Efficient Multiscale Platelets Modeling Using Supercomputers

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1. INTRODUCTION

Advances in medical imaging techniques and computational methods have enabled accurate simulations of subject-specific blood flows at the level of blood cell and in complex arterial networks [1]. Those advances in studying blood flow dynamics have in turn improved cardiovascular devices (CVS) design, a process relying heavily on numerical simulations. While the advent of these devices has provided life-saving solutions to millions of patients globally, thrombogenic risk potential of these devices remains an impediment [2]. Thrombosis formation on the surface of these implantable devices is initialized by chain reactions of platelets disorders. However, quantitative analysis of the platelet shape change is, at best, confined in the laboratory experiments. Successfully computer-modeling such intricate phenomena and analyzing stress field of platelets activation will help design vascular diseases drugs and implantable blood recirculating devices. Nevertheless, untangling the mechanical stimuli to trigger platelet activation is full of physical, mathematical and computational challenges.

First of all, physical insights are essential for developing an accurate platelet predictive model with parameters matching laboratory mechanical and thermodynamic blood properties. Secondly, efficient simulations require modeling not just the flow dynamics but process pertinent to flow-induced platelet-mediated blood clotting. As such, multiple scales must be considered to characterize system behavior and the associated efficient modeling tools must be developed for high-resolution low-cost studies of complex biological problems. In addition to model construction, achieving high computing speed is another challenge for completing simulation of a certain physical timeframe. Yet the large gap in the space and time scales and modeling algorithm complexities limit computing speed. At last, porting simulations to accelerators and optimizing performance is not a trivial task.

Advances are needed to enable breakthroughs in multiscale platelets modeling. These advances include: (1) accurate mathematical models for each scale considered; (2) stable spatial and temporal interfacing methods; (3) robust algorithms that capable of both extracting main features and of quantifying possible errors; and (4) parallel solvers for each model and be scalable to tens of thousands of computer processors, and be portable to heterogeneous architectures.

2. METHODS AND RESULTS

This work is to present computational methodology that will simulate the millisecond-scale hematology with heterogeneous supercomputing. This poster will cover:

2.1 Multiscale Model

A multiscale model for solving this multicomponent biological problem is developed and implemented for simulation on supercomputers. In this model, three simulation domains are identified: platelet domain, blood flow domain and interfacing domain [3, 4]. For platelet domain, the microscopic method using coarse-grained molecular dynamics (CGMD) is employed to emulate components of platelets such as pathogenic membranous morphology and cytoskeletal filaments. For blood flow domain, the mesoscopic method using dissipative particle dynamics (DPD) is employed to address the bulk transfer of viscous blood flows in arterials with adjustable flow Reynolds numbers. For interfacing domain, to mimic friction between platelets surface membranes and surrounding blood flows, we proposed a hybrid force filed containing the stochastic and random terms from DPD and Lenard-Jones potential from MD [3]. Through massive supercomputing and parameterizing experiments, the mechanical properties such as platelet membrane viscoelasticity, flow compressibility and viscosity can be resembled by model parameters [5].

2.2 Multiple Time-Stepping Algorithm

In order to accommodate the multiple spatial scales in our platelet model, adaptive multiple time-stepping (MTS) algorithm with four-level integrators to connect the corresponding temporal scales is developed [6]. The four-level integrator can be adjusted via three loop factors to optimize accuracy and computing speeds, resulting in huge speedup of computation while maintaining stability and accuracy.

2.3 GPU Acceleration and Performance Analysis

In order to reduce the burden of inter-processor communication, we exploit a double-punch speedup strategy, i.e., the algorithmic MTS algorithm and GPGPU acceleration [7]. Porting intensive computation workloads to systems with accelerators help reduce the inter-process communication costs on CPU-only systems. We analyze the performance of multiscale platelet-mediated simulations on two supercomputers: Tianhe-2 and CS-Storm (a high-density multi-accelerator system). The performance results manifest the possibility of simulating the millisecond-scale hematology at resolutions of nanoscale platelets and mesoscale bio-flows using millions of particles.

3. CONCLUSIONS AND FUTURE WORK

Multiscale models, numerical algorithms, and advanced hardware will enable solution of new classes of problems in science, engineering, and medicine. My research is at the center of such

development. Future work is to build larger platelets aggregation simulation system to predict blood clotting mechanics, rheology, and dynamics, to better understand thrombosis pathologies. Achievement of such goal will enable efficient predictive simulations for initial thrombogenicity study and may provide a useful guide for exploring mechanisms of other complex biomedical problems at disparate spatiotemporal scales.

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