TFAWS Active Thermal Paper Session

A volume of fluid numerical algorithm for simulating multiphase incompressible flows with large density discontinuities

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Outline

- Multiphase flow applications
- Modeling multifluid flows with volume of fluid (VOF)
  - Numerical algorithm
  - Volume fraction advection schemes
  - Test problems
- Multifluid flows with large, discontinuous density jumps
  - Difficulties, solution, and test problems
- Incorporating additional interfacial physics
  - Surface tension
  - Wall adhesion
- Conclusion

Multiphase flow applications

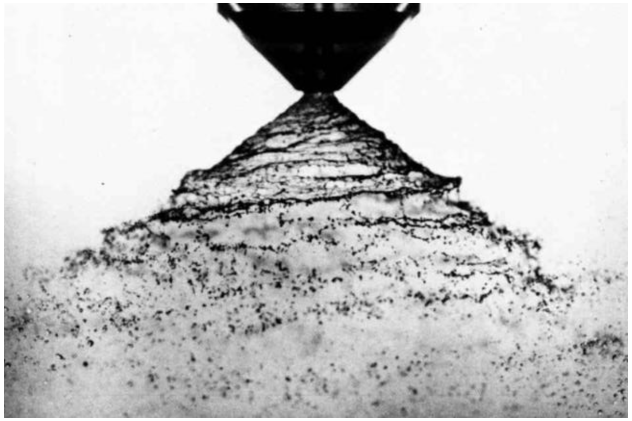
Multiphase flow is the simultaneous flow of material in different phases or in the same phase but with different flow properties

Liquid-Gas (multifluid)
- Atomization of cryogenic propellant
- Fuel sloshing in tanks
- Lubrication systems

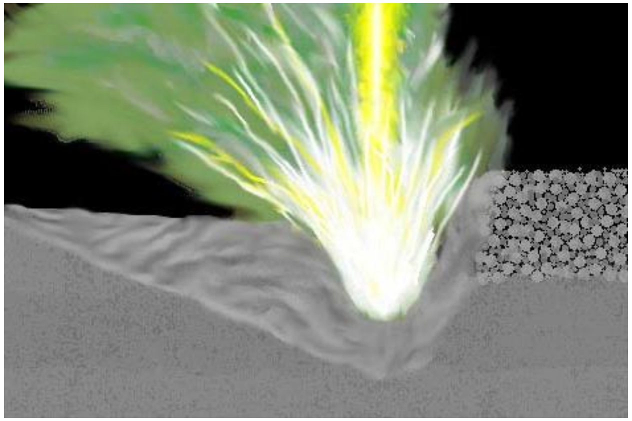
Liquid-Liquid (multifluid)
- Oil dispersion in water
- Microfluidics

Gas-Solid
- Particle-laden rocket plumes
- Dust storms

Liquid-Gas-Solid
- Additive manufacturing
- Nuclear and chemical reactors



Liquid jet atomization (Van Dyke, M., 1982)



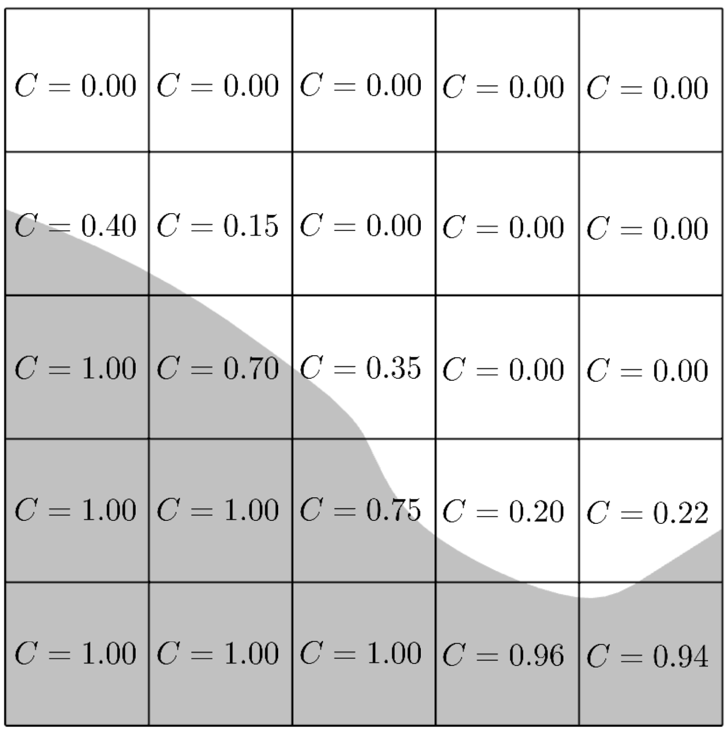
Melt pool in laser additive manufacturing (www.stratonics.com)

Modeling multiphase flow with VOF

Volume of Fluid (VOF) method:

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = \nabla p + \nabla\cdot\mu(\nabla\mathbf{u}+\nabla\mathbf{u}^T) + \mathbf{F}_B \quad \text{on } \Omega \quad \forall t\in(0,T)$$

$$\nabla\cdot\mathbf{u} = 0 \quad \text{on } \Omega \quad \forall t\in(0,T)$$



VOF representation of a fluid interface

$$\rho = C\rho_1 + (C-1)\rho_2$$
$$\mu = C\mu_1 + (C-1)\mu_2$$

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

Symbol	Variable
$\mathbf{u}$	Velocity
p	Pressure
ρ	Density
μ	Dynamic viscosity
$\mathbf{f}$	Acceleration due to body force
C	Cell volume fraction

Pressure-velocity coupling

Two-step projection method:

1. Calculate provisional velocity ($\mathbf{u}^*$) ignoring pressure gradient term

$$\frac{(\rho\mathbf{u})^* - (\rho\mathbf{u})^n}{\Delta t} = -\mathbf{A}_h^n + \mathbf{D}_h^n + \mathbf{F}_B^n$$

$$\mathbf{A}_h^n = \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}),$$
$$\mathbf{D}_h^n = \nabla\cdot\mu\big(\nabla\mathbf{u}+\nabla\mathbf{u}^T\big)^n$$

2. Solve Poisson equation for pressure

$$\nabla\cdot\left(\frac{1}{\rho^{n+1}}\nabla\, p^{n+1}\right) = \frac{1}{\Delta t}\nabla\cdot\mathbf{u}^*$$

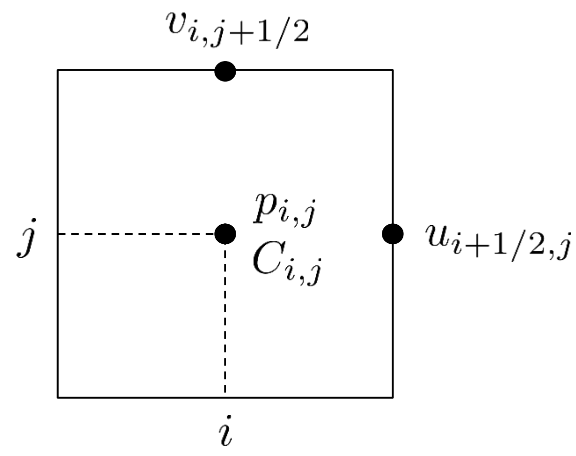
3. Correct provisional velocity to be divergence-free

$$\frac{(\rho\mathbf{u})^{n+1} - (\rho\mathbf{u})^*}{\Delta t} = -\frac{1}{\rho^{n+1}}\nabla\, p^{n+1}$$

Numerical approach

Discretization

- Finite volume on staggered, Cartesian grid
- Van Leer's scheme for convective term

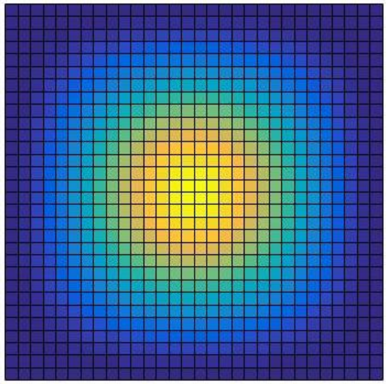


Elliptic solver

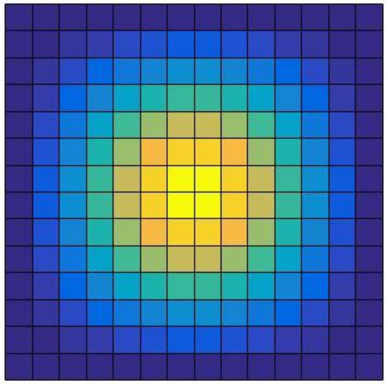
- Geometric multigrid

$$\nabla^2 p = f \qquad \boxed{p_{i,j}^{k+1} = \frac{1}{4}(p_{i-1,j}^{k+1} + p_{i+1,j}^{k} + p_{i,j-1}^{k+1} + p_{i,j+1}^{k}) - \frac{h^2}{4} f_{i,j}}$$

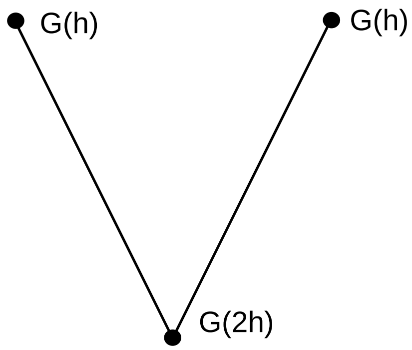
Gauss-Seidel



G(h)



G(2h)



Two-grid V-cycle

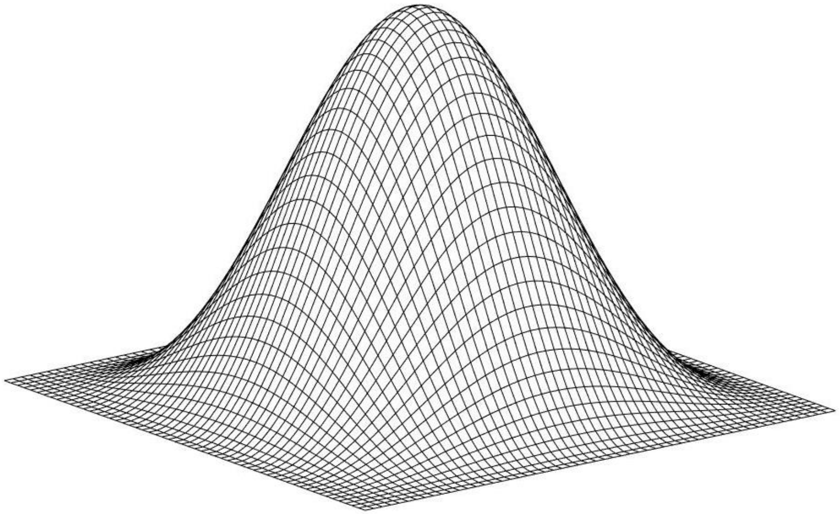
Elliptic PDE solver

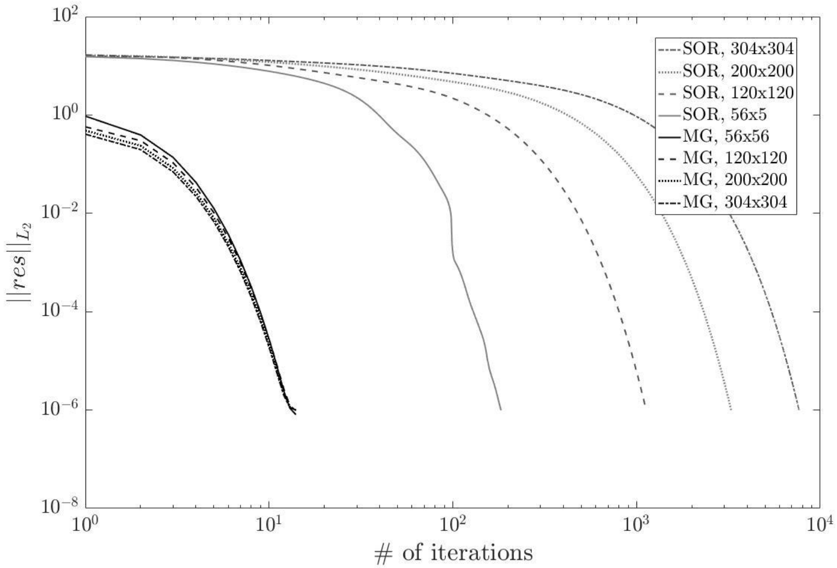
Multigrid test problem

$$\nabla \cdot \beta \nabla \phi = \theta$$

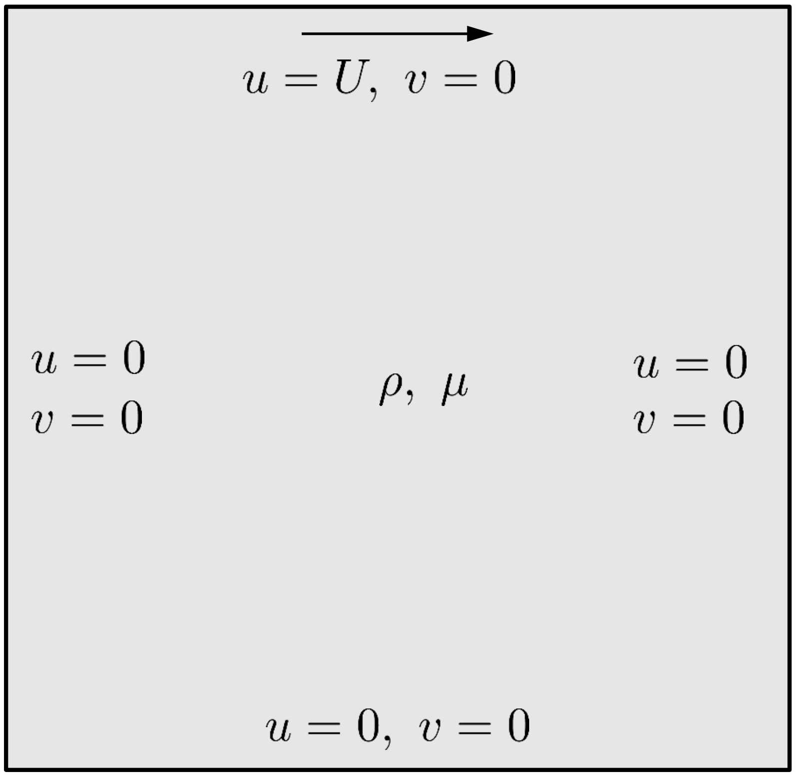
$$\beta = -1, \quad \theta = -2\pi^2 \big(\cos(2\pi x) \sin(\pi y) + \cos(2\pi y) \sin(\pi x) \big)$$

$$\phi = 0 \text{ on } \partial\Omega$$





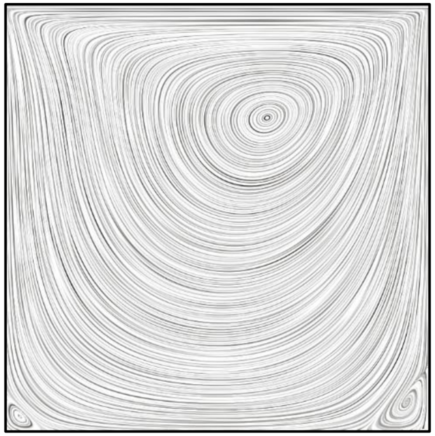
Lid-driven cavity



$Re = 40{,}000$

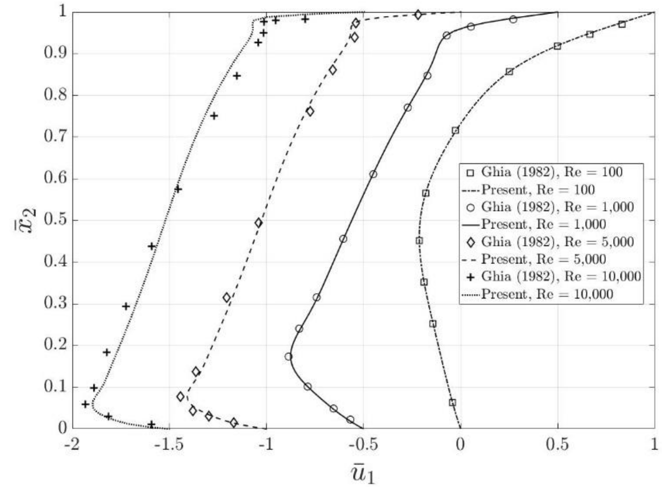
Single-phase flow test

Lid-driven cavity



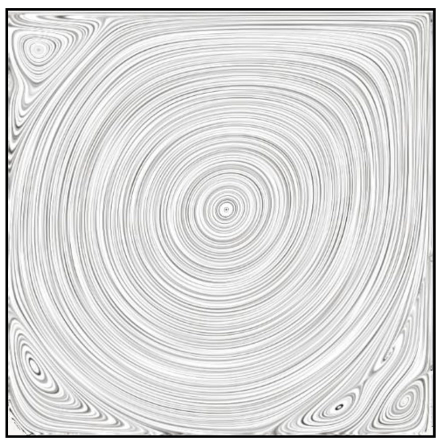
$Re = 100$

$Re = 1{,}000$

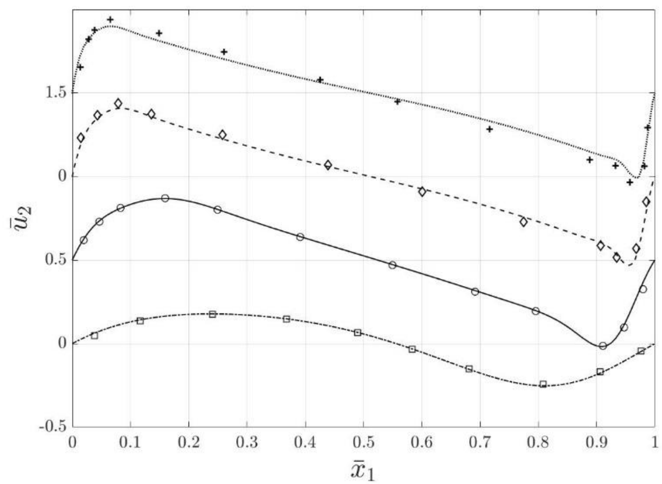


Horizontal velocity profile along centered vertical transect

$Re = 5{,}000$



$Re = 10{,}000$

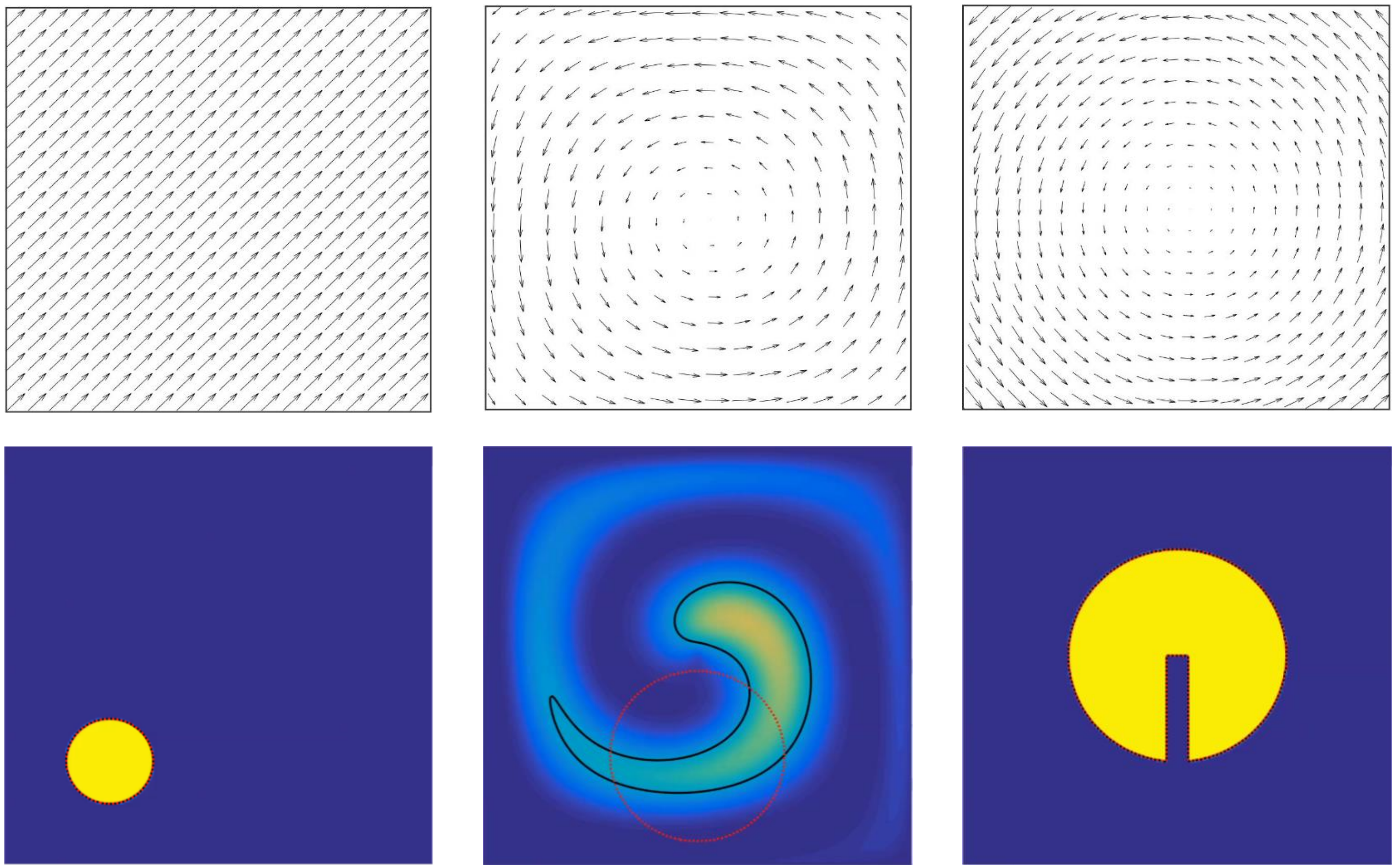


Vertical velocity profile along centered horizontal transect

VOF – Volume fraction advection

Solving $\frac{\partial C}{\partial t} + \nabla \cdot (C\mathbf{u}) = 0$ with upwind finite differences

Translational Flow	Shearing Vortex	Rigid-Body Vortex
$u = 1,\ v = 1$	$u = \sin(\pi x)\cos(\pi y),\ v = -\sin(\pi y)\cos(\pi x)$	$u = 0.5 - y,\ v = x - 0.5$



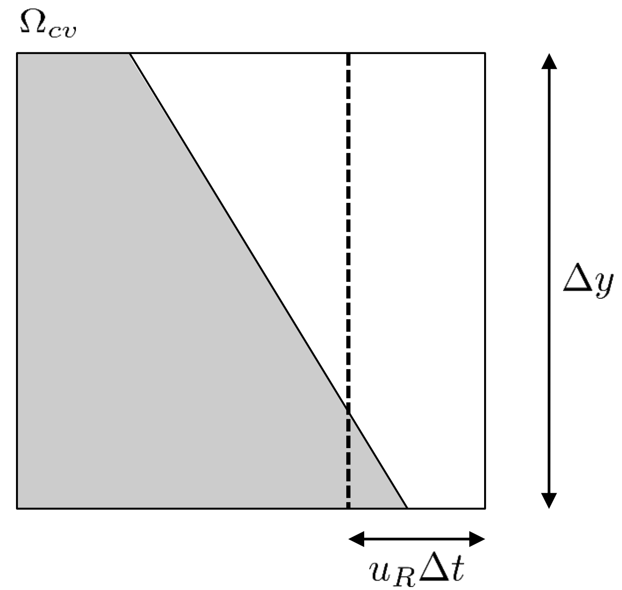
VOF – Volume fraction advection

Finite volume approach

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

$$\frac{1}{V_{\Omega_{cv}}} \iint_{\Omega_{cv}} \left(\frac{\partial C}{\partial t} + \nabla \cdot (C\mathbf{u}) \right) d\Omega = 0$$

$$\frac{\partial C}{\partial t} + \frac{1}{V_{\Omega_{cv}}} \oint_{\partial\Omega_{cv}} \Big(C(\mathbf{u} \cdot \hat{\mathbf{n}}) \Big) ds = 0$$



$$\frac{C^{n+1} - C^n}{\Delta t} = -\frac{1}{\Delta x \Delta y} \left(u_R C \Delta y - u_L C \Delta y + v_T C \Delta x - v_B C \Delta x \right)$$

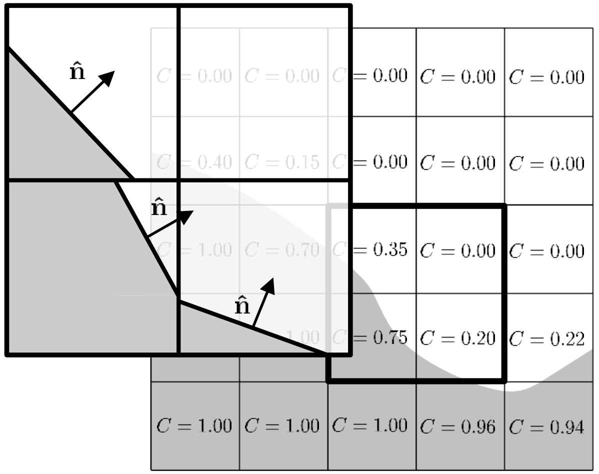
$$\boxed{\begin{aligned} C^* &= C^n - \frac{1}{\Delta x \Delta y} \left(FV_R - FV_L \right) \\ C^{n+1} &= C^* - \frac{1}{\Delta x \Delta y} \left(FV_T - FV_B \right) \end{aligned}}$$

Piecewise Linear Interface Calculation (PLIC)

1. Reconstruct interface
   - Calculate interface normal vector

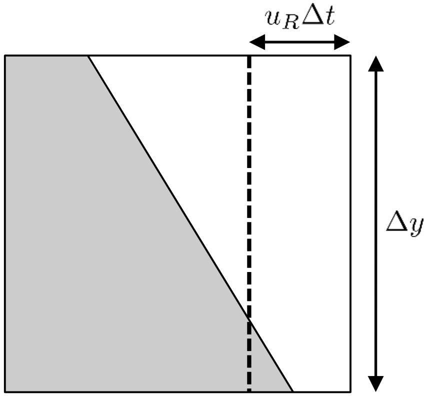
$$\hat{\mathbf{n}} = \frac{-\nabla C}{||\nabla C||}$$

   - Cut cell using volume fraction

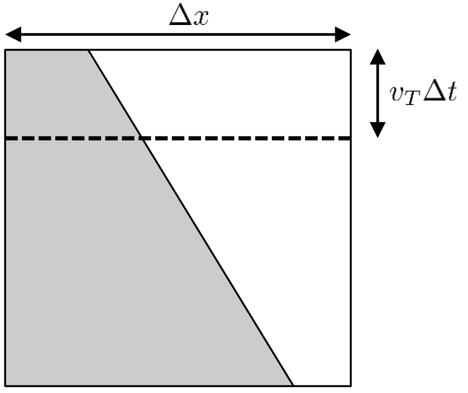


VOF representation of a fluid interface

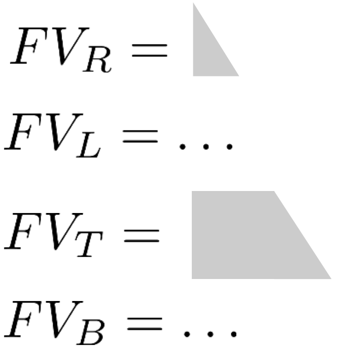
2. Compute fluxed volumes



Right face



Top face



VOF – Volume fraction advection

Solving $\frac{\partial C}{\partial t} + \nabla \cdot (C\mathbf{u}) = 0$ with PLIC

Translational Flow

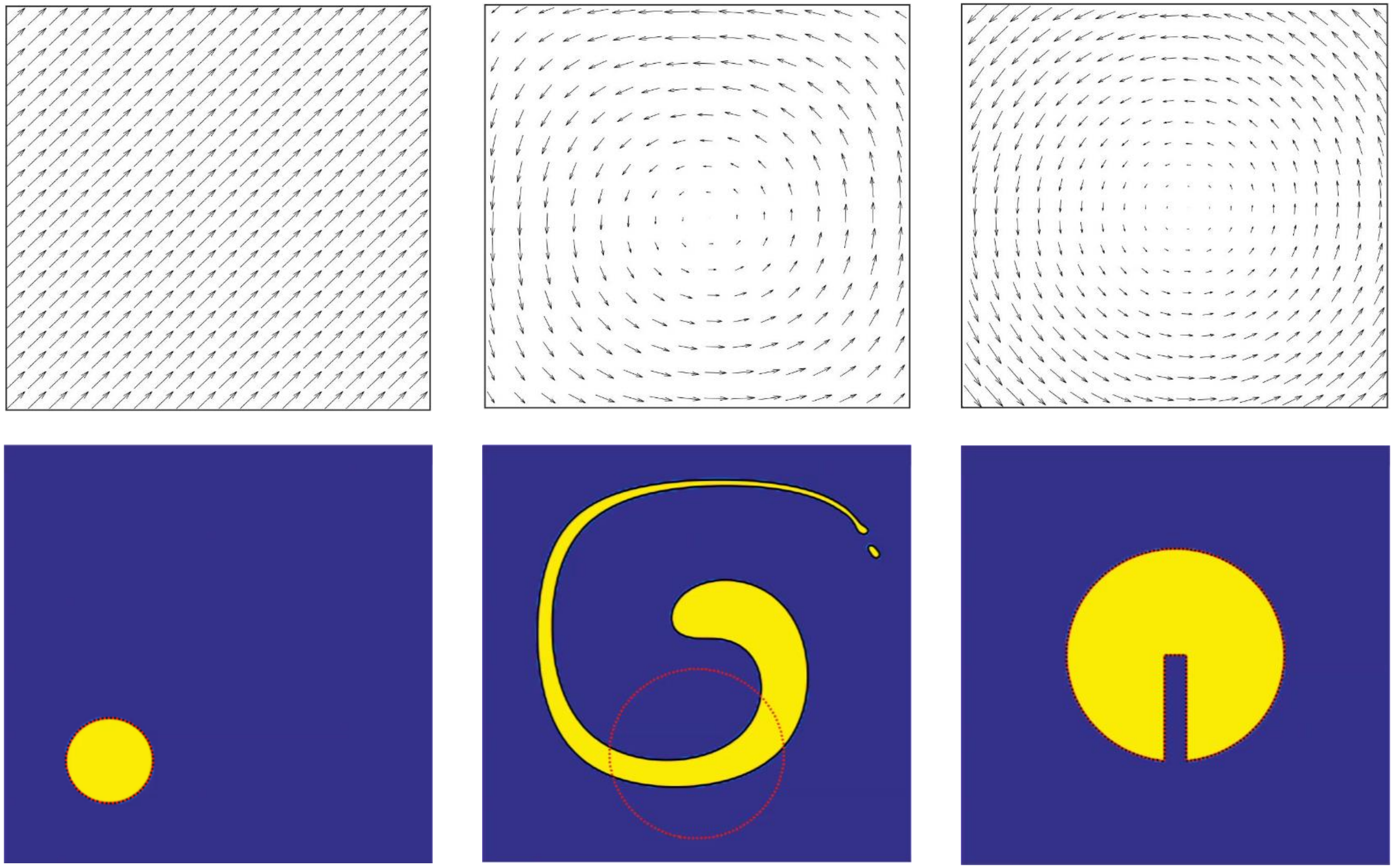
$u = 1,\ v = 1$

Shearing Vortex

$u = \sin(\pi x)\cos(\pi y),\ v = -\sin(\pi y)\cos(\pi x)$

Rigid-Body Vortex

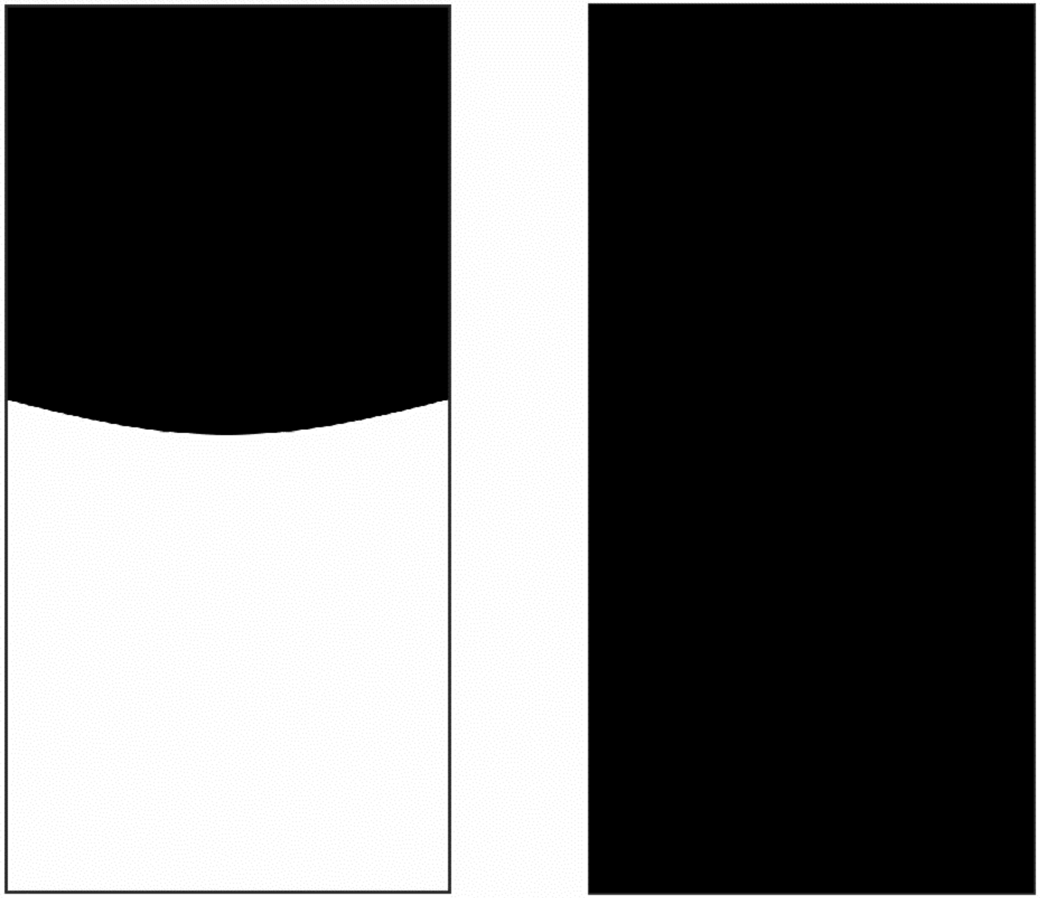
$u = 0.5 - y,\ v = x - 0.5$



Multifluid flow test (small density ratio)

Rayleigh-Taylor Instability

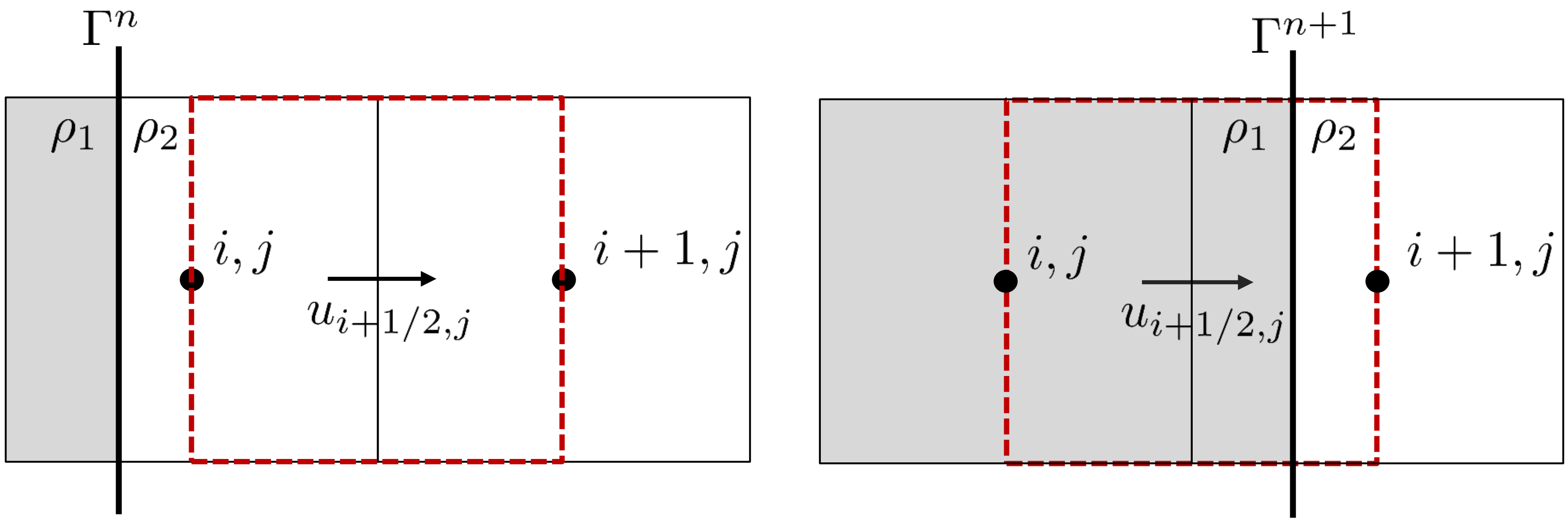
$$\rho_1/\rho_2 = 1.25$$



Volume Fraction

Velocity Magnitude

Difficulties due to large density ratio



$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \cancel{\nabla p} + \cancel{\nabla \cdot} \tau + \cancel{\mathbf{F}}_B$$

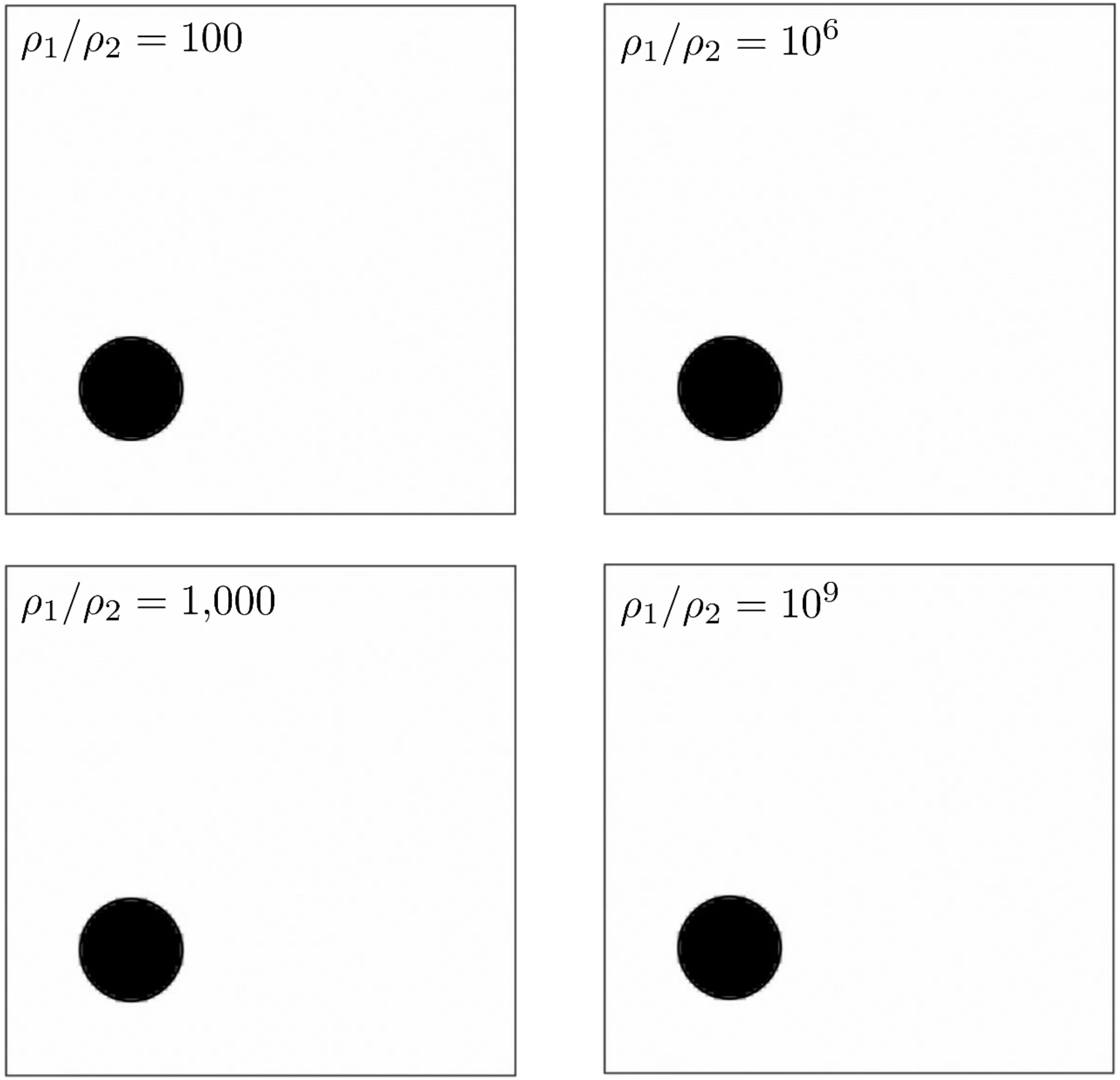
$$\frac{(\rho \mathbf{u})^*_{i+1/2,j} - (\rho \mathbf{u})^n_{i+1/2,j}}{\Delta t} = -\nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u})^n_{i+1/2,j}$$

$$\rho_{i+1/2,j} = \frac{1}{2}(\rho_{i+1,j} + \rho_{i,j})$$

Is this a good approximation?

Large density ratio flow tests

$u_0 = 1,\ v_0 = 1$

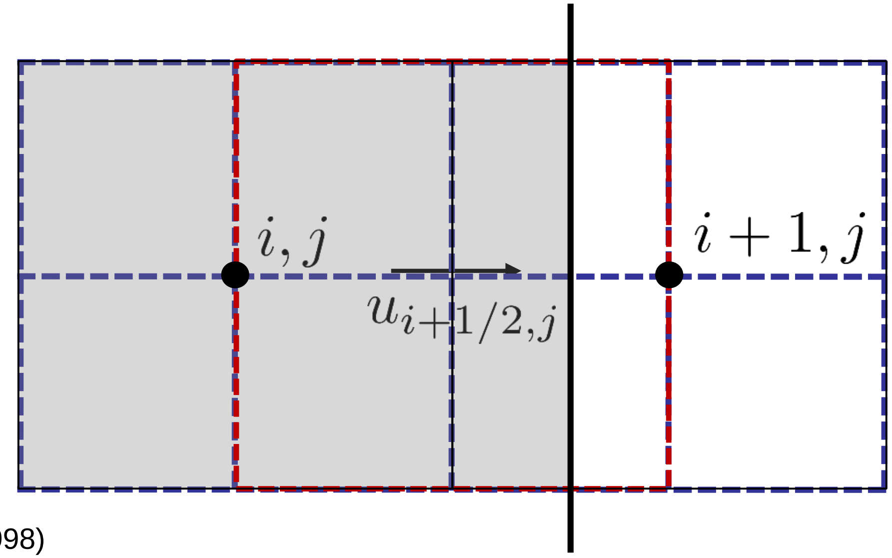


Consistent mass-momentum advection

$$(\rho\mathbf{u})^*_{i+1/2,j} - (\rho\mathbf{u})^n_{i+1/2,j} = -\Delta t \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u})^n_{i+1/2,j}$$

$$\frac{\Delta t}{V_{\Omega_{cv}}}\iint_{\Omega_{cv}} \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u})^n_{i+1/2,j} d\Omega = \frac{\Delta t}{V_{\Omega_{cv}}}\oint_{\partial\Omega_{cv}} \rho\mathbf{u}(\mathbf{u}\cdot\hat{\mathbf{n}})ds$$

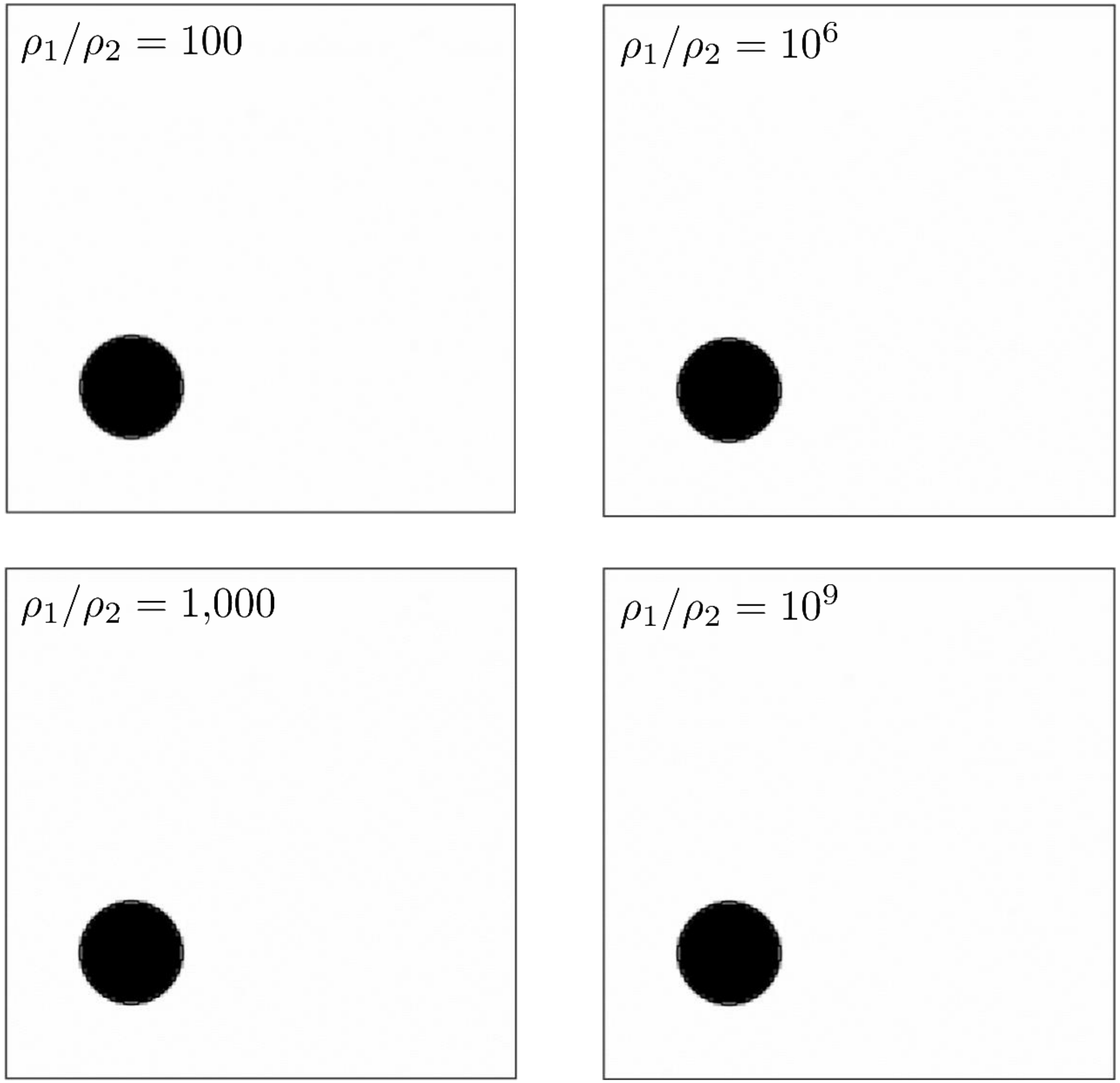
$$(\rho\mathbf{u})^*_{i+1/2,j} - (\rho\mathbf{u})^n_{i+1/2,j} = -\frac{1}{\Delta x\Delta y}\left(\underbrace{\langle\rho\mathbf{u}_{i+1,j}\Delta t\Delta y\rangle}_{m_{i+1,j}}\mathbf{u}_{i+1,j} - \underbrace{\langle\rho\mathbf{u}_{i,j}\Delta t\Delta y\rangle}_{m_{i,j}}\mathbf{u}_{i,j}\right)$$



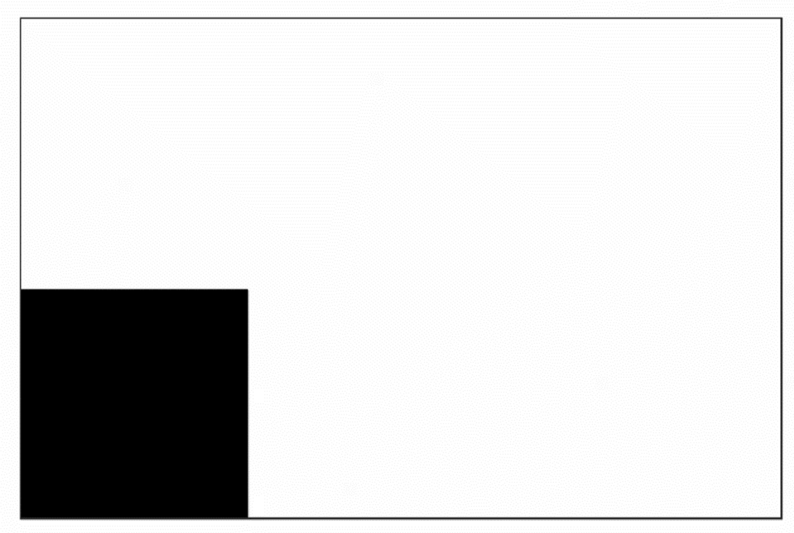
(Rudman, M., 1998)

Large density ratio flow tests

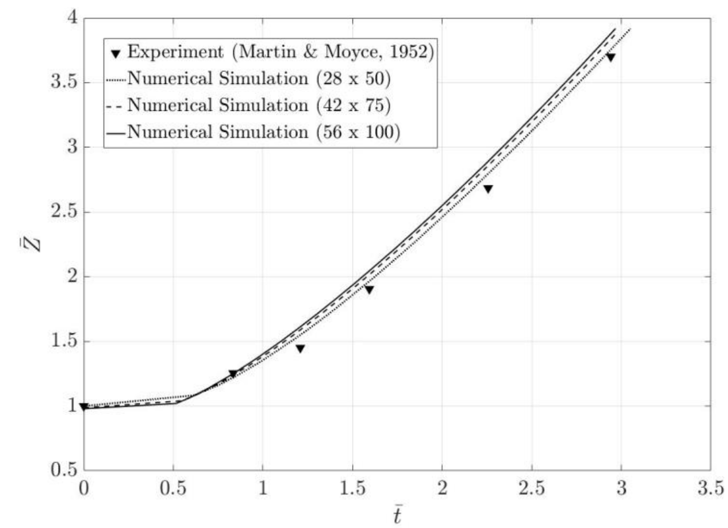
$u_0 = 1, \; v_0 = 1$



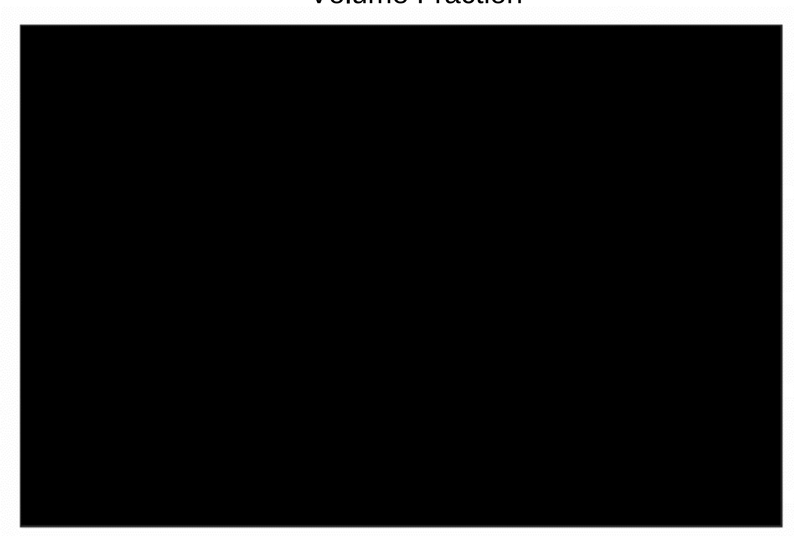
Collapsing water column (dam break)



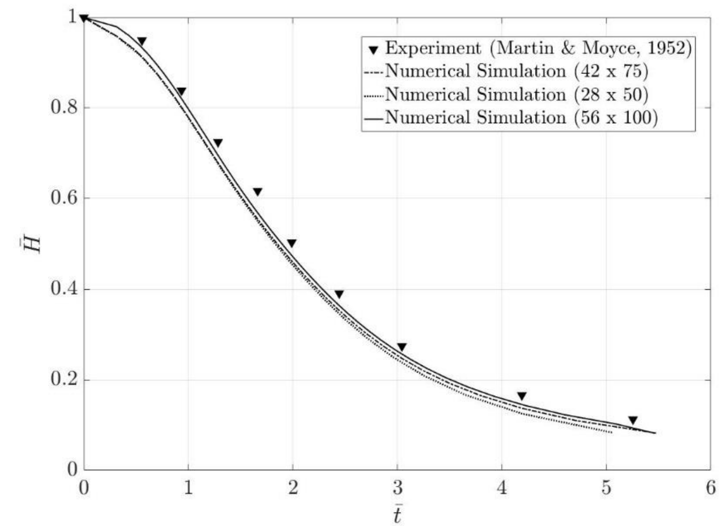
Volume Fraction



Surge front with time



Velocity Magnitude

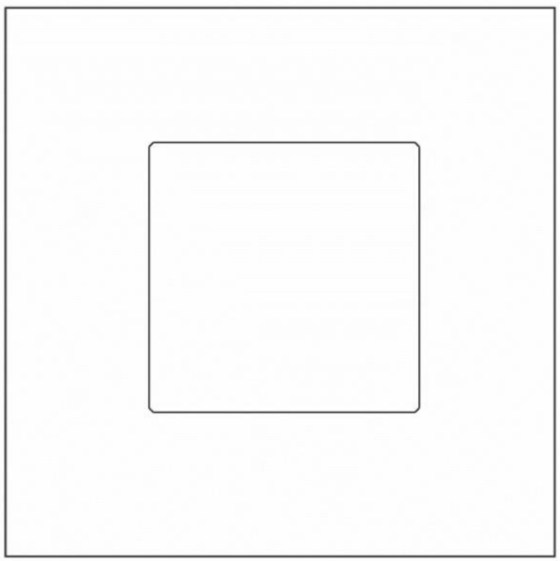


Column height with time

Continuum surface force (CSF) method

(Brackbill J.U., Kothe, D.B., and Zemach, C., 1991)

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = \nabla p + \nabla\cdot\tau + \mathbf{F}_B + \mathbf{F}_{ST}, \quad \mathbf{F}_{ST} = \sigma\kappa\nabla C, \quad \kappa = -\nabla\cdot\hat{\mathbf{n}}$$

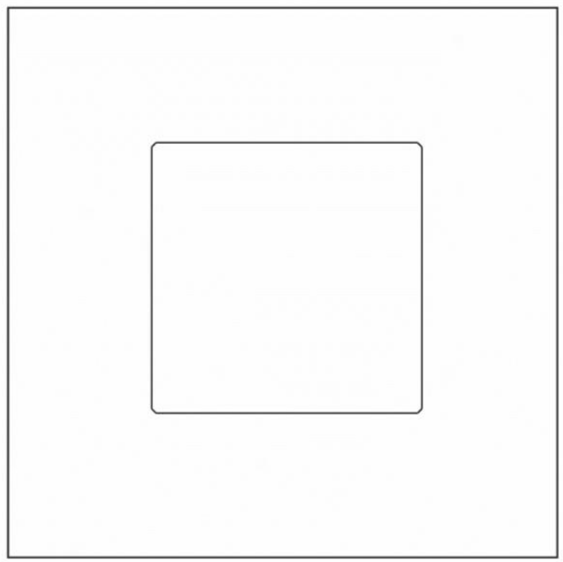


Glycerin

$\rho = 1{,}260\ \mathrm{kg/m^3}$

$\mu = 0.950\ \mathrm{Pa\cdot s}$

$\sigma = 0.064\ \mathrm{N/m}$

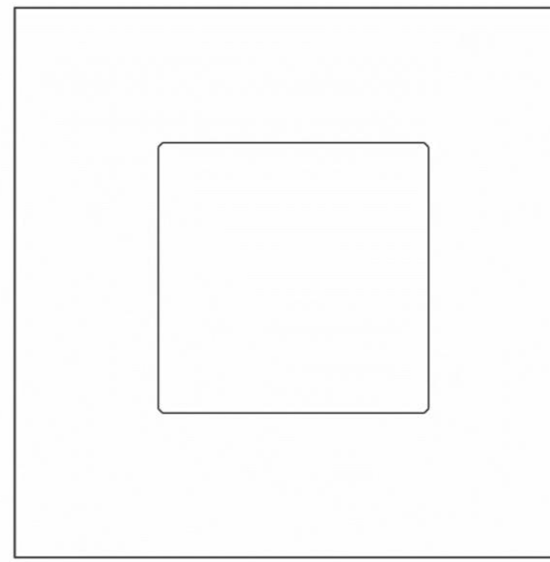


Engine Oil

$\rho = 856.7\ \mathrm{kg/m^3}$

$\mu = 0.122\ \mathrm{Pa\cdot s}$

$\sigma = 0.036\ \mathrm{N/m}$



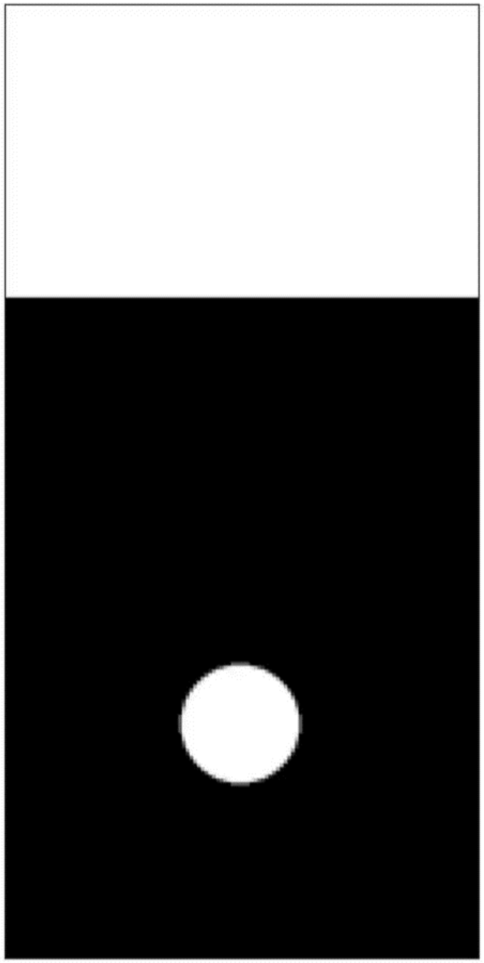
Liquid Hydrogen

$\rho = 70.8\ \mathrm{kg/m^3}$

$\mu = 1.35\times 10^{-5}\ \mathrm{Pa\cdot s}$

$\sigma = 1.93\times 10^{-3}\ \mathrm{N/m}$

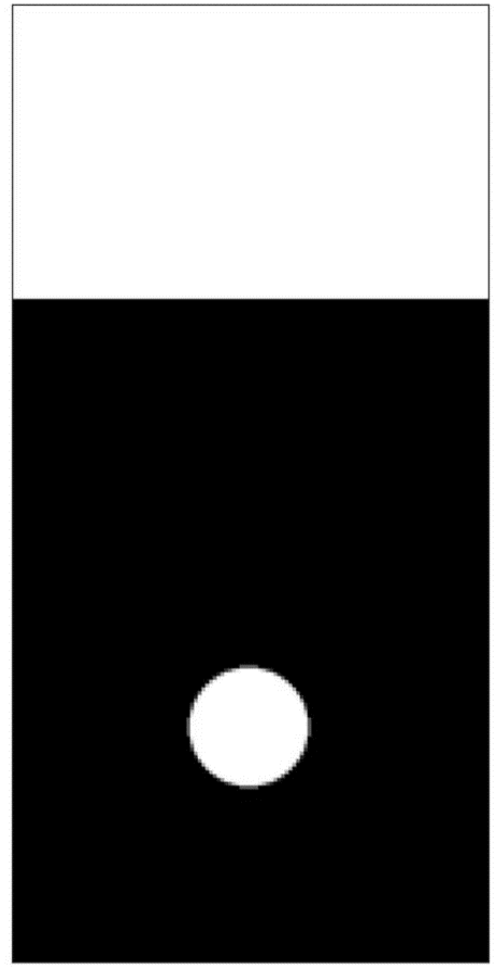
Rising bubble in quiescent liquid



$\rho_o/\rho_i = 1{,}000$

$\mu_o/\mu_i = 100$

$Bo = \infty$



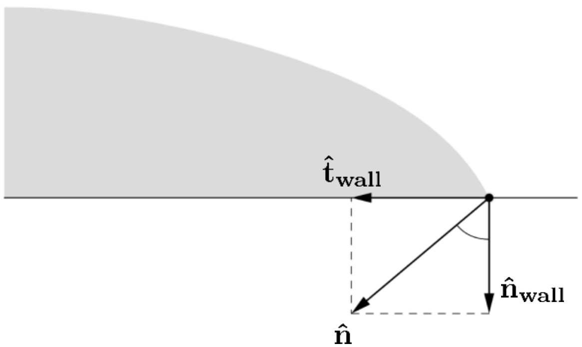
$\rho_o/\rho_i = 1{,}000$

$\mu_o/\mu_i = 100$

$Bo = 5.983$

Wall adhesion

Contact angle treatment

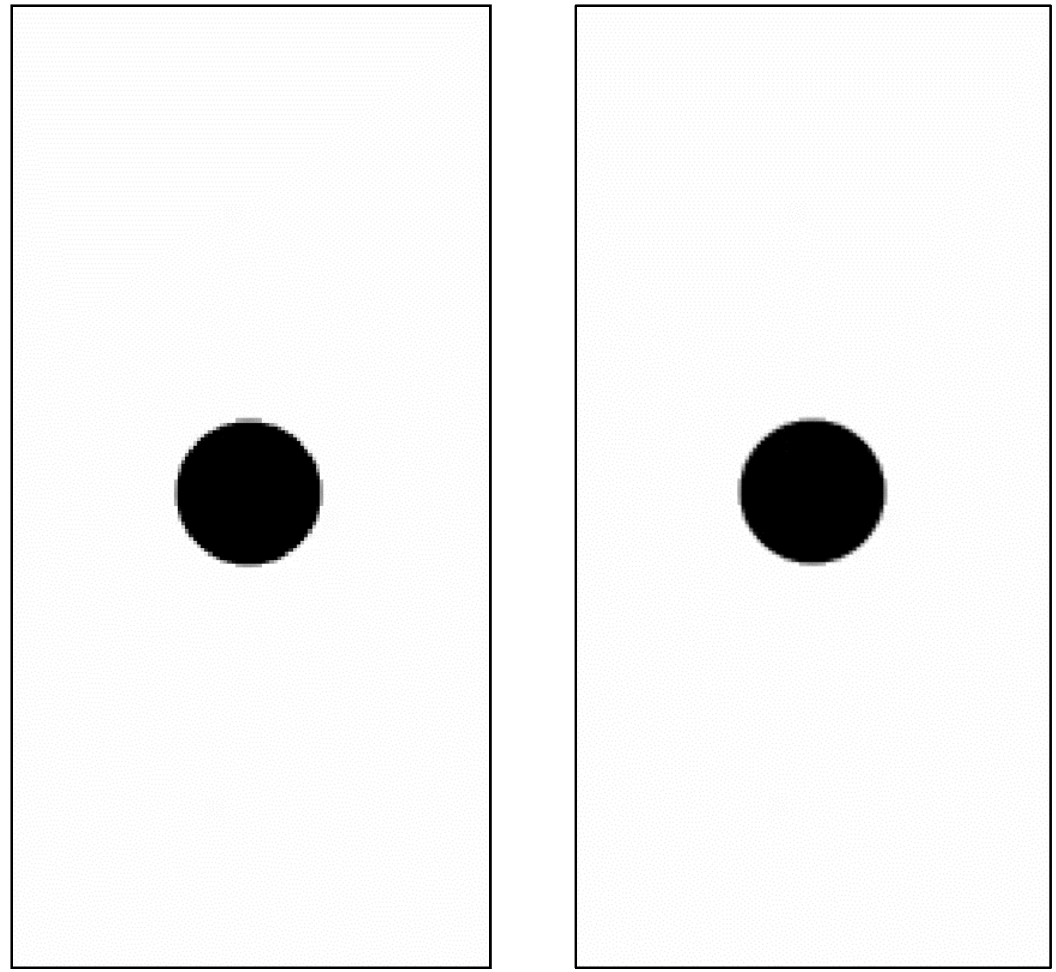


$$\mathbf{F}_{ST} = \sigma \kappa \nabla C$$

$$\kappa = -\nabla \cdot \hat{\mathbf{n}}$$

$$\hat{\mathbf{n}} = \hat{\mathbf{n}}_{\mathbf{wall}} \cos \theta_c + \hat{\mathbf{t}}_{\mathbf{wall}} \sin \theta_c$$

$Bo = 0.2759$



$\theta_c = 70°$ $\theta_c = 170°$

Conclusion

Summary

- VOF method for modeling interfacial flows with large density jumps requires:
  1. Scalar advection scheme that preserves sharp interfaces
  2. Tight coupling between mass and momentum advection

Future work

- Extend to three-dimensions
- Incorporate rigid-body dynamics module for fluid-object interaction
- Employ framework to investigate interfacial flow problems in additive manufacturing, aerospace, energy, biomedical, and other applications

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  - Natalie Pippolo

Bibliography

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