Computing foaming flows: from microfluidic crystals to breaking waves

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Two types of bubble interaction

- thin liquid film
- film drainage
- stable film
- film rupture
- coalescence
- collision or stable structure

- surfactants
- Marangoni effect
- viscous flow of liquid
Foaming flows
Numerical model
Two-component incompressible flow

- Navier-Stokes equations

\[ \nabla \cdot \mathbf{u} = 0 \]
\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) = -\nabla p + \nabla \cdot \left( \mu \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right) + \sigma \kappa \mathbf{n}_S \delta_S \]

- Advection of volume fraction

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

\[ \rho = (1 - \alpha)\rho_1 + \alpha\rho_2 \]
\[ \mu = (1 - \alpha)\mu_1 + \alpha\mu_2 \]

Discretization
- Finite volume on Cartesian grid
- Bell-Colella-Glaz projection [Bell1989]
- Embedded boundaries for complex domains [Colella2006]
- Particles for curvature estimation [Karnakov2020]
Standard volume-of-fluid

- All bubbles in one volume fraction field

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

- Cannot describe overlapping interfaces
- At a distance below one cell, bubbles *always coalesce*
Multi-marker volume-of-fluid

- Each bubble in separate field

\[
\frac{\partial \alpha_i}{\partial t} + (\mathbf{u} \cdot \nabla) \alpha_i = 0 \quad i = 1, \ldots, N
\]

- Describes overlapping interfaces
- Bubbles \textbf{never coalesce}

\begin{align*}
\text{total volume fraction} & \quad \alpha = \sum_{i=1}^{N} \alpha_i \\
\text{surface tension} & \quad \mathbf{f}_\sigma = \sigma \sum_{i=1}^{N} \kappa_i \mathbf{n}_S^{(i)} \delta_S^{(i)}
\end{align*}

- Complexity \(\mathcal{O}(N_{\text{cells}} N)\)
- Expensive with many bubbles

Coyajee and Boersma,
Foaming flows: state of the art

- Multi-marker volume-of-fluid
  Coyajee and Boersma, 2009  Cifani, 2016
  Expensive with many closely packed bubbles

- Voronoi Implicit Interface Method
  Saye and Sethian, 2011
  Only dry foams. Liquid between bubbles disappears

- Color-gradient lattice Boltzmann
  Montessori et al. 2021
  Artificial compressibility and density ratio close to 1
Proposed method

- Multilayer volume-of-fluid (Multi-VOF) [arXiv:2103.01513]
- Bubbles have unique colors
- Layer = volume fraction + color
- Only uses 4 layers

- Standard discretizations apply to stencil values assembled locally for each color

- Bubbles never coalesce

- Complexity $\mathcal{O}(N_{\text{cells}})$
- No dependency on the number of bubbles
Software
Aphros

Finite volume solver for incompressible flows with surface tension

github.com/cselab/aphros

- C++14
- Based on the Cubism library, Gordon Bell prize 2013 for high throughput computation [Rossinelli2013]
- Parallelized with MPI and OpenMP
- Multiphysics: electrochemistry, nucleation and growth of bubbles, Lagrangian particles
Applications
Drop impact on a liquid-liquid interface

Water-glycerin drop falling in silicon oil

present simulation

simulation multi-marker VOF [Coyajee2009]

experiment [Mohamed-Kassim2003]

Mean curvature flow

- \( n \) triple junctions under mean curvature flow
  \[ u = \kappa n_S \]

- Exact solution for area growth
  [Mullins1956]
  \[ \frac{dA}{dt} = 2\pi \left( \frac{n}{6} - 1 \right) \]

- Compared to VIIM [Saye2012]
  - more accurate at low resolutions
  - slower convergence rate
  - describes wet foams

\[ t = 0 \quad t = 0.06 \]

\[ n = 4 \quad n = 8 \]
Microfluidic crystals

differences from experiment:
lower density ratio (10), lower viscosity (0.25 mPa·s), shorter channel

gas inlet
fixed pressure $P$

liquid inlets, fixed flow rate

gas thread separated at regular intervals

width 1000 μm

height 100 μm

Raven and Marmottant. Microfluidic crystals: dynamic interplay between rearrangement waves and flow. PRL, 2009
Microfluidic crystals

- Structures with fewer bubbles have higher flow resistivity

Simulation experiment [Raven2009]

- Spontaneous transitions

$P = 216\, \text{Pa}$ hex-one

$P = 194\, \text{Pa}$ hex-two

$P = 149\, \text{Pa}$ hex-three

$P = 140\, \text{Pa}$ hex-four

Gas flow rate (mL/h)

Inlet pressure (Pa)
Bidisperse foam generation

difference from experiment: lower density ratio [20]

Vecchiolla, Giri, and Biswal. Bubble–bubble pinch-off in symmetric and asymmetric microfluidic expansion channels for ordered foam generation. Soft matter, 2018
Bidisperse foam generation

- Injected bubbles are monodisperse
- Every 2nd bubble splits in two

[Vecchiolla2018]
Foaming waterfall

- Mesh 768x384x384
- 13000 cores, 24 hours, Piz Daint
Foaming waterfall

- Bubbles show features of foam: thin membranes (lamellae) and triple lines (Plateau borders).

- Bubble size distribution matches a theoretical scaling law [Garret2000].
Gallery of interactive simulations

github.com/cselab/aphros

set string title "Coalescence of bubbles"
set string visual "
vorticity {
    set vect values -2 0 2
    set vect colors $Blue $White $Red
}

volume fraction {
    set vect values 0 1
    set vect colors $Yellow $Yellow
    set vect opacities 0 1
}
"

set double extent 0
set double sigma 1
set double rho2 0.01
set double nu2 0.01

set string init_vf list
set string list_path "inline
sphere 3 1 4 1
sphere 5 1 4 1"

mesh (64,64)
applied config of 422 characters

Hostname 
emscripten 1
InvVF: Reading inline list of primitives from list_path
Read 2 primitives
global mesh=64,64
surface tension dt=0.0125291
viscosity dt=15.625
Found events:

step=0 t=0.000000000 dt=4.040000000e-06 wt=0.02200000
......iter=1, diff=4.0400000000000000e+00
......adv=6.0000000000-0.0000000000

demos: drops | electrochemistry
videos: waves | waterfall | coalescence

ETH Zurich, CSElab
Summary

- Multi-VOF for coalescence prevention
  arXiv:2103.01513

- Software Aphros
  github.com/cselab/aphros

Thank you!
References

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  Bubble–bubble pinch-off in symmetric and asymmetric microfluidic expansion channels for ordered foam generation. Soft matter. 2018
  The connection between bubble size spectra and energy dissipation rates in the upper ocean. Journal of physical oceanography. 2000