Enhanced Discretization and Space-Time Refinement in Moving-Boundary Flow Simulation

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Outline

• Why moving boundaries?
  • melt flow processes
  • solid mechanics

• Which frame of reference?
  • Lagrangian, Eulerian, mixed

• How to follow the interface?
  • tracking and capturing

• Enhanced surface discretization
  • NEFEM, IGA

• Space-time refinement
  • simplex space-time grids
Why Moving Boundaries?

- **Fluid:**
  - filling
  - swelling
  - solidification

- **Solid:**
  - shrinking
  - deformation
Which Frame of Reference?

- **Lagrangian:**
  - frame attached to moving material
  - no inflow or outflow of material
- **Eulerian:**
  - frame fixed in space
  - material flows relative to the frame
- **Lagrangian-Eulerian:**
  - neither Lagrangian nor Eulerian
  - Lagrangian and Eulerian as special cases
How to Follow the Interface?

Interface tracking

- interface = grid boundary
- deforming ALE grid

Interface capturing

- cut interface cell
- empty cell
- fixed Eulerian grid
Interface Tracking

• Advantages:
  • low discretization errors at the interface
  • easy inclusion of interface effects

• Disadvantages:
  • deformation limited if no remeshing
  • projection errors if remeshing

• Arbitrary Lagrangian-Eulerian (ALE), space-time finite elements
Interface Capturing

• Advantages:
  • easy handling of large deformations
  • allows topology changes

• Disadvantages:
  • high discretization errors at the interface
  • load imbalance

• Particle methods, volume-of-fluid, level-set, phase field
Interface Capturing • Level Set

- **Level set function** \( \phi(x, t) \)
  - fluid A domain \( \phi < 0 \)
  - fluid B domain \( \phi > 0 \)
  - interface \( \phi = 0 \)

- Due to Osher and Sethian (1988)
- Advected with fluid velocity:

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0
\]

- Determines material properties at integration point:

\[
\rho, \mu(\phi) = \begin{cases} 
\rho_A, \mu_A, & \phi(x, t) < 0 \\
\rho_B, \mu_B, & \phi(x, t) > 0 
\end{cases}
\]
Interface Capturing • Level Set Reinitialization

• Initial value is signed distance function
• Signed-distance property **degrades**:
• How to reinitialize?
  • search for closest interface node
  • narrow band search
  • iterative solution of Eikonal equation

• Mass conservation is not guaranteed
Interface Capturing • Level Set Sharpening

• XFEM-based integration:

level set  linearization  quadrature

• Adaptive refinement:
Interface-Tracking Problem

• Three governing equations
  • kinematic condition
  • interior mesh update
  • incompressible Navier-Stokes

• Solved within nonlinear iteration loop
  
  begin time step loop
    begin nonlinear iteration loop
      solve elevation equation
      solve deformation equation
      solve flow equation
    end loop
  end loop
Governing Equations: Flow

- Incompressible Navier-Stokes equations:

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \mathbf{f} \right) - \nabla \cdot \mathbf{\sigma} = 0 \quad \text{on } \Omega_t \quad \forall t \in (0, T) \]

\[ \nabla \cdot \mathbf{u} = 0 \quad \text{on } \Omega_t \quad \forall t \in (0, T) \]

- Constitutive equation:

\[ \mathbf{\sigma} = -\rho \mathbf{I} + \mathbf{T}, \quad \mathbf{T} = 2\mu \mathbf{\varepsilon}(\mathbf{u}), \quad \mathbf{\varepsilon}(\mathbf{u}) = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \]

- Boundary conditions:

\[ \mathbf{u} \cdot \mathbf{e}_d = g_d \quad \text{on } (\Gamma_t)_{g,d}, \quad d = 1 \ldots n_{sd} \]

\[ \mathbf{n} \cdot \mathbf{\sigma} \cdot \mathbf{e}_d = h_d \quad \text{on } (\Gamma_t)_{h,d}, \quad d = 1 \ldots n_{sd} \]

- For plastics flow:
  - Navier-Stokes → Stokes
  - Newtonian fluid → shear-thinning or viscoelastic (Giesekus, Oldroyd-B)
Galerkin Least-Squares Formulation: Flow

• Find $u^h \in (S_u^h)_n$, $p^h \in (S_p^h)_n$ such that $\forall w^h \in (V_u^h)_n$, $\forall q^h \in (V_p^h)_n$:

$$\int_{Q_n} w^h \cdot \rho \left( \frac{\partial u^h}{\partial t} + u^h \cdot \nabla u^h - f \right) dQ + \int_{Q_n} \varepsilon(w^h) : \sigma(p^h, u^h) dQ$$

$$+ \int_{Q_n} q^h \nabla \cdot u^h dQ + \int_{\Omega_n} (w^h)_n^+ \cdot \rho ((u^h)_n^+ - (u^h)_n^-) d\Omega$$

$$+ \sum_e \int_{Q_n^e} \tau_{\text{mom}} \frac{1}{\rho} \left[ \rho \left( \frac{\partial w^h}{\partial t} + u^h \cdot \nabla w^h \right) - \nabla \cdot \sigma(q^h, w^h) \right]$$

$$\cdot \left[ \rho \left( \frac{\partial u^h}{\partial t} + u^h \cdot \nabla u^h - f \right) - \nabla \cdot \sigma(p^h, u^h) \right] dQ$$

$$+ \sum_e \int_{Q_n^e} \tau_{\text{cont}} \nabla \cdot w^h \rho \nabla \cdot u^h dQ = \int_{(P_n)_h} w^h \cdot h^h dP.$$

• Notation:

$$(u^h)_n^\pm = \lim_{\varepsilon \to 0} u(t_n \pm \varepsilon)$$
Governing Equations: Deformation

• Displacements \( \mathbf{v}(\mathbf{x}, t) \) governed by linear elasticity:

\[
\nabla \cdot \mathbf{\sigma}_m(\mathbf{v}) = 0 \quad \text{on } \Omega_t \quad \forall t \in (0, T),
\]

\[
\mathbf{\sigma}_m(\mathbf{v}) = \lambda_m \left( \text{tr } \mathbf{\varepsilon}_m(\mathbf{v}) \right) \mathbf{I} + 2\mu_m \mathbf{\varepsilon}_m(\mathbf{v}),
\]

\[
\mathbf{\varepsilon}_m(\mathbf{v}) = \frac{1}{2} \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right).
\]

• Boundary conditions:

\[
\mathbf{v} \cdot \mathbf{e}_d = g_{m,d} \quad \text{on } (\Gamma_t)_{g_{m,d}}, \quad d = 1 \ldots n_{sd},
\]

\[
\mathbf{n} \cdot \mathbf{\sigma}_m \cdot \mathbf{e}_d = h_{m,d} \quad \text{on } (\Gamma_t)_{h_{m,d}}, \quad d = 1 \ldots n_{sd}.
\]

• Mesh update:

\[
\mathbf{x}(t_{n+1}) = \mathbf{x}(t_n) + \mathbf{v}.
\]
Galerkin Formulation: Deformation

• Find \( \mathbf{v}^h \in (\mathcal{S}_\mathbf{v}^h)_n \) such that \( \forall \delta \mathbf{v}^h \in (\mathcal{V}_\mathbf{v}^h)_n \):

\[
\int_{\Omega_n} \mathbf{\varepsilon}_m(\delta \mathbf{v}^h) : \mathbf{\sigma}_m(\mathbf{v}^h) d\Omega = \int_{(\Gamma_n)_h,m} \delta \mathbf{v}^h \cdot \mathbf{h}_m^h d\Gamma.
\]

• Coefficients \( \lambda_m \) and \( \mu_m \) adjusted to stiffen small cells:

\[
\lambda_m = \frac{\lambda_0}{\left( f + (1 - f) \left| \frac{\partial x}{\partial \xi} \right| \right)}, \quad \mu_m = \frac{\mu_0}{\left( f + (1 - f) \left| \frac{\partial x}{\partial \xi} \right| \right)}.
\]

• Alternate approaches:
  ▶ geometric (Masud, 1997 & 2007),
  ▶ stress-based (Oñate et al., 2000),
  ▶ ...
Governing Equations: Elevation

- Kinematic condition at the free surface:

\[ u \cdot n = \dot{v} \cdot n. \]

- One condition but two or three unknowns per node
- Whether explicitly stated or not, equivalent to:

\[ \frac{\partial \phi}{\partial t} = \frac{u \cdot n}{e \cdot \nabla} \phi + u_y. \]

where \( \phi \) is the generalized elevation along direction \( e \)
- Often applied point-wise; OK in tanks, but not in channels or jets:
Galerkin Least-Squares Formulation: Elevation

• Find $\phi^h \in S_\phi$ such that $\forall \psi^h \in V_\phi$:

$$\int_{Q_{\uparrow\uparrow}} \psi^h \left( \frac{\partial \phi^h}{\partial t} + u_x \frac{\partial \phi^h}{\partial x} - u_y \right) dQ_{\uparrow\uparrow} + \sum_{e_{\uparrow\uparrow}} \int_{Q_{\uparrow\uparrow}^e} \tau_{DC} \frac{\partial \psi^h}{\partial x} \cdot \frac{\partial \phi^h}{\partial x} dQ_{\uparrow\uparrow}$$

$$+ \sum_{e_{\uparrow\uparrow}} \int_{Q_{\uparrow\uparrow}^e} \tau_{GLS} \left[ \frac{\partial \psi^h}{\partial t} + u_x \frac{\partial \psi^h}{\partial x} \right] \cdot \left[ \frac{\partial \phi^h}{\partial t} + u_x \frac{\partial \phi^h}{\partial x} - u_y \right] dQ_{\uparrow\uparrow} = 0.$$

• Stabilization and DC parameters, using residual $R(\phi^h)$:

$$\tau_{GLS} = \frac{\Delta_{\uparrow\uparrow}}{2 \left| u_x \right|}, \quad \tau_{DC} = \delta \Delta_{\uparrow\uparrow}^2 R(\phi^h).$$
Example: Olmsted Dam

- Spillway of Olmsted dam on Ohio River
- Experiments in a scale model at ERDC:
  - Periodic spillway section
- Obstacles dissipate flow energy and reduce erosion:
Example: Olmsted Dam

- Computed using 418K tetrahedra and 1000 time steps:
Example: Olmsted Dam

- Mesh adapts to free surface movement:
Example: Olmsted Dam

• Quasi-steady state reached without remeshing

• Stream-wise component of velocity shown
• Hydraulic jump position accurately predicted
Example: Olmsted Dam

- Comparison of space-time (left) and level-set with XFEM (right)

Sauerland et al., Computers and Fluids, 87 (2013) 41–49
NURBS-Enhanced Finite Elements (Huerta et al.)

- Most elements are standard finite elements
- Elements on the NURBS boundary represent the exact geometry

NEFEM in Die Swell

- Transient Stokes equations; parabolic inflow; no slip on the walls
- FEM: linear space-time elements
- NEFEM: linear space-time approximation; geometry with cubic NURBS

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<th>NEFEM Swell Factor</th>
<th>FEM Swell Factor</th>
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Isogeometric Analysis (Hughes et al.)

- Analogous to isoparametric concept

- IGA uses NURBS to represent both the geometry and the unknown:

$$u^h = \sum_{i=1}^{n} R_{i,p}(\theta) u_i$$

Spline-Based Coupling for Fluid-Structure-Interaction

- Standard FE
- IGA + NEFEM
- IGA + Standard FE
Storage Tanks

- plant with industrial storage tanks
- stability under earthquakes (seismic loading) is an important design requirement

pressure bumps  diamond-shaped buckling  elephant footing
Storage Tanks

Requirements

- free-surface flow
- deformable domain with arbitrary wall shapes
- deformable structure

Methods

- interface tracking
- NURBS-enhanced finite elements
- arbitrary boundary description through NURBS
- Isogeometric Analysis for elastodynamics
3D Cylindrical Tank

• Liquid-filled storage tank subjected to seismic excitation

• Linear FEM for fluid, IGA shell for solid
3D Cylindrical Tank • Fluid Flow Field

• Fluid velocity (left) and mesh deformation (right) in rigid tank:

• Notice mesh nodes sliding across the NURBS edge
3D Cylindrical Tank • Structural Solution

- Structural deformation without excitation

maximal and minimal deformation

- Excitation started after equilibrium reached

equilibrium vertical displacement
surface grid point height in rigid (red) and flexible (blue) tank
Mesh Generation for Space-Time

• Hughes and Hulbert (1988), Maubach (1991):

Fig. 1. Space-time mesh for a two-material elastic rod problem.

• 3D case presents obvious difficulties...
Prisms versus Simplices

- Standard prismatic extensions of 3D elements:
  - 3d6n
  - 4d8n

- Simplex elements required for fully-unstructured meshes:
  - 3d4n
  - 4d5n
Prisms to Simplices

• Start with prismatic 4D mesh
• Add temporal refinement nodes along the spines:

• Perturb temporal coordinates:

• Delaunay triangulation using, e.g., qhull package
Final Steps

• Sliver elimination:

• Temporally refined 3D space-time mesh for 2D cylinder:
Test Case: Gaussian Hill in 2D and 3D

• Initial profile:

\[ u(x, 0) = \frac{5}{7} \exp \left\{ - \left( \frac{x - x_0}{\ell} \right)^2 \right\} \]

advected according to:

\[ \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0 \]

with \( a = 1 \) and \( \nu = 1/30000 \)

• Spatial meshes in 2D and 3D:

• Numerical solutions at \( t = 0.6 \) compared to exact solution
Test Case: Gaussian Hill in 2D

• GLS with C-N (left), prisms (middle) and tetra space-time with $C = 1$

• GLS with C-N (left), prisms (middle) and tetra space-time with $C = 3$
Test Case: Gaussian Hill in 3D

- GLS with pentatope space-time with $C = 1 \sim 3$

- Space-time edge for $(x, 0, 0)$ also shown

- Flow examples in the next talk of Violeta Karyofylli
Summary

• Why moving boundaries?
  • during melt flow: filling, swelling
  • after melt flow: solidification, shrinkage

• Which frame of reference?
  • Lagrangian
  • Eulerian and mixed

• How to follow the interface?
  • interface tracking: ALE, space-time
  • interface capturing: MAC, VOF, level set, phase field

• Enhanced surface discretization
• Space-time refinement
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