Blood Clot Formation Modelling with LAMMPS: Thrombosis versus Hydrodynamic Stress

學生：醫工四 B11508002 陳楷霖

指導教授：張書瑋、周佳靚

Introduction

- **Modeling thrombosis:** Thrombosis is a multiscale process driven by mechanical interactions among platelets, red blood cells, and blood flow. Clot growth is determined by the balance between adhesion force and hydrodynamic stress. [1]
- **Mechanistic regulation of clot stability:** By systematically varying flow speed and adhesion strength, our simulation shows how hydrodynamic stress and inter-particle forces regulate clot growth and its local stress evolution.
- **Particle-based simulation framework:** In this study, we utilize a LAMMPS-based particle model that enables controlled investigation of adhesion with interatomic potential and flow forces. This approach captures collective mechanical behavior at the microscale under varying flow conditions. [2]

Materials & Methods

- **LAMMPS-based Modeling:**

We developed a two-dimensional particle-based model using LAMMPS, where blood components are represented as Lennard–Jones particles under Poiseuille flow. Vessel walls, a damaged wall region (clot seed), red blood cells, and platelets are explicitly modeled with distinct interaction rules. [3]

- **Multistage Modeling**

To capture clot formation beyond initial attachment, we introduced a multistage modeling strategy where platelet activation and interaction strengths are updated sequentially.

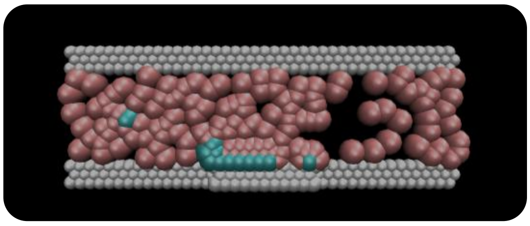
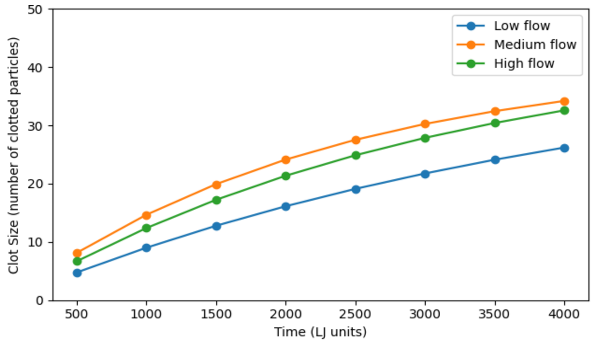


Fig. 1. A middle frame of the proposed LAMMPS-based model of thrombosis

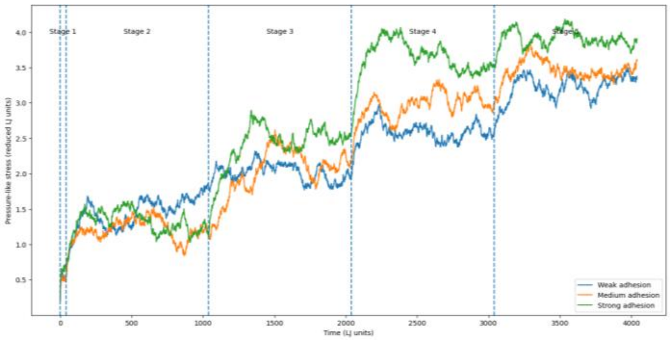
Results & Discission

- **Clot Sizes under different flow strengths**



Medium flow consistently produces the largest clot throughout the simulation, followed by high flow, while low flow results in the smallest clot at all time points.

- **Stress Evolution during different stages**



Stronger adhesion produces higher stress levels due to more effective force transmission within the clot, also demonstrating that increasing adhesion strength enhances the magnitude of mechanical stress sustained by the clot during multistage development.

Conclusion

From our experiments, several things can also be inferred:

- ***Slower blood flow doesn't lead to larger clots***

Clot size is maximized at intermediate flow strength, where particle transport to the injury site is efficient without excessive shear.

- ***Thicker blood experience higher mechanical stress***

Stronger adhesion enhances internal force transmission and rigidity, allowing clots of similar size to sustain markedly different mechanical loads.

- ***Drinking less water accelerates clot formation by increasing adhesion***

Reduced hydration can increase effective adhesion between blood components, leading to faster clot stabilization and higher mechanical stress.

References

[1] Fogelson, A. L., & Neeves, K. B. (2015). Fluid Mechanics of Blood Clot Formation. Annual Review of Fluid Mechanics, 47, 377–403. https://doi.org/10.1146/annurev-fluid-010814-014513

[2] Fedosov, Dmitry A, Caswell, B., & Karniadakis, G. E. (2025). General coarse-grained red blood cell models: I. Mechanics. ArXiv.org. https://arxiv.org/abs/0905.0042

[3] Xiao, L., Liu, Y., Chen, S., & Fu, B. (2016). Simulation of Deformation and Aggregation of Two Red Blood Cells in a Stenosed Microvessel by Dissipative Particle Dynamics. Cell Biochemistry and Biophysics, 74(4), 513–525. https://doi.org/10.1007/s12013-016-0765-2