A Multiple Time Stepping Algorithm for Efficient Multiscale Modeling of Platelets Flowing in Blood Plasma

Na Zhang, Peng Zheng, Li Zhang, Danny Bluemstein, Yuefan Deng.1,3
1 Department of Applied Mathematics and Statistics, Stony Brook University, NY, 11794
2 Department of Biomedical Engineering, Stony Brook University, NY 11794
3 National Supercomputer Center in Jinan, Shandong, China.

Motivations
Cardiovascular diseases and thrombosis burden in implantable blood recirculating devices account for near 30% of all deaths globally and 35% in the US annually. Thrombosis in vascular diseases and implants is potentiated by an interaction of platelets with an injured wall or foreign surface. However, numerical simulations of flow-induced platelet-mediated thrombosis is an immense computational and algorithmic challenge due to the modeling complexity and disparate spatiotemporal scales of the mechanisms occur.

Methodologies
- Mathematical Models – Study mechanical and dynamics properties of blood flow and platelets;
- Coupling Method – Interface disparate spatial scales of blood flow and platelets and simulate flow-induced platelet-mediated thrombosis under various flows;
- Multiscale Multiple Time Stepping (MTS) Algorithm – 300x reduction in computing time over standard MTS for solving multiscale models

Multiscale Models

<table>
<thead>
<tr>
<th>Scale</th>
<th>Nanoscale</th>
<th>Mesoscale</th>
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<tbody>
<tr>
<td>Microfluidics</td>
<td>Platelet Cell</td>
<td>Blood Plasma</td>
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Methods
Coarse Grained Molecular Dynamics (CGMD) Dispersive Particle Dynamics (DPD)

Time-Step: 0~100 ns
Length: 1~2 μm

Model Abstraction

![Model Abstraction](image)

Figure 3 Integrated multiscale multiple time stepping algorithm for particle-based platelets flowing in blood plasma model. We decompose the whole integrator process into four levels: (1) DPD-modified blood plasma (which has the largest time step Δt ≈ 10−7 s); (2) DPD-CGMD modeled deformable platelet membrane at contact region of two scales; (3) CGMD modeled platelet of non-bonded components; (4) CGMD modeled platelet of bonded component (which needs the most frequent update, Δt ≈ 10−3 s). Jump factors are introduced to make trade-off between speed and accuracy.

Overview
Our group has developed a multiscale multiple time stepping algorithms for the multiscale models.

Figure 4 Multiple Scales in the Model

Force Fields

\[ F^P = \sum_i \left( \frac{\partial}{\partial r_i} \left( \sum_j k(r_{ij}) \frac{q_i q_j}{r_{ij}} \right) \right) \]

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\[ F^\phi = -\nabla \phi \left( \sum_j k(r_{ij}) \frac{q_i q_j}{r_{ij}} \right) \]

Where \( F^p \) and \( F^\phi \) are the conservative, dispersive, and random force acting on fluid flow.

Accuracy vs. Computing Speed for Multiscale Simulations

![Accuracy vs. Computing Speed for Multiscale Simulations](image)

References

Contact Information
Na Zhang: na.zhang@stonybrook.edu