Phase field methods
for
flows with elastic membranes

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

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

Texas A&M

A. Mohan, K. Rajagopal

University of Pittsburgh

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

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
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

- 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 12 µm 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
Outline

- A phase field model for two immiscible fluids
- Introduction of membrane into framework
- Example Simulations
- Conclusions
## Interface Descriptions

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<td>Immersed interface</td>
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<td>Fictitious Domain</td>
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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
Equations governing fluid motion

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

\[
\rho (v_t + (v \cdot \nabla) v) - \text{div}(T) = \rho f
\]
\[
\rho_t + \text{div}(\rho v) = 0
\]

- Assumptions:
  - Newtonian behavior
  \[
  T = -pI + \mu \left( \nabla v + (\nabla v)^T \right)
  \]
  - Incompressible fluid
  \[
  \text{div}(v) = 0
  \]
**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
    \[
    \rho = \left(\frac{1}{2} + \phi\right) \rho_1 + \left(\frac{1}{2} - \phi\right) \rho_2
    \]
The phase variable

- Key observation for immiscible fluids:
  - In the Lagrangian description, \( \phi \) is independent of time
    \[
    \phi(x(X,t), t) = \phi_r(X)
    \]
  - The material time derivative is zero, or
    \[
    \phi_t + v \cdot \nabla \phi = 0
    \]
Equations governing two-fluid motion

\[ \phi_t + v \cdot \nabla \phi = 0 \]

\[ \rho(\phi) \left( v_t + (v \cdot \nabla) v \right) - \text{div} \left( T(\phi) \right) = \rho(\phi) f \]

\[ \text{div}(v) = 0 \]

“Balance of mass”

Balance of momentum

- Time schemes:

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

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

\[ \text{div}(v^n) = 0 \]
Numerical scheme

Solve for Interface + Solve for Flow

Interface

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

Scalar Convection Equations for $\varphi$

Discontinuous Galerkin in space and time

High-order in space
Piecewise constant in time

Solution for $\varphi$ at $t = t^n$

Velocities

Solution for $\varphi$ 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 \(\Phi\) : 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
• Conclusions
Notation

- An elastic body:

\[ F = \frac{\partial x_i}{\partial X_\alpha} \]
- Membrane Motion: \( \chi_s : S_r \rightarrow S(t) \)
- Differential: \( d\chi_s : TS_r \rightarrow TS(t) \)

- Membrane Deformation Gradient: If \( v \in TS_r(X) \subset \mathbb{R}^3 \)
  \[
  d\chi_s v = F_s v \in \mathbb{R}^3 \quad \text{where} \quad F_s = F(I - N \otimes N)
  \]
Membrane stresses: Sharp Interface Model

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

\[
\int_{\Omega} \left[ \rho(\phi) \left( v_t + (v \cdot \nabla) v \right) \cdot w + p \div(w) + \mu(\phi) D(v) \cdot D(w) \right] d\Omega
\]

\[
\int_{S(t)} \left( \frac{1}{J_s} \right) D\mathbf{w}(F_s) \cdot (\nabla w) F_s = \int_{\Omega} \rho(\phi) f \cdot w
\]

- 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
  \[
  S(t) = x \in \Omega \mid \phi(x, t) = 0
  \]

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

  \[
  \int_{S_r} (...)dA = \int_{S(t)} (...) (1/J_s)da
  \]

  \[
  = \int_{\Omega} (...) (1/J) |F^T \nabla \phi| dx
  \]

- Recall: \( J = \text{det}(F) = 1 \) if \( \text{div}(v) = 0 \)
The governing equations

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

\[ \phi_t + v \cdot \nabla \phi = 0 \]

Membrane Rotation
\[ \begin{cases} 
(R_s)_t + (v \cdot \nabla)R_s = W(v)R_s \\
(E_s)_t + (v \cdot \nabla)E_s = R^T_s D(v)R_s 
\end{cases} \]

Membrane Strain
\[ \text{Convection Equations} \]

\[ \text{Navier-Stokes Equations} \]

\[ \text{Membrane Stress} \]
\[ \begin{align*}
\rho(\phi) (v_t + (v \cdot \nabla) v) - \text{div} \left(-pI + \mu(\phi)D(v)\right) \\
- \text{div} \left(4R_s C(E_s)R^T_s\right) = \rho(\phi)f
\end{align*} \]
The governing equations

Initial Conditions:

Phase Function \( \phi(x, 0) = \phi_0(x) \)

Membrane Rotation \( R_s(x, 0) = (I - N \otimes N) |\nabla \phi(x, 0)|^{1/4} \)

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

\[
\phi_t + v \cdot \nabla \phi = 0
\]

\[
\begin{align*}
\left( R_\phi \right)_t + (v \cdot \nabla) R_\phi &= W(v) R_\phi \\
\left( E_\phi \right)_t + (v \cdot \nabla) E_\phi &= R_\phi^T D(v) R_\phi
\end{align*}
\]

\[
\text{div}(v) = 0
\]

\[
\rho(\phi) \left( v_t + (v \cdot \nabla) v \right) - \text{div} \left( -p I + \mu(\phi) D(v) \right) - \text{div} \left( 4 R_\phi^T C \left( E_\phi \right) R_\phi^T \right) = \rho(\phi) f
\]

Membrane Rotation

Membrane Strain

Convection Equations

Navier-Stokes Equations

Membrane Stress
The governing equations

Time discretization schemes:

\[ \phi_t + v^{n-1} \cdot \nabla \phi = 0 \]
\[ R_t + (v^{n-1} \cdot \nabla) R = W(v^{n-1}) R \]
\[ E_t + (v^{n-1} \cdot \nabla) E = (R^n)^T D(v^n) R^n \]

\[ \text{div}(v^n) = 0 \]
\[ \rho^{n-1} \left( \frac{v^n - v^{n-1}}{\tau} + (v^{n-1} \cdot \nabla) v^n \right) \text{div} (-p^n I + \hat{\mu} D(v^n)) \]
\[ -\text{div} \left( R^n C(E^n)(R^n)^T \right) = \rho f^{n+1/2} \]

Membrane Stress
Numerical Scheme

Solve $\phi$ equation for $\phi_h^n$
Discontinuous Galerkin in time, space

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

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

$\phi_h^n, \phi_h^{n-1}$

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

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

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

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• Introduction of membrane into framework
• Example Simulations
• Conclusions
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

<table>
<thead>
<tr>
<th></th>
<th>No Membrane</th>
<th>Membrane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase Variable</td>
<td></td>
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<tr>
<td>U-Velocities</td>
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<tr>
<td>V-Velocities</td>
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<tr>
<td>Divergence</td>
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<tr>
<td>Strains</td>
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</tbody>
</table>

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

$t \in (0, 10)$
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

- 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

\[ \lambda_1 = \lambda_2 = 2.5 \times 10^3 \]
\[ t \in (0,3) \]
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 (Δt=0.005)
  - 32 processors of Lemieux

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

\[ \lambda_1 = \lambda_2 = 2.5 \times 10^4 \]
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 ($\Delta t=0.01$)

- **Problem Size:**
  - DOF’s in $\Phi$ 262,144
  - DOF’s in $v,p$ 112,724
Outline

- A phase field model for two immiscible fluids
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- Conclusions
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

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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: $\rho_f = 0.5$  $\rho_a = 1.0$
  - Imposed Velocity Field: $u_r = 0$
    $$u_\theta = r^2$$
  - Simulation Information:
    - 40 x 40 quadrilateral biquartic elements ($\Delta h = 0.05$)
    - 4000 time steps ($\Delta t=0.0025$)

$t \in [0, 20]$
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 $\varphi, R$ at $t = t^{n-1}$
- Solution for $v, E$ at $t = t^{n-1}$
- Scalar & Tensor Convection Equations for $\varphi, R$
- Discontinuous Galerkin in space and time
- High-order in space
  - Piecewise constant in time
- Solution for $\varphi, R$ at $t = t^n$

**Velocities**
- Solution for $\varphi, R$ 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 $t = t^n$
Solve $\phi$ equation for $\phi^n_h$

Discontinuous Galerkin in time, space

**Weak Form:**

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

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

**Discrete Scheme:**

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

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

$$= \int_K \phi_{h^-}(t^{n-1}) \psi_h(t^{n-1})$$
Numerical Scheme

\[(R_s)_t + (v \cdot \nabla)R_s = W(v)R_s\]

**Weak Form:**

\[\int_{\Omega} R_s \cdot S d\Omega \bigg|_{t=0}^{T} - \int_{0}^{T} \int_{\Omega} (R_s \cdot S_t + R_s \cdot (v \cdot \nabla) S) \, d\Omega \, dt \]
\[= - \int_{0}^{T} \int_{\Omega} (W(v)R_s \cdot S) \, d\Omega \, dt \]
\[+ \int_{0}^{T} \int_{\partial\Omega_{out}} R_s \cdot S (v \cdot n) \, ds \, dt = - \int_{0}^{T} \int_{\partial\Omega_{in}} R_{sin} \cdot S (v \cdot n) \, ds \, dt\]

**Discrete Scheme:**

\[\int_{K} R_h(t^n)S_h(t^n) - \int_{t^{n-1}}^{t^n} \int_{K} R_h ((S_h)_t + (v^{n-1} \cdot \nabla) S_h) + W(v^{n-1})R_h \cdot S_h \]
\[+ \int_{t^{n-1}}^{t^n} \int_{\partial K} ((v^{n-1} \cdot n)^{+} R_h + (v^{n-1} \cdot n)^{-} R_{h-}) S_h \]
\[= \int_{K} R_{h-}(t^{n-1})S_h(t^{n-1})\]
Numerical Scheme

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

\[
\rho^{n-1} (v_t + (v^{n-1} \cdot \nabla) v^n) - \text{div} (-p^n I + \hat{\mu} D(v^n)) = 0
\]

\[
-\text{div} \left( R^n C (E^n)(R^n)^T \right) = \rho f^{n+1/2}
\]

\[
-(R^n)^T D(v^n) R^n + E_t + (v^{n-1} \cdot \nabla) E = 0
\]
Physics-Based Preconditioning

\[
\begin{bmatrix}
A_{uu} & A_{uE} \\
A_{Eu} & A_{EE}
\end{bmatrix}
\begin{bmatrix}
u \\
E
\end{bmatrix} =
\begin{bmatrix}
F_u \\
F_E
\end{bmatrix}
\]

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

\[
\hat{S} = \hat{A}_{uu} - A_{uE}\hat{A}_{EE}^{-1}A_{Eu}
\]

\[
\hat{A}_{EE} = \int_K E_h(t^n)S_h(t^n) - \int_{t^{n-1}}^{t^n} \int_K E_h \left((F_h)_t + (v^{n-1} \cdot \nabla) F_h \right)
\]
The falling drop example

- **Simulation Information:**
  - 60 x 60 elements
    - For discontinuous Galerkin calculations: biquartic basis functions
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  - 2000 time steps (\(\Delta t=0.005\))
  - 64 processors of Lemieux

- **Problem Size:**
  - DOF’s in \(\Phi\) 57,600
  - DOF’s in \(R\) 230,400
  - DOF’s in \(v,p\) 33,000
  - DOF’s in \(E\) 230,400

\[ t \in (0,10) \]
\[ \lambda_1 = \lambda_2 = 2.5 \times 10^4 \]
## Effect of Preconditioner

Isogranular comparison for simulations without the membrane

<table>
<thead>
<tr>
<th>PEs</th>
<th>Elements</th>
<th>DOF</th>
<th>iterations</th>
<th>Time (s)</th>
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<tbody>
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<td>Time Steps</td>
<td>( \phi )</td>
<td>N-S</td>
<td>( \phi )</td>
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<tr>
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Effect of Preconditioner

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Isogranular comparison for simulations with the membrane