Numerical Simulation of Capillary Waves

Comparative Study of Volume of Fluid and Level Set Methods

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Background and Motivation

Liquid Properties

- Surface tension

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- Viscosity

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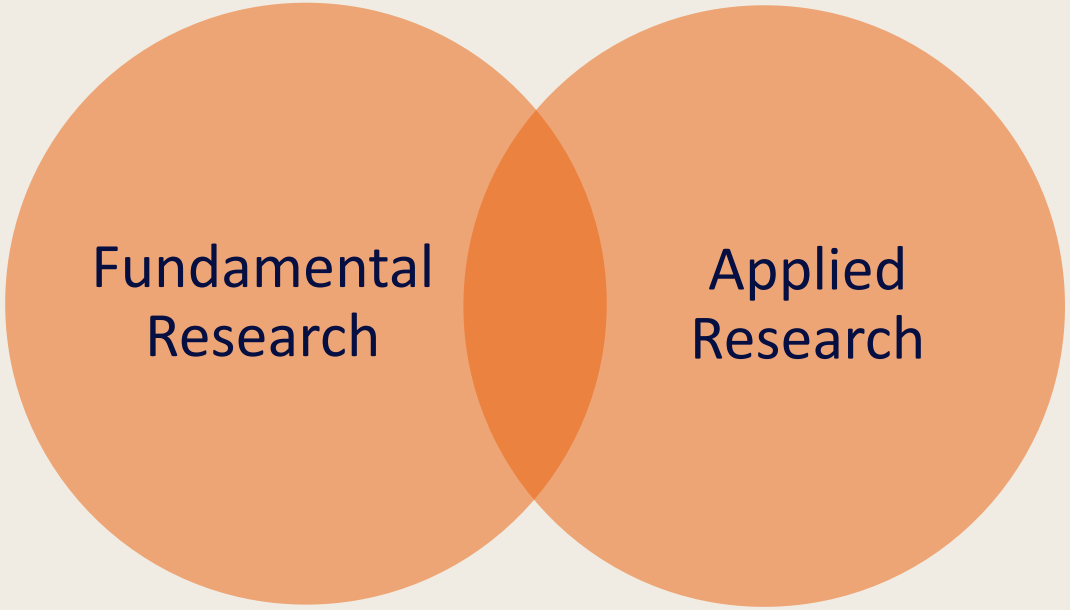
Need of Measurement

- Quantification of properties
- Fundamental research
  - Fluid and interface behavior
- Applied research
  - Modeling
  - Simulation
  - Monitoring
  - Control
- Applications
  - Chemical & process
  - Energy
  - Biomedical etc.



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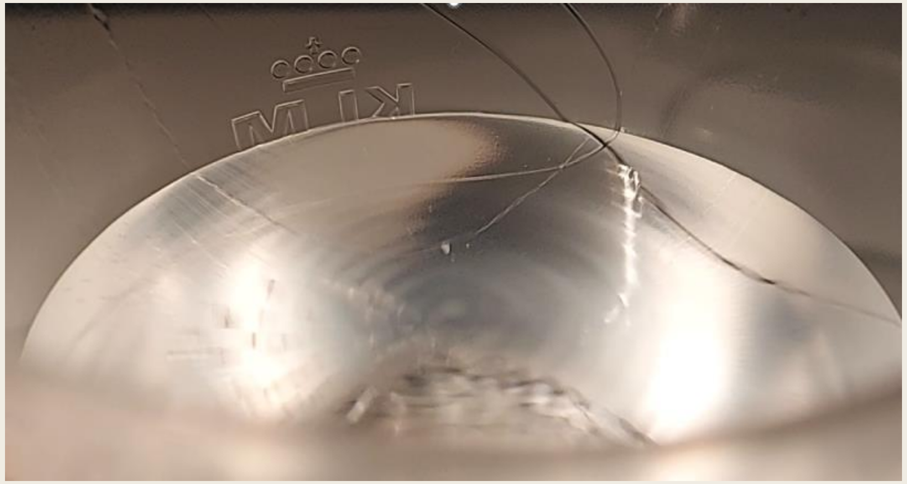
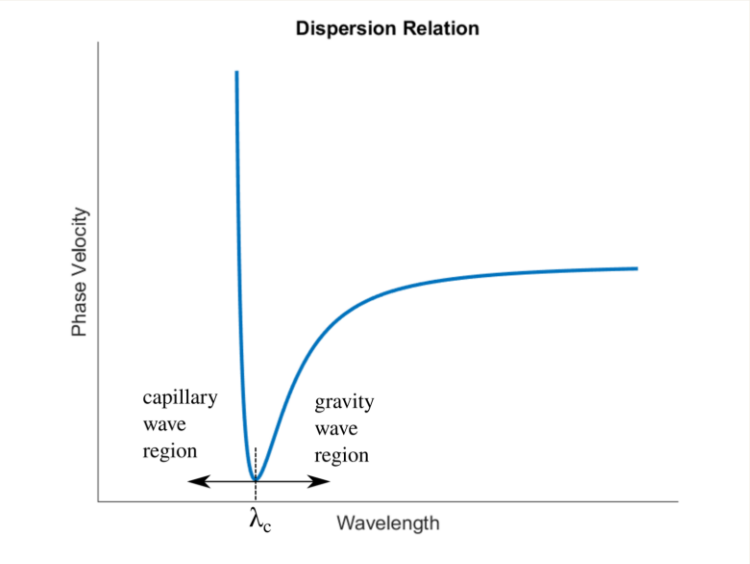
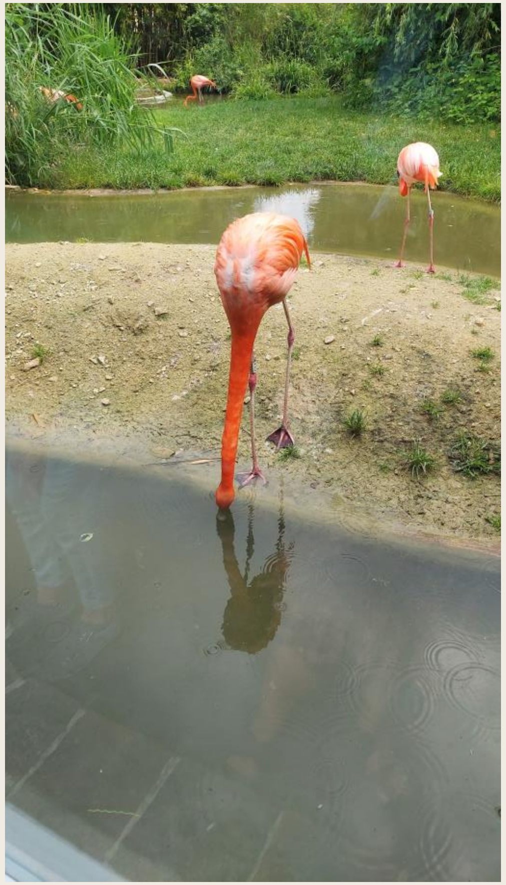
Capillary Waves

- Interfacial tension is dominant force
- Characterized by tiny amplitude and high frequency
- Linear wave theory (dispersion eq.)

$$\omega^2 = k\left(g + \frac{k^2\sigma}{\rho}\right)\tanh(kh)$$



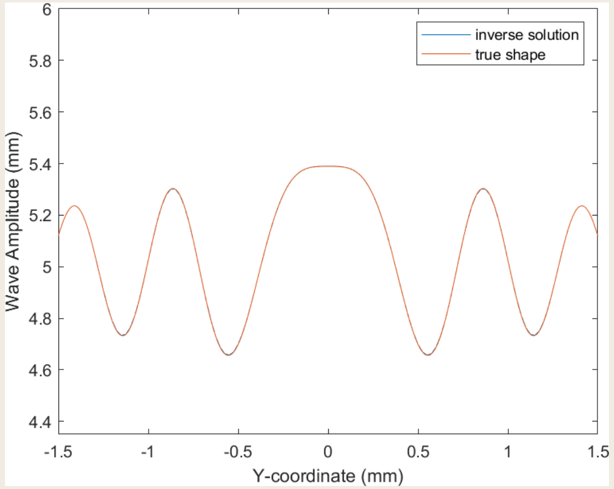


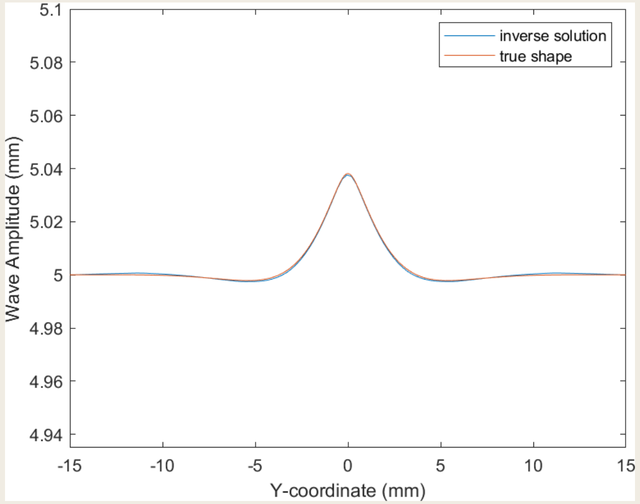


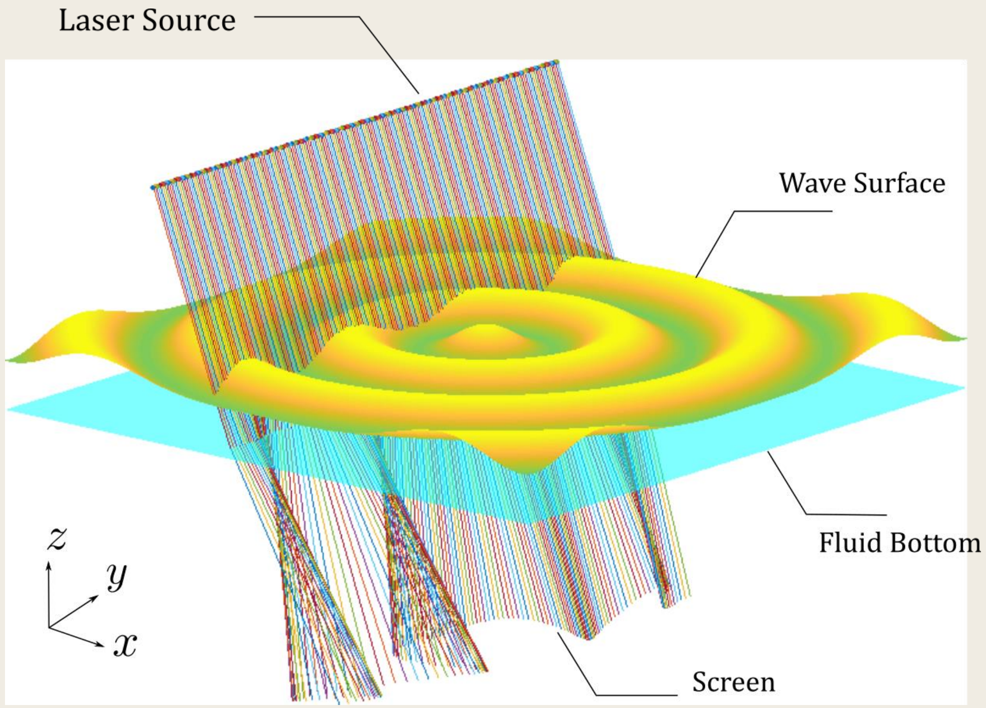
New Method of Measurement

- Using refraction as magnifier
- Geometric optics
  - Forward and inverse ray-tracing problem
- MATLAB code
  - Constrained and unconstrained numerical optimization

Mukim et al., AIP Advances, 2022



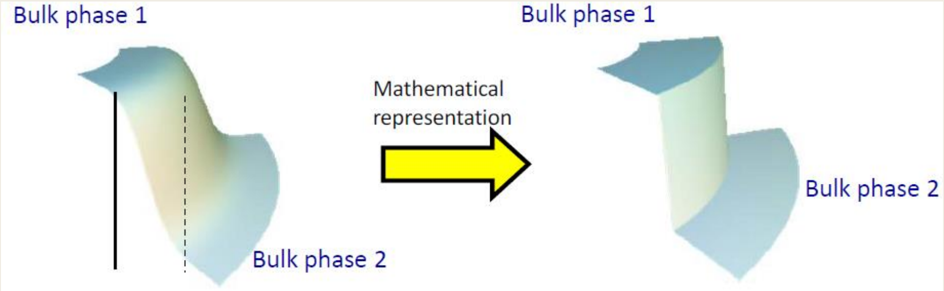




Numerical Simulations

Numerical Simulation

- Objectives
  - Verify linear wave theory in experimental setup
  - Help in design of experiment
- Transient, incompressible, isothermal, immiscible two-phase flow
- One-fluid formulation of two-phase modeling approaches
  - Volume of Fluids (VoF)
  - Level Set (LS)
- Interface capturing mechanism, curvature calculation for interfacial tension force
- Contact angle effects are neglected



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Numerical Simulation

- Continuity equation

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

- Momentum equation

$$\frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\mathbf{uu}) = \frac{1}{\rho}\left(\boldsymbol{\nabla} p + \boldsymbol{\nabla} \cdot \left[\mu\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{T}\right)\right] + \rho \mathbf{g} + \mathbf{f}_{\mathbf{st}}\right)$$

- CSF (continuous surface force) formulation for interfacial tension force (no Marangoni flow)

$$\mathbf{f}_{\mathbf{st}} = \sigma \kappa \delta_s \mathbf{n}$$

- Accurate calculation of interfacial tension force depends on
  - Curvature
  - Surface normal
  - Numerical approximation of Dirac delta function

Volume of Fluids

- Volume fraction

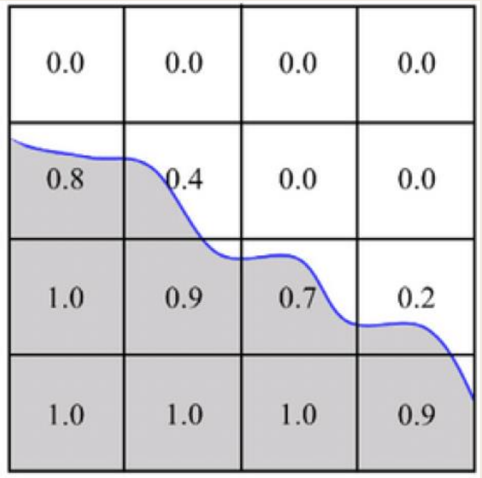
$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0$$

- Volume averaged fluid properties
- Interfacial tension

$$\mathbf{f_{st}} = \sigma \kappa \delta_s \mathbf{n}, \kappa = -\nabla \cdot \mathbf{n} = -\nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right)$$

- Interface capture
  - interFoam (algebraic)
    - Artificial compression for sharpness of interface
    - Boundedness $0 \leq \alpha \leq 1$ ensured by MULES
  - interIsoFoam (geometric)
    - Based on isoAdvector method
    - More accurate face flux calculation

- Pros and cons
  - Slightly difficult to implement
  - Conservative
  - Sharpness and accuracy depends on interface compression and capturing methods



Level Set

- Level set variable phase initialization

$$\phi\Big|_{t=0} = \begin{cases} \left(1 + e^{\varsigma/\epsilon}\right)^{-1} & \text{fluid 1} \\ \left(1 - e^{\varsigma/\epsilon}\right)^{-1} & \text{fluid 2} \end{cases}$$

- Interface advection

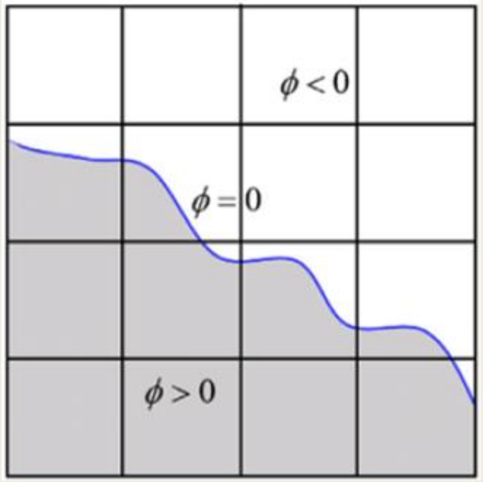
$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla}\phi = \gamma \boldsymbol{\nabla} \cdot \left(\epsilon \boldsymbol{\nabla}\phi - \phi(1-\phi)\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \right)$$

- Volume averaged density and viscosity
- Interface advection

$$\mathbf{f_{st}} = \sigma\kappa\delta_s\mathbf{n}, \delta_s = 6|\boldsymbol{\nabla}\phi||\phi(\phi-1)|$$

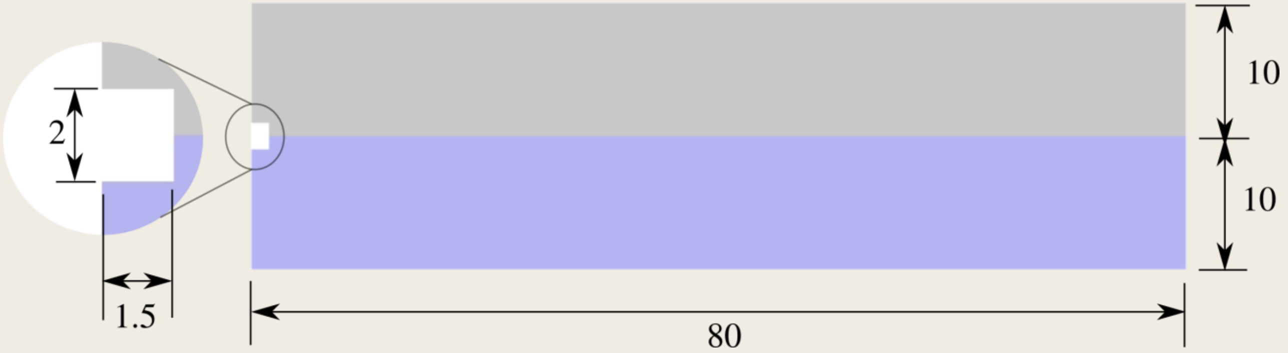
$$\kappa = -\boldsymbol{\nabla}\cdot\mathbf{n} = -\boldsymbol{\nabla}\cdot\left(\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}\right)$$

- Pros and cons
  - Easy to implement
  - Highly accurate interfacial normal and curvature
  - Non-conservative (conservative level set available in COMSOL but faces issues with convergence and/or computational time)



Numerical Setup

- Planar symmetric setup
- Material properties
  - Water-air
- Numerical experiments
  - Frequency **20** & 40 Hz
  - Interfacial tension 20 & **70** mN/m
- Amplitude 0.2 mm
- Mesh size
  - dx = 0.1 mm, dy = 0.02 and 0.1 mm
- Graded mesh
- Dynamic mesh motion



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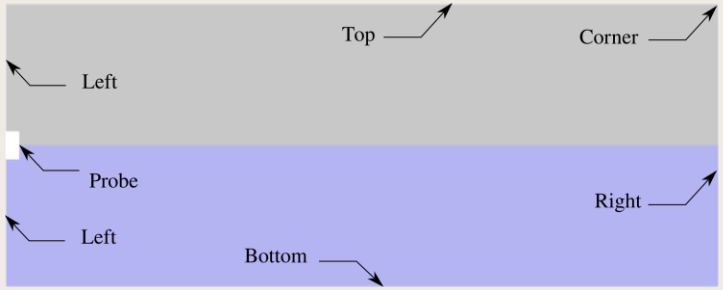
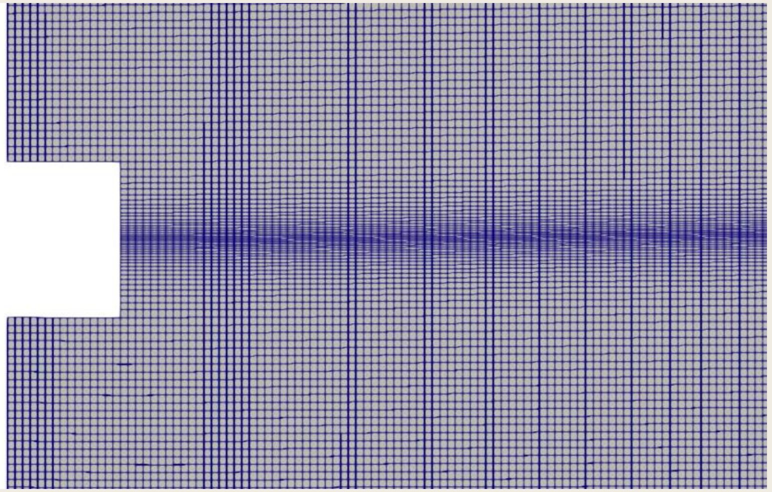
Numerical Setup

- Boundary conditions





OpenFOAM

Name	U	p_rgh	alpha.water	pointDisplacement
Left	symmetryPlane	symmetryPlane	symmetryPlane	symmetryPlane
Bottom	noSlip	fixedFluxPressure	zeroGradient	fixedValue
Right	noSlip	fixedFluxPressure	zeroGradient	fixedValue
Top	pressureInletOutlet Velocity	totalPressure	inletOutlet	fixedValue
Probe	movingWallVelocity	fixedFluxPressure	zeroGradient	oscillatingDisplacement

COMSOL

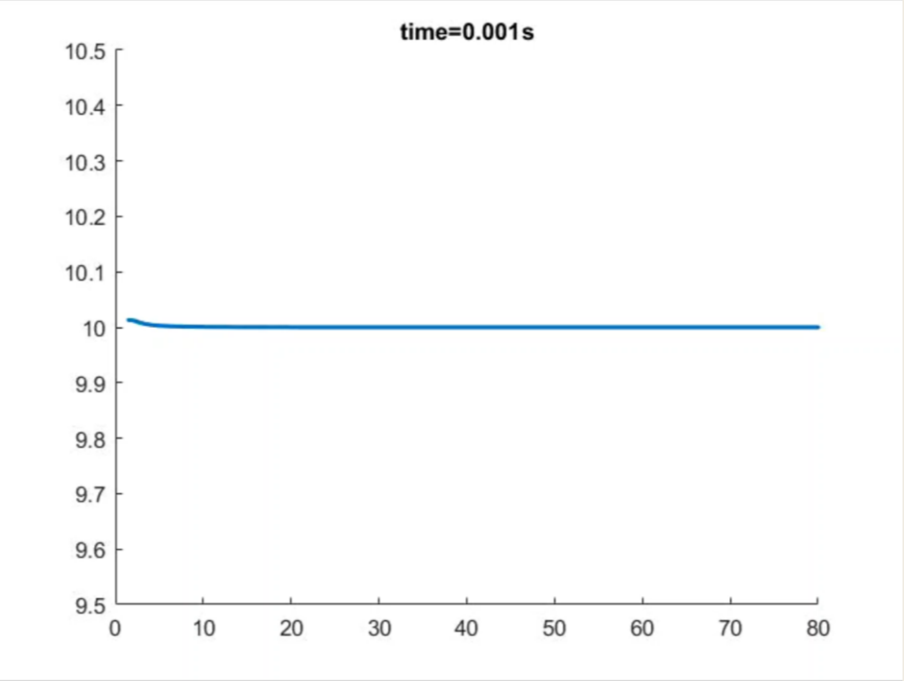
Name	Moving Mesh	Laminar Flow	Level Set
Left	Symmetry	Symmetry	Symmetry
Bottom	-	Wall	No Flow
Right	-	Wall	No Flow
Top	-	Outlet	Outlet
Probe	Prescribed Displacement	Wall	No Flow
Corner	-	Pressure Point Constraint	-

Results

Results

- Volume fraction

- Post-processing with MATLAB
  - Isosurface



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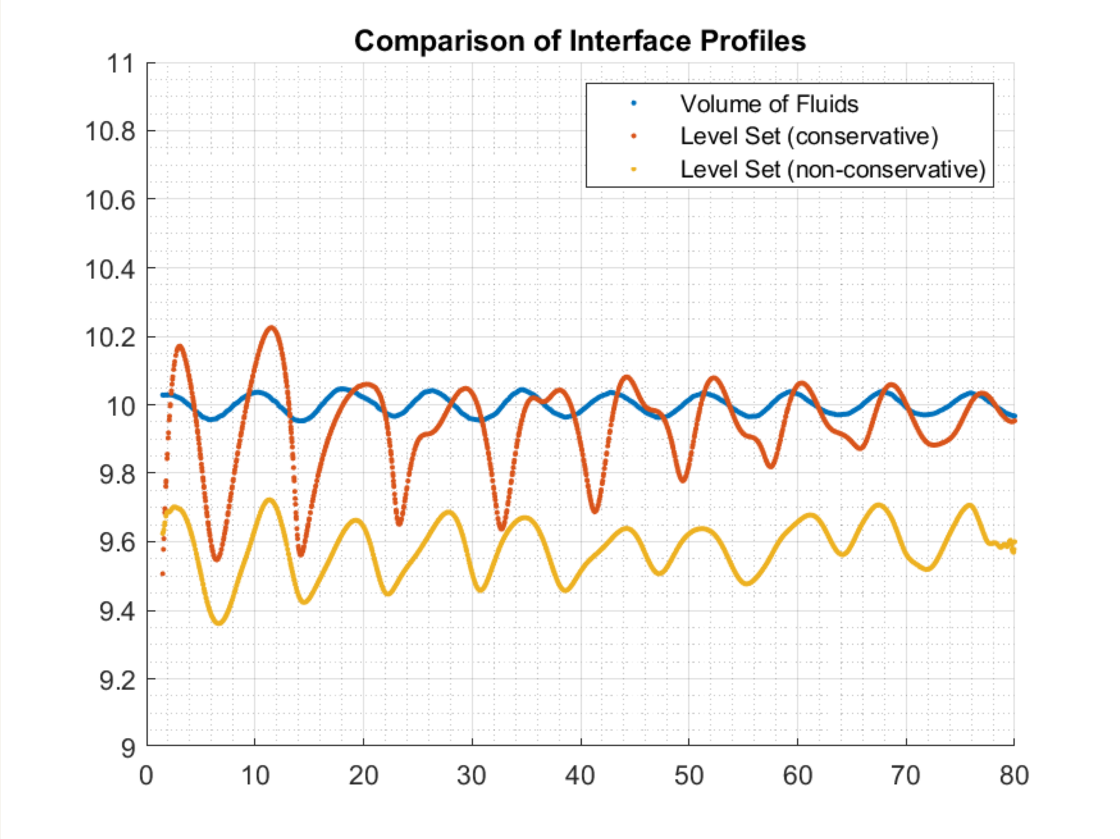
Results

Frequency (Hz)	$\lambda_{analytical}$ (mm)	λ_{VoF} (mm)	λ_{LS_nc} (mm)	$Error_{VoF}$ (%)	$Error_{LS\_nc}$ (%)
20	11.8	12.2	11.5	3.38	2.54
40	6.85	6.7	6.7	2.18	2.18

Surface Tension (mN/m)	$\lambda_{analytical}$ (mm)	λ_{VoF} (mm)	λ_{LS_nc} (mm)	$Error_{VoF}$ (%)	$Error_{LS\_nc}$ (%)
20	8.4	8.0	8.0	4.76	4.76
70	11.8	12.2	11.5	3.38	2.54



Conclusion

Conclusion

- Planar symmetry with dynamic mesh motion implemented successfully in OpenFOAM and COMSOL Multiphysics
- One-way fluid-structure interaction coupling achieved by dynamic mesh motion to transmits the velocity to the liquid
- Both VoF and LS have similar error values, but need more simulations for confidence
- Reflection of waves results in slight change in wavelength
- VoF interface profile closely matches with predicted analytical results (important for next step of simulation)
- Conservative LS shows improved mass conservation but higher amplitude in interface shapes


Thank you!