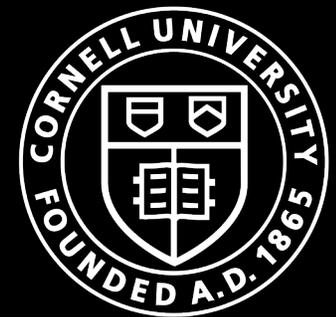


# An enhanced volume of fluid framework for multi-scale atomization modeling



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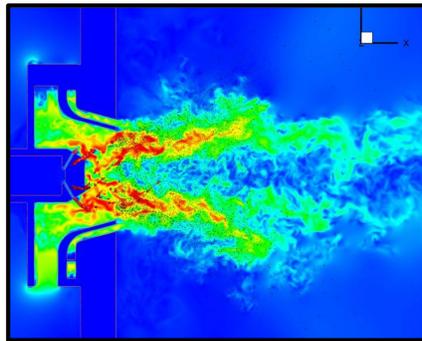


Joseph Giliberto, Zonghao Zou, and Olivier Desjardins  
Sibley School of Mechanical and Aerospace Engineering  
Cornell University

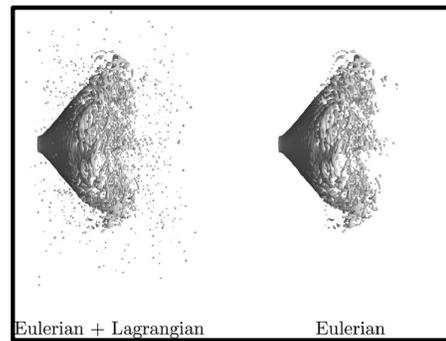


# Spray atomization modeling

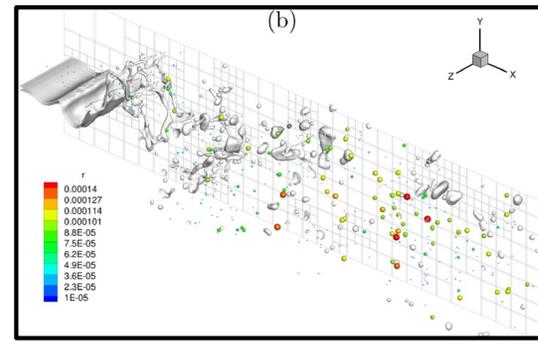
- Spray atomization is a critical process in many applications
- Detailed near-field spray diagnostics are very challenging
- CFD studies of spray atomization are becoming commonplace
  - Enabled by growing computational resources & improved numerics



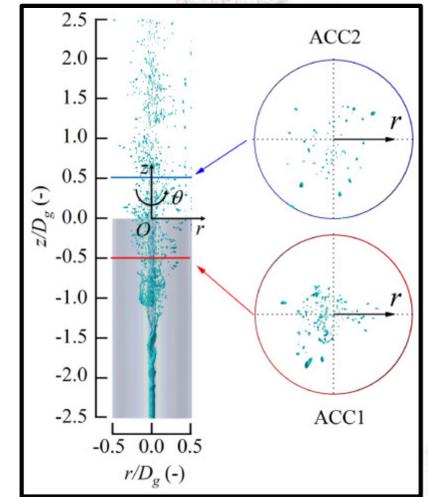
Li et al. (2013)



Evrard et al. (2019)



Zuzio et al. (2019)

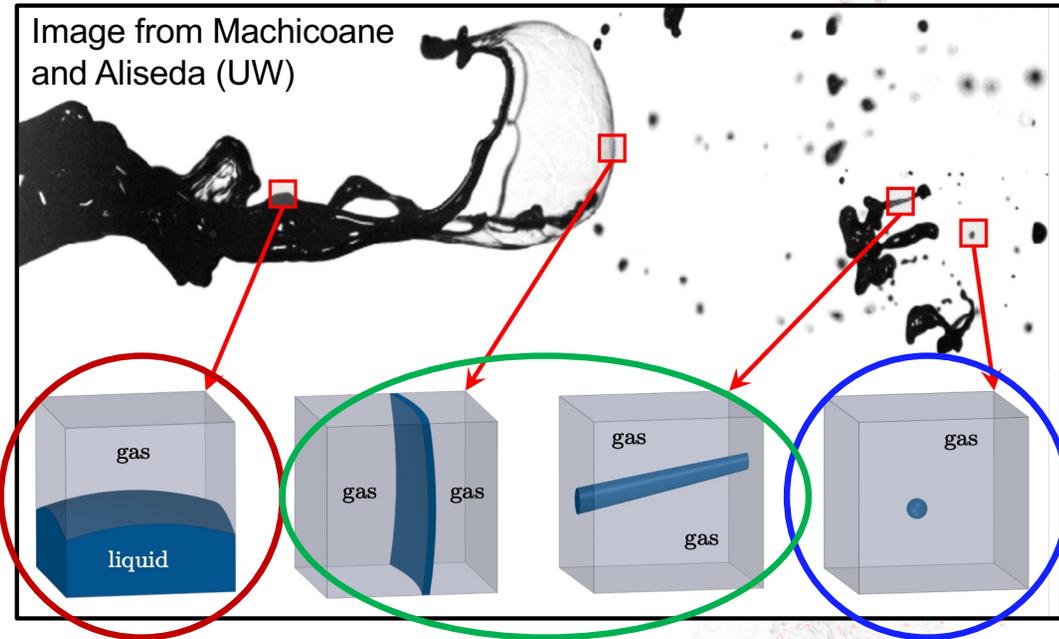


Wen et al. (2022)

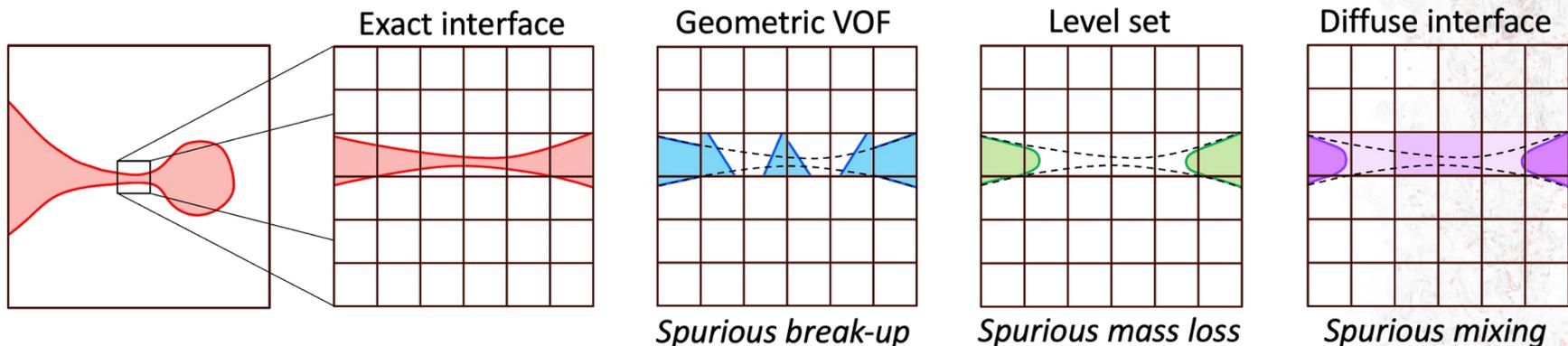
- **Standard practice**
  1. Use **Eulerian interface capturing** to predict interface deformation and break-up
  2. Convert resulting droplets to **Lagrangian representation** for easier and faster tracking
- **Yet computational predictions of drop size in sprays have remained elusive**

# Limitations of classical framework

- Spray atomization gives rise to a wide range of interfacial topologies
  - **Eulerian interface capturing** works well for well-resolved regions
  - **Lagrangian particle tracking** works well for small drops
  - **Films and ligaments** cannot inherently be represented by either method



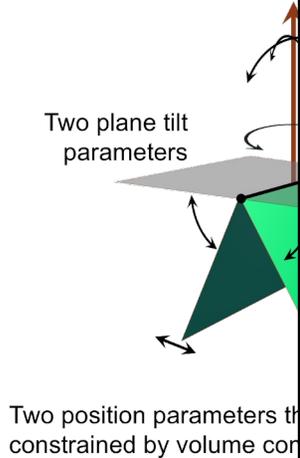
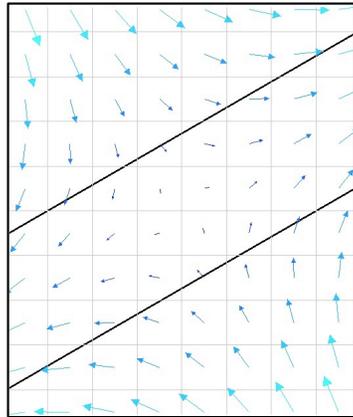
- Insufficient resolution of films and ligaments lead to catastrophic numerical errors



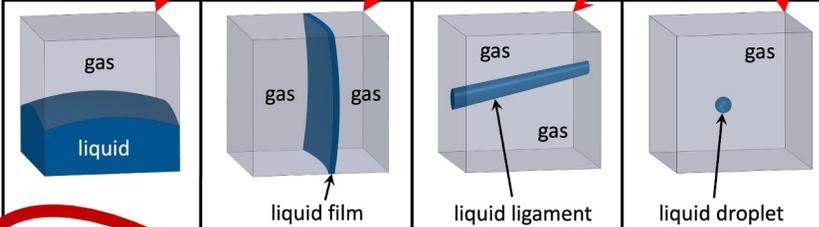
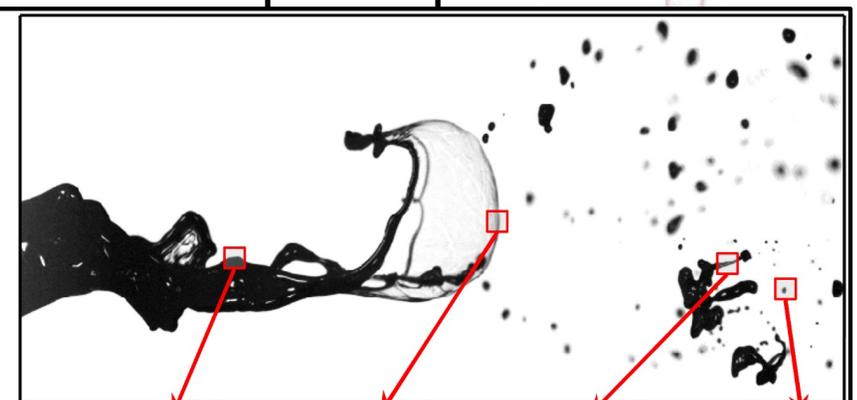
- Mesh refinement is **not a solution** because (1) key molecular scale processes are missing, (2) break-up is still numerical, and (3) the cost becomes enormous...

# Eulerian sub-grid scale film and droplet

- For VOF, reconstructing the interface with PLIC enables SGS film capturing, eliminating



- Reconstructing the interface with piecewise linear interface capturing (PLIC) enables SGS ligament capturing, eliminating



PLIC				
R2P				
PPIC				
Lagrangian droplet tracking				

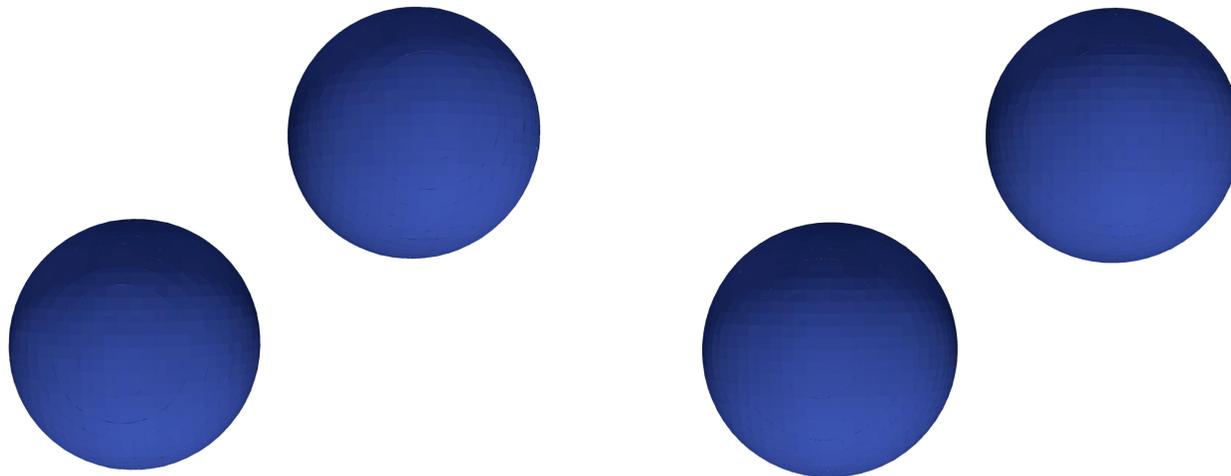
The table is mostly crossed out with red 'X' marks. A large red circle highlights the first row of the table. A red 'X' is also present over the 'PLIC' row. A red circle highlights the 'Lagrangian droplet tracking' row, with a red 'X' over the droplet image.

**FUTURE WORK  
Renewal proposal**



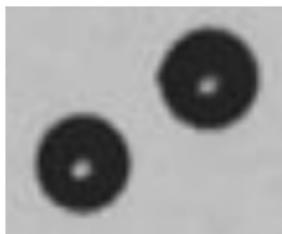
# Modeling bouncing droplets

$\rho_l/\rho_g$	$\mu_l/\mu_g$	$D/\Delta x$	$We_l$	$B = \chi/D$
622	116.5	23.04	14.4	0.42

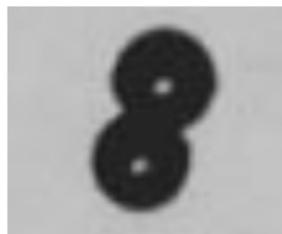


**VOF with R2P film capturing  
(no model)**

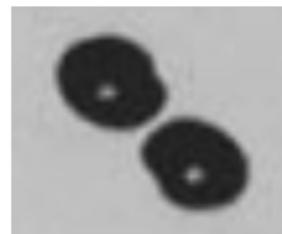
**Standard VOF**



(a)  $t = 0$  ms

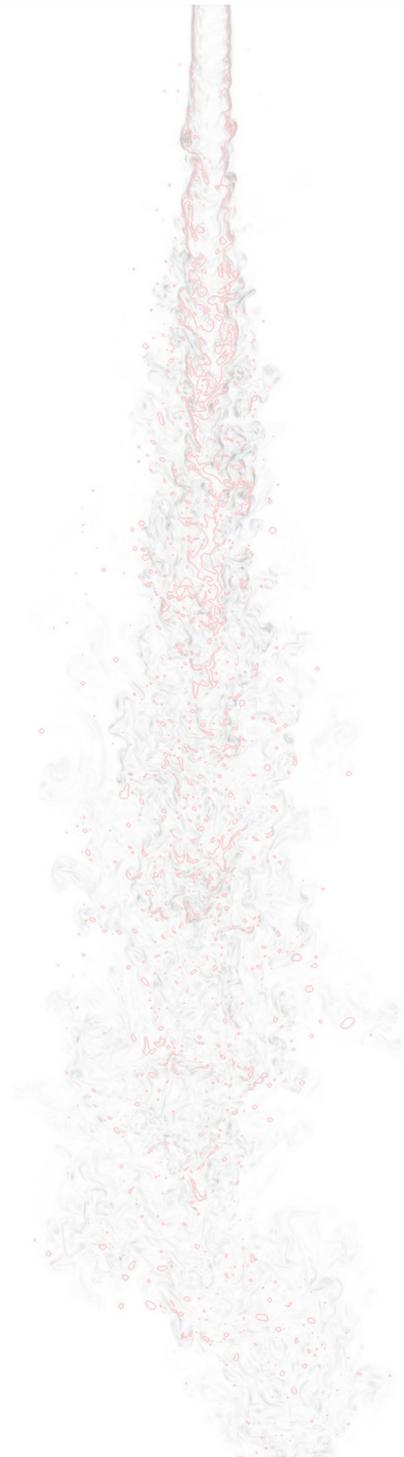


(b)  $t = 18$  ms



(c)  $t = 38$  ms

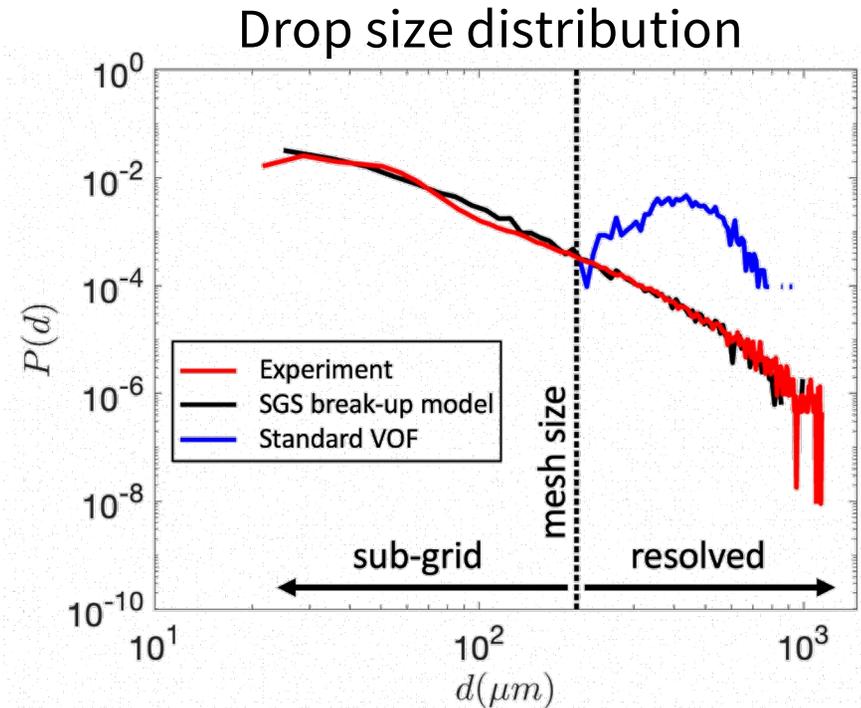
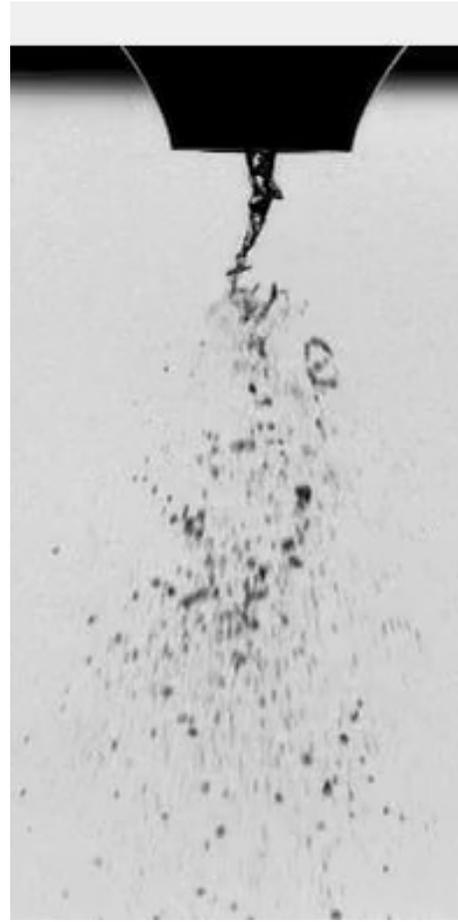
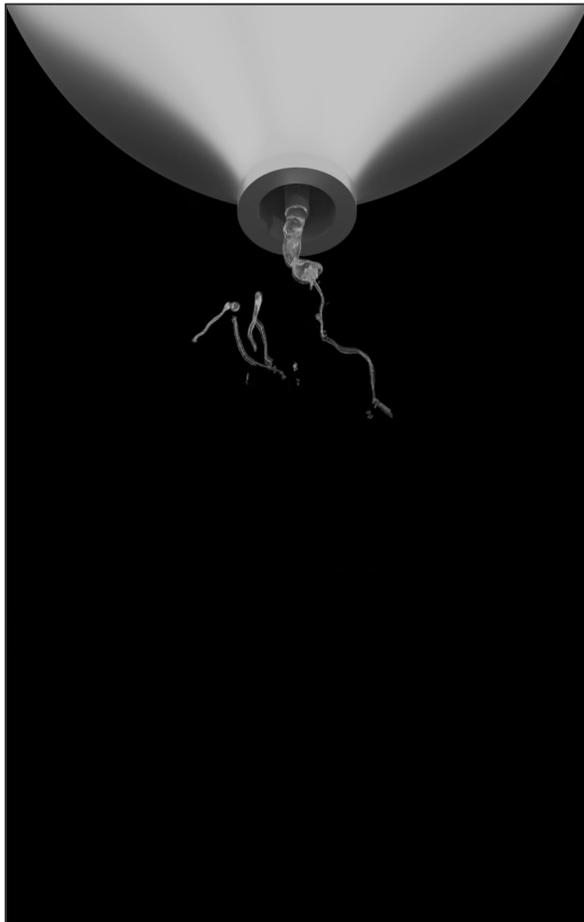
Bouncing expected  
(Qian & Law, 1997)



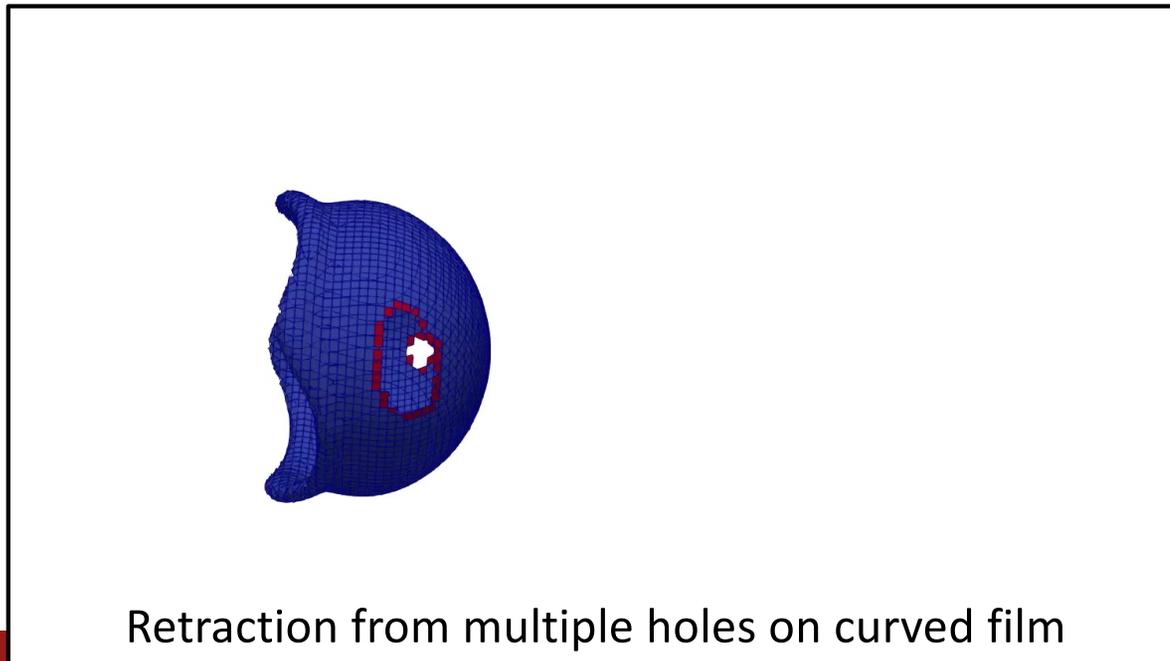
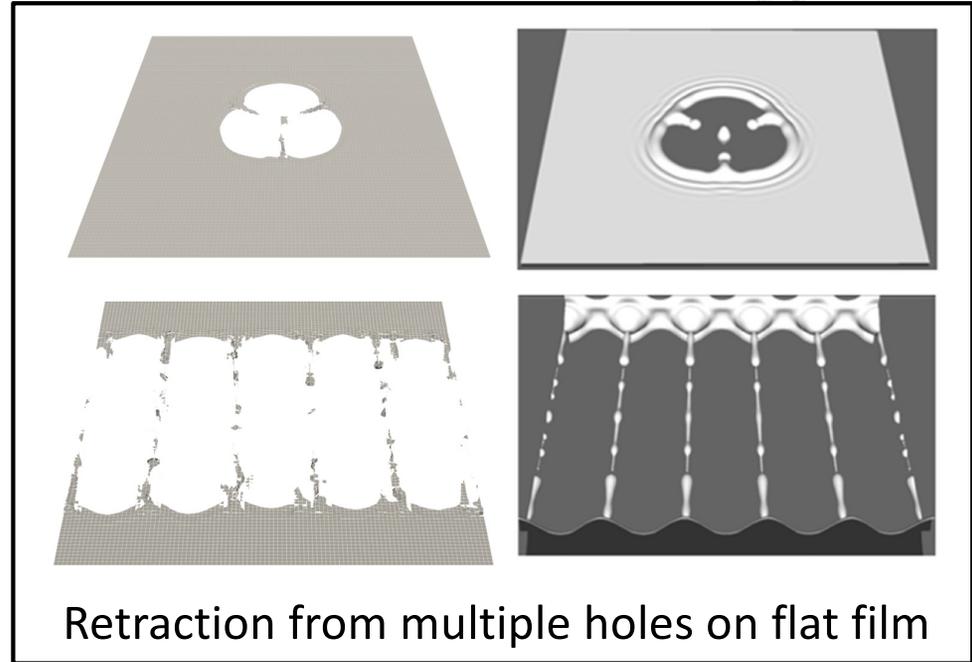
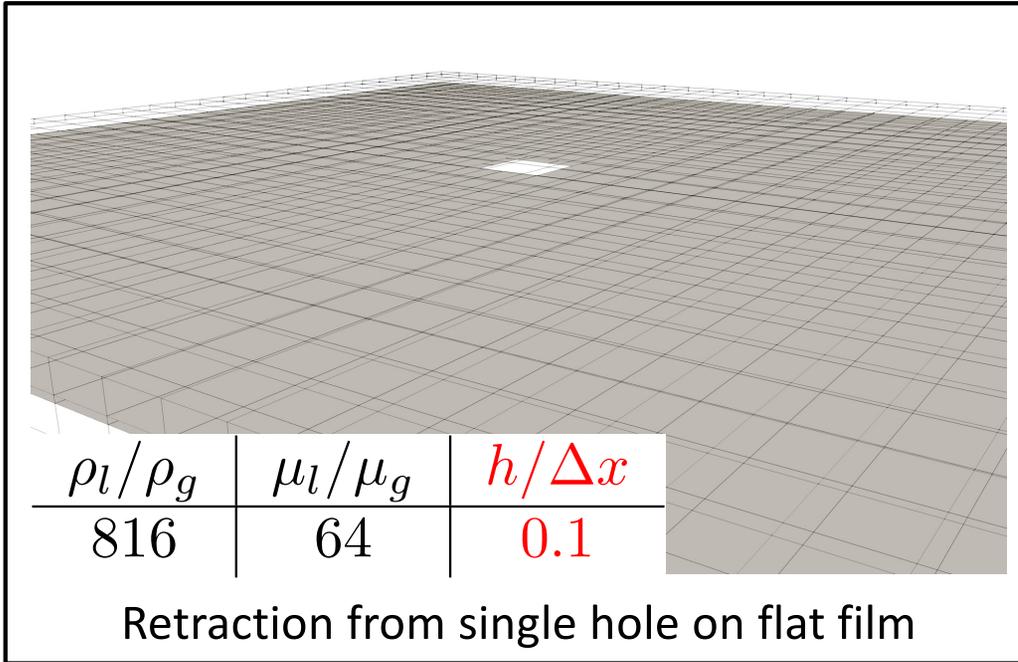


# Application to bag break-up in air-blast atomization <sup>1</sup>

$Re_g \equiv \frac{4Q_g}{\sqrt{4\pi A_g} v_g}$	$Re_l \equiv \frac{\rho_l U_l d_l}{\mu_l}$	$M \equiv \frac{\rho_g U_g^2}{\rho_l U_l^2}$	$We \equiv \frac{\rho_g (U_g - U_l)^2 d_l}{\sigma}$	$\rho^* \equiv \frac{\rho_l}{\rho_g}$	$\mu^* \equiv \frac{\mu_l}{\mu_g}$
21400	1200	6.4	39.1	815	65



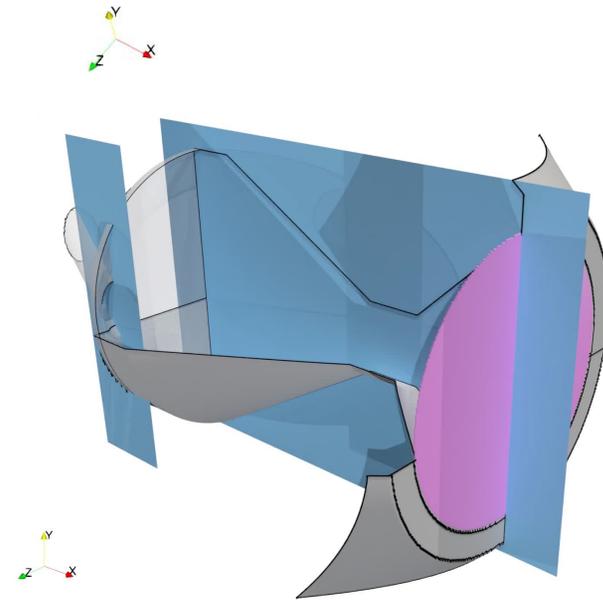
# Sub-filter modeling of film retraction





# Application to Research Simplex Atomizer (RSA)

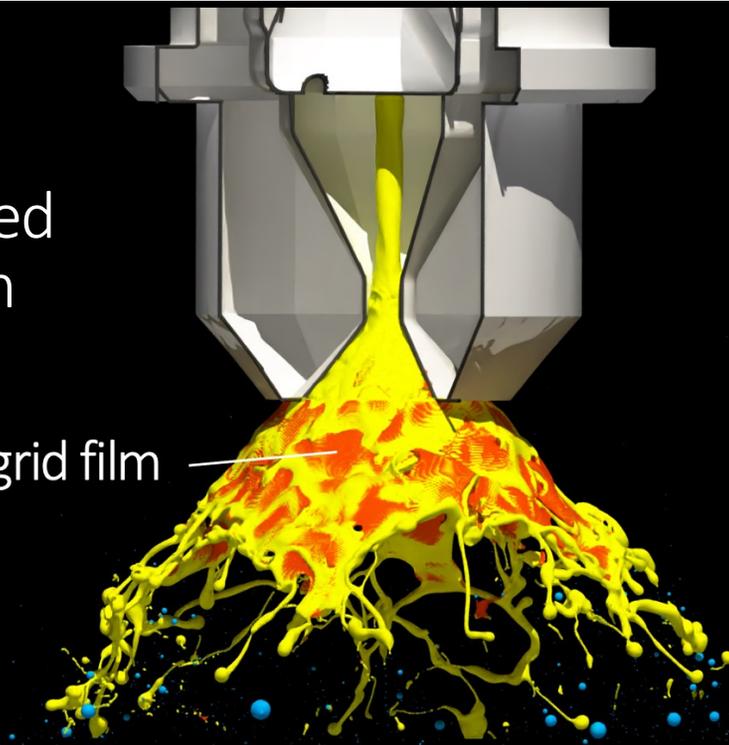
- Canonical simplex atomizer geometry that has been studied both experimentally<sup>1,2,3</sup> and numerically<sup>4</sup>
- **Experimental test conditions**<sup>2</sup>
  - MIL-PRF-7024 Type II calibration fluid
  - Injection pressure: 50 and 100 bar
- **Simulation information**
  - Domain size: 1 cm<sup>3</sup>
  - Uniform Cartesian mesh
  - Dirichlet inflow on inlet pipes
  - Atomizer geometry modeled with volumetric direct forcing immersed boundary method



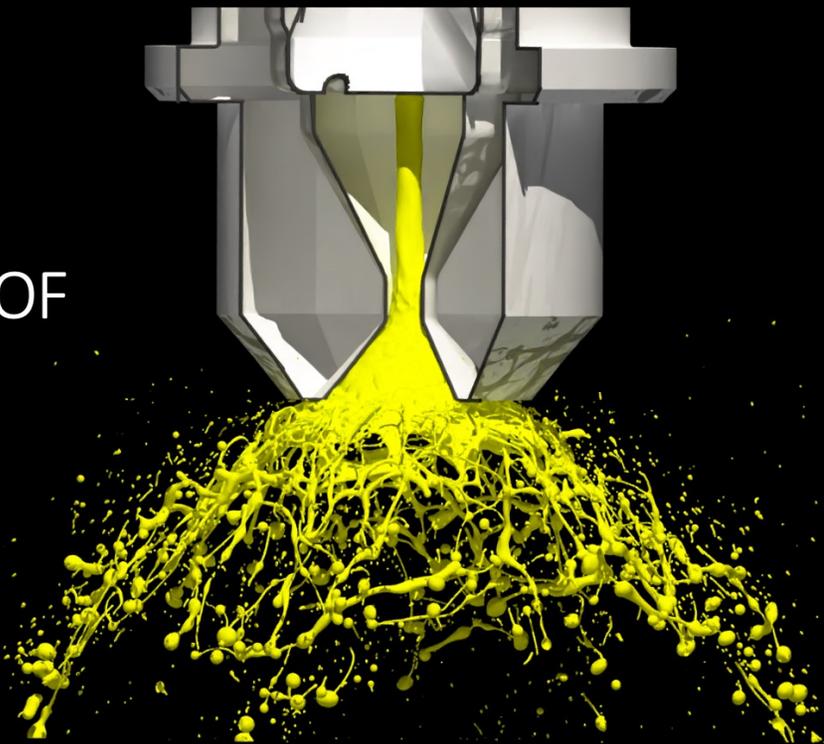
Liquid	$\rho_l$ (kg/m <sup>3</sup> )	$\mu_l$ (mPa · s)	$\sigma$ mN/m	Method	$\Delta$ ( $\mu$ m)
Water	1000	1.137	72.8	PLIC-NET	78, 39, 20, 16, 13
MIL-C	770	0.924	24	PLIC-NET, R2P	20

VOF enhanced  
with R2P film  
capturing

sub-grid film

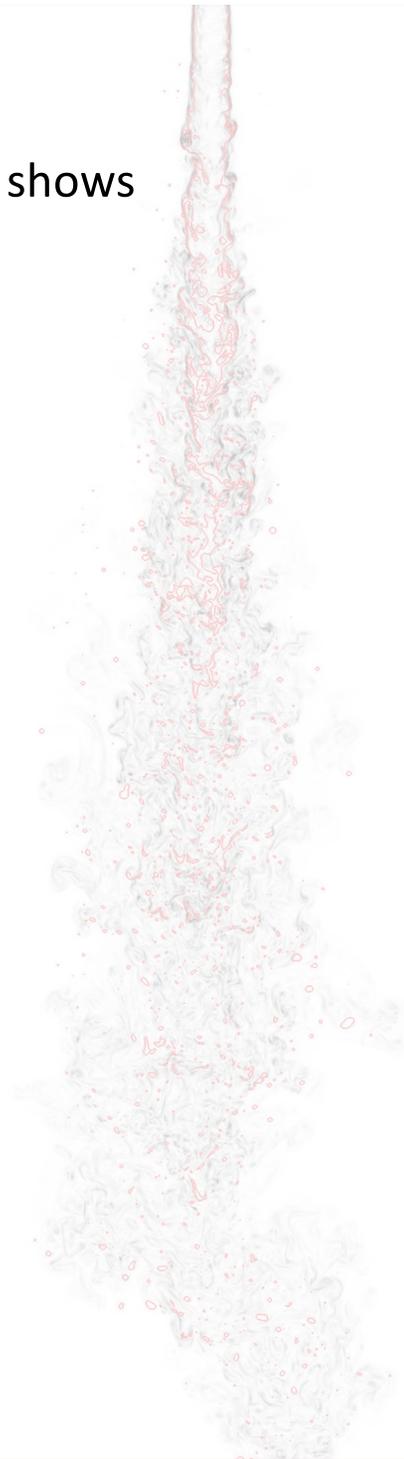
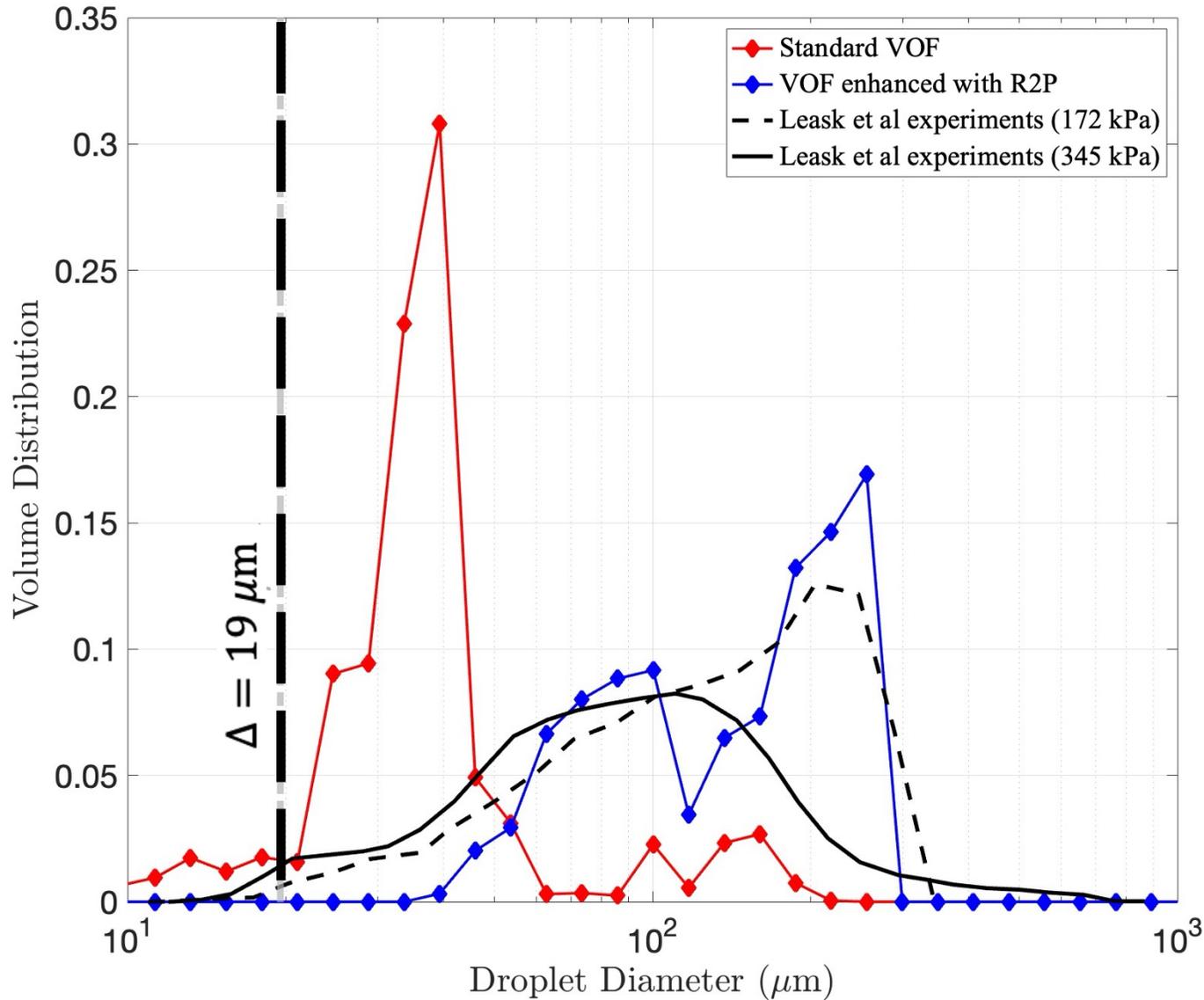


Standard VOF



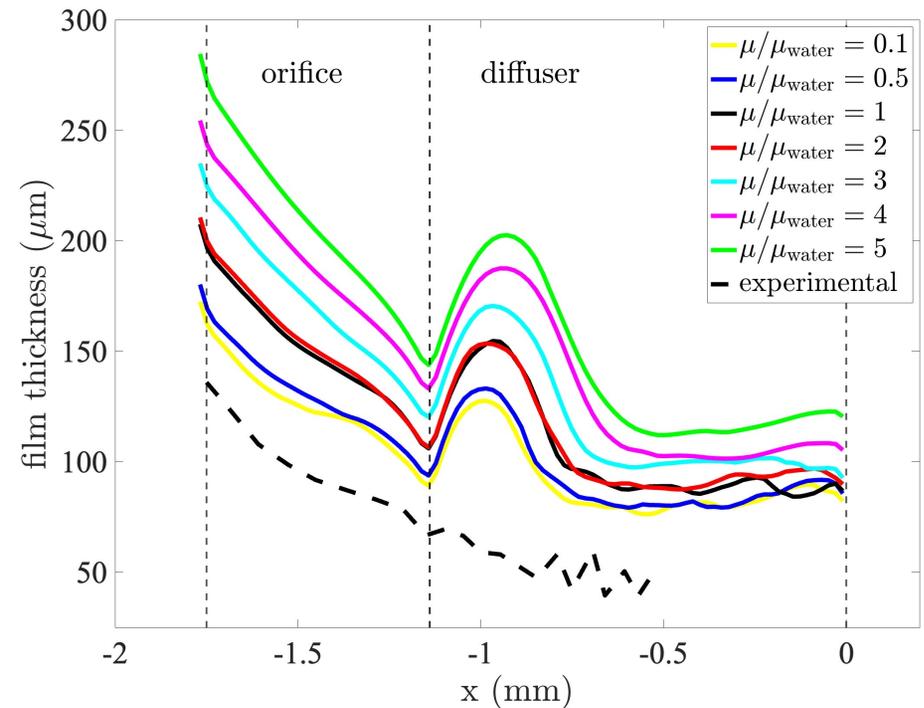
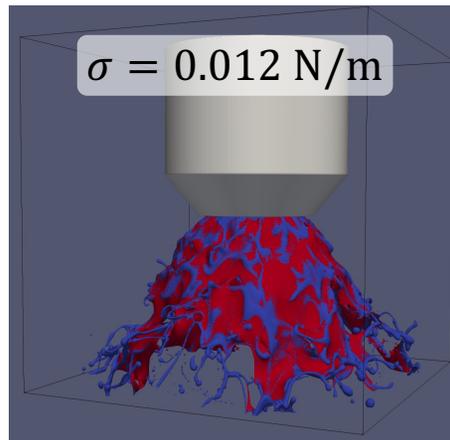
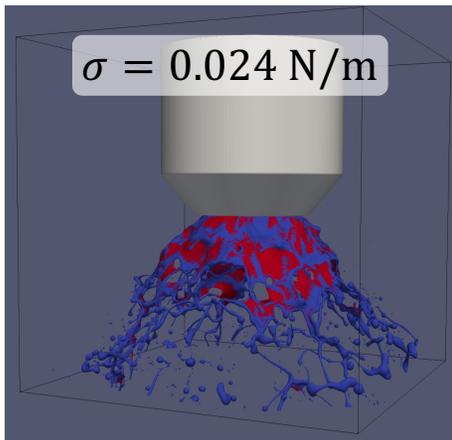
# RSA results – Drop sizes

- Our approach **captures well the drop size distribution**, while standard VOF shows accumulation of droplet diameter near mesh resolution



# Summary and perspectives

- Improvements to interface reconstruction methods **enable SGS capturing** of thin films and ligaments (soon!)
- **Volume-filtered framework** allows elucidating unclosed SGS terms
- Physics-informed models for **SGS film break-up and retraction** proposed and demonstrated in realistic simplex atomizer
- Results show **good qualitative & quantitative predictions**, although film thickness mismatch in the atomizer is under investigation
- **Effect of viscosity and surface tension** on film formation is being quantified



# Availability

- **Open-source software**

- Github for **NGA2** flow solver

<https://www.multiphasecf.com>

<https://github.com/desjardi/NGA2>

- Github for **IRL** VOF library

<https://github.com/robert-chiodi/interface-reconstruction-library>

- **Commercial software**

- With the help of Fausto Di Muzio (Nestlé), in discussion with Siemens/StarCCM+

