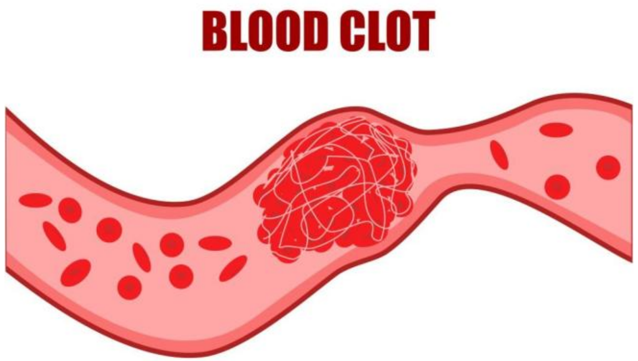
Department of Biomedical Engineering,

National Taiwan University

Blood clot formation modelling using LAMMPs:

Thrombosis (血栓形成) v.s. Hydrodynamic stress



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Introduction

- Objective:
  - ❑ Model the formation of blood clots in veins/arteries using a molecular dynamics approach in LAMMPS.
  - ❑ Use big and small spheres to represent RBCs and platelets.
  - ❑ Study how ***flow speed and adhesion strength*** influence clot growth and local pressure on the seed region.

** 純探討血液凝結導致的血栓

其他狀況（血管/粥狀動脈硬化、其他物理性阻塞...etc）不納入模擬與比較

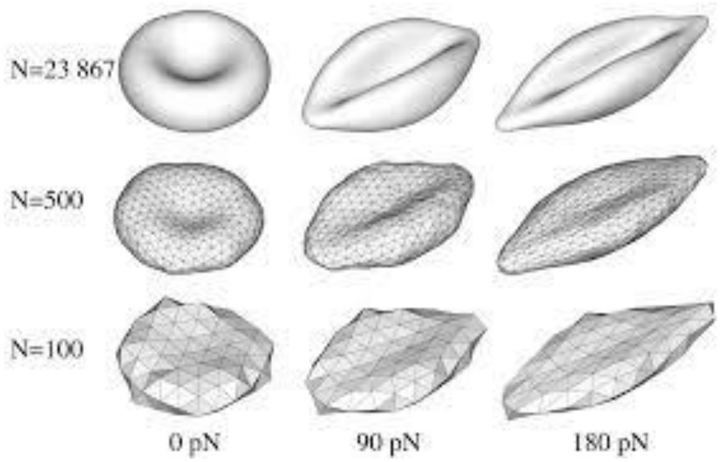
Introduction

- Research Background

  - Coarse-grained blood flow modeling

    → Using spheres, beads or shapes to represent RBCs [1]

    → More about blood flow modelling and RBC mechanics [2,3]



  - *Blood flow simulation* + *Thrombosis simulation* [4]

  - *Simulate blood flow and thrombosis (using interatomic potential) with LAMMPS*

Introduction

- Research Question:

Under different *flow speed* , *adhesion strength*:

- ❑ Clot size v.s. pressure overtime?
- ❑ How does different adhesion strength influence clot formation speed?
- ❑ What can be inferred from the results?

e.g. veins form faster than artery? 濃稠血液 forms clots easier?

Methodology

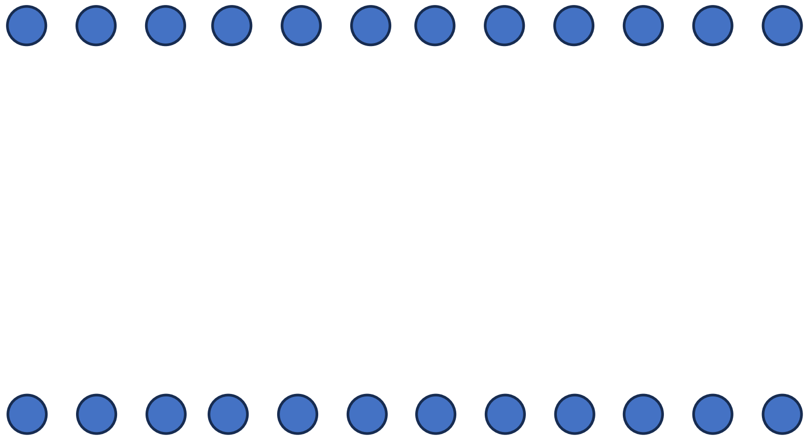
- Model Design

```
# Simulation box
region box block 0 60 0 20 0 2   # x: flow, y: vein height, z: thin
create_box 4 box

# Define top/bottom walls as fixed atoms
region lower_wall block 0 60 0 1 0 2
region upper_wall block 0 60 19 20 0 2
create_atoms 4 region lower_wall
create_atoms 4 region upper_wall

group lower_wall region lower_wall
group upper_wall region upper_wall

# Freeze wall atoms
fix freeze_lower lower_wall setforce 0.0 0.0 0.0
fix freeze_upper upper_wall setforce 0.0 0.0 0.0
```



Methodology

- Model Design

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# Freeze wall atoms
fix freeze_lower lower_wall setforce 0.0 0.0 0.0
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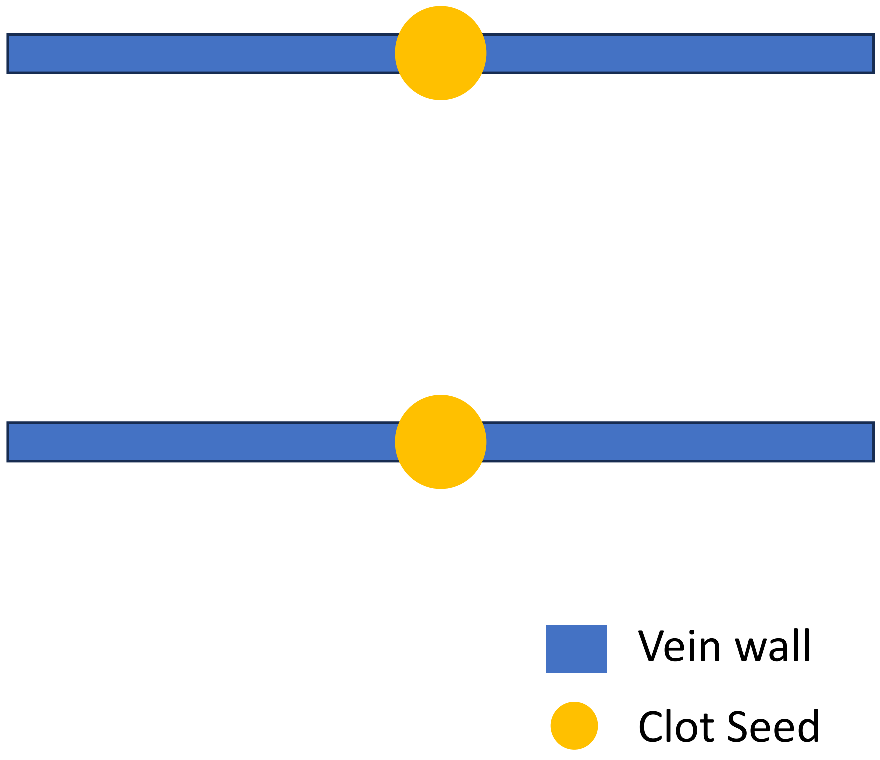
```

```
#clot seed
create_atoms 4 single 30 10 1
create_atoms 4 single 30 12 1
group seeds type 4
fix freeze_seeds seeds setforce 0.0 0.0 0.0
```



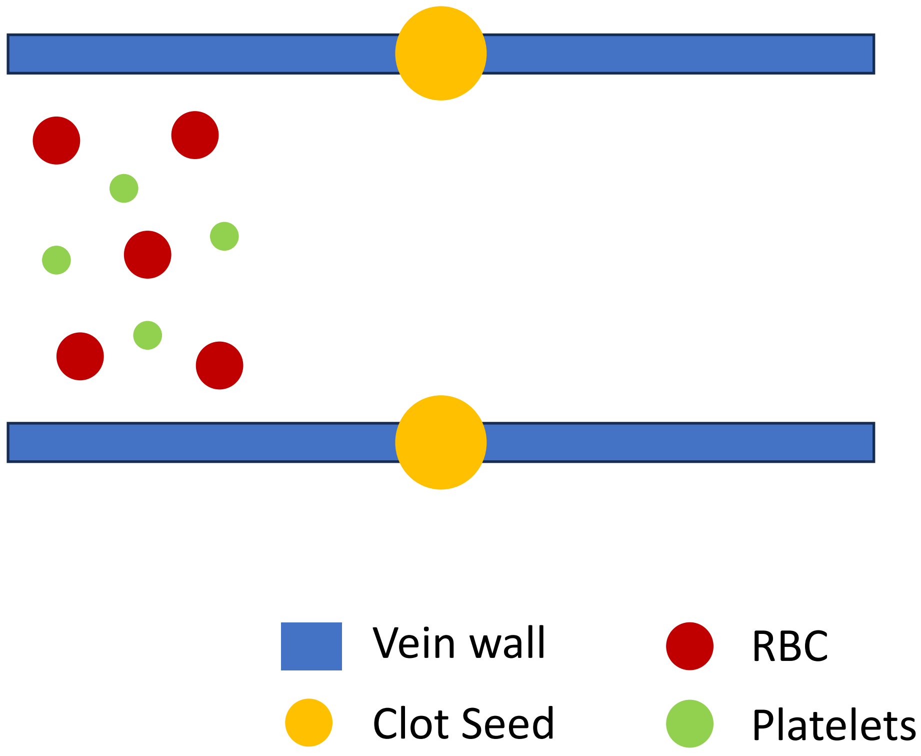
Methodology

- Model Design

```
# Atom style and types
atom_style atomic
units lj

# Masses for different particle types
mass 1 3.0      # RBCs (larger particles)
mass 2 1.5      # Platelets (smaller particles)
mass 3 1.0      # Solvent/plasma
mass 4 10.0     # Fixed seed (injury site)
```

```
# initial velocities
compute         mobile flow temp
velocity        flow create 1.0 482748 temp mobile
fix             1 all nve
fix             2 flow temp/rescale 200 1.0 1.0 0.02 1.0
fix_modify      2 temp mobile
```



Methodology

- Model Design

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# initial velocities
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velocity         flow create 1.0 482748 temp mobile
fix              1 all nve
fix              2 flow temp/rescale 200 1.0 1.0 0.02 1.0
fix_modify       2 temp mobile
```
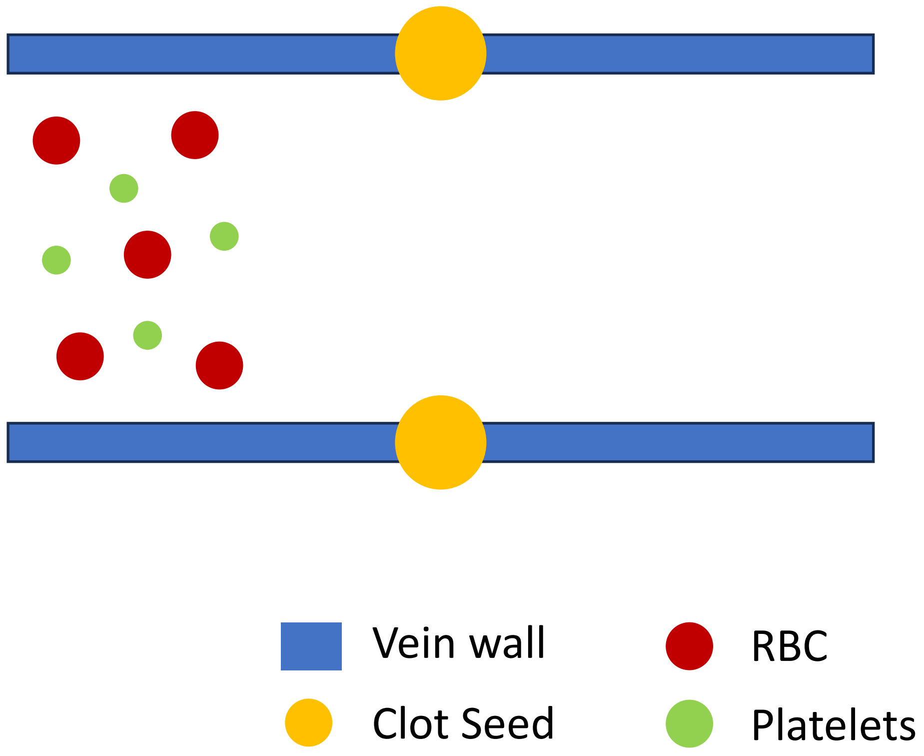

```
# hybrid pair potentials
pair_style hybrid/overlay lj/cut 2.5 morse 1.0

# Repulsion between general particles
pair_coeff * * lj/cut 1.0 1.0 2.5

# Adhesion: platelet-seed attractive force
pair_coeff 2 4 morse 2.0 2.0 1.0  # D0=2.0, alpha=2.0, r0=1.0
```



Methodology

- Model Design

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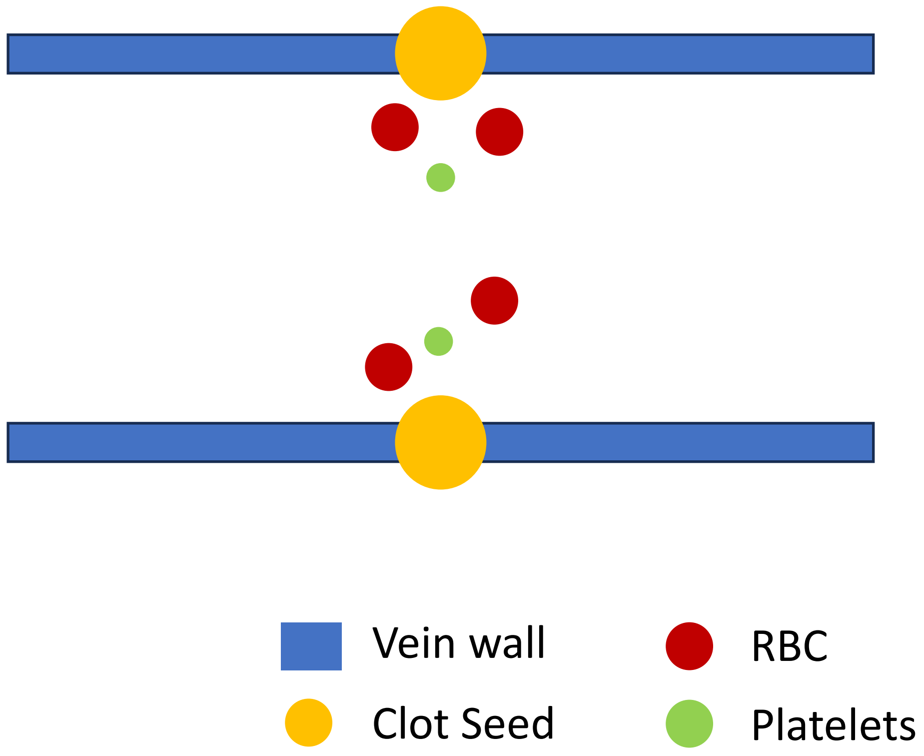
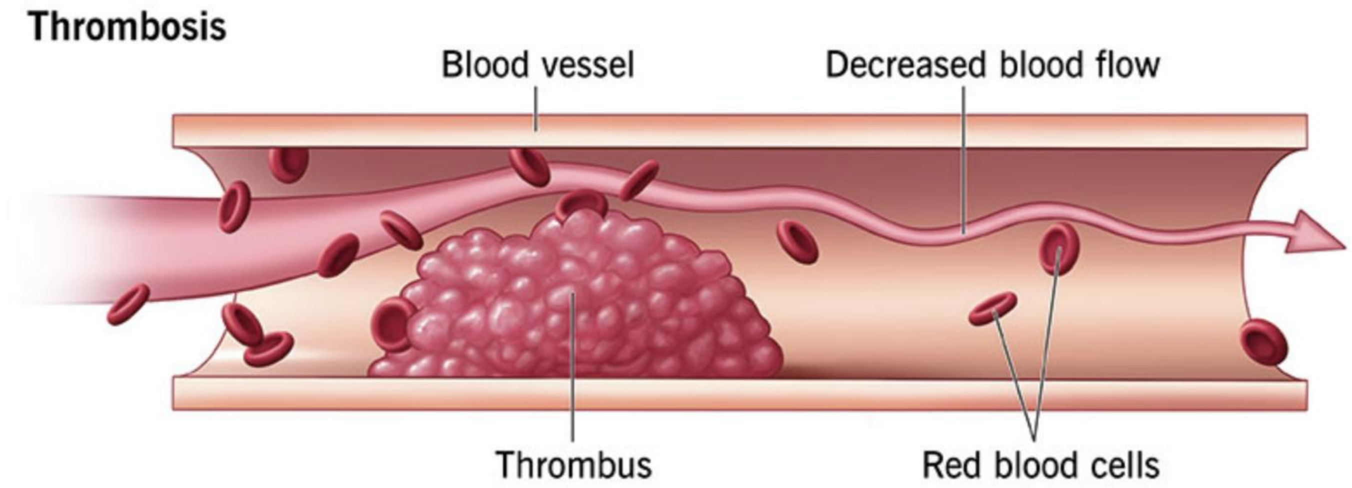


Methodology

- Post-processing
  - Plot clot ***particle number vs. time*** → clot growth rate.
  - **Calculate pressure rise over time** as clot blocks flow.

Expected Results

- *Clot size* **α** *Pressure*
- Higher adhesion → faster nucleation and more stable clot
- Veins form clots easier (slower blood flow speed → adhesion dominant)



References

[1] Fedosov, D. A., Caswell, B., & Karniadakis, G. E. (2010). A Multiscale Red Blood Cell Model with Accurate Mechanics, Rheology, and Dynamics. *Biophysical Journal*, *98*(10), 2215–2225. https://doi.org/10.1016/j.bpj.2010.02.002

[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

[4] Moiseyev, G., & Bar-Yoseph, P. Z. (2013). Computational modeling of thrombosis as a tool in the design and optimization of vascular implants. *Journal of Biomechanics*, *46*(2), 248–252. https://doi.org/10.1016/j.jbiomech.2012.11.002

Thank you for listening!