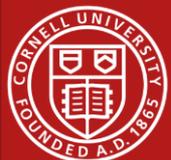


# High-Fidelity Numerical Modeling of Spray Droplet Formation

*An enhanced volume of fluid framework  
for multi-scale atomization modeling*

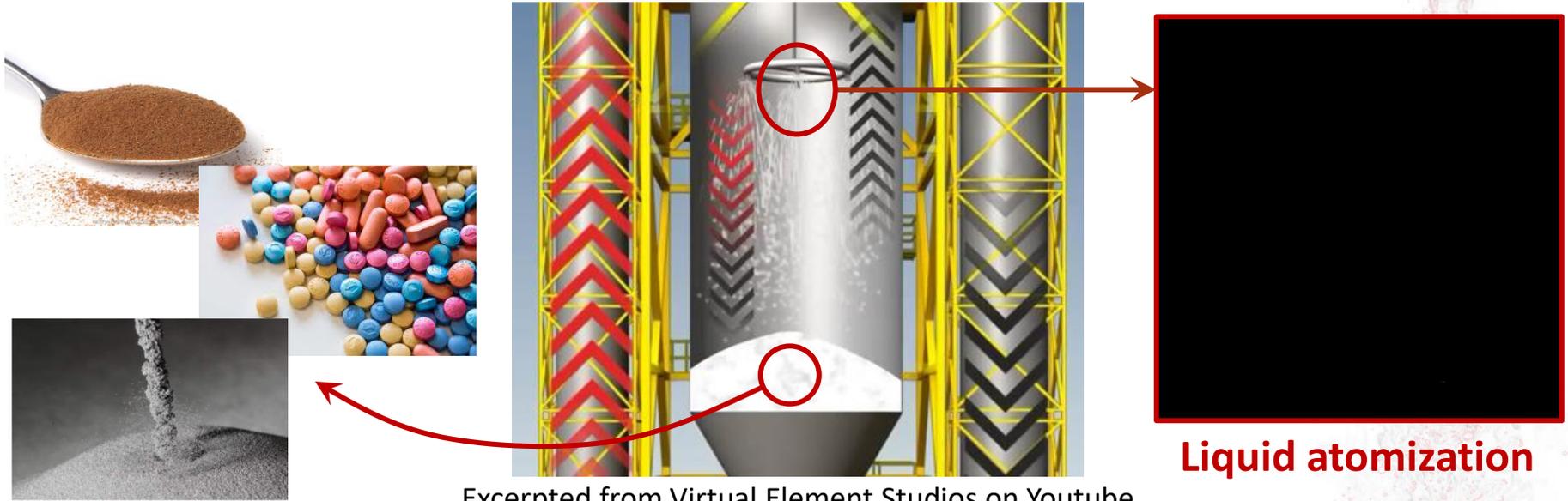
IFPRI ANNUAL GENERAL MEETING  
JUNE 2024

Olivier Desjardins and Joseph Giliberto  
Sibley School of Mechanical and Aerospace Engineering  
**Cornell University**



Cornell University  
Computational Thermo-Fluids  
Laboratory

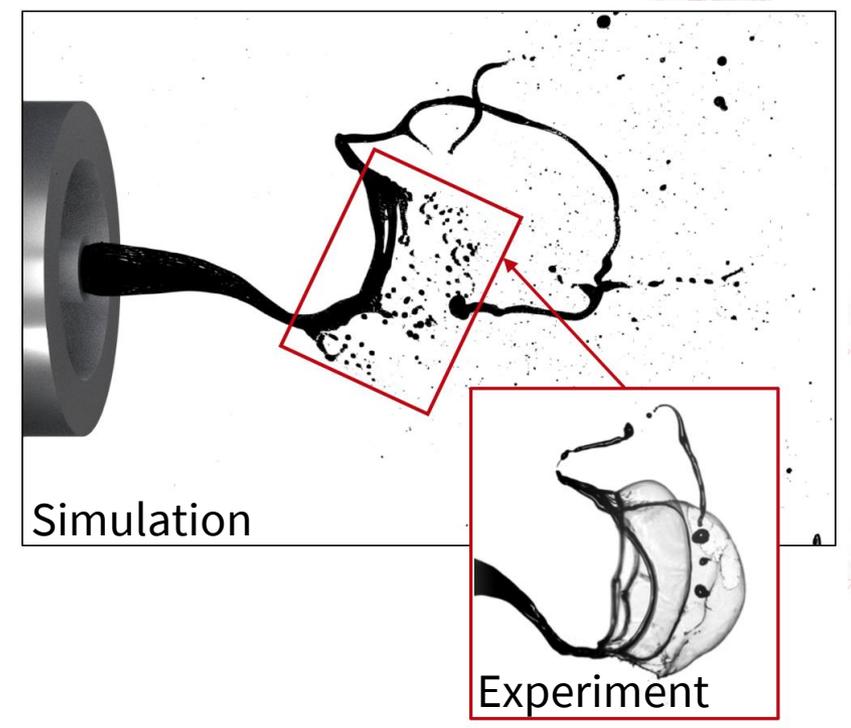
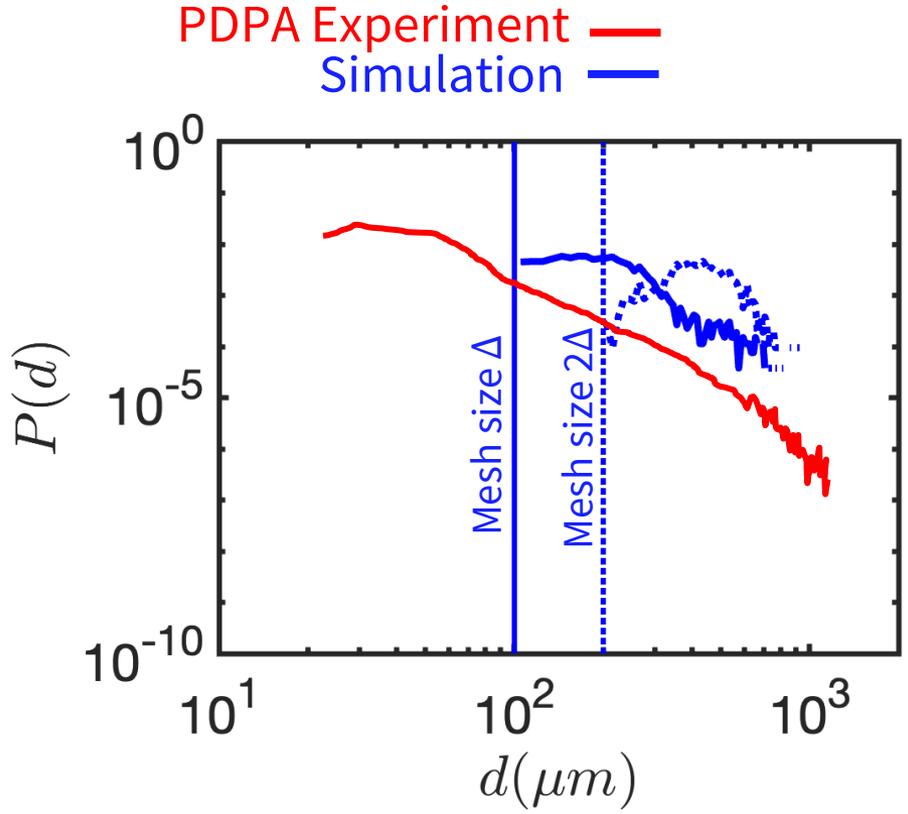
# Motivation – Atomizing complex fluids



Excerpted from Virtual Element Studios on Youtube

- Many industrial processes such as spray drying for powder production rely on **atomizing complex fluids** into a spray
- Process optimization depends on ability to **predict and control spray formation** – often achieved through phenomenological models or lab-scale testing
- **Complex liquid rheology** adds significant challenges: high effective viscosity, shear-rate-dependent viscosity, viscoelasticity, viscoplasticity

# Drop size statistics are not well predicted



# Project objective and proposed work plan

- Objective

**Assess and enhance ability of our novel high-fidelity multiscale spray atomization model for complex fluids**

- Proposed work plan

## Year 1

- Assess influence of high viscosity fluid in air-blast configuration
- Identify experimental datasets for complex fluid atomization

## Year 2

- Compare against experimental data
- Assess performance of our strategy

## Year 3

- Implement non-Newtonian fluid model
- Improve modeling closures for complex fluids

# Project objective and proposed work plan

- Objective

**Assess and enhance ability of our novel high-fidelity multiscale spray atomization model for complex fluids**

- Proposed work plan and accomplishments **in Year 1 and Year 2**

## Year 1

**in pressure-swirl configuration**

- **Assess influence of high viscosity fluid** ~~in air-blast configuration~~
- **Identify experimental datasets for complex fluid atomization**

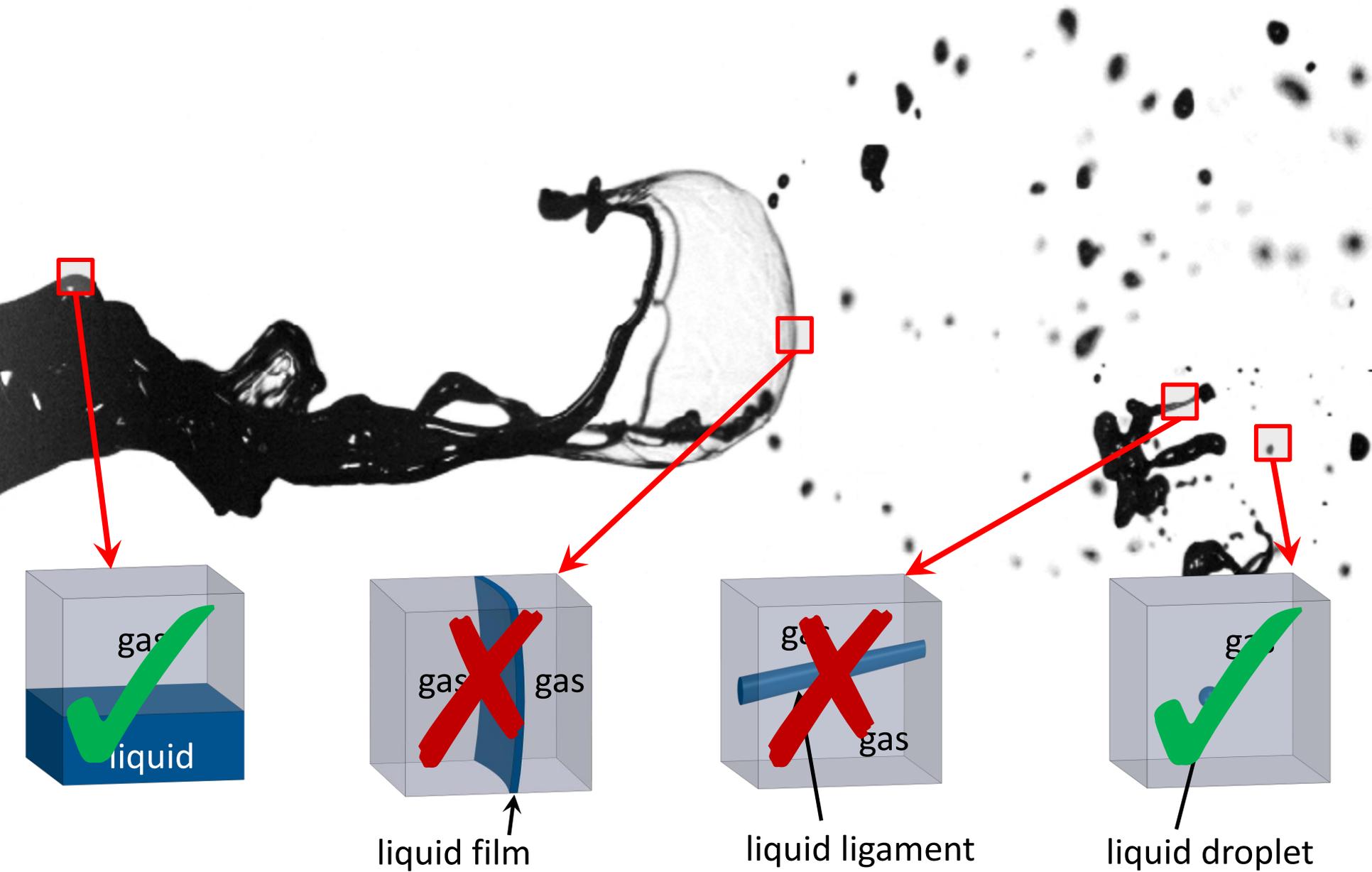
## Year 2

- Compare against experimental data
- **Assess performance of our strategy**

## Year 3

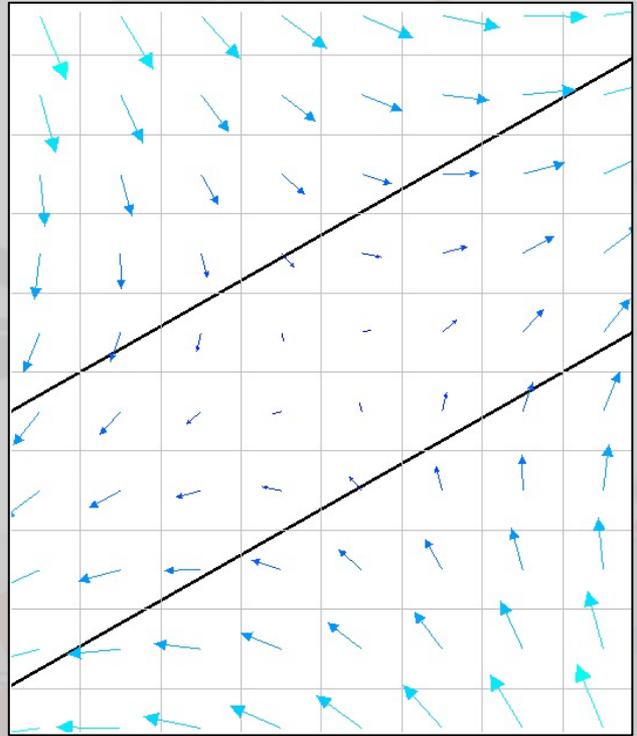
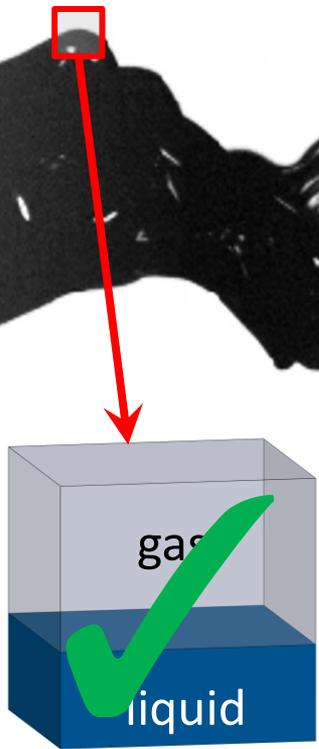
- **Implement non-Newtonian fluid model**
- **Improve modeling closures for complex fluids**

# Limitations of classical mathematical framework

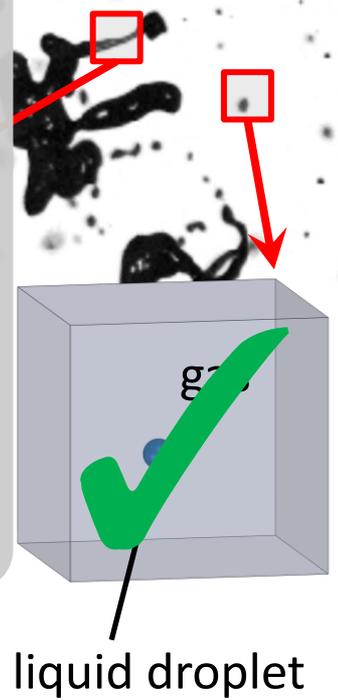


# Limitations of classical mathematical framework

Standard Eulerian methods require all interfacial structures **to be fully resolved**



Liquid film in stagnation flow  
↑ liquid film      ↓ liquid ligament



liquid droplet

# Numerical break-up in Eulerian interface capturing

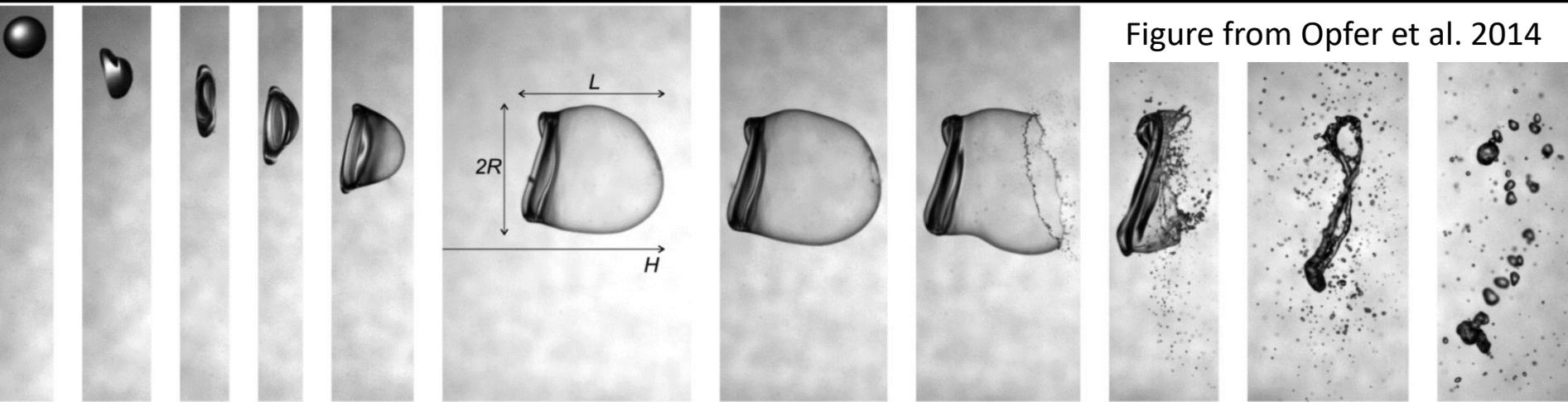
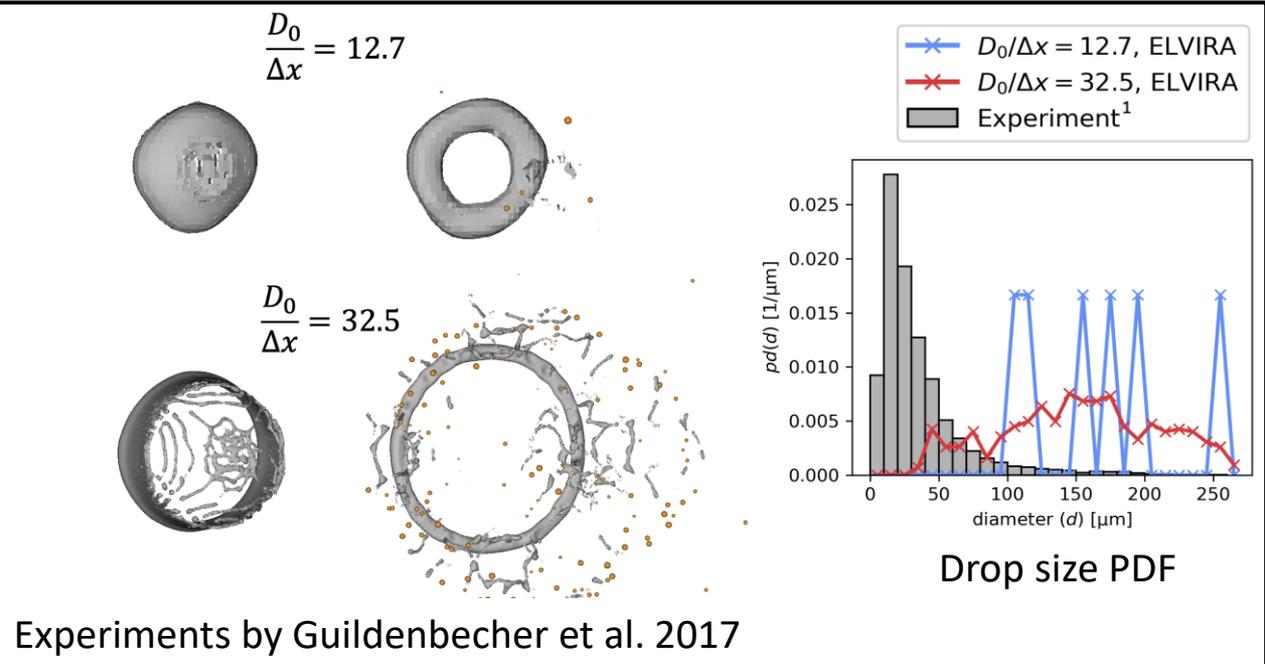


Figure from Opfer et al. 2014



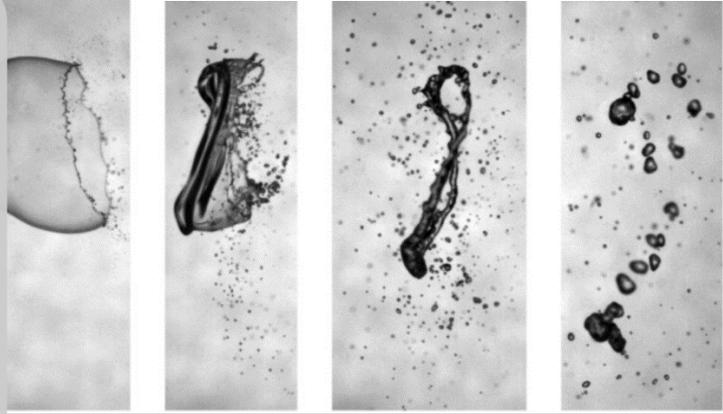
Experiments by Guildenbecher et al. 2017

# Numerical break-up in Eulerian interface capturing

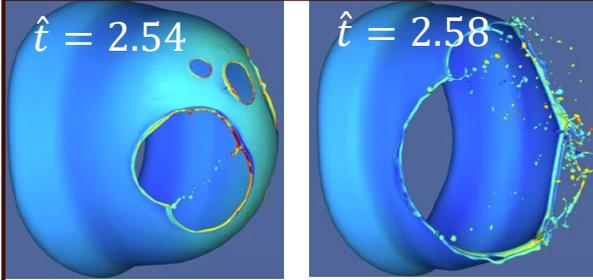
## The problem

- Spurious numerical break-up happens at limit of mesh resolution
- Exemplified here with VOF-PLIC, but common to all Eulerian interface capturing techniques (algebraic VOF, level set, diffuse interface...)

Figure from Opfer et al. 2014



- **We are unable to predict drop size pdf because break-up is due to numerical errors instead of appropriate microscale physics**
- **Striking with films but also true for ligaments**
- **Not addressed via mesh refinement**
  - **Missing key molecular scale processes**
  - **Break-up still purely numerical**
  - **Enormous cost**

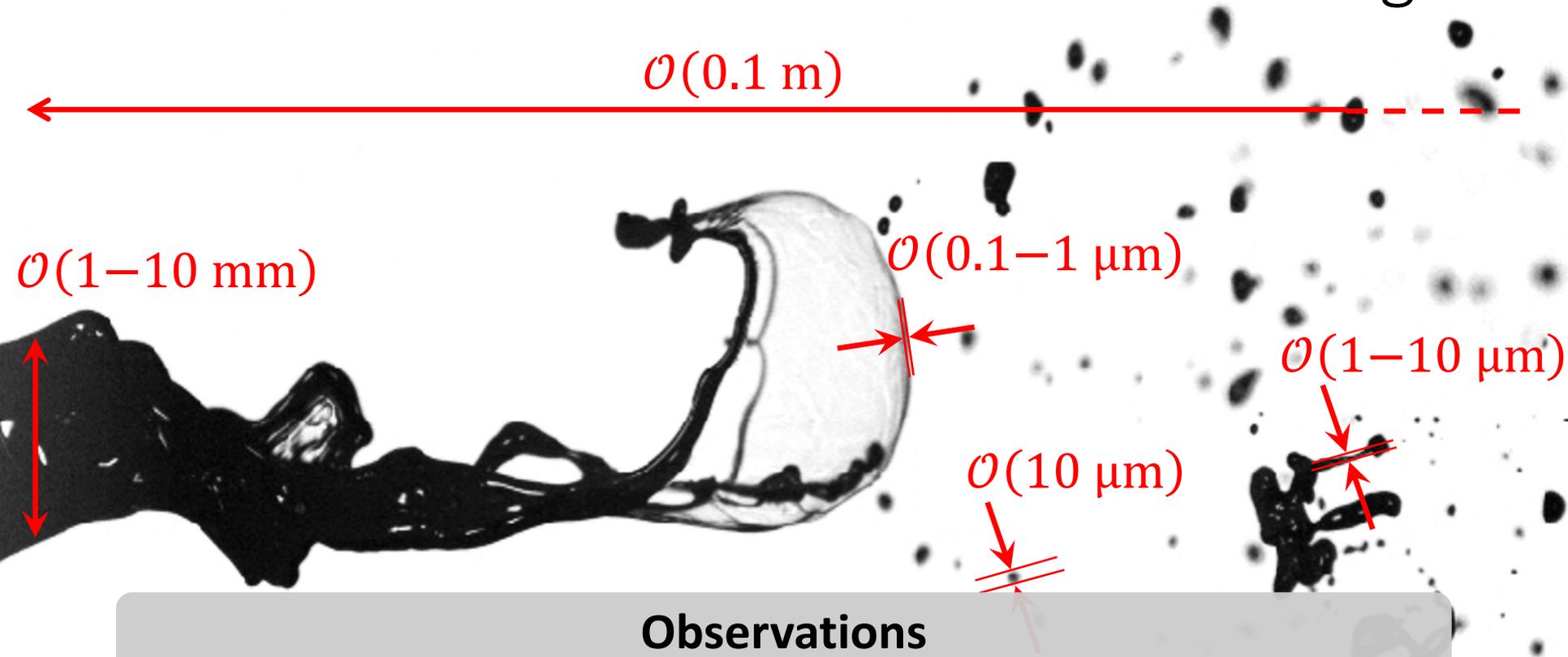


2048 cells per diameter  
4.3 million core-hours  
*“Film break-up due to numerical cut-off”*

Experiments by Gueldenbecher et al. 2017

Preprint by Ling & Mahmood

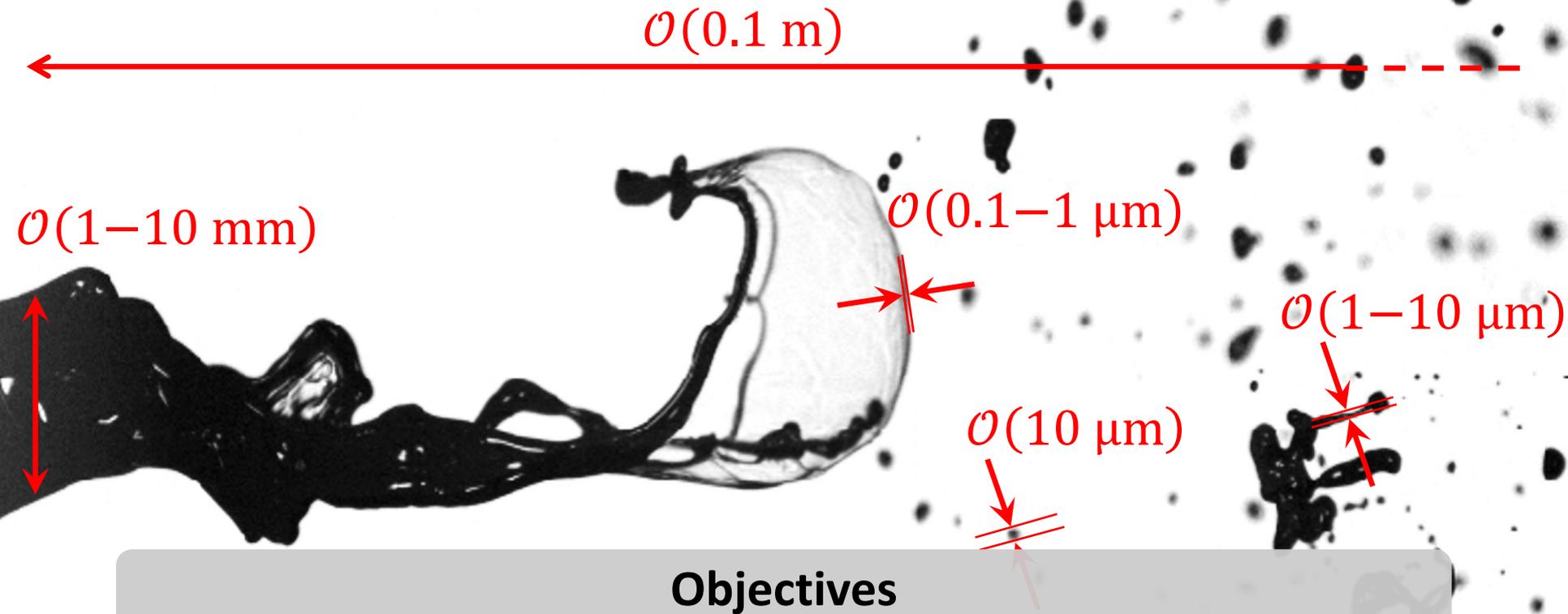
# Enhanced VOF to enable multi-scale modeling



## Observations

1. Highly **multi-scale**, from molecular (van der Waals) to full spray
2. Once surface tension dominates (i.e., below the Kolmogorov–Hinze scale), **interface shapes are simple**: near-planar, film, ligament, drop
3. Extensive **theories exist to describe microscale dynamics** of surface tension-driven flows and break-up (e.g., Rayleigh–Plateau, Taylor–Culick, and Rayleigh–Taylor instabilities)

# Enhanced VOF to enable multi-scale modeling

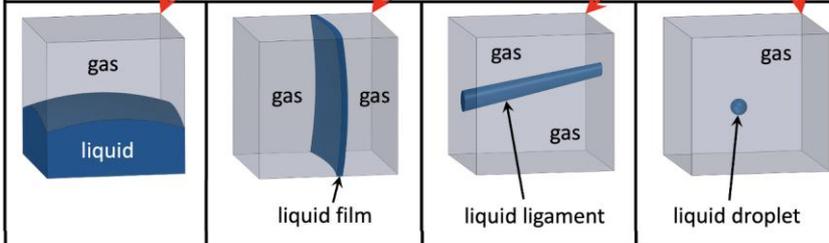
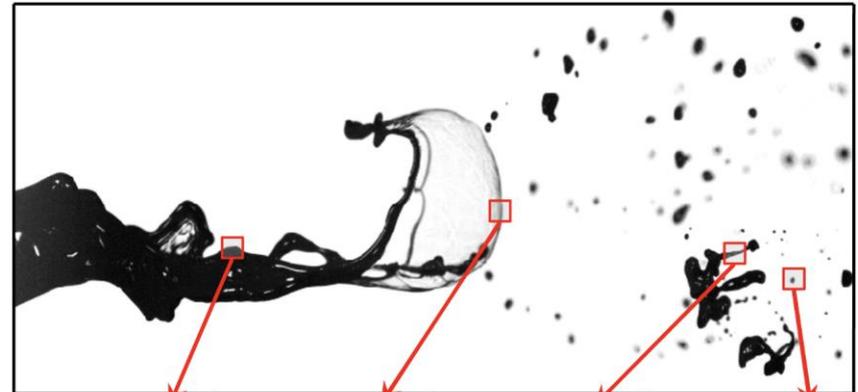


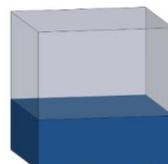
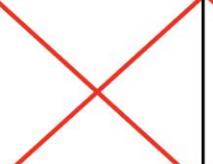
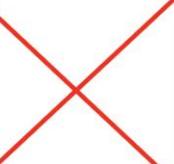
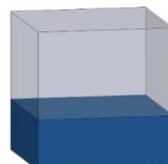
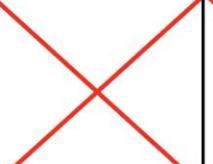
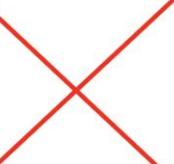
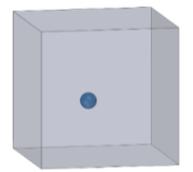
## Objectives

- Enhance Eulerian interface capturing in order to
  - Eliminate numerical break-up
  - Enable sub-grid scale capturing of the simple interface shapes that are expected in surface tension-dominated flows
- Advance mathematical framework to model sub-grid scale dynamics by exploiting existing theories for surface tension-driven flows

# Enhanced VOF (eVOF)

*Enabling multi-scale modeling*

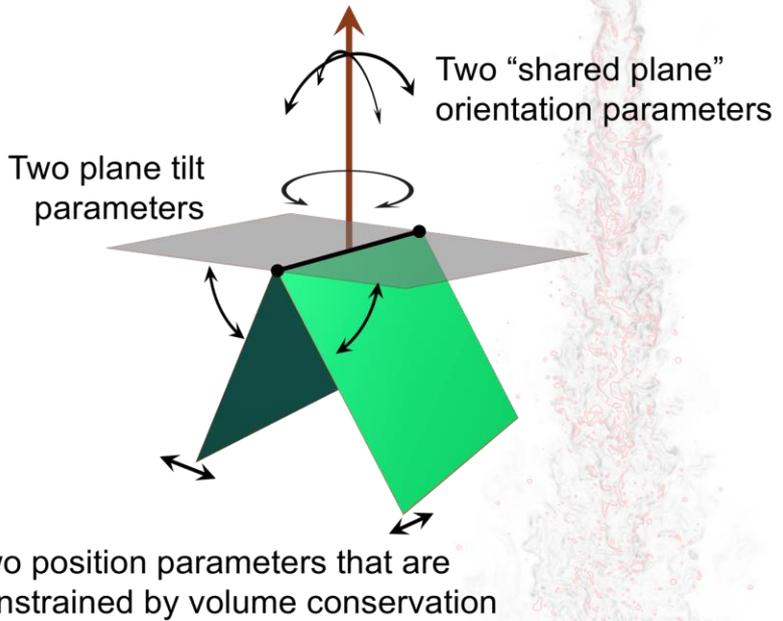


				
PLIC				
Lagrangian droplet tracking				

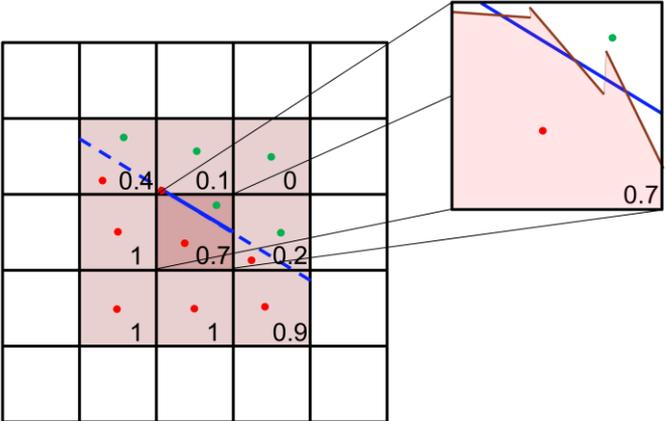
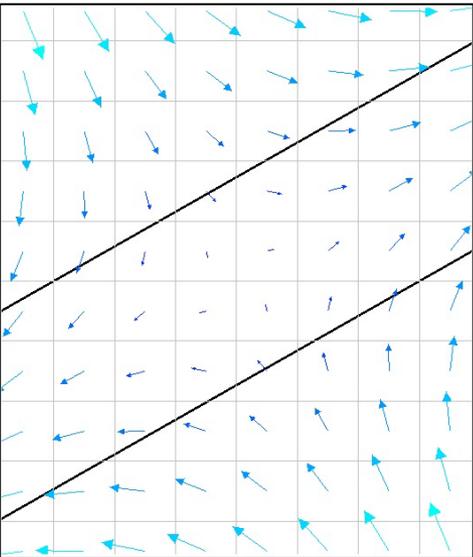


# Eulerian sub-grid scale film capturing

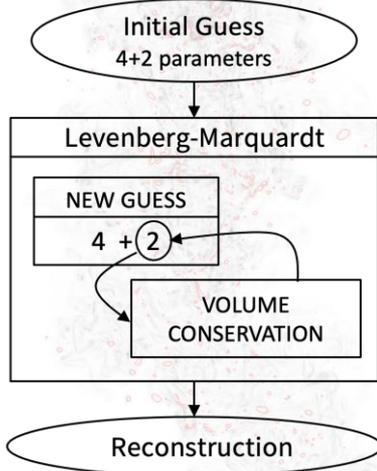
- Simple idea is to allow for **two interfaces to coexist in each cell**
  - **Reconstruction with 2 Planes (R2P)** <sup>1</sup>
  - Available as open-source library (<https://www.multiphasecf.com>)



- Effectively eliminates numerical topology change for films



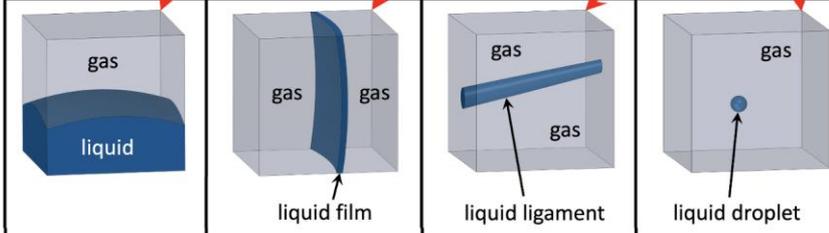
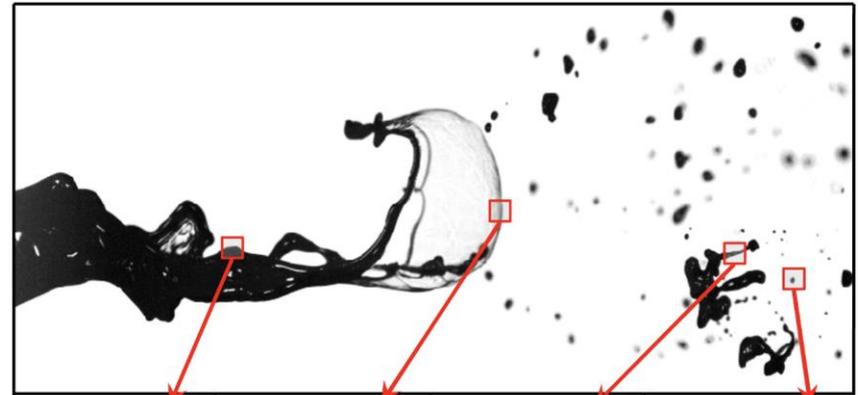
$$e_r = \underbrace{\|w_\alpha^T(\alpha^t - \tilde{\alpha}^t)\|}_{\text{Volume error same as (E)LVIRA}} + \underbrace{\|w_l^T(c^t - \tilde{c}^t)\| + \|w_g^T(c^g - \tilde{c}^g)\|}_{\text{Centroid error generalization of MOF}} + \underbrace{\|w_\Sigma^T(\Sigma - \tilde{\Sigma})\|}_{\text{Surface area error limiter on surface energy}}$$

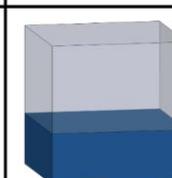
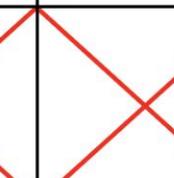
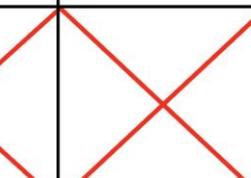
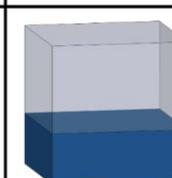
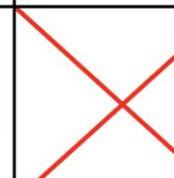
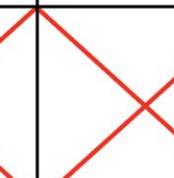
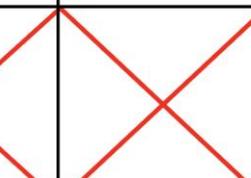
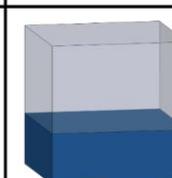
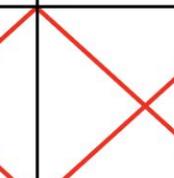
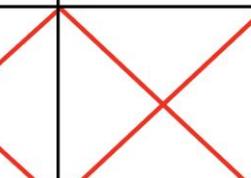
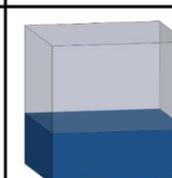
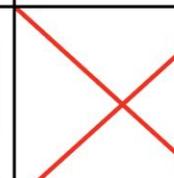
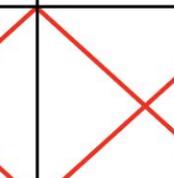
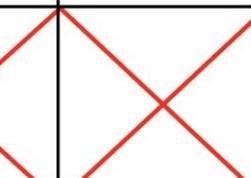


<sup>1</sup> Han, Chiodi, and Desjardins, *J. Comp. Phys*, in review

# Enhanced VOF (eVOF)

*Enabling multi-scale modeling*

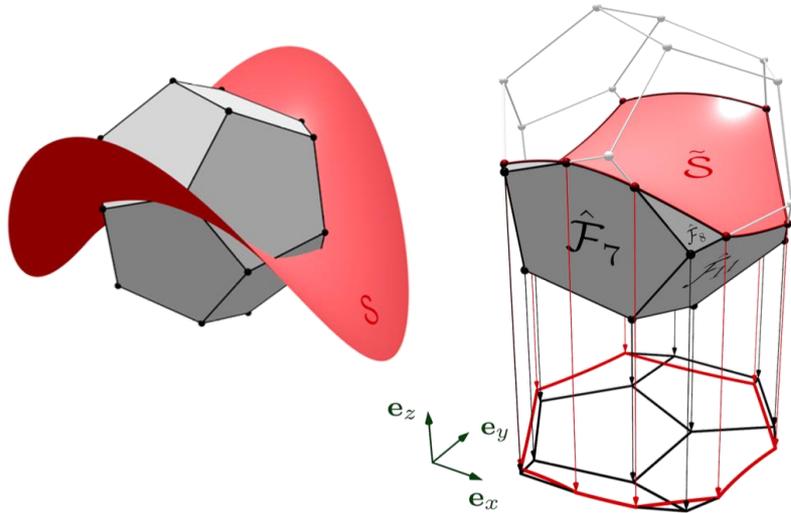


				
PLIC				
R2P				
Lagrangian droplet tracking				



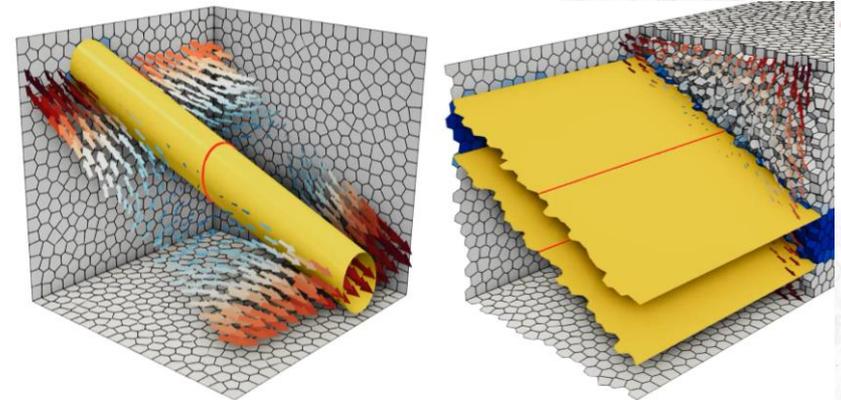
# Eulerian capturing of sub-grid scale topologies

- Another idea is to enable **paraboloid interface in each cell**
  - **Piecewise-Parabolic Interface Calculation (PPIC)**<sup>1</sup>
  - Available as open-source library (<https://www.multiphasecfd.com>)



Exact moment calculation based on sum of 1D integrals over straight lines or conic section arcs  
*Kromer & Bothe, JCP (2023)*  
*Evrard et al., SIAM J. Sci. Comput. (2023)*

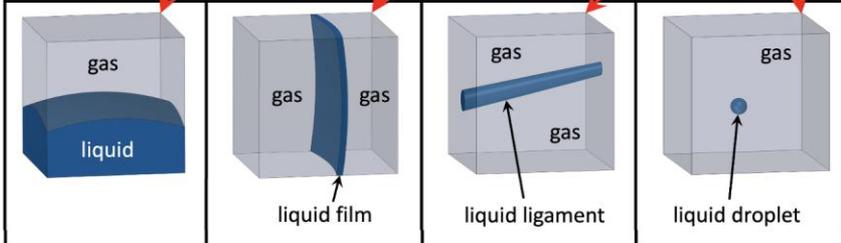
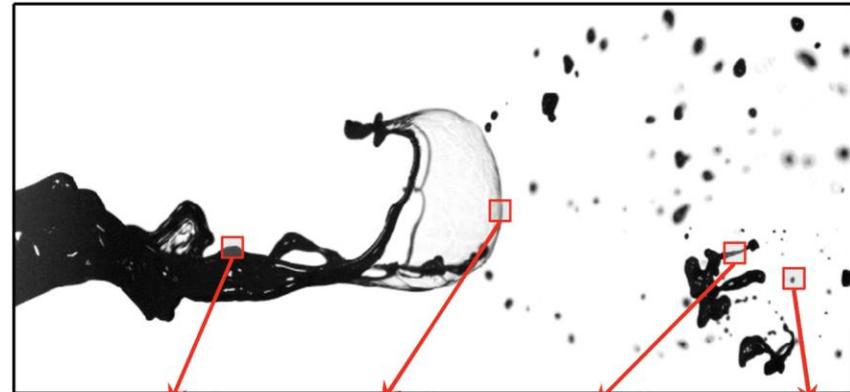
- Able to directly represent sub-grid scale films and ligaments



<sup>1</sup> Evrard, Chiodi, van Wachem, Desjardins, *SIAM J. Sci. Comput.* (2023)

# Enhanced VOF (eVOF)

*Enabling multi-scale modeling*

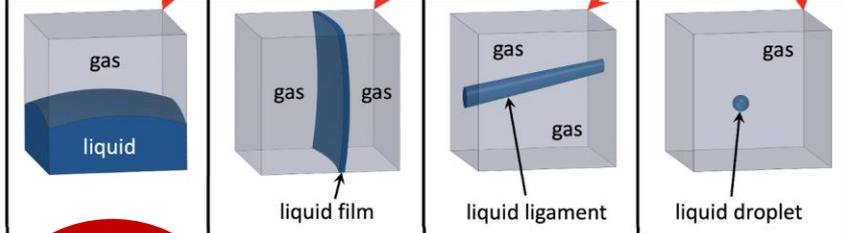
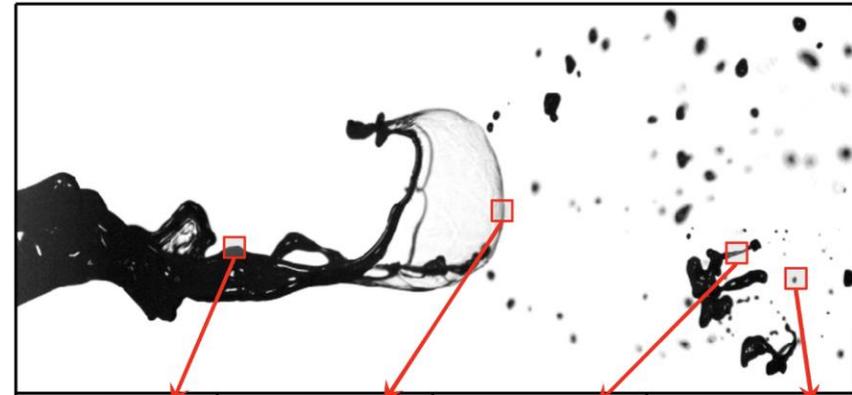


PLIC				
R2P				
PPIC				
Lagrangian droplet tracking				

# Enhanced VOF (eVOF)

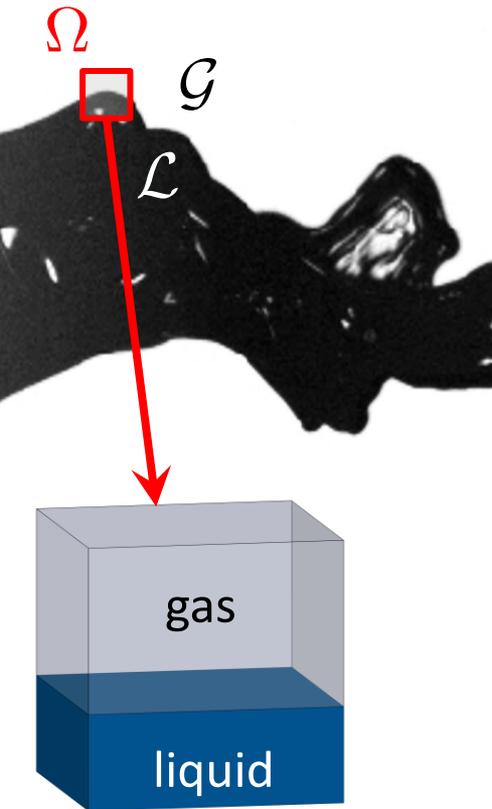
## Enabling multi-scale modeling

- So far, eVOF provides
  - **SciML-enabled PLIC-R2P hybrid**
  - *Ligaments with PPIC are work-in-progress*
  - Robust capturing of sub-grid structures
  - Spurious numerical break-up eliminated
- However, sub-grid scale structures are essentially not seen by the flow solver
  - Need to reintroduce physics explicitly
  - Assume surface tension-dominated flow
  - Rely on theory for guidance
- In the rest of the talk, we will demonstrate **several sub-grid scale models**



PLIC				
R2P				
PPIC				
Lagrangian droplet tracking				

# Volume-filtered framework for enhanced VOF



## Liquid distribution function

$$\psi(\mathbf{x}, t) = \begin{cases} 1, & \text{if } \mathbf{x} \in \mathcal{L}, \\ 0, & \text{if } \mathbf{x} \in \mathcal{G}. \end{cases}$$

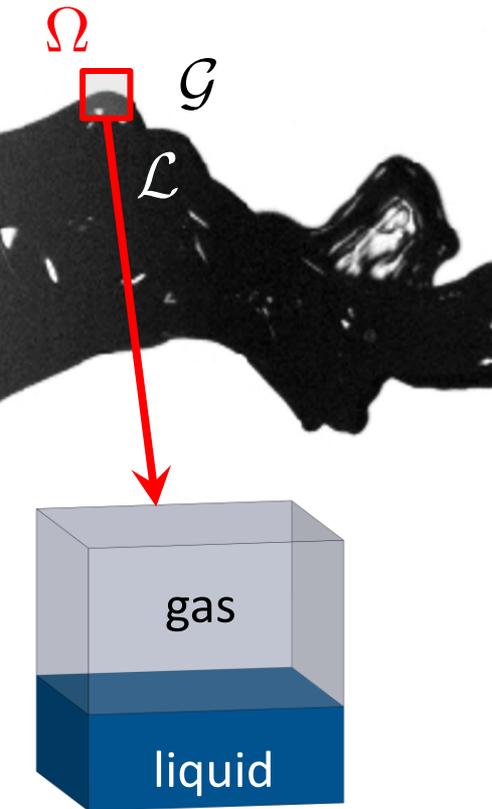
## Volume filtering operators

$$\bar{f} = \frac{\int_{\Omega} f \, d\mathbf{x}}{\int_{\Omega} d\mathbf{x}}$$

$$\bar{f}^l = \frac{\int_{\Omega} f \psi(\mathbf{x}, t) \, d\mathbf{x}}{\int_{\Omega} \psi(\mathbf{x}, t) \, d\mathbf{x}} = \frac{\int_{\Omega \cap \mathcal{L}} f \, d\mathbf{x}}{\int_{\Omega \cap \mathcal{L}} d\mathbf{x}}$$

$$\bar{f}^g = \frac{\int_{\Omega} f (1 - \psi(\mathbf{x}, t)) \, d\mathbf{x}}{\int_{\Omega} (1 - \psi(\mathbf{x}, t)) \, d\mathbf{x}} = \frac{\int_{\Omega \cap \mathcal{G}} f \, d\mathbf{x}}{\int_{\Omega \cap \mathcal{G}} d\mathbf{x}}$$

# Volume-filtered framework for enhanced VOF



## Continuity equation

$$\nabla \cdot \bar{\mathbf{u}} = 0$$

## Liquid volume fraction transport equation

$$\frac{\delta}{\delta t} \bar{\psi} = 0$$

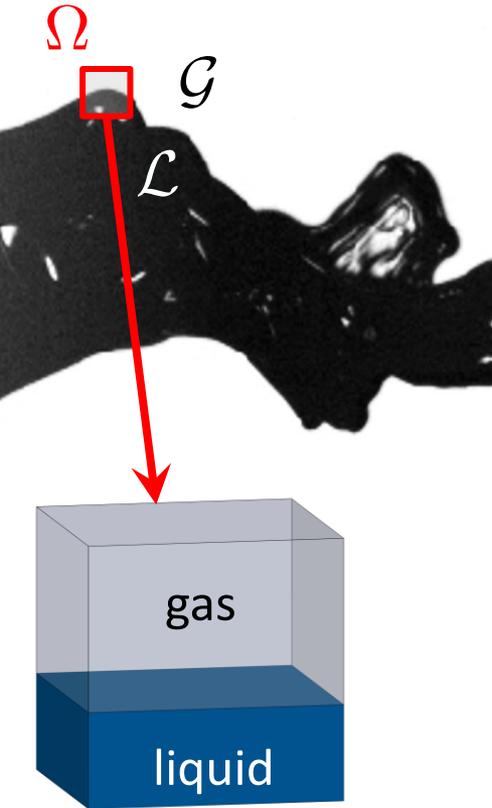
## Phasic barycenter transport equations

$$\frac{\delta}{\delta t} \bar{\mathbf{x}}^l = \bar{\mathbf{u}}^l \quad \frac{\delta}{\delta t} \bar{\mathbf{x}}^g = \bar{\mathbf{u}}^g$$

## Navier-Stokes equation

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) &= -\nabla \bar{p} + \overline{\sigma \kappa \mathbf{n} \delta} \\ &+ \nabla \cdot [\bar{\mu} (\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T)] \\ &+ \tau_t + \nabla \cdot (\tau_c + \tau_v) \end{aligned}$$

# Volume-filtered framework for enhanced VOF



## Continuity equation

$$\nabla \cdot \bar{\mathbf{u}} = 0$$

## Liquid volume fraction transport equation

$$\frac{\delta}{\delta t} \bar{\psi} = 0$$

## Phasic barycenter transport equations

$$\frac{\delta}{\delta t} \bar{\mathbf{x}}^l = \bar{\mathbf{u}}^l \quad \frac{\delta}{\delta t} \bar{\mathbf{x}}^g = \bar{\mathbf{u}}^g$$

## Navier-Stokes equation

$$\begin{aligned} \frac{\partial \bar{\rho} \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) = & -\nabla \bar{p} + \overline{\sigma \kappa \mathbf{n} \delta} \\ & + \nabla \cdot [\bar{\mu} (\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T)] \\ & + \bar{\tau}_t + \nabla \cdot (\bar{\tau}_c + \bar{\tau}_v) \end{aligned}$$

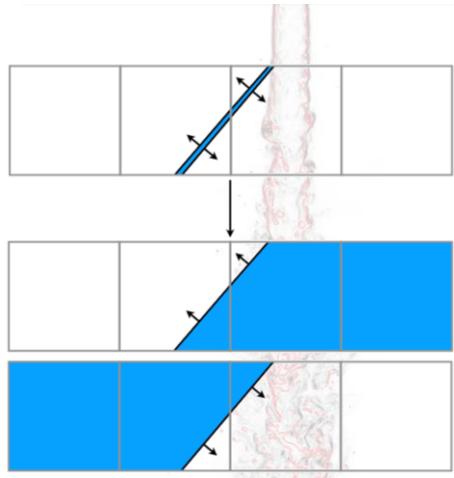
Non-trivial closed term

Unclosed terms

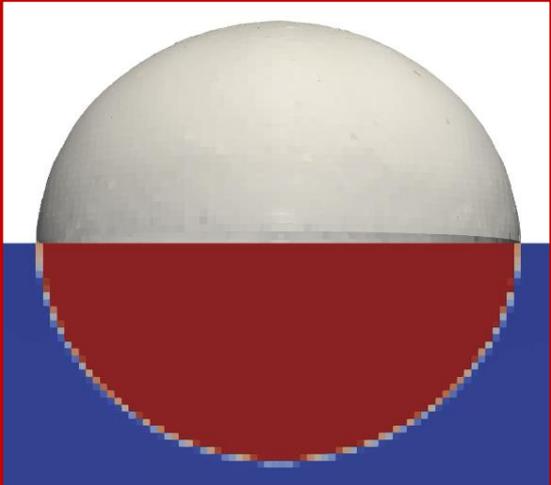
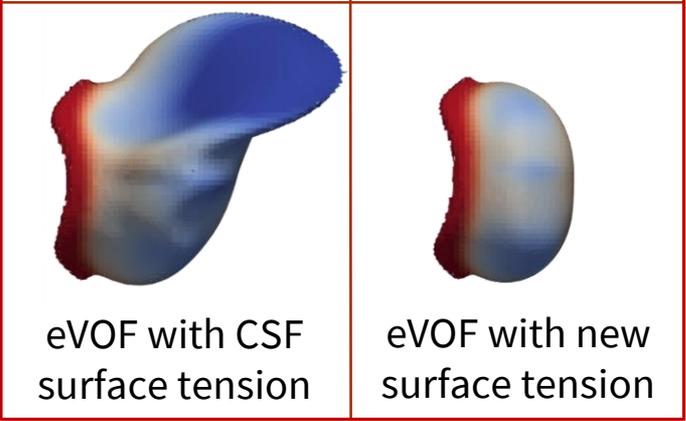
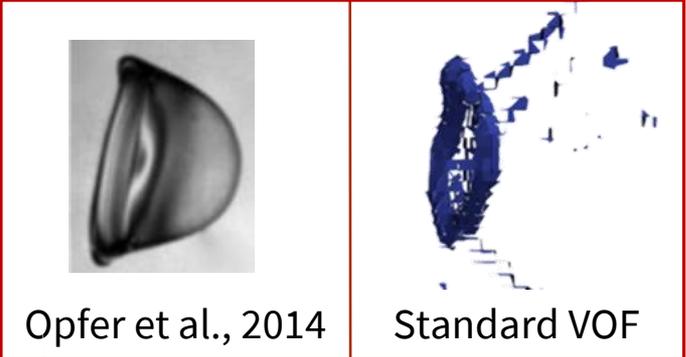
# SGS surface tension in eVOF

- Compared to standard VOF, eVOF enables thin film capturing
- Standard implementations of surface tension (e.g., based on volume fraction gradient) fail due to vanishing volume fraction

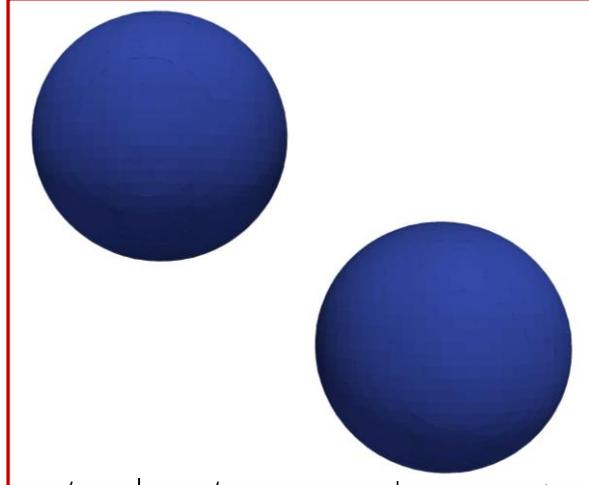
$$\overline{\sigma \kappa n \delta} \neq \sigma \kappa \nabla \alpha$$



- Developed new discretization compatible with multiple interfaces per cell



Oscillation period  
 $7.87 \times 10^{-3}$  s (simulation)  
 $7.85 \times 10^{-3}$  s (theory by Grinfeld, 2012)  
 Thin-film bubble oscillation

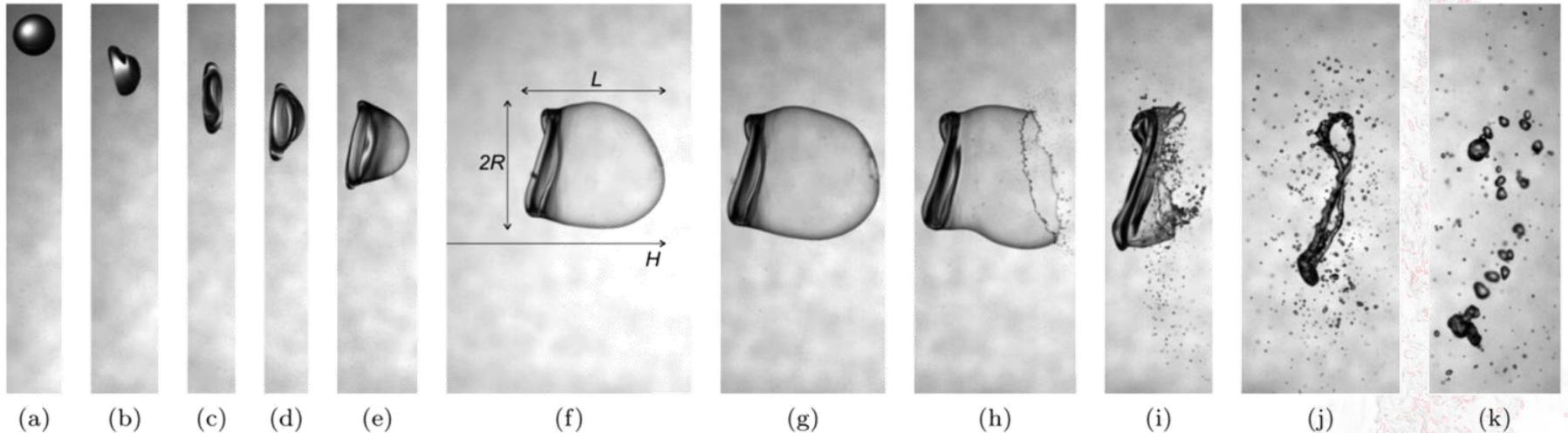


$\rho_l / \rho_g$	$\mu_l / \mu_g$	$We_l$	$B = \chi / D$
622	116.5	14.4	0.42

Bouncing expected (Qian & Law, 1997)  
 Glancing droplet collisions

# Break-up modeling in eVOF

## *Low viscosity*



### Assumptions

1. Ignore temporal, convective, and viscous SGS terms
2. Assume  $\bar{\mathbf{u}} \approx \bar{\mathbf{u}}^l \approx \bar{\mathbf{u}}^g$  except at the edge of films
3. At edge of film, assume that break-up dynamics are dominating
  - Model droplet shedding from retracting rim
  - Based on theory of Wang and Bourouiba (2018)
  - Hole nucleation based on local film thickness criterion

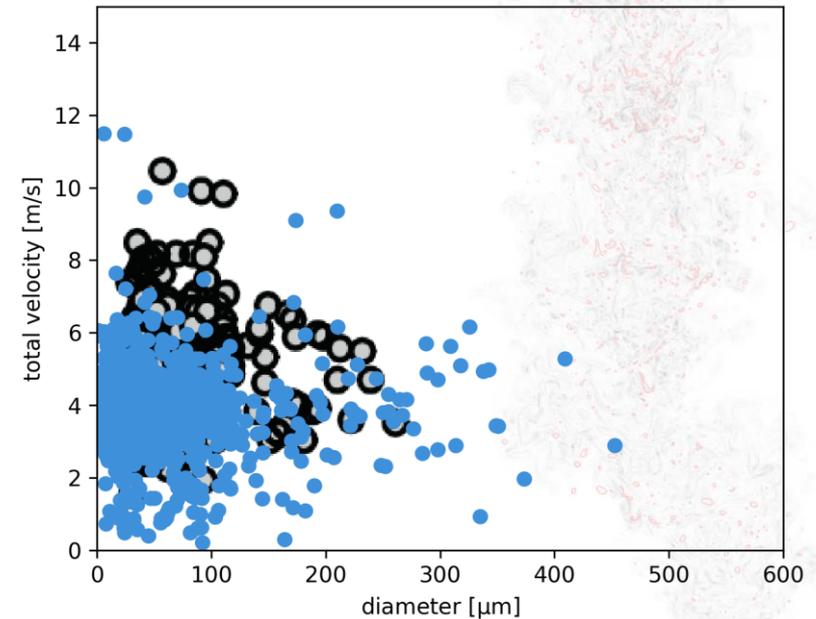
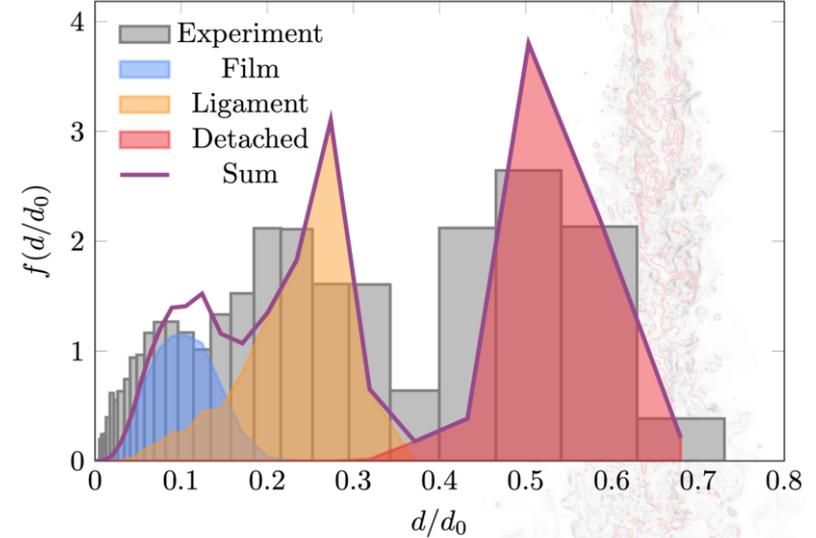
# Break-up modeling in eVOF

## *Low viscosity*

- Experiments by Guildenbecher et al. (2017)
- Simulations with 25 cells per diameter
- $TI = 1.9\%$ , statistics over 45 realizations

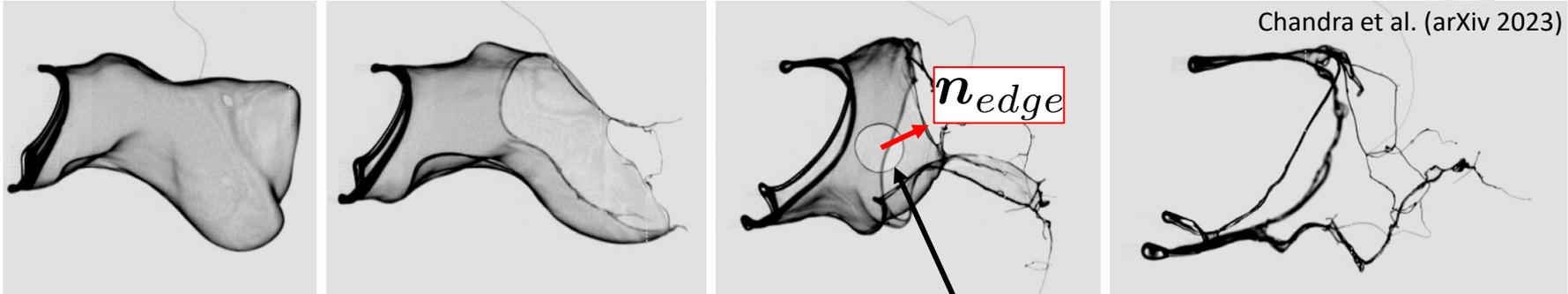


$\rho_l/\rho_g$	$\mu_l/\mu_g$	$Oh$	$We_g$	$Re_g$
657.5	66.7	0.00542	13.8	1778



# Film retraction modeling in eVOF

## *High viscosity and viscoelasticity*



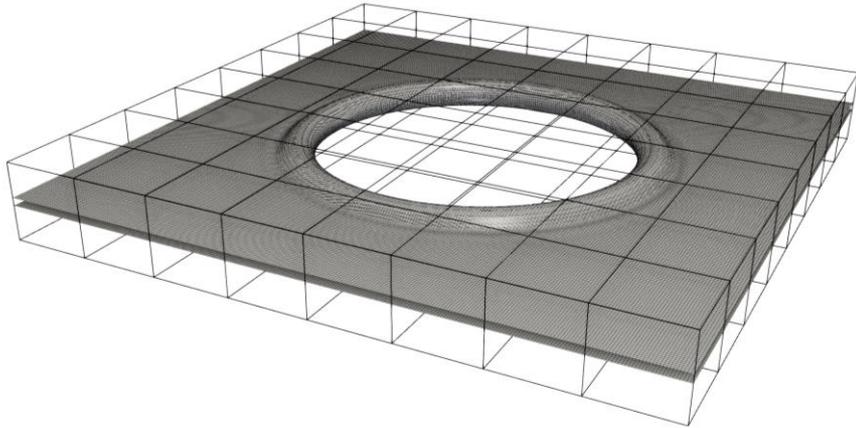
### Assumptions

$$U_{TC} = \sqrt{\frac{2\sigma}{\rho_l h}}$$

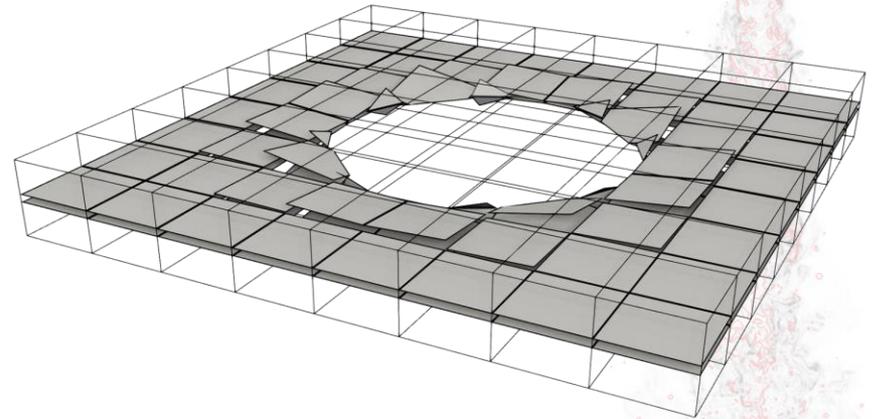
1. Ignore temporal, convective, and viscous SGS terms
2. Assume  $\bar{\mathbf{u}} \approx \bar{\mathbf{u}}^l \approx \bar{\mathbf{u}}^g$  except at the edge of the film
3. At edge of film, assume that viscous **Taylor–Culick retraction** is dominating
  - $\bar{\mathbf{u}} \approx \bar{\mathbf{u}}^g$  and  $\bar{\mathbf{u}}^l - \bar{\mathbf{u}}^g \approx U_{TC} \mathbf{n}_{edge}$
  - Distribute velocity using a **Stokeslet solution** to conserve mass
  - Hole nucleation based on local film thickness criterion

# Film retraction modeling in eVOF

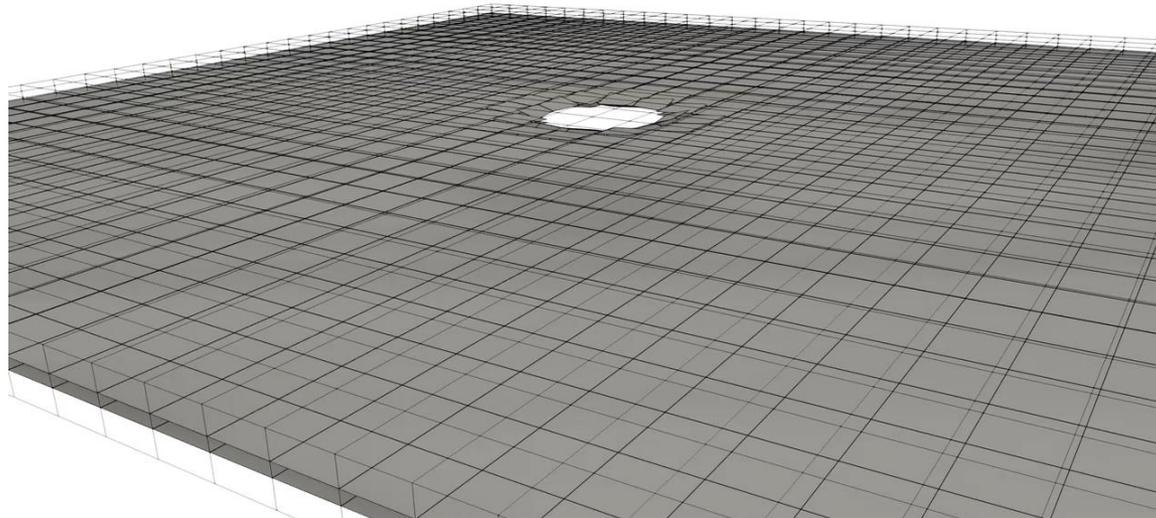
*High viscosity and viscoelasticity*



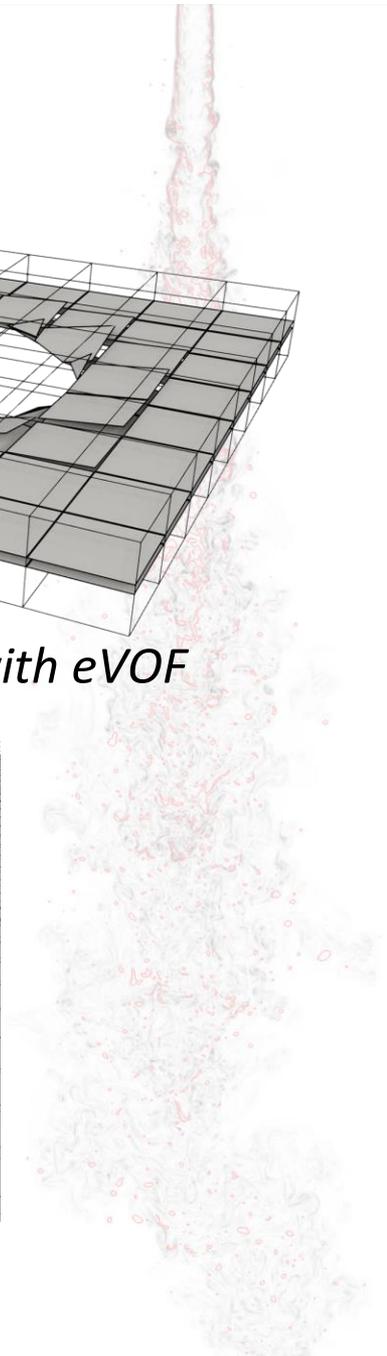
*Fully resolved film with standard VOF*



*Fully sub-grid film with eVOF*



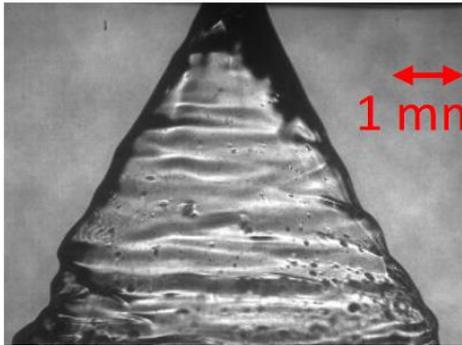
*Fully sub-grid retracting film with eVOF and  
Taylor–Culick/stokeslet slip velocity model*



# Film retraction modeling in eVOF

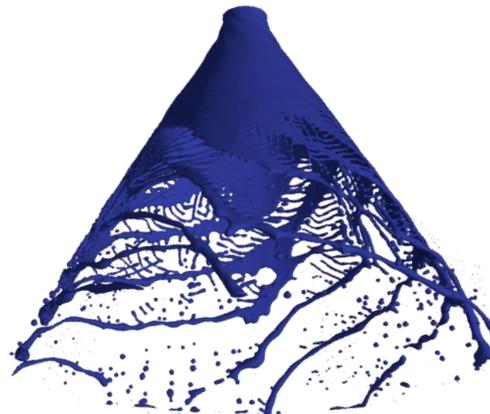
*High viscosity and viscoelasticity*

Experimental<sup>1</sup>



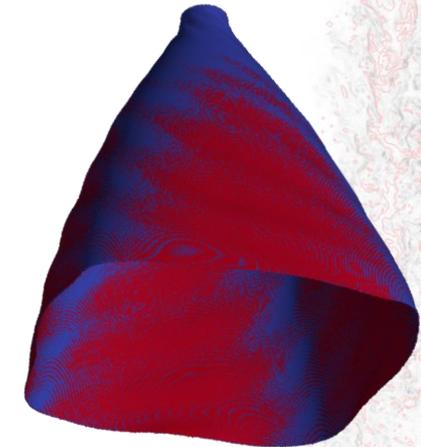
Chen & Ashgriz, *IJMF* (2022)

VOF



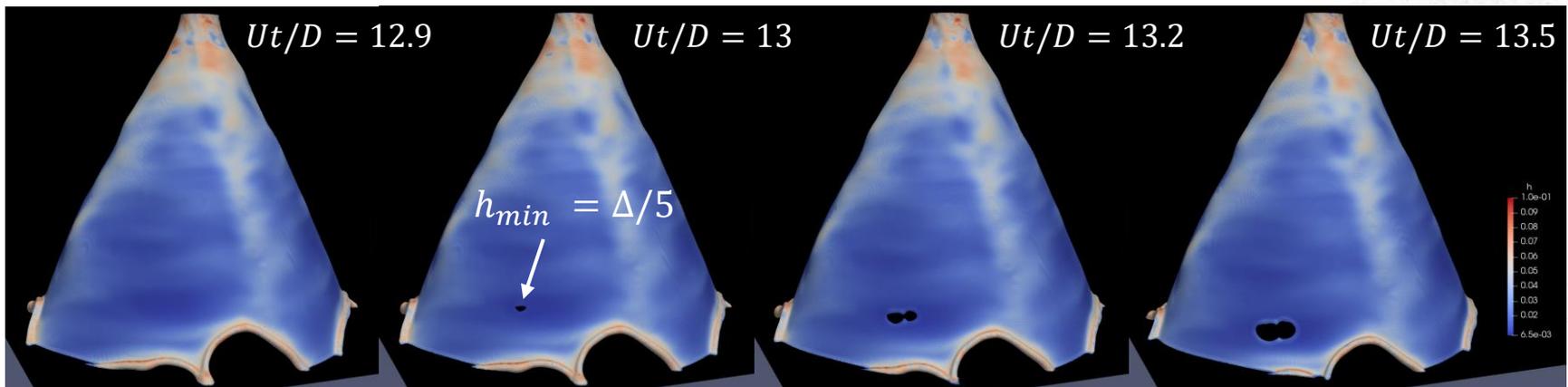
*Spurious break-up*

eVOF



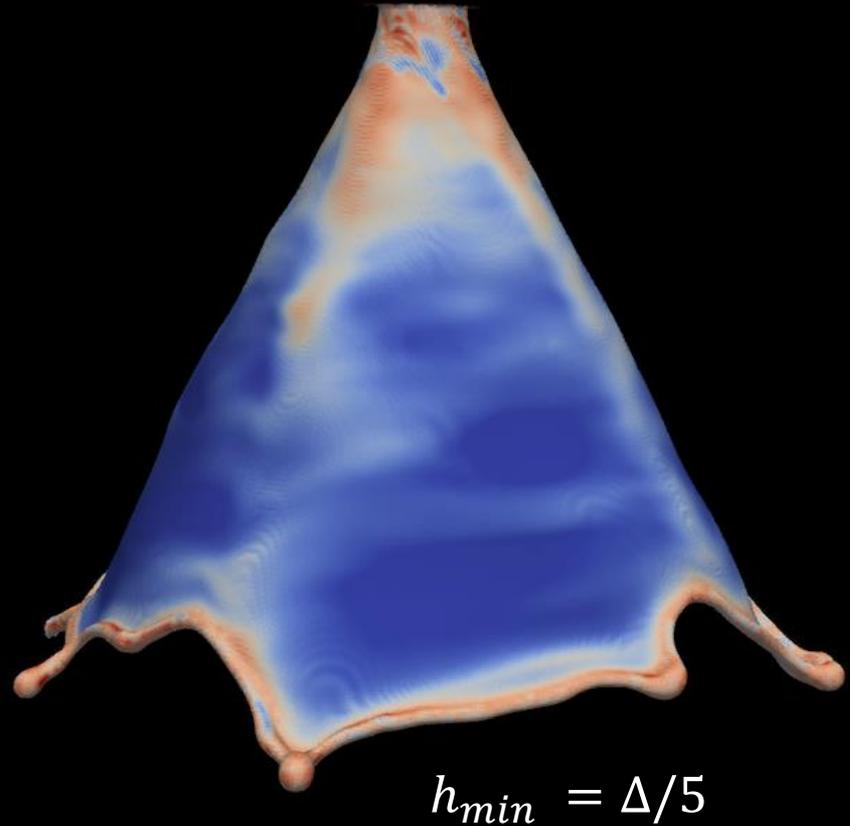
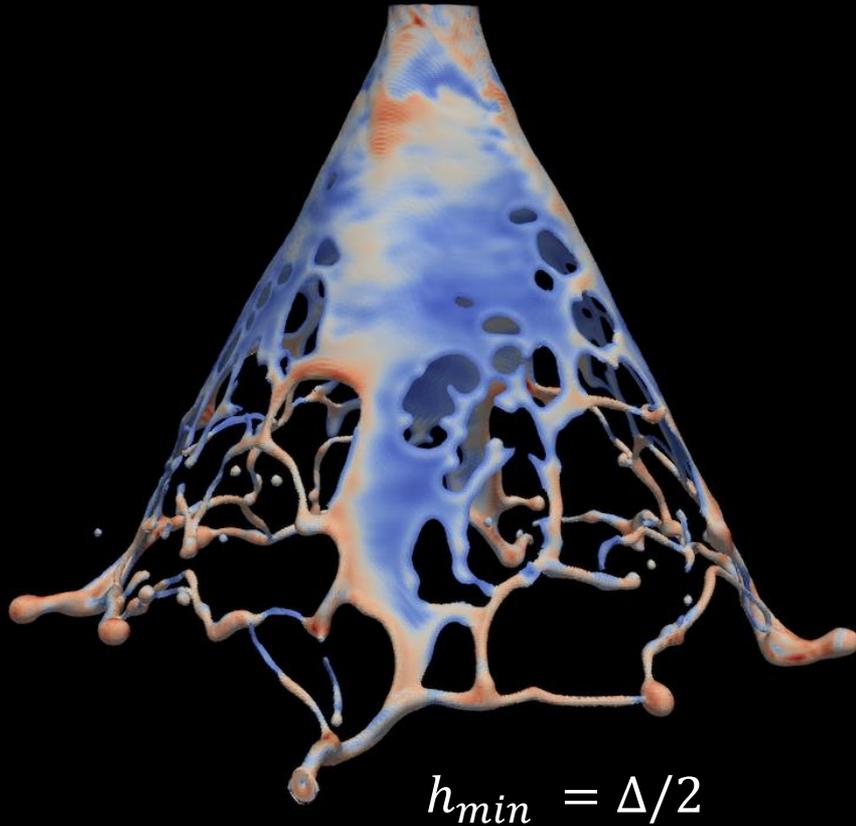
*No break-up*

## eVOF with sub-grid scale hole nucleation and film retraction



# Film retraction modeling in eVOF

*High viscosity and viscoelasticity*



- Mesh resolution no longer controls the onset of break-up
- Instead, onset of break-up is controlled by hole nucleation model

# Conclusions

- **Algorithmic advances in VOF methods such as R2P and PPIC enable efficient tracking of simple sub-grid scale interfacial features without numerical break-up**
- Interface is assumed to **remain very simple at the sub-grid scale** (e.g., flat sheets and straight ligaments)
  - Not well-suited for representing turbulent interfacial corrugations at the sub-grid scale, but appropriate if surface tension dominates (i.e., if Kolmogorov–Hinze scale is mesh-resolved)
- Requires development of **novel models for sub-grid scale interface dynamics**
  - Surface tension across film, hole nucleation, film retraction, ligament rupture, ligament retraction, drag on ligament, etc...
- This approach may provide an efficient strategy for handling highly stable sheets and ligaments in **high-viscosity and viscoelastic fluids**

