AI Meets HPC: Learning the Cell Motion in Biofluids

Ziji Zhang[1], Peng Zhang[1], Changnian Han[1], Guojing Cong[2], Chih-Chieh Yang[2], Yuefan Deng[1]

[1]Applied Mathematics and Statistics Department, Stony Brook University, Stony Brook, NY 11794, USA and [2]IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598, USA

Introduction & Motivation

Background: The rotation of an ellipsoidal particle immersed in a viscous flow is described by the Jeffery orbits equation [1]: $\dot{\phi}(\dot{\gamma}t) = \frac{1}{2}(\Lambda \cos 2\phi + 1)$. But, its accuracy is insufficient: it does not always agree with experimental results. We use **platelet simulation** in the blood as a representative example which is related to cardiovascular diseases and COVID-19 [2-3].

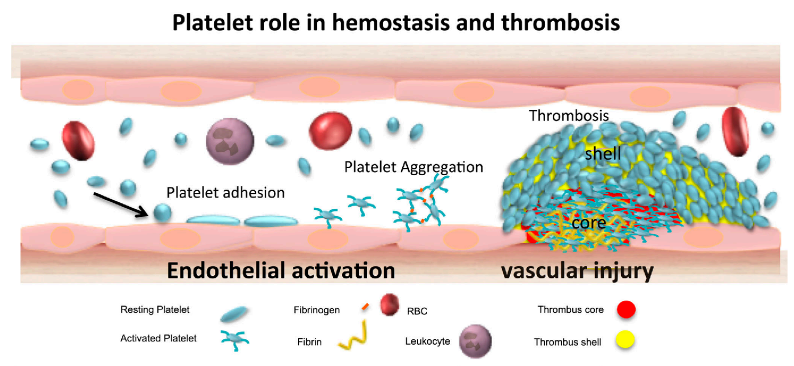


Figure: Platelet plays a key role in the formation of thrombosis. [2]

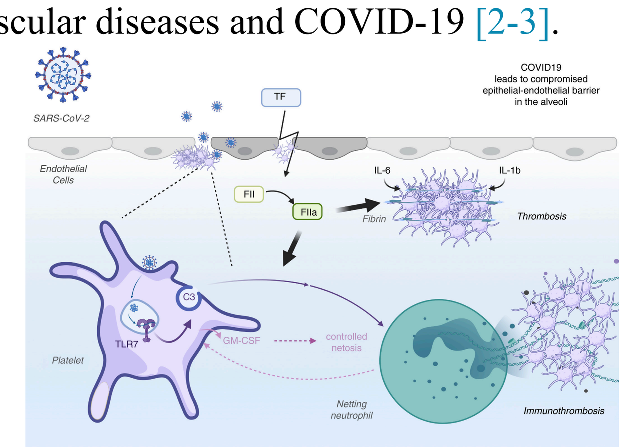


Figure: Platelet functions at COVID-19. [3]

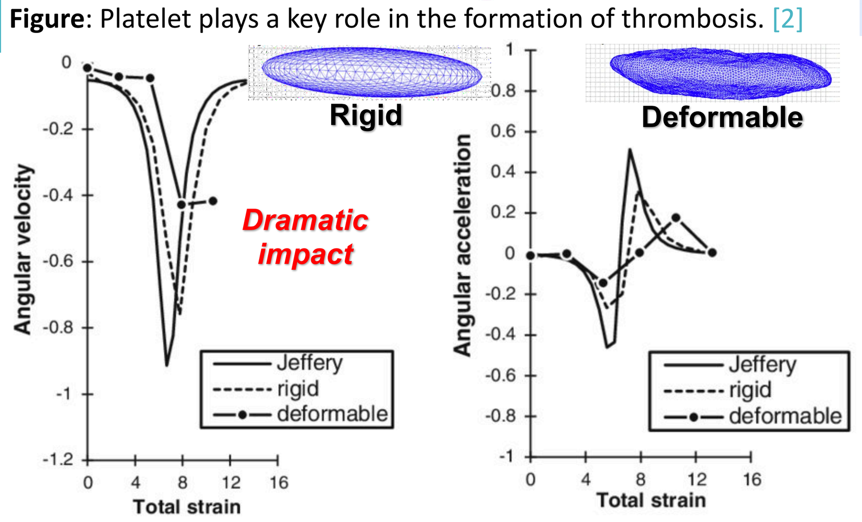


Figure: Comparisons of simulation results and Jeffery orbits. [4]

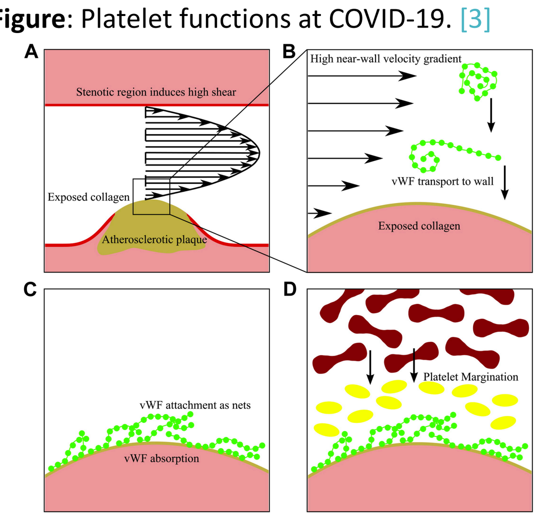


Figure: High shear thrombosis and stenosis. [5]

Motivation:

- ❑ Generalizing the 100-year-old Jeffery orbits equation to describe the cell dynamics in biofluids with atomic resolution.
- ❑ Introducing the details of dynamic fluid-structure interaction (FSI) in modeling.
- ❑ Learning through one of fastest supercomputers for the basic dynamics of cell motion.

HPC for Ground Truth

Validation: We model the motion of platelets using **multiscale modeling** (MSM), which considers rotation of deformable platelets in viscous blood flows at the nano-to-microscales.

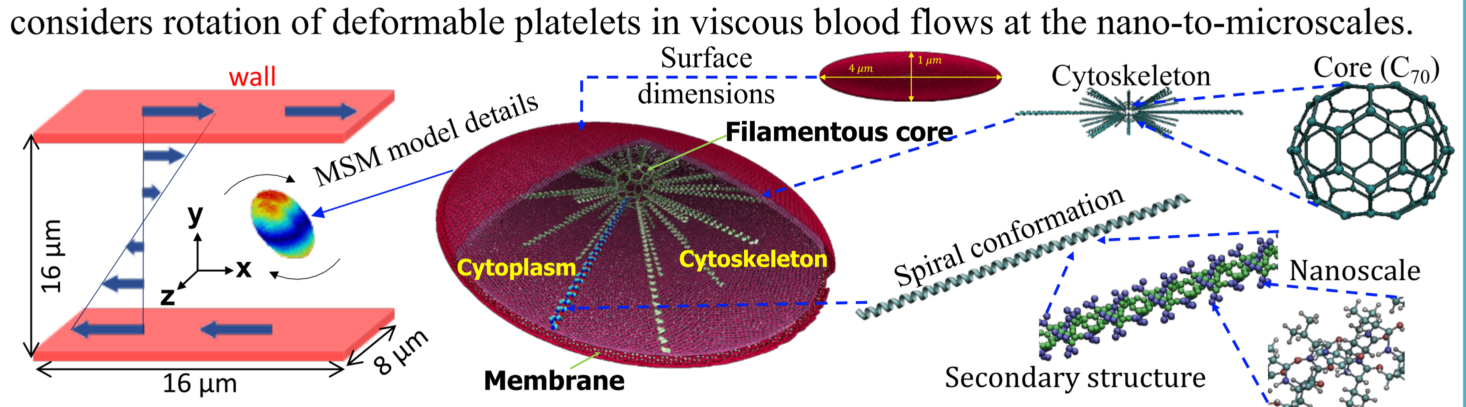


Figure: The system uses a total of 1,265,719 atoms: 1,091,360 atoms in flow and 140,303 atoms in platelet. In platelet, we use 40,446 atoms for cytoskeleton, 32,853 for cytoplasm and 67,004 for membrane.

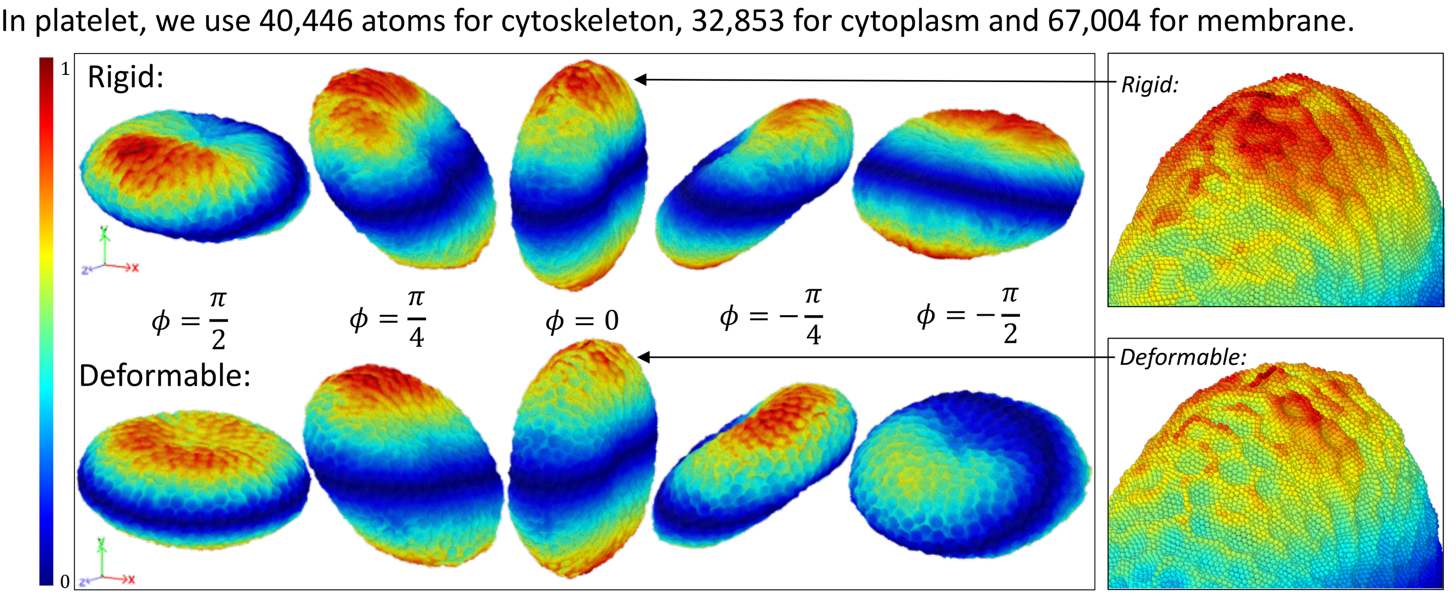


Figure: Velocity distribution for different positions of the rotation process, for rigid and deformable platelet body setups (left side). Zoom in to show the velocity distributions on membrane (right side).

Online Learning for Equation of Motion

A generalized Jeffery orbits equation (G-JOE) of motion

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

- **Output variable**
  - Rotation angular velocity
  - Prediction of cell dynamics
- **Input variable**
  - Rotation angle
  - Represent the cell motion
- **Global variable**
  - Dimensionless time
  - $\dot{\gamma}$: shear rate of flow
- **Learnable parameter**
  - Deviation from oblate
  - Initial value: 1
- **Learnable parameter**
  - Deforming capability
  - Initial value: 0
- **Learnable parameter**
  - Fluid-structure interaction
  - Initial value: -1
- **Constant value**
  - From original Jeffery orbits
  - $\frac{e^2-1}{e^2+1}$, e: initial aspect ratio

Figure: The detailed parameter explanations of generalized Jeffery orbits equation

A novel biomechanics-informed online learning framework

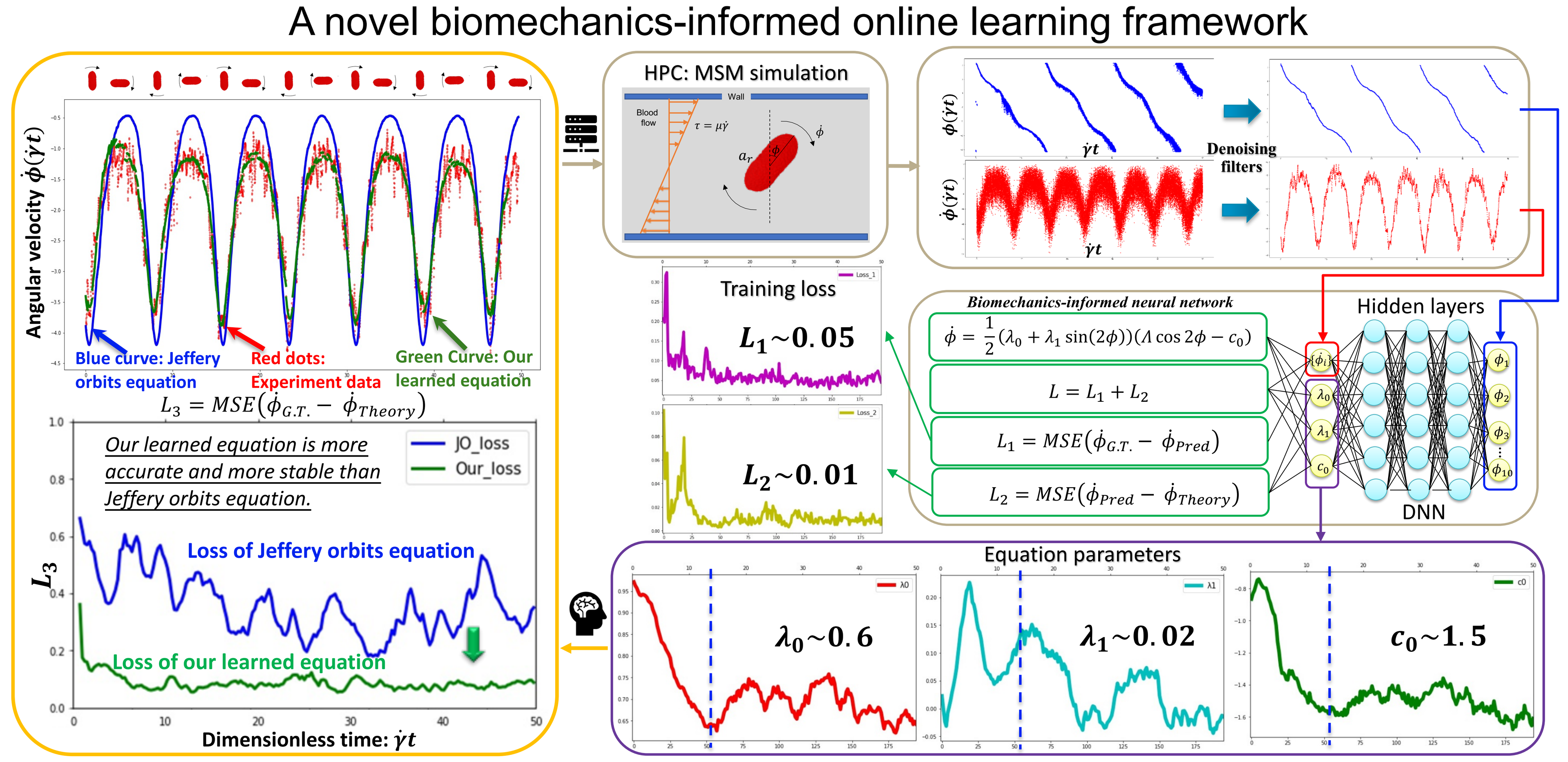


Figure: The BIOL provides a novel methodology framework for deriving equation parameters and consummate our modeling of dynamic system.

Online Learning for Parameters

Application: We provide a **fast and accurate** way to determine FSI parameters in modeling, simplifying the dynamic systems and reducing the computation load.

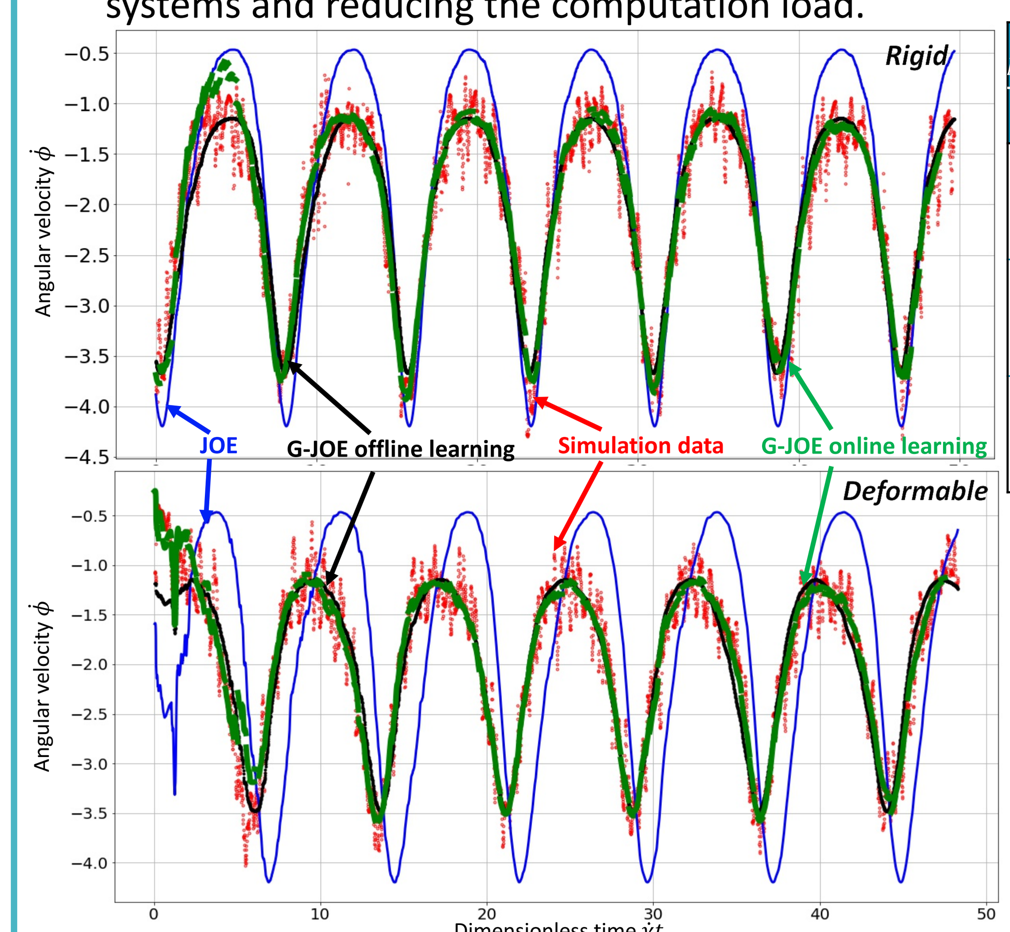


Figure: Angular velocity prediction comparisons under 50 dyne/cm².

$\frac{MSE(\dot{\phi}_{G.T.} - \dot{\phi}_{Theory})}{\dot{\gamma}t}$	Shear stress ($dyne/cm^2$), Rigid (R), Deformable (D)			
	50	100	200	300
Original Jeffery orbits	R: 0.305, D: 1.141	R: 0.654, D: 2.226	R: 0.967, D: 3.758	R: 0.742, D: 9.261
Generalized Jeffery orbits	**R: 0.081, D: 0.053**	**R: 0.085, D: 0.084**	**R: 0.138, D: 0.285**	**R: 0.302, D: 0.247**
Improved accuracy	R: 276.5%, D: 2052.8%	R: 669.4%, D: 2518.8%	R: 600.7%, D: 1218.6%	R: 145.7%, D: 3649.4%

Online Learning Results:

- ❖ Generalized Jeffery orbits equation is more **accurate** than original Jeffery equation.
- ❖ Online learning results are **consistent** with offline learning, but **adaptive** and **timely**.
- ❖ The deformable simulation will generate more noise data, but online learning could **robustly** denoise and predict.

Conclusions & Future Work

Conclusions:

- ❖ The values of equation parameters are derived **consistently** for different flow conditions.
- ❖ Online learning could **adaptively** learn simulations even begin with numerical artifacts.
- ❖ MSM + BIOL could **save 90% of simulation time** without losing significant accuracy.

Future work: Intelligent Supercomputing

- ❖ *More than HPC*: we analyze our BIOL workflow and develop the AI + HPC framework.
- ❖ *Future computing:* we work with IBM for the design of future HPC architecture.

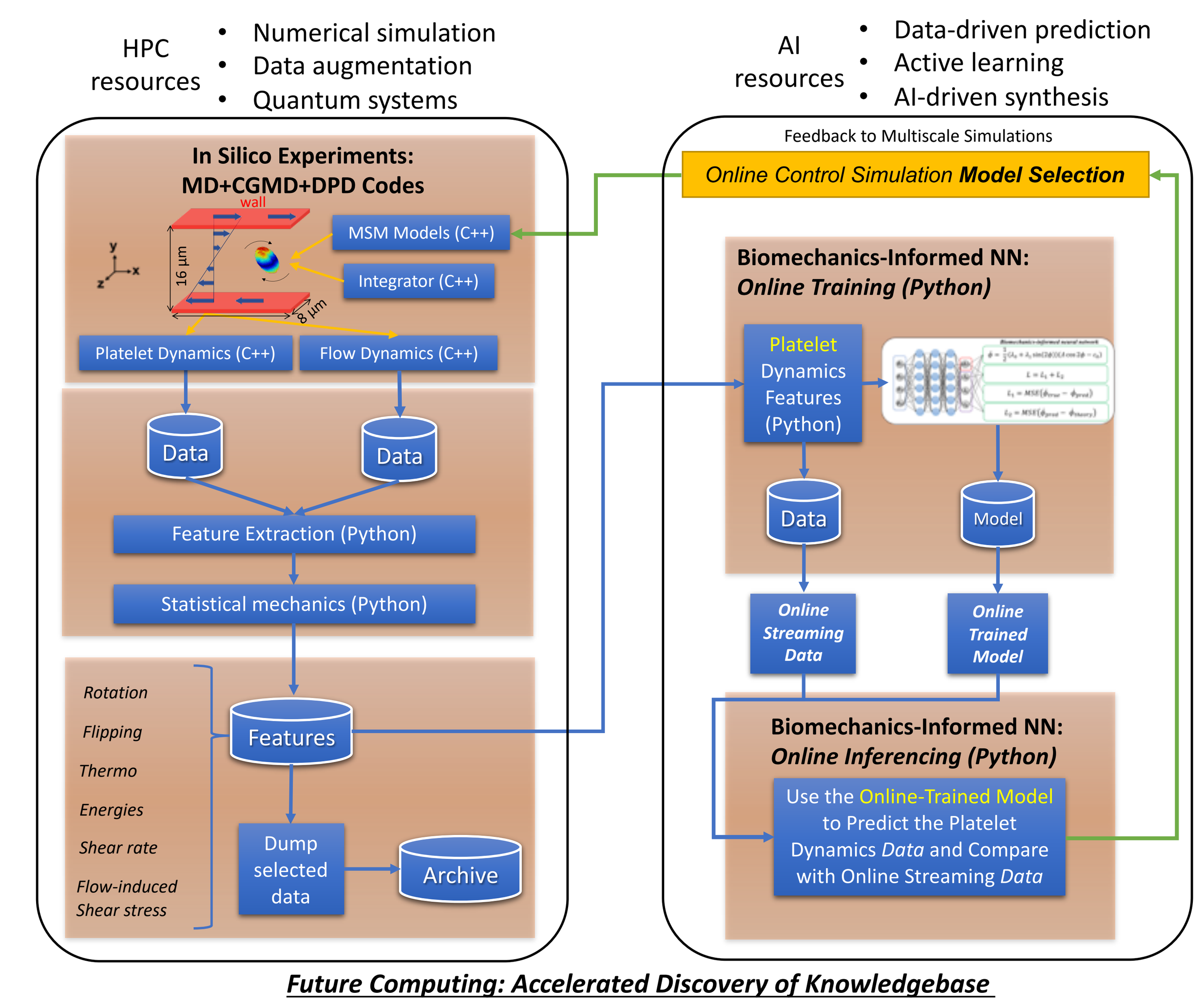
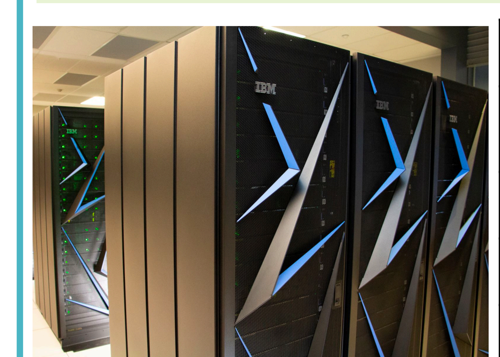


Figure: Proposed future computing architecture: accelerated discovery of knowledgebase

The IBM Supercomputer AiMOS



Processor: IBM POWER9 20C 3.45GHz	**GPUs:** 1512 NVIDIA Volta GV100 (6/node)
Nodes: 252	**Power Consumption:** 512.08 kW
Cores: 130,000	**Interconnect:** Dual-rail Mellanox EDR Infiniband
Memory: 128,000 GB	**Linpack Performance (Rmax):** 8,339 TFlop/s
Nmax: 3,809,280	**Theoretical Peak (Rpeak):** 11,032 TFlop/s

Acknowledgements

- The project is supported by the SUNY-IBM Consortium Award, IPDyna: Intelligent Platelet Dynamics, FP00004096 (PI: Y. Deng, Co-I: P. Zhang).
- All simulations were conducted on AiMOS supercomputer at Rensselaer Polytechnic Institute and the WSC cluster at the IBM T.J Watson center through an IBM Faculty Award FP0002468 (PI: Y. Deng).
- We would like to thank Dr. James Sexton from IBM for his 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)