- In this module, we will deal with advanced modeling capabilities.
- Advanced modeling capabilities rely a lot in physical models, such as, turbulence, multiphase flows, porous media, combustion, radiation, heat transfer, phase change, acoustics, cavitation, and so on.
- Therefore, it is extremely important to get familiar with the theory behind the models.

"Essentially, all models are wrong,
but some are useful"

G. E. P. Box

George Edward Pelham Box
18 October 1919 – 28 March 2013. Statistician, who worked in the areas of quality control, time-series analysis, design of experiments, and Bayesian inference. He has been called *"one of the great statistical minds of the 20th century"*.

What is a multiphase flow?

- A multiphase flow is a fluid flow consisting of more than one phase component and have some level of phase separation above molecular level.
- Multiphase flows exist in many different forms.
- Two phase flows can be classified according to the state of the different phases:
    - Gas-Liquid mixture.
    - Gas-Solid mixture.
    - Liquid-Solid mixture.
    - Immiscible liquid-liquid.

Multiphase flows in industry and nature

- Multiphase flows are very common in industry and in nature, the following are a few examples depending on the state of the different phase.

- **Gas–particle flows:**
  - Natural: sand storms, volcanoes, avalanches, rain droplets, mist formation.
  - Biological: aerosols, dust particles, smoke (finely soot particles),
  - Industrial: pneumatic conveyers, dust collectors, fluidized beds, solid propellant rockets, pulverized solid particles, spray drying, spray casting.

- **Liquid–solid flows:**
  - Natural: sediment transport of sand in rivers and sea, soil erosion, mud slides, debris flows, iceberg formation.
  - Biological: blood flow, eyes, lungs.
  - Industrial: slurry transportation, flotation, fluidized beds, water jet cutting, sewage treatment plants, bio-reactors.

Multiphase flows in industry and nature

- Multiphase flows are very common in industry and in nature, the following are a few examples depending on the state of the different phase.

- **Gas–liquid flows:**
    - Natural: ocean waves.
    - Biological: blood flow, eyes, lungs.
    - Industrial: boiling water and pressurized water nuclear reactors, chemical reactor, desalination systems, sewage treatment plants, boilers, heat exchangers, internal combustion engines, liquid propellant rockets, fire sprinkler suppression systems.

- **Liquid–liquid flows:**
    - Industrial: emulsifiers, fuel-cell systems, micro-channel applications, extraction systems.

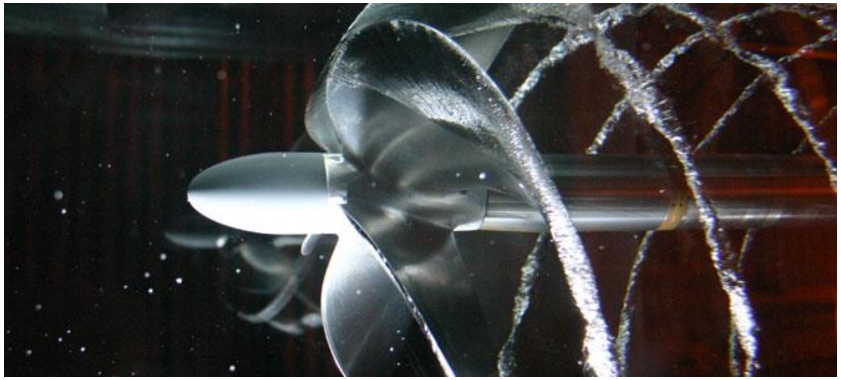
- **Gas–liquid–solid flows:**
    - Industrial: air lift pumps, fluidized beds, oil transportation

Examples of multiphase flows

Municipal and industrial water treatment
http://www.asiapacific.basf.com/apex/AP/en/upload/Press2010/BASF-Water-Chem-2010-Paper-Chem-2010-Intex-Shanghai

Cargo ship wake
http://developeconomies.com/development-economics/how-to-get-america-back-on-track-free-trade-edition/

Siltation & Sedimentation
http://blackwarriorriver.org/siltation-sedimentation/



Propeller cavitation
http://www.veempropellers.com/features/cavitationresistance

Examples of multiphase flows

Cooling Towers
https://whatiswatertreatment.wordpress.com/what-are-the-systems-associated-with-water-treatment-and-how-are-they-treated/103-2/

Volcano eruption
http://americanpreppersnetwork.com/2014/08/preparing-volcano-eruption.html

Fermentation of beer and spirits
http://www.distillingliquor.com/2015/02/05/how-to-make-alcohol-and-spirits/

Coastal structures – Waves interaction.
http://californiabeachblog.blogspot.it/2013_10_01_archive.html

Classifying multiphase flows according to phase morphology

- **Disperse system**: the phase is dispersed as non-contiguous isolated regions within the other phase (the continuous phase) . When we work with a disperse phase we say that the system is dispersed: disperse-continuous flow.
- **Separated system**: the phase is contiguous throughout the domain and there is one well defined interphase with the other phase. When we work with continuous phases we say that the system is separated: continuous-continuous flow.

Dispersed system

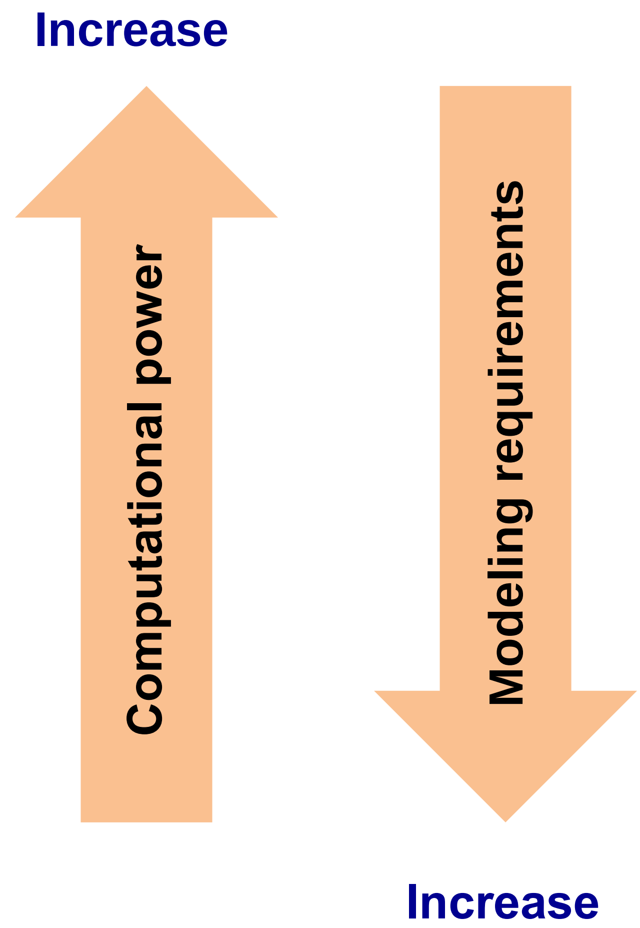
Separated system

Why simulating multiphase flows is challenging?

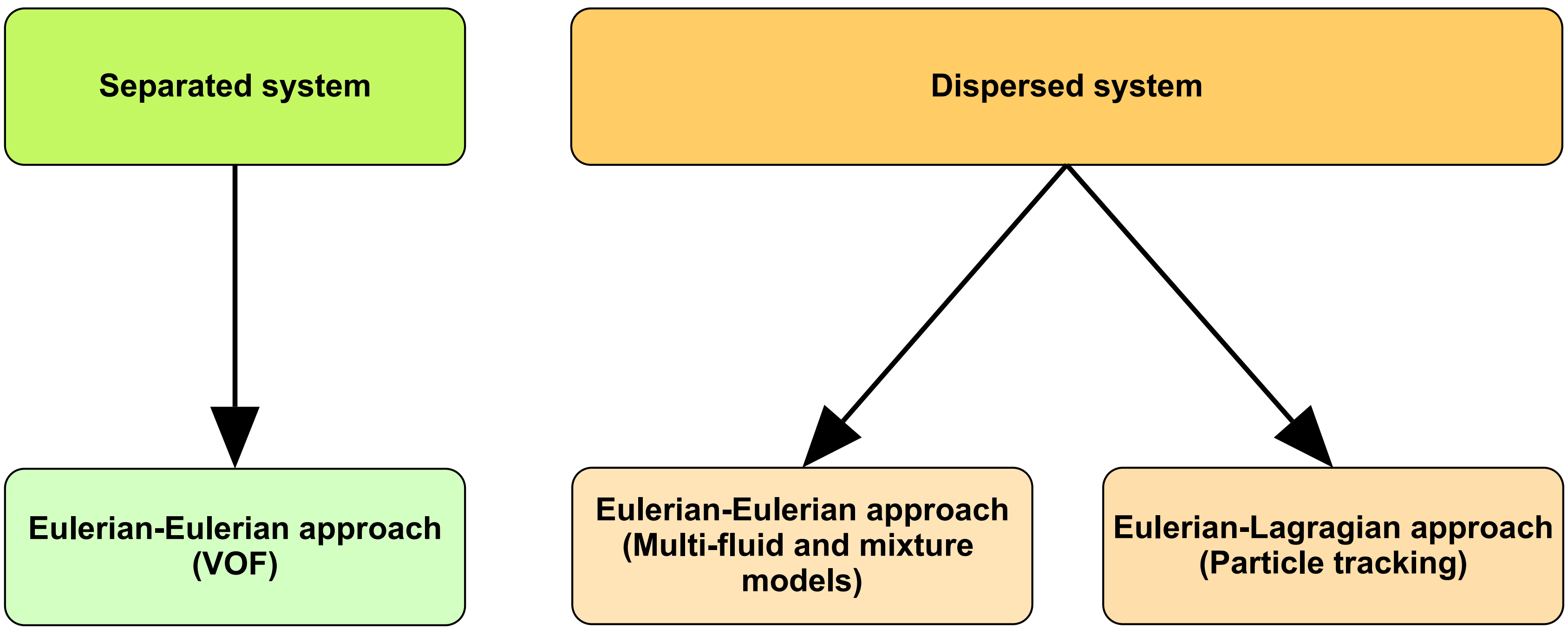
- Simulating multiphase flows is not an easy task.
- The complex nature of multiphase flows is due to:
    - More than one working fluid.
    - The transient nature of the flows.
    - The existence of dynamically changing interfaces.
    - Significant discontinuities (fluid properties and fluid separation).
    - Complicated flow field near the interface.
    - Interaction of small scale structures (bubbles and particles).
    - Different spatial-temporal scales.
    - Dispersed phases and particle-particle interactions.
    - Mass transfer and phase change.
    - Turbulence.
    - Many models involved (drag, lift, heat transfer, turbulence dispersion, frictional stresses, collisions, kinetic theory, and so on).

How to treat the wide range of behaviors in multiphase flows

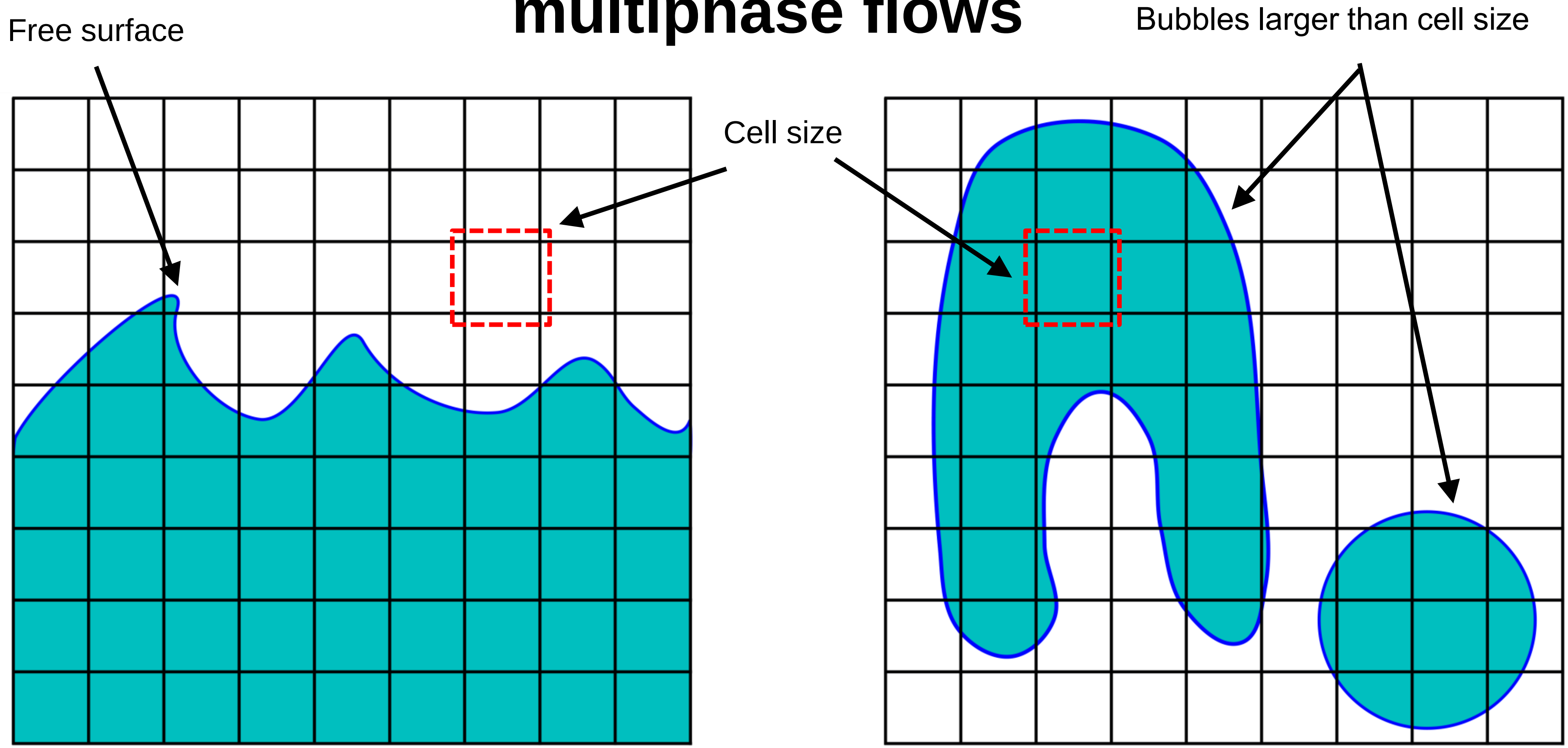
- **Fully resolved:** solves complete physics. All spatial and temporal scales are resolved.
- **Eulerian-Lagrangian:** solves idealized isolated particles that are transported with the flow. One- or two-way coupling is possible. Can account for turbulence, momentum transfer, and mass transfer.
- **Eulerian-eulerian:** solves two or more co-existing fluids. The system can be dispersed or separated, and can account for turbulence, momentum transfer, and mass transfer.



How to treat the wide range of behaviors in multiphase flows



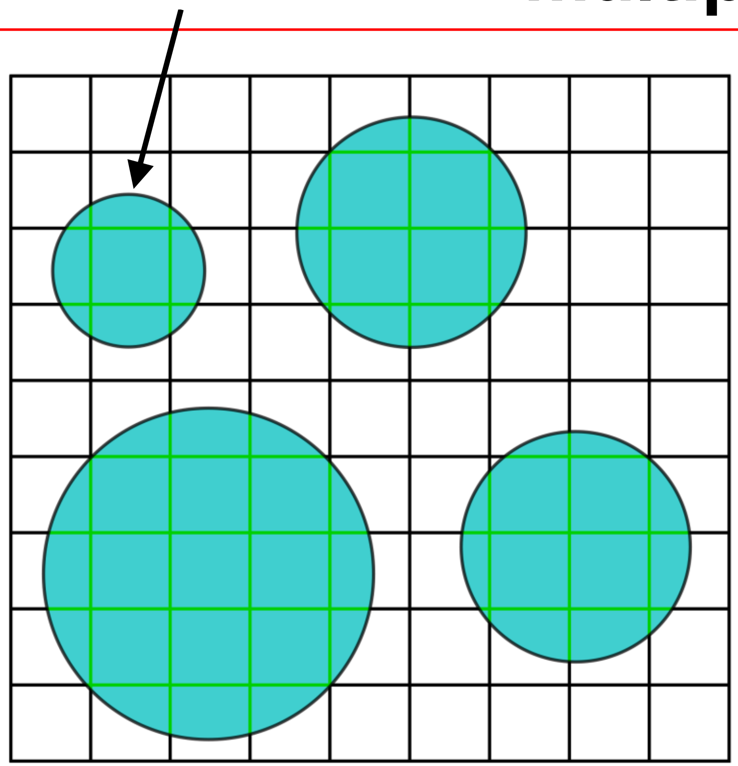
How to treat the wide range of behaviors in multiphase flows



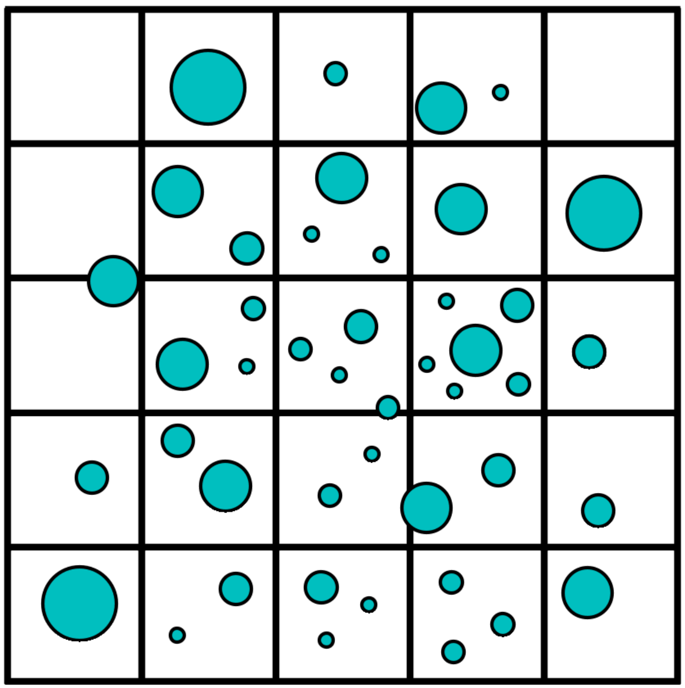
- Applicability of the VOF method to separated systems (non-interpenetrating continua).
- In the illustrations, the free surface and bubbles are track/resolve by the mesh.
- The smaller the features we want to track/resolve, the smaller the cells should be.

How to treat the wide range of behaviors in multiphase flows

Not ok. Only one cell to resolve the bubble.

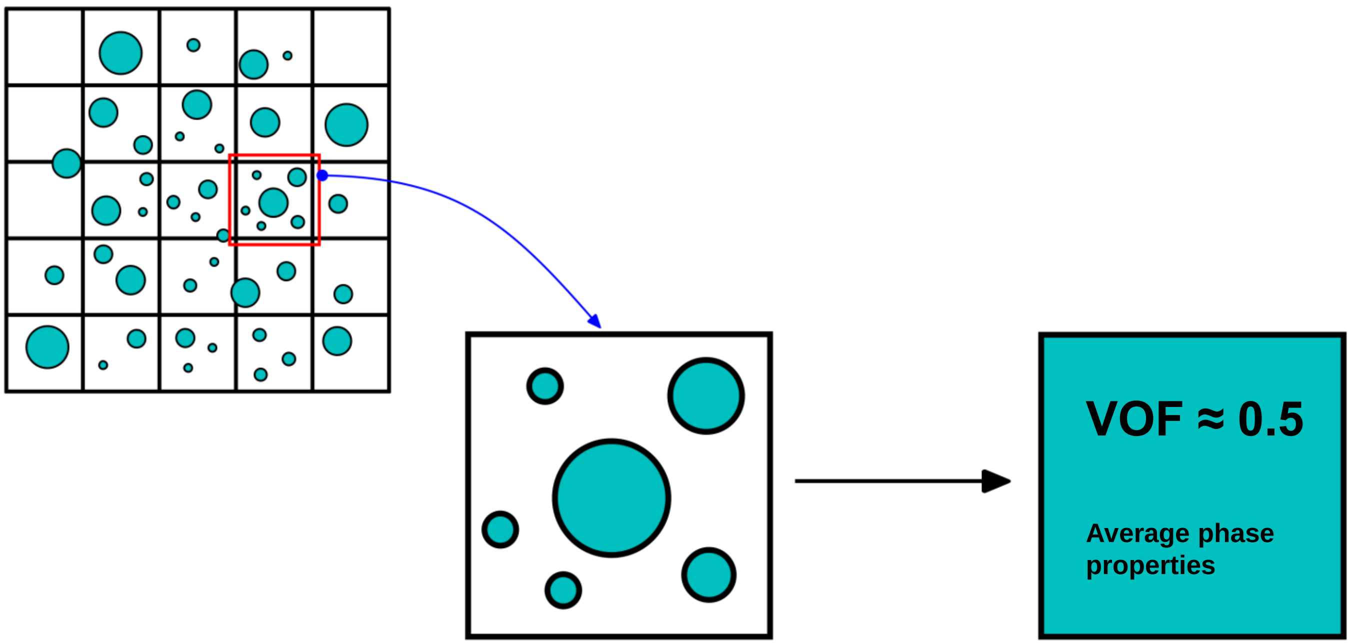


- Bubbles, droplets and/or particles bigger than grid scales (GS), can be resolved using VOF.
- To resolve a bubble you will need at least two cells in every direction



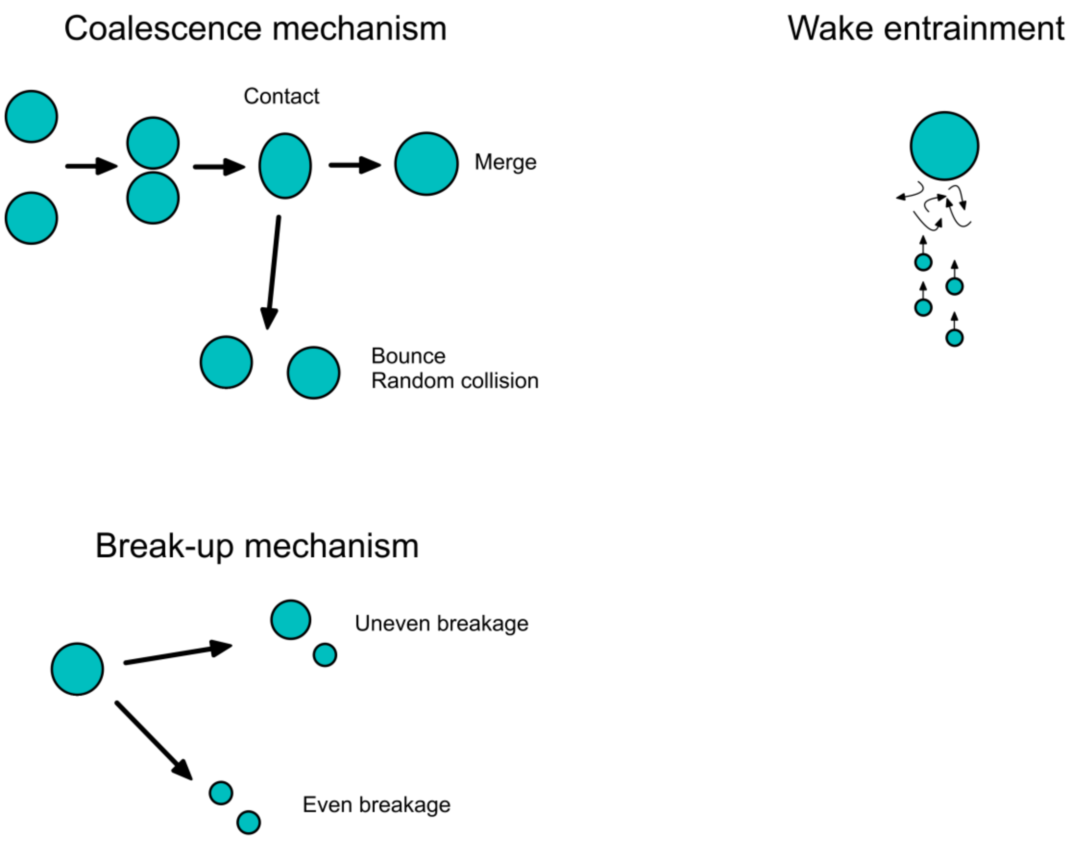
- Bubbles, droplets and/or particles smaller than grid scales (sub-grid scales or SGS), can not be resolve using the VOF method.
- We need to use models.

How to treat the wide range of behaviors in multiphase flows



- Dispersed phase in a continuous phase.
- In this case, the VOF method is not able to handle bubbles smaller than grid scales.
- Multi-fluid and mixture models are able to model bubbles smaller than grid scales by averaging the phase properties in the discrete domain.

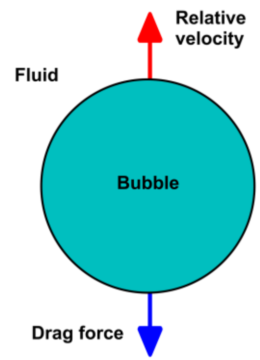
How to treat the wide range of behaviors in multiphase flows

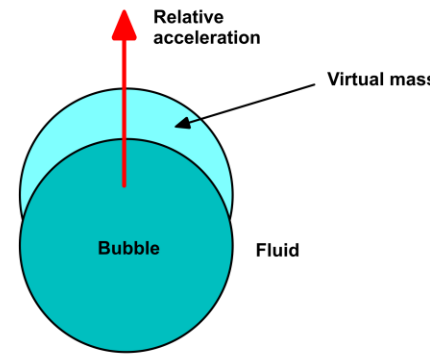


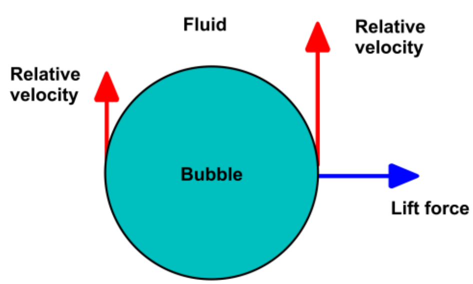
- Multi-fluid and mixture approaches can model bubble coalescence, bubble break-up and wake entrainment in dispersed systems

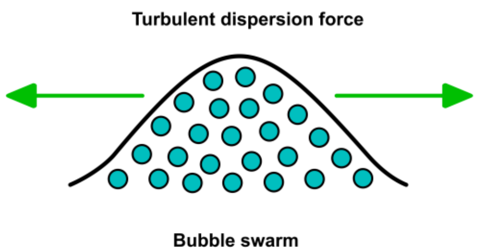
How to treat the wide range of behaviors in multiphase flows

- When using multi-fluid and mixture approaches interfacial momentum transfer models must be taken into account in order to model mass transfer and phases interaction.
- As for turbulence modeling, there is no universal model.
- It is up to you to choose the model that best fit the problem you are solving.
- Depending on the physics involved, you will find different models and formulations
- You need to know the applicability and limitations of each model, for this, refer to the literature.

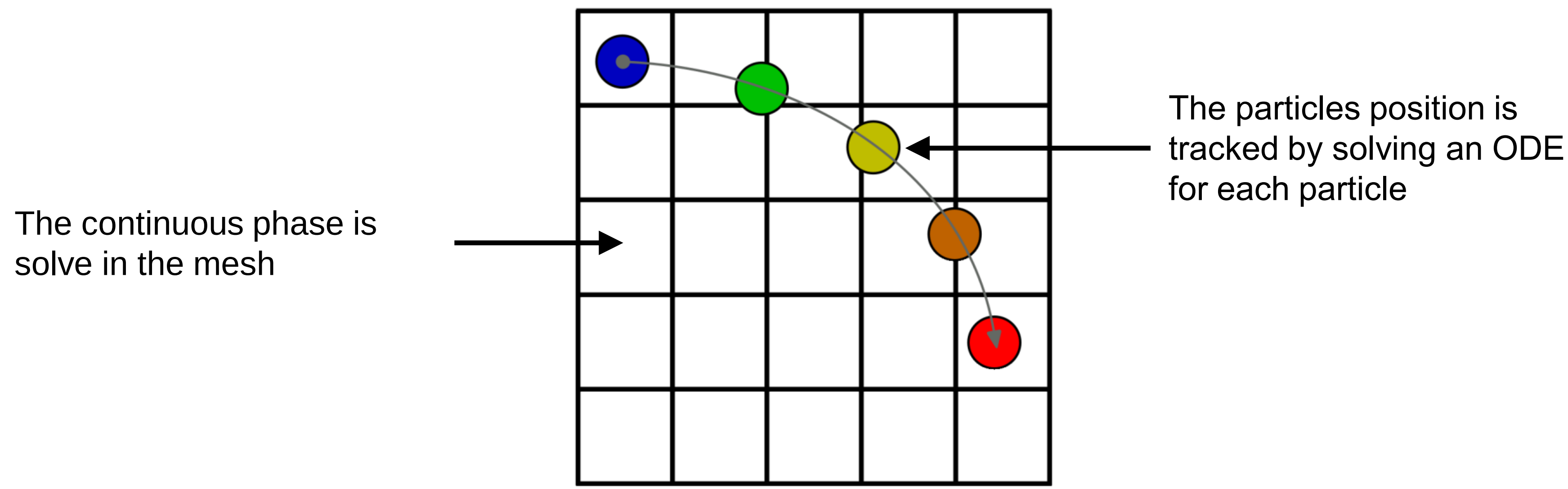








How to treat the wide range of behaviors in multiphase flows

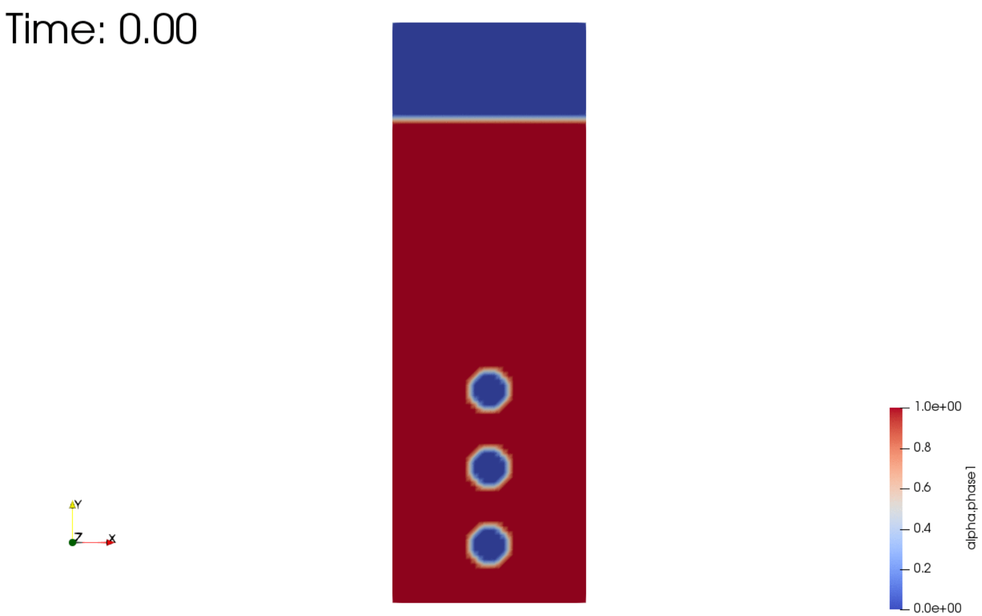


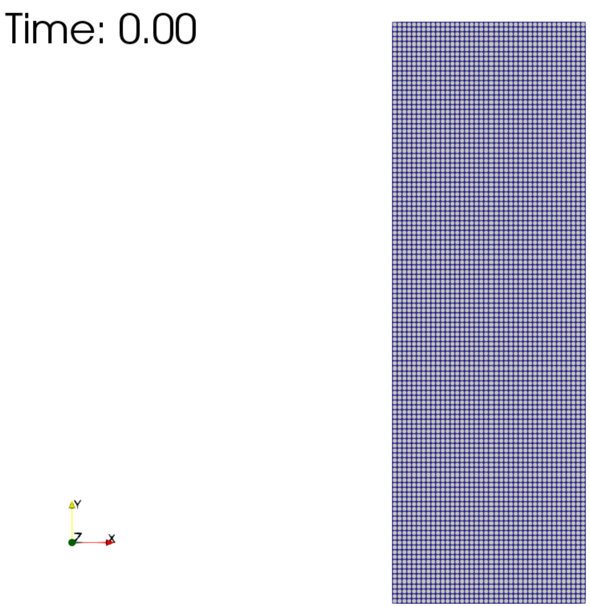
- In the Eulerian-Lagrangian framework, the continuous phase is solved in an Eulerian reference system and the particles or dispersed phase is solved in a Lagrangian reference system.
- The particles can be smaller or larger than the grid size.
- The particles can be transported passively or they can be coupled with the fluid governing equations.
- It accounts for particle interaction and mass transfer.
- The particles can interact with the boundaries and have a fate.

Numerical approaches for multiphase flows

Eulerian-Eulerian (VOF)	Eulerian-Eulerian (Dispersed systems)	Eulerian-Lagrangian
• Non-interpenetrating continua. • Continuous phases: Eulerian. • Fluid properties are written on either side of the interface (no averaging). • Solves one single set of PDEs: mass, momentum, energy.	• Interpenetrating continua. • Continuous phase: Eulerian. • Dispersed phase: Eulerian. • Phase-weighted averages. • Solves PDEs for all phases (including interphase transfer terms): mass, momentum, energy. • It can deal with gas-liquid, gas-solid, and liquid-solid interactions.	• Continuous phase: Eulerian. • Dispersed phase: Lagrangian. • Solves ODEs for particle tracking (for every single particle). • Solves a set of PDEs for the continuous phase: mass, momentum, energy. • Phase interaction terms (including interphase transfer terms).

Numerical approaches for multiphase flows



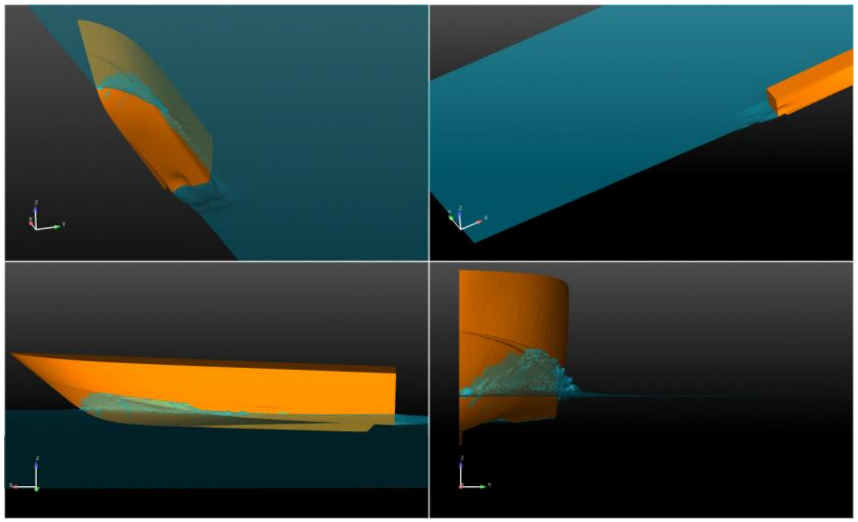


http://www.wolfdynamics.com/training/mphase/image2.gif

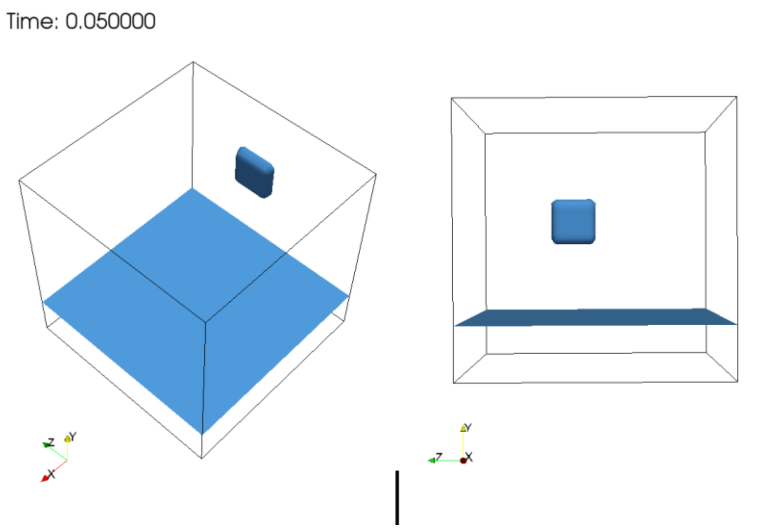
http://www.wolfdynamics.com/training/mphase/image3.gif

- Simulation showing free surface tracking, bubble tracking, bubble coalescence, bubble break-up and wake entrainment using the VOF method.
- In this simulation the free surface and bubbles are capture by using AMR. However, the smallest bubble that can be resolved is at the smallest grid size.

Numerical approaches for multiphase flows



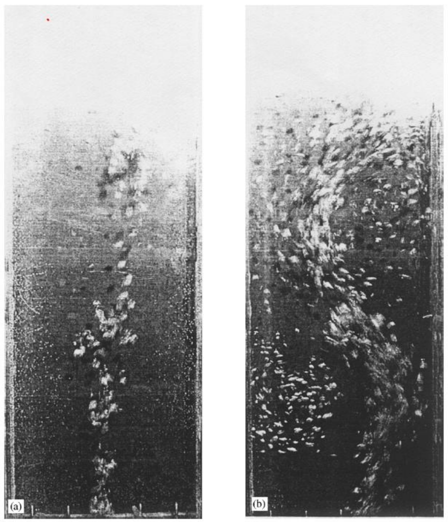
www.wolfdynamics.com/training/mphase/image10.gif

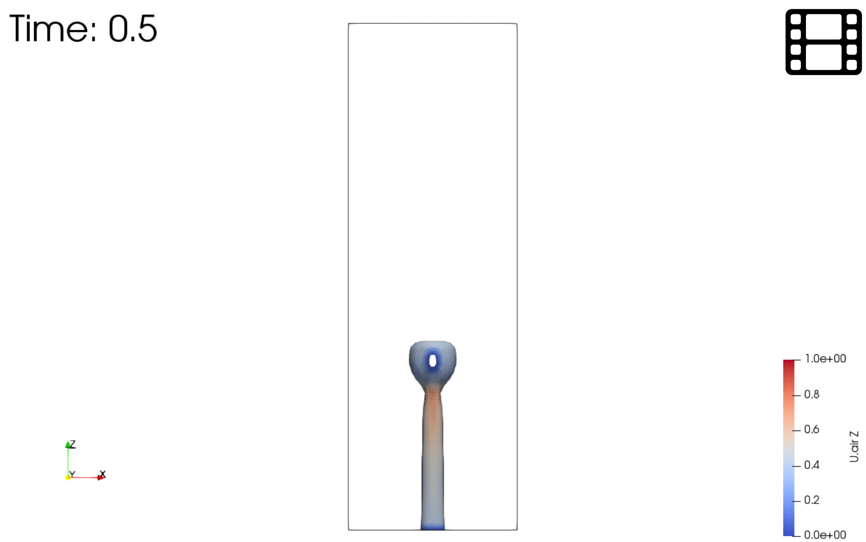


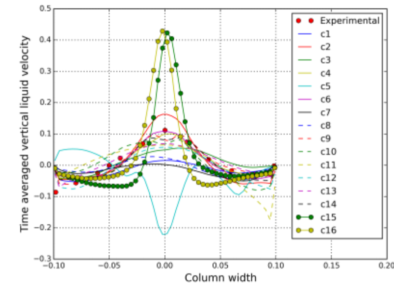
http://www.wolfdynamics.com/training/mphase/image16.gif

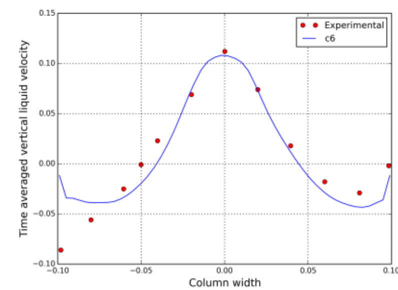
- Simulations showing free surface tracking using the VOF approach
- The left image corresponds to a simulation with rigid body motion and accurate surface tracking using the VOF method.

Numerical approaches for multiphase flows









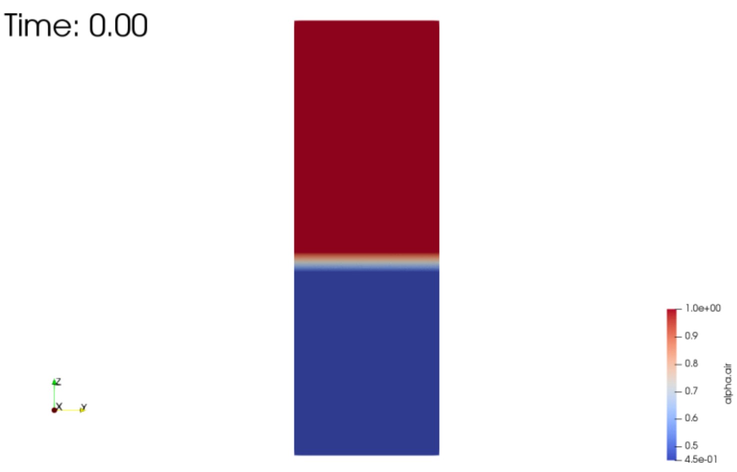
http://www.wolfdynamics.com/training/mphase/image18.gif

- Eulerian-Eulerian simulation (gas-liquid).
- The bubbles are not being solved, instead, the interaction between phase is being averaged.

References:

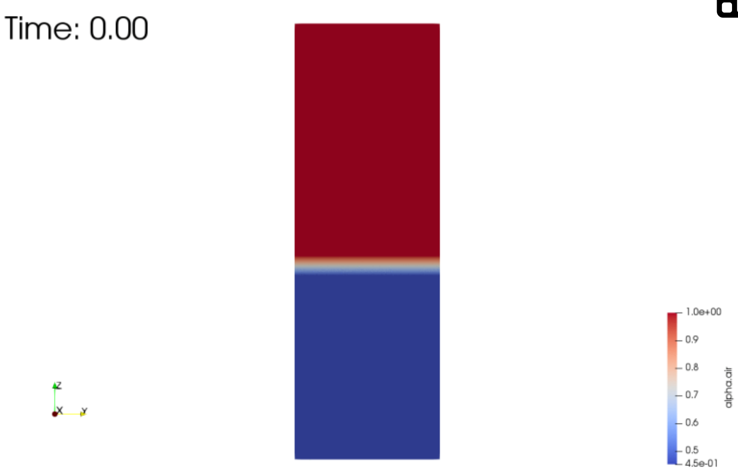
[1] Vivek V. Buwa, Vivek V. Ranade, Dynamics of gas–liquid flow in a rectangular bubble column: experiments and single/multi-group CFD simulations. Chemical Engineering Science 57 (2002) 4715 – 4736

Numerical approaches for multiphase flows



twoPhaseEulerFoam
Air volume fraction
Turbulent case

http://www.wolfdynamics.com/training/mphase/image42.gif

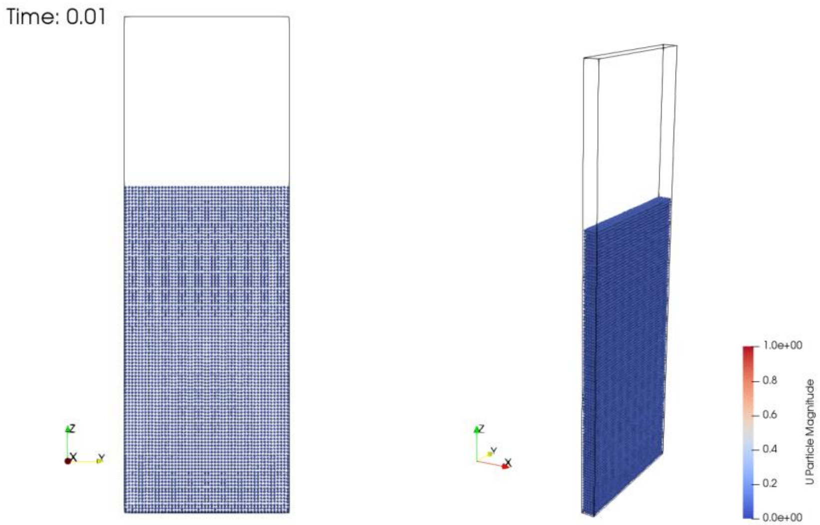


twoPhaseEulerFoam
Air volume fraction
Laminar case

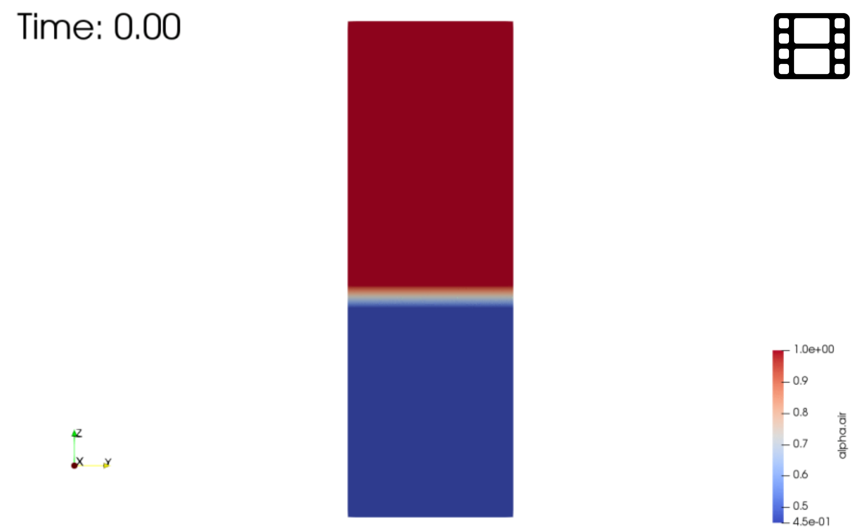
http://www.wolfdynamics.com/training/mphase/image41.gif

- Eulerian-Eulerian simulations using the Eulerian-Granular KTGF approach (solid-gas).
- The granular phase is simulated as continuous phase.
- In these simulations we can observe the influence of turbulence modeling in the solution.

Numerical approaches for multiphase flows



DPMFoam
Particle-particle interactions colored by velocity magnitude (particles not to scale)
http://www.wolfdynamics.com/training/mphase/image43.gif



twoPhaseEulerFoam
Air volume fraction
Turbulent case
http://www.wolfdynamics.com/training/mphase/image42.gif

- Comparison of an Eulerian-Lagrangian simulation and an Eulerian-Eulerian simulation (gas-solid).
- In the Eulerian-Lagrangian approach we track the position of every single particle. We also solve the fate and interaction of all particles.
- In the Eulerian-Eulerian approach we solve the granular phase as a continuous phase.
- The computational requirements of the Eulerian-Eulerian simulation are much lower than those for the Eulerian-Lagrangian simulation.

Volume-of-Fluid (VOF) governing equations for separated systems

- The incompressible, isothermal governing equations can be written as follows,

Source terms:
- Porous media
- Coriolis forces
- Centrifugal forces
- Mass transfer
- and so on …

$$\nabla \cdot \mathbf{U} = 0$$

Surface tension - Continuum surface force (CSF)

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) = -\nabla p + \nabla \cdot \tau + \rho g + f_\sigma + \rho S$$

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot \mathbf{U}\gamma + \nabla \cdot (\mathbf{U}_r \gamma (1 - \gamma)) = 0 \longrightarrow$$

Phase transport equation and interface tracking with surface compression

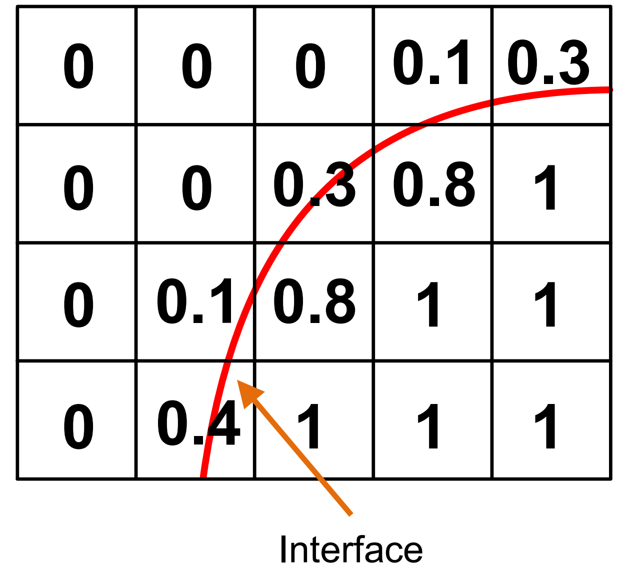
$$0 < \gamma < 1 \longrightarrow$$

Volume fraction (bounded quantity)

- You can see the volume fraction γ as a pointer that indicates what phase (with the corresponding physical properties), is inside each cell of the computational domain.

Volume-of-Fluid (VOF) governing equations for separated systems

- For example, in the case of two phases where phase 1 is represented by $\gamma = 1$ and phase 2 is represented by $\gamma = 0$; a volume fraction value of 1 indicates that the cell is fill with phase 1; a volume fraction of 0.8 indicates that the cell contains 80% of a phase 1; and a volume fraction of 0, indicates that the cell is fill with phase 2.



- The values between 0 and 1 can be seen as the interface between the phases.

- The fluid properties can be written on either side of the interface as follows,

$$\rho = \gamma_1 \rho_1 + (1 - \gamma_1)\rho_2$$

$$\mu = \gamma_1 \mu_1 + (1 - \gamma_1)\mu_2$$

Eulerian-Eulerian governing equations for dispersed systems

- The Eulerian-Eulerian approach solves the governing equations for each phase, it treats the phases as interpenetrating continua.
- The incompressible, isothermal governing equations with interface tracking can be written as follows,

Surface tension - Continuum surface force (CSF)

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{U}_k) = 0$$

Interface forces or momentum transfer.
Bubbles interaction models

$$\frac{\partial (\alpha_k \rho_k \mathbf{U}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{U}_k \mathbf{U}_k) = -\nabla \cdot (\alpha_k \tau_k) - \alpha_k \nabla p + \alpha_k \rho_k \mathbf{g} + \mathbf{M}_k + f_\sigma + \mathbf{S}_k$$

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \mathbf{U}_k \alpha_k \rho_k + \nabla \cdot (\mathbf{U}_r \alpha_k \rho_k (1 - \alpha_k)) = 0$$

$$\sum_k \alpha_k = 1.0 \qquad \rho_m = \sum_k \alpha_k \rho_k \qquad \mathbf{U}_m = \frac{\sum_k \alpha_k \rho_k \mathbf{U}_k}{\rho_m}$$

Source terms:
- Porous media
- Coriolis forces
- Centrifugal forces
- Mass transfer
- and so on …

Eulerian-Lagrangian governing equations

- In the Eulerian-Lagrangian framework, the continuous phase is solved in an Eulerian reference system and the particles or dispersed phase is solved in a Lagrangian reference system.
- The particles can be transported passively, or they can be coupled with the fluid governing equations (they can modify the fluid field).
- The particles can interact with the boundaries, they can escape, bounce, stick, or form a wall film.
- This formulation accounts for particle interaction and mass transfer.
- The governing equations can be written as follows,

$$m\frac{d\mathbf{U}}{dt} = \mathbf{F}_{drag} + \mathbf{F}_{pressure} + \mathbf{F}_{virtual\,mass} + \mathbf{F}_{other}$$

$$+$$

Any of the Eulerian formulations (single or multi-phase)

On the multiphase flows models

- In OpenFOAM®, there are many interfacial momentum transfer models implemented.
- There are also many models for Eulerian-Lagrangian methods.
- No need to say that turbulence also applies to multiphase flows.
- We want to remind you that there is no universal model, it is up to you to choose the model that best fit the problem you are solving.
- You need to know the applicability and limitations of each model, for this, refer to the literature.
- Remember, you have the source code so feel free to explore it.

Multiphase solvers in OpenFOAM®

- OpenFOAM® comes with many solvers and models that can address a wide physics.
- When dealing with multiphase flows in OpenFOAM®, you can use VOF, Eulerian-Eulerian, Eulerian-Eulerian with VOF, and Eulerian-Lagrangian methods.
- The solution methods can account for turbulence models, interface momentum transfer models, mass transfer models, particle interaction models and so on.
- It is also possible to add source terms, deal with moving bodies or use adaptive mesh refinement.

- You will find the source code of all the multiphase solvers in the directory:
  - **`OpenFOAM-6/applications/solvers/multiphase`**

- You will find the source code all the particle tracking solvers in the directory:
  - **`OpenFOAM-6/applications/solvers/lagrangian`**

Multiphase solvers in OpenFOAM®

- These are the multiphase solvers that you will use most of the time in OpenFOAM®.

- The VOF approach:
    - interFoam family solvers

- The Eulerian-Eulerian approach:
    - twoPhaseEulerFoam, multiphaseEulerFoam

- The Eulerian-Granular KTGF (kinetic theory of granular flows) approach.
    - twoPhaseEulerFoam

- The Eulerian-Lagrangian framework,
    - DPMFoam, MPPICFoam

Multiphase solvers in OpenFOAM®

- Remember, you should always conduct production runs using a second order discretization scheme.
- Most of multiphase flows are transient, so you need to use transient methods.
- You also need to add new entries in the dictionaries *fvScheme* and *fvSolution*.
- The new entries, correspond to the new terms and equations used by the solver.
- You also need to set the initial and boundary conditions and assign the physical properties.
- Hereafter we will only address how to select physical properties for the VOF method. However, the procedure is similar for other solvers.
- In the training material, you will find many tutorials addressing the different approaches.

Selecting physical properties and advanced physics

- In the directory **`constant`** you will find the dictionaries used to select physical properties and advanced physics.
- The following dictionaries are compulsory:
  - *`g`*: in this dictionary you set the gravity field.
  - *`transportProperties`*: in this dictionary you set the transport properties for each phase.
  - *`turbulenceProperties`*: in this dictionary you set the turbulence model.
- The dictionary *`transportProperties`* requires special attention, as it is in this dictionary where we set the transport properties for each phase.
- We also give a name to the phases in the dictionary *`transportProperties`*.
- These dictionaries are standard for the VOF solvers (interFoam and so on).
- If you are using a different solver (e.g., twoPhaseEulerFoam), you will need to use additional dictionaries where you define the interfacial models and so on.

Selecting physical properties and advanced physics

- If you are using the solver interFoam, the *transportProperties* dictionary should looks like this one:

The first phase is always considered the primary phase

Phases naming convention. The name of the phases is chosen by the user.

phase1 properties

phase2 properties

Surface tension between phase1 and phase2

```
phases (phase1 phase2);

phase1
{
        transportModel   Newtonian;
        nu               nu [ 0 2 -1 0 0 0 0 ] 1e-06;
        rho              rho [ 1 -3 0 0 0 0 0 ] 1000;
}

phase2
{
        transportModel   Newtonian;
        nu               nu [ 0 2 -1 0 0 0 0 ] 1.48e-05;
        rho              rho [ 1 -3 0 0 0 0 0 ] 1;
}

sigma sigma [ 1 0 -2 0 0 0 0 ] 0.07;
```

Selecting physical properties and advanced physics

- In the directory **0** you will find the dictionaries used to define the boundary conditions and initial conditions of all field variables (including the volume fraction)
- When you create the dictionaries for the boundary conditions and initials conditions for the volume fraction (or alpha), you use the same naming convention as in the dictionary *transportProperties*.
- That is to say, if you are naming you primary phase phase1, you should create the dictionary *alpha.phase1*.
- This dictionary will contain the initial and boundary conditions of the volume fraction

Some useful bibliographical references

- **Computational Techniques for Multiphase Flows**
  G. H. Yeoh, J. Tu. 2009, Butterworth-Heinemann
- **Multiphase Flow Analysis Using Population Balance Modeling: Bubbles, Drops and Particles**
  G. H. Yeoh, C. P Cheung, J. Tu. 2013, Butterworth-Heinemann
- **Turbulence Modeling for CFD**
  D. Wilcox. 2006, DCW Industries.
- **Error analysis and estimation in the Finite Volume method with applications to fluid flows.**
  H. Jasak. PhD Thesis. 1996. Imperial College, London.
- **Computational fluid dynamics of dispersed two-phase flows at high phase fractions**
  H. Rusche. PhD Thesis. 2002. Imperial College, London.
- **Towards the numerical simulation of multi-scale two-phase flows**
  H. Marschall. PhD Thesis. 2011. Technische Universität München.
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