial data, is one of the hard problems in computational fluid dynamics!
The sharp marker function $H$ can be approximated in several different ways for computational purposes. Below we show a smoothed marker function, $I$, the volume of fluid approximation, $C$, and a level set representation, $\phi$. 
In 1D, using upwind and LW. The solution quickly deteriorates. Modern advection methods help, but not completely.
Methods that use the “one-field” or “weak” formulation of the Navier-Stokes equations
Volume of Fluid
To advect a discontinuous marker function, first consider 1D advection. Using simple upwind leads to excessive diffusion due to averaging the function over each cell, before finding the fluxes.

**Upwind**
Since the marker function only takes on two values, 0 and 1, the advection can be made much more accurate by “reconstructing” the function in each cell before finding the fluxes, integrated over time:

\[
\int_t^{t+\Delta t} F_{j+1/2} \, dt = \begin{cases} 
0, & \Delta t \leq (1-f_j)h/U, \\
 h - (f_j + U\Delta t), & \Delta t > (1-f_j)h/U
\end{cases}
\]

One-dimensional Volume-Of-Fluid
While VOF works extremely well in one-dimension, there are considerable difficulties extending the approach to higher dimensions. The basic problem is the “reconstruction” of the interface in each cell, given the volume fraction in neighboring cells.

In the SLIC method the interface was taken to be perpendicular to the advection direction.

In the Hirt/Nichols method the interface was taken to be parallel to one axis.

In PLIC the interface is a line with arbitrary orientation.

Once the interface has been reconstructed, the marker function is advected by geometric considerations.
Moving Interface Problems—Fundamentals

Original

SLIC

Hirt/Nichols

VOF

PLIC
Level Set Methods
Identify the interface as a “level-set” of a smooth function

Advect the level set function by

\[ \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \]

use

\[ \mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \quad \mathbf{u} \cdot \mathbf{n} = u_n \]

to get

\[ \frac{\partial \phi}{\partial t} + u_n |\nabla \phi| = 0 \]
The level set function can be arbitrarily smooth. To identify each fluid it is necessary to construct a marker function with a narrow transition zone.

The marker function can be generated by (for example):

\[
I(\phi) = \begin{cases} 
0 & \text{if } \phi < -\alpha h \\
\frac{1}{2}(1 + \frac{\phi}{\alpha h} + \frac{1}{\pi} \sin(\pi \frac{\phi}{\alpha h})) & \text{if } |\phi| \leq \alpha h \\
1 & \text{if } \phi > \alpha h 
\end{cases}
\]

The delta function is generated as the derivative of the marker function:

\[
\delta = \nabla I = \frac{dI}{d\phi} \nabla \phi
\]
The level set function for two circles, as a distance function
For most applications, the shape of the level set functions must remain the same close to the interface.

To keep the interface shape the same, it is necessary to “reinitialize” the level set function. This is usually done by making it a distance function.

At each time step, solve:

$$\frac{\partial \phi}{\partial \tau} + \text{sgn}(\phi)(|\nabla \phi| - 1) = 0$$
Other Methods for the Advection of the Marker Function
The CIP (Constrained Interpolation Polynomial) Method (Yabe)

In addition to advecting the marker function $f$, its derivative is advected by fitting a third order polynomial through the function and its derivatives.

Start with
\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0
\]

Introduce
\[
g = \frac{\partial f}{\partial x}.
\]

In 1D, the advection of the derivative is given by
\[
\frac{\partial g}{\partial t} + u \frac{\partial g}{\partial x} = 0
\]

Therefore, the derivative is translated with velocity $u$, just as the function. In 2D splitting is used to separate translation and deformation.
The CIP method results in very accurate advection and for a sharp interface it greatly reduces overshoots, but does not eliminate them completely.
The phase field Method (Jaqcmin)

Solve modified Navier-Stokes equations, developed by thermodynamic considerations at the microscale

$$\rho_0 \frac{Du}{Dt} = -\nabla S + \mu \nabla^2 u - c \nabla \phi + g \rho(c)$$

and

$$\frac{Dc}{Dt} = \kappa \nabla^2 \phi$$

The energy function can take several different forms, for example, if:

$$\phi = \beta \frac{d\psi(c)}{dc} - \alpha \nabla^2 c$$

and

$$\psi(c) = (c + 1/2)^2 (c - 1/2)^2$$

Then it can be shown that surface tension and interface thickness are:

$$\sigma = \sqrt{\alpha \beta / 18}$$

and

$$\epsilon \approx 4.164 \sqrt{\alpha / \beta}$$
Standard Tests for advection
Zalasak’s test: A notched circular blob is advected by a solid body rotation, measuring how the blob deteriorates
Moving Interface Problems—Fundamentals

From Kothe & Rider

Markers

High order advection (PPM)

Level Set

PLIC
Surface Tension
Singular interface forces are approximated by a smoothed delta function that becomes “more singular” as the smoothing is reduced.

\[ k = -\nabla \cdot \mathbf{n} \]

\[
\frac{\partial H}{\partial t} + \mathbf{u} \cdot \nabla H = 0
\]
The curvature is found from the normal field

\[ k = -\nabla \cdot \mathbf{n} \]

But the direction of the force is found from the marker function

\[ f_{i,j} = (\sigma \kappa)_{i,j} \nabla I_{i,j} \]

Numerical approximation for the normal

\[ n_{i,j}^x = \frac{1}{h} (f_{i+1,j+1} + 2f_{i+1,j} + f_{i+1,j-1} - f_{i-1,j+1} - 2f_{i-1,j} - f_{i-1,j-1}) \]

\[ n_{i,j}^y = \frac{1}{h} (f_{i+1,j+1} + 2f_{i,j+1} + f_{i-1,j+1} - f_{i+1,j-1} - 2f_{i,j-1} - f_{i-1,j-1}) \]
Summary

The “one-fluid” formulation of the Navier-Stokes equations was originally used in the MAC method. It does remain one of the most versatile way of following the motion of flows with sharp interfaces. The conservation equations can be discretized in many ways, similarly to the equations for smooth flows. To advect the marker function identifying the different fluids and to incorporate surface tension, several different but related methods have been developed, all of which are capable of producing high quality results.