THE UNIVERSITY OF CHICAGO

COMPUTATIONAL AND APPLIED MATHEMATICS COLLOQUIUM

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Machine Learning for Intelligent Multiscale Modeling of Platelet Dynamics

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Jones 226, 5747 South Ellis Avenue

ABSTRACT

Multiscale modeling in biomedical engineering is gaining momentum because of progress in supercomputing, applied mathematics, and quantitative biomedical engineering. For example, scientists in various disciplines have been advancing, slowly but steadily, the simulation of blood including its flowing and the physiological properties of such components as red blood cells, white blood cells, and platelets. Platelet activation and aggregation stimulate blood clotting that results in heart attacks and strokes causing nearly 20 million deaths each year. To reduce such deaths, we must discover new drugs. To discover new drugs, we must understand the mechanism of platelet activation and aggregation. To model platelets' dynamics involves setting the basic space and time discretization in huge ranges of 5-6 orders of magnitudes, resulting from the relevant fundamental interactions at atomic, to molecular, to cell, to fluid scales. To achieve the desired accuracy at the minimal computational costs, we must select the correct physiological parameters in the force fields such as the Morse potential and Hooke's law as well as the spatial and temporal discretization, by machine learning. We demonstrate our preliminary results of speeding up a multiscale two-platelet aggregation simulation, while maintaining sufficient accuracy, by nearly one order of magnitude, compared with traditional algorithm that uses the smallest of all temporal and spatial scales in order to capture the finest details of the dynamics. We present our analyses of the accuracies and efficiencies of the representative modeling. We will also outline the general methodologies of multiscale modeling of cells at atomic resolutions.

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