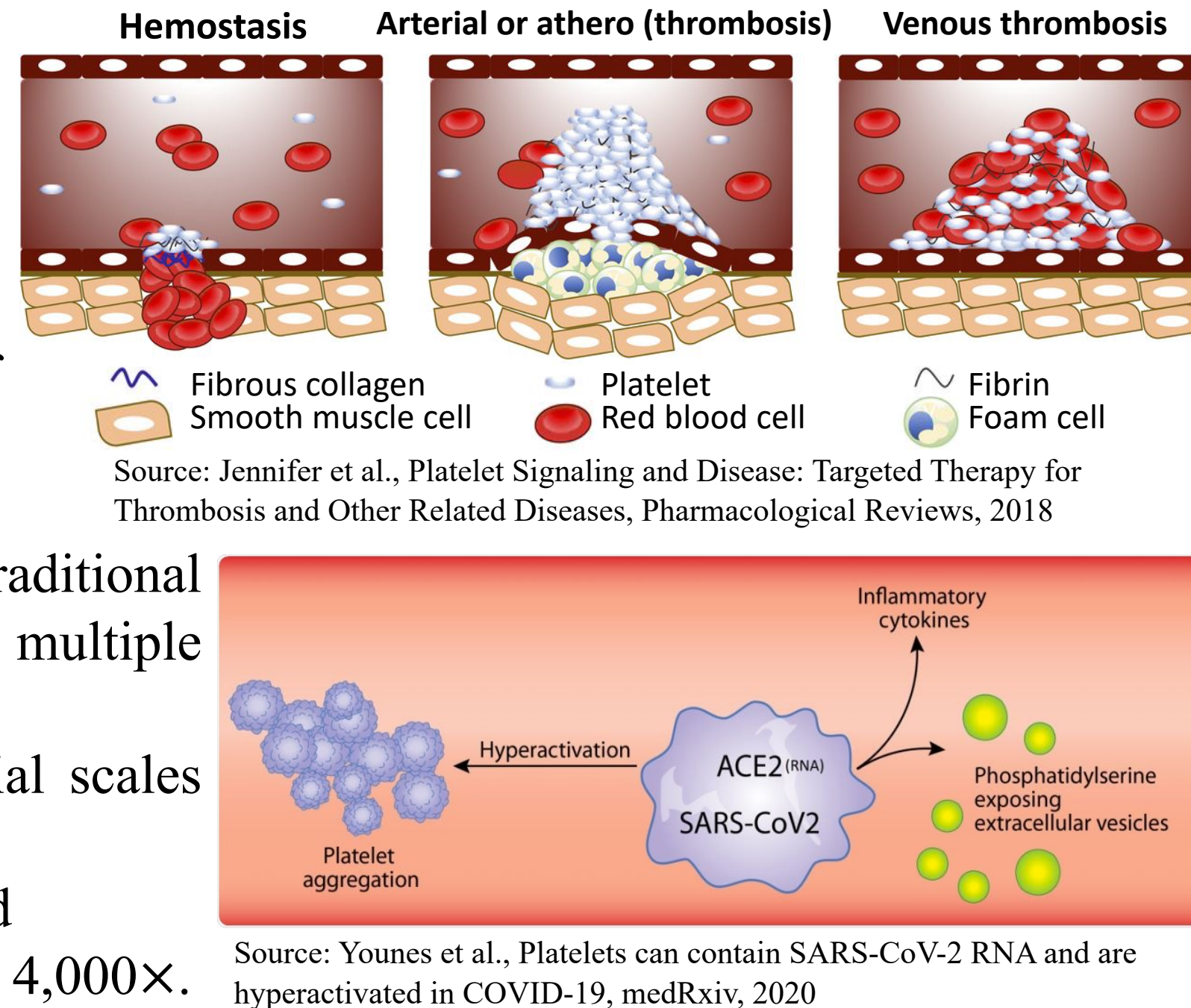


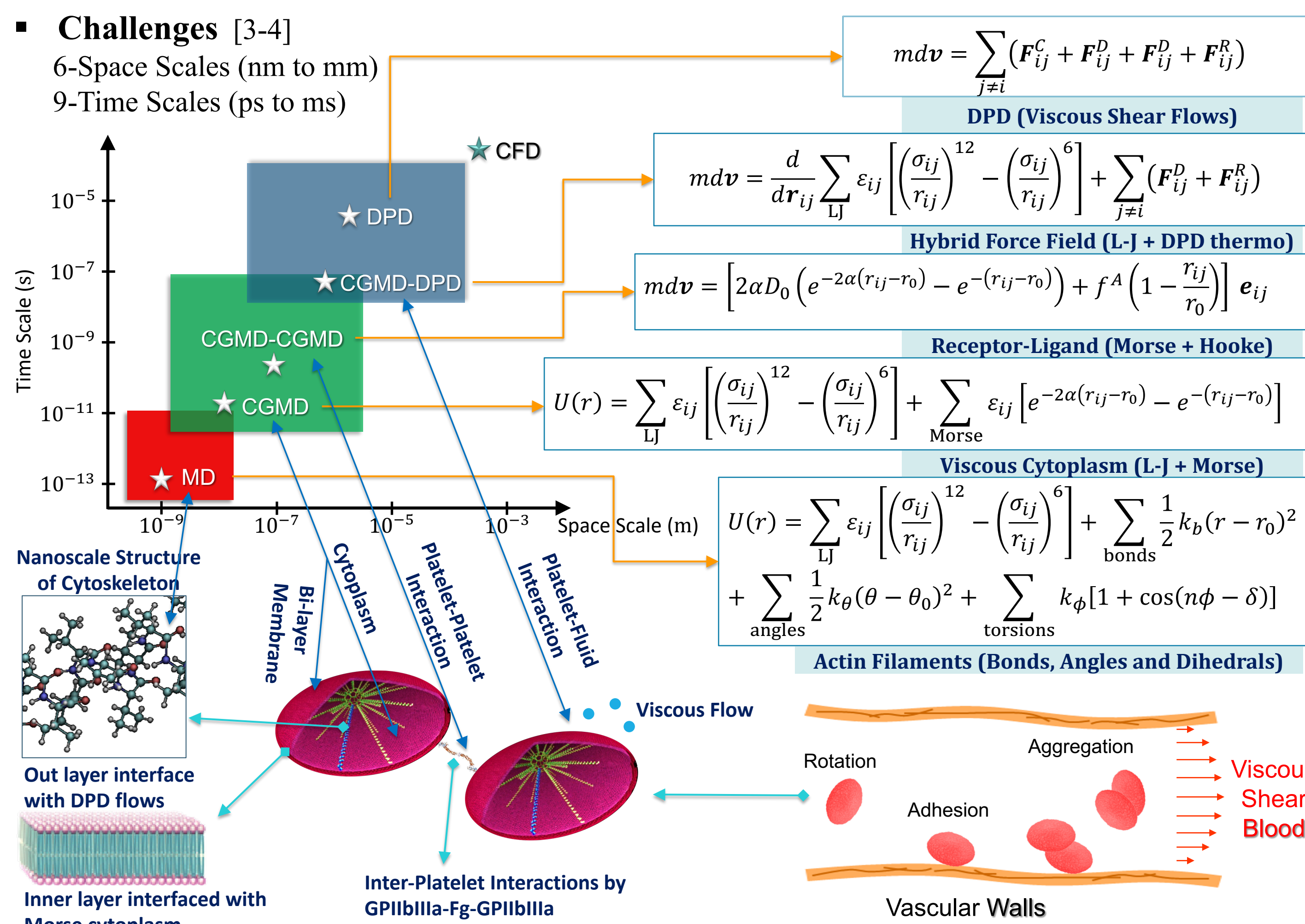
Introduction and Significance

Platelet activation, adhesion, and aggregation are complex dynamical processes that cause physiological reactions including thrombosis formation, a cause of heart diseases and stroke. During the current pandemic of COVID-19, microthrombi in the arteries and veins are observed in most severely ill patients [1]. Comparing to traditional approaches, our AI-guided adaptive multiple time stepping algorithm (AI-MTS) can

- model interactions covering 6 spatial scales and 9 temporal scales,
- detect system dynamics changes, and
- speed up numerical simulations over 4,000×



The Structure of Multiscale Bioscience



Related Work and Simulation Experiments

Related Work in Multiscale Modeling (MSM) Algorithms

Algorithms	Models	Rationale	Timestep Sizes
STS	MD/MSM	highest resolution	single, static
RESPA [2]	MD	split forces	multiple, static
MTS [3]	MSM	split component	multiple, static
AI-MTS	MSM	adapt to states by AI	multiple, dynamic

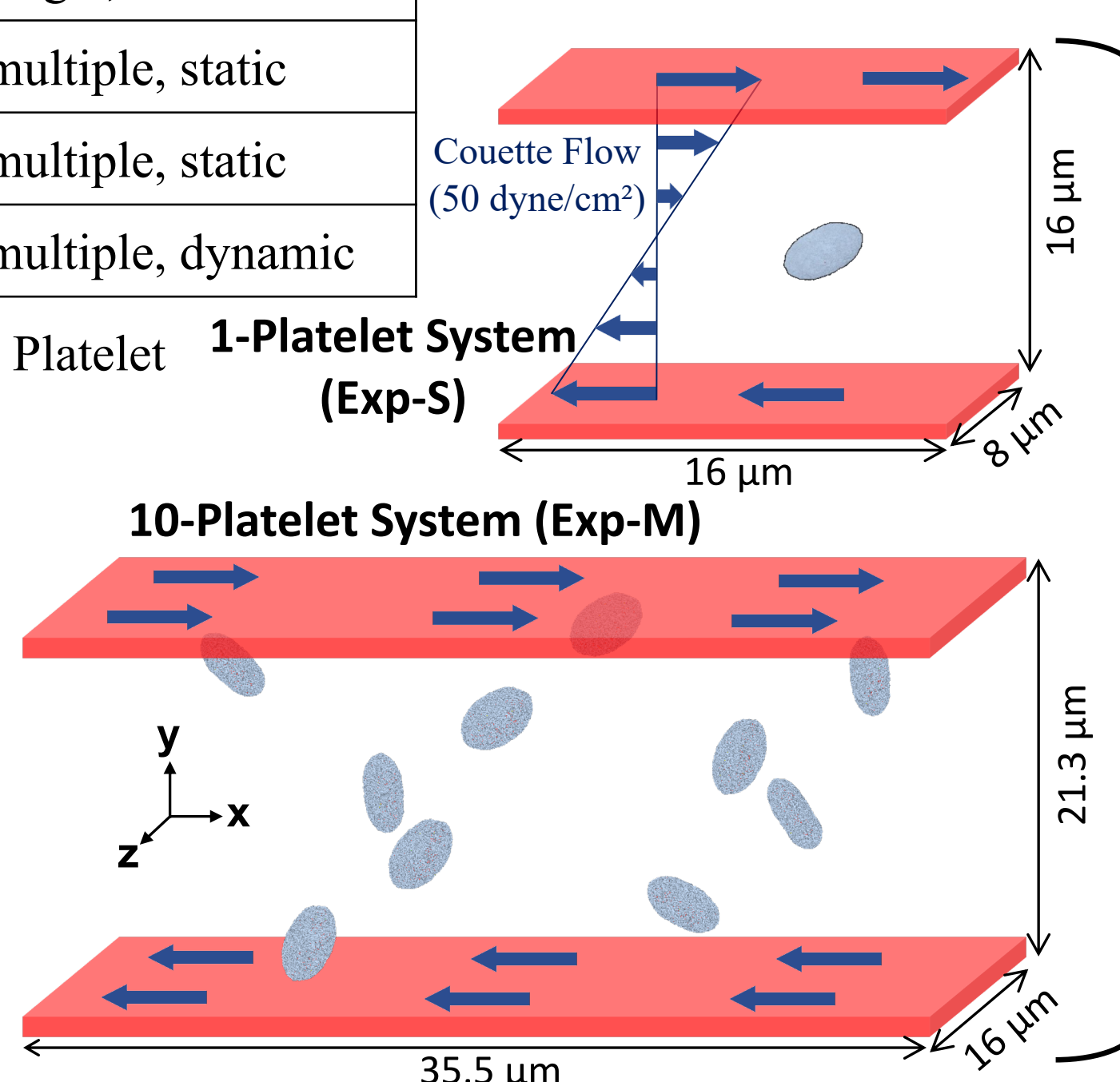
The Number of Particles in Various Components of a Platelet

Membrane	Cytoplasm	Cytoskeleton	Total
67,004	32,853	40,446	140,303

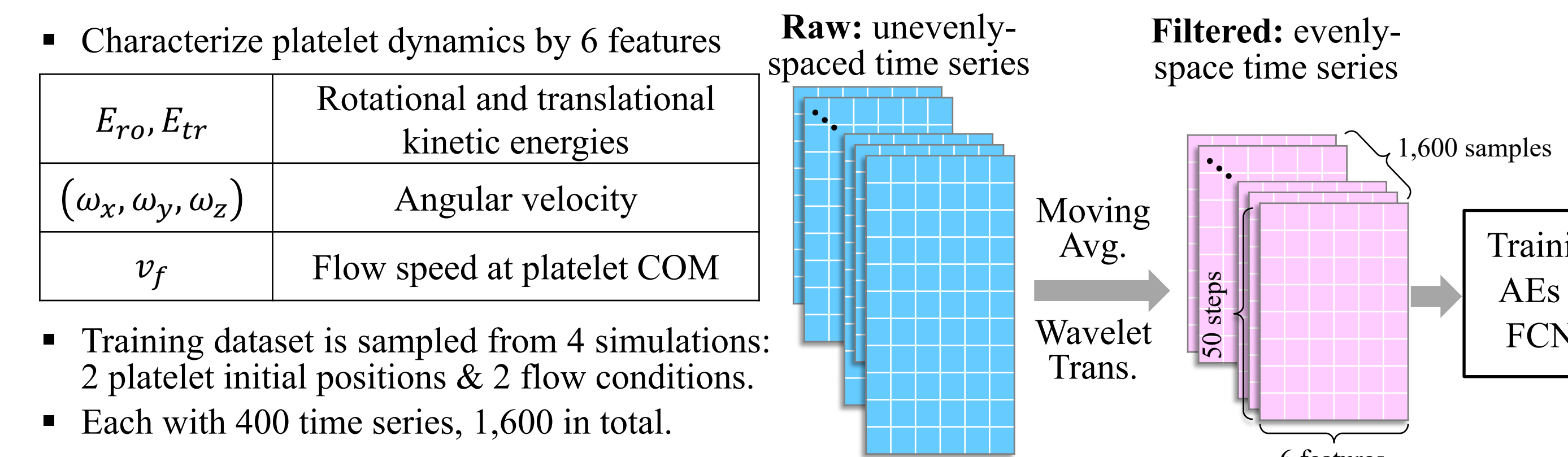
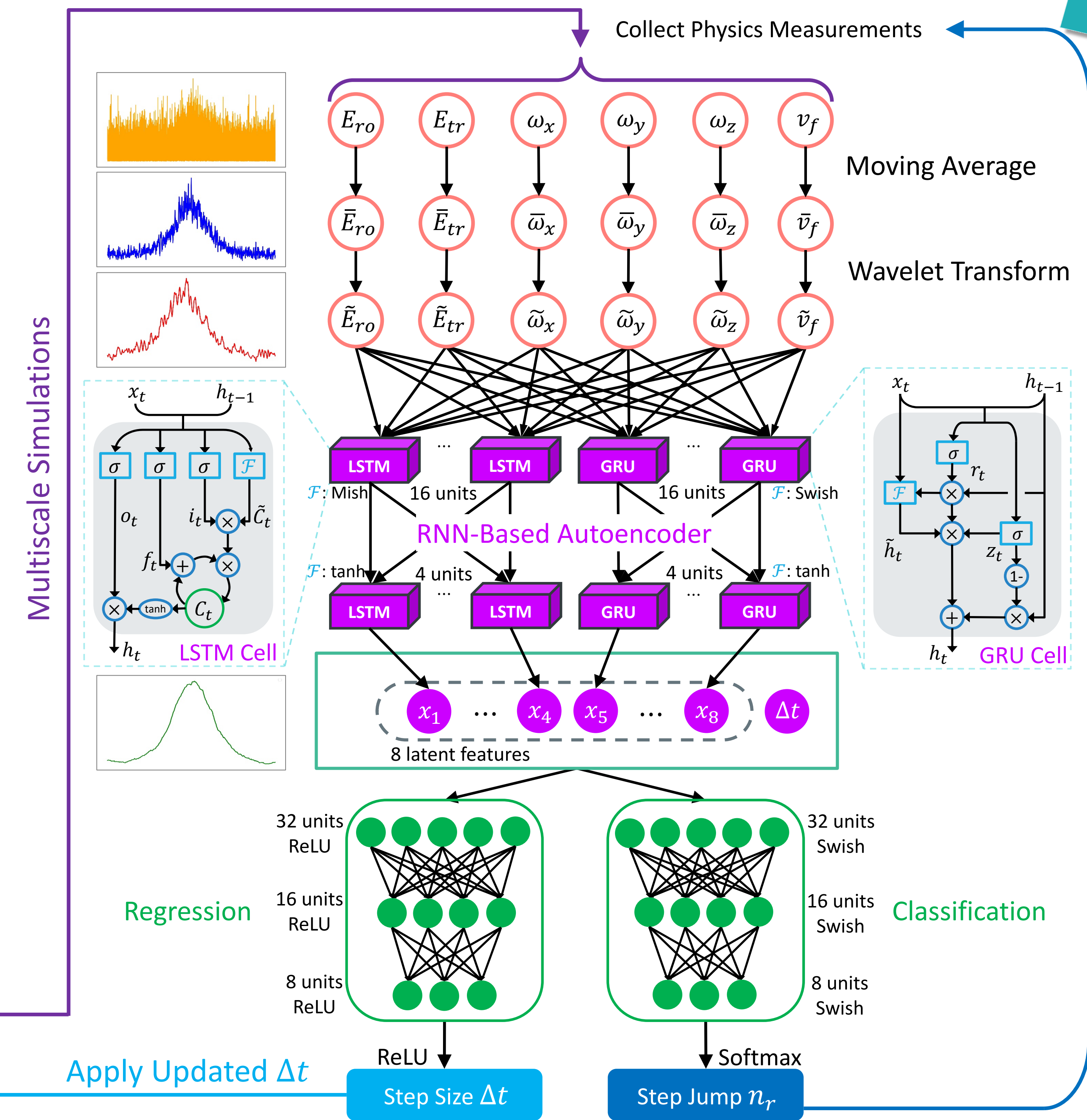
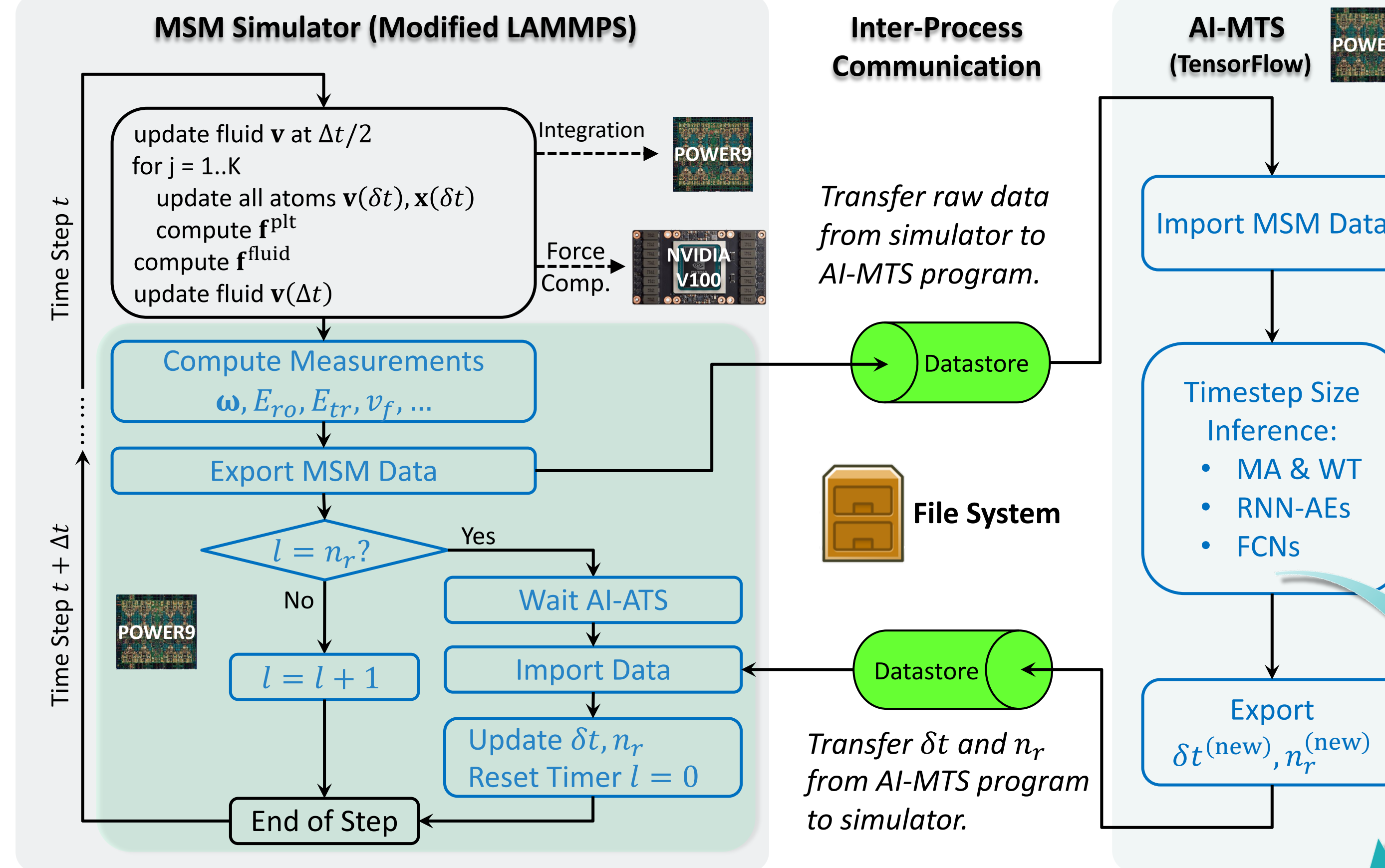
The Parameters for Two Experiments

System	# Platelet Particles	# Fluid Particles	# Total
Exp-S	140,303	1,125,408	1,265,711
Exp-M	1,403,030	6,568,840	7,971,870

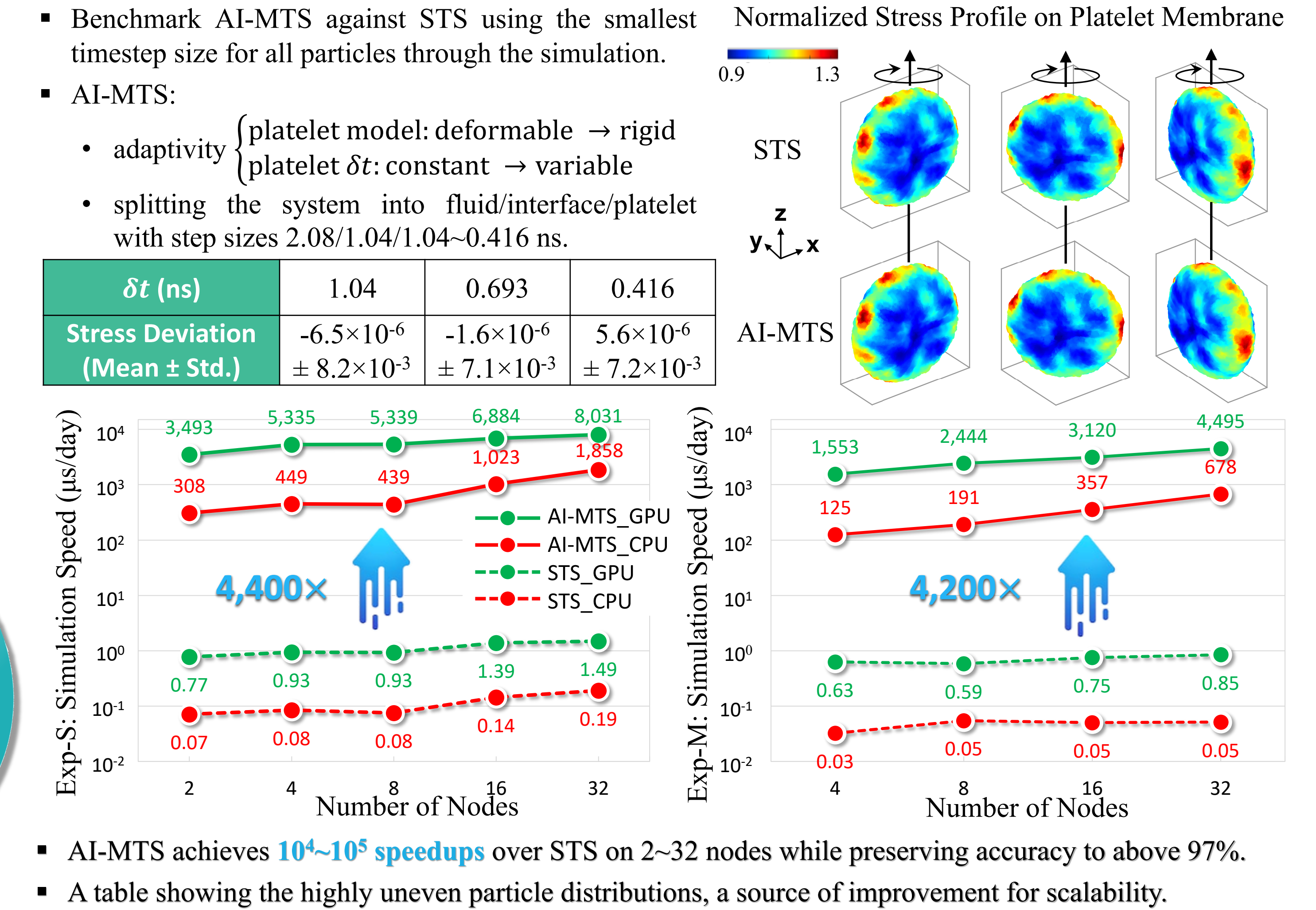
AI-MTS enables adaptive time stepping by AI to the underlying system states in MSM simulations on HPC.



AI-Enabled Multiscale Modelling



Performance Analysis



# Nodes	2	4	8	16	32	4	8	16	32
# Particles	15,255	7,741	3,852	1,916	945	45,557	22,751	11,345	5,630
Min	15,255	7,741	3,852	1,916	945	45,557	22,751	11,345	5,630
Avg	17,597	8,789	4,394	2,197	1,098	55,360	27,680	13,840	6,920
Max	72,072	62,819	47,792	29,655	20,474	100,561	111,333	75,258	66,275

The HPC Experiment Platform

AiMOS Supercomputer @ Rensselaer Polytechnic Institute

System contains 252 nodes, each with:

	CPU	GPU
Model	2 × IBM Power 9	6 × NVIDIA Tesla V100
Memory	256 GB per CPU	32 GB per GPU
Performance	0.5 TFlop/s per CPU	6.7 TFlop/s per GPU



Conclusions and Future Work

- AI-MTS provides a novel integration of machine learning with multiscale modeling in reducing redundant computations while preserving sufficient accuracy, by adapting integration timestep sizes.
- AI-MTS helps realize a speedup of 3–4 orders of magnitude by intelligently managing the disparity in temporal scales for complex applications involving multi-physics.
- AI-MTS encapsulates the beauty and power of the integrated machine learning with HPC.
- AI-MTS will be examined to enable holistic minimizations of load imbalance and communication.

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- [1] Y. Zaid, et al., "Platelets can contain SARS-CoV-2 RNA and are hyperactivated in COVID-19", *medRxiv*, 2020.
- [2] M. E. Tuckerman, et al., "Molecular Dynamics Algorithm for Multiple Time Scales: Systems with Long Range Forces", *J. Chem. Phys.*, 94 (1991) 6811–6815.
- [3] P. Zhang, et al., "A Multiple Time Stepping Algorithm for Efficient Multiscale Modeling of Platelets Flowing in Blood Plasma", *J. Comput. Phys.*, (284) 668–686, 01/2015.
- [4] C. Han, et al., "Artificial Intelligence for Accelerating Time Integrations in Multiscale Modeling", *J. Comput. Phys.*, 2020 (under revision).