



## Biomedical Informatics Grand Rounds



**Peng Zhang, PhD;**

**Research Scientist, Stony Brook University**

### Multi-Scale Modeling and Machine Learning for Biomedical Studies

**Wednesday, September 18, 2019 3 pm—4 pm**  
**Health Science Center L2-3B**

#### **Abstract:**

We introduce a new platform for integrating multiscale modeling and machine learning for accurate elucidation of the complex interactions between living tissues and mechanical stimuli, represented by the vexing problem of shear-induced platelets activation and resultant thrombosis. The coupling of the disparate spatial-temporal scales between the macroscopic transport and the molecular-level events poses a major modeling and computing challenge. This platform addresses the mechano-biological linkages by incorporating meso scale Dissipative Particle Dynamics (DPD) of viscous blood flow, interfaced with micro-scale Coarse-Grained Molecular Dynamics (CGMD) of platelets' viscoelastic bilayer membranes and atomic-scale Molecular Dynamics (MD) of intra-platelet structural and functional components (cytoplasm, microtubules and cytoskeleton). The multiple scales of the model are dynamically coupled: by passing the information between the subsystems of these scales. To handle 3-4 orders of magnitude disparity in the temporal scales between micro- and molecular-scale methods, I developed a new multiple time-stepping (MTS) algorithm that demonstrated 3000x reduction in computing time over standard methods benchmarked on three architecturally different supercomputers. Guided by machine learning involving a LSTM (long short-term memory) neural network, the MTS algorithm adjusts the time-stepping sizes for efficient and accurate modeling. Additionally, for enabling quantified validation for model credibility with *in-vitro* experiments, I developed a multi-agent learning system that predicts the platelet dynamics and morphological changes from high-speed dynamic microscopy imaging in circulation microchannels under various chemical agonists and flow stresses. The multi-scale modeling and machine-learning platform enables complete and accurate studies of the systems as complex as biomedicine.

#### **Bio:**

Peng Zhang is a research scientist at Stony Brook University. He received his Ph.D. in Applied Mathematics from Stony Brook University, after completing his M.S. in Parallel Computing and B.S. in Mathematics from Nankai University with honors. His research focuses on the development of efficient and accurate problem-solving technologies for applications in science and engineering by coupling mathematical models, algorithms including machine learning, and software suites. He published more than 30 papers in applied mathematics, high performance computing, biomedical engineering and biosciences, plus two book chapters in big data. He has five awarded patents in US and China. He received two XSEDE Research Awards in 2014 and 2015. He has co-supervised and is co-supervising 7 doctoral students. He has presented more than 20 lectures at international conferences and seminars such as BMES, SB3C and SC. He has taught a variety of courses at Stony Brook University, including numerical algebra, parallel computing, computer algorithms and applications of complex analysis.

**\*\*CME Credit Available\*\***

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