

AI Meets HPC: Learning the Cell Motion in Biofluids

Ziji Zhang
Applied Mathematics Department
Stony Brook University
Stony Brook, NY, USA
ziji.zhang@stonybrook.edu

Peng Zhang
Applied Mathematics Department
Stony Brook University
Stony Brook, NY, USA
peng.zhang@stonybrook.edu

Changnian Han
Applied Mathematics Department
Stony Brook University
Stony Brook, NY, USA
changnian.han@stonybrook.edu

Guojing Cong
IBM Thomas J. Watson Research Center
Yorktown Heights, NY, USA
gcong@us.ibm.com

Chih-Chieh Yang
IBM Thomas J. Watson Research Center
Yorktown Heights, NY, USA
chih.chieh.yang@ibm.com

Yuefan Deng
Applied Mathematics Department
Stony Brook University
Stony Brook, NY, USA
yuefan.deng@stonybrook.edu

Abstract—We generalized the century-old Jeffery orbits equation, by a novel biomechanics-informed online learning framework using simulation data at atomic resolutions, to a new equation of motion for flowing cells to account for the fluid conditions and the cell deformable structures. To validate, we examined the motions, dominantly rotations, of a human platelet in viscous blood flow at various shear stresses and platelet deformability. With the flow and platelet parameters learned from our framework, the new equation captures motions of the platelet accurately. This learned equation will help reduce greatly the complexity of simulating cells in biofluids and, in the case of platelets, of analyzing blood clot formation.

Keywords—Cell equation of motion, multiscale modeling, online learning, future computing.

I. INTRODUCTION AND MOTIVATION

The highly celebrated 100-year-old Jeffery orbits equation (JOE) [1] that described the motion of an ellipsoidal rigid-body, *i.e.*, an oblate, immersed in a steady viscous shear flow is being generalized to characterize the motion of living cells such as human platelets that resemble an oblate in the flowing blood, with the aid of HPC and machine learning. The JOE demonstrates that oblates tumble with infinitely many marginally stable periodic orbits, while small perturbations of the flow conditions or the oblate shape may lead to substantial variations in the motion, which is evident in our modeling the motion of blood cells using multiscale modeling (MSM). Zhang *et al.* [2] compared the multiscale particle-based simulation results of an oblate-like platelet with the JOE solution in Couette flows. Platelets are commonly modeled as rigid bodies although, in reality, a platelet is quite far from rigid. The JOE, as expected, describes rigid platelets accurately and fails badly to capture the essential details of the motion of a true, *i.e.*, deformable, platelet because the JOE omitted the intricate fluid-platelet interactions and the dynamics of the platelet deformability.

The dynamics of platelet motion plays an important role in the formation of thrombosis, a common pathology underlying cardiovascular diseases, which accounts for over 30% of all deaths globally [3, 4]. And it has a potential role in triggering deaths from the infection of COVID-19 [5]. As a practical application of adapting our equation and the biomechanics-informed online learning (BIOL) framework, we discover the

equation of motion, and the associated parameters, for deformable platelets flowing in blood.

II. ONLINE LEARNING FOR EQUATION OF MOTION

A new equation of motion, the generalized JOE (G-JOE), is introduced to relate the angular velocity $\dot{\phi}$ with rotational angle and three parameters $\{\lambda_0, \lambda_1, c_0\}$. The G-JOE describes an oblate spheroid, whose axis of symmetry is defined by the unit vector \mathbf{n} . The polar angle of the spheroid, concerning a fixed lab frame whose origin is at the oblate center, is θ while ϕ is the azimuthal angle. The major and minor axis length is denoted by a and b respectively, so the aspect ratio is $e = a/b > 1$. The spheroid is immersed in a laminar motion linear shear flow, whose origin is at the center of the platelet to eliminate any constant translation. In our case, platelet with an oblate-like shape tumbling at the xy plane with $\theta = \pi/2$ and $\dot{\theta} = 0$ for simplicity. This G-JOE considers more realistic physics conditions than the classical theory:

$$\dot{\phi}(\dot{\gamma}t) = \frac{1}{2}(\lambda_0 + \lambda_1 \sin(2\phi))(\Lambda \cos(2\phi) - c_0) \quad (1)$$

where $\Lambda = (e^2 - 1)/(e^2 + 1)$; λ_0 describes its shape-deviation from a perfect oblate; and λ_1 accounts for the platelet's dynamic deformation to applied stresses. It aims to capture the deforming capability of blood cells and can also be considered as inherent vibration magnitude. c_0 is the fluid-structure interaction term.

The BIOL framework determines the parameters and consummates the introduction of the equation of motion. We also correlate the learning process with MSM simulations that provide the ground truth, transferring streaming data, comparing results, and providing termination conditions.

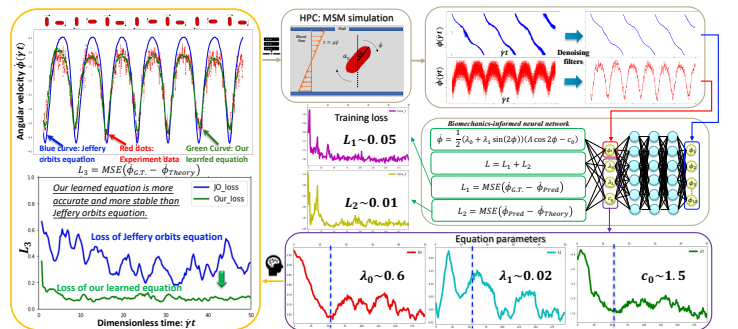


Fig. 1 The biomechanics-informed online learning framework

We select rotation angle ϕ , which is a conformation-based length unit, as input to the neural network. The output angular velocity $\dot{\phi}$ implies the biomechanical properties of the interest object, implicitly incorporated by a neural network. Instead of simply treating a neural network as a “black box”, we design the principle functions with conceptual explanations and use the neural network, with feed-forward fully connected layers, to optimize the learnable parameters, both in the neural network and in the G-JOE. Using the known biomechanical properties, we select the features informed by the dynamical system to enable guided learning.

III. HPC FOR GROUND TRUTH

We model the motion of platelets using multiscale modeling (MSM), which considers the rotation of deformable platelets in viscous blood flows at the nano-to-micron length scales. The simulated system uses total 1,265,719 atoms of which 1,091,360 for the flow and 140,303 for the platelet. Representing the inter-platelet components, we used 40,446 and 32,853 atoms for the cytoskeleton and the cytoplasm, respectively, and 67,004 atoms for the platelet membrane that interacts with the flow. We examined the platelet motion under 50, 100, 200, 300 dyne/cm² using rigid and deformable conformations respectively (Fig. 2). All numerical simulations are implemented by modified LAMMPS package on RPI’s AiMOS supercomputer and the IBM’s WSC Cluster consisting of IBM AC-922 nodes.

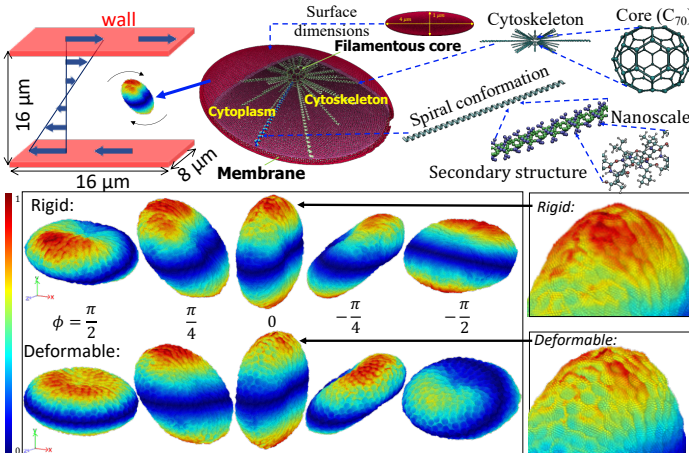


Fig. 2 Ground truth from MSM simulation results with the aid of HPC

IV. ONLINE LEARNING FOR PARAMETERS

We examined the angular velocities, calculated by the JOE and predicted by the G-JOE, and compared them with the MSM-simulated results via month-long HPC calculations. Under all experimental conditions, the results from the G-JOE are far more accurate than those of the JOE. The mean squared errors between predictions and ground truth are calculated and the G-JOE improved 3~20 times accuracy.

The deformable body simulation setup generates more noisy streaming data because the rotation axis is instantaneous during the simulation process. Our online learning adaptively learns simulations with, understandably, initial inaccuracies. As expected, the longer we learn, the more accurate our predictions become. Compared with traditional offline learning, online

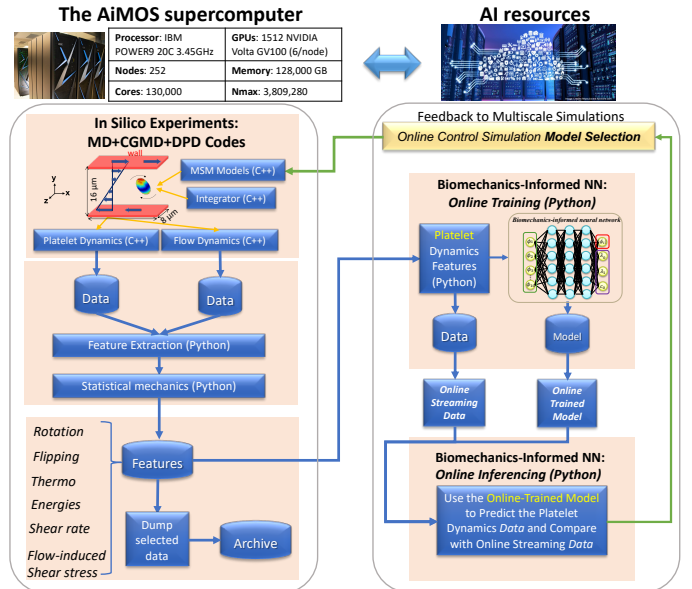


Fig. 3 Future computing HPC+AI architecture: accelerating intelligent discovery of knowledgebase

learning offers consistent results with offline learning while providing a host of other advantages.

V. CONCLUSIONS AND FUTURE WORK

Applying our G-JOE and the BIOL framework, we studied the cell motion in biofluids exemplified by platelet flowing in blood. The platelet-specific parameters thus predicted enable accurate description of the motion of realistic platelets at various flow conditions. This mathematics- and science-informed intelligent system provides a novel architecture to help deepen the study of the complex systems. As a start, our work may stimulate collaboration with IBM to explore the future computing architecture for synergistically integrating HPC with AI.

ACKNOWLEDGMENTS

We thank the SUNY-IBM Consortium for supporting IPDyna (PI: Y. Deng, Co-I: P. Zhang), RPI for AiMOS supercomputer and IBM for WSC cluster through an IBM Faculty Award (PI: Y. Deng), and Dr. J. Sexton for inspiring discussions.

REFERENCES

- [1] G. B. Jeffery, "The motion of ellipsoidal particles immersed in a viscous fluid," *Proceedings of the Royal Society of London. Series A, Containing papers of a mathematical and physical character*, vol. 102, no. 715, pp. 161-179, 1922.
- [2] P. Zhang *et al.*, "Multiscale particle-based modeling of flowing platelets in blood plasma using dissipative particle dynamics and coarse grained molecular dynamics," *Cell. Mol. Bioeng.*, vol. 7, no. 4, pp. 552-574, 2014.
- [3] E. J. Benjamin *et al.*, "Heart disease and stroke Statistics-2019 update a report from the American Heart Association," *Circulation*, 2019.
- [4] L. D. Casa *et al.*, "Role of high shear rate in thrombosis," *J. Vasc. Surg.*, vol. 61, no. 4, pp. 1068-1080, 2015.
- [5] M. Koupenova, "Potential Role of Platelets in COVID - 19: Implications for Thrombosis," *Res. Pract. Thromb. Haemost.*, 2020.
- [6] Z. Zhang *et al.* "Generalized Jeffery Orbits Equation for Deformable Spheroid," *J. Comput. Phys.*, 2020. (submitted)