The Role of Linear Stability in Primary Atomization using High Fidelity Spray A Simulations

Arpit Agarwal & Prof. Mario F. Trujillo

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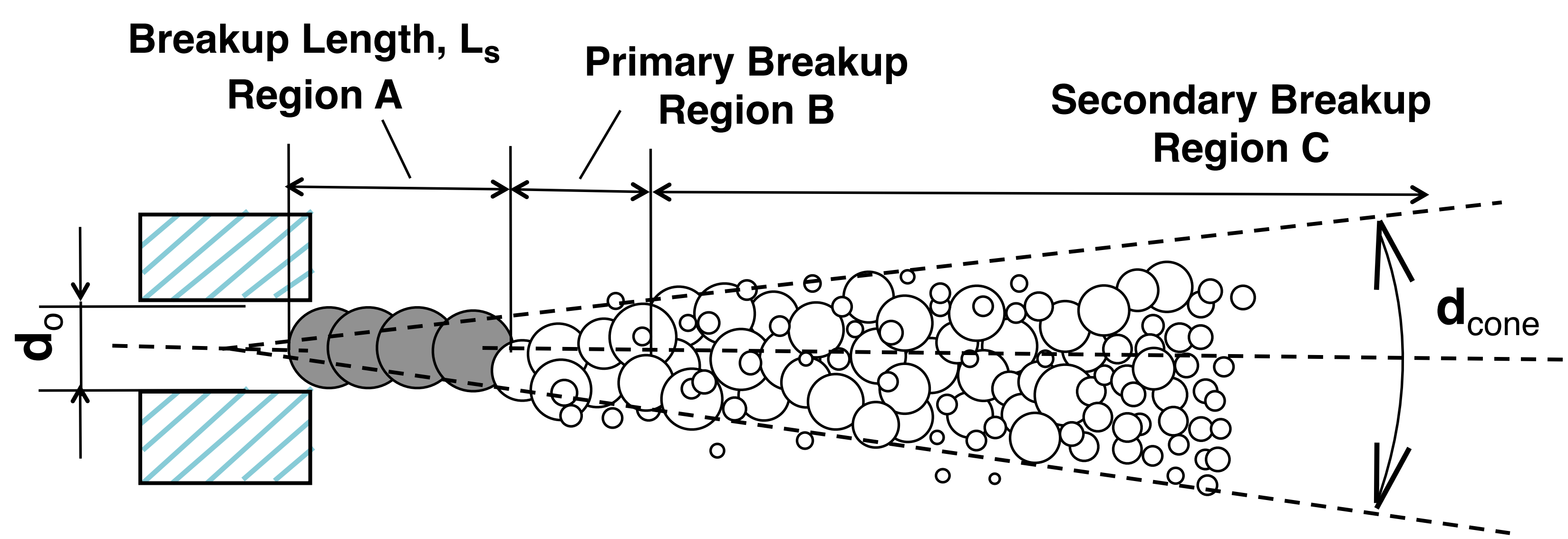
est 1946

Lag.-Eul. Spray Model Framework

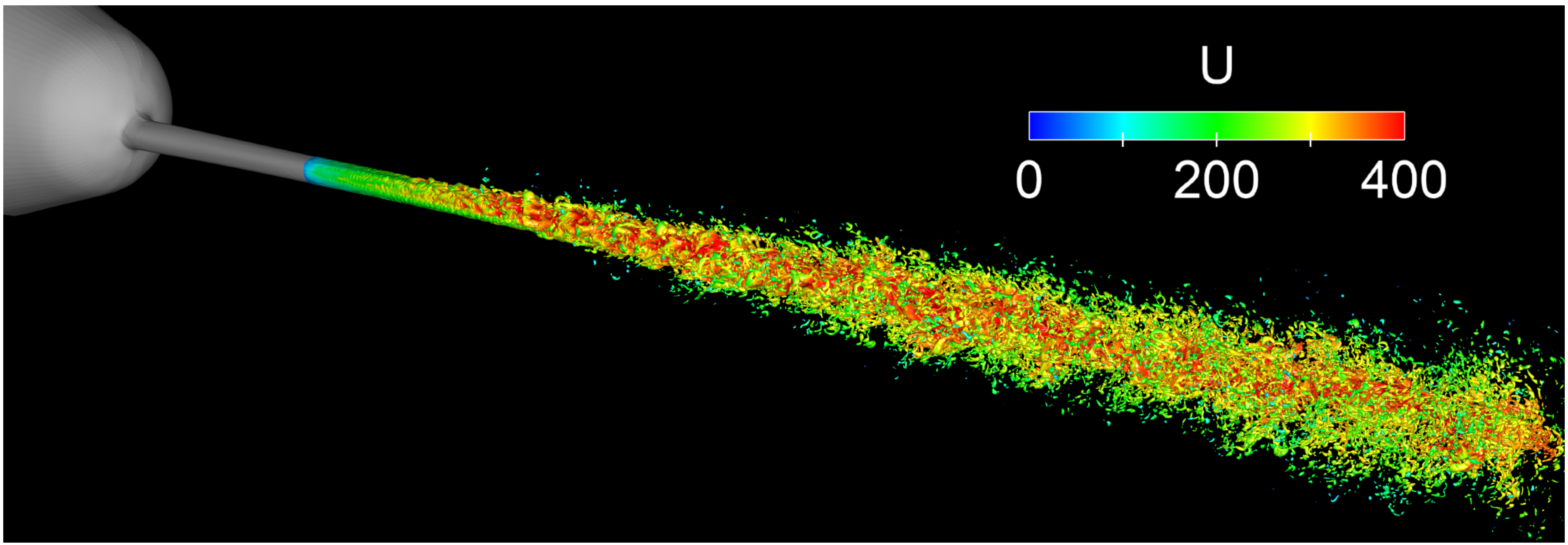
- Cascading effect of liquid breakup - SMDs, momentum coupling etc.
- Breakup usually completely unresolved - heavy reliance on models
- KH/RT models have dominated in the last 2-3 decades



- KH/RT and related models have problems; they are sensitive to: model constants, nozzle conditions, grid resolution, liquid properties

Interfacial instabilities: Three Aspects

- Extent of validity of linear-based instability theory (KH is a subset)
- Surface disturbances: Linear theory vs. VoF sims. in the near field
- Role of fastest & most violent modes and primary atomization



Revisiting models in lieu of high spatio-temporal resolution data

Outline

- Simulation Overview
  - Spray A geometry
  - Domain and Grid Setup, Grid stats
- Validation Exercise
  - Projected Mass Density Metrics
- Results
  - Metrics & Surface Disturbances
  - Implications for Primary Atomization
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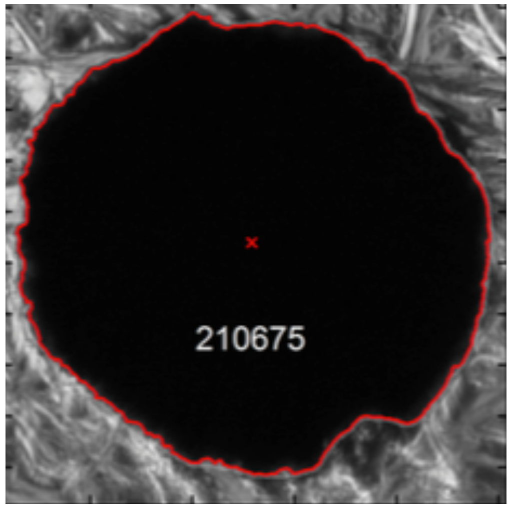
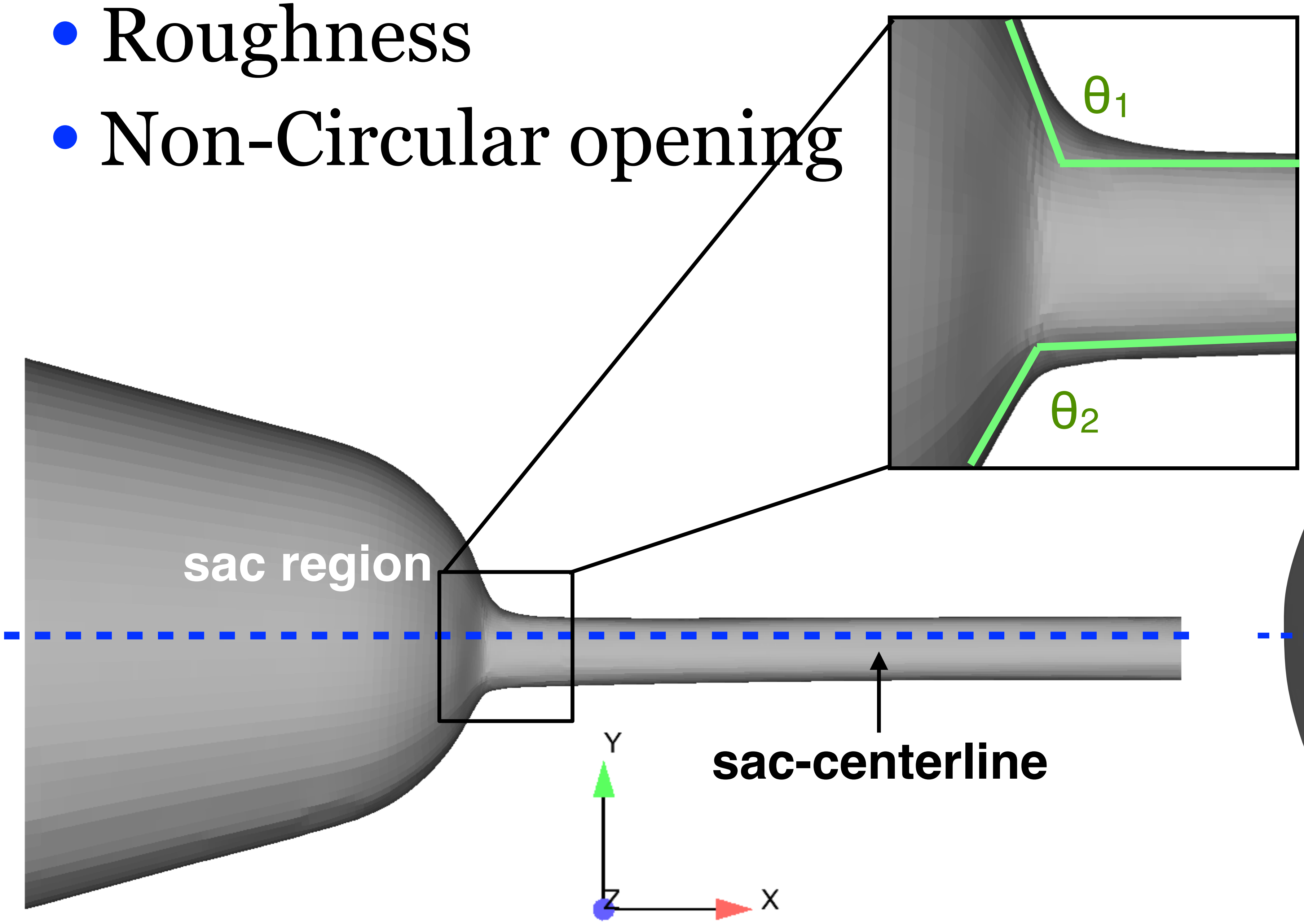
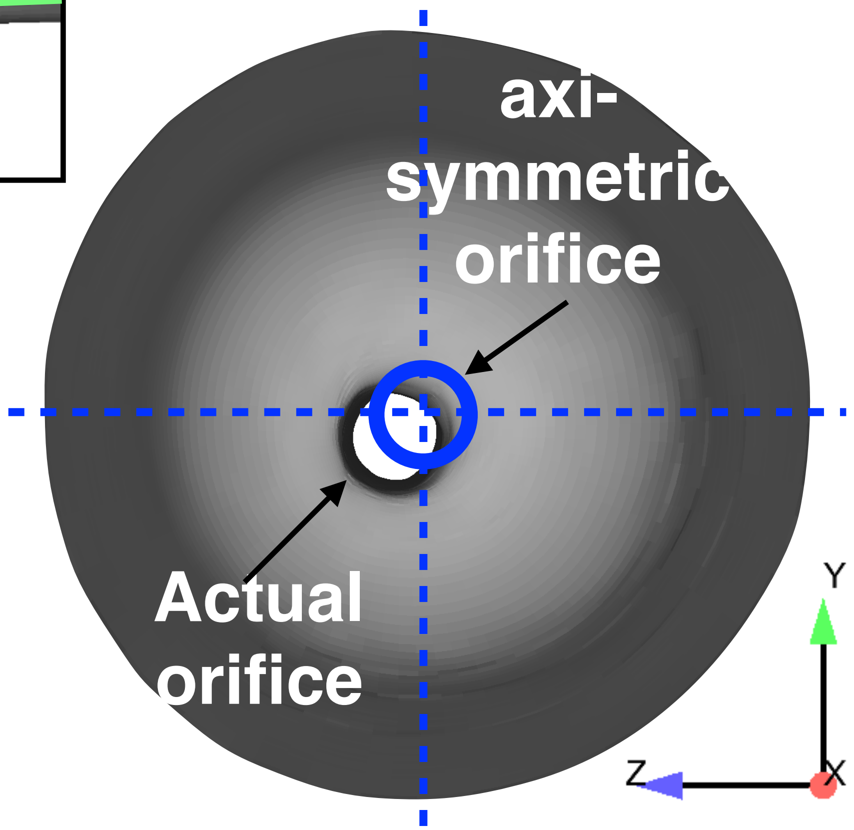
ECN SprayA - Asymmetries & Imperfections

- Off-center orifice
- Tapering orifice
- Roughness
- Non-Circular opening



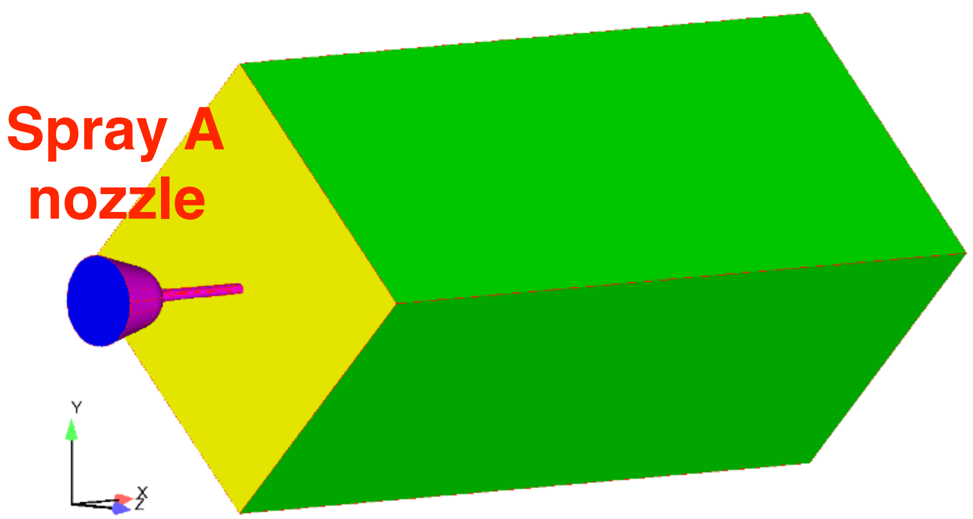
Optical scan of the orifice exit [1]

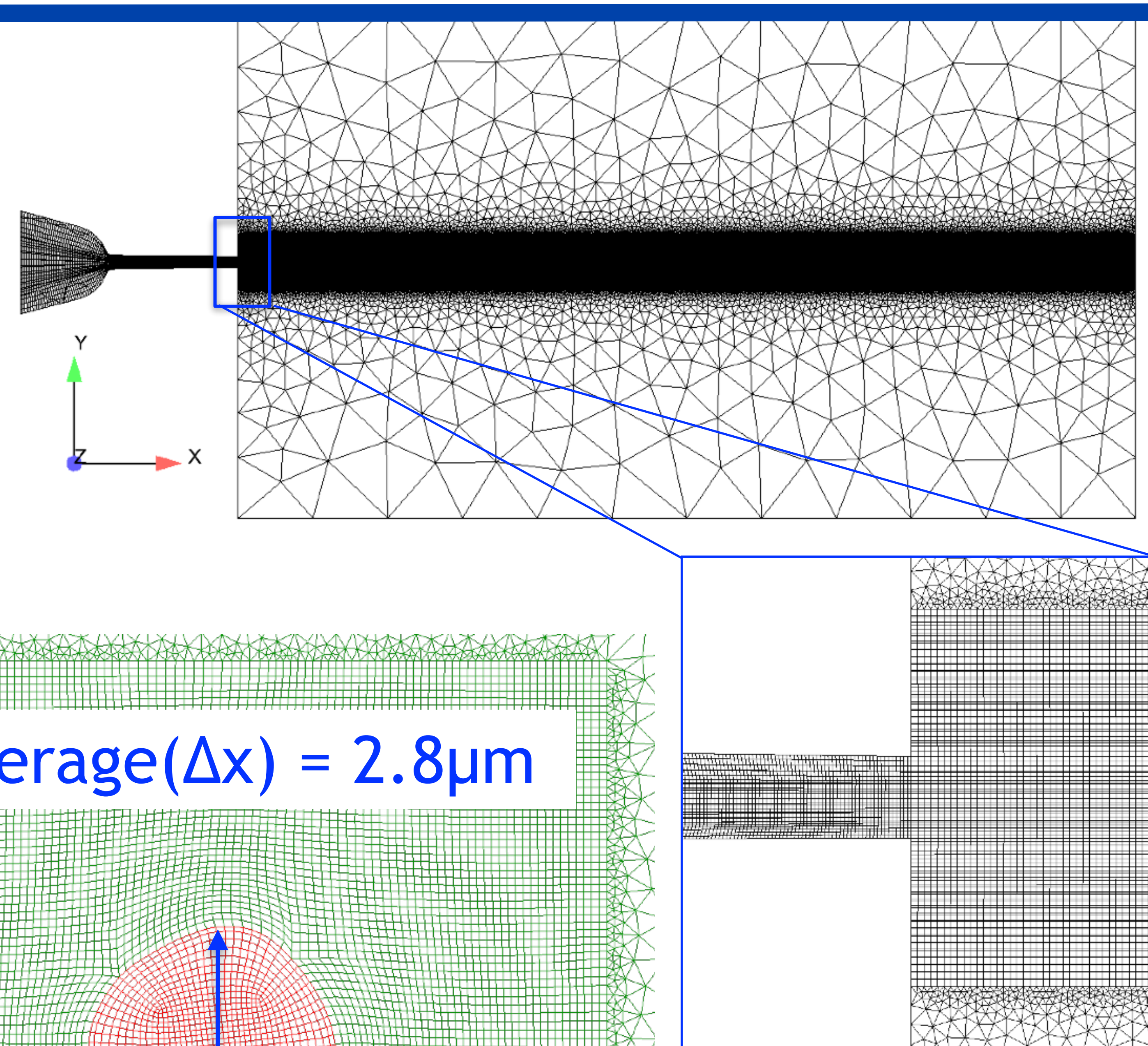


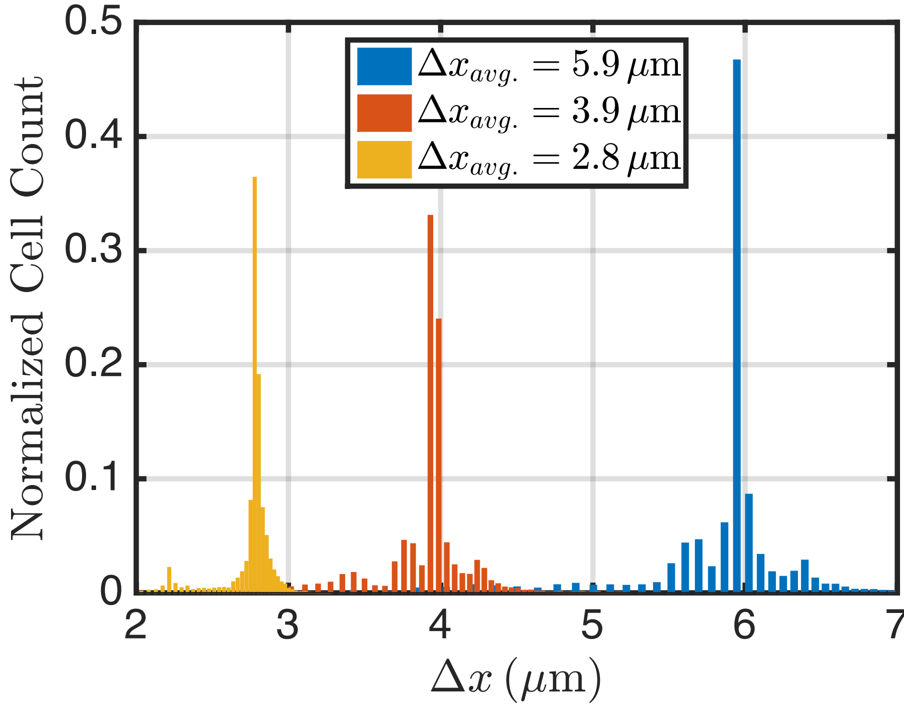


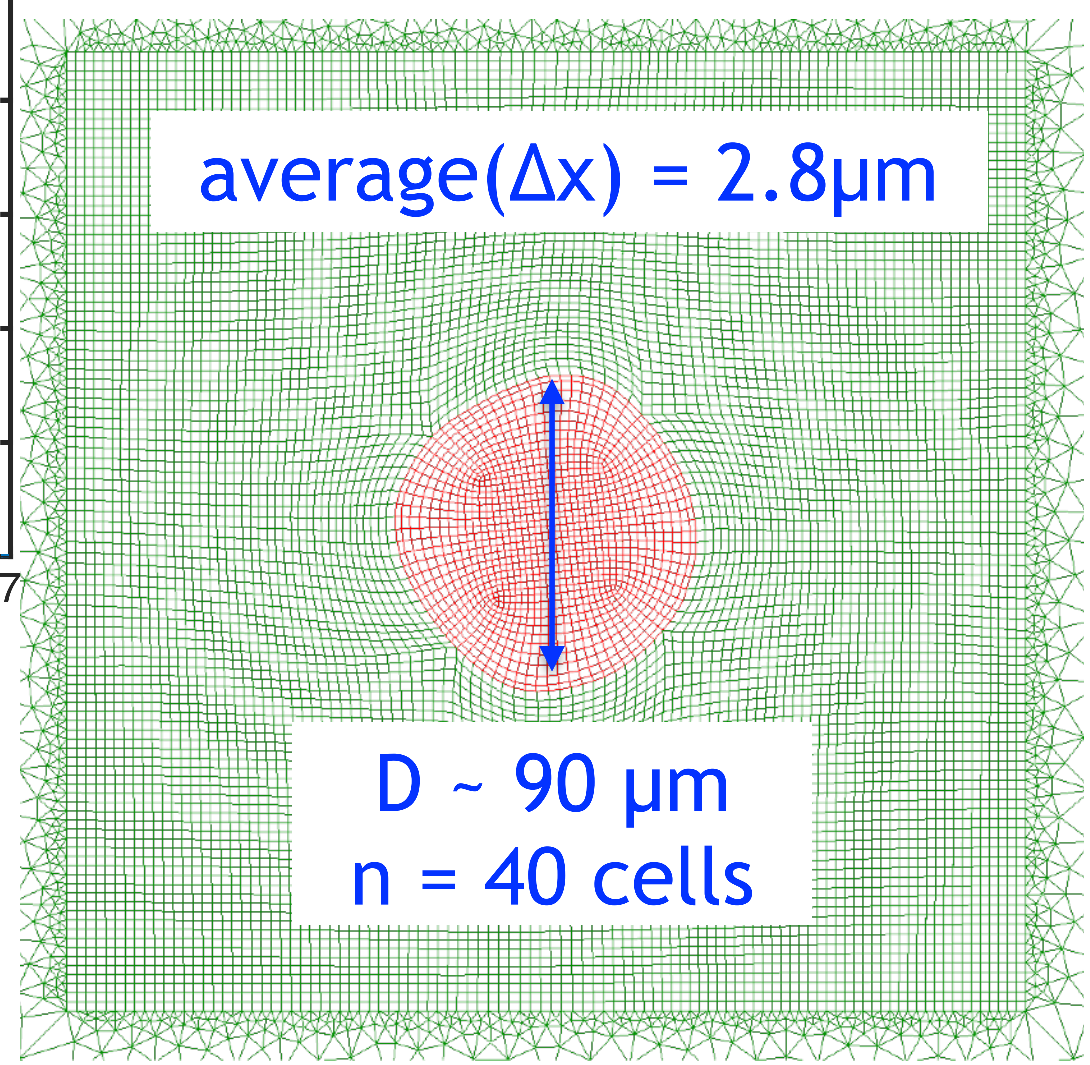
[1] Kastengren, Alan L., et al. Atomization and Sprays (2012).
[2] https://ecn.sandia.gov/diesel-spray-combustion/computational-method/meshes/

Boundary Fitted Grids: $\Delta x = 2.8\mu m$









- High quality, boundary fitted grid
- VoF simulations (`interFOAM`)
- No models

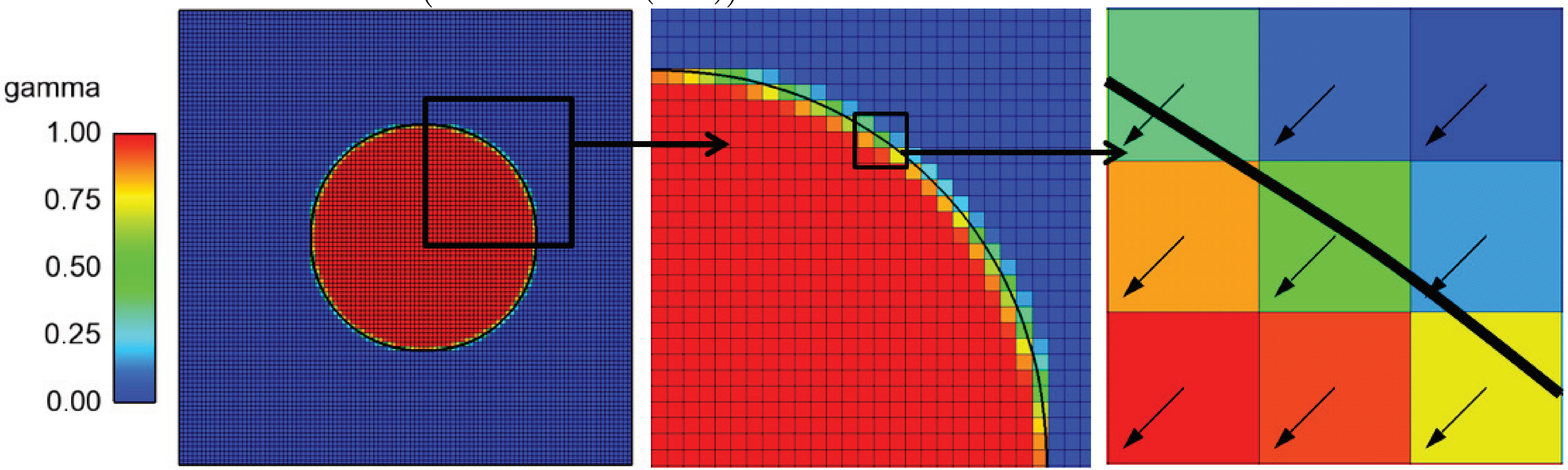
Algebraic VoF (aVoF) (interFoam [4,5])

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

$$\frac{\alpha_i^{n+1} - \alpha_i^n}{\Delta t} + \frac{1}{|\Omega_i|} \sum_{f \in \partial\Omega_i} (F_u + \lambda_M F_c) = 0$$

$$F_u = \phi_f \alpha_{f,upwind} \,, \quad \phi_f = \mathbf{u}_f \bullet \mathbf{S}_f \qquad F_c = \phi_f \alpha_{f,vanLeer} + \phi_{rf} \alpha_{rf} (1 - \alpha_{rf}) - F_u$$

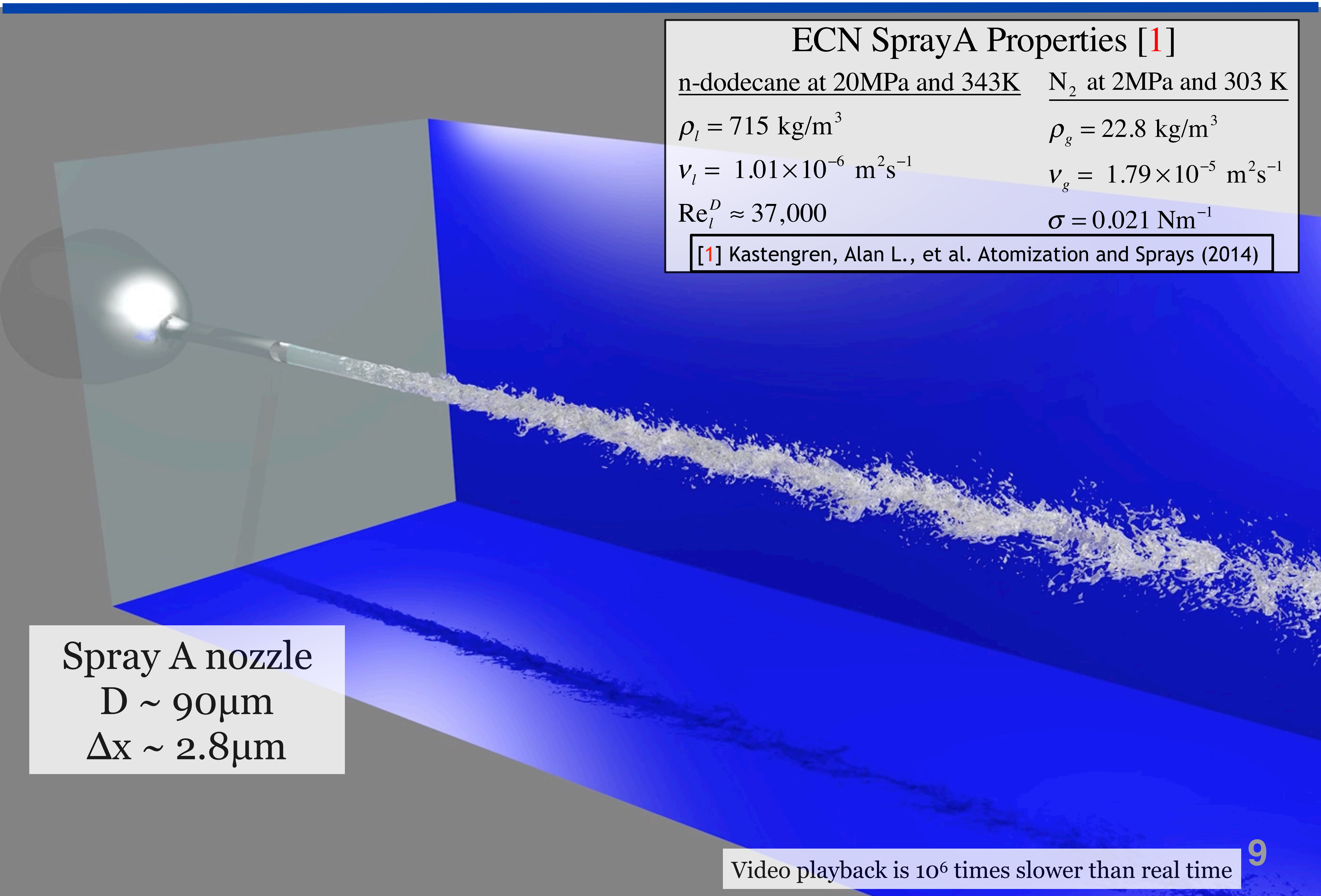
$$\text{with } \phi_{rf} = \min_{\Omega i}\left(C_\gamma \frac{|\phi_f|}{\mathbf{S}_f}, \max_{\Omega}\left(\frac{|\phi_f|}{\mathbf{S}_f} \right) \right) (\mathbf{n}_\Gamma \bullet \mathbf{S}_f) \quad \text{where } \mathbf{n}_\Gamma = \text{interface normal}$$



Original developers:
[1] Hrvoje Jasak, PhD Thesis, 1996
[2] Onno Ubbink, PhD Thesis, 1997
[3] Henrik Rusche, PhD Thesis, 2003

Documentation and testing:
[4] www.openfoam.org
[5] Deshpande, Anumolu, & Trujillo (Comput. Sci. Disc.,2012)

Illustration of the Spray



ECN SprayA Properties [1]

n-dodecane at 20MPa and 343K	N_2 at 2MPa and 303 K
$\rho_l = 715\ \text{kg/m}^3$	$\rho_g = 22.8\ \text{kg/m}^3$
$\nu_l = 1.01\times10^{-6}\ \text{m}^2\text{s}^{-1}$	$\nu_g = 1.79\times10^{-5}\ \text{m}^2\text{s}^{-1}$
$\text{Re}_l^D \approx 37{,}000$	$\sigma = 0.021\ \text{Nm}^{-1}$

[1] Kastengren, Alan L., et al. Atomization and Sprays (2014)

Spray A nozzle
D ~ 90μm
Δx ~ 2.8μm

Video playback is 10^6 times slower than real time

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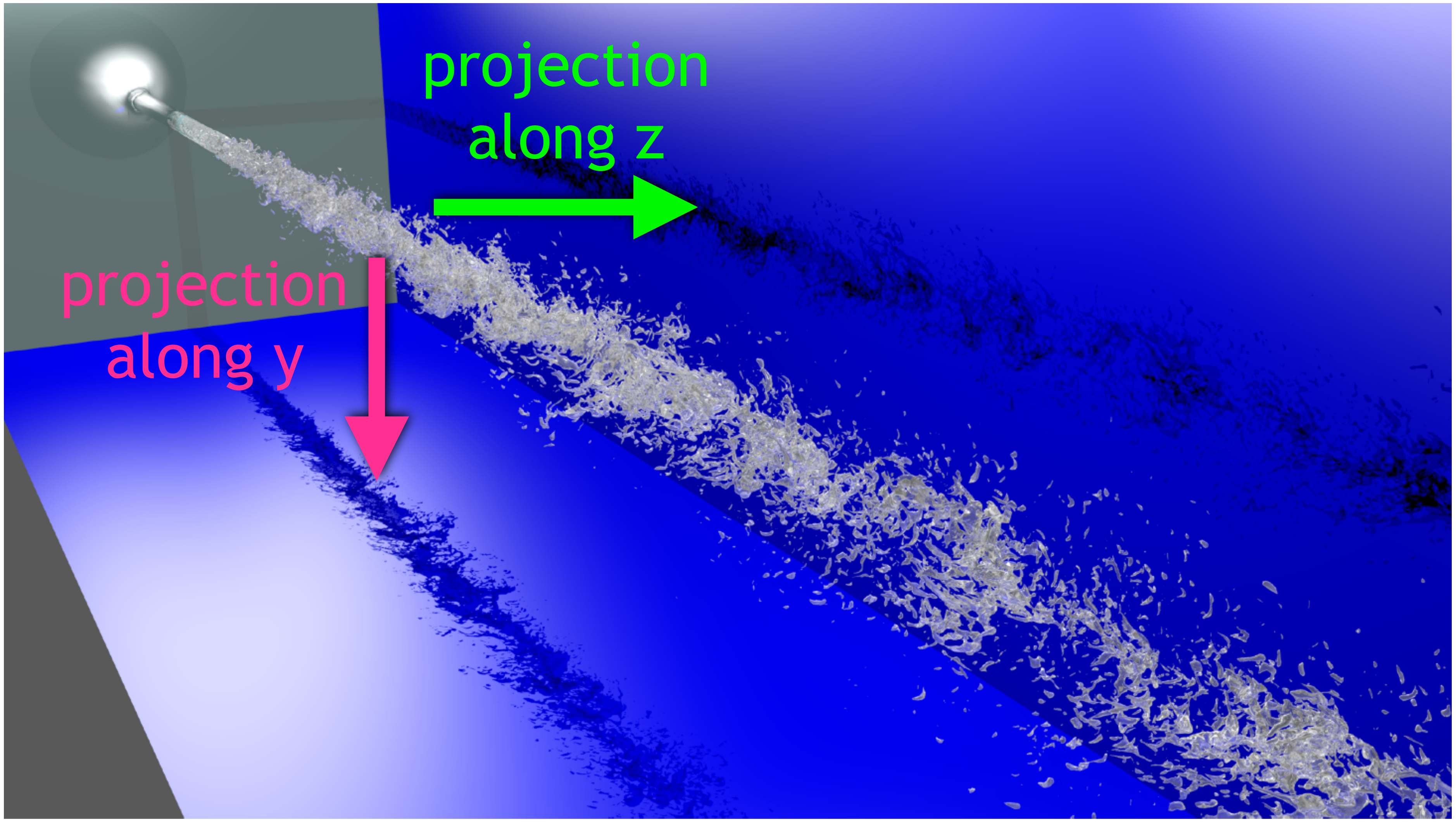
Experimental Validation

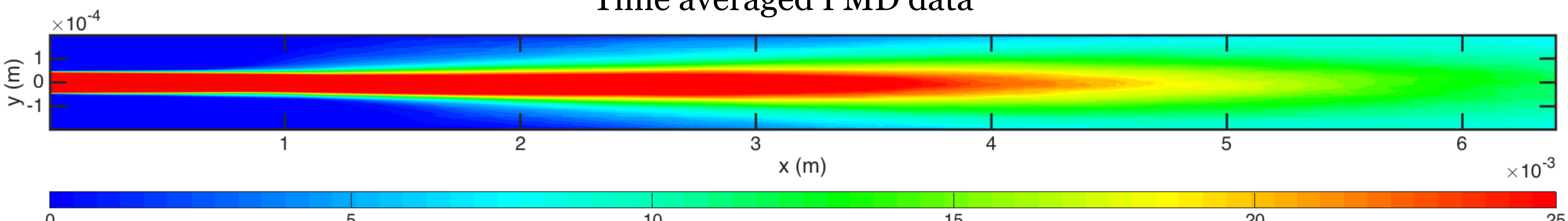


Projected Mass Density:

$$\Phi(z,x) = \rho_l \int_{-\infty}^{\infty} \langle \alpha(x,y,z) \rangle dy$$

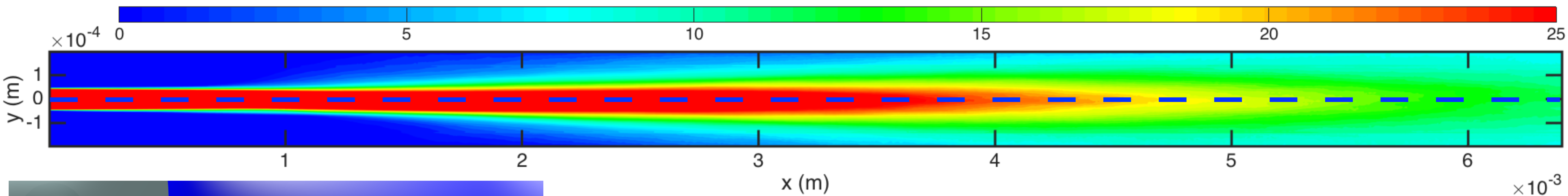
$$\Phi(y,x) = \rho_l \int_{-\infty}^{\infty} \langle \alpha(x,y,z) \rangle dz$$

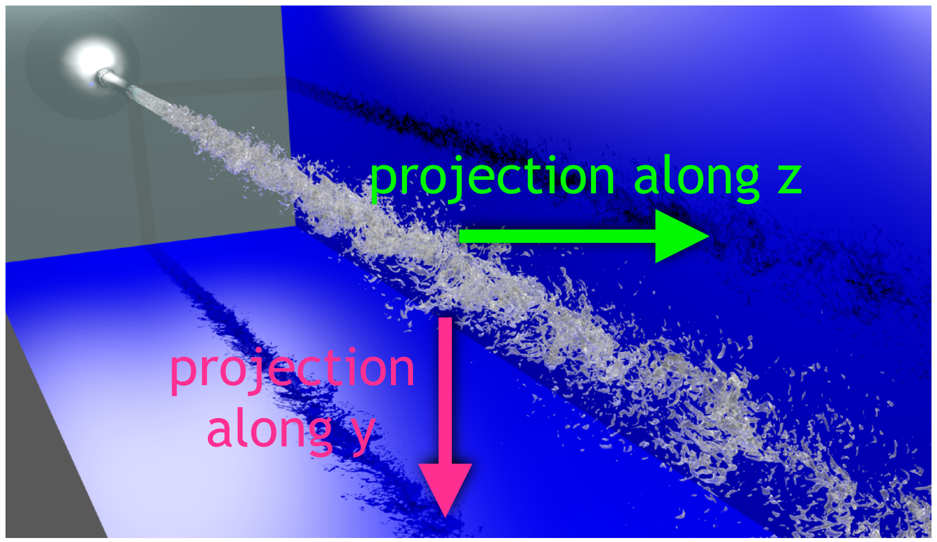
Time averaged PMD data

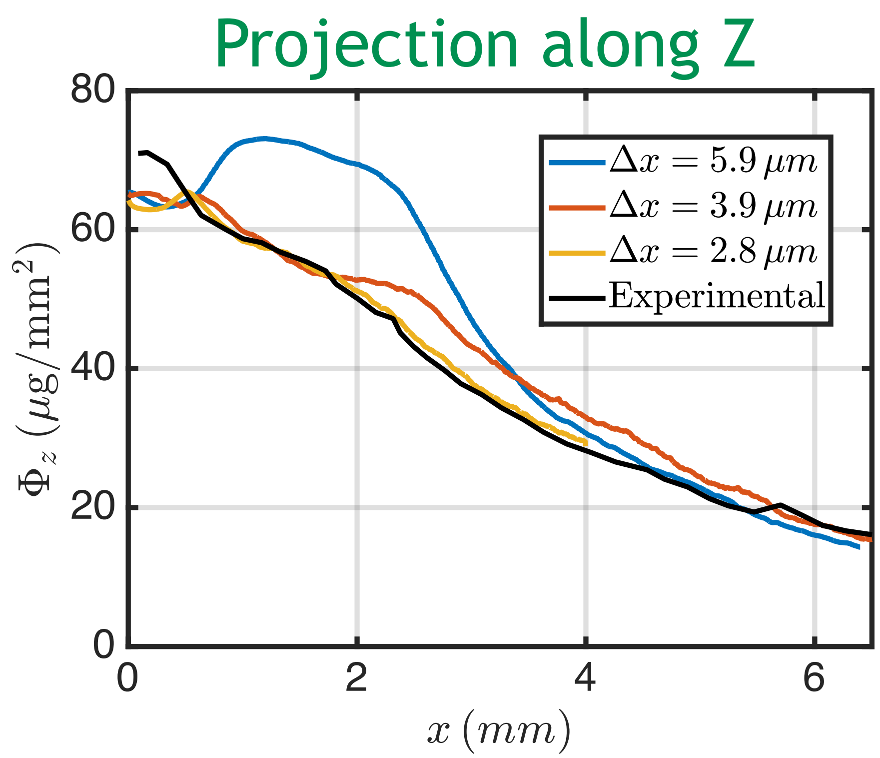


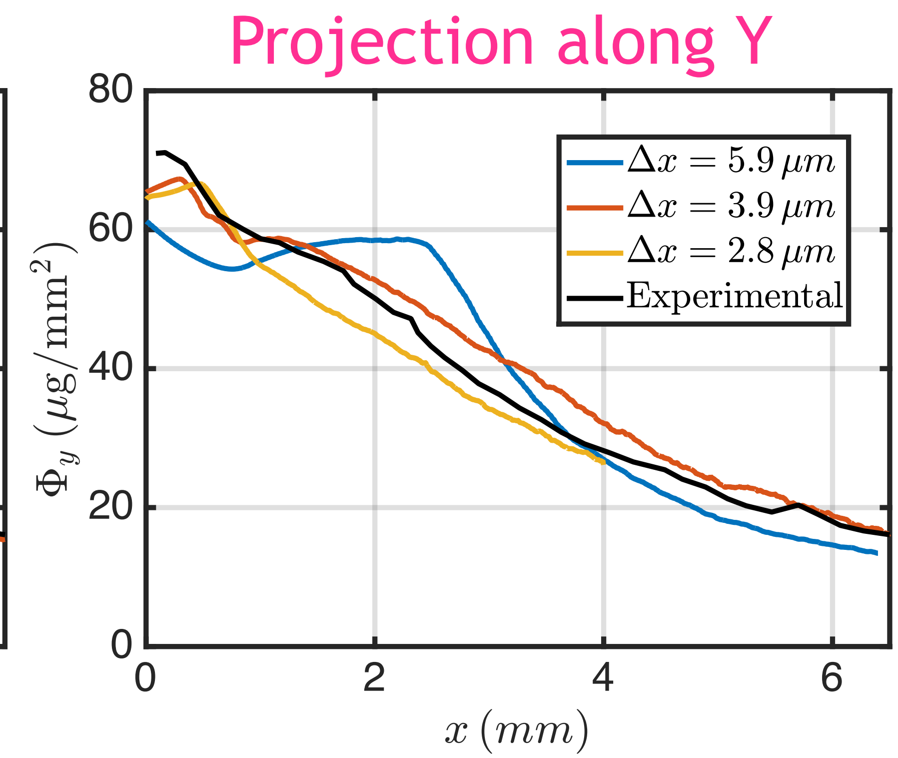
Time averaging:
$t_0 = 25\mu s;\ t_f = 50\mu s$

Experimental Validation









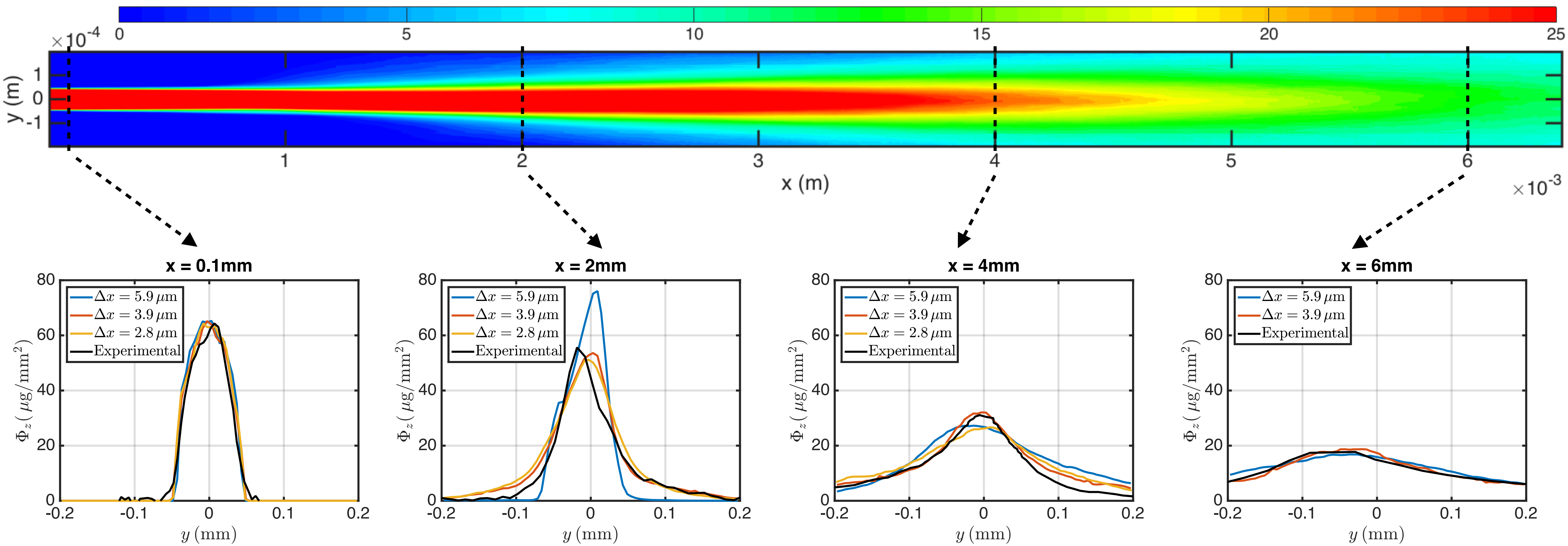
Error Values

Δx	φ_z	φ_y
5.9 µm	10.7%	7.3%
3.9 µm	4.4%	3.5%
2.8 µm	2.0%	5.0%

- Asymmetric spray - Different projections give slightly different mass density values
- Asymmetry extensively reported in literature as well
- Decent agreement for finer grids

[1] Kastengren, Alan L., et al. ICLASS Paper (2012)
[2] Kastengren, Alan L., et al. Atomization and Sprays (2014)

Experimental Validation



Error Values				
Δx	**x = 0.1mm**	**x = 2mm**	**x = 4mm**	**x = 6mm**
5.9 μm	4.7%	7.7%	5.2%	1.7%
3.9 μm	3.8%	3.7%	2.5%	1.1%
2.8 μm	3.9%	4.6%	4.0%	-

- Accurate liquid mass distribution - indicates that flow profile is captured well in the simulations

[1] Kastengren, Alan L., et al. ICLASS Paper (2012).
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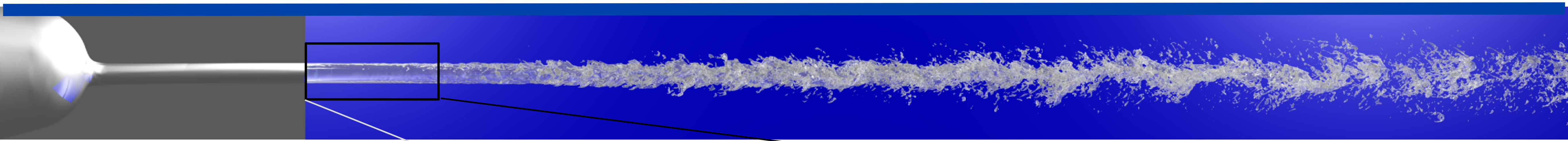
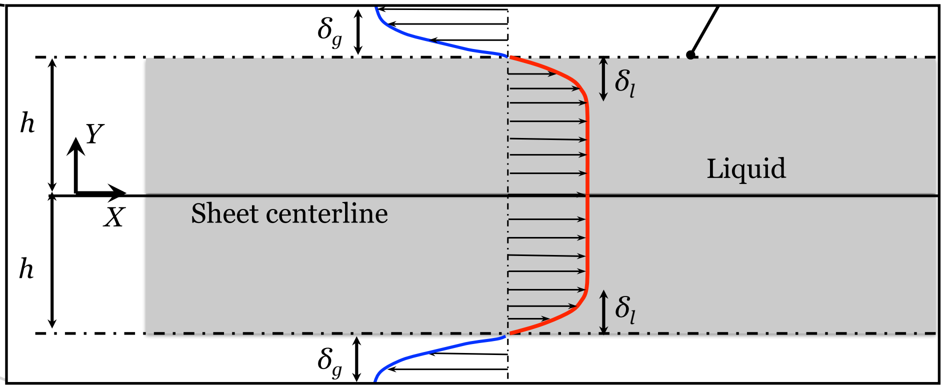
Three Assumptions in Linear Theory





N.S. Momentum Equation

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} + \tilde{\mathbf{U}}\cdot\nabla\tilde{\mathbf{U}} = -\frac{1}{\rho}\nabla\tilde{P} + \nu\nabla^2\tilde{\mathbf{U}}$$

↓

Velocity Decomposition

Substitute $\tilde{\mathbf{U}} = \mathbf{U} + \mathbf{u}$ and $\tilde{P} = P + p$

$$\underbrace{\left(\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U}\cdot\nabla\mathbf{U} + \frac{\nabla P}{\rho} - \nu\nabla^2\mathbf{U}\right)}_{=0\ \because\ \text{base flow satisfies momentum equation}} + \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{U}\cdot\nabla\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{U} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\frac{\nabla p}{\rho} + \nu\nabla^2\mathbf{u}$$

↓

Perturbation Mom. Eqn.

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{U}\cdot\nabla\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{U} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u}$$

↓

Simplifying Assumptions

- Perturbation Velocity: Perturbations are small $\therefore$ non-linear terms are negligible
- Base Velocity:
  - Base velocity is completely streamwise (V=W=0)
  - Base velocity is fully developed in x $\left(\frac{\partial U}{\partial x} = 0\right)$

↓

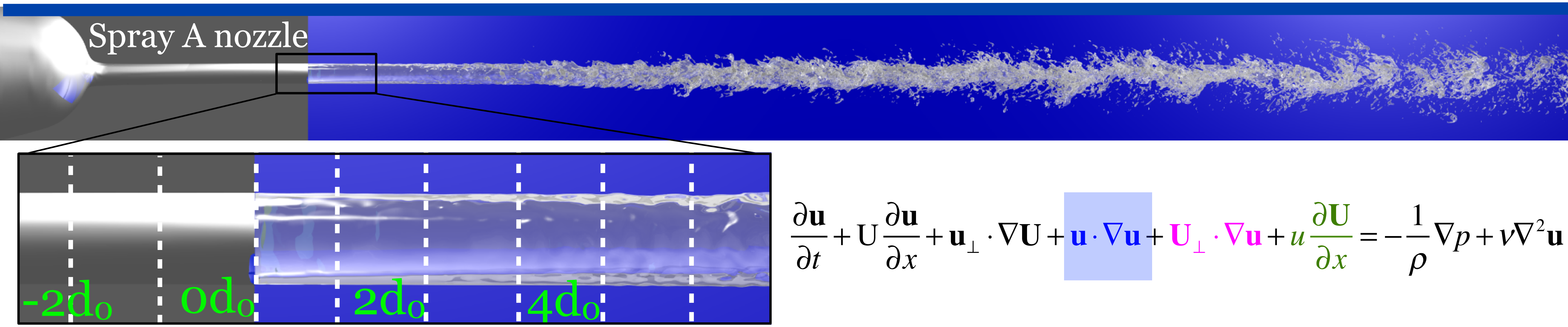
Expanded Perturbation Mom. Eqn.

$$\frac{\partial \mathbf{u}}{\partial t} + \underbrace{U\frac{\partial \mathbf{u}}{\partial x} + \mathbf{u}_\perp\cdot\nabla U}_{\text{advection terms present in the conventional system}} + \underbrace{\left(\mathbf{u}\cdot\nabla\mathbf{u} + \mathbf{U}_\perp\cdot\nabla\mathbf{u} + u\frac{\partial \mathbf{U}}{\partial x}\right)}_{\text{Advection terms ignored in the conventional system}} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u}$$

↓

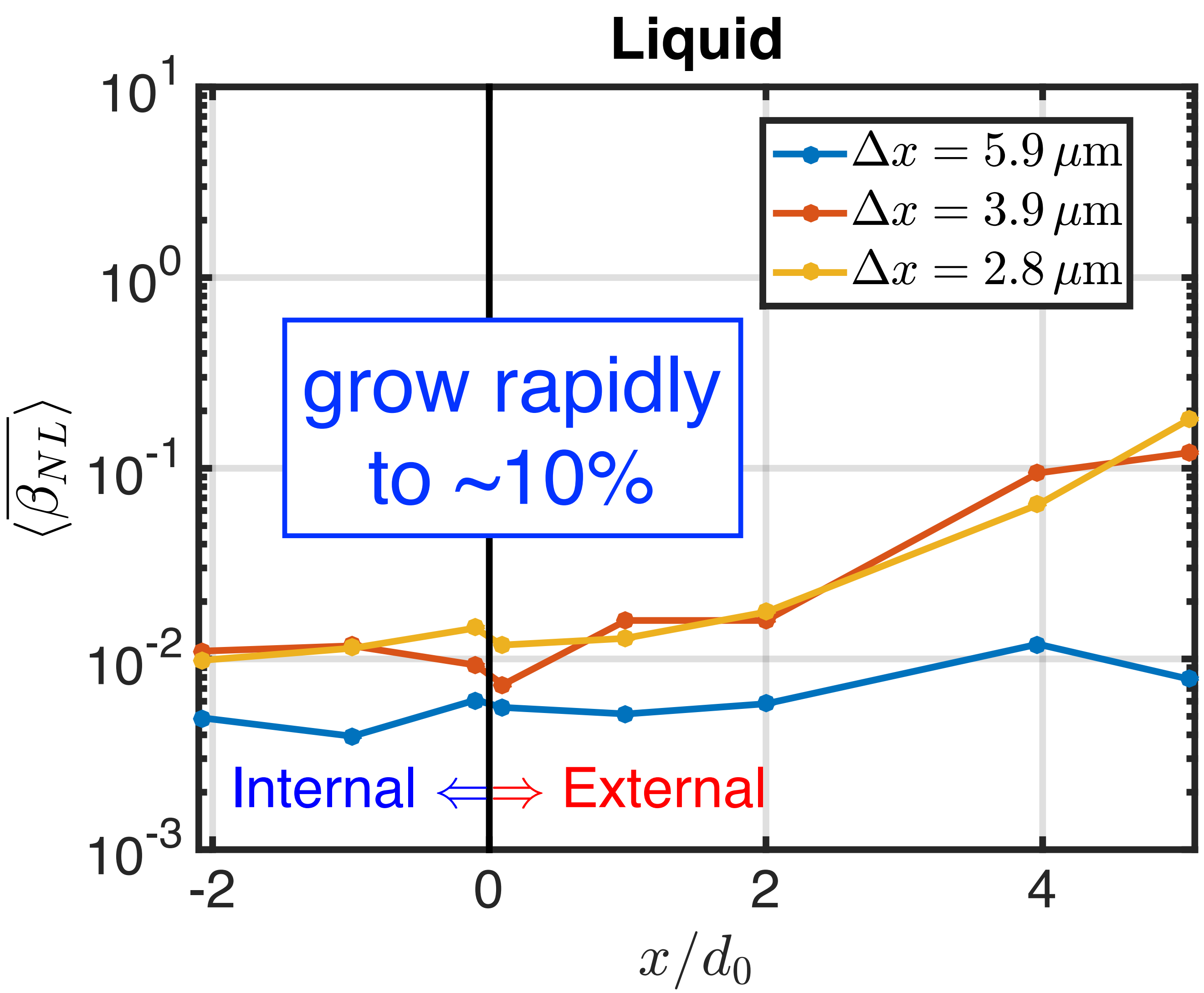
Orr-Sommerfeld Equation → **Impose solution form** → **Identify dominant modes** → **KH/RT model(s)**

Extent of Validity of Linear Theory



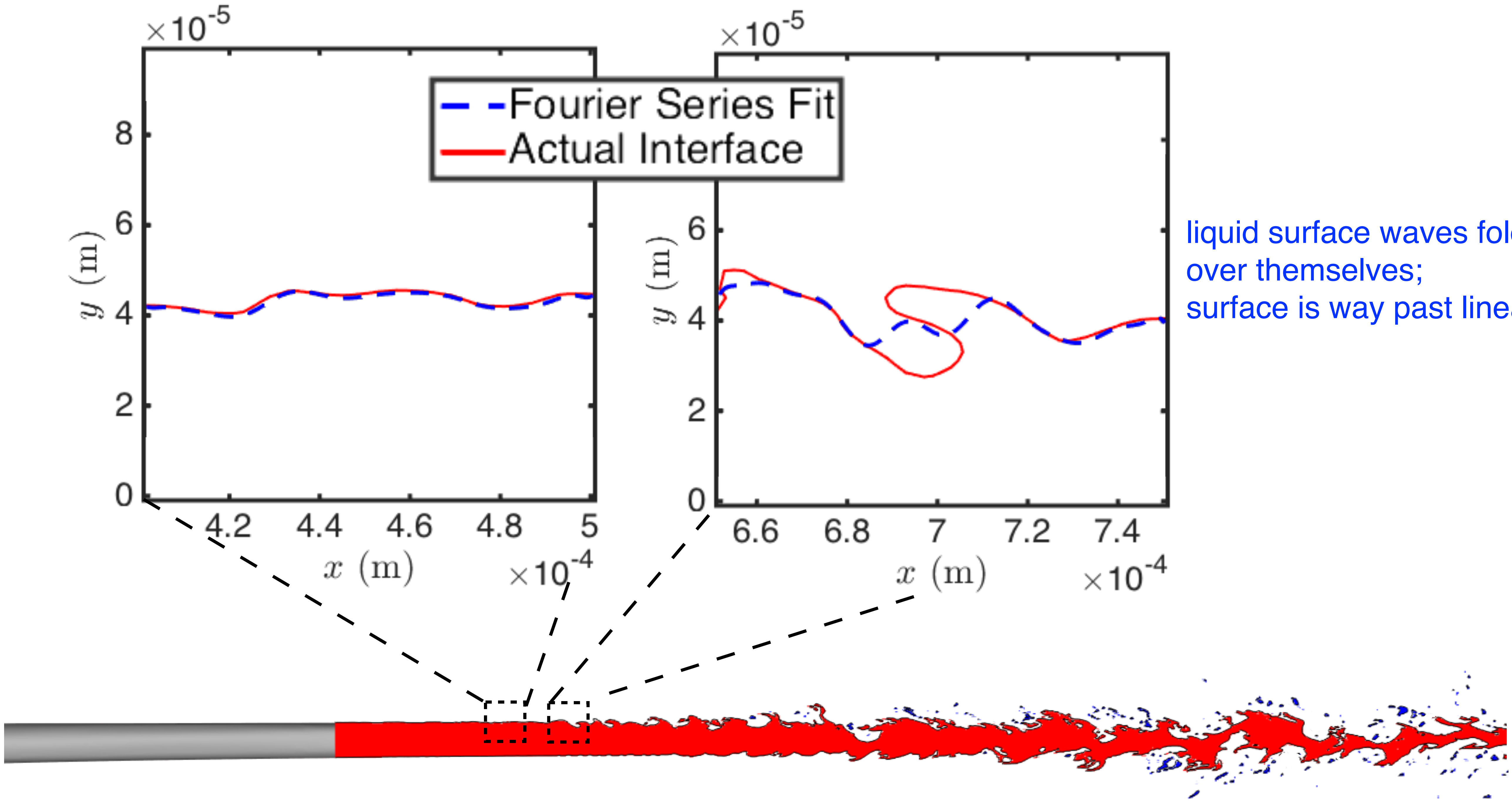
$$\frac{\partial \mathbf{u}}{\partial t} + U\frac{\partial \mathbf{u}}{\partial x} + \mathbf{u}_{\perp}\cdot\nabla\mathbf{U} + \mathbf{u}\cdot\nabla\mathbf{u} + \mathbf{U}_{\perp}\cdot\nabla\mathbf{u} + u\frac{\partial \mathbf{U}}{\partial x} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u}$$

Non-linear perturbation terms



- Strong, exponential growth in non-linearities
- Assumptions may not be valid beyond $5d_o$

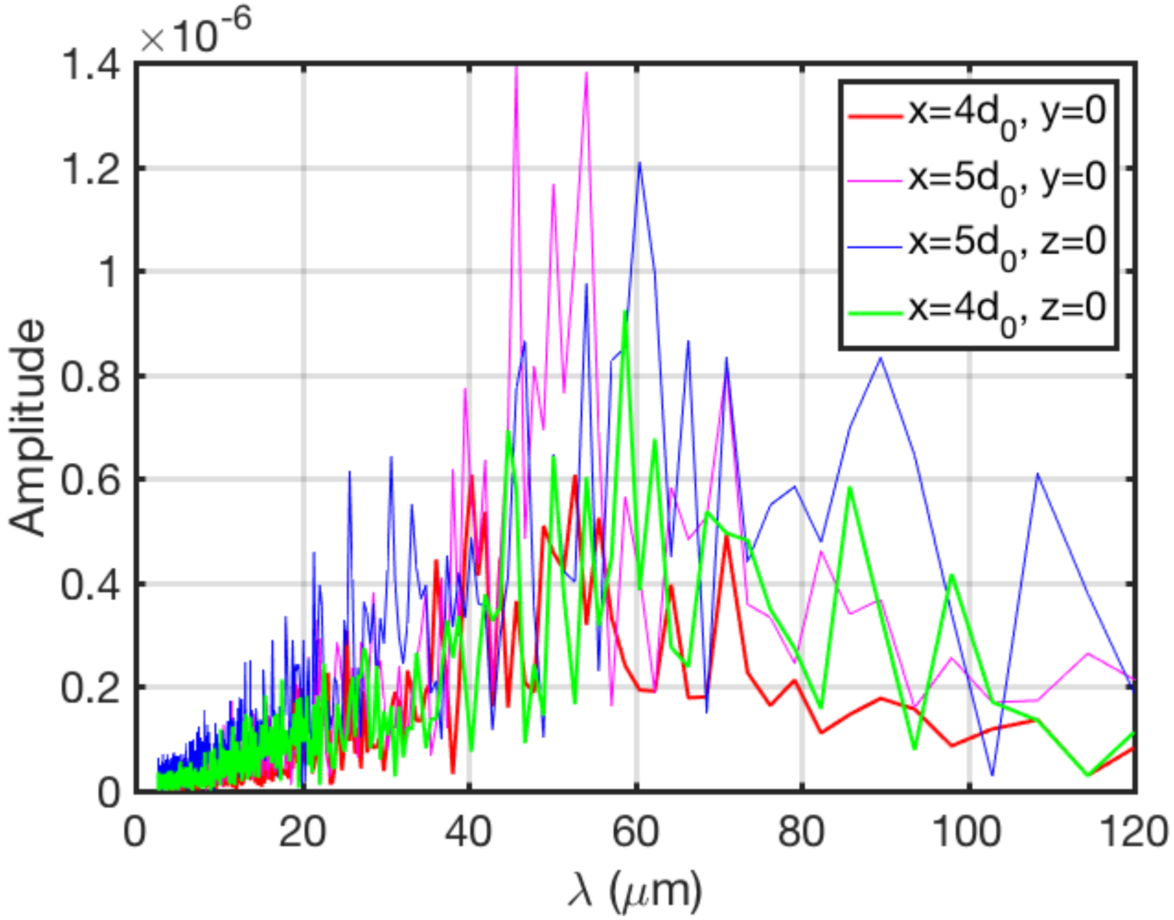
Quick Departure of Surface from Linear Prescription



liquid surface waves fold over themselves; surface is way past linearity

- Surface becomes non-linear very early ($x \cong 7d_o$)

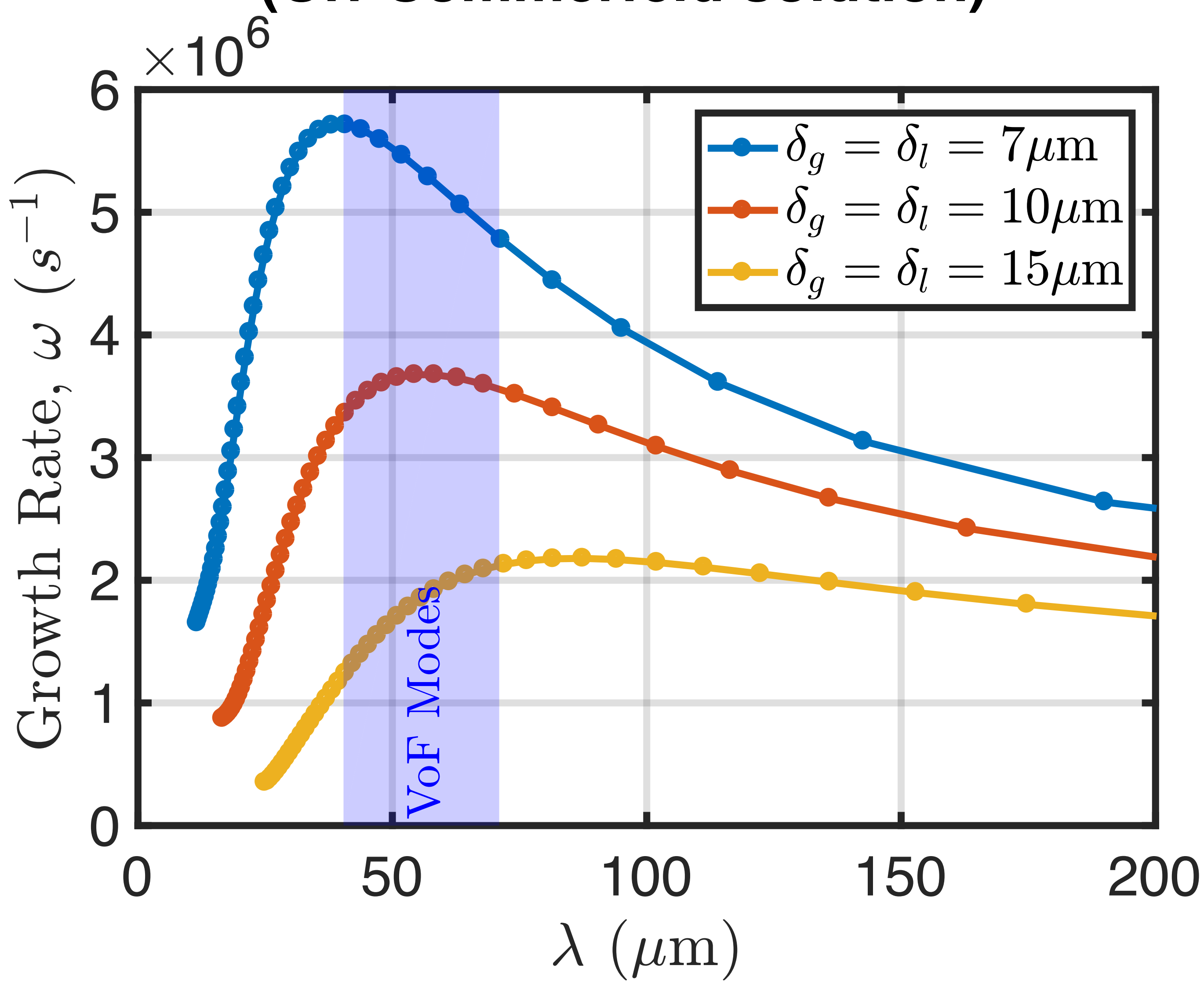
VoF Perturbations vs. Linear Theory Prediction



Disturbance modes in VoF simulations

- $\lambda = {U_\xi}/{freq.}$,where $U_\xi \cong 412$ m/s

Disturbance modes from linear stability theory (Orr Sommerfeld solution)



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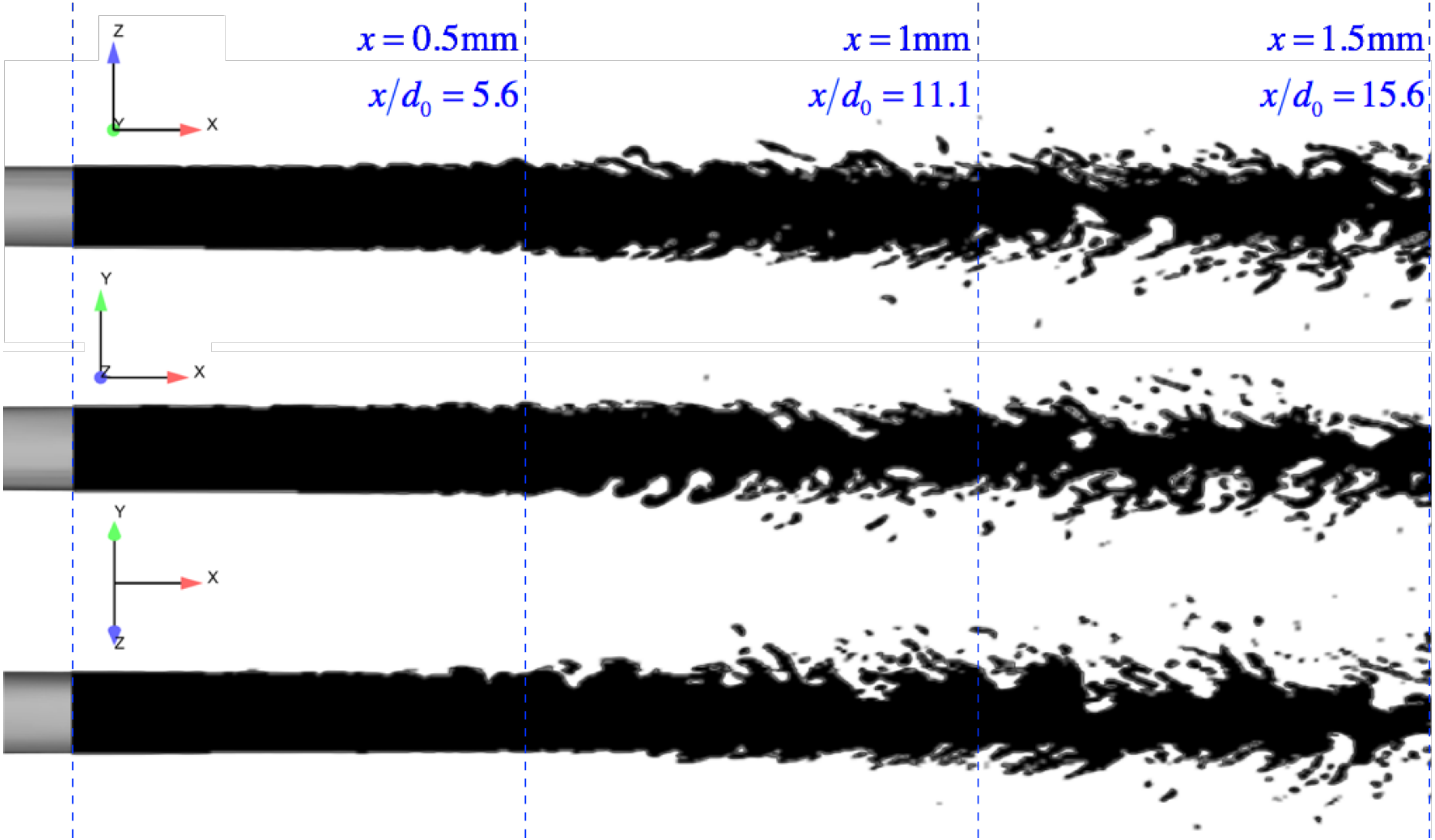
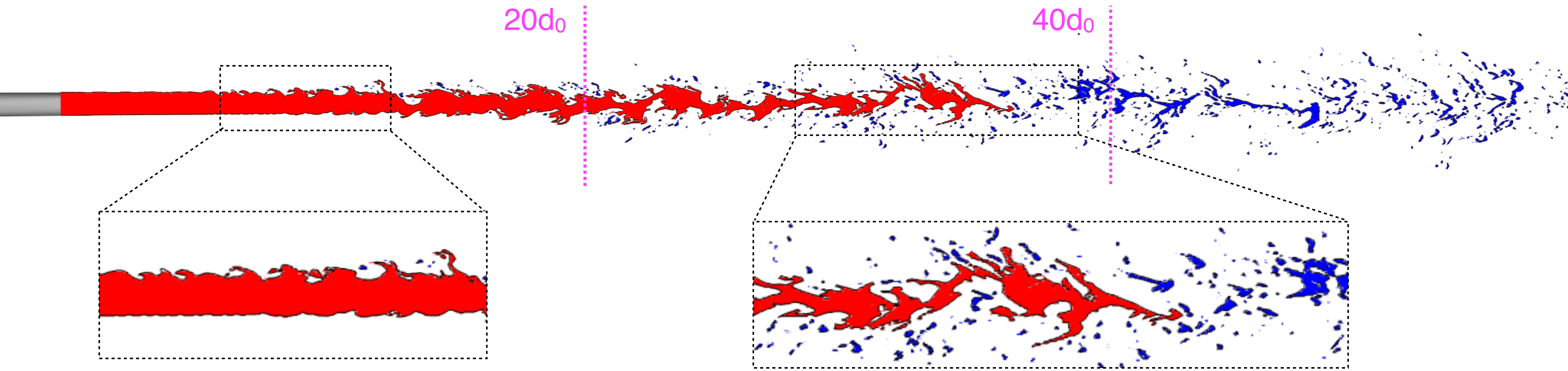
Instability limited to stripping of surface



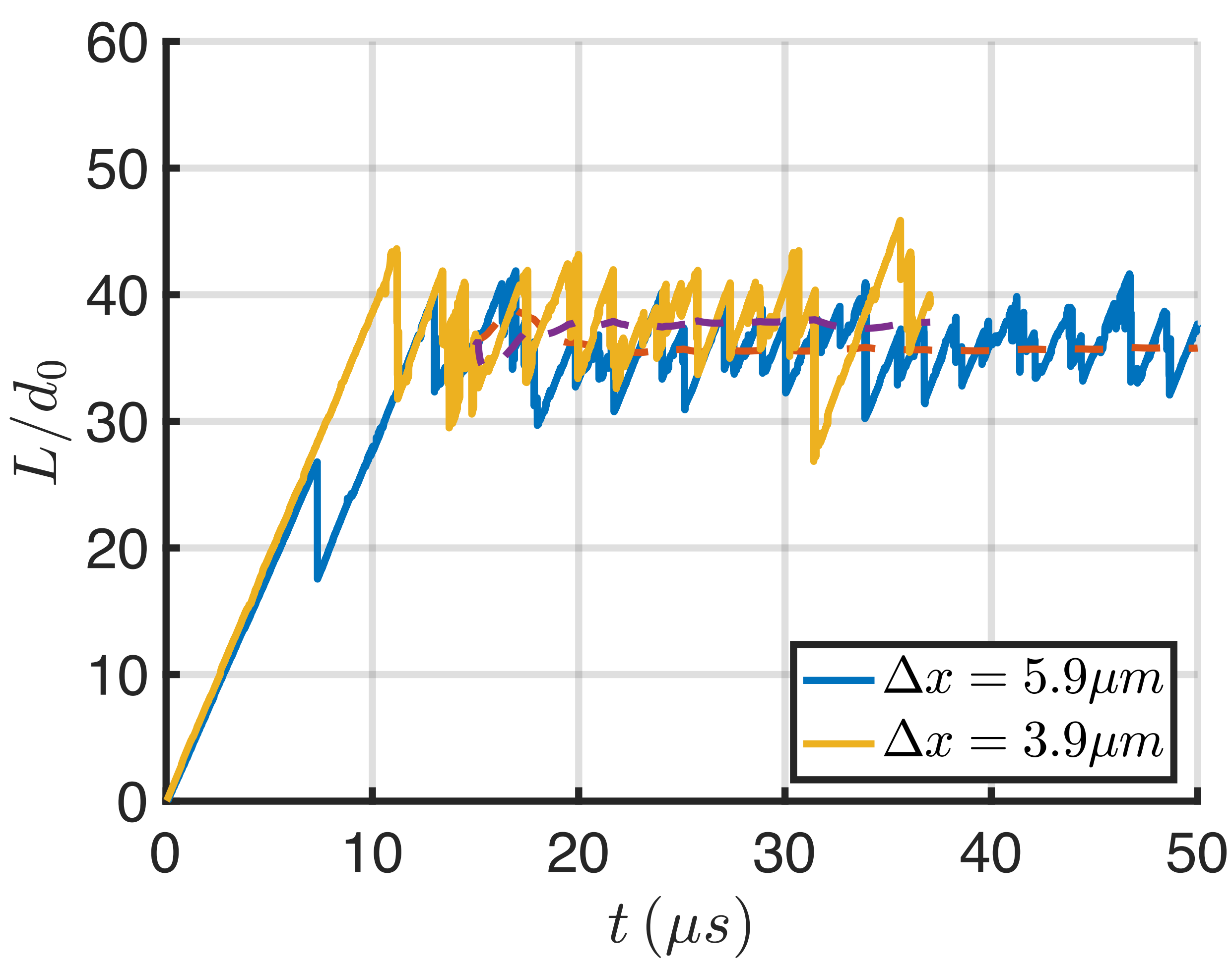
- Action of surface instability is limited to stripping of the surface
- Core of the fluid column remains unperturbed for much longer (15 diameters)

Do Surface Disturbances Cause Primary Atomization?



Surface breakup; core undisturbed

Liquid core severed



- Breakup happens in the form of large-scale oscillations about $30d_0$ downstream of surface breakup
- Surface disturbances may not be directly responsible for destruction of liquid core [1, 2]

[1] Deshpande, Gurjar, Trujillo (2015). Physics of Fluids
[2] Marmottant, Villermaux (2004) Journal of Fluid Mechanics

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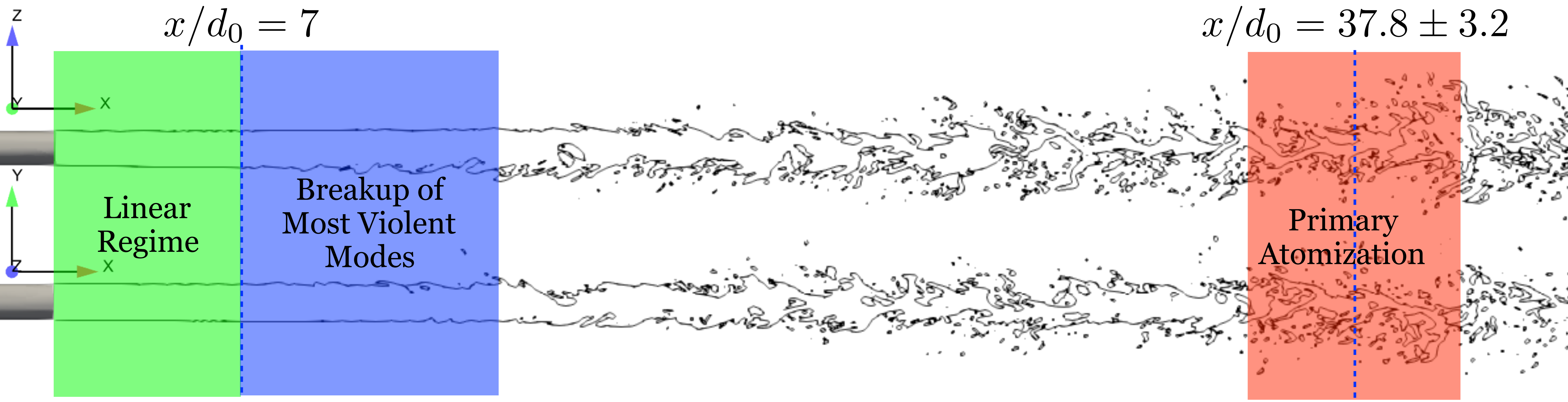
Conclusions



- Linear Regime:
  - Non-linearities exhibit strong, exponential growth, 10% by $x=4d_0$
  - Initial unstable modes are predicted well by linear-theory
- Surface Breakup:
  - Unstable modes break up the surface relatively early ($x=7d_0$ to $10d_0$)
- Primary Atomization:
  - Complete destruction of core happens ~$30d_0$ downstream
  - Surface disturbances may not be directly responsible for destruction of liquid core [1-2]

[1] Deshpande, Gurjar, Trujillo (2015). Physics of Fluids
[2] Marmottant, Villermaux (2004) Journal of Fluid Mechanics

Thank you!

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A Closer Look at Linear Stability Theory in Modeling Spray Atomization

Check for updates

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ABSTRACT

The common Lagrangian-Eulerian modeling of liquid sprays is largely based on linear stability theory, where the associated growth rates and most unstable wavelengths are used in prescribing initial Lagrangian droplet characteristics. Using highly-resolved VoF simulations, the present work is aimed at examining the extent to which this linear stability and associated flow characteristics hold in a realistic spray configuration under normal operating conditions using the ECN spray A geometry. This involves a comparison between linear stability wavelength predictions, originating from two-phase Orr-Sommerfeld solutions, and those obtained from the VoF simulations. The results show that within the first 4 diameters beyond the orifice, the non-linear components of the Navier-Stokes have grown to 10% of the corresponding linear part in both the liquid and the gas phase, and continue to grow exponentially. The non-axial and non-fully developed flow profiles are particularly significant even within one diameter but do not develop as strongly as the non-linear components. Linear stability theory is able to adequately capture the initial surface disturbances, and there is reasonable agreement with VoF simulations, despite the fact that the base flow is not exactly the conventional one. A main finding from the work shows that while the most unstable modes are captured in the simulations and agree with theoretical predictions, these modes are *not* directly responsible for fragmenting the liquid core or causing primary atomization. Their action is limited to breaking up the surface of the jet, while the liquid core of the jet remains intact for another 20 jet diameters downstream.