Quadrature-based moment methods for polydisperse multiphase flows

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Collaborators

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- Dr. Bo Kong – US DOE Ames Laboratory

Students

- Jeffrey C. Heylmun – Ph.D. Student – Iowa State University
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- Ehsan Madadi-Kandjani – Ph.D. Student (graduated) – Now at U.T. Austin

What are polydisperse multiphase flows?

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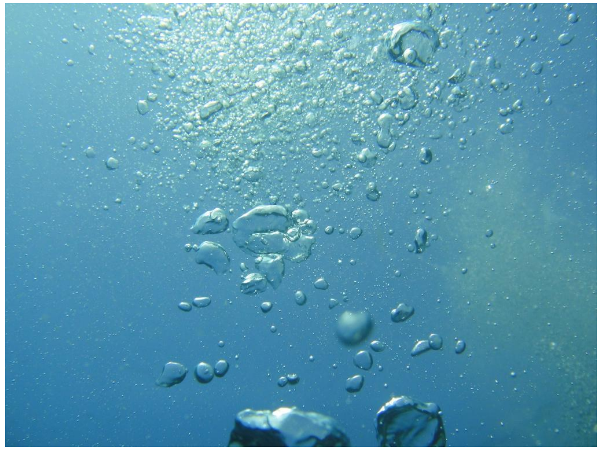
Disperse multiphase flows

We limit our attention to disperse multiphase flows

- One phase is composed by discrete elements, such as bubbles, droplets or particles: discrete phase
- The other one is assumed to be continuous (at least in the majority of the system): continuous phase



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Bubbly flow
- Bubbles are discrete entities
- The liquid is continuous
- Disperse

Free-surface flow
- Multiphase
- Not disperse

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Spray
- Droplets are discrete
- The gas (air) is continuous
- Disperse

Challenges in describing polydisperse multiphase flows [1]

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Different locations may have very different flow conditions

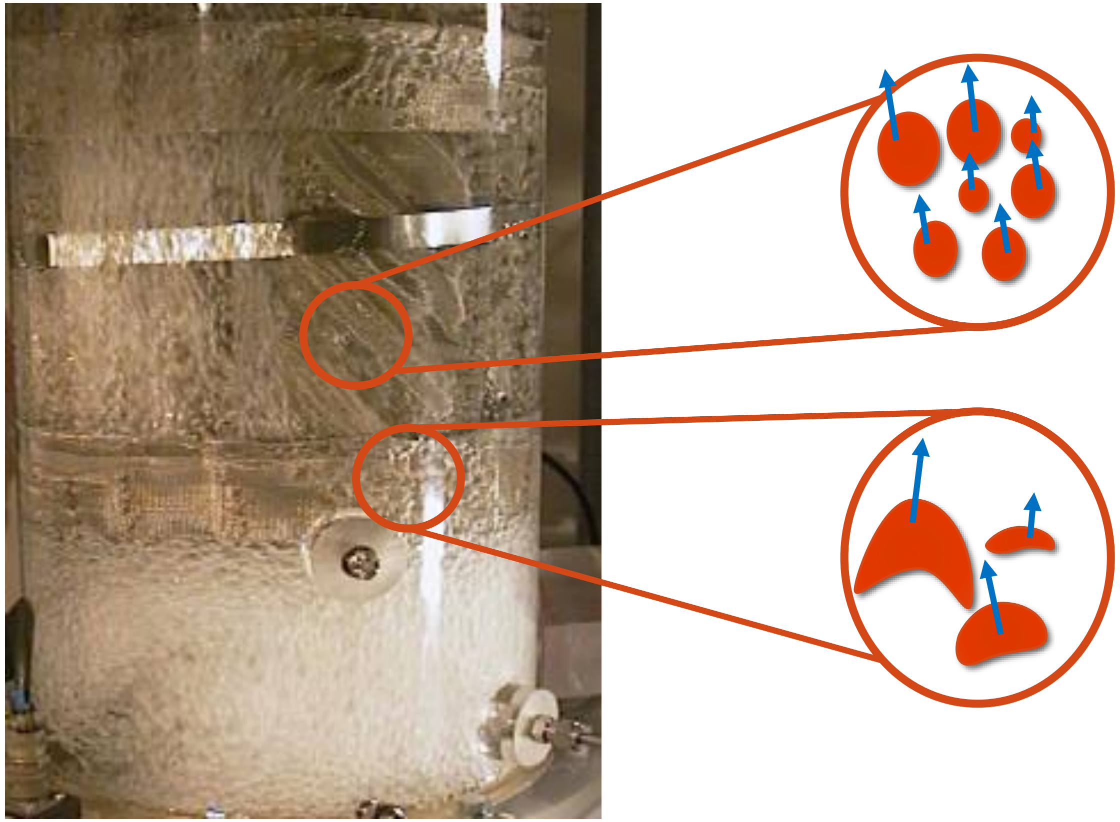
Different physical phenomena determine the local flow behavior

Flow conditions depend also on time

Dilute
- Mostly particle advection
- Lower frequency of particle collisions

Dense
- Frequent collisions among particles
- At particularly high concentrations, friction among particles

Challenges in describing polydisperse multiphase flows [1]



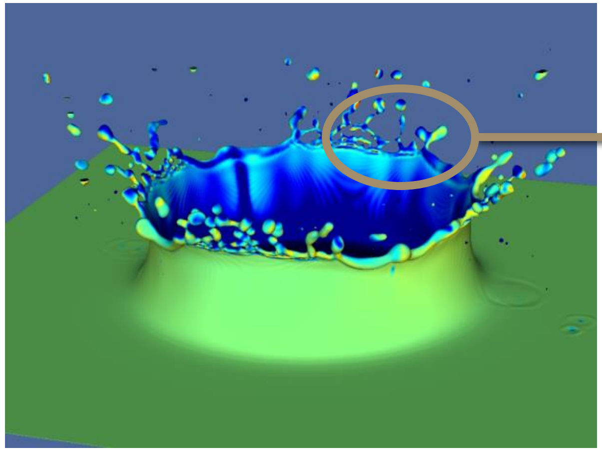
Polydispersity

- Size distribution
- Shape distribution
- Property (density, …) distribution

Polycelerity

- Bubbles with different size move at different velocities

Challenges in describing polydisperse multiphase flows [3]



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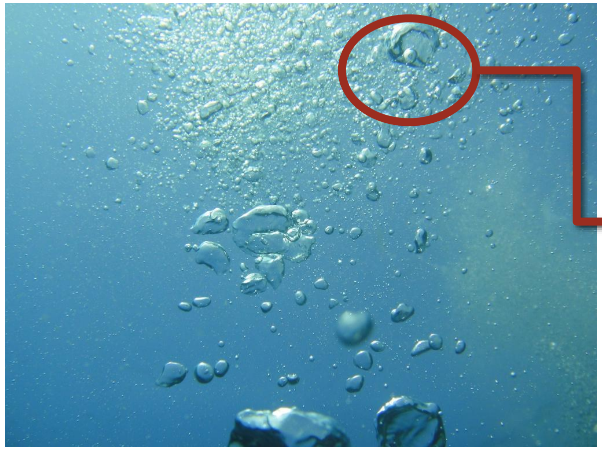
Breakup
- Liquid jets originate drops
- Bubbles break in smaller bubbles
- Particles can fragment or undergo erosion and form smaller particles



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Coalescence/Aggregation
- Bubbles (or drops) merge to form larger bubbles
- Particles aggregate and form bigger particles, possibly changing shape

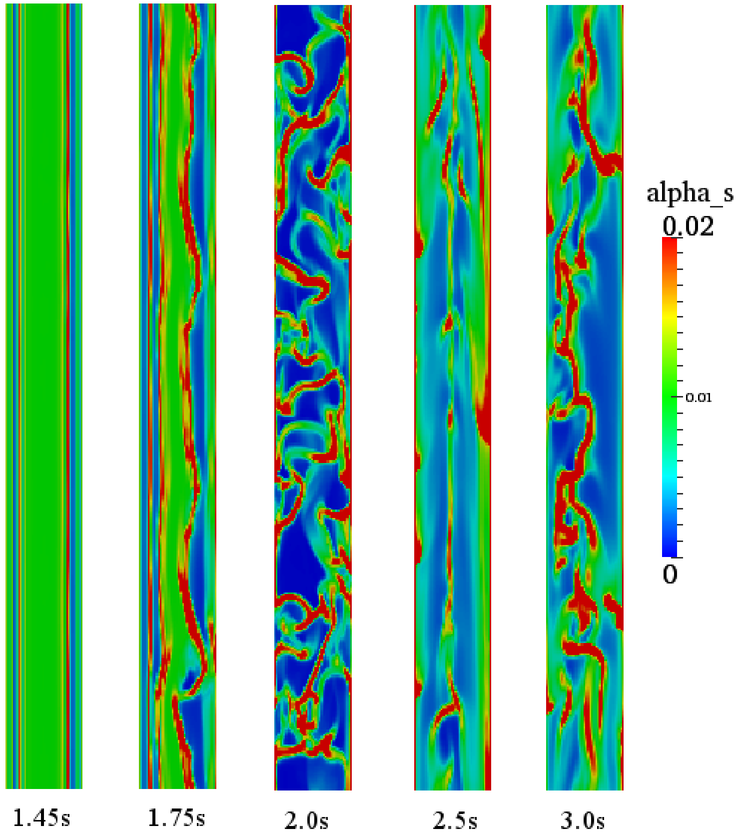
Challenges in describing polydisperse multiphase flows [4]

If particles have significant inertia, they tend to segregate

Causes

- Interaction between fluid and particles
- Interaction among particles

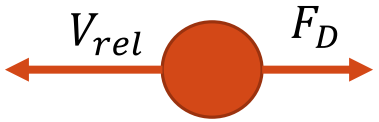
Complex interaction between phases (fluid-solid, fluid-fluid)



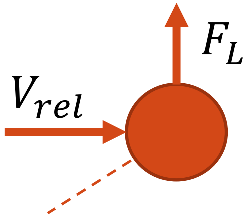
Forces

Several forces act on a particle or a bubble in a fluid, among which:

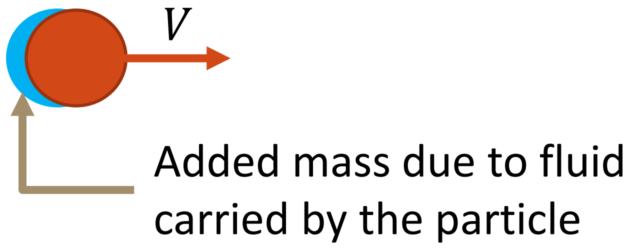
- Drag force
  - Parallel to the direction of relative motion



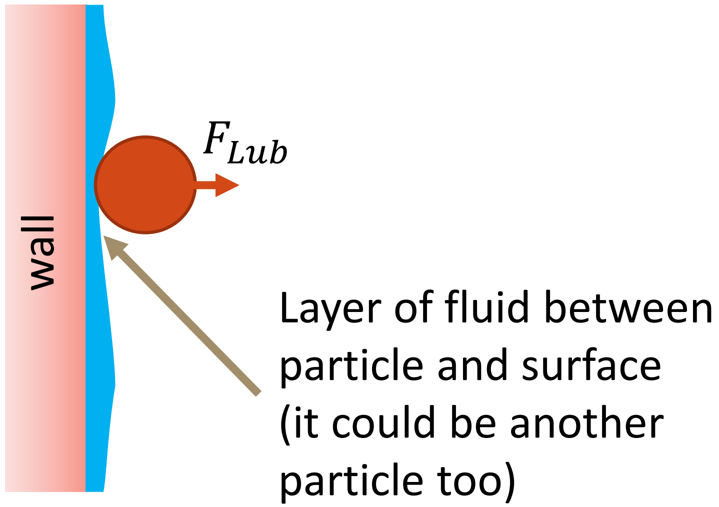
- Lift force
  - Perpendicular to the direction of relative motion



- Added (or virtual) mass



- Lubrication



Modeling multiphase flows: why?

Investigating multiphase flows is complex

- Experiments are expensive
  - Cost of building the equipment
  - Cost of running the experiments (instruments, chemicals, personnel)
- Experiments may be dangerous or not possible
  - Toxic chemicals, difficult to use in a laboratory
  - Dangerous situations to study extreme cases: explosions, nuclear accidents, contamination
- Experiments can't always access the entire range of relevant parameters
  - Difficulties of optical measurements
  - Sometime only average measurements when tomographic techniques are used

Modeling: a complementary approach to experiments

- A model needs to reliably reproduce experiments
- It can also inform on what experiments should be performed to fill a knowledge gap
- Once tested (validated), it can become a tool to design and optimize engineering applications

Increased insight and knowledge of the physical phenomena

→

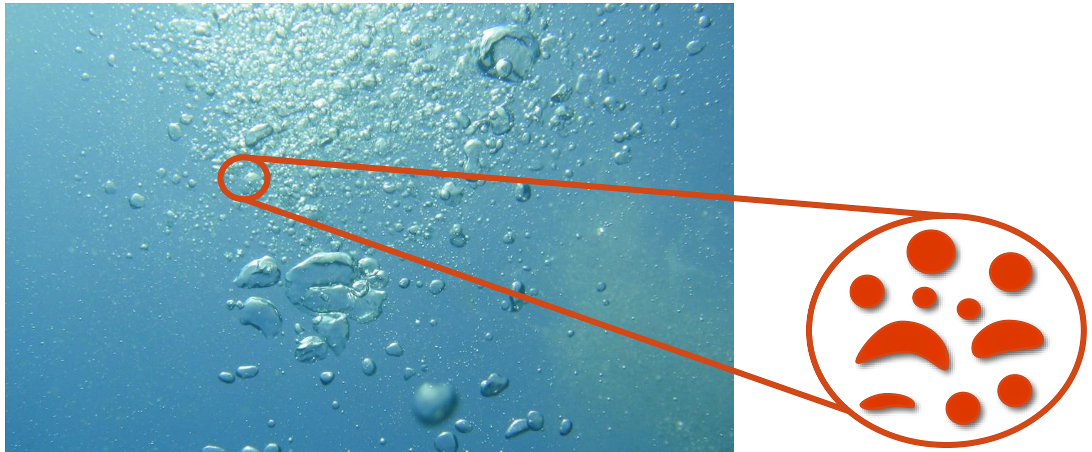
More effective and rapid engineering design

Aspects of modeling

Predictive computational model for polydisperse multiphase flows for engineering applications

- Description of the physics
  - Forces
  - Turbulence
  - Property transfer and chemistry
  - Polydispersity
- Numerical approach
  - Accuracy
  - Robustness
  - Computational time
- Implementation
  - Ease of use
  - Dissemination

A mathematical framework to describe multiphase flows



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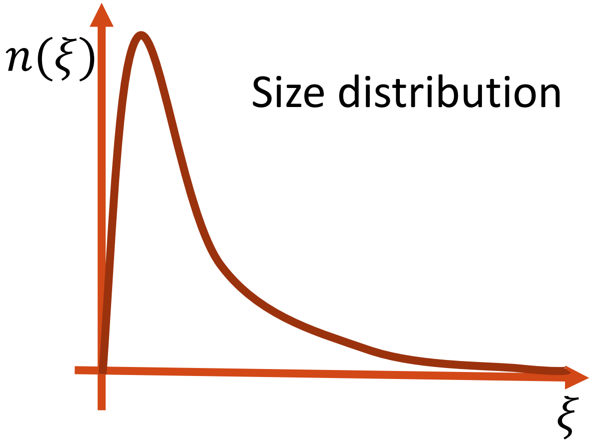
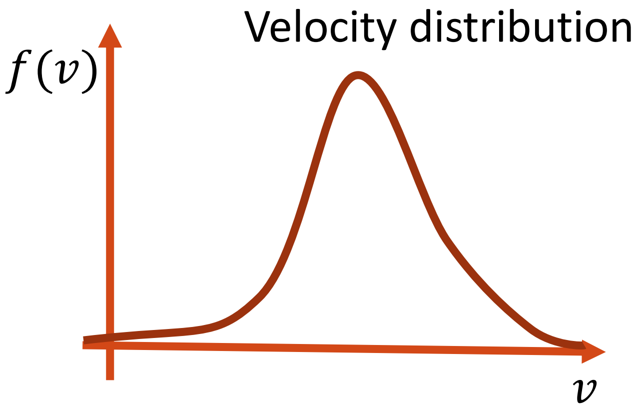
We want to describe the evolution in space and time of a population of particles

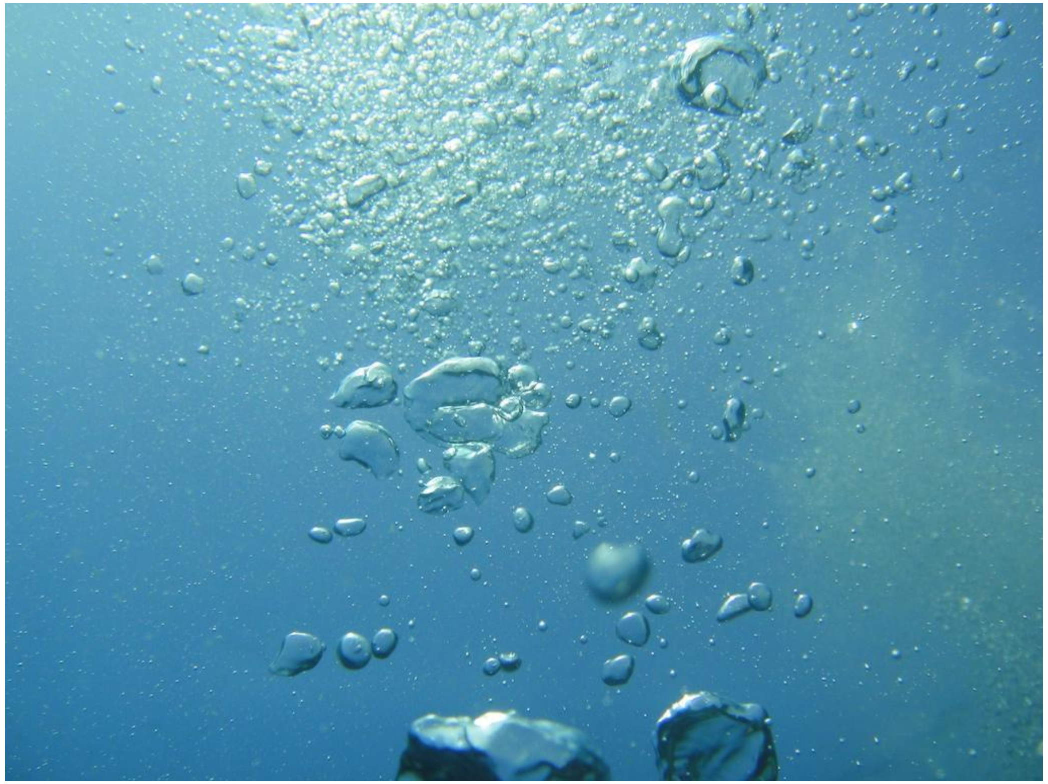




Size and velocity are not independent

Joint size-velocity distribution $f(\mathbf{x}, t; \xi, \mathbf{v})$

Evolution of $f(\mathbf{x}, t; \xi, \mathbf{v})$



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Advection

- Translates the distribution in space but does not change the shape

Local changes

- Coalescence
- Breakup
- Nucleation (formation of new particles)
- Evaporation
- …

External forces

- Induce acceleration

What equation describes this evolution?

Generalized population balance

The behavior of a population of particles or bubbles can be described by means of a number density function (NDF) $f(\mathbf{x}, t, \xi, \mathbf{v})$ which evolves according to the equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot \left[(\mathbf{A} + \mathbf{g}) f \; - \mathcal{D}_{\mathrm{dis}} \frac{\partial \ln(n)}{\partial \mathbf{x}} f \right] + \frac{\partial}{\partial \xi} [G(\xi) f] = \mathbb{C}(\xi, \mathbf{v})$$

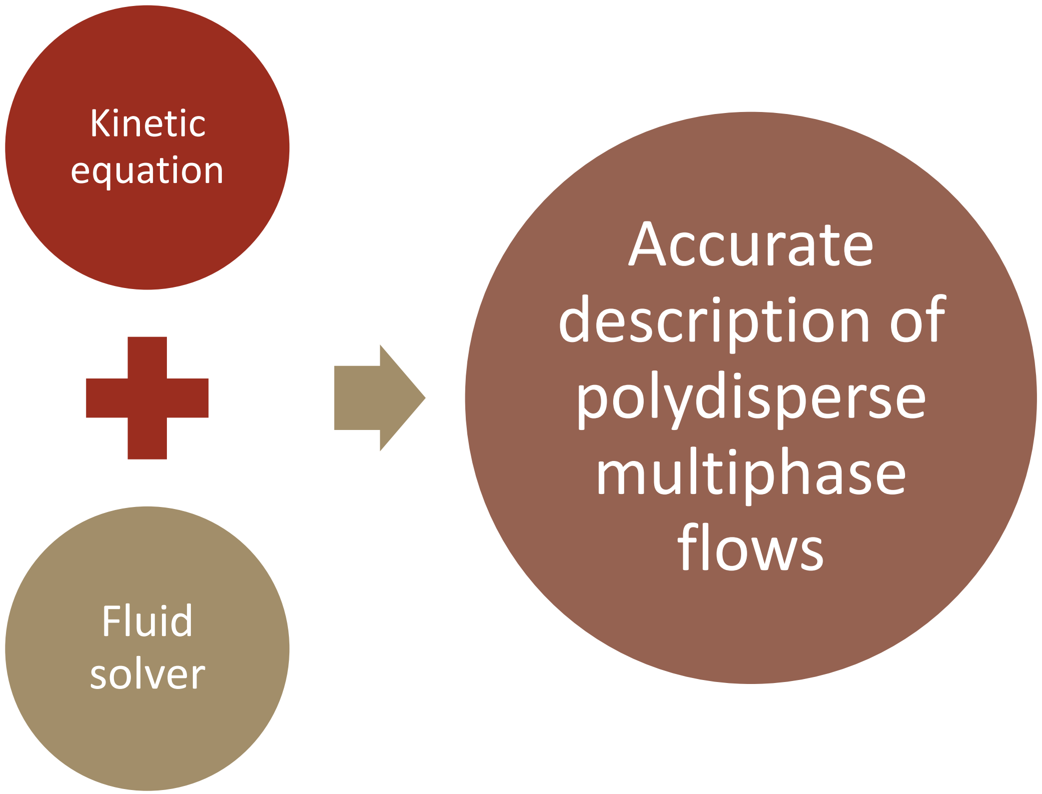
where:

- $\mathbf{A}$ is the acceleration due to forces (drag, lift, added mass, …) acting on bubbles, excluding the gravitational acceleration
- $\mathbf{g}$ is the gravitational acceleration
- $\mathcal{D}_{\mathrm{dis}}$ is the dispersion coefficient
- $\mathbb{C}(\xi, \mathbf{v})$ accounts for interactions between bubbles (i.e. breakup, coalescence)

The bubble size distribution is the marginal NDF:

$$n(\xi) = \int_{\mathbb{R}^3} f(\mathbf{x}, t, \xi, \mathbf{v}) \mathrm{d}\mathbf{v}$$

Kinetic equation for bubble populations [2]



However:

- The NDF $f(\mathbf{x}, t, \xi, \mathbf{v})$ has a high dimensionality
  - 3 spatial dimensions
  - 1 temporal dimension
  - 1 (at least) internal coordinate describing bubble mass or size
  - 3 velocity component
- Direct discretization is prohibitively expensive for applications: 7 dimensions + time
- Lagrangian description of bubbles
  - Accurate
  - Costly
  - Numerical difficulties due to strong coupling with the fluid phase
- In engineering applications accurately it may not be necessary to know the NDF exactly, but some of its properties may be sufficient

Moment methods – Basic concepts

In moment methods:

- The idea of solving for the NDF is abandoned
- A set of moments of the NDF are transported:

$$m_{p,i,j,k}(\mathbf{x},t) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^+} \xi^p u_{\mathrm{x}}^i u_{\mathrm{y}}^j u_{\mathrm{z}}^k f(\mathbf{x},t,\xi,\mathbf{v})\mathrm{d}\xi\mathrm{d}\mathbf{U}$$

where

- p is the order of the moment with respect to the size coordinate ξ
- i, j, k are the orders of the moments with respect to the velocity components

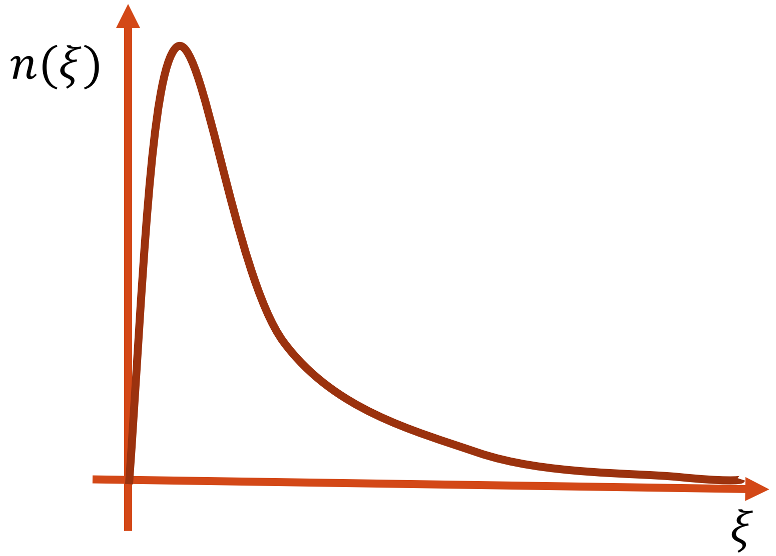
Applying the definition of joint moment to the kinetic equation, partial differential equations for the spatio-temporal evolution of the moments of the NDF are found.

$$\frac{\partial m_{p,i,j,k}}{\partial t} + \nabla \cdot \mathcal{P}_{p,i,j,k} = \mathcal{S}_{p,i,j,k}$$

What is the meaning of moments?

Moments are statistics of the distribution

- Some common examples
  - Mean
  - Variance
  - Skewness
  - Kurtosis
- In the context of moment methods for multiphase flows
  - Particle volume fraction
  - Particle mean velocity
  - Particle velocity variance
  - Mean, variance and other statistics of the size distribution



A first class of problems: non-inertial particles

Particles with negligible inertia compared to the fluid

- Nanoparticles

They follow the fluid motion

The model equation simplifies

Univariate NDF: $f(\mathbf{x}, t, \xi, \mathbf{v}) \rightarrow n(t, \mathbf{x}; \xi)$

$$\frac{\partial m_{p,i,j,k}}{\partial t} + \nabla \cdot \mathcal{P}_{p,i,j,k} = \mathcal{S}_{p,i,j,k} \quad \Longrightarrow \quad \frac{\partial m_p}{\partial t} + \nabla \cdot \mathcal{P}_p(\boxed{U_f}) = \mathcal{S}_p$$

Fluid velocity

A challenge: preserving moments

Let’s take a look at the moment transport equations:

$$\frac{\partial m_p}{\partial t} + \nabla \cdot \mathcal{P}_p = \mathcal{S}_p$$

This equation can be solved numerically by splitting it into two consecutive steps:

$$\frac{\partial m_p}{\partial t} + \nabla \cdot \mathcal{P}_p = 0$$

Advection

$$\frac{\partial m_p}{\partial t} = \mathcal{S}_p$$

Integration of source terms

Both steps may lead to invalid vectors of moments

Realizability problem

Realizable moment advection

When solving

$$\frac{\partial m_p}{\partial t} + \nabla \cdot \mathcal{P}_p = 0$$

the adoption of traditional numerical methods of order higher than one may lead to invalid (unrealizable sets of moments).

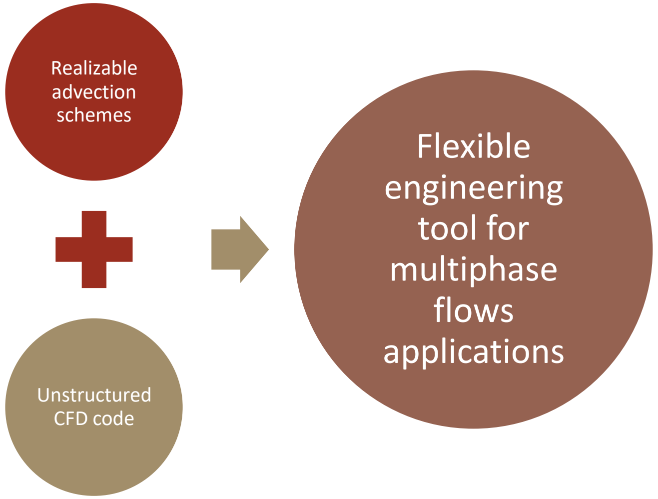
In simple terms, we say a moment vectors is realizable if it corresponds to a NDF:

- Not all N-dimensional vectors are the first N moments of a NDF!

$$\begin{cases} m_0 > 0 \\ m_0 m_2 - m_1^2 > 0 \\ \dots \end{cases}$$

Challenge:

- Obtain accurate solutions of moment transport equations
- Maintain realizability of the set of transported moments
- Formulate a method that can be used for complex engineering problems with non-trivial geometries



Realizable finite-volume advection scheme

If we consider moments of distributions defined on the positive real axis (i.e. size distribution), one approach to formulate realizable advection schemes is the following:

- Define the scheme as a function of quantities which are bounded in a know interval and related to the moments

$$m_p \Leftrightarrow \zeta_k$$

  - The ζ_k quantities are positive if the moments are realizable
- Re use ζ_k to reconstruct the moments on the cell faces and define the advection flux
- Re-use of traditional MUSCL reconstruction
- Additional limitation needed when near the boundary of the moment space

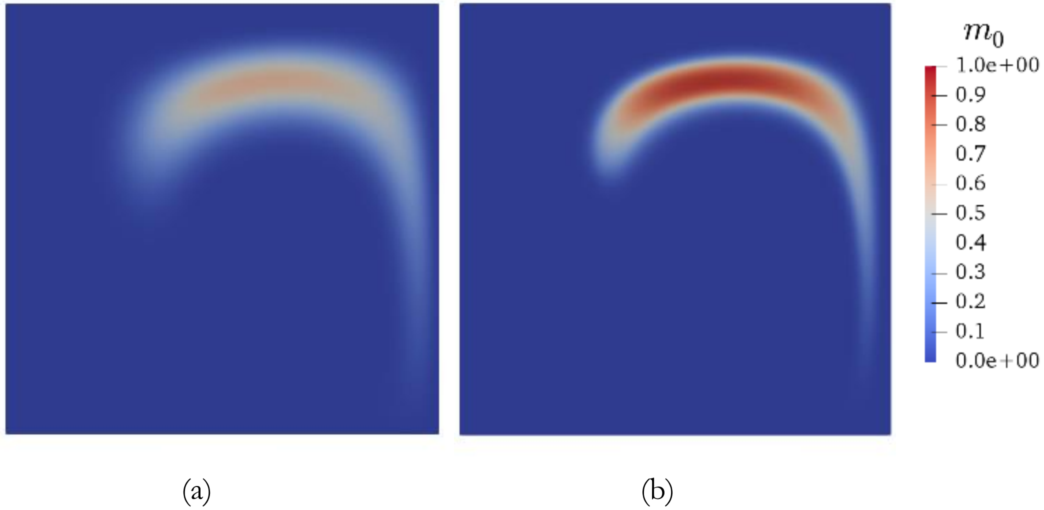
[1] H. Dette, W.J. Studden, Matrix measures, moment spaces and Favard's theorem for the interval [0,1] and [0,∞), Linear Algebra and Its Applications. 345 (2002) 169–193. doi:10.1016/S0024-3795(01)00493-1.
[2] M. Skibinsky, Extreme nth moments for distributions on [0, 1] and the inverse of a moment space map, Journal of Applied Probability. 5 (1968) 693–701. doi:10.2307/3211931.

Implementation of realizable advection into OpenQBMM

We have implemented realizable moment advection into the open-source CFD code OpenFOAM®

- Work based on the scheme developed by Laurent and Nguyen at EM2C
- F. Laurent, T.T. Nguyen, Realizable second-order finite-volume schemes for the advection of moment sets of the particle size distribution, Journal of Computational Physics. 337 (2017) 309–338. doi:10.1016/j.jcp.2017.02.046.

Fully unstructured grid to fit applications with complex geometries



Comparison of zero-order moment field obtained on a 128^2 grid at t = 0.8, with:

(a) first-order advection scheme

(b) second-order realizable scheme

Realizable integration of source terms

Realizability problems happen also when integrating source terms:

$$\frac{\partial m_p}{\partial t} = \mathcal{S}_p$$

Some time-integrators (Euler, Runge-Kutta SSP) ensure realizability if source term is linear, but most are not.

Constraint of small time-steps to make sure the set of moments is realizable

↓

Excessive computational time

Solution

- Adapt the time-step based on the realizability criterion
- Realizable ODE solver of Nguyen et al. (2016)
  - T.T. Nguyen, F. Laurent, R.O. Fox, M. Massot, Solution of population balance equations in applications with fine particles: Mathematical modeling and numerical schemes, Journal of Computational Physics. 325 (2016) 129–156. doi:10.1016/j.jcp.2016.08.017.
- Reduction of computational cost
  - A factor of 10 in aggregation and breakup cases
  - From hours to minutes
- Implementation into OpenQBMM
  - A. Passalacqua, F. Laurent, E. Madadi-Kandjani, J.C. Heylmun, R.O. Fox, An open-source quadrature-based population balance solver for OpenFOAM, Chemical Engineering Science. 176 (2018) 306–318. doi:10.1016/j.ces.2017.10.043.

A little more inertia: bubbles

Bubbles tend to have small inertia, but not negligible

They don't strictly follow the fluid motion

It is acceptable to assume that, locally, bubbles with the same size move with the same velocity

This corresponds to rewriting the NDF as

$$f(\mathbf{x}, t, \xi, \mathbf{v}) = n(\mathbf{x}, t, \xi)\delta(\mathbf{x}, t, \mathbf{v} - \mathbf{U}(\xi))$$

where:

- $n(\mathbf{x}, t, \xi)$ is the bubble mass distribution
- $\delta(\mathbf{x}, t, \mathbf{v} - \mathbf{U}(\xi))$ is a Dirac delta distribution
- $\mathbf{U}(\xi)$ is the bubble velocity conditioned on the bubble mass

We need to define a procedure to reconstruct $n(\mathbf{x}, t, \xi)$ and determine $\mathbf{U}(\xi)$ from the moments to close the moment evolution equations

Moment transport equations

With the mono-kinetic assumption, we can:

- Close the bubble mass distribution considering $2N$ moments in bubble mass

$$M_p = m_{p,0,0,0}, \qquad p \in \{0, 1, \dots, 2N-1\},$$

$$\frac{\partial M_p}{\partial t} + \nabla \cdot \mathcal{U}_p = \int_{\mathbb{R}^+} \xi^p \mathbb{C}(\xi) \mathrm{d}\xi$$

- Find the functional form of $\mathbf{U}(\xi)$ from the first-order velocity moments:

$$\boldsymbol{\mathcal{U}}_p = (m_{p,1,0,0}, m_{p,0,1,0}, m_{p,0,0,1}), \; p \in \{0, 1, \dots, N-1\}$$

$$\frac{\partial \boldsymbol{\mathcal{U}}_p}{\partial t} + \boxed{\nabla \cdot \mathcal{P}_\mathrm{p}} = M_p \mathbf{g} + \int_{\mathbb{R}^+} n(\xi) \xi^p \left(\mathbf{A}(\xi) - \mathcal{D}_{\mathrm{dis}} \nabla \ln\left(n(\xi)\right)\right) \mathrm{d}\xi$$
$$+ \frac{\alpha_\mathrm{b} g_0}{\tau_\mathrm{c}} \left(M_p \mathbf{U}_b - \mathcal{U}_p\right) + \int_{\mathbb{R}^+} n(\xi) \xi^p \mathbf{U}(\xi) \mathbb{C}(\xi)\, \mathrm{d}\xi$$

$$\boxed{\mathcal{P}_p = \int_{\mathbb{R}^+} n(\xi) \xi^p \mathbf{U}(\xi) \otimes \mathbf{U}(\xi) \mathrm{d}\xi}$$

Closure of the moment equations [1]

The moment equations are unclosed:

- Terms containing the NDF
- Moment fluxes

We close these terms by means of Gaussian quadrature:

- The bubble mass NDF is written as weighted sum of Dirac delta distributions:

$$n(\xi) = \sum_{\alpha=0}^{N-1} w_\alpha \delta(\xi - \xi_\alpha)$$

which leads to:

$$M_p = \sum_{\alpha=0}^{N-1} w_\alpha \xi_\alpha^p$$

Weights and abscissae are found from the $2N$ moments $M_p, p \in \{0, \dots, 2N-1\}$.

$$M_p, p \in \{0, \dots, 2N-1\}$$

Inversion algorithm

$$(w_\alpha, \xi_\alpha), \alpha \in \{0, \dots, N-1\}$$

J.C. Wheeler, Modified moments and Gaussian quadratures, Rocky Mountain J. Math. 4 (1974) 287–296. doi:10.1216/RMJ-1974-4-2-287.

Closure of the moment equations [2]

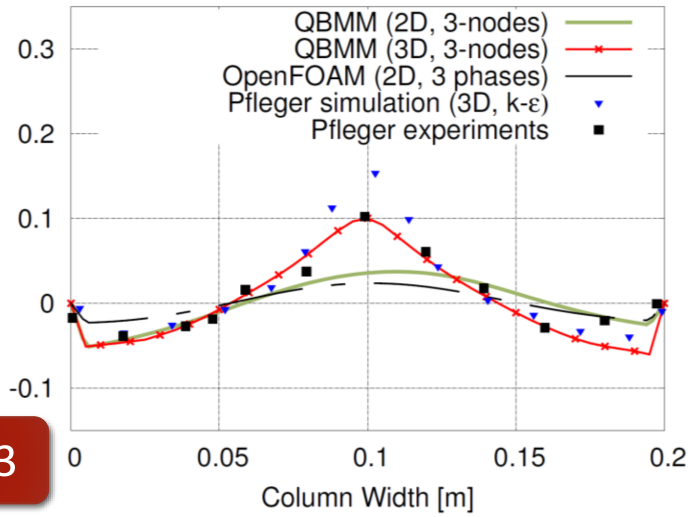
For each size node α, the velocity conditioned on size $\mathbf{U}_\alpha$ are found from the velocity moments $\mathcal{U}_p$ using the conditional quadrature method of moments by solving the family of linear systems:

$$\begin{bmatrix} \boldsymbol{\mathcal{U}}_0 \\ \boldsymbol{\mathcal{U}}_1 \\ \vdots \\ \boldsymbol{\mathcal{U}}_{N-1} \end{bmatrix} = \begin{bmatrix} \mathrm{w}_0 & 0 & \dots & 0 \\ 0 & \mathrm{w}_1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \mathrm{w}_{\mathrm{N}-1} \end{bmatrix} \begin{bmatrix} 1 & 1 & \dots & 1 \\ \xi_0 & \xi_1 & \dots & \xi_{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ \xi_0^{N-1} & \xi_1^{N} & \dots & \xi_{N-1}^{N-1} \end{bmatrix} \begin{bmatrix} \mathbf{U}_0 \\ \mathbf{U}_1 \\ \vdots \\ \mathbf{U}_{N-1} \end{bmatrix}$$

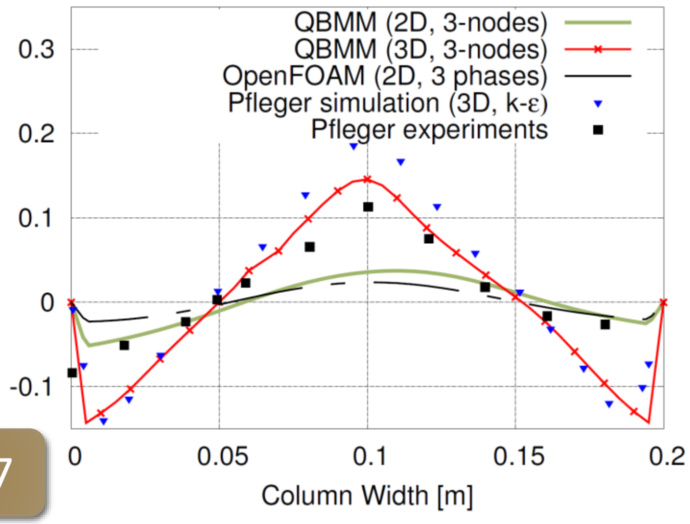
Reconstruction of $\mathbf{U}(\xi)$

C. Yuan, R.O. Fox, Conditional quadrature method of moments for kinetic equations, Journal of Computational Physics. 230 (2011) 8216–8246. doi:10.1016/j.jcp.2011.07.020.

Polydisperse gas-liquid flow



H = 0.13



H = 0.37

Same bubble colum as in the monodisperse case

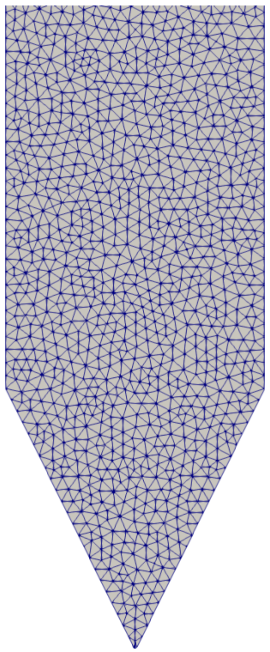
Three bubble sizes:

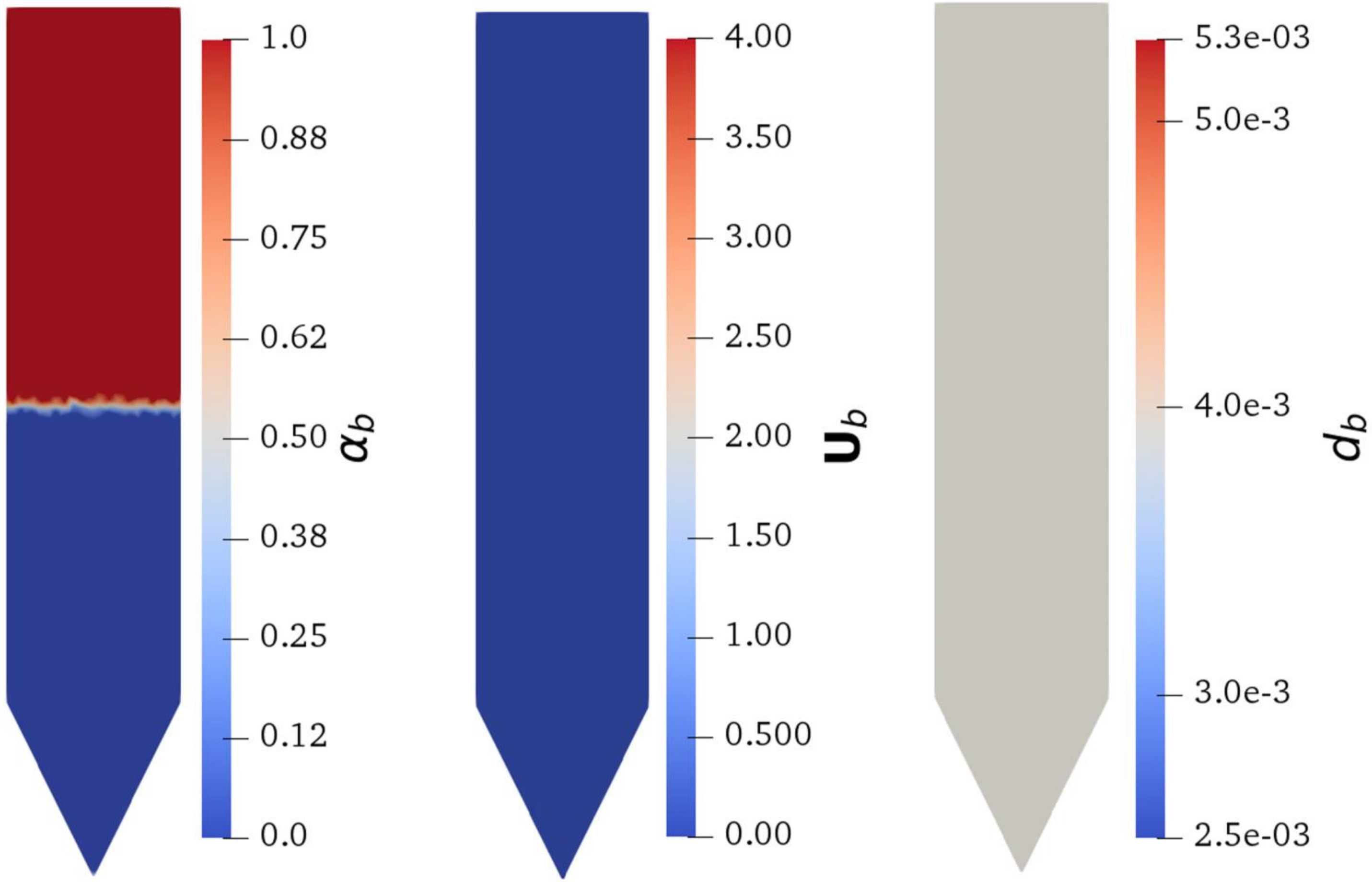
- 1.0 mm
- 2.5 mm
- 4.0 mm
- Equal volume fractions and inlet velocities to match the mean bubble diameter in experiments

An example in a complex geometry

Mixing vessel

- Coalescence and breakup
- $U_{g,\text{inlet}} = 10\ \text{m/s}$





OpenQBMM

The source code of the solver used in this project is part of OpenQBMM, an open-source framework for quadrature-based moment methods based on OpenFOAM.

The code is available at:

- Website: www.openqbmm.org
- GitHub repository: https://github.com/OpenQBMM

If you use OpenQBMM, **cite it**! Software citations are as important as citations of papers.

- DOI for OpenQBMM: 10.5281/zenodo.591651 (all versions)
- Specific DOI for a release: https://github.com/OpenQBMM/OpenQBMM/releases

Questions?