Level-Set and Phase-Field Methods: Application to Moving Interfaces and Two-Phase Fluid Flows

Maged Ismail

Claremont Graduate University
& Keck Graduate Institute

KECK GRADUATE INSTITUTE of Applied Life Sciences

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Claremont GRADUATE UNIVERSITY

Outline

- Background & Motivation
- Level Set Method
- Sharp-Interface Phase-Field Method
- Conservative Level Set Method
- Mathematical Formulation for Two-phase Flows
- Conclusions & Future Work
- Acknowledgments
- References

Background & Motivation

- **Tracking of moving interfaces**

  - Wide range of scientific and engineering applications
  (e.g. two-phase fluid flows, melting and solidification, computer graphics, image segmentation

  - Typically two types of approaches to simulate moving interfaces:

    - Particle Methods (Lagrangian, explicit)

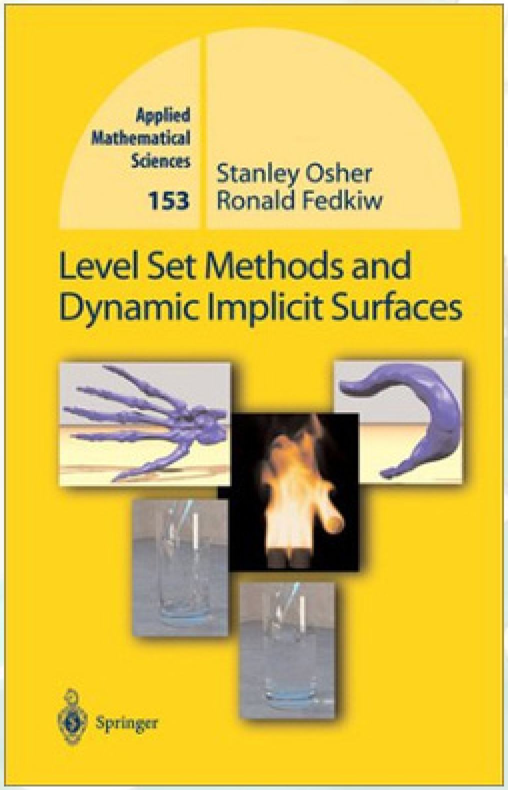
      can't handle topological changes, sharp corners…

    - Level Set Methods (Eulerian, implicit)

      today's topic

Level Set Method

- An implicit method for capturing the evolution of an interface.
- History: Devised by Sethian and Osher (J. Computational Physics,1988) as a simple and versatile method for computing and analyzing the motion of an interface in two or three dimensions.
- Based upon representing an interface as the zero level set of some higher dimensional function.



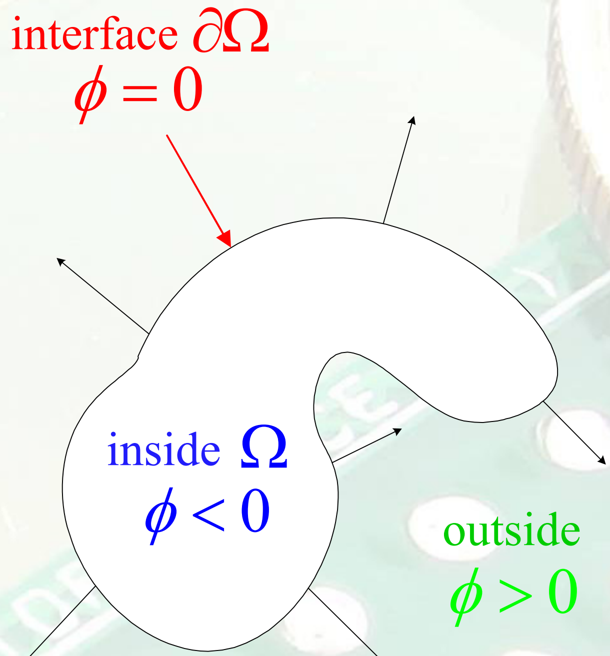
Level Set Method

- **Basic idea**

  To track the evolution of a moving interface:

  ▪ Recast problem with one additional dimension – the distance from the interface.

$$\phi(x,t) = \begin{cases} +d(x,t) & x \notin \Omega \\ 0 & x \in \partial\Omega \\ -d(x,t) & x \in \Omega \end{cases}$$



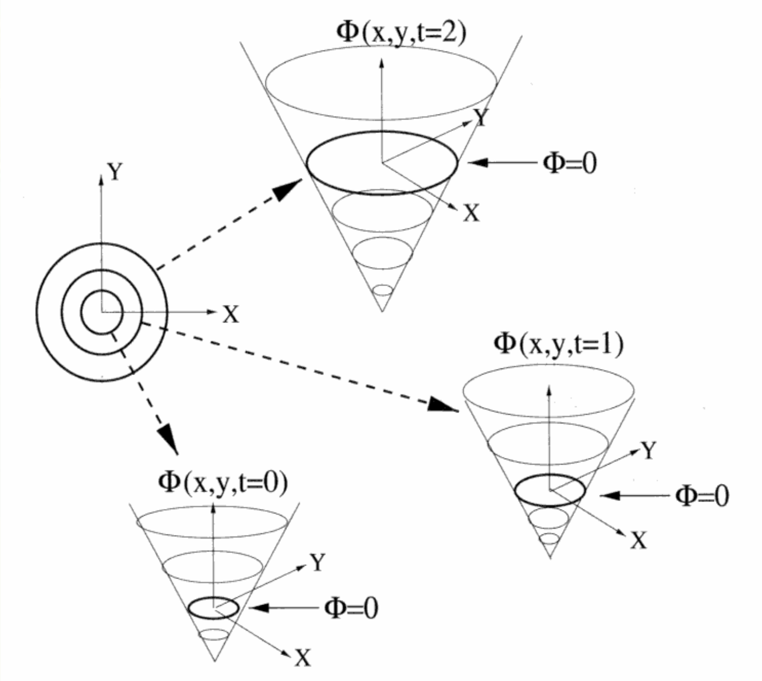
Level Set Method

- The interface always lies at the zeroth level set of the function ϕ
- *i.e.*, the interface is defined by the implicit equation $\phi_t\left(x, y\right) = 0$
- To advance the interface:

Given a velocity field, $\boldsymbol{u}$

The evolution equation becomes:

$$\boxed{\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0}$$



- Interfacial geometric quantities can be easily calculated using ϕ

$$\mathbf{n} = \nabla \phi / |\nabla \phi|, \kappa = \nabla \cdot \mathbf{n}$$

Level Set Method

- **Advantages:**
  - capable of capturing topological changes
  - intrinsic geometric properties are easy to determine
  - relatively easy to implement
  - accurate high order computational schemes exist

- **Difficulties:**
  - computationally expensive
  - re-initialization is needed to maintain the signed distance function
  - not conservative

  loss or gain of mass (area) due to numerical diffusion

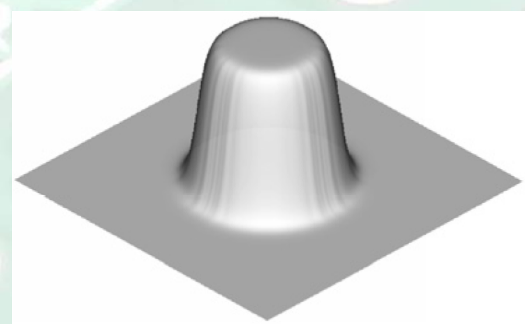
Sharp-Interface Phase-Field Method

- Based on: Sun, Y., and Beckermann, C., "Sharp Interface Tracking Using the Phase-Field Equation," J. Computational Physics, 2007.
- Instead of signed distance function, the phase field function is assumed to be

$$\phi = -\tanh\left(\frac{x}{\sqrt{2}W}\right) \quad \Longrightarrow \quad \phi \to \begin{cases} +1 & \text{inside} \\ \text{smooth transition} & \text{near the interface} \\ -1 & \text{outside} \end{cases}$$

- Using same interface advection equation

$$\boxed{\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0}$$



Sharp-Interface Phase-Field Method

- However, using $\boldsymbol{u} = \boldsymbol{u}_e + (a - b\kappa)\boldsymbol{n}$
  and $\kappa = \nabla \cdot \boldsymbol{n} = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) = \frac{1}{|\nabla \phi|} \left[\nabla^2 \phi - \frac{(\nabla \phi \cdot \nabla)|\nabla \phi|}{|\nabla \phi|} \right]$
- The following evolution equation can be derived

$$\frac{\partial \phi}{\partial t} + a|\nabla \phi| + \boldsymbol{u}_e \cdot \nabla \phi = b\left[\nabla^2 \phi + \frac{\phi(1-\phi^2)}{W^2} - |\nabla \phi| \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) \right]$$

- Descritized using finite difference method
- Simple forward Euler for time discretization (explicit)
- spatial discretization…

Sharp-Interface Phase-Field Method

- Laplacian (9-point finite-difference stencil):

$$\nabla^2 \phi_{i,j} = \frac{2\left(\phi_{i+1,j} + \phi_{i,j+1} + \phi_{i-1,j} + \phi_{i,j-1} - 4\phi_{i,j}\right) + 0.5\left(\phi_{i+1,j+1} + \phi_{i+1,j-1} + \phi_{i+1,j-1} + \phi_{i-1,j-1} - 4\phi_{i,j}\right)}{3\Delta x^2}$$

- Norm of the gradient (central difference):

$$\left|\nabla \phi\right|_{i,j} = \frac{1}{\Delta x}\sqrt{\frac{\left(\phi_{i+1,j} - \phi_{i-1,j}\right)^2}{4} + \frac{\left(\phi_{i,j+1} - \phi_{i,j-1}\right)^2}{4}}$$

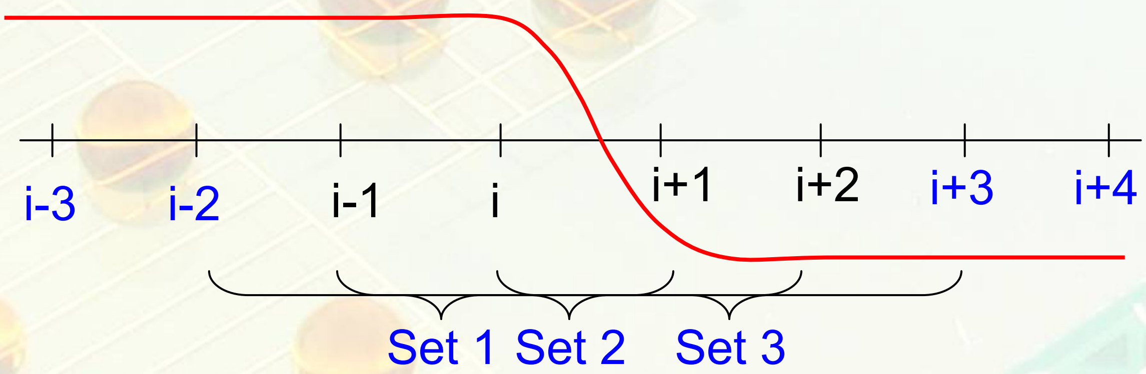
- Curvature (???):

$$\nabla \cdot \left(\frac{\nabla \phi}{\left|\nabla \phi\right|}\right)_{i,j} = \frac{1}{\Delta x}\left(\begin{aligned} &\frac{\phi_{i+1,j} - \phi_{i,j}}{\sqrt{\left(\phi_{i+1,j} - \phi_{i,j}\right)^2 + \left(\phi_{i+1,j+1} + \phi_{i,j+1} - \phi_{i+1,j-1} - \phi_{i,j-1}\right)^2 / 16}} - \frac{\phi_{i,j} - \phi_{i-1,j}}{\sqrt{\left(\phi_{i,j} - \phi_{i-1,j}\right)^2 + \left(\phi_{i-1,j+1} + \phi_{i,j+1} - \phi_{i-1,j-1} - \phi_{i,j-1}\right)^2 / 16}} \\ &+ \frac{\phi_{i,j+1} - \phi_{i,j}}{\sqrt{\left(\phi_{i,j+1} - \phi_{i,j}\right)^2 + \left(\phi_{i+1,j+1} + \phi_{i+1,j} - \phi_{i-1,j+1} - \phi_{i-1,j}\right)^2 / 16}} - \frac{\phi_{i,j} - \phi_{i,j-1}}{\sqrt{\left(\phi_{i,j} - \phi_{i,j-1}\right)^2 + \left(\phi_{i+1,j-1} + \phi_{i+1,j} - \phi_{i-1,j-1} - \phi_{i-1,j}\right)^2 / 16}} \end{aligned} \right)$$

Sharp-Interface Phase-Field Method

- Hyperbolic term $\boldsymbol{u}_e \cdot \nabla \phi$
  (3rd order Essentially-Non-Oscillatory scheme)

Need 4 points to discretize $\nabla \phi$ with third order accuracy



This often leads to oscillations at the interface

Fix: pick the best four points out of a larger set of grid points to avoid/minimize oscillations ("essentially-non-oscillatory")

Sharp-Interface Phase-Field Method

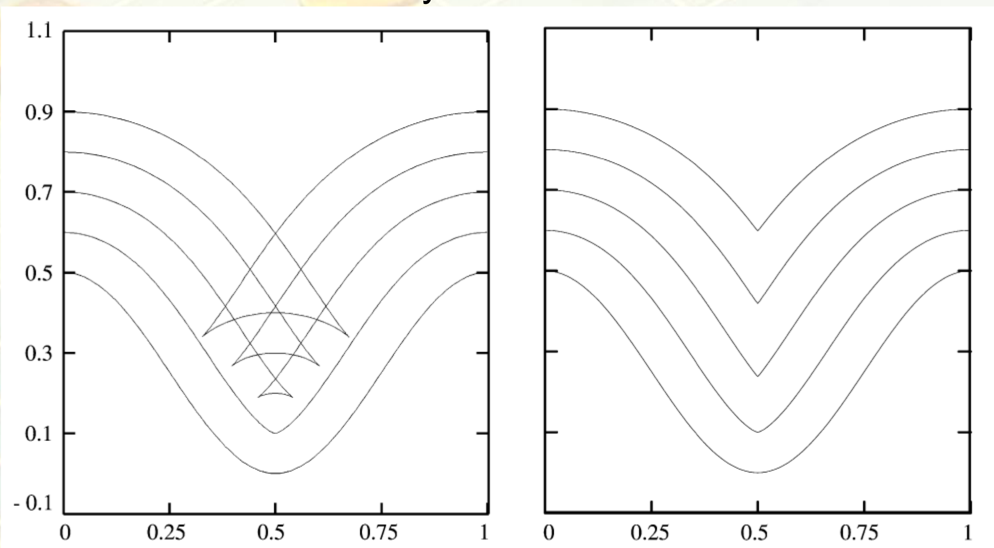
- **Results**

  - Interface motion with a constant normal speed

  periodic cosine curve propagating with normal speed of unity

$$\gamma(0) = \left[1 - s, (1 + \cos 2\pi s)/4\right], \quad 0 \le s \le 1$$

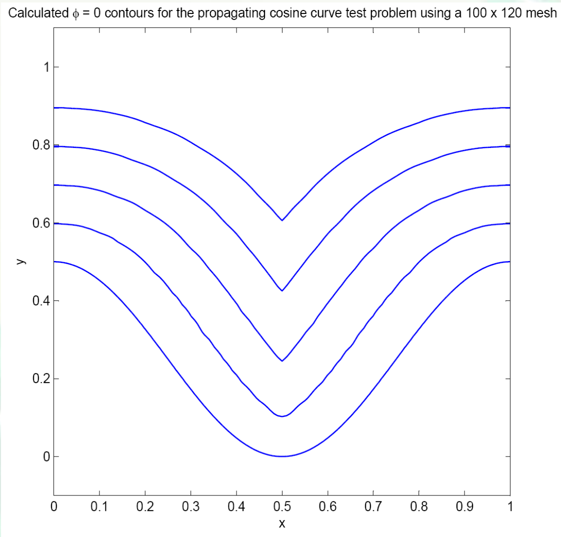
Analytical solutions

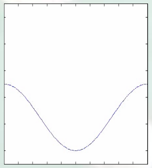


Swallowtail solution

Weak solution (meaningful)

Numerical solution



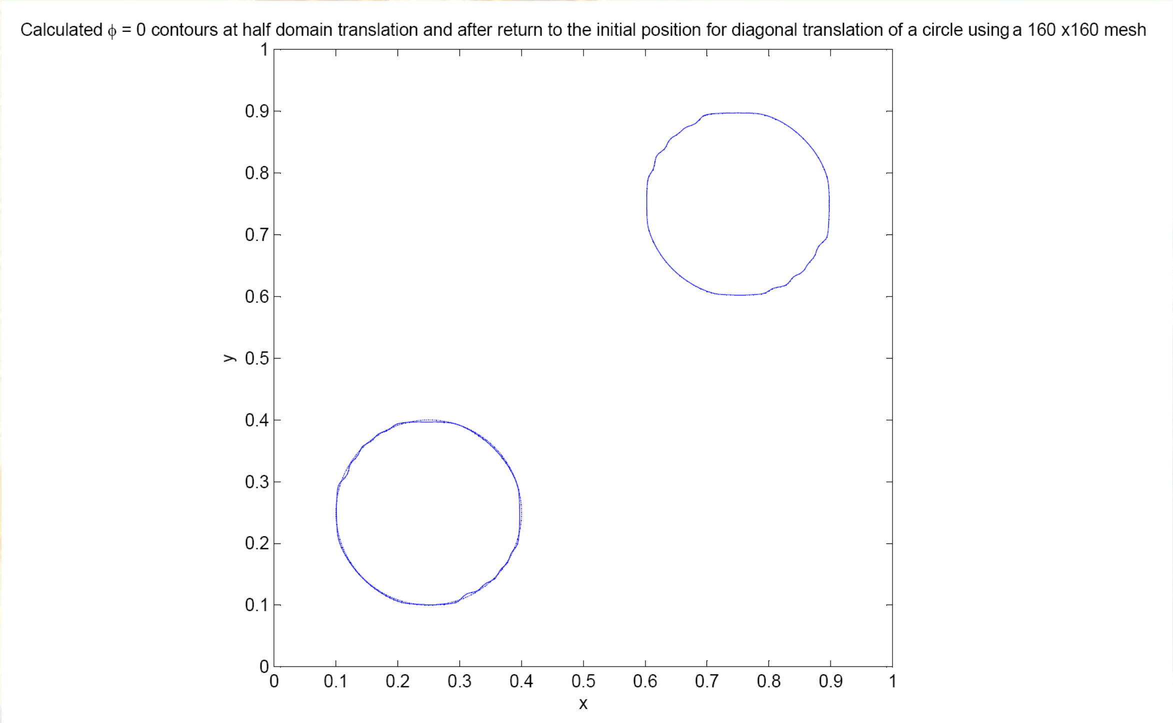


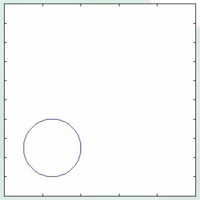
Sharp-Interface Phase-Field Method

- **Results**

  - Interface motion due to external flow fields

  (Diagonal translation of a circle)





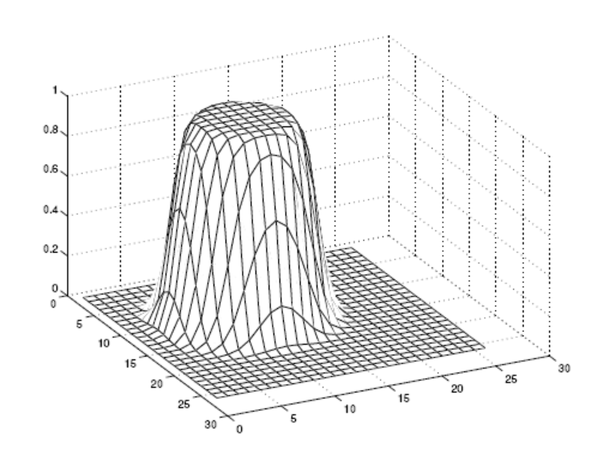
Conservative Level Set Method

- Based on :Olsson, E., Kreiss, G., A conservative level set method for two phase flow, Journal of Computational Physics, 2005.
- **Level set function** ϕ
  smeared out Heaviside instead of signed distance function

$$\phi = H_{sm}\left(\phi_{sd}\right) = \begin{cases} 0, & \phi_{sd} < -\varepsilon, \\ \dfrac{1}{2} + \dfrac{\phi_{sd}}{2\varepsilon} + \dfrac{1}{2\pi}\sin\left(\dfrac{\pi\phi_{sd}}{\varepsilon}\right), & -\varepsilon \le \phi_{sd} \le \varepsilon, \\ 1, & \phi_{sd} > \varepsilon, \end{cases}$$

where $\left|\phi_{sd}\left(\boldsymbol{x}\right)\right| = d\left(\boldsymbol{x}\right) = \min_{\boldsymbol{x}_\Gamma \in \Gamma}\left(\left|\boldsymbol{x} - \boldsymbol{x}_\Gamma\right|\right)$

- **Interface represented by** $\phi = 0.5$



Conservative Level Set Method

- **Evolution equation of** ϕ

  - **Standard level set method** $\dfrac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = 0$

    ▪ loss or gain of mass (area) due to numerical diffusion

    ▪ interface shape is not preserved

  - **Modified equation (non-conservative form):** add

    ▪ shape preserving artificial compression

    ▪ artificial diffusion to smear the profile (avoid discontinuities)

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

Conservative Level Set Method

- **Modified equation (conservative form)**

▪ divergence free velocity field

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

▪ shape of the level set function stabilized across the interface

▪ exact numerical conservation of the integral of ϕ

▪ the above equation can be split into two steps:

Advection + Reinitialization

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) = 0 \quad , \quad \frac{\partial \phi}{\partial \tau} = \gamma \left[\nabla \cdot \left(\varepsilon \nabla \phi - \phi (1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \right]$$

Mathematical Modeling of Two-phase Flows

- **Incompressible Navier-Stokes equations ($10^6 prize)**

Conservation of mass (Continuity equation):

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

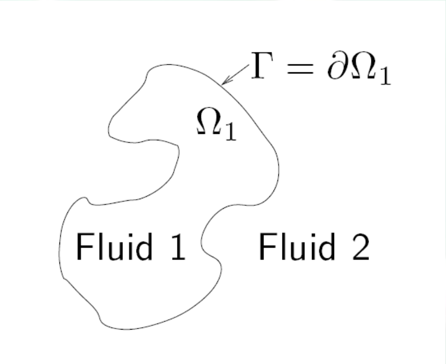
Conservation of linear momentum (Newton's 2nd law):

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{t}} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) = -\nabla p + \nabla\cdot\left(\mu\left(\nabla\boldsymbol{u} + \left(\nabla\boldsymbol{u}\right)^T\right)\right) + \rho\boldsymbol{g} + \sigma\kappa\delta\boldsymbol{n} + \boldsymbol{F}$$

density and dynamic viscosity depend on ϕ

$$\rho = \rho_1 + \left(\rho_2 - \rho_1\right)\phi$$

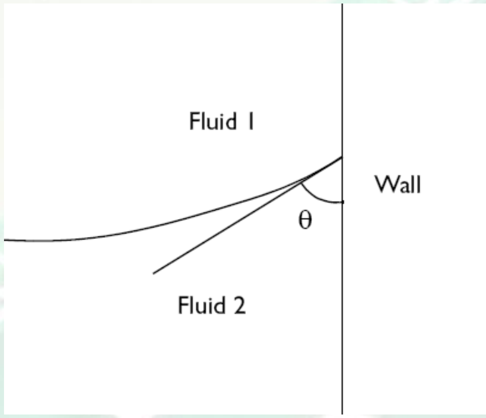
$$\mu = \mu_1 + \left(\mu_2 - \mu_1\right)\phi$$



Numerical Simulation

- COMSOL Multiphysics 3.3a (formerly FEMLAB)
- solving the NS eqns coupled with the modified conservative / non-conservative level-set equation using finite-element method
- computational time for each case ~ 1-6 hours on Pentium 4, 3GHz processor with 2GB of RAM
- special treatment of moving three-phase contact-line

wetted wall boundary condition:



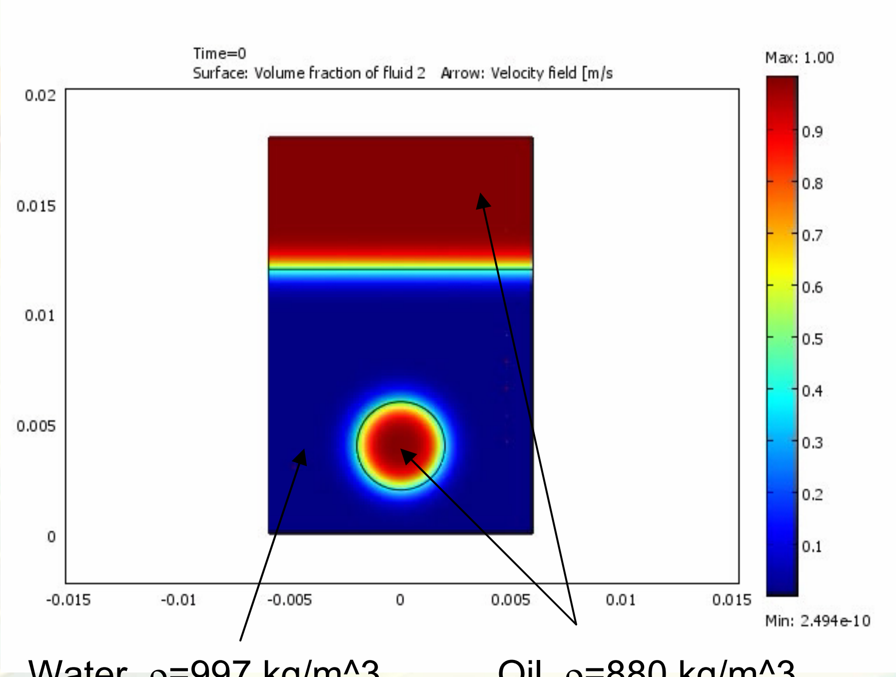
- enforces slip $\boldsymbol{u} \cdot \boldsymbol{n}_{\text{wall}} = 0$
- adds a frictional force $\boldsymbol{F}_{\text{fr}} = -\frac{\eta}{\beta} \boldsymbol{u}$
- adds the weak boundary term

$$\int_{\partial\Omega} \text{test}(\boldsymbol{u}) \cdot \left[\sigma \left(\boldsymbol{n}_{\text{wall}} - (\boldsymbol{n} \cos\theta) \right) \delta \right] dS$$

Results

- **Rising bubble**
  oil bubble rising up through water

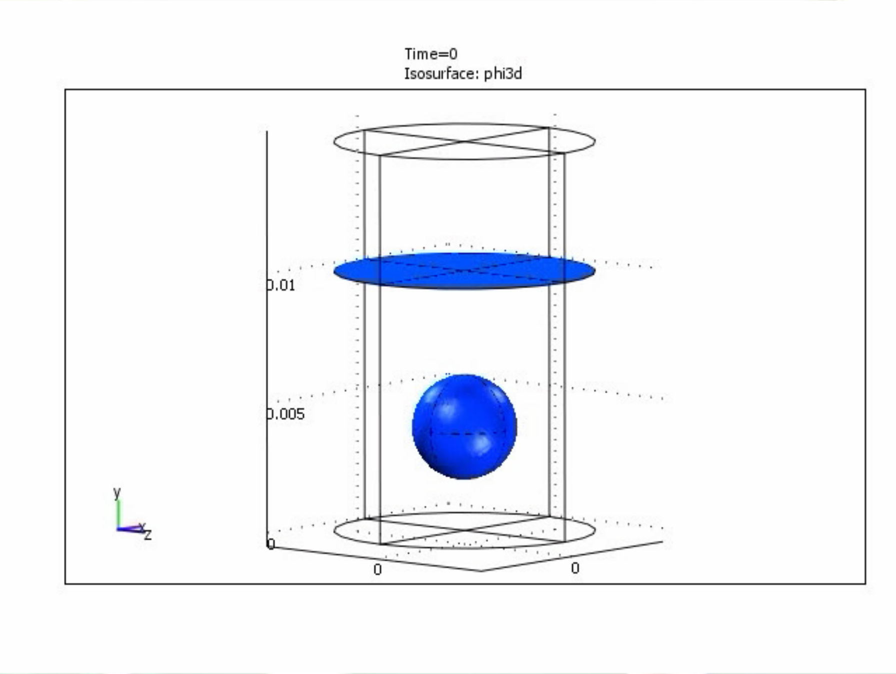
2D case



Water, ρ=997 kg/m^3

Oil, ρ=880 kg/m^3

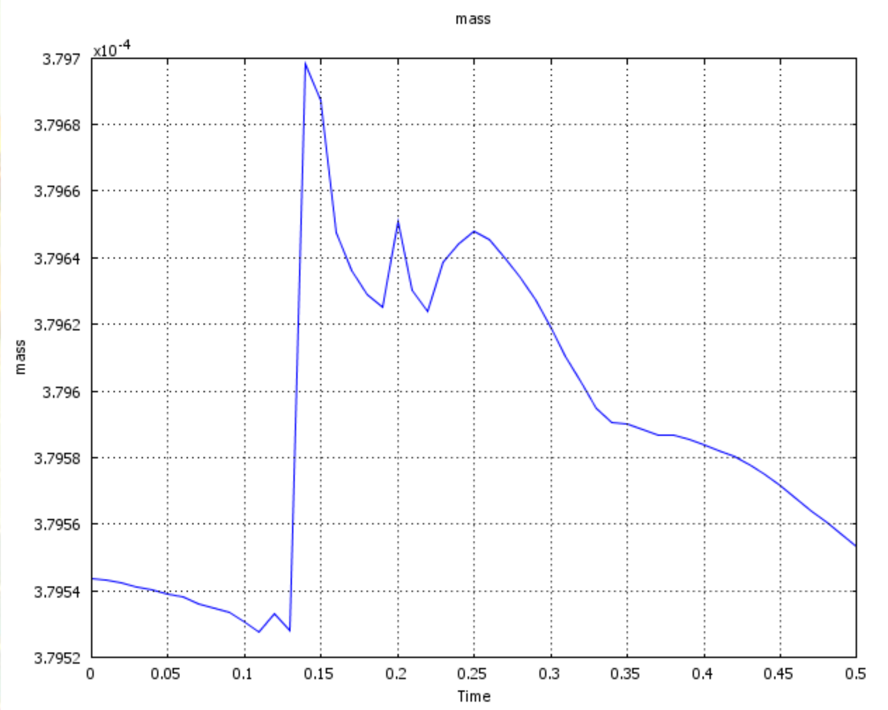
2D axisymmetric (revolved to 3D)



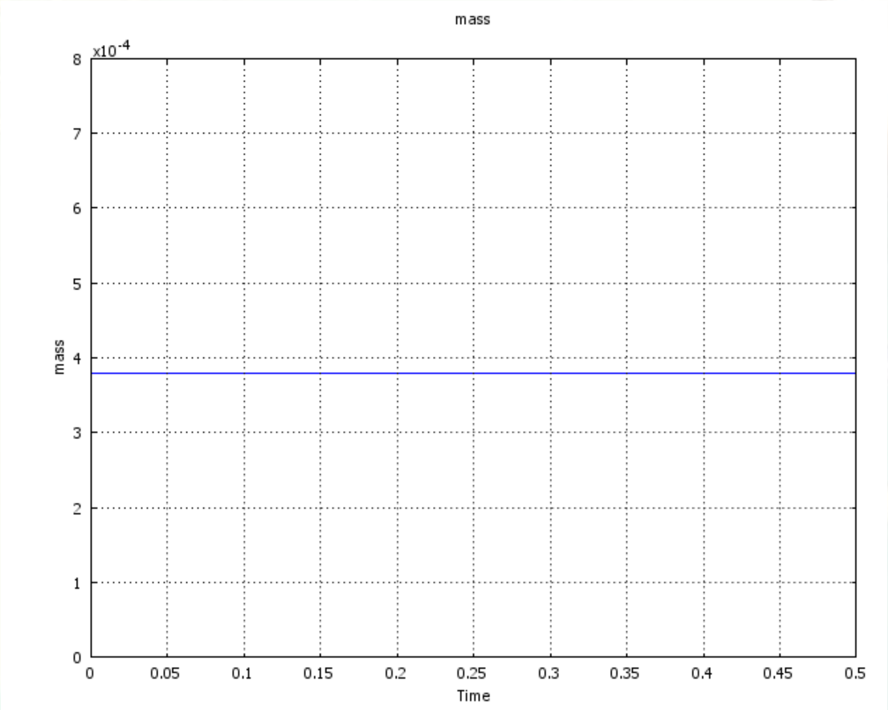
Results (cont.)

- **Rising bubble**

  mass conservation (axisymmetric case)



Non-conservative

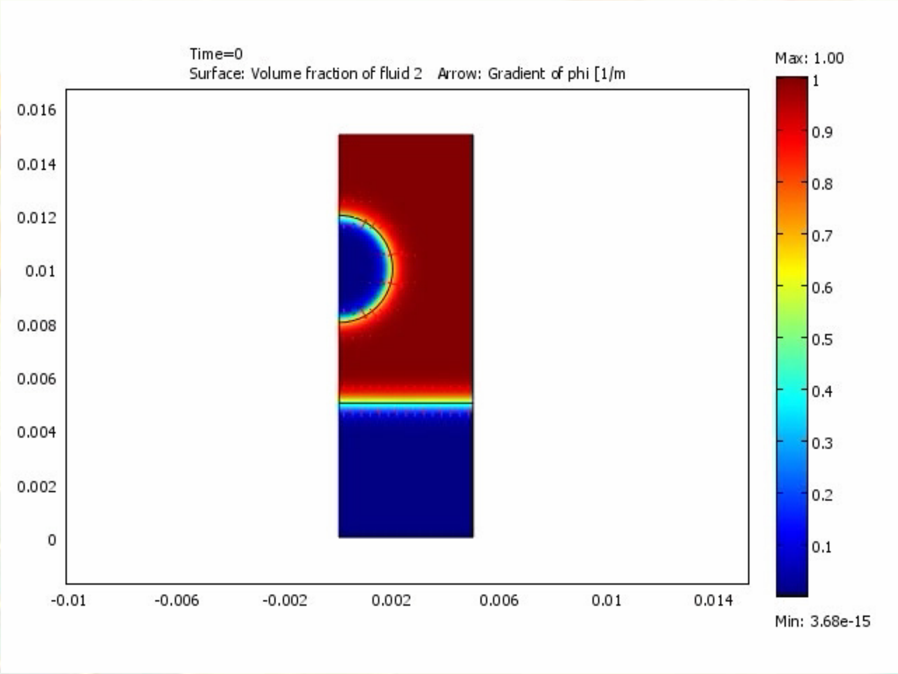


Conservative

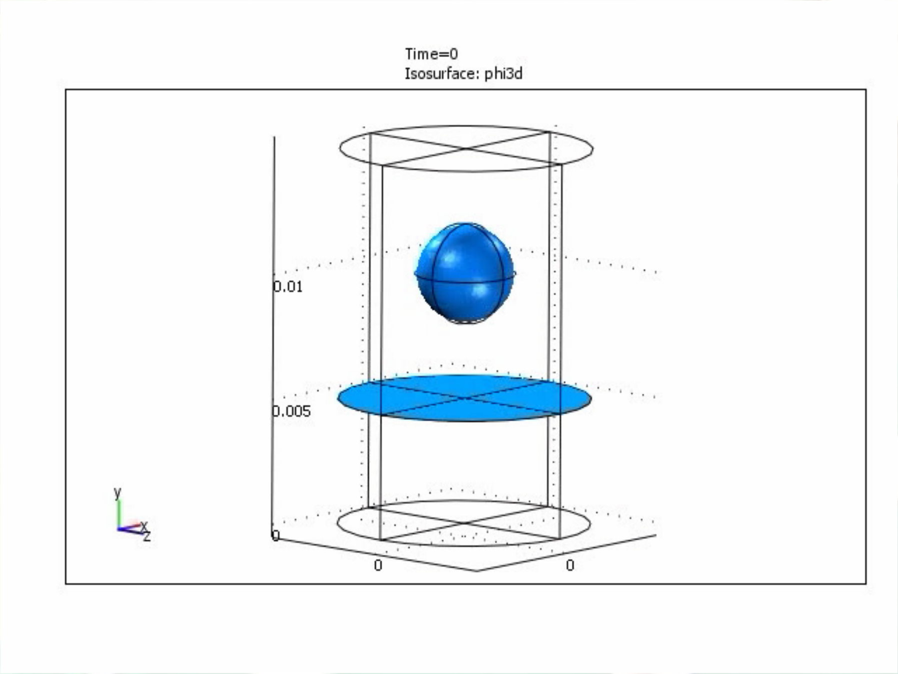
Results (cont.)

- **Falling droplet**

2D axisymmetric

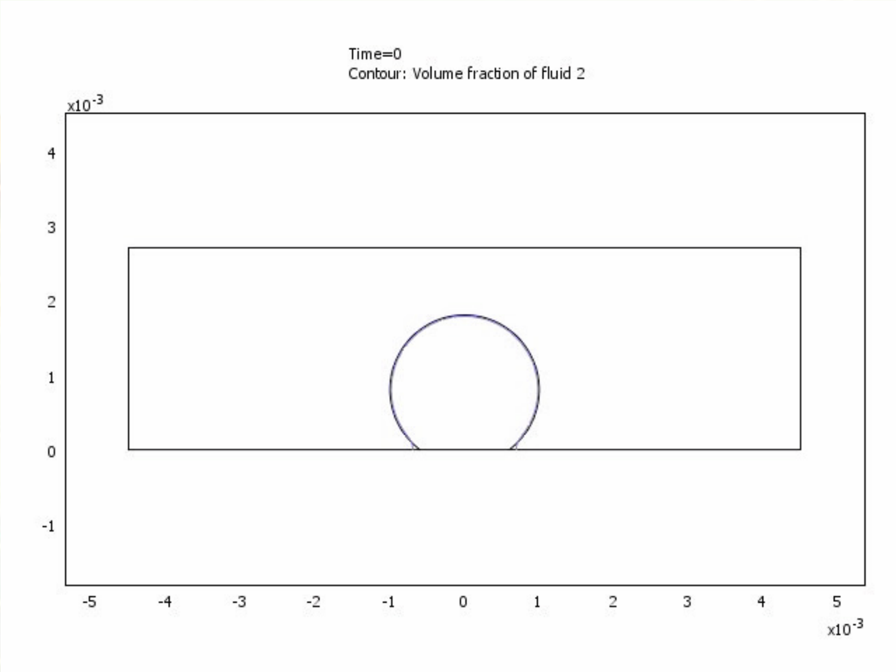


2D axisymmetric (revolved to 3D)

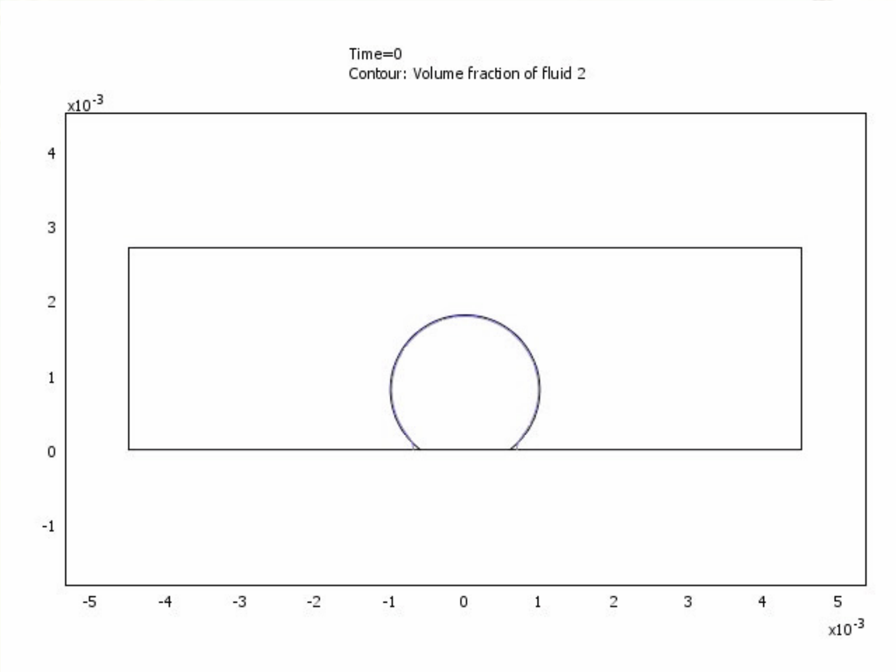


Results (cont.)

- **Droplet spreading** (moving contact lines!)



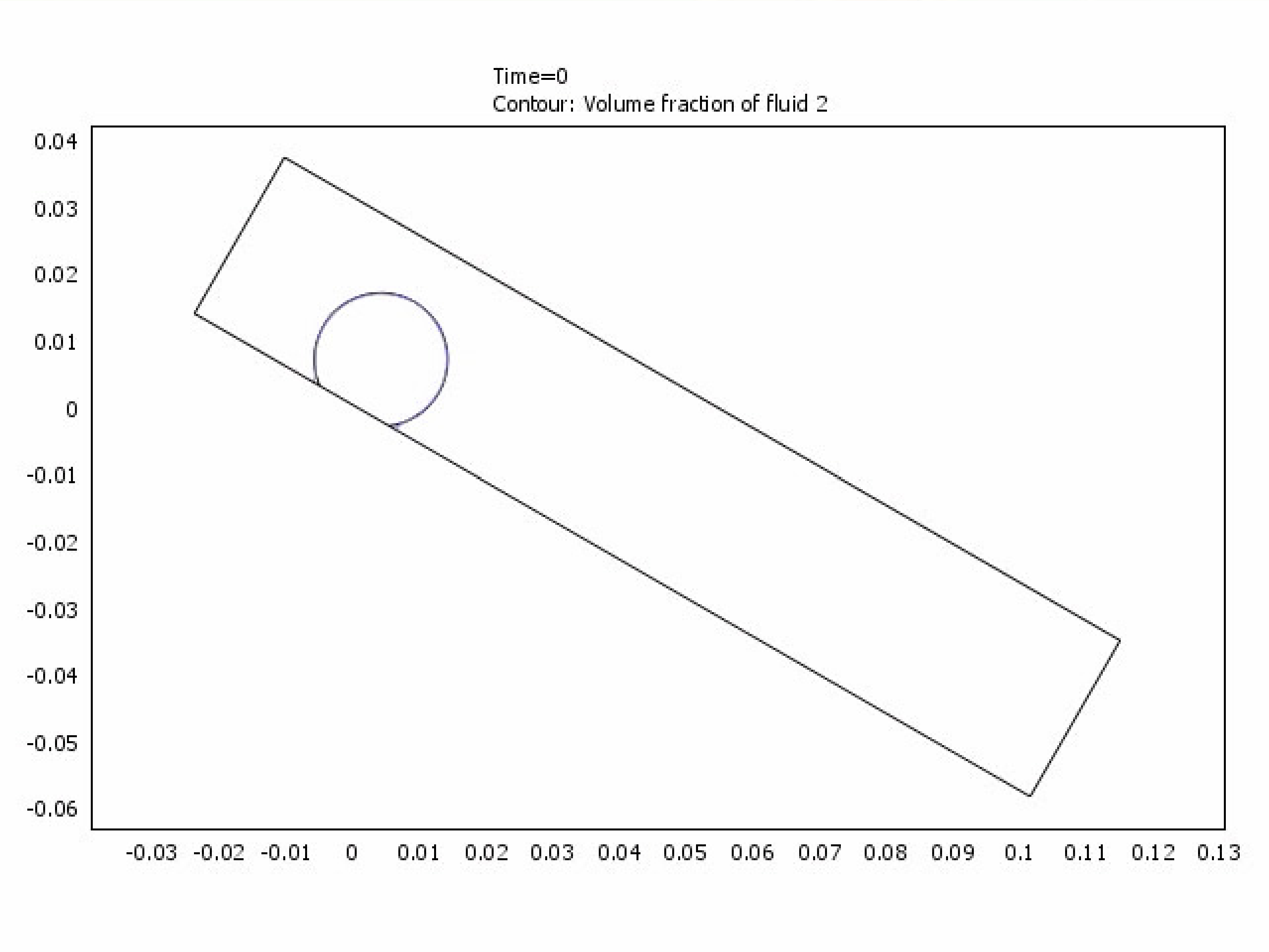
zero gravity



with gravity

Results (cont.)

- **Droplet sliding/spreading down an inclined plane**



Conclusions

- Several variants of the standard level-set method exist.
- Sharp-interface phase-field method implemented in Matlab using FD discretization and used for tracking propagating interfaces.
- Conservative level-set method tested on several two-phase flow benchmark cases.
- Problems with moving contact-line also considered.

Future Work

- Validation with published experimental/analytical results
- Implementing the sharp-interface phase-field method in COMSOL Multiphysics
- Application to droplet-microfluidics
- Extension to three-dimensional cases (parallel-computing!)
- Funding…proposals

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- Support from KGI/CGU

References

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- Sun, Y., Beckermann, C., 2007, Sharp Interface Tracking Using the Phase-Field Equation, Journal of Computational Physics, Vol. 220, pp. 626-653.

Questions

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Thank you!