Phase field methods for flows with elastic membranes

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June 20, 2005

Howes Scholar Presentation

Mechanics, Algorithms, & Computing

Carnegie Mellon

Sangria Project: simulation of flows with dynamic interfaces on multi-teraflops computers

Information Technology Research

Carnegie Mellon

J. Antaki, A. Cunha, G.Blelloch, E. Börner, O. Ghattas, J. Hill, C. Kadow, I. Malcevic, G. Miller, I.Pagani, S. Pav, N. Walkington

University of Pittsburgh

G. Burgreen, B. Griffith, M. Kameneva, R. Kormos, E. Sorenson, J. Wu

Texas A&M

A. Mohan, K. Rajagopal

University of Washington

S. Green, G. Turkiyyah

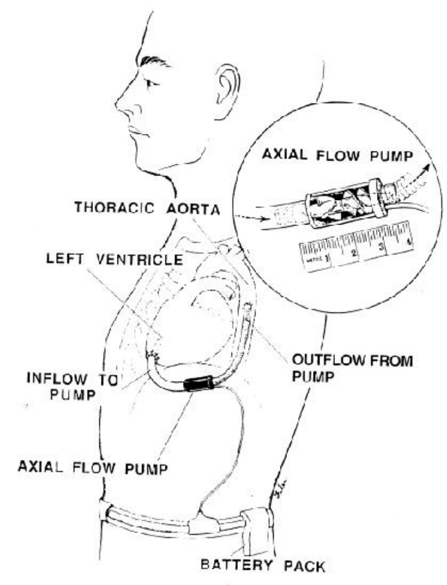
Motivation

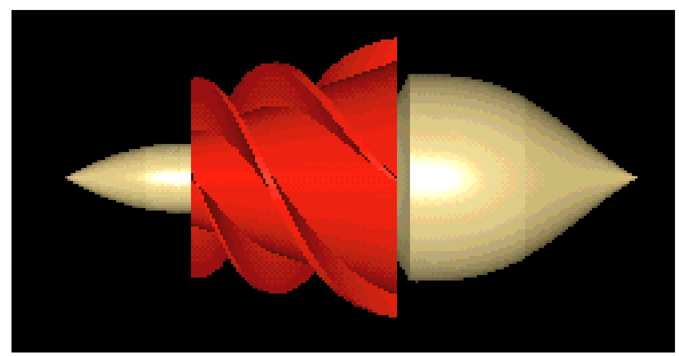
- 80,000 Americans awaiting organ transplantation; 8% can expect to die while waiting
- Artificial organs are the only hope for the majority in the foreseeable future
- Cut-and-try design is expensive, time-consuming, suboptimal
- Computer modeling and simulation permit computational testing and optimization of proposed designs prior to the initiation of expensive animal and clinical trials
- Computer modeling provides greater insight into the behavior of such systems, leading to superior designs

http://www.mirm.pitt.edu

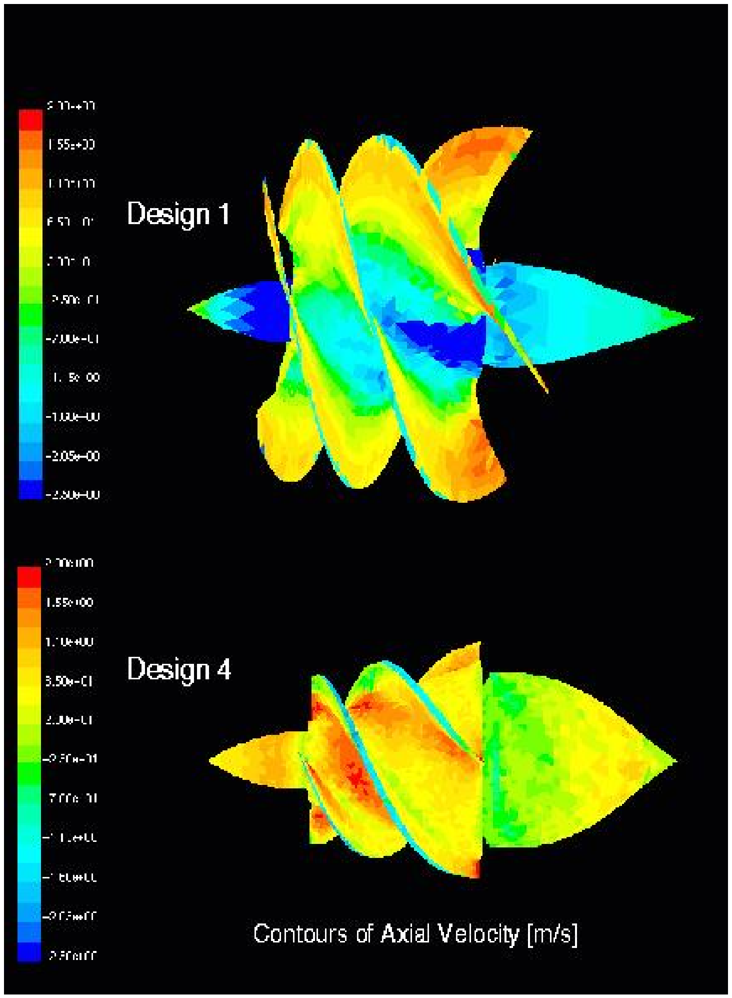
Motivating problem: hemodynamic devices

- "Streamliner" left ventricular assist device under development at UPMC
- Led by Jim Antaki
- Numerous advantages
  - Small size
  - Reliability
  - Low power consumption
  - Less invasive
  - Magnetic bearings
- Design challenge
  - Overcome tendency to shear red blood cells
- First animal implantation July 1998: 7X reduction in blood damage over previous prototype





Motivating problem: hemodynamic devices



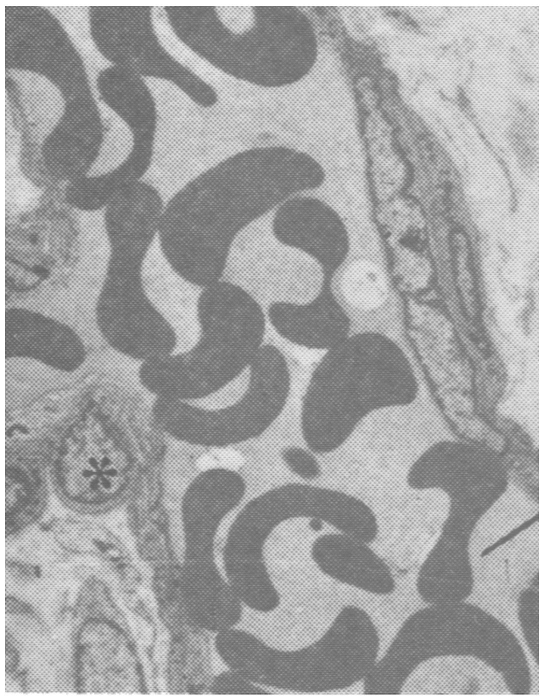
G. Burgreen and J. Antaki, 1996

- Extensive CFD modeling and optimization by Greg Burgreen
- Simulations based on macroscopic homogeneous flow models (Navier-Stokes)
- Major reductions in
  - stagnated flow regions (reduces thrombosis)
  - shear stresses (reduces hemolysis)
- But model is homogeneous: incapable of predicting variation in RBC concentration
- Are regions of high shear devoid of RBCs?
  - Bearing journals
  - Blade tip regions
- Macroscopic models fail in such regions; length scales too small

Motivation

- Microstructural blood flow modeling
  - large relative motion between cells
  - large deformations of cellular membranes

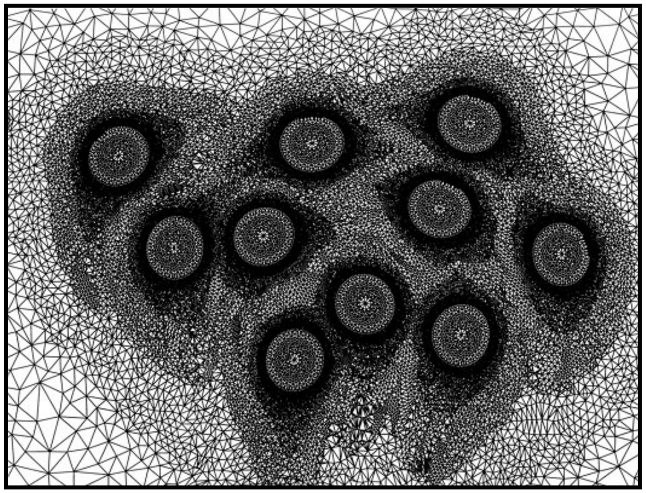
Electron micrograph of blood flow in 12μm ateriole (Rodin, 1972)



Computational model of fluid-solid mixture (Malcevic, 2001)

Challenges

- Physical
  - Continuum mechanics models for elastic interfaces in fluid flow
  - Stable numerical approximations for resulting fluid-structure interaction problem



- Algorithmic
  - Defining the interface between the cell and plasma in time
  - Parallel numerical algorithms for the coupled system
  - Implementation and scaling on parallel machines

Outline

- A phase field model for two immiscible fluids
- Introduction of membrane into framework
- Examples
- Conclusions

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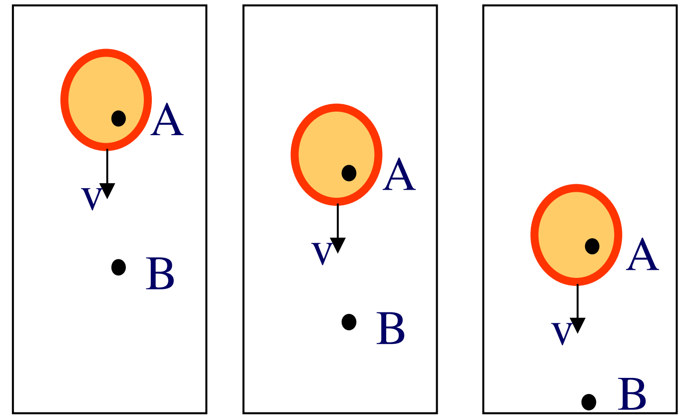
Interface Descriptions

Coordinate Framework	Interface Description: Implicit	Interface Description: Explicit
Lagrangian		Overset Meshes Domain Decomposition <u>Interface-Conforming Grids</u>
Eulerian	Volume of fluid <u>Level-Set</u> Phase field	Immersed boundary <u>Immersed interface</u> Fictitious Domain

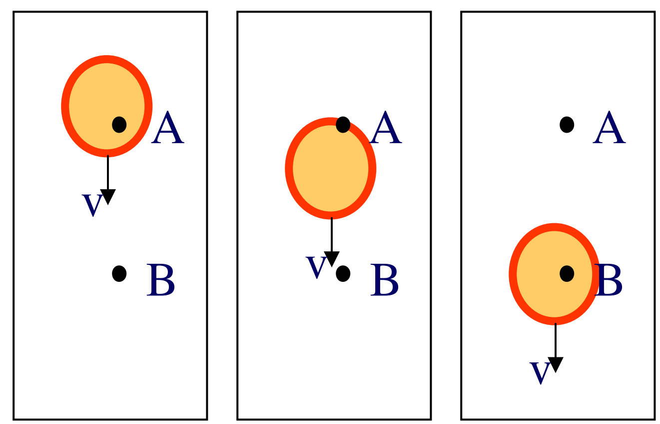
Coordinate Frameworks

- Lagrangian description
  - Interface representation embedded in material description of flow
  - Interfaces are well-resolved and remain sharp
  - Mesh convects and deforms with flow
  - But mesh quickly becomes distorted, and dynamic remeshing becomes necessary
  - Particularly difficult in parallel, 3D
- Eulerian description
  - Fixed grid
  - Straightforward in parallel
  - Interfaces approximately resolved through some other means

Lagrangian (material) framework



Eulerian (spatial) framework



Equations governing fluid motion

- For all fluids, we require that the *balance of momentum* and the *balance of mass* hold.

$$\rho\left(v_t + (v\cdot\nabla)\,v\right) - div\,(T) = \rho f$$

$$\rho_t + div(\rho v) = 0$$

- Assumptions:
  - Newtonian behavior $\quad T = -pI + \mu\,\overbrace{\left(\nabla v + (\nabla v)^T\right)}^{D(v)}$
  - Incompressible fluid $\quad div(v) = 0$

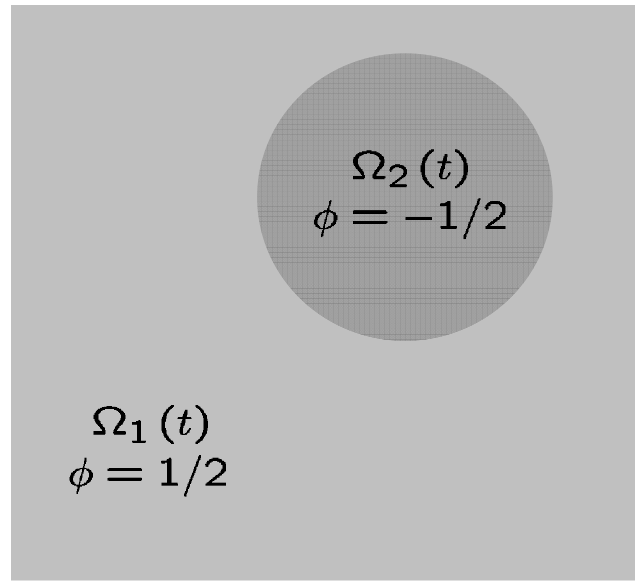
The phase variable

- Definition of the phase variable:
  - Consider a domain with two immiscible fluids
  - To resolve the material properties, introduce the variable

$$\phi = \begin{cases} +1/2 & x \in \Omega_1(t) \\ -1/2 & x \in \Omega_2(t) \end{cases}$$

  - Material properties at a spatial point (x, t) are then defined as

$$\rho = \left(\tfrac{1}{2} + \phi\right)\rho_1 + \left(\tfrac{1}{2} - \phi\right)\rho_2$$



The phase variable

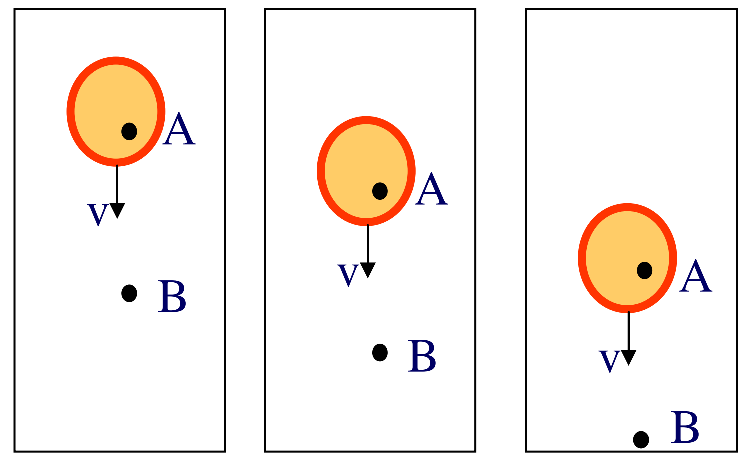
- Key observation for immiscible fluids:
  - In the Lagrangian description, ϕ is independent of time

$$\phi\left(x\left(X,t\right),t\right)=\phi_r\left(X\right)$$

  - The material time derivative is zero, or

$$\phi_t+v\cdot\nabla\phi=0$$

Lagrangian (material) framework



Equations governing two-fluid motion

Strongly coupled equations

$$\phi_t + v \cdot \nabla\phi = 0 \quad \Big\} \text{ “Balance of mass”}$$

$$\left.\begin{aligned} \rho(\phi)\left(v_t + (v \cdot \nabla)\, v\right) - div\,(T(\phi)) &= \rho(\phi) f \\ div(v) &= 0 \end{aligned}\right\} \text{Balance of momentum}$$

Non-linear term

- Time schemes:

$$\phi_t + v^{n-1} \cdot \nabla\phi \; = 0$$

$$\rho^{n-1}\left(\frac{v^n - v^{n-1}}{\tau} + \left(v^{n-1} \cdot \nabla\right) v^n\right) - div\left(\widehat{T}\right) = \widehat{\rho} f^{n+1/2}$$

$$div(v^n) = 0$$

Numerical scheme

Solve for Interface + Solve for Flow

Interface

Solution for φ at $t = t^{n-1}$
Solution for v at $t = t^{n-1}$

Scalar Convection Equations for φ

Discontinuous Galerkin in space and time

High-order in space
Piecewise constant in time

Solution for φ at $t = t^{n}$

Velocities

Solution for φ at $t = t^{n}$
Solution for v at $t = t^{n-1}$

Navier-Stokes Equations

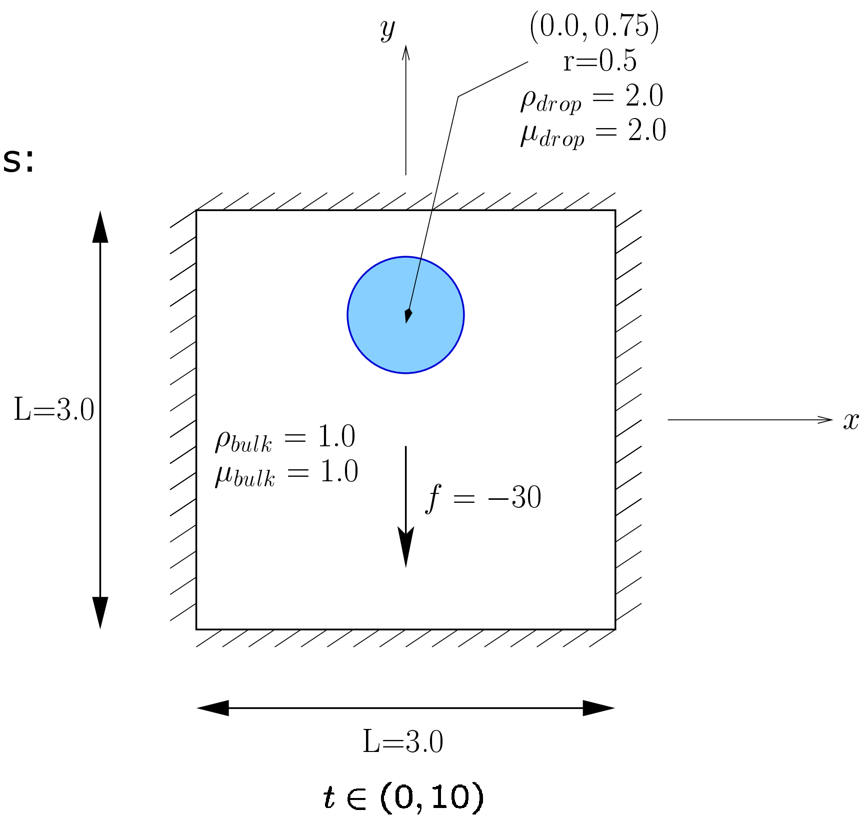
Galerkin in space
Backward Euler in time

Quadratic in v
Linear in p

Solution for v at $t = t^{n}$

The falling drop example

- Simulation Information:
  - 60 x 60 elements
    - For discontinuous Galerkin calculations: biquartic basis functions
    - For standard Galerkin calculations: Taylor-Hood elements
  - 2000 time steps ($\Delta t=0.005$)
  - 4 processors of Lemieux (Alpha cluster at PSC)



- Problem Size:
  - DOF's in Φ : 57,600
  - DOF's in v,p: 33,000

Outline

- A phase field model for two immiscible fluids
- Introduction of membrane into framework
- Example Simulations
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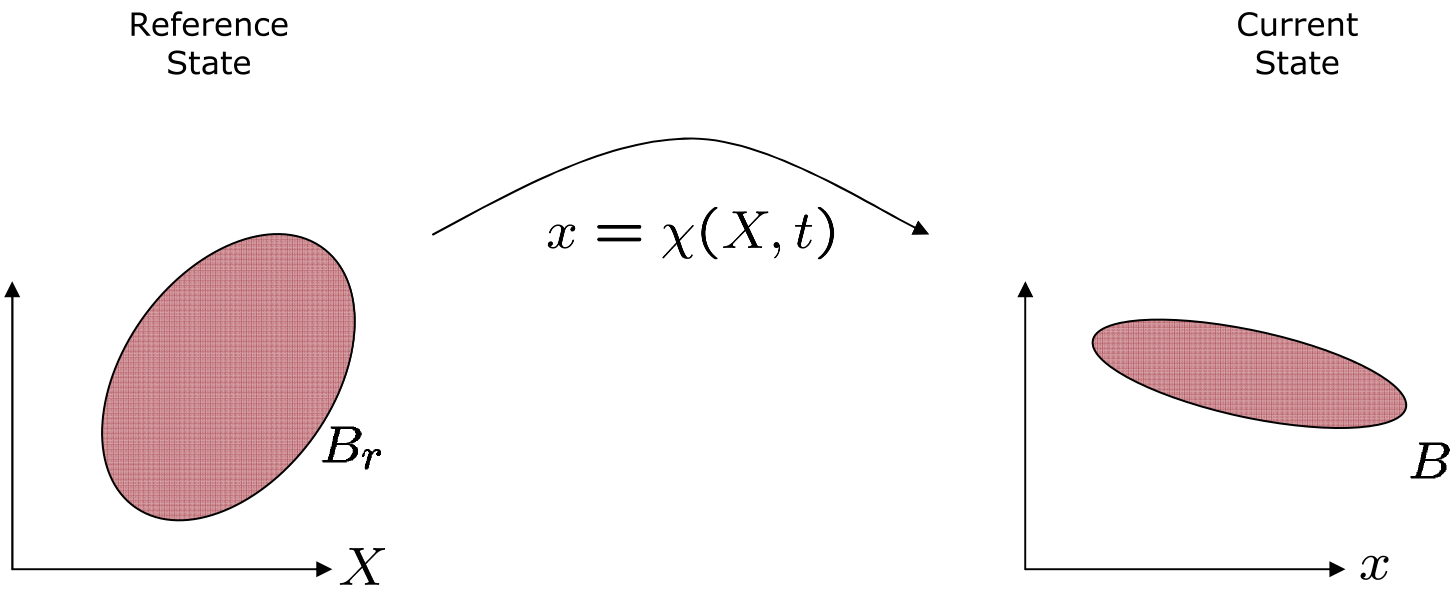
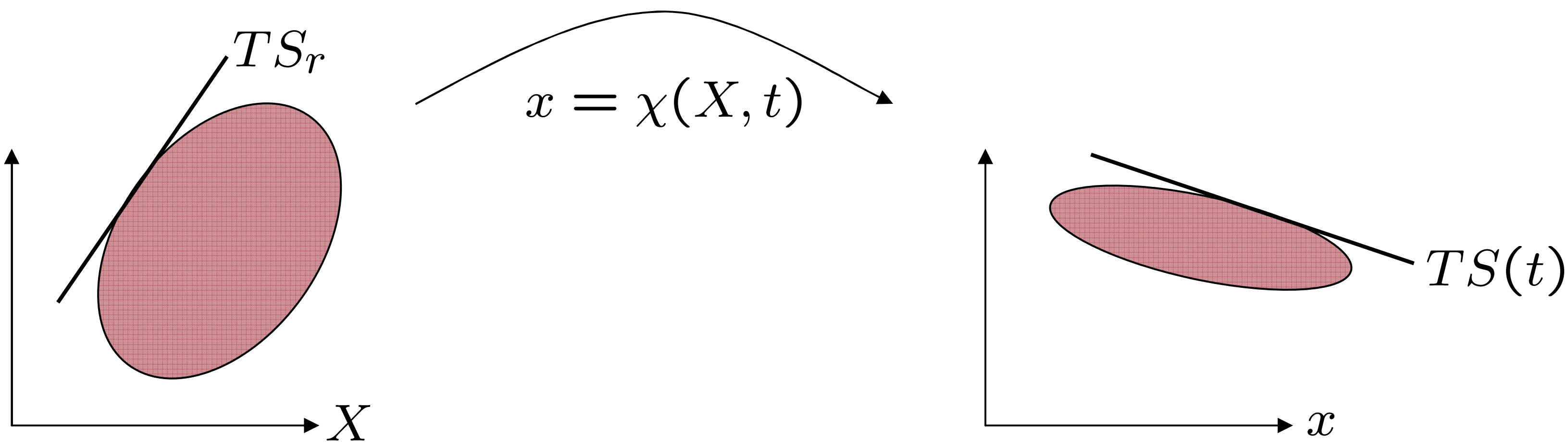
Notation

- An elastic body:



$$F = \partial x_i / \partial X_\alpha$$

Differential Geometry



- Membrane Motion: $\chi_s : S_r \rightarrow S(t)$
- Differential: $d\chi_s : TS_r \rightarrow TS(t)$

- Membrane Deformation Gradient: If $v \in TS_r(X) \subset \Re^3$

$$d\chi_s v = F_s v \in \Re^3 \quad \text{where } F_s = F(I - N \otimes N)$$

Membrane stresses: Sharp Interface Model

- The momentum equation can be written in weak form as, including the Cauchy stress,

$$\int_\Omega [\rho(\phi)\,(v_t + (v\cdot\nabla)v)\cdot w + p\,div(w) + \mu(\phi)D(v)\cdot D(w)]\,d\Omega$$

$$\int_{S(t)} (1/J_s)D\mathcal{W}(F_s)\cdot(\nabla w)F_s = \int_\Omega \rho(\phi)f\cdot w$$

- The evolution of the membrane deformation gradient is

$$F_{st} + (v\cdot\nabla)F_s = (\nabla v)F_s$$

Membrane stresses: Phase field Approximation

- Level Set Representation

$$S(t) = x \in \Omega \,|\, \phi(x,t) = 0$$

- Phase field Approximation of Surface: $-1/2 < \phi < 1/2$

$$\int_{S_r} (\ldots) dA = \int_{S(t)} (\ldots)(1/J_s) da$$

$$= \int_{\Omega} (\ldots)(1/J)|F^T \nabla \phi| dx$$

- Recall: $J = det(F) = 1$ if $div(v) = 0$

The governing equations

Eulerian form of conservation of momentum and mass eqns for a viscous incompressible fluid with a membrane at the interface

$$\left.\begin{aligned} &\phi_t + v \cdot \nabla\phi = 0 \\ &\begin{array}{r} \text{Membrane Rotation} \\ \text{Membrane Strain} \end{array} \left\{\begin{aligned} &(R_s)_t + (v\cdot\nabla)R_s = W(v)R_s \\ &(E_s)_t + (v\cdot\nabla)E_s = R_s^T D(v) R_s \end{aligned}\right. \end{aligned}\right\} \text{Convection Equations}$$

$$\left.\begin{aligned} &div(v) = 0 \\ &\rho(\phi)\left(v_t + (v\cdot\nabla)\, v\right) - div\left(-pI + \mu(\phi)D(v)\right) \\ &\qquad \underbrace{-div\left(4R_s\ \mathsf{C}\,(E_s)R_s^T\right)}_{\text{Membrane Stress}} = \rho(\phi) f \end{aligned}\right\} \text{Navier-Stokes Equations}$$

The governing equations

Initial Conditions:

Phase Function	$\phi(x,0) = \phi_0(x)$
Membrane Rotation	$R_s(x,0) = (I - N \otimes N)\,\lvert\nabla\phi(x,0)\rvert^{1/4}$
Membrane Strain	$E_s(x,0) = 0$
Velocities/Pressures	$v(x,0) = v_0(x)$

The governing equations

Eulerian form of conservation of momentum and mass eqns for a viscous incompressible fluid with a membrane at the interface

$$\phi_t + v \cdot \nabla \phi = 0$$

Membrane Rotation

Membrane Strain

$$\begin{cases} (R_s)_t + (v \cdot \nabla) R_s = W(v) R_s \\ (E_s)_t + (v \cdot \nabla) E_s = R_s^T D(v) R_s \end{cases}$$

Convection Equations

$$div(v) = 0$$

$$\rho(\phi)\left(v_t + (v \cdot \nabla)\, v\right) - div\left(-pI + \mu(\phi) D(v)\right)$$

$$\underbrace{-div\left(4R_s\ \mathsf{C}(E_s) R_s^T\right)}_{\text{Membrane Stress}} = \rho(\phi) f$$

Navier-Stokes Equations

The governing equations

Time discretization schemes:

$$\phi_t + v^{n-1} \cdot \nabla\phi = 0$$

$$R_t + (v^{n-1} \cdot \nabla)R = W(v^{n-1})R$$

$$E_t + (v^{n-1} \cdot \nabla)E = (R^n)^T D(v^n) R^n$$

$$div(v^n) = 0$$

$$\rho^{n-1}\left(\frac{v^n - v^{n-1}}{\tau} + \left(v^{n-1} \cdot \nabla\right) v^n\right) - div\left(-p^n I + \widehat{\mu} D(v^n)\right) - div \underbrace{\left(R^n \; \mathsf{C}(E^n)(R^n)^T\right)}_{\text{Membrane Stress}} = \widehat{\rho} f^{n+1/2}$$

Numerical Scheme

Solve ϕ equation for ϕ_h^n
Discontinuous Galerkin in time, space

ϕ_h^n, ϕ_h^{n-1}

Compute $\bar{\rho}$ and $\bar{\mu}$

$\bar{\rho}, \bar{\mu}, \rho^{n-1}$

Solve R_s equation for $R_{s_h}^n$
Discontinuous Galerkin in time, space

$R_{s_h}^n, R_{s_h}^{n-1}$

Solve coupled momentum, strain equation for v_h^n and $E_{s_h}^n$
Galerkin in space, Backward Euler in time; Discontinuous Galerkin in space, time

- PETSc library of linear solvers, preconditioners used
- Parallel implementation in all cases

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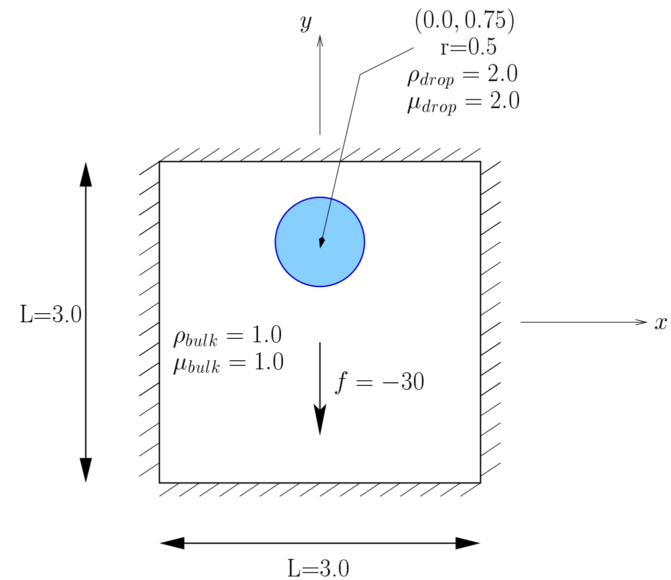
The falling drop example

- Simulation Information:
  - 60 x 60 elements
    - For discontinuous Galerkin calculations: biquartic basis functions
    - For standard Galerkin calculations: Taylor-Hood elements
  - 2000 time steps (Δt=0.005)
  - 64 processors of Lemieux

- Problem Size:
  - DOF's in Φ 57,600
  - DOF's in R 230,400
  - DOF's in v,p 33,000
  - DOF's in E 230,400

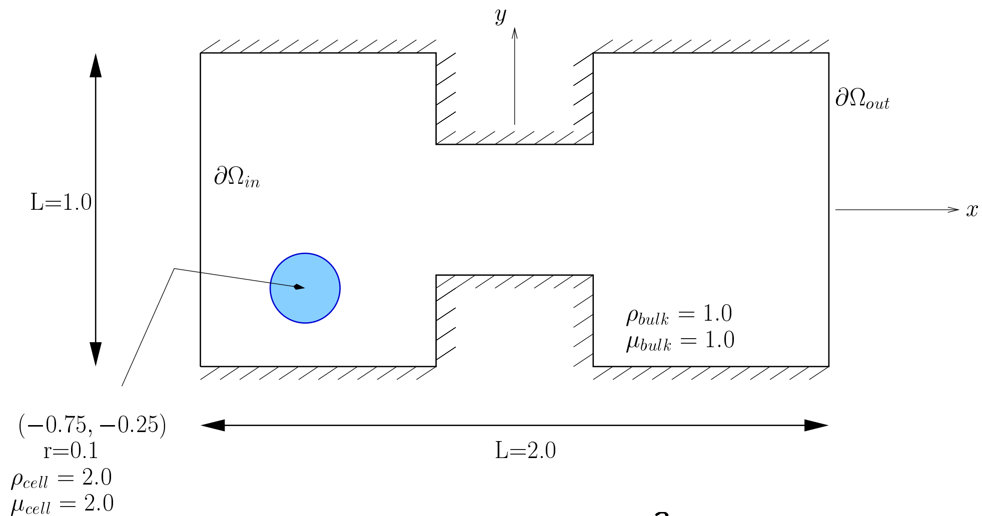


$$t \in (0, 10)$$
$$\lambda_1 = \lambda_2 = 2.5 * 10^4$$

	No Membrane	Membrane
Phase Variable		
U-Velocities		
V-Velocities		
Divergence		
Strains		

The channel problem

- Simulation Information:
  - 2720 elements (h=0.025)
    - For discontinuous Galerkin calculations: biquartic basis functions
    - For standard Galerkin calculations: Taylor-Hood elements
  - 4800 time steps (Δt=0.0006)
  - 32 processors of Lemieux



$$\lambda_1 = \lambda_2 = 2.5 * 10^3$$
$$t \in (0, 3)$$

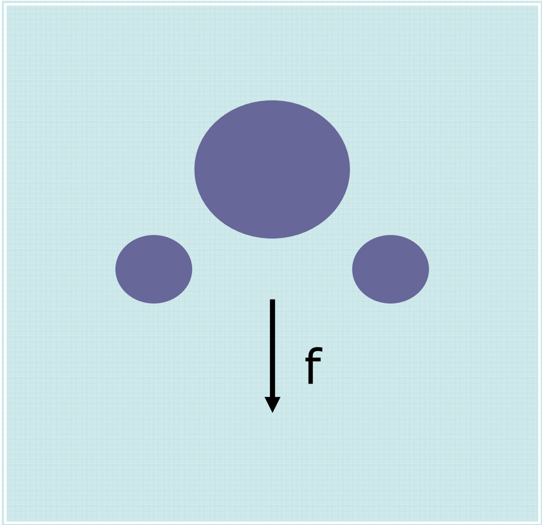
- Problem Size:
  - DOF's in Φ 43,500
  - DOF's in R 174,100
  - DOF's in v,p 27,000
  - DOF's in E 174,100

	No Membrane	Membrane
Phase Variable		
U-Velocities		
V-Velocities		
Divergence		
Strains		

Multiple bodies under gravity

- Simulation Information:
  - 60 x 60 elements
    - For discontinuous Galerkin calculations: biquartic basis fns.
    - For standard Galerkin calculations: Taylor-Hood elements
  - 2000 time steps ($\Delta t=0.005$)
  - 32 processors of Lemieux

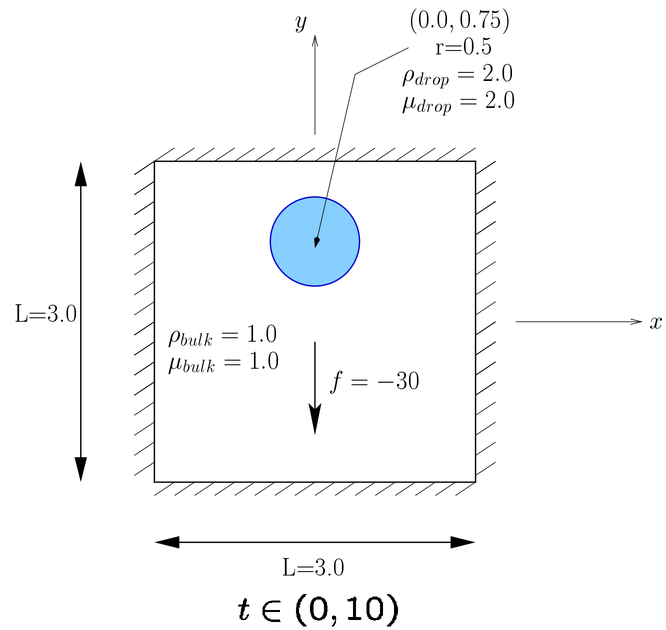
- Problem Size:
    - DOF's in Φ : 57,600
    - DOF's in R : 230,400
    - DOF's in E,v,p: 263,400



$$\lambda_1 = \lambda_2 = 2.5 * 10^4$$

The falling drop example, revisited

- Simulation Information:
  - 16 x 16 x 16 elements
    - For discontinuous Galerkin calculations: triquartic basis functions
    - For standard Galerkin calculations: Taylor-Hood elements
  - 1000 time steps (Δt=0.01)



- Problem Size:
  - DOF's in Φ 262,144
  - DOF's in v,p 112,724

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Conclusions

- Physical Advantages
  - Incorporation of an elastic membrane into an Eulerian flow description
- Numerical & Computational Advantages:
  - Fixed mesh never requires remeshing
  - Not required to explicitly track the interface
  - All steps highly parallel
  - Parallel preconditioner that respects strong fluid-membrane coupling
  - Little change required to extend to 3-D

Research challenges

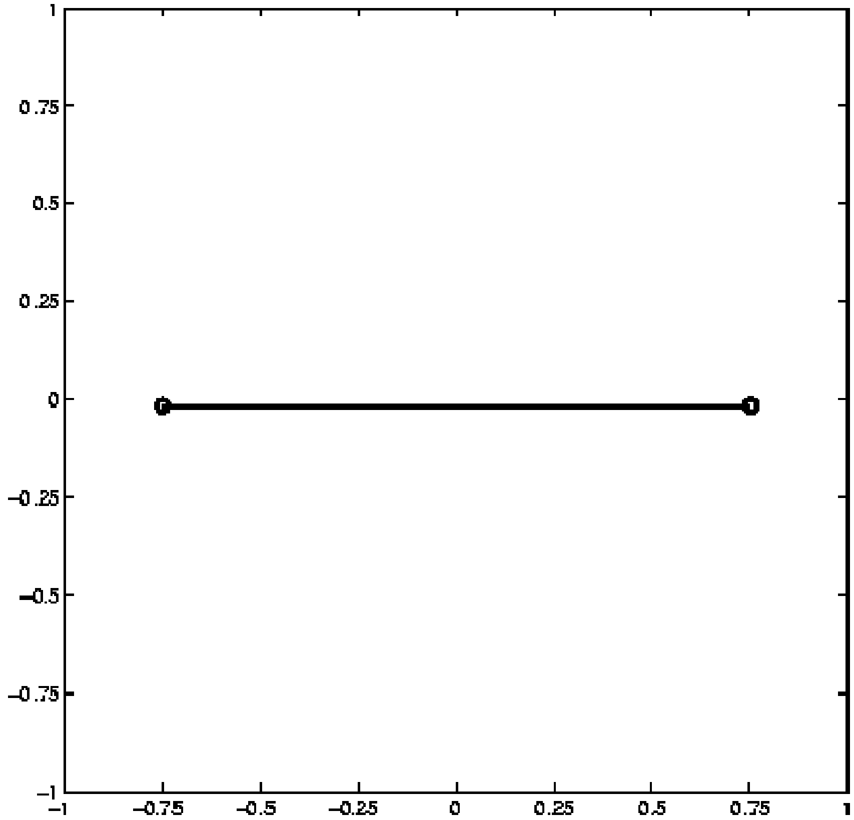
- Mechanics
  - Addition of a phase field approximation of surface tension
  - Incorporation of bending stiffness into membrane model
  - Experimental validation of elastic membrane
- Numerics
  - Scalability study of algorithm and implementation
  - Implementation of adaptive *p*- and *h*-refinement in space
  - Improvement of time discretization

Acknowledgements

- N. Walkington and O. Ghattas
- Funding:
  - DOE Computational Science Graduate Fellowship
  - Sangria Project: NSF-ITR ACI 0086093

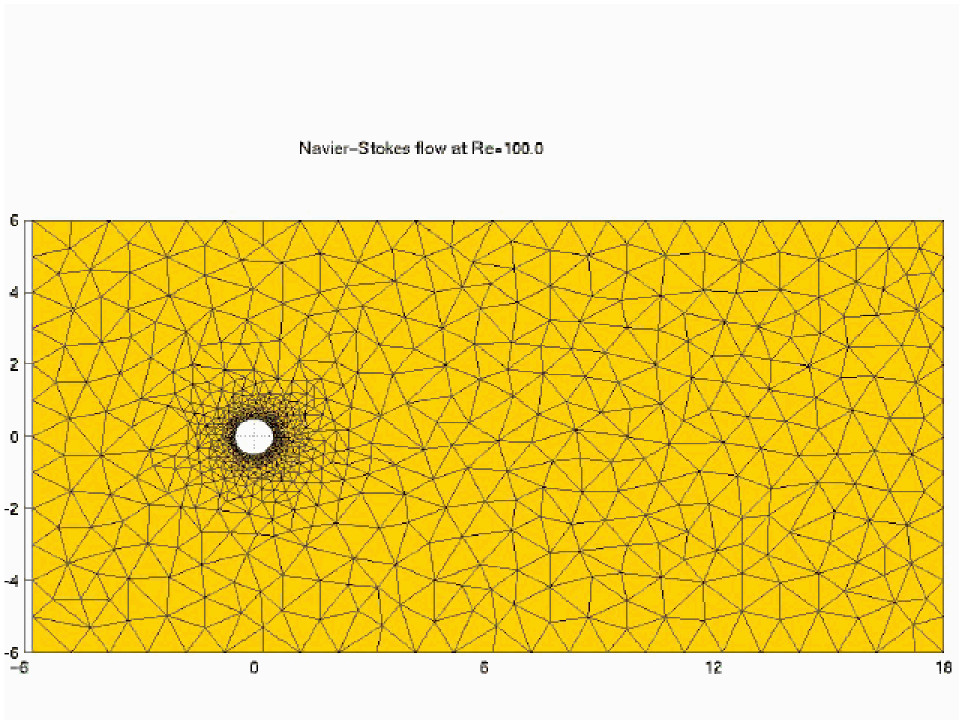
Questions

Immersed Interface Example



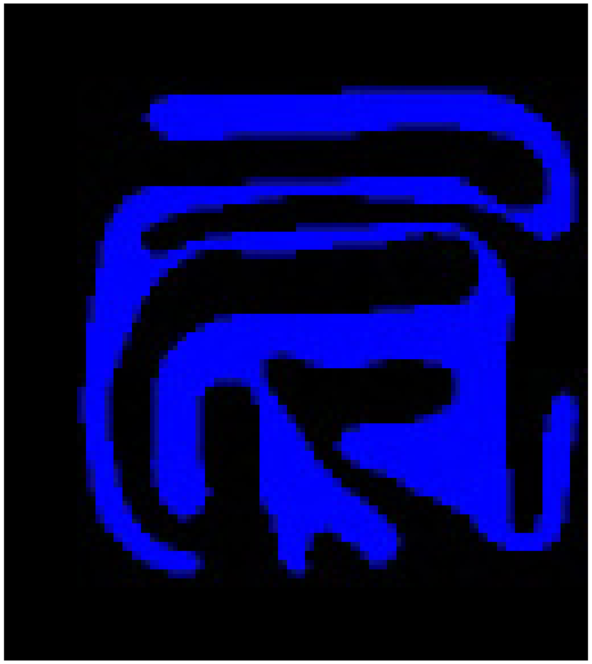
Long Lee (UNC) and Randy Leveque (UW)

Interface Conforming Example



Ivan Malcevic (CMU)

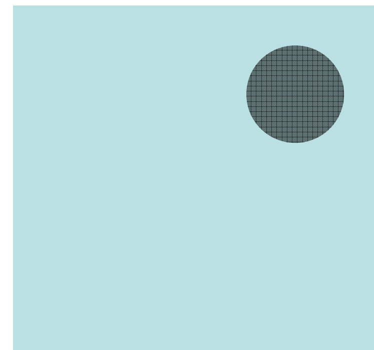
Level Set Example



J. Sethian (UC-Berkeley)

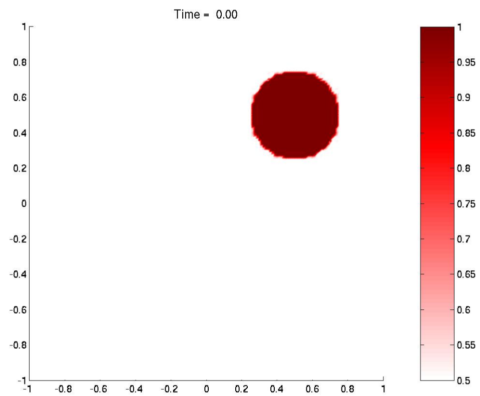
Time discretization

- Reversibility of Spiraling Fluid
  - Geometry: $\Omega = \{(x,y) \mid -1 \leq x \leq 1, -1 \leq y \leq 1\}$
  - Material Properties: $\rho_f = 0.5 \qquad \rho_s = 1.0$
  - Imposed Velocity Field: $u_r = 0$
    $u_\theta = r^2$
  - Simulation Information:
    - 40 x 40 quadrilateral biquartic elements (Δh = 0.05)
    - 4000 time steps (Δt=0.0025)

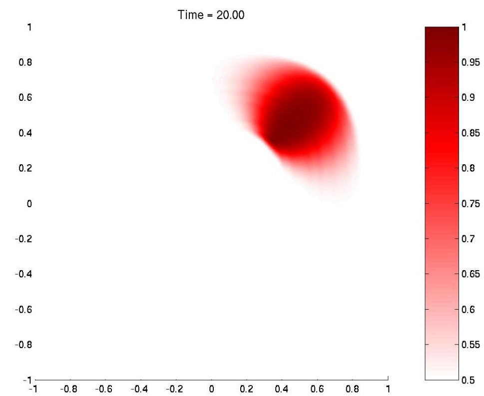


$t \in [0, 20]$

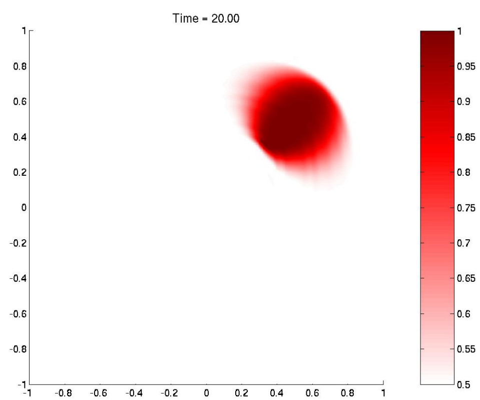
Time discretization



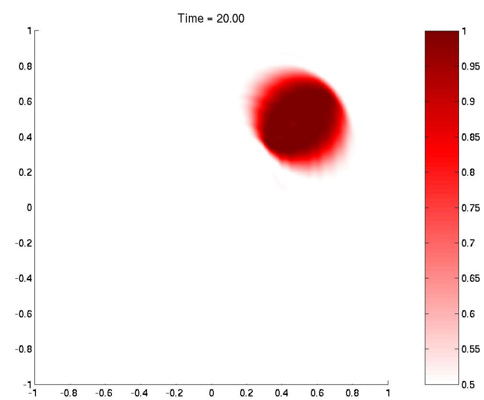
Initial Position (t = 0)



Final Position (t = 20)
4000 Time Steps



Final Position (t = 20)
8000 Time Steps



Final Position (t = 20)
16000 Time Steps

Numerical scheme

Solve for Interface + Solve for Flow

Interface

Solution for φ, R at $t= t^{n-1}$
Solution for v, E at $t= t^{n-1}$

Scalar & Tensor Convection Equations for φ, R

Discontinuous Galerkin in space and time

High-order in space
Piecewise constant in time

Solution for φ, R at $t = t^{n}$

Velocities

Solution for φ, R at $t=t^{n}$
Solution for v, E at $t= t^{n-1}$

Coupled Navier-Stokes & Strain Equations

Galerkin in space (v)
Backward Euler in time (v)
D-G in space, time (E)

Taylor-Hood for v,p
High-order in space for E

Solution for v, E at $t = t^{n}$

Numerical Scheme

Solve ϕ equation for ϕ_h^n
Discontinuous Galerkin in time, space

$$\phi_t + v \cdot \nabla \phi = 0$$

Weak Form:

$$\int_\Omega \phi \psi d\Omega \Big|_{t=0}^{T} - \int_0^T \int_\Omega \phi \left(\psi_t + v \cdot \nabla \psi\right) d\Omega dt + \int_0^T \int_{\partial\Omega_{out}} \phi \psi v \cdot n \, ds \, dt$$

$$= -\int_0^T \int_{\partial\Omega_{in}} \phi_{in} \psi v \cdot n \, ds \, dt$$

Discrete Scheme:

$$\int_K \phi_h(t^n)\psi_h(t^n) - \int_{t^{n-1}}^{t^n} \int_K \phi_h \left((\psi_h)_t + v^{n-1} \cdot \nabla \psi_h\right)$$

$$+ \int_{t^{n-1}}^{t^n} \int_{\partial K} \left(\left(v^{n-1} \cdot n\right)^+ \phi_h + \left(v^{n-1} \cdot n\right)^- \phi_{h_-}\right) \psi_h$$

$$= \int_K \phi_{h_-}(t^{n-1})\psi_h(t^{n-1})$$

Numerical Scheme

$$(R_s)_t + (v \cdot \nabla) R_s = W(v) R_s$$

Solve R_s equation for $R^n_{s_h}$

Discontinuous Galerkin in time, space

Weak Form:

$$\int_\Omega R_s \cdot S d\Omega \Big|_{t=0}^{T} - \int_0^T \int_\Omega \left(R_s \cdot S_t + R_s \cdot (v \cdot \nabla)\, S\right) d\Omega dt$$
$$- \int_0^T \int_\Omega \left(W(v) R_s \cdot S\right) d\Omega dt$$
$$+ \int_0^T \int_{\partial\Omega_{out}} R_s \cdot S\,(v \cdot n)\; ds\, dt = - \int_0^T \int_{\partial\Omega_{in}} R_{s_{in}} \cdot S\,(v \cdot n)\; ds\, dt$$

Discrete Scheme:

$$\int_K R_h(t^n) S_h(t^n) - \int_{t^{n-1}}^{t^n} \int_K R_h \left((S_h)_t + \left(v^{n-1} \cdot \nabla\right) S_h\right) + W(v^{n-1}) R_h \cdot S_h$$
$$+ \int_{t^{n-1}}^{t^n} \int_{\partial K} \left(\left(v^{n-1} \cdot n\right)^+ R_h + \left(v^{n-1} \cdot n\right)^- R_{h\_}\right) S_h$$
$$= \int_K R_{h\_}(t^{n-1}) S_h(t^{n-1})$$

Numerical Scheme

Solve coupled momentum, strain equation for v_h^n and $E_{s_h}^n$

Galerkin in space, Backward Euler in time; Discontinuous Galerkin in space, time

$$\underbrace{\rho^{n-1}\left(v_t + \left(v^{n-1}\cdot\nabla\right)v^n\right) - div\left(-p^n I + \widehat{\mu} D(v^n)\right)}_{A_{uu}} \underbrace{-div\left(R^n\, \mathsf{C}(E^n)(R^n)^T\right)}_{A_{uE}} = \widehat{\rho} f^{n+1/2}$$

$$\underbrace{-(R^n)^T D(v^n) R^n}_{A_{Eu}} \quad \underbrace{+E_t + (v^{n-1}\cdot\nabla)E}_{A_{EE}} = 0$$

Physics-Based Preconditioning

$$\begin{bmatrix} A_{uu} & A_{uE} \\ A_{Eu} & A_{EE} \end{bmatrix} \left\{ \begin{array}{c} u \\ E \end{array} \right\} = \left\{ \begin{array}{c} F_u \\ F_E \end{array} \right\}$$

$$P = \begin{bmatrix} \widehat{S}^{-1} & 0 \\ -\widehat{A}_{EE}^{-1} A_{Eu} \widehat{S}^{-1} & \widehat{A}_{EE}^{-1} \end{bmatrix} \begin{bmatrix} I & -A_{uE}\widehat{A}_{EE}^{-1} \\ 0 & I \end{bmatrix}$$

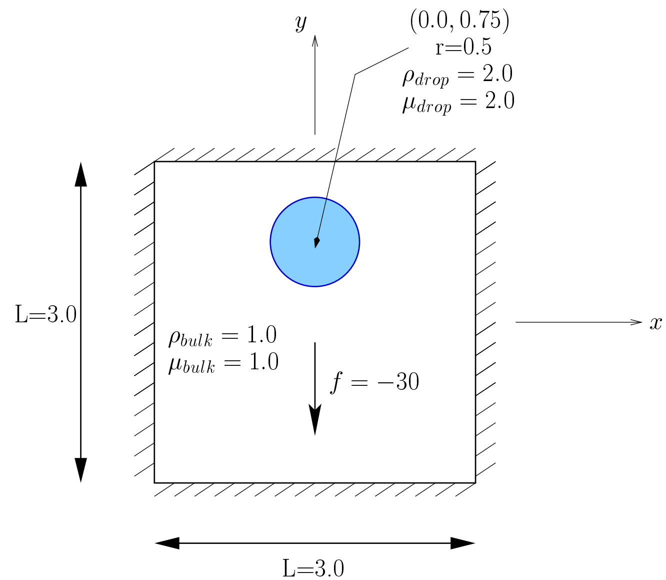
$$\widehat{S} = \widehat{A}_{uu} - A_{uE}\widehat{A}_{EE}^{-1} A_{Eu}$$

$$\widehat{A}_{EE} = \int_K E_h(t^n) S_h(t^n) - \int_{t^{n-1}}^{t^n} \int_K E_h \left((F_h)_t + \left(v^{n-1} \cdot \nabla \right) F_h \right)$$

The falling drop example

- Simulation Information:
  - 60 x 60 elements
    - For discontinuous Galerkin calculations: biquartic basis functions
    - For standard Galerkin calculations: Taylor-Hood elements
  - 2000 time steps (Δt=0.005)
  - 64 processors of Lemieux

- Problem Size:
  - DOF's in Φ 57,600
  - DOF's in R 230,400
  - DOF's in v,p 33,000
  - DOF's in E 230,400



$t \in (0, 10)$

$\lambda_1 = \lambda_2 = 2.5 * 10^4$

	No Membrane	Membrane
Phase Variable		
U-Velocities		
V-Velocities		
Divergence		
Strains		

Effect of Preconditioner

PEs	Elements Time Steps	DOF ϕ N-S	iterations ϕ	iterations N-S	Time (s)
1	16 x 16	4,096	2.96	10.28	25
	75	2,467			
4	32 x 32	16,384	4.11	23.57	72
	150	9,539			
8	45 x 45	32,400	4.90	30.76	136
	225	18,678			
16	64 x 64	65,536	4.34	44.34	228
	300	37,507			
32	91 x 91	132,496	4.66	60.88	467
	450	75,442			

Isogranular comparison for simulations without the membrane

Effect of Preconditioner

PEs	Elements Time Steps	DOF ϕ R N-S	iterations ϕ	 R	 N-S	Time (s)
1	8 x 8 38	1,024 2,467 659	1.34	1,36	20.21	32
4	16 x 16 75	4,096 16,384 2,467	3.93	3.97	40.85	97
16	32 x 32 150	16,384 65,536 9,539	4.20	4.20	72.40	335
32	45 x 45 225	32,400 129,600 18,678	4.03	4.06	112.90	919
64	64 x 64 300	65,536 262,144 37,507	4.05	4.13	137.62	1522

Isogranular comparison for simulations with the membrane