# A Molecular Model for Platelets at Multiple Scales and Simulations on Supercomputers

**ACM Student Research Competition (SRC) Poster**


**Li Zhang[1], Yuefan Deng[1,2] (Advisor)**

[1]Department of Applied Mathematics & Statistics, Stony Brook University, Stony Brook, NY 11794, USA

[2]National Supercomputer Center in Jinan, Shandong Computer Science Center, Jinan, Shandong 250101, PRC


## Introduction

A molecular model at multiscale for human platelets is designed and implemented on large-scale supercomputers. The essence of this research involves development of a platelet model and studies of the model numerically. The molecular model for human blood platelets characterizes the principal physiological functions of several key components of a single platelet. As such, the model will require simulations at spatial scales as small as a typical molecule and as big as a complete cell, spanning several orders of magnitude in space and time. To simulate the dynamics accurately and efficiently, multiscale must also be considered. All in all, a more realistic model will require massive computations. This research will be enabled by the rising power of supercomputing in solving the most crushingly difficult problems in many fields including biomedical engineering. Numerical experiments with our model require considerations of large number of particles and the physiological phenomena at multiscale and thus demand development of the-state-of-the-art parallel algorithms, the main thrust of this work.

## Supercomputing Methodologies

### Packages

LAMMPS, NAMD, VMD, HEMD*

*HEMD: in house algorithms package, which is built in and developed by our own group for multiscale simulations.

### Platforms

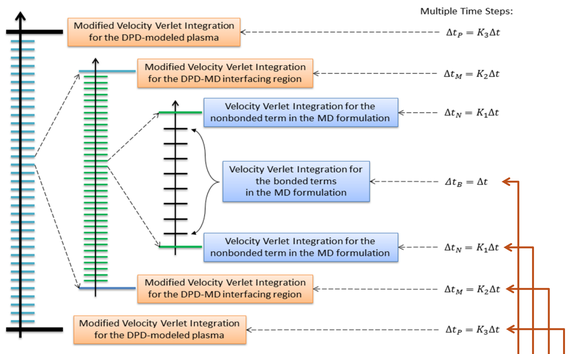
*Seawulf Cluster, Galaxy* (Stony Brook University)

*Sunway Blue Light System* (National Supercomputing Center in Jinan, China)

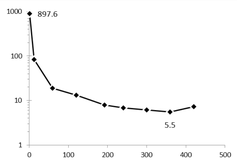
*Stampede* (Texas Advanced Computing Center)

### Algorithms

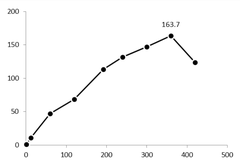
Temporal l Interfacing Algorithm – Multiscale Multiple Time Stepping




### Performances

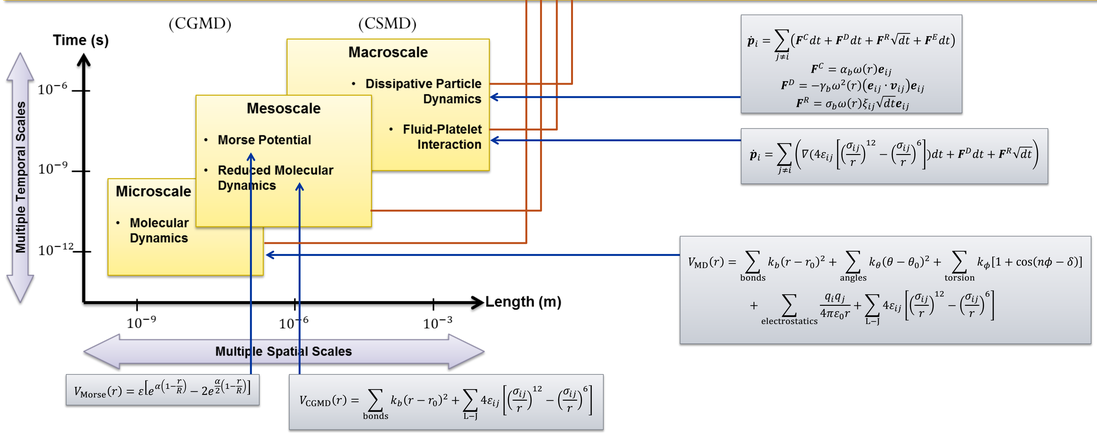



Parallel speeds (wallclock time): vs. number of processor cores

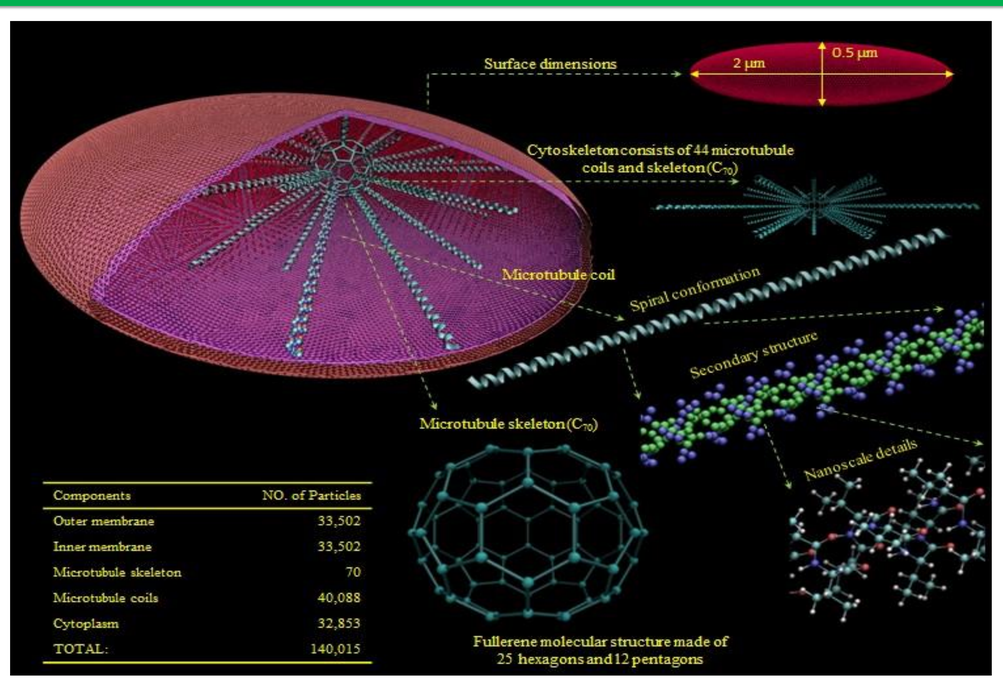



Speedups vs. number of processor cores

## Multiscale Modeling




## Structures and Constituents

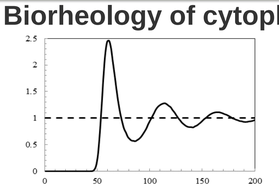



| Components | NO. of Particles |
|---|---|
| Outer membrane | 33,502 |
| Inner membrane | 33,502 |
| Microtubule skeleton | 70 |
| Microtubule coils | 40,088 |
| Cytoplasm | 32,853 |
| TOTAL: | 140,015 |

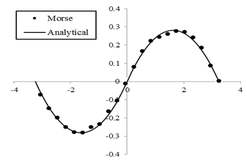
## Simulation Results

### Cytoplasm

**Biorheology of cytoplasm**




Radial Distribution Function $g(r)$ vs. the distance in nanometer r (nm)

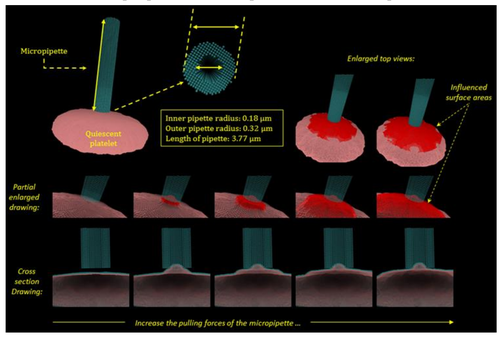



Counter Poiseuille flows velocity (m/s) vs. position

### Membrane

**Elasticity of membrane**

- micropipette aspiration experiment

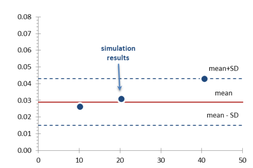



**Shear Modulus**

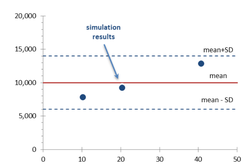
$$\mu_s = \frac{r_{in}^2}{2.45}\left(\frac{\Delta P}{L_s}\right)$$

**aspiration pressure**

$$\Delta P = \frac{F_{ext}}{\pi r_t^2}$$

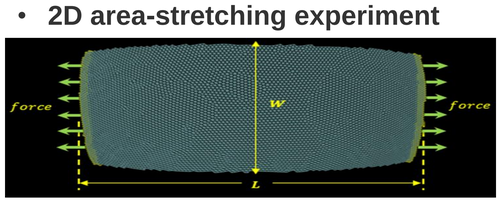



Shear elastic modulus $\mu_s$ (dyn/cm) vs. external force $F$ (pN)



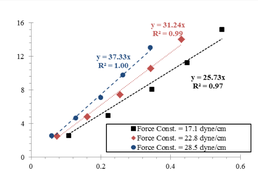

Shear elastic modulus normalized by membrane thickness $\mu_{sn}$ (dyn/cm²) vs. external force $F$ (pN)

- 2D area-stretching experiment

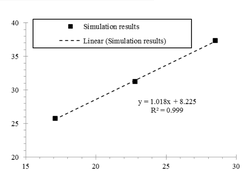



**Young's Modulus**

$$Y_m = \frac{S_{ext}}{\Delta L/L}$$

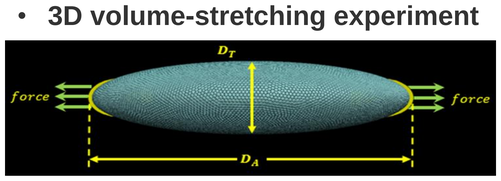


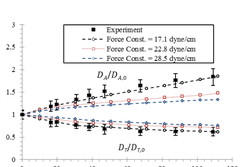

membrane-stretching response: stress (μN/m) vs. strain (ΔL/L)




Young's modulus of the membrane (μN/m) vs. the spring force constants (dyn/cm)

- 3D volume-stretching experiment

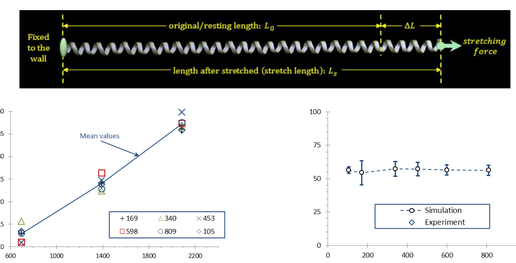



Platelet stretching response: the diameter change ratios vs. stretching force (pN)

### Filaments

**Stiffness of filaments**



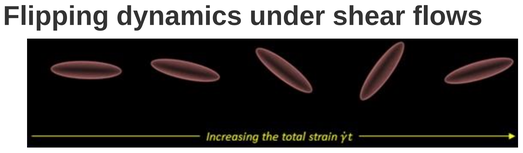

Length change $\Delta L$ (nm) vs. stretching force $F$ (pN)

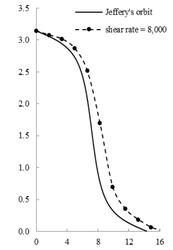



The stiffness $F/\Delta L$ (in pN/nm) vs. resting length $L_0$ (in nm)

### Biophysics

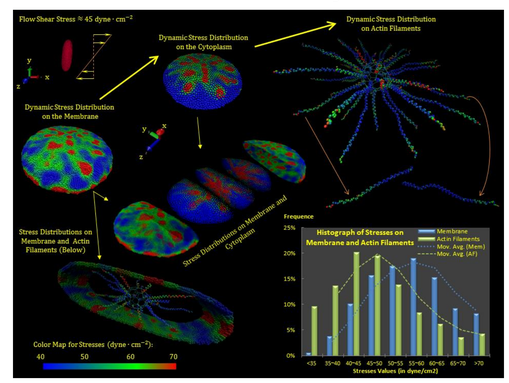
- Flipping dynamics under shear flows



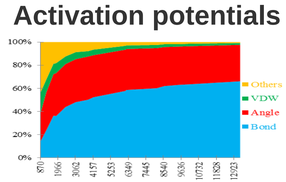




Rotation angle $\phi(\dot{\gamma}t)$ (radian) vs. total strain $\dot{\gamma}t$

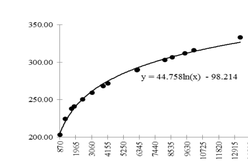
- Mechanotransduction analysis




- Activation potentials




Energy distribution in filaments extensive percentage vs. $\Delta E$ (kcal/mol)




Total length change in filaments extensive length vs. $\Delta E$ (kcal/mol)


**CONTACTS:**

**Li Zhang**

**– li.zhang.2@stonybrook.edu**

**Yuefan Deng (Advisor)**

**– yuefan.deng@stonybrook.edu**