Direct Numerical Simulations of Multiphase Flows-2

Governing Equations

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1. We start our development of a numerical method for simulations of multifluid and multiphase flows by a short discussion of the governing equations.

Here we will focus on:

Incompressible isothermal flow

The “one-fluid” formulation of the governing equations

2. The development described here focuses on incompressible flows, since for many problems of practical interest this is an excellent approximation, and we start by developing a method for isothermal flows. The governing equations can be written in many different forms and those different forms provide the natural starting point for different numerical methods. Here, we will focus on the integral form of the equations and the so-called single fluid formulation where we write one set of equations for the whole flow field, including the different fluids.

Governing Equations

3. We start by a summary of the derivation of the governing equations.

DNS of Multiphase Flows

The flow is predicted using the governing physical principles:

Conservation of mass. If the density of a material particle does not change, we have incompressible flow

Conservation of momentum. For incompressible flow the pressure is adjusted to enforce conservation of volume

Conservation of energy. For isothermal flow as we will be concerned with here, the energy equation is not needed

Geometric relationships that specify the motion of fluid particles. For flow consisting of two or more fluids where each fluid has constant properties, we only need to know how the interface moves

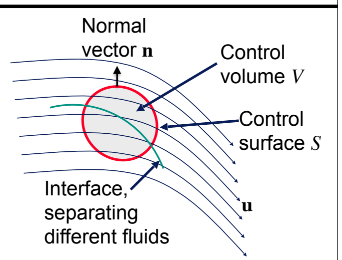
4. The governing equations are mathematical statements of the physical principles that we use to predict the evolution of the flow. For fluid mechanics problems we generally use the principle of conservation of mass, conservation of momentum and conservation of energy. Here we assume that the density of a material particle does not change as its location changes and this leads to incompressible flow, where the volume of any small fluid blob remains constant. For incompressible flows the pressure, used in the momentum equations, has a special role, since it must take on whatever value needed to enforce incompressibility. For isothermal flow the special role of the pressure allows us to leave out the energy equation but for problems where the temperature changes, we will need to bring it back. For flows consisting of two fluids with different properties we also need to solve an equation specifying what part of the domain is occupied by which fluid, or where the interface separating the different fluids, is.

DNS of Multiphase Flows

Conservation of mass

The increase of mass inside a control volume is equal to the net inflow of mass (inflow minus outflow). The normal is the outward pointing normal so inflow is negative and outflow is positive:

$$\frac{\partial}{\partial t}\int_V \rho dv = -\oint_S \rho \mathbf{u}\cdot\mathbf{n} ds$$



Notice that the control volume may contain an interface separating fluids with different material properties, such as density.

5. The conservation of mass equation is derived by applying the conservation of mass principle to a small control volume. Consider a control volume, fixed in space and of a arbitrary but fixed shape. We denote the control volume by V and the control surface which separates the control volume from its surrounding by S. The mass conservation principle states that the rate of change of the total mass in the control volume, the time derivative of the integral of the density over the control volume, is equal to the net in or outflow into the control volume, represented by the surface integral of density times the normal velocity. Since we take the normal to be positive pointing outward and inflow adds to mass and outflow decreases the mass, we need a minus sign in front of the surface integral. Notice that the control volume can contain an interface so the density can be different on different parts of the control surface.

DNS of Multiphase Flows

The divergence (or Gauss's) theorem can be used to convert surface integrals to volume integrals and vice versa.

$$\int_V \nabla\cdot\mathbf{u} dv = \oint_S \rho\mathbf{u}\cdot\mathbf{n} ds$$

Applying it to the right hand side of the mass conservation equation gives

$$\frac{\partial}{\partial t}\int_V \rho dv = -\int_V \nabla\cdot\rho\mathbf{u} dv$$

or, bringing the time derivative under the integral and collecting all terms under one integral sign

$$\int_V \Big(\frac{\partial \rho}{\partial t} + \nabla\cdot\rho\mathbf{u}\Big) dv = 0$$

6. Using the divergence theorem and that the control volume is fixed in space, so the time derivative can be moved under the integral sign, the mass conservation equation can be written as one volume integral over the rate of change of the density plus the divergence of the mass flux, or the density times the velocity.

DNS of Multiphase Flows

The mass conservation equation equation is

$$\int_V \Big(\frac{\partial \rho}{\partial t} + \nabla\cdot\rho\mathbf{u}\Big)dv = 0$$

Expanding the divergence

$$\int_V \Big(\frac{\partial \rho}{\partial t} + \mathbf{u}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{u}\Big)dv = 0$$

The first two terms are the convective derivative

$$\frac{D\rho}{\partial t} = \frac{\partial \rho}{\partial t} + \mathbf{u}\cdot\nabla\rho$$

So we can write

$$\int_V \Big(\frac{1}{\rho}\frac{D\rho}{Dt} + \nabla\cdot\mathbf{u}\Big)dv = 0$$

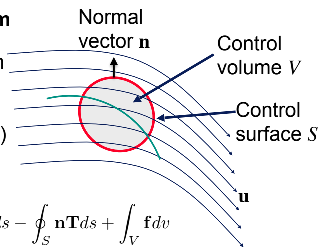
If $D\rho/Dt = 0$ then $\int_V \nabla\cdot\mathbf{u}dv = 0$ or $\boxed{\oint_S \mathbf{u}\cdot\mathbf{n}ds = 0}$ Volume is conserved!

7. We then expand the divergence and realizing that the first two terms are the convective derivative—partial rho with respect to time plus the velocity times the gradient of rho—so we can write the conservation of mass equation as the volume integral of the convective derivative of rho, divided by rho, plus the divergence of the velocity. If the density of a material particle remains constant, as it does for incompressible flows, then the first term is zero and we are left with the volume integral of the divergence of the velocity being equal to zero. Applying the divergence theorem, this can be restated as the surface integral over the control surface of the normal velocity being equal to zero. Or, the volume inflow into a control volume is balanced by the outflow for incompressible flows.

DNS of Multiphase Flows

Conservation of momentum

The increase of momentum inside a control volume is equal to the net inflow of mass (inflow minus outflow) plus surface and volume forces



$$\frac{\partial}{\partial t}\int_V \rho\mathbf{u}dv = -\oint_S \rho\mathbf{u}\mathbf{u}\cdot\mathbf{n}ds - \oint_S \mathbf{n}\mathbf{T}ds + \int_V \mathbf{f}dv$$

Stress Tensor

$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D}$ Incompressible, Newtonian fluid

Deformation Tensor

$\mathbf{D} = \frac{1}{2}\Big(\nabla\mathbf{u} + \mathbf{u}^T\Big)$ or, in component form: $D_{i,j} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big)$

8. The momentum equation is derived in the same way. We focus on an arbitrary control volume, of a fixed shape and fixed in space. The rate of change of momentum in the control volume is given by the net inflow of momentum—the first term on the left where rho u is the momentum and multiplying that by the normal velocity gives the flux through the boundary—plus surface and volume forces, given by the second and third term. For the surface forces we assume a Newtonian fluid where the stress is given by the pressure, acting normal to the control surface plus the viscous stresses given by the viscosity time the rate of deformation tensor, which is the symmetric part of the velocity gradient tensor. The full stress tensor also has stresses from compressing the fluid but for incompressible fluid this is zero and is therefore not included here.

DNS of Multiphase Flows

The body force term generally includes gravity, but can also include other forces. Here, surface tension is treated as a body force so we write:

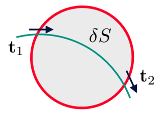
$$\int_V \mathbf{f}dv = \int_V \rho\mathbf{g}dv + \int_V \mathbf{f}_\sigma dv$$

The evaluation of the gravity term is straightforward and how to find the surface tension is discussed below.

9. The body force generally includes gravity, and for immiscible multiphase flows we usually also have surface tension. We will give the specific form for the surface tension shortly, but here simply split the body force into two parts. For more complex situations we can have additional body forces, such as due to electric or magnetic forces, or we may have body forces such as centripetal and Coriolis forces that appear because we are in moving frame of reference.

Surface Tension

The force on a control volume enclosing a segment of the interface is the difference in the tension where the interface enter the control volume and where it exists



$$\mathbf{F}_\sigma = (\sigma \mathbf{t})_2 - (\sigma \mathbf{t})_1$$

Using

$$\mathbf{t}_2 - \mathbf{t}_1 = \int_{\delta S} \frac{\partial \mathbf{t}}{\partial s} ds \quad \text{and} \quad \frac{\partial \mathbf{t}}{\partial s} = \kappa \mathbf{n}$$

Assuming constant surface tension σ.

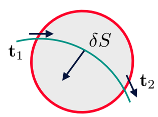
Gives

$$\mathbf{F}_\sigma = \int_{\delta S} \sigma \frac{\partial \mathbf{t}}{\partial s} ds = \int_{\delta S} \sigma \kappa \mathbf{n} ds$$

Notice that $\mathbf{F}_\sigma$ is the total force on the control volume due to the tension in the interface

10. For two-dimensional flow, tension on the interface is given simply by sigma times the tangent vector, here denoted by bold lowercase t. The force on a control volume enclosing a segment of the interface is the difference in the tension where the interface enter the control volume and where it exists, or sigma t at 2 minus sigma t at 1. We can represent the total force on the control volume in several ways. We will, in particular, use that the difference in sigma t at the endpoints can be written as an integral over the part of the interface that is inside the control volume, which we denote by delta S. Using that the derivative of the tangent vector with respect to arch length s, gives the curvature times the normal to the interface, bold n, and taking the surface tension to be constant, we can write the total force as the integral of sigma times the curvature times the normal, over the part of the interface that is inside the control volume.

Multiply by a one dimensional delta function and integrate over the control volume to get the total surface force on the control volume



$$\mathbf{F}_\sigma = \int_V \sigma \kappa \mathbf{n} \delta_S ds$$

The different ways in which we can write the surface force leads to different numerical approximations and in the numerical code we will write we will use a different form.

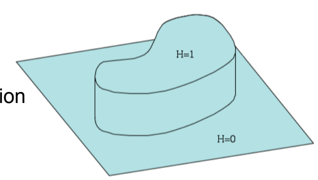
11. We can convert the integral over the part of the interface inside the control volume to an integral over the control volume by multiplying by a one dimensional delta function that is zero everywhere except at the interface. Although we will not use this form for the numerical code, it is very common and sometimes useful in theoretical discussions, such as those at the end of this lecture.

We are concerned with the flow of two or more fluids with different properties, such as density and viscosity.

For immiscible fluids, the interface separating the different fluids remains sharp for all time.

Identify each fluid by a marker function H

$$H(\mathbf{x}) = \begin{cases} 1 \text{ in fluid } 1 \\ 0 \text{ in fluid } 2 \end{cases}$$



The material properties are functions of the marker function

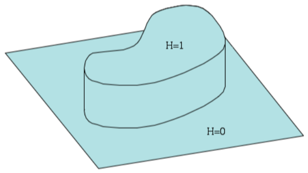
$$\rho = H\rho_1 + (1-H)\rho_2$$
$$\mu = H\mu_1 + (1-H)\mu_2$$

12. For flows with two or more fluids of different but constant properties we generally need to know what fluid is where. Thus, we need a marker function that is updated as the flow evolves. The various material properties can then be set as functions of the marker function. For two fluids we use a step function that is one in one fluid and zero in the other and the properties take one of two possible values.

DNS of Multiphase Flows

If the density of each material particle remains constant, the material derivative of the density is zero

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = 0$$



Substituting

$$\rho = H\rho_1 + (1-H)\rho_2$$

$$H(\mathbf{x}) = \begin{cases} 1 \text{ in fluid } 1 \\ 0 \text{ in fluid } 2 \end{cases}$$

Substituting and using that

$$\frac{D\rho_1}{Dt} = \frac{D\rho_2}{Dt} = 0$$

Gives

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

In some cases we simply use the density as the indicator function

13. To update the marker function we start with the mass conservation equation and substitute the expression for density as a function of the marker function. Using that the convective derivative of the densities is zero, we immediately get that the marker function is governed by the same equation, namely that the convective derivative is zero, or the marker moves with the fluid. That is, of course, something that we could have seen coming. If the material properties are constant in each fluid, as is the case here, the advection of the marker function becomes considerably simpler and we only need to know where the interface is.

DNS of Multiphase Flows

Summary: the governing equations in integral form.

Momentum conservation (the Navier-Stokes equations)

$$\frac{\partial}{\partial t}\int_V \rho \mathbf{u} dv = -\oint_S \rho \mathbf{u}\mathbf{u} \cdot \mathbf{n} ds$$
$$-\oint_S p\mathbf{n} ds + \oint_S \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \cdot \mathbf{n} ds + \int_V \rho \mathbf{g} dv + \int_V \sigma \kappa \mathbf{n} \delta_S ds$$

Conservation of volume (from the mass conservation equation since the flow is incompressible)

$$\oint_S \mathbf{u} \cdot \mathbf{n} ds = 0$$

Motion of the indicator function and updating properties

$$\frac{\partial H}{\partial t} + \mathbf{u} \cdot \nabla H = 0 \qquad \begin{aligned} \rho &= H\rho_1 + (1-H)\rho_2 \\ \mu &= H\mu_1 + (1-H)\mu_2 \end{aligned}$$

V: Control volume
S: Control surface

14. To sum up, the equations that we will be solving are the momentum equations for the two velocity components, subject to the constrain that the fluid are incompressible so that the volume flow in and out of a control volume balances, and the advection equation for the marker function, which will then give the material properties of the fluid.

DNS of Multiphase 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 governing equations can also be written in differential form using using generalized functions

15. Let me conclude the introduction of the governing equations by making a few points: First of all, the conservation equations for mass and momentum apply to any flow situations, including flows of multiple immiscible fluids. Secondly, for multiphase flows, each fluid generally has properties that are different from the other fluids and the location of each fluid must therefore be tracked. And third, we usually have additional physics that must be accounted for at the interface, such as surface tension. The governing equations can also be written in differential form using generalized functions, as I will discuss briefly in the next few slides.

DNS of Multiphase Flows

The "One-Fluid" Approach— The Governing Equations in Differential Form

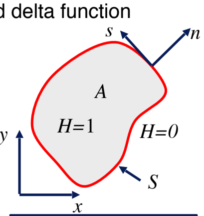
16. Although we work with the integral form of the governing equations here, since that leads directly to a finite volume method, many authors prefer to start from the differential form. Indeed, my guess is that more papers start from the differential form than the integral form, even when finite volume methods are used.

DNS of Multiphase Flows

Generalized functions: Step function and delta function

$$H(x,y,t) = \int_{A(t)} \delta(x-x')\delta(y-y')da'$$

$$\nabla H = \int_A \nabla[\delta(x-x')\delta(y-y')]\; da'$$
$$= -\int_A \nabla'[\delta(x-x')\delta(y-y')]\; da'$$
$$= -\oint_S [\delta(x-x')\delta(y-y')\mathbf{n}\; ds'$$
$$= -\int_S [\delta(x-x')\delta(y-y')\mathbf{n}\; ds'$$
$$= -\int_S \delta(s)\delta(n)\mathbf{n}\; ds'$$
$$= -\delta(n)\mathbf{n}$$



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

Using:

$$\delta(x-x')\delta(y-y') = \delta(s)\delta(n)$$

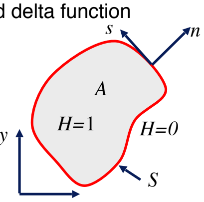
17. Since the marker function is discontinuous and the surface tension is singular, we need to work with generalized function to be able to write down the differential form. To do so we need to define the Heaviside step function in such a way that we can find its gradient. A particularly simple way is to define it as the area integral over the multiplication of two one-dimensional delta functions. Here x' and y' are the integration variables and x and y are the coordinates of the point where we are sitting. If x and y are inside the area, the x and y will be equal to x' and y' and the integral will be one but if x and y are outside the area, then the integral will be zero. The gradient is with respect to x and y so we can bring it under the integral. However, since the gradient is anti-symmetric with respect to the primed and unprimed variables, we can change the gradient to the gradient with respect to the primed variables, changing the sign. We now apply the divergence theorem, to write the integral as a surface integral (or a contour integral in 2D), and since the delta functions are zero everywhere except where x,y are equal to x',y', we can drop the circle on the integral.

DNS of Multiphase Flows

Generalized functions: Step function and delta function

$$H(x,y,t) = \int_{A(t)} \delta(x-x')\delta(y-y')da'$$

$$\nabla H = \int_A \nabla[\delta(x-x')\delta(y-y')]\; da'$$
$$= -\int_A \nabla'[\delta(x-x')\delta(y-y')]\; da'$$
$$= -\oint_S [\delta(x-x')\delta(y-y')\mathbf{n}\; ds'$$
$$= -\int_S [\delta(x-x')\delta(y-y')\mathbf{n}\; ds'$$
$$= -\int_S \delta(s)\delta(n)\mathbf{n}\; ds'$$
$$= -\delta(n)\mathbf{n}$$



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

Using:

$$\delta(x-x')\delta(y-y') = \delta(s)\delta(n)$$

17-Cont.: By introducing local coordinates, n in the normal direction and s in the tangential direction, we can integrate over the tangent direction and thus are left with the results that the gradient of the Heaviside function is equal to a delta function times the local normal. Here we take the normal to be positive pointing away from the H=1 region so we need a minus sign.

DNS of Multiphase Flows

The governing equations in differential form are derived in a standard way by consider the integral form for arbitrary control volume and insisting that the integrand is zero. In conservative form the equations are:

Conservation of Momentum

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p + \nabla \cdot \mu(\nabla \mathbf{u} + \nabla^T \mathbf{u}) + \rho \mathbf{g} + \underbrace{\sigma \kappa \mathbf{n}_f \delta(n)}_{\text{Singular interface term}}$$

Conservation of Mass

$\nabla \cdot \mathbf{u} = 0$ Incompressible flow

Equation of State:

$\frac{D\rho}{Dt} = 0; \quad \frac{D\mu}{Dt} = 0$ Constant properties following a material point

Alternatively, we have:

$$\frac{DH}{Dt} = \frac{\partial H}{\partial t} + \mathbf{u} \cdot \nabla H = 0$$

$$\rho = \rho_1 H + (1-H)\rho_2$$

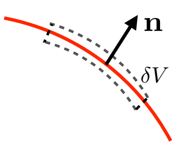
$$\mu = \mu_1 H + (1-H)\mu_2$$

18. By applying the standard argument to the integral form, that the equations hold for an arbitrary control volume so the integrand must be zero, we get the differential form of the conservation equations. These equations are essentially the same as for single-phase flow, except the material properties are step-functions and we must add a singular surface tension term. The momentum equations must, of course, be supplemented by the incompressibility condition and advection equations for the material properties. We generally refer to this form of the equations as the one-fluid, or one-field, formulation.

DNS of Multiphase Flows

The "one-fluid" formulation implicitly contains the proper interface jump conditions. Integrating each term over a small control volume centered on the interface:

$$\underbrace{\int_{\delta V} \frac{D\rho \mathbf{u}}{Dt} dv}_{=0} = \underbrace{-\int_{\delta V} \nabla p dv}_{[-p]\mathbf{n}} + \underbrace{\int_{\delta V} \nabla \cdot \mu(\nabla \mathbf{u} + \nabla^T \mathbf{u}) dv}_{[\mu(\nabla \mathbf{u} + \mathbf{u}^T)]\mathbf{n}} + \underbrace{\int_{\delta V} \rho \mathbf{g} dv}_{=0} + \underbrace{\int_{\delta V} \kappa \sigma \mathbf{n} \delta(n) dv}_{\kappa \sigma \mathbf{n}}$$



The non-zero terms give the

Jump Condition:

$$[-p + \mu(\nabla \mathbf{u} + \mathbf{u}^T)] = -\kappa \sigma \mathbf{n}$$

19. It is important to keep in mind that the one-fluid form of the governing equations contains no approximations beyond the standard continuum equations. They do, in particular, include the jump conditions that we would have to apply at an interface if we solved separate equations for each fluid region. We can extract the jump conditions by integrating the one fluid equations over a small "pill box" containing the interface. The box follows the interface, which moves with the fluid velocity, so we combine the first two terms into the convective derivative and then integrate. Most of the terms have a finite value and go to zero as the size of the box goes to zero. The singular terms, however, do not do that and we are left with a statement that says that the jumps in the pressure and the viscous stresses are balanced by the surface tension. We note that we need to modify this argument slightly if there is mass transfer across the interface, such as for evaporation and condensation and if the surface tension is not constant.

DNS of Multiphase Flows

We can also show that the "one-fluid" formulation contains the equations written separately for each fluid and the jump conditions:

Write:

$$\mathbf{u} = H_1 \mathbf{u}_1 + H_2 \mathbf{u}_2$$

$$p = H_1 p_1 + H_2 p_2$$

$$\rho = H_1 \rho_1 + H_2 \rho_2$$

Use

$$H_1 H_2 = 0$$

$$H_i H_i = H_i, \quad i = 1, 2$$

and substitute into the momentum equation to get

$$H_1(\mathbf{x})\underbrace{(\ldots\ldots)}_{=0} + H_2(\mathbf{x})\underbrace{(\ldots\ldots)}_{=0} + \delta(\mathbf{x}_f)\underbrace{(\ldots\ldots)}_{=0} = 0$$

Momentum equation in phase 1 — Momentum equation in phase 2 — Interface conditions

The terms multiplied by the different generalized functions must each vanish separately

20. We can also show that the "one-fluid" formulation contains the equations written separately for each fluid and the jump conditions by writing every variable as a function of the marker function and substituting into the one-fluid equations. By grouping terms depending on whether they are multiplied by H 2, H 1, or a delta function and using that each group must be equal to zero separately, we recover the equations for each region plus the jump conditions.

DNS of Multiphase Flows

Solution Strategies

21. Once we have the governing equations and have decided on which form, such as the integral form, to use, we need a solution strategy. There are several possibilities.

DNS of Multiphase Flows

To solve for the flow, the governing equations are discretized both in space and time. The computational domain is divided into a finite number of control volumes (finite volume methods) or a finite number of points is used to represent the flow (finite difference methods).

For flows involving moving interfaces, solution methods can be divided in two major categories

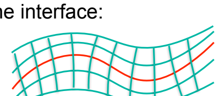
1. Solving separate equations in each fluid using a **moving** grid aligned with the interface, and applying boundary conditions at the interface:

2. Solving one set of equations for the whole domain on a **fixed** grid and incorporate the boundary conditions into the equations

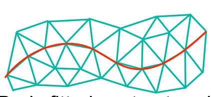
22.To solve for the flow, the governing equations need to be discretized both in space and time. To do so we divide the computational domain into a finite number of control volumes for finite volume methods or use a finite number of points to represent the flow if we are using finite difference methods. For flows with moving interfaces, solution methods can be divided in two major categories. We can solve separate equations in each fluid using a moving grid aligned with the interface where we apply the appropriate boundary conditions. Or, we can solve one set of equations for the whole domain on a fixed grid and incorporate the boundary conditions directly into the governing equations.

DNS of Multiphase Flows

Solving separate equations in each fluid using a **moving** grid aligned with the interface, and applying boundary conditions at the interface:

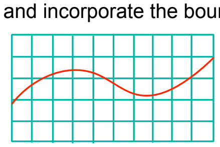


Body fitted structured grid

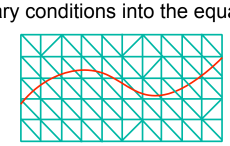


Body fitted unstructured grid

Solving one set of equations for the whole domain on a **fixed** grid and incorporate the boundary conditions into the equations



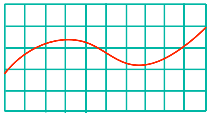
Stationary structured grid



Stationary unstructured grid

23. These alternatives are shown schematically here. In the left column we use structured grids where the layout determines the relationship of each control volume to its neighbors, and on the right we use unstructured grids, where the shape and layout of the control volumes are arbitrary and we need to explicitly store information about their layout. In the top row we align gridlines or control volume boundaries with the interface but in the bottom row the interface is independent of the grid lines. While the grids in the bottom row are usually stationary, the grids in the top row must change with time, if the interface is moving.

DNS of Multiphase Flows



Here we solve one set of equations for the whole domain on a fixed grid and incorporate the boundary conditions into the equations

The one-fluid formulation allows us to treat multi-phase flows in more or less the same way as single phase flows.

The main differences are:

The density and viscosity change discontinuously across the interface and have to be updated as the interface moves

Surface tension needs to be evaluated and added to the Navier-Stokes equations

24. In our case we will use regular structured grids where the interface can have an arbitrary orientation with respect to the grid lines. This overall strategy is, by far, the most common and so far the most successful approach to simulating flows with sharp interfaces. Even after we settle on this approach there are a number of alternative methods. Roughly speaking the questions are what numerical method we use to solve the Navier-Stokes equations and how do we track the interface separating the different fluids. These are somewhat separate questions and in the next lectures we will first develop a code to solve the Navier-Stokes equations and then present a few of the possibilities that are available for tracking the interface. We will then pick one of them to implement in the flow solver.