Modelling soft bodies with immersed boundaries

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Outlook

• Why do we need immersed boundaries?
• How can we use immersed boundaries?
• Applications
• Conclusion and future prospects
Why do we need immersed boundaries?
Simulation of blood flow (on cellular level)

Components:

- blood plasma ✓
- blood cells ✗
- channel boundaries ✓
Red blood cell

- elastic
- preferred shape
- fixed volume and surface area
ESPResSo

- soft-matter simulations
- molecules, atoms with their own mass
- interacting with bonds and potentials
- LBM
- closed objects with their own particle management
How can we use immersed boundaries?
Immersed boundary method

- discretization of object's boundary
- IB points
  - triangular mesh
  - elastic forces
  - interaction with fluid
Elastic forces*

LOCAL
• Constant local area constraint
• Surface strain constraint – stretching
• Curvature constraint – bending

NONLOCAL
• Constant volume constraint
• Constant global area constraint

* Dupin et al., Modeling the flow of dense suspensions of deformable particles in three dimensions Physical Review E 75 (6), 066707
Interaction with the fluid

Combination of LBM and IBM
Model of blood plasma

- Fluid dynamics – lattice-Boltzmann method (LBM)

\[
    f_i(\vec{x} + \vec{e}_i \delta_t, t + \delta_t) = f_i(\vec{x}, t) - \frac{(f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t))}{\tau} + F_i(\vec{x}, t)
\]

- Discrete velocities
- Fixed grid
- Parallelizable
- Explicit integration scheme: propagation + collision
Fluid – particle interaction

**Immersed boundary method**

- Fluid:
  - fixed grid
  - lattice-Boltzmann equation

- Blood cell:
  - boundary points are free in space
  - Newton equations

Drag force:
\[ F = K(u_f - u_p) \]
Fluid – particle interaction

**Immersed boundary method**

- Fluid:
  - fixed grid
  - lattice-Boltzmann equation

- Blood cell:
  - boundary points are free in space
  - Newton equations

external Force for LBM-equation
Calibration of immersed elastic objects

- elastic properties
- interaction with fluid
Calibration of elastic properties

- 5 parameters from elastic forces (stretching, bending, local area, global area, volume)

<table>
<thead>
<tr>
<th>force exerted on cell</th>
<th>67pN</th>
<th>130pN</th>
<th>193pN</th>
</tr>
</thead>
<tbody>
<tr>
<td>axial diameter $d_{ax}^0$</td>
<td>12.34</td>
<td>14.17</td>
<td>15.3</td>
</tr>
<tr>
<td>transverse diameter $d_{tr}^0$</td>
<td>5.05</td>
<td>4.53</td>
<td>4.29</td>
</tr>
</tbody>
</table>

Calibration of elastic properties

Optimal values of elasticity parameters for a healthy RBC.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stretching $k_s$</td>
<td>0.008</td>
</tr>
<tr>
<td>Bending $k_b$</td>
<td>0.0016</td>
</tr>
<tr>
<td>Local area $k_{al}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Global area $k_{eg}$</td>
<td>1.0</td>
</tr>
<tr>
<td>Volume $k_v$</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Calibration of IB – fluid interaction

- mass of IB points
- mesh density of IB points
- friction coefficient (drag force intensity on IB point)


Initial velocity $v_0$ of the sphere/ellipsoid
Calibration of IB – fluid interaction

- mass of IB points
- mesh density of IB points
- friction coefficient (drag force intensity on IB point)


fluidic drag force slows down the sphere/ellipsoid
Calibration of IB – fluid interaction

![Graph showing the relationship between mass of IB points and volume of ellipsoid](image.png)
Applications
Circulating tumor cells (CTCs)
Prognostic value

• Counting of CTCs:
  – medical checkups
  – control therapies
  – recognize new tumors developing

• Genetic/molecular characterization
  – gain information about main tumor and metastatic development
  – understanding evolution of cancer
Filter methods

- SIZE
  - different sizes and elasticities of blood cells

- ANTIBODY
  - surfaces covered with antibodies
Technical challenge

• CTCs are very rare (1-100 CTC per billions of blood cells)
• every single CTC is important
• CTCs change over time
• similar size and affinity properties to ordinary blood cells
New promising technologies

(a)

(b)

(c)

blood inflow

blood outflow

Conclusion

• Closed objects with their own particle management
• Calibration of elastic boundary and interaction with the fluid
• Applications: blood cells, bacteria, air bubbles, (magnetic) beads, dust ........

• Speed/Performance
108 Red Blood Cells
43200 IB-points
200 x 100 x 300
6 Mio. LB cells
16 CPUs Intel Xeon
X5650 @ 2.67GHz
1 GPU Tesla
M2075 6 GB
500.000 timesteps
> 19 days simulation
Remember

• Today 14:00 - Hands-On: Immersed Boundary Conditions

• Thursday 11:00 – Lecture
  Recent and Future Developments of ESPResSo
Thank you for your attention!

http://cell-in-fluid.weebly.com/

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