Fluid-Structure Interactions in Phase Field Models

22.091, Introduction to Modeling and Simulation
Massachusetts Institute of Technology

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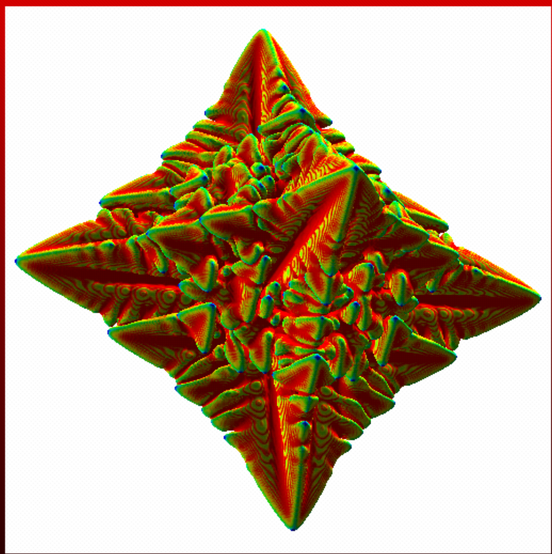
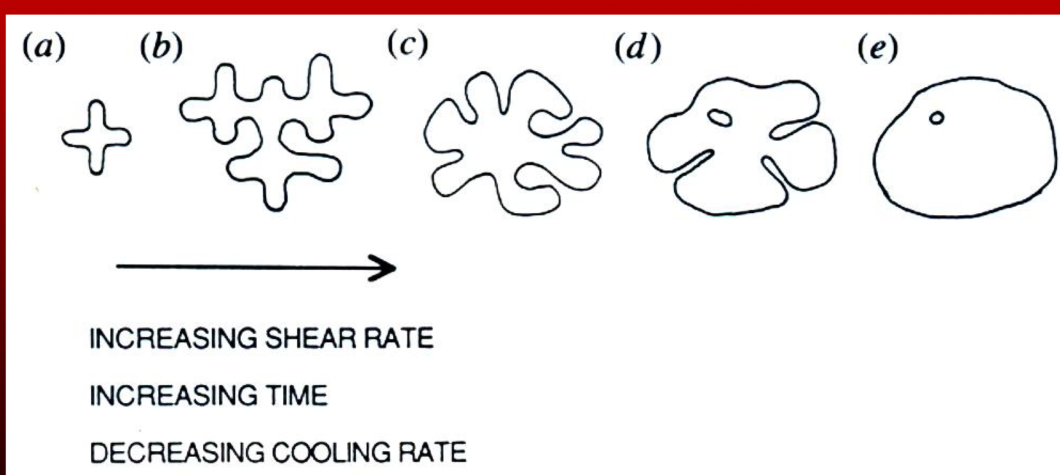
Dendrite modeling



James Warren, NIST

Floating Crystals

Motivation: dendrites move, rotate, deform



Flemings, 1991

Recall: oscillating liquid droplet

Add convection to Cahn-Hilliard conservation equation

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = \nabla \kappa \cdot \nabla \left(\beta \Psi'(\phi) + \alpha \nabla^2 \phi \right) + \kappa \left(\beta \nabla^2 \Psi(\phi) + \alpha \nabla^2 \nabla^2 \phi \right)$$

Navier-Stokes

$$\frac{D\vec{u}}{Dt} = -\nabla p + \nu \nabla^2 \vec{u} + \rho \vec{g} + F_{int}$$

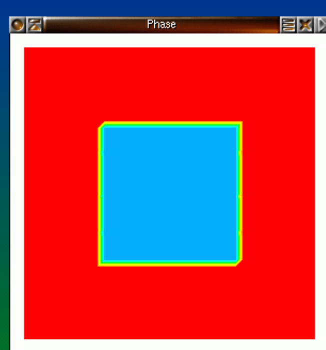
Coupling between phase, velocity

$$F_{int} = -\phi \nabla \mu$$

Velocity-Phase Coupling

Oscillating liquid drop benchmark

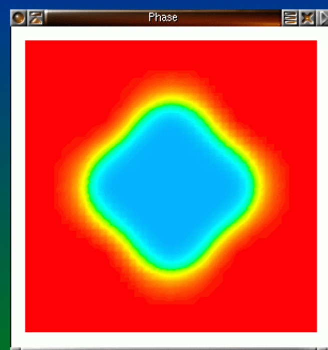
Results: 40x40, t=0



Velocity-Phase Coupling

Oscillating liquid drop benchmark

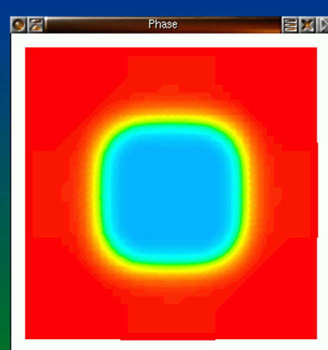
Results: 40x40, t=0.0127



Velocity-Phase Coupling

Oscillating liquid drop benchmark

Results: 40x40, t=0.0257



Fluid-Structure Interactions

Solve very different equations in fluid, solid

- Fluid: Navier-Stokes, calculate velocities

$$\nabla \cdot \vec{v} = 0$$
$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \eta \nabla^2 \vec{v} + \vec{F}$$

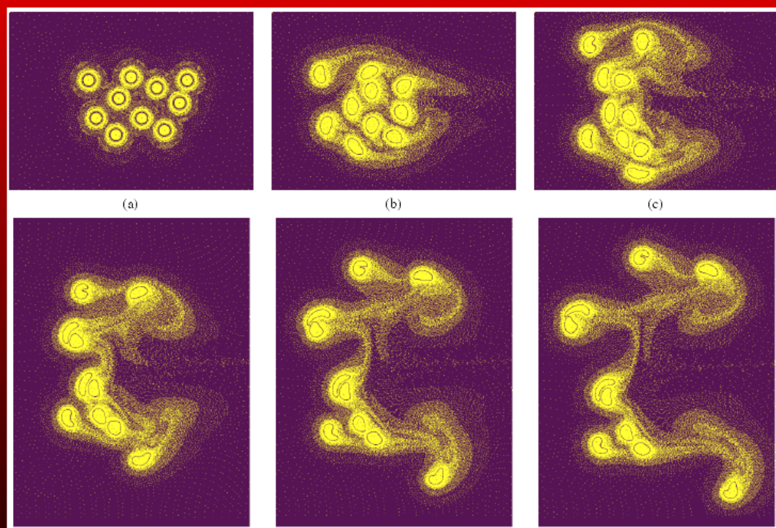
- Solid: calculate displacements

$$\nabla \cdot \sigma + \vec{F} = 0$$
$$\sigma_{ij} = c_{ikjl}\epsilon_{kl}$$
$$\epsilon_{kl} = u_{k,l} + u_{l,k}$$

- Match displacements, tractions at interfaces

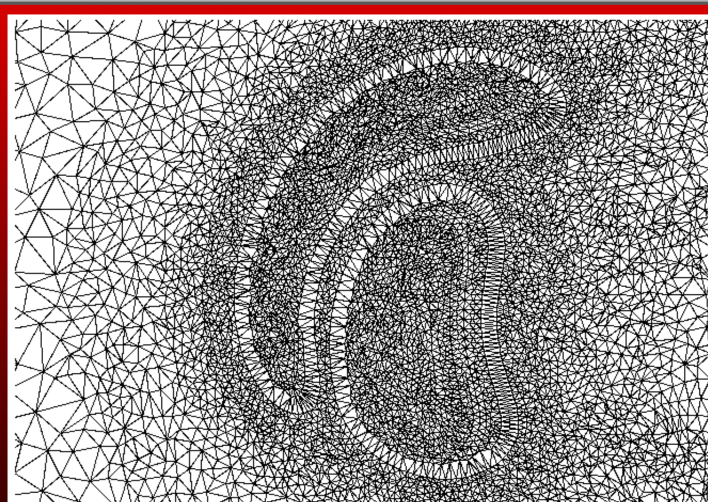
Applications: aeroelasticity, flexible constraints, motion of particles

Blood Cell Motion and Deformation



Cells are viscoelastic, fluid is viscous

Mesh for Blood Flow Model



Dynamic mesh Lagrangian method

Requires a sharp interface

Combining the Two Approaches

Dynamic mesh Lagrangian fluid-structure interactions:

- Nodes move with the fluid or solid
- Certain nodes make up the (sharp) interface
- Matter cannot cross the interface
- Different equations in different phases

Phase Field:

- No sharp boundary between fluid and solid
- Same equation everywhere

Combination:

- Like deformation mechanics: mixed strain
- Here: mixed-stress

$$\rho \frac{D\vec{v}}{Dt} = \nabla \cdot [p(\phi)\sigma_e + (1 - p(\phi))\sigma_f] + \vec{F}$$

Combining the Two Approaches

First cut: assume incompressible fluid, solid

- Incompressible continuity equation everywhere
- Pressure enforces incompressibility

$$\sigma = -PI - p(\phi)\tau_e - (1 - p(\phi))\tau_f, P = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

- In fluid, recovers classical Newtonian shear

$$\tau_f = -\eta(\nabla\vec{v} + \nabla\vec{v}^T)$$

- In solid, pure shear, Poisson ratio is 1/2

$$\tau_e = -G\gamma_e$$

- Coupling between velocity, elastic strain

$$\frac{\partial \gamma_e}{\partial t} = \nabla\vec{v} + \nabla\vec{v}^T$$

Field variables: velocity, pressure, elastic shear strain

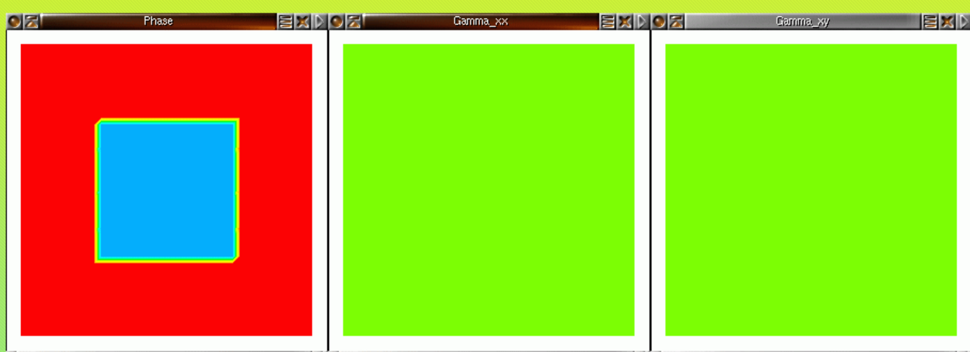
Why Elastic Shear Strain?

- Allows for particle agglomeration
- Relevant to the local state of the material
- Avoids small differences between large displacements
- Two independent components in 2-D, five in 3-D
- Reset to zero when phase falls below threshold (here 0.1)

Phase Field + Fluid-Structure Results

Oscillating solid drop

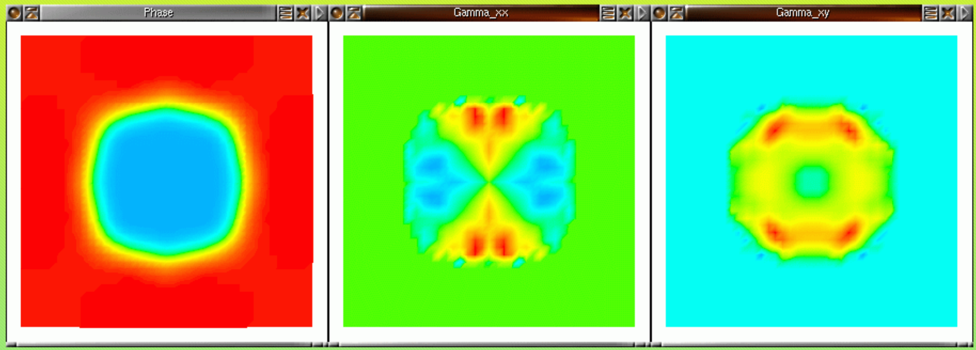
Results: 40x40, t=0



Phase Field + Fluid-Structure Results

Oscillating solid drop

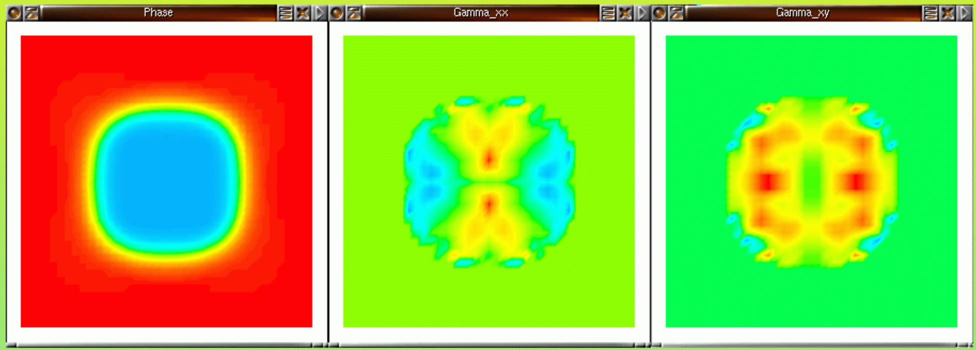
Results: 40x40, t=0.0078



Phase Field + Fluid-Structure Results

Oscillating solid drop

Results: 40x40, t=0.0257



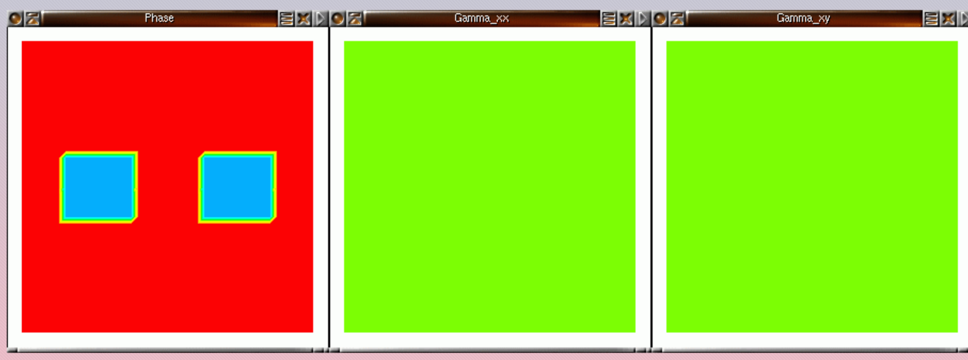
Reasons for rounding:

- High diffusivity (to quickly establish interface)
- Strain convection central differencing -> numerical diffusion!

Phase Field + Fluid-Structure Results

Impinging particles in stagnation flow

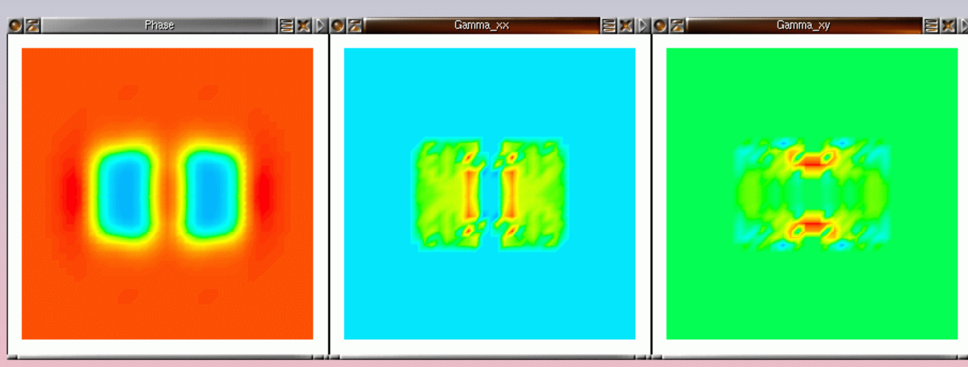
Results: 40x40, t=0



Phase Field + Fluid-Structure Results

Impinging particles in stagnation flow

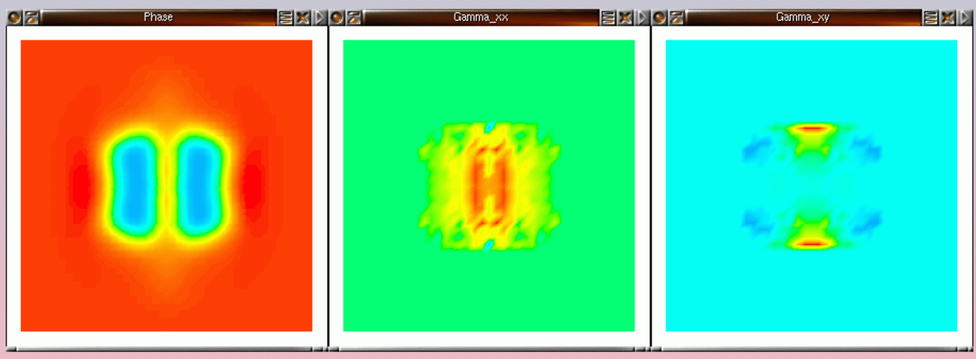
Results: 40x40, t=0.0035



Phase Field + Fluid-Structure Results

Impinging particles in stagnation flow

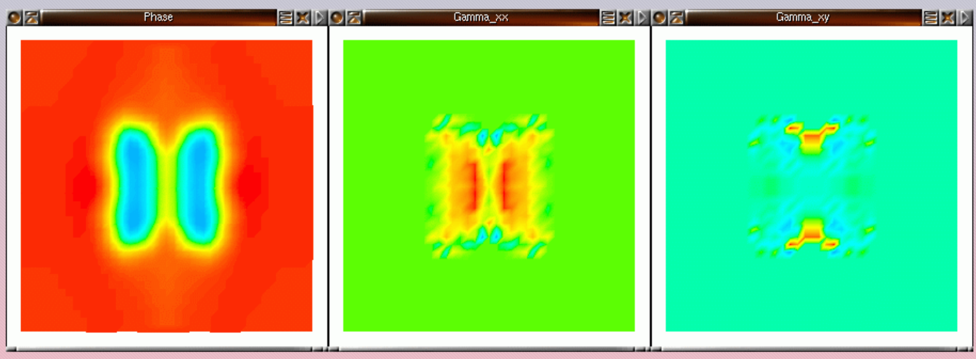
Results: 40x40, t=0.0067



Phase Field + Fluid-Structure Results

Impinging particles in stagnation flow

Results: 40x40, t=0.0091



Solute liquid trapped at interface eventually diffuses away

Current Focus

- Improve shear strain convection (upwind), add rotation
- Explore behavior at interface
  - Artificial erosion of solid?
- Behavior for very different fluid/solid properties
- Anisotropic systems
  - Rotate crystalline orientation using vorticity
- Floating 3-D dendrites!

Conclusions

- ”Mixed stress” formulation permits combination of phase field, fluid-structure interactions methodologies
- Elastic strain is overlaid on fluid velocity to provide solid behavior
- Formulation demonstrated using isotropic Cahn-Hilliard system
- Straightforward extension to anisotropic systems and 3-D
- Toward Modeling Solidification of Crystals Floating in a Moving Liquid