Unified models for Mixing Fluids

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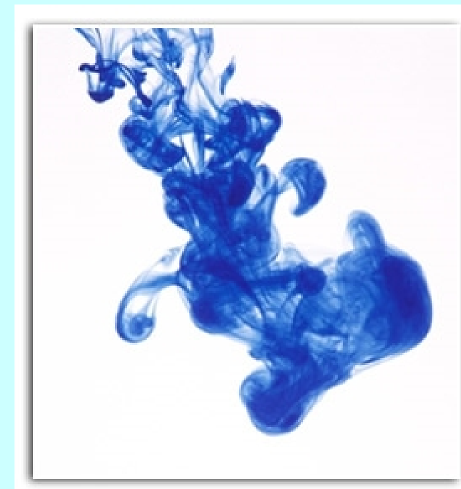
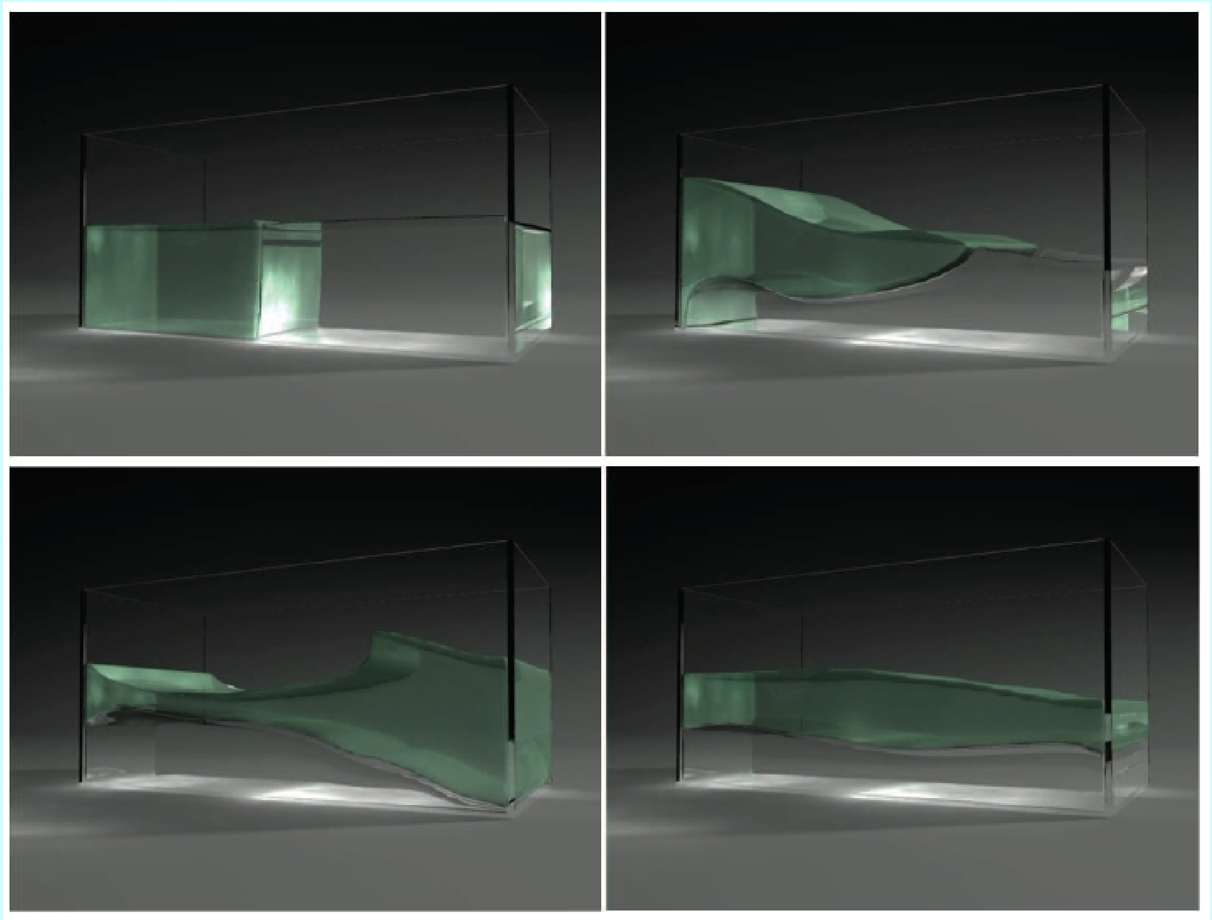
Unified Models for Mixing Fluids

- Large density interface problems in fluids:
  - drop formation
  - puddles on surface
  - separation of dissimilar fluids
- We will look at 2 different solutions for this problem



A Unified Handling of Immiscible and Miscible Fluids



CASA
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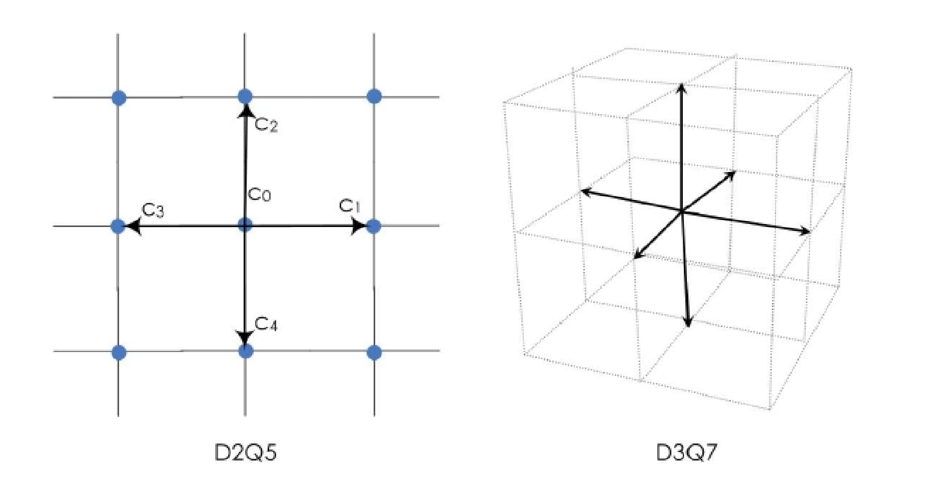
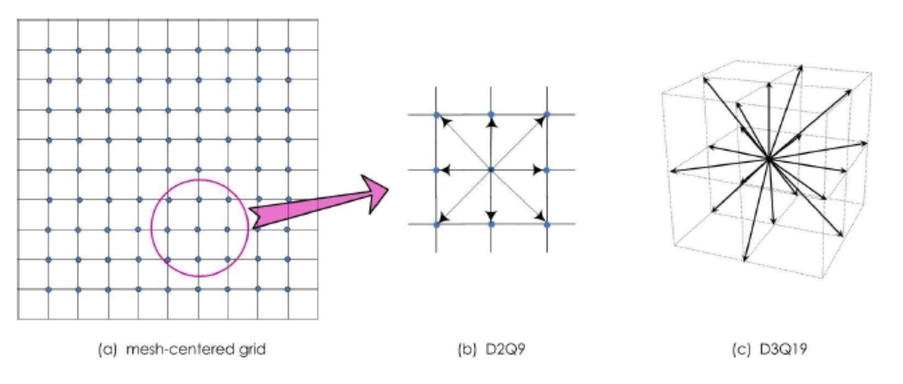
A Unified Handling of Immiscible and Miscible Fluids

- Uses chemical potential energy formulations to alter time-varying concentration fields
- The concentration fields determine the interfaces
- Uses Lattice Boltzmann method

What is the Lattice Boltzmann Method?





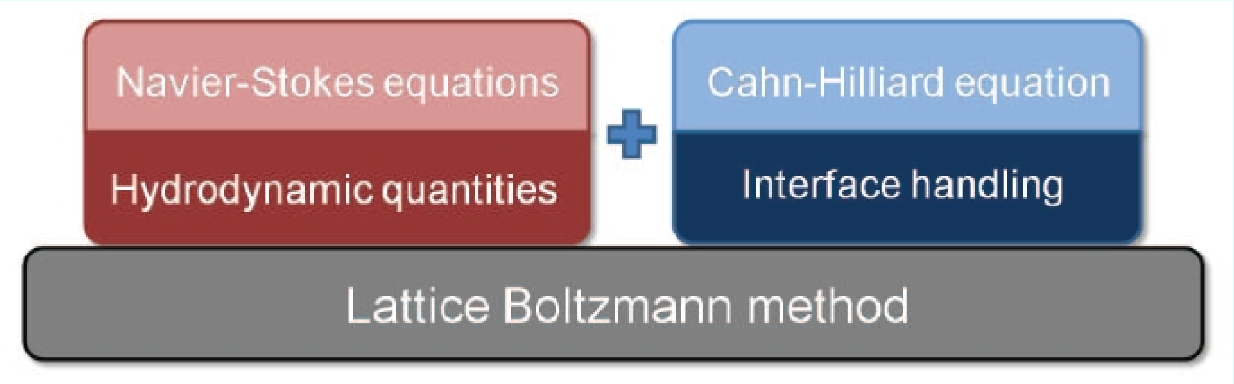
- Simulates a Newtonian fluid with collision models (A Newtonian fluid flows no matter how fast it is stirred, i.e. water, not pudding)
- Simulated particles move between neighboring nodes of a discrete lattice
- "the viscous flow behavior emerges automatically from the intrinsic particle streaming and collision processes" -- Wikipedia

Why use the Lattice Boltzmann Method?

- Local dynamics (like SPH) reduce computation
- Easy to model multiphase models by modifying the collision process
- No need for ad-hoc reinitialization of particles or creation of fictitious particles (as in level-set methods)
- Easy to adapt for parallelization

Solution with the Lattice Boltzmann Method

- Use the Lattice Boltzmann method to solve both C-H & N-S eqns



- Concentration Field with normalized values [0,1] represents how much of a substance exists in the space
  - .5 is high potential
  - 0,1 are low potential
- The isosurface represents interface between fluids

$$\{x \mid c(x,t) = 0.5\}$$

Solution with the Lattice Boltzmann Method

- Concentration field evolution is governed by the Cahn-Hilliard equation
- Models steady decrease of free energy of miscibility
- In other words: segregation of separate fluids over time
- Free energy

$$\mathcal{F}(C) = \int_\Omega [B(C) + I(C)]\, dx,$$

- Interfacial energy

$$I = \frac{1}{2}\kappa|\nabla c(\mathbf{x},t)|^2$$

- Bulk energy (zero for miscible fluids)

$$B = c^2(1-c)^2,$$

Solution with the Lattice Boltzmann Method

- C-H equation for N fluids

$$\frac{DC}{Dt} = M \triangle \Upsilon,$$

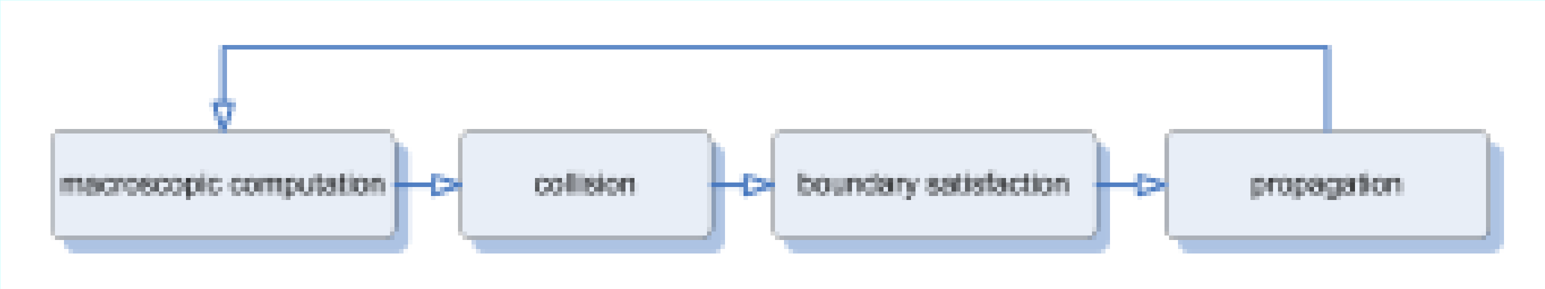
$$\Upsilon = (\mu_1, \mu_2, \ldots, \mu_n)$$

$$\mu_i = \frac{\delta F}{\delta c_i} = \frac{\partial f}{\partial c_i} - \kappa_i \triangle c_i$$

- Need to solve (N-1) C-H eqns for N fluids
- For surface tension, they multiply chemical potential by concentration and sum over all the fluids

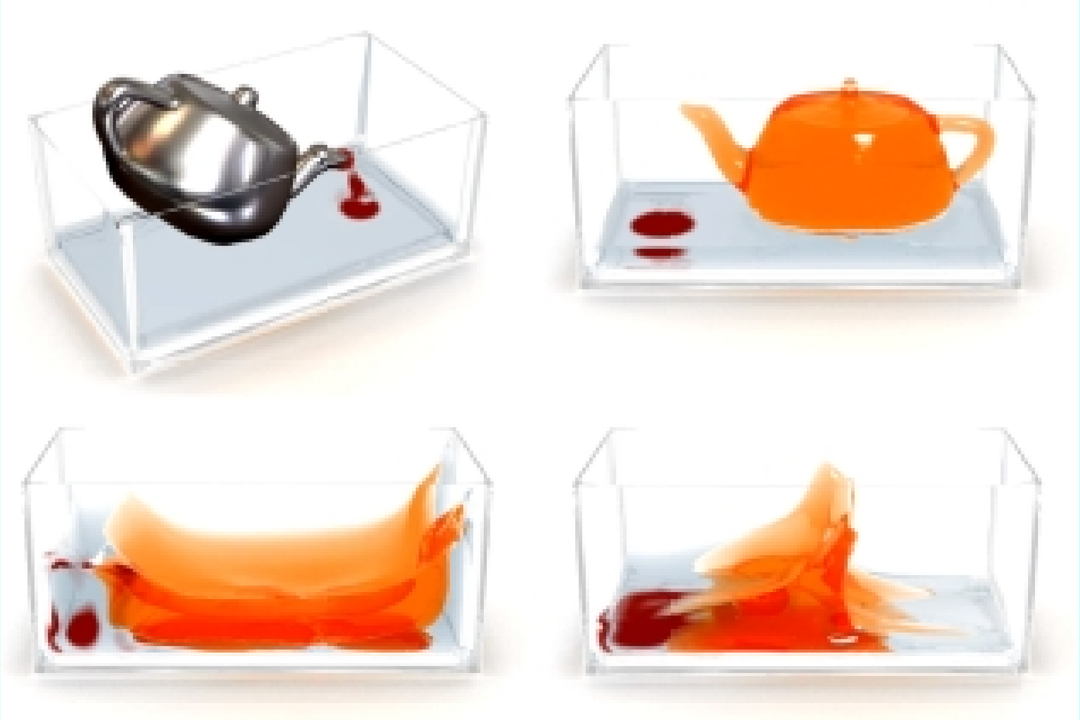
$$\sum_i \mu_i \nabla c_i$$

Solution with the Lattice Boltzmann Method



- LBM computation process is as follows:
- Macroscopic computation (density, velocity, and concentration are calculated from distribution functions)
- Collision (Bhatnagar-Gross-Krook method)
- Boundary condition satisfaction
- Propagation (move to neighboring nodes)
- Repeat for next time step...

Results



Contributions

- Unified handling of multiple miscible and immiscible fluids
- Guaranteed conservation of concentration
- Handles fluids with very low viscosity
- Easily & massively parallelizable

Density Contrast SPH Interfaces

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What is Smoothed Particle Hydrodynamics?

- A Lagrangian method (mesh-free) where information moves with particles, not through a grid
- Particles have smoothing length which defines their neighborhood
- Their properties are smoothed over this length using a kernel function (cubic spline or Gaussian)
- Properties are summed based on properties of particles in neighborhood
- Sum is weighted by distance and density and kernel function

What is Smoothed Particle Hydrodynamics?

- Basic SPH equation for any property A

$$A(\mathbf{r}) = \sum_j \frac{m_j}{\rho_j} A_j W(\mathbf{r} - \mathbf{r}_j, h),$$

- Example of using it for density

$$\rho_i = \sum_j m_j W(\mathbf{r}_{ij}, h)$$

- For fluid simulation using Navier-Stokes eqns we want to find pressure and viscosity fields
- Gradient example

$$\nabla A(\mathbf{r}) = \sum_j m_j \frac{A_j}{\rho_j} \nabla W(|\mathbf{r} - \mathbf{r}_j|, h).$$

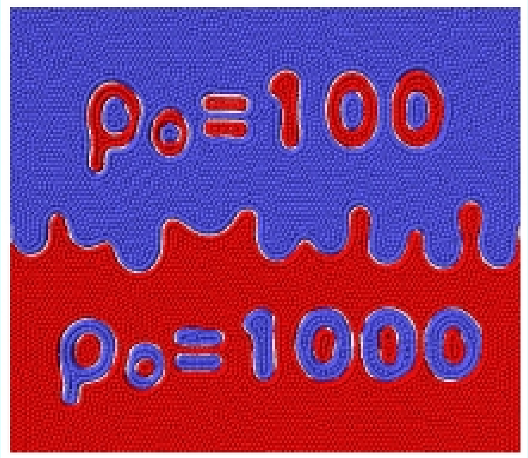
What is Smoothed Particle Hydrodynamics?

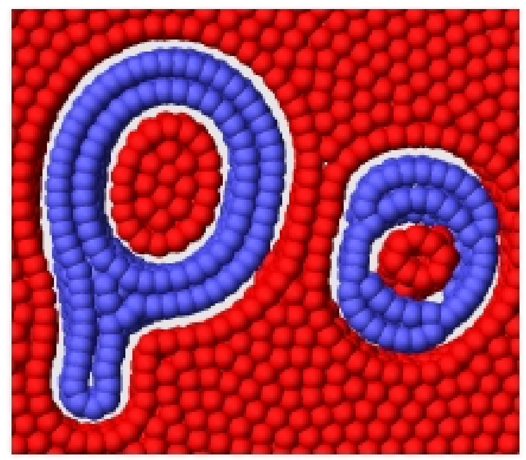
- Pressure $$p_i = \frac{k\rho_0}{\gamma}((\frac{\rho_i}{\rho_0})^\gamma - 1)$$
- Pressure Force $$\mathbf{F}_i^{pressure} = -\frac{m_i}{\rho_i}\sum_j \frac{m_j}{\rho_j}\frac{p_i + p_j}{2}\nabla W(\mathbf{r}_{ij}, h)$$
- Viscosity Force $$\mathbf{F}_i^{viscosity} = \frac{m_i}{\rho_i}\sum_j \frac{\mu_i + \mu_j}{2}\frac{m_j}{\rho_j}(\mathbf{v}_j - \mathbf{v}_i)\nabla^2 W(\mathbf{r}_{ij}, h),$$

What is Smoothed Particle Hydrodynamics?

- Pros
  - Conservation of mass for free
  - Lends itself to adaptivity by changing smoothing length locally (based on density)
  - Implicitly models fine detail (droplets)
- Cons
  - Adaptivity can only be based on density b/c it is Lagrangian in nature
  - Mesh generation

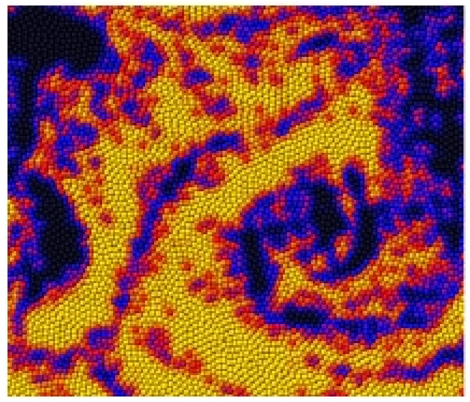
Problems with standard SPH





- Rest densities and masses of neighboring particles that vary within the smoothing length can cause:
  - unphysical density/pressure variations
  - unnatural interface tensions
  - numerical instabilities

Problems with standard SPH

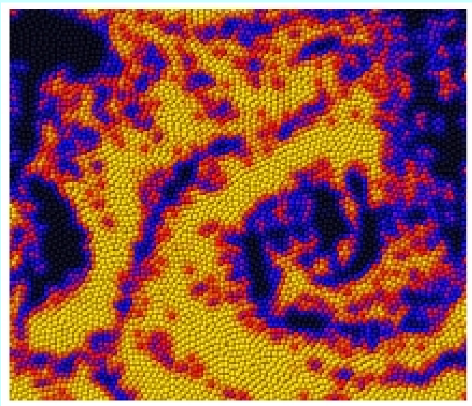


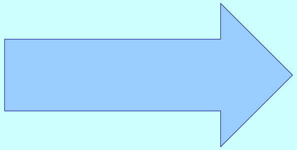
Standard SPH Density

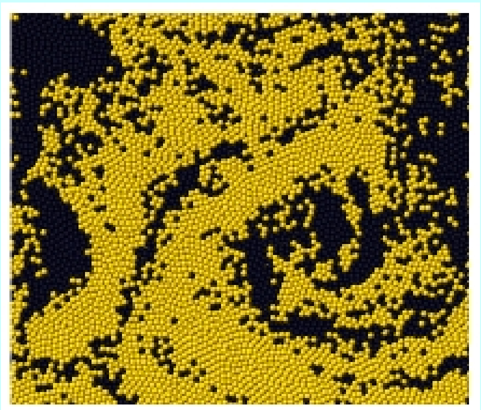
- Standard density summation is a problem when neighbors have different rest densities (and thus different masses)
- Close to interface, particle density is over/under-estimated (smoothed)
- Bad densities lead to false pressure which in turn leads to wrong interface tension which creates a large gap at interface (or worse -- instability)
- Numerical instabilities occur when density ratios > 10 exist (smaller time steps don't help)

Solution to standard SPH problems

- Compute density based on particle number density
- Derive new formulas for pressure, pressure forces, and viscous forces
- Add a new interface tension model







Solution to standard SPH problems

Solution to standard SPH problems:

- New Particle Density $\delta_i = \sum_j W(\mathbf{r}_{ij}, h).$ (each particle assumes neighbors have same rest density & mass as themselves)
- Adapted Density

$$\rho_i = \sum_j m_j W(\mathbf{r}_{ij}, h) \quad \Rightarrow \quad \tilde{\rho}_i = m_i \delta_i = m_i \sum_j W(\mathbf{r}_{ij}, h).$$

- Adpated Volume $V_i = \frac{m_i}{\tilde{\rho}_i} = \frac{1}{\delta_i}.$

Solution to standard SPH problems

Solution to standard SPH problems:

- Adapted Pressure

$$p_i = \frac{k\rho_0}{\gamma}((\frac{\rho_i}{\rho_0})^\gamma - 1) \quad \Rightarrow \quad \tilde{p}_i = \frac{k\rho_0}{\gamma}((\frac{\tilde{\rho}_i}{\rho_0})^\gamma - 1)$$

- Pressure Gradient Term

$$a = -\frac{\nabla p}{\delta m} \quad \Rightarrow \quad a = -\frac{\nabla \tilde{p}}{\delta m}$$

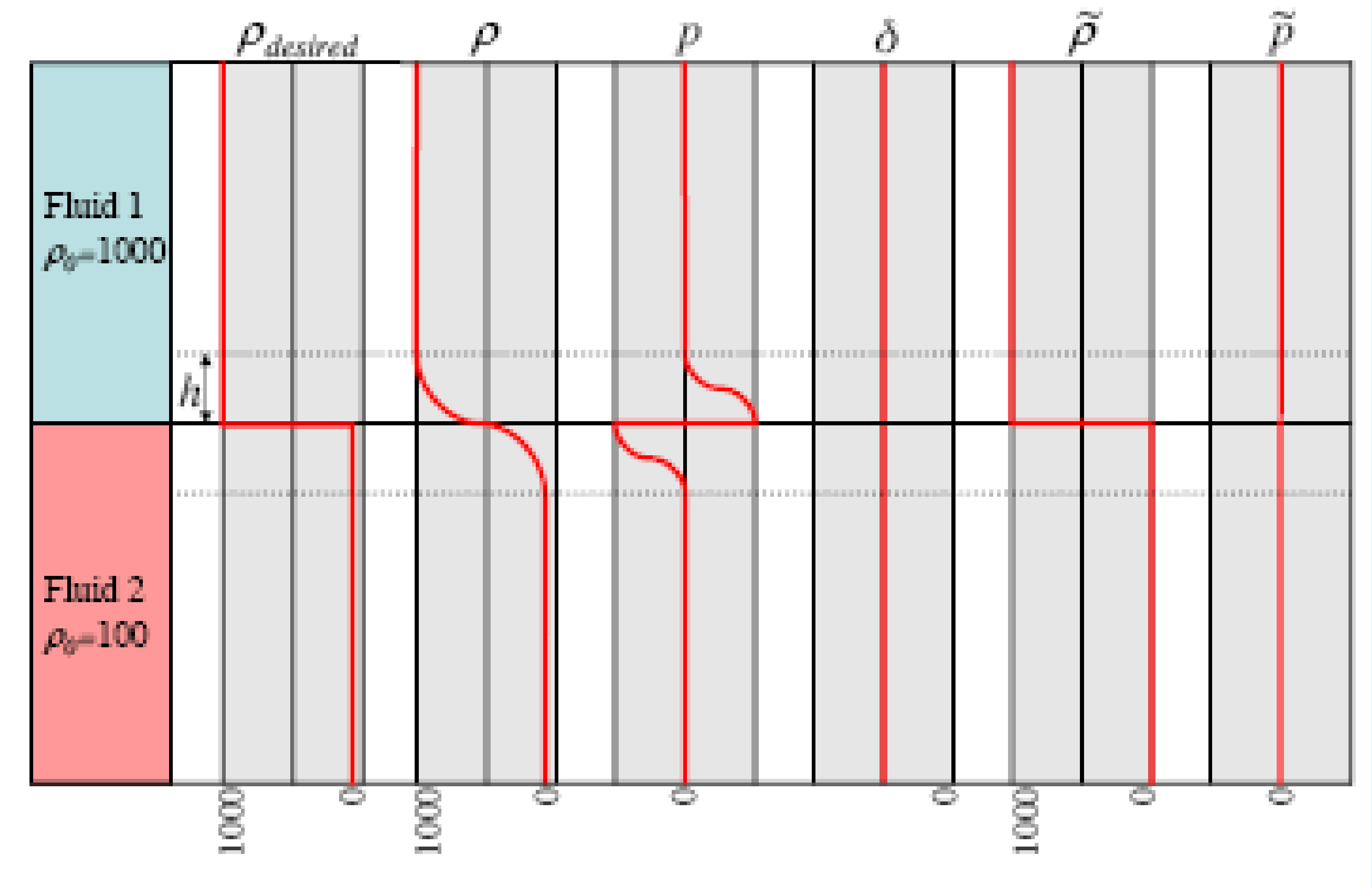
- Pressure Force

$$\mathbf{F}_i^{pressure} = -\frac{m_i}{\rho_i}\sum_j \frac{m_j}{\rho_j}\frac{p_i + p_j}{2}\nabla W(\mathbf{r}_{ij}, h) \quad \Rightarrow \quad \mathbf{F}_i^{pressure} = -\frac{1}{\delta_i}\sum_j \frac{1}{\delta_j}\frac{\tilde{p}_i + \tilde{p}_j}{2}\nabla W(\mathbf{r}_{ij}, h)$$

- Viscous Forces

$$\mathbf{F}_i^{viscosity} = \frac{m_i}{\rho_i}\sum_j \frac{\mu_i + \mu_j}{2}\frac{m_j}{\rho_j}(\mathbf{v}_j - \mathbf{v}_i)\nabla^2 W(\mathbf{r}_{ij}, h), \quad \Rightarrow \quad \mathbf{F}_i^{viscosity} = \frac{1}{\delta_i}\sum_j \frac{\mu_i + \mu_j}{2}\frac{1}{\delta_j}(\mathbf{v}_j - \mathbf{v}_i)\nabla^2 W(\mathbf{r}_{ij}, h)$$

Solution to standard SPH problems



New Interface Tension Model

- Interface Tension force

$$\mathbf{F}^{interface} = \frac{1}{\delta_i}\sigma\kappa\mathbf{n}$$

- Define a colorfield (non-zero at each particle position) to compute curvature and normals
- Smoothed, normalized colorfield

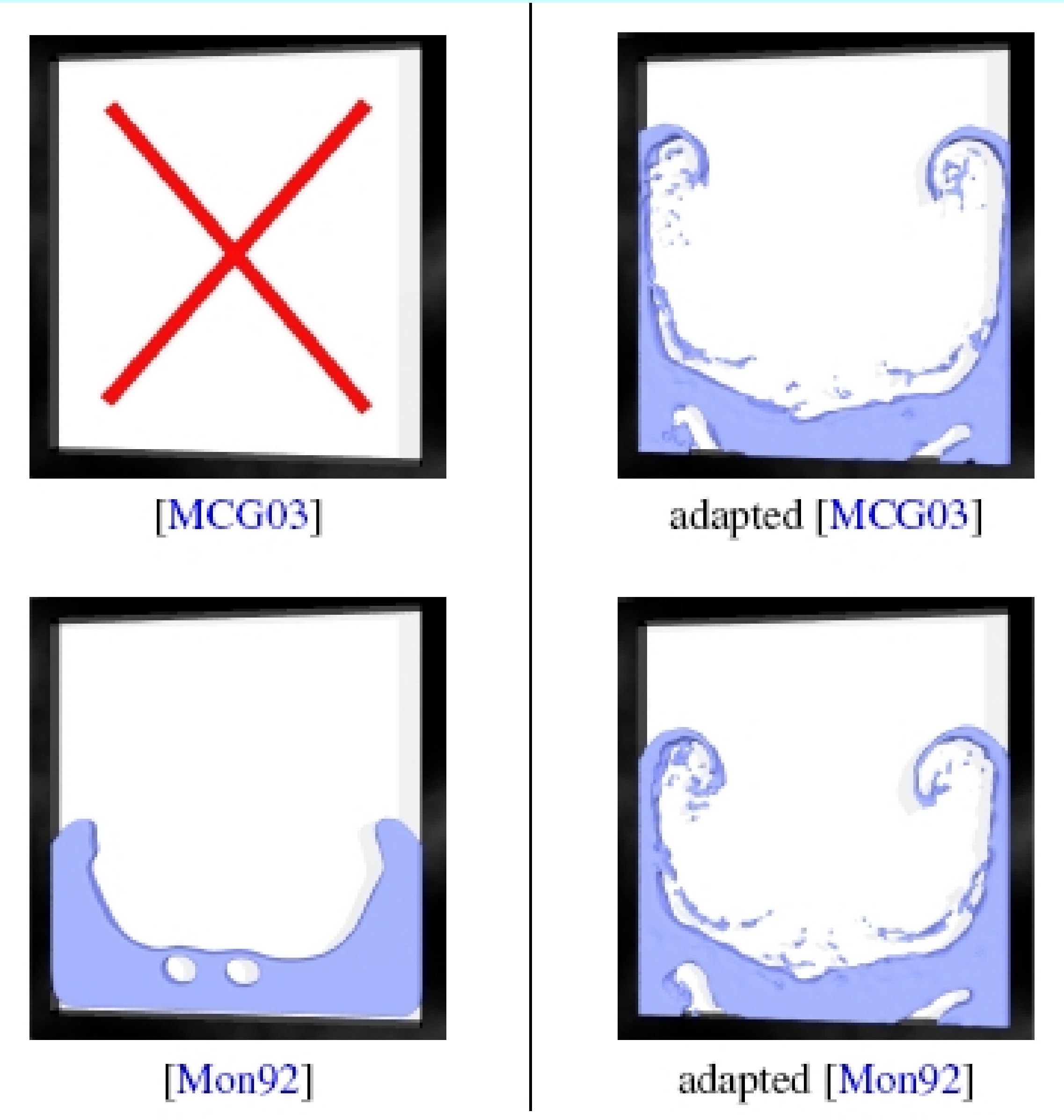
$$<c>_i = \frac{\sum_j \frac{1}{\delta_j} c_j W(\mathbf{r}_{ij}, h)}{\sum_j \frac{1}{\delta_j} W(\mathbf{r}_{ij}, h)}$$

- SPH formulations of normal and curvature using the colorfield

$$\mathbf{n}_i = \sum_j \frac{1}{\delta_j}(<c>_j - <c>_i)\nabla W(\mathbf{r}_{ij}, h)$$

$$\kappa = \frac{-\sum_j \frac{1}{\delta_j}(\hat{\mathbf{n}}_j - \hat{\mathbf{n}}_i)\cdot\nabla W(\mathbf{r}_{ij}, h)}{\sum_j \frac{1}{\delta_j} W(\mathbf{r}_{ij}, h)}$$

Results



Contributions

- Unified handling of multiple miscible and immiscible fluids
- Solves physically incorrect interface problems inherent in basic SPH
- Solves numerical instability problems
- ... and does so without increasing computational costs
- User can select desired amount of interface tension