Multi-Scale Platelet Surrogate Modeling via Neural Operators: Toward Next-Generation Thrombosis Care

Marco Laudato[1] and Luca Manzari[2]
[1]FLOW Research Center, Department of Engineering Mechanics, KTH Royal Institute of Technology, Stockholm, Sweden
[2]PDC Center for High-Performance Computing, KTH Royal Institute of Technology, Stockholm, Sweden
[1] Email: laudato@kth.se

Summary

Precise modeling of platelet biomechanics is crucial for understanding thrombosis progression and informing clinical decisions. We develop a surrogate model for single platelet behavior using a Deep Operator Network (DeepONet). This approach captures the entire platelet dynamic response in a blood shear flow environment while drastically reducing computational cost. Preliminary results show that the method can resolve the entire time evolution of the platelet with minimal error, below 2%, while enabling real-time stress accumulation predictions. The synergy of HPC-based frameworks (LAMMPS) with DeepONet allows for clinically relevant simulations for improved thrombosis risk assessment. Close collaboration with clinical partners ensures that these insights translate directly into practical therapeutic applications, demonstrating the transformative potential of advanced computational biomechanics.

Introduction

The mechanical activation of platelets under high shear stress is a critical trigger in thrombosis, a major cause of morbidity and mortality worldwide. While computational models have provided critical insights into platelet biomechanics, bridging these models to the clinic demands near real-time predictions. This project addresses this challenge by integrating large-scale high-performance computing (HPC) simulations with cutting-edge deep learning approaches. This synergy enables precise, rapid predictions of platelet dynamics in various physiological and pathological contexts, paving the way for personalized thrombosis medicine.

Methods

Platelet dynamics in shear flow were simulated using LAMMPS, an open-source molecular dynamics engine well-suited for modeling complex fluid-structure interactions at sub-platelet scale. Each simulation provided spatiotemporal data on platelet deformation and stress accumulation under physiologically relevant flow conditions. A Deep Operator Network (DeepONet) was then employed to learn the operator mapping from flow parameters to platelet responses. Training utilized HPC-generated datasets, ensuring that the model captured a wide range of shear rates and biological variability. By encoding the underlying governing equations in its architecture, DeepONet allowed for efficient and accurate inference of platelet displacement and stress distribution, significantly reducing the computational burden compared to traditional solvers.

Results and Discussion

Initial studies [1] reproduced both the onset and final displacement of single platelets in shear flow with high accuracy, offering key insights into how platelets deform under varying flow conditions. Recent experiments extended this capability, enabling the surrogate model to capture full platelet dynamics throughout the entire simulation time span with an error below 2% (see Figure 1, left panel). Moreover, the DeepONet framework provided real-time predictions of accumulated stress on platelets, a critical indicator of potential damage or activation pathways (see Figure 1, right panel). These advances highlight the system's potential for clinical applications, where quick, precise modeling can support personalized assessments of thrombosis risk and guide targeted therapeutic strategies. Close collaboration with clinicians ensures that future developments align with patient-centered outcomes.

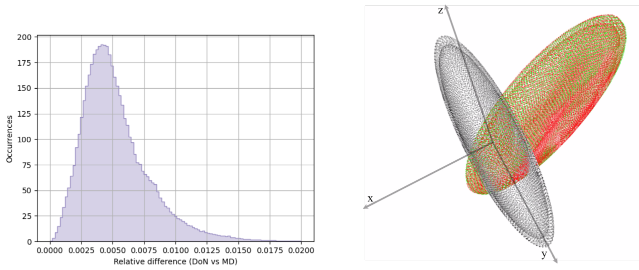

Figure 1: *(left panel)* Distribution of the relative differences between the neural operator prediction and the ground truth. The maximum relative difference is 2%, while the mode of the distribution is approximately 0.5%. *(right panel)* Comparison of the deformed platelet configuration predicted by DeepONet and that obtained from particle dynamics simulations using LAMMPS. The green points represent the DeepONet predictions and red points indicate the ground truth simulation results. The gray points correspond to the platelet initial configuration.

Conclusions

DeepONet-based surrogate modeling offers a transformative step toward real-time, patient-specific thrombosis risk assessment. By uniting HPC simulations with advanced neural networks, the THRONE project paves the way for accessible, clinically relevant computational tools that support precision medicine approaches in thrombosis care.

Acknowledgments

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References

[1] Laudato, M., Manzari, L., & Shukla, K. High-Fidelity Description of Platelet Deformation Using a Neural Operator. arXiv preprint arXiv:2412.00747. (2024). *arXiv preprint 2412.00747.*