Immersed Boundary Methods for Fluid-Structure Interaction

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• Develop an efficient numerical method for studying the motion of solid and deformable particles in complex fluid domain using uniform mesh
Governing equations

- The viscous incompressible Navier-Stokes equations

\[
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) = -\nabla p + \mu \nabla^2 u + f + \rho \hat{f},
\]

\[\nabla \cdot u = 0,\]

- Immersed boundary exerts singular force on the fluid

\[
f(x, t) = \int_{\Gamma(t)} F(q, r, s, t) \delta(x - X(q, r, s, t)) \, dq \, dr \, ds
\]

- Immersed boundary moves with the fluid velocity

\[
\frac{dX(q, r, s, t)}{dt} = \int_\Omega u(x, t) \delta(x - X(q, r, s, t)) \, dx
\]
Projection method

Step 1: Compute an intermediate velocity field $u^*$ by solving

$$\frac{u^* - u^n}{\Delta t} = - (u \cdot \nabla u)^{n+\frac{1}{2}} + \frac{1}{\rho} \left( \frac{\mu}{2} \left( \nabla^2 u^* + \nabla^2 u^n \right) - \nabla p^{n-\frac{1}{2}} + (f^{n+\frac{1}{2}}) + \hat{f}^{n+\frac{1}{2}} \right).$$

Step 2: Compute a pressure update $\phi^{n+1}$ by solving the Poisson equation

$$\nabla^2 \phi^{n+1} = \rho \frac{\nabla \cdot u^*}{\Delta t},$$

Step 3: Update pressure and velocity field

$$u^{n+1} = u^* - \frac{1}{\rho} \Delta t \nabla \phi^{n+1},$$

$$p^{n+1/2} = p^{n-1/2} + \phi^{n+1} - \frac{\mu}{2\rho} (\nabla \cdot u^*).$$
Thin-Shell Kinematics

Reference configuration

Deformed configuration

Reference configuration

Deformed configuration

\[
\phi(\xi^1, \xi^2, \xi^3) = \bar{x}(\xi^1, \xi^2) + \xi^3 \bar{a}_3(\xi^1, \xi^2) \quad \text{with} \quad -\frac{h}{2} \leq \xi^3 \leq \frac{h}{2}
\]

\[
\phi(\xi^1, \xi^2, \xi^3) = x(\xi^1, \xi^2) + \xi^3 \eta(\xi^1, \xi^2)\bar{a}_3(\xi^1, \xi^2)
\]

\[
\eta = \frac{h}{\bar{h}} \quad \text{Thickness stretch}
\]
Equilibrium deformation of hyperelastic shell

\[ \bar{a}_\alpha = \bar{X}(\xi^1, \xi^2)_\alpha, \quad a_\alpha = X(\xi^1, \xi^2)_\alpha. \]

\[ g_\alpha = a_\alpha + \xi^3 a_{3,\alpha}, \quad g_3 = a_3, \]

\[ g_\alpha = a_\alpha + \xi^3 (\eta a_3)_\alpha, \quad g_3 = \eta a_3, \]

\[ \bar{g}_i \cdot \bar{g}^j = \delta^j_i \text{ and } g_i \cdot g^j = \delta^j_i. \]

stress resultant

\[ n^i = \int_{-h/2}^{h/2} \tau \cdot g^i \bar{v} d\xi^3, \]

moment resultant

\[ m^\alpha = \int_{-h/2}^{h/2} \tau \cdot g^\alpha \xi^3 \bar{v} d\xi^3, \]

bending stress

\[ q^{\alpha \beta} = \frac{\partial H}{\partial \kappa_{\alpha \beta}} = 2 \kappa_B (\kappa_m - \kappa_m^R) g^{\alpha \beta}. \]
Equilibrium deformation of hyperelastic shell

At equilibrium:
\[ \delta \Pi = \delta \Pi_{\text{int}} + \delta \Pi_{\text{ext}} = 0 \]

Variation of potential energy of the internal forces:
\[ \delta \Pi_{\text{int}} = \int_{\Omega_S} \frac{\partial W}{\partial \mathbf{F}} : \delta \mathbf{F} \, d\Omega_S + \int_{\Gamma} \frac{\partial H}{\partial \kappa_{\alpha\beta}} \delta \kappa_{\alpha\beta} \, d\Gamma \]

Mooney-Rivlin strain energy function:
\[ W = c_1 (I_1 - 3) + c_2 (I_2 - 3) \]

Helfrich bending energy function:
\[ H = 2 \kappa_B (\kappa_m - \kappa_m^R)^2 \]

Internal force at node I:
\[ \mathbf{f}_I = \int_{\Gamma} \begin{bmatrix} n^\alpha \cdot \frac{\partial a_\alpha}{\partial \mathbf{x}_I} + \eta n^3 \cdot \frac{\partial a_3}{\partial \mathbf{x}_I} + m^\alpha \cdot \left( \eta \frac{\partial a_3}{\partial \mathbf{x}_I} \right) \end{bmatrix} \, d\Gamma \]
\[ + \int_{\Gamma} q^{\alpha\beta} \begin{bmatrix} \left( \frac{\partial a_\alpha}{\partial \mathbf{x}_I} \right) \cdot a_3 + a_{\alpha,\beta} \cdot \frac{\partial a_3}{\partial \mathbf{x}_I} \end{bmatrix} \, d\Gamma \]

Le et al. J. Comp. Phys. 228: 8427, 2009
Spatial discretization of the thin-shell

Flat triangle

$$x_h = \sum_{I=1}^{3} N^I \left( \xi^1, \xi^2 \right) x_I$$

A six-node curved triangle

$$x_h = \sum_{I=1}^{6} N^I \left( \xi^1, \xi^2 \right) x_I$$

Triangular patch

$$x_h = \sum_{I=1}^{12} N^I \left( \xi^1, \xi^2 \right) x_I$$
Subdivision of Spline Curves

- Refinement of control polygon:

  New midpoints:  \( x_{2i+1}^{j+1} = \left( x_i^j + x_{i+1}^j \right) / 2 \)

  Current nodes:  \( x_{2i}^{j+1} = \left( x_{i-1}^j + 6x_i^j + x_{i+1}^j \right) / 8 \)

- Limiting node positions:

  Current nodes:  \( x_i^{j,\infty} = \left( x_{i-1}^j + 4x_i^j + x_{i+1}^j \right) / 6 \)
Loop’s subdivision scheme

Control-Mesh    One Refinement    Two Refinements

Surface $C^2$ continuous everywhere except at irregular nodes (nodes that do not have six neighbors)
Loop’s subdivision scheme

- Compute locations of new vertices as weighted average of original vertices

- Local neighborhood gives compact support

- Limiting node positions computed by similar scheme
Subdivision elements: Regular patches

- Evaluate for arbitrary \( v, w \) by linear operation \( x(v, w) = x\Phi c(v, w) \), with local node locations \( x \) and monomial coefficients \( c(v, w) \)

\[
c(v, w) = (1, v, w, v^2, vw, w^2, v^3, v^2w, vw^2, w^3, v^4, v^3w, v^2w^2, vw^3, w^4)^T
\]

- Precomputed constant matrix \( \Phi \)

\[
x_h = \sum_{I=1}^{12} N^I (v, w) x_I
\]

\( N^I \equiv \text{Quartic Box-splines} \)
Subdivision elements: Irregular patches

Regular patches

Numerical results: Capsule in shear flow

Shear rate $\dot{\gamma}$

Dimensionless shear rate: $G = \frac{\mu \dot{\gamma} a}{E}$

Deformation parameter: $D_{xz} = \frac{L - D}{L + D}$
Numerical results: Capsule in shear flow

Spherical capsule in shear flow:

Deformation parameter

Inclination angle

- $D_{xz}$
- $\theta / \pi$

Parameters:

- $G = 0.2$
- $G = 0.1$
- $G = 0.05$
- $G = 0.025$
- $G = 0.01$
- $G = 0.005$

Methods:

- present
- analytical

- BEM
- LBM
Red blood cell in shear flow

Tumbling

Swinging

Swinging

Tumbling

Transition

Phase diagram

Inverse dimensionless shear rate

Viscosity ratio

Swinging

Tumbling

Transition
Multiple cells flowing in microvessel
If an Eulerian background grid node coincides with the rigid boundary,
The MLS is a method for reconstructing continuous functions from a set of random points (a cloud of nodes) via the calculation of a weighted least squares (WLS) measure biased towards the region around the interpolation point.
u(x) is approximated by determining the vector a(x) that minimizes the weighted residual:

\[ R = \sum_{i=1}^{n} W(x - x_i) \left[ p^T(x_i) a(x) - u(x_i) \right]^2, \]

\[ W(x - x_i) = \begin{cases} \frac{2}{3} - 4r^2 + 4r^3, & r \leq 0.5 \\ \frac{4}{3} - 4r + 4r^2 - \frac{4}{3}r^3, & 0.5 < r \leq 1.0 \\ 0, & \text{otherwise}, \end{cases} \]

where \( r = \|x - x_i\|/r_s \)

Minimizing the residual with respect to a(x) leads to the following system of equations:

\[ A(x) a(x) = B(x) u_s \]

\[ u_s = [u_1 \quad u_2 \quad \ldots \quad u_n]^T \]

\[ A(x) = \sum_{i=1}^{n} W(x - x_i) p(x_i) p^T(x_i), \]

\[ B(x) = [W(x - x_1) p(x_1) \quad \ldots \quad W(x - x_n) p(x_n)]^T, \]

\[ u(x) = \sum_{i=1}^{n} \Phi_i(x) u_i = \Phi^T(x) u_s \]

\[ \Phi^T(x) = p^T(x) A(x)^{-1} B(x) \]

Treatment of the deformable boundaries

Distribution operator:

\[ f(x, t) = \sum_{l=1}^{NL} F_l(X_l, t) D_h \left( x - X_l(t) \right) \Delta S_l \]

Interpolation operator:

\[ \frac{dX(t)}{dt} = \int_{\Omega} u(x, t) \delta(x - X(t)) dx \]

\[ \delta_h(x) = \frac{1}{h^3} \phi \left( \frac{x_1}{h} \right) \phi \left( \frac{x_2}{h} \right) \phi \left( \frac{x_3}{h} \right) \]

\[ \phi(r) = \begin{cases} \frac{1}{4} \left( 1 + \cos \left( \frac{\pi r}{2} \right) \right), & |r| \leq 2, \\ 0, & \text{otherwise} \end{cases} \]

With MLS shape function:

\[ f_k = \frac{1}{h^3} \sum_{l=1}^{NL} \Phi^l_k(X_l) F_l \Delta S_l \]

\[ U_l(X_l) = \sum_{k=1}^{ne} \Phi^l_k(X_l) u_k \]
Treatment of the deformable boundaries

Conservation of elastic power:

\[
\sum_{k=1}^{tne} f_k \cdot u_k h^3 = \sum_{k=1}^{tne} \sum_{l=1}^{NL} \Phi_k^l F_l \Delta S_l \cdot u_k = \sum_{l=1}^{NL} F_l \cdot \left( \sum_{k=1}^{tne} \Phi_k^l u_k \right) \Delta S_l = \sum_{l=1}^{NL} F_l \cdot U_l \Delta S_l ,
\]

\[
\sum_{k=1}^{ne} \Phi_k^l (X_l) = 1
\]

Total force:

\[
\sum_{k=1}^{tne} f_k h^3 = \sum_{k=1}^{tne} \sum_{l=1}^{NL} \Phi_k^l F_l \Delta S_l = \sum_{l=1}^{NL} \left( \sum_{k=1}^{tne} \Phi_k^l \right) F_l \Delta S_l = \sum_{l=1}^{NL} F_l \Delta S_l
\]

Torque identity between the Eulerian and Lagrangian meshes

\[
\sum_{k=1}^{tne} x_k \times f_k h^3 = \sum_{k=1}^{tne} x_k \times \sum_{l=1}^{NL} \Phi_k^l F_l \Delta S_l = \sum_{l=1}^{NL} \left( \sum_{k=1}^{tne} x_k \Phi_k^l \right) \times F_l \Delta S_l = \sum_{l=1}^{NL} X_l \times F_l \Delta S_l .
\]

\[
\sum_{k=1}^{ne} \Phi_k^l (X_l) x_k = X_l
\]
Results - Pressure-driven flow

\[ u_z(r) = U_{\text{max}} \left[ 1 - \left( \frac{r}{R} \right)^2 \right], \text{ where } U_{\text{max}} = -\frac{R^2}{4\mu} \frac{dp}{dz} \]
Elastic capsule in shear flow
### Deterministic Lateral Displacement

**Equations:**

\[
Ca = \frac{\mu u_{\text{max}}}{E_s} \quad Re = \frac{\rho u_{\text{max}} a}{\mu}
\]

\[
R/a = 1.875, \frac{\lambda}{a} = 6.25 \quad L_z = 3.125a
\]

\[
L_y = 12.5a
\]

\[
\frac{d}{\lambda} = 0.125 \text{ and } 0.2 \quad L_x = 8\lambda \text{ and } 5\lambda.
\]

**Diagram Notes:**

- \( \lambda \) and \( \lambda/d = 8 \text{ and } 5 \)

- \( d/\lambda = 0.125 \text{ and } 0.2 \)

- \( L_x = 8\lambda \text{ and } 5\lambda \)
Deterministic Lateral Displacement

(a) $\lambda/d = 5$

(b) $\lambda/d = 8$
Deterministic Lateral Displacement

Time: 0.0

$Ca = 0.6$
Deterministic Lateral Displacement

Time: 0.0

$Ca = 0.1$. 

Deterministic Lateral Displacement

\[ Ca = 0.6 \]
Deterministic Lateral Displacement

\[ Ca = 0.1. \]
DLD – Inclination angle

\[ Ca = 0.43 \]
\[ \lambda/d = 11 \]

\[ Ca = 0.21 \]

\[ Ca = 0.07 \]

Average transverse velocity
DLD – Phase diagram

- **displaced**
- **zig-zag**
Deterministic Lateral Displacement

Part (a) $\lambda/d = 5$

Part (b) $\lambda/d = 8$
Conclusions

• Thin shell model and the Immersed Boundary method are very effective in handling viscous flow problems involving multiple elastic capsules.

• Subdivision surfaces have been employed to generate smooth force

• Moving Least Square reconstruction was implemented in the framework of the direct-forcing approach to allow more rigid and fluid points entering the reconstruction process