AI-Guided Adaptive Multiscale Modelling of Platelet Dynamics

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1 INTRODUCTION

Thromboembolism is the major cause of life-threatening cardiovascular diseases and stroke and a serious complication for implantable blood recirculating devices [1]. Platelets play an essential role in the thrombosis initiation, which is initiated by the reaction of platelets activation and aggregation. During the current pandemic of COVID-19, microthrombi is observed in arteries, veins, and microvascular circulation of severely ill patients [4]. Limitations in analyzing fine-grained details in laboratory experiments obstruct the quantitative study on the platelet responses under flow-induced blood clotting. We developed a multiscale modeling (MSM) platform for platelets in shear blood flow to efficiently characterize such an intricate system spanning multiple spatiotemporal scales [5]. The conventional algorithm uses the most conservative timestep size (Δt) for all particles, leading to massive redundant computations at top scales. RESPA [3] proposed to split the force computations by interaction ranges and apply different Δt's in molecular dynamics models. We introduced a multiple time stepping algorithm (MTS) [6] to simulate a MSM of platelet by integrating various components with disparate Δt's. Multiple Δt's in these approaches are pre-determined empirically based on spatial scales splitting. The essential challenge remains in adapting Δt to the constantly varying system dynamics. Our artificial intelligence (AI)-guided MTS (AI-MTS) is a response to this challenge.

2 ADAPTIVE MULTIPLE TIME STEPPING ALGORITHM

We developed a multiscale particle-based biophysical model of platelets in shear blood flow [6]. The hydrodynamics of viscous flow is simulated by dissipative particle dynamics (DPD) at the mesoscopic scale and the platelet constituents are modeled by coarse-grained molecular dynamics (CGMD) at the microscopic scale. The fluid-platelet interface is characterized by a hybrid force field containing dissipative and random terms from top-scale DPD and Lenard-Jones potential from bottom-scale CGMD. The disparate spatial scales are accommodated by splitting the system into the fluid and the platelet. To handle the temporal scales, an AI-MTS integrator is developed with a factor K indicating the timestep size ratio between that of the fluid Δt and of the platelet δt, where Δt is a large constant value for fluid particles advancing at the top scale and δt is a variable adapted to the platelet dynamics. We characterize the platelet motion by six physics measurements including three velocity components, two kinetic energies, and the surrounding flow speed at the platelet center of mass.

To analyze platelet dynamics in terms of these six target measurements, we construct a neural network-based learning architecture (Figure 1) [2]: (1) a 2-stage denoising filters containing moving averaging and wavelet transformation to reduce high-frequency oscillations in the raw data; (2) two recurrent neural network-based autoencoders to extract latent features; and (3) two fully connected networks to predict δt and step jump n_r, the number of steps until the next inference. Networks were trained by the data sampled from four experiments, from the combinations of two platelet initial positions with two flow conditions, with 400 samples per experiment.

The AI-MTS inference integrates the AI program with the MSM simulator. The simulator carries out time integration and exports measurements to datastore. Once the AI program is triggered, it imports the measurements and processes through the pipeline. At a time, a pair of new δt and n_r is transferred back to the simulator

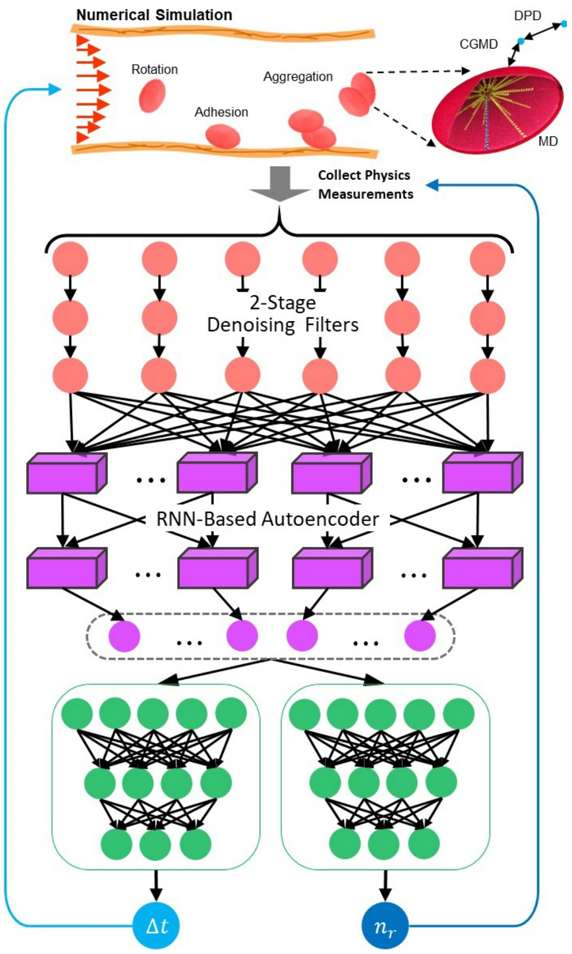

Figure 1: AI-guided MTS framework.

through the other datastore, where δt is used to update K and n_r is used as a dynamic time trigger for the next inference.

3 PERFORMANCE ANALYSIS

The AI-MTS is benchmarked against the standard tine stepping algorithm (STS) on a 1-platelet system consisting of 1.2 million particles and a 10-platelet system of 8 million particles. The STS uses the most conservative Δt for all particles through the entire simulation. The AI-MTS applies the characteristic Δt to the fluid and automatically regulates platelet δt to adapt to its dynamics by AI-guided inference. All numerical experiments were conducted on the AiMOS supercomputer of AC922 nodes. The accuracy of the AI-MTS is assessed by examining the platelet physical states while the speed performance of CPU-only experiments is measured over the STS. We observe a speedup of more than 4,000 (Figures 2-3) while preserving accuracy to above 97%. By implementing force computations and neighbor lists rebuilding on GPUs, we achieved an additional speedup of 5~10. The highly uneven particle distributions among processes is a source of improvement for scalability.

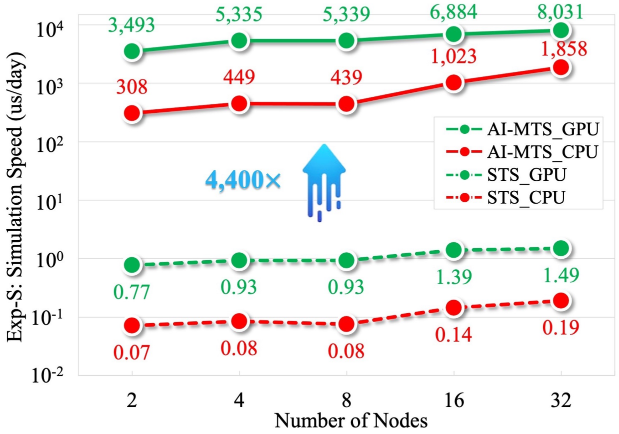

Figure 2: Speed performance of the 1-platelet system.

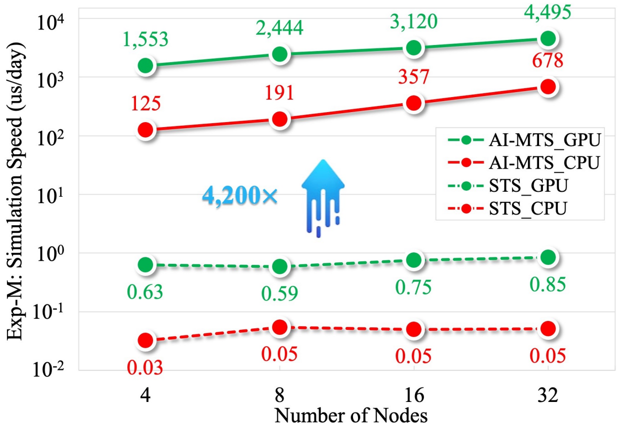

Figure 3: Speed performance of the 10-platelet system.

4 CONCLUSIONS AND FUTURE WORK

Our AI-MTS demonstrates its present values and additional potential of adaptively eliminating massive manual labor and unnecessary computing and enabling studies of complex problems with medical applications. Our platform will help gain insights into platelet-mediated thromboembolism by incorporating more realistic interactions in a larger system including inter-platelet interactions in aggregation, platelet-vessel interactions in adhesion, and intra-platelet rearrangement upon activation. Going through more stress tests and a more detailed analysis of its computation and communication workload, our further optimized platform may exemplify the realization of the potential of coupling HPC with AI.

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REFERENCES

[1] Danny Bluestein. 2006. Towards optimization of the thrombogenic potential of blood recirculating cardiovascular devices using modeling approaches. *Expert Review of Medical Devices* 3 (May 2006), 267–270. https://doi.org/10.1586/17434440.3.3.267

[2] Changnian Han, Peng Zhang, Danny Bluestein, Guojing Cong, and Yuefan Deng. 2020. Artificial Intelligence for Accelerating Multiscale Modeling. *J. Comput. Phys.* (2020). (under revision).

[3] Mark E Tuckerman and Bruce J Berne. 1991. Molecular Dynamics in Systems with Multiple Time Scales: Systems with Stiff and Soft Degrees of Freedom and with Short and Long Range Forces. *J. Chem. Phys.* 95, 11 (1991), 8362–8364. https://doi.org/10.1063/1.461263

[4] Younes Zaid, Florian Puhm, Isabelle Allaeys, Abdallah Naya, Mounia Oudghiri, Loubna Khalki, Youness Limami, Nabil Zaid, Khalid Sadki, Rafiqua Ben El Haj, Wissal Maher, Lamiae Belayachi, Bouchra Belefquih, Amina Benouda, Amine Cheikh, Yahia Cherrah, Louis Flamand, Fadila Guessous, and Eric Boilard. 2020. Platelets can Contain SARS-CoV-2 RNA and are Hyperactivated in COVID-19. *medRxiv* 50 (June 2020). https://doi.org/10.1101/2020.06.23.20137596

[5] Peng Zhang, Li Zhang, Marvin J. Slepian, Yuefan Deng, and Danny Bluestein. 2017. A Multiscale Biomechanical Model of Platelets: Correlating with In-Vitro Results. *J. Biomech.* 50 (Jan. 2017), 26–33. https://doi.org/10.1016/j.jbiomech.2016.11.019

[6] Peng Zhang, Na Zhang, Yuefan Deng, and Danny Bluestein. 2015. A Multiple Time Stepping Algorithm for Efficient Multiscale Modeling of Platelets Flowing in Blood Plasma. *J. Comput. Phys.* 284 (March 2015), 668–686. https://doi.org/10.1016/j.jcp.2015.01.004