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.

**Introduction**

**Supercomputing Methodologies**

LAMMPS, NAMD, VMD, HEMD

*HEMD: in-house algorithms package, which is build 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)

**Simulation Results**

**Cytoplasm**

- Bioregulation 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 $E_s$ (dyn/cm) vs. external force $F$ (pN)
  - Shear elastic modulus normalized by membrane thickness $E_{th}$ (dyne/cm²) vs. external force $F$ (pN)

**Biophysics**

- Flipping dynamics under shear flows
- Mechanotransduction analysis

**Structures and Constituents**

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

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