

Machine Learning for Adaptive Discretization in Massive Multiscale Biomedical Modeling

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ABSTRACT

For multiscale problems, traditional time stepping algorithms use a single smallest time stepsize in order to capture the finest details; using this scale leads to a significant waste of computing resources for simulating coarse-grained portion of the problem. To improve computing efficiency for multiscale modeling, we propose a novel state-driven adaptive time stepping (ATS) algorithm to automatically adapt the time stepsizes to the underlying biophysical phenomena at multiple scales. In this, we use a machine-learning based solution framework to classify and label these states for regulating the time stepsizes. We demonstrate the values of our ATS algorithm by assessing the accuracy and efficiency of a multiscale two-platelet recruitment aggregation simulation. By comparing with traditional algorithm for this simulation, our ATS algorithm significantly improves the efficiency while maintaining accuracy. Our novel ATS algorithm presents a more efficient framework for solving massive multiscale biomedical problems.

CCS CONCEPTS

• **Computing methodologies** → **Machine learning**; **Neural networks**; **Multiscale systems**;

KEYWORDS

machine learning, multiscale modeling, adaptive time stepping, parallel computing

1 INTRODUCTION

Multiscale modeling (MSM) is a method that multiple models at different scales are considered simultaneously to describe particle properties or behaviors on one scale by parameters from other scales. Traditional time stepping algorithm uses the smallest time stepsize through the entire simulation to ensure sufficient motions at shortest temporal scales are caught. However, the redundant computations at top scales leads to a significant waste computing resources. Although the MSM provides a way to describe sufficient details at disparate spatial scales, there is no time stepping algorithms that adapts temporal scales to diversities of spatial scales. To bridge this gap, we propose a novel state-driven adaptive time-stepping (ATS) algorithm. This proposed ATS algorithm aims to adapt time

stepsizes to underlying biophysical phenomena. To demonstrate the performance for our ATS algorithm, numerical experiments are conducted on our previous developed multiscale model for platelet recruitment aggregation [2]. Accuracy and efficiency are presented and compared with traditional methods.

2 ADAPTIVE TIME STEPPING ALGORITHM

We developed a particle-based multiscale model of platelets employing Dissipative Particle Dynamics (DPD) and Coarse-Grained Molecular Dynamics (CGMD) methods to characterize initiation of thrombosis in shear flow [3, 4]. The hydrodynamics of viscous blood flow is simulated using DPD at mesoscopic scale ranged from mm to μm and μs timescale; the platelet is modeled with CGMD to simplify the atomistic model at microscopic scale coupling with ns to ps timescale in Figure 1. The platelet recruitment aggregation evolves through several phases at different spatial and temporal scales [1]. To detect state changes, we establish a machine-learning based solution framework to learn and regulate time stepsizes in Figure 2. This algorithm considers particles' positions and momenta as inputs. We describe phases by the most significant attributes of states from inputs at first two layers. Then these attributes are

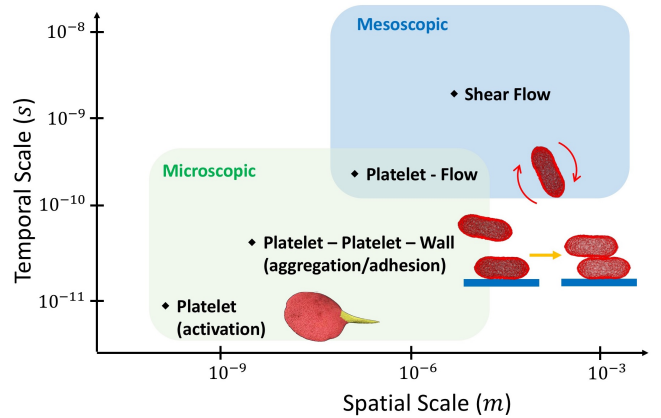


Figure 1: Multiple scales of modeling platelet in shear flow.

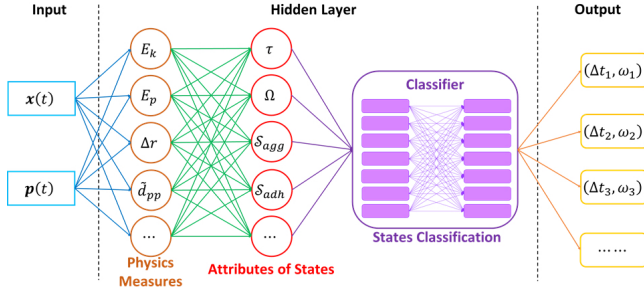


Figure 2: Machine learning framework of ATS algorithm.

categorized by a neural network and labeled by a vector of two components: time stepsize Δt and state examination frequency ω . In $1/\omega$ steps, the simulation proceeds with a new time stepsize. By the end of these steps, ATS algorithm re-adjusts the time stepsizes. State examination frequency is determined by change rate of state.

3 ACCURACY AND EFFICIENCY ANALYSIS

We simulated a microchannel to study interactions of two platelets in Poiseuille flow. The simulation dimensions are $35.6 \times 16 \times 35.6$ (length $\times$ height $\times$ width) in μm . No slip boundary conditions are applied on the top and bottom walls and periodic boundary conditions are applied along x - and z -directions. We tested our ATS algorithm against the reference system using STS algorithm. For accuracy analysis, we employed absolute error as $\epsilon_a = |\eta_{ats} - \eta_{sts}|$ and relative error normalizing absolute error by the reference measures as $\epsilon_r = \epsilon_a / |\eta_{sts}|$. Figure 3 shows relative errors along the time of system kinetic energy and distance between center of mass of two platelets in ATS and STS simulations. The final states of the aggregation process by both algorithms are consistent with each other as the morphological comparison in Figure 4. For efficiency analysis, we measured the speed in wall clock time per state. Our ATS captures 5 state changes with 3 different time stepsizes listed in Table 1. Figure 5 plots the time stepsizes used in both algorithms and compares simulation time and speedup achieved in each state. During recruitment stage (state 1-4), ATS algorithm improves efficiency through using large stepsizes; in stabilization stage (state 5), there is a need to capture the micro-structural changes at nm -length scale thus the stepsize has to be the smallest at both ATS and STS algorithms. Compared with the STS system, the ATS algorithm achieves a great speedup at recruitment and initiation of aggregation while maintaining $\geq 95\%$ accuracy in platelets dynamics.

4 DISCUSSIONS

We develop an ATS algorithm that can significantly improve the efficiency of multiscale simulations by dynamically regulating time stepsizes coupling with biophysical states across multiple scales. This novel ATS algorithm establishes a machine-learning based framework to characterize each state by most significant attributes for adjusting time stepsizes. This work presents a preliminary study for initial formation of platelet recruitment aggregation using ATS algorithm. Shear-induced platelet-mediated thrombosis formation is a more advanced system that contains more platelets and more complex biophysical processes, and incorporates multiple events

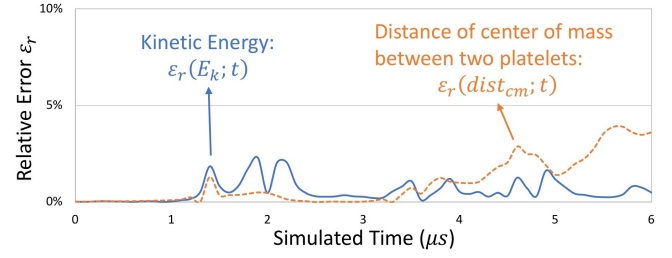


Figure 3: Accuracy analysis in energy and center of mass.

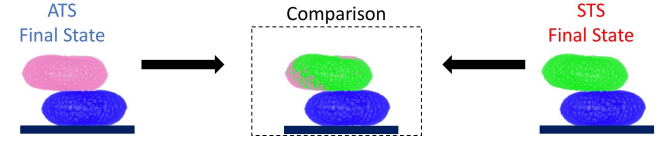


Figure 4: Morphological comparison at final state.

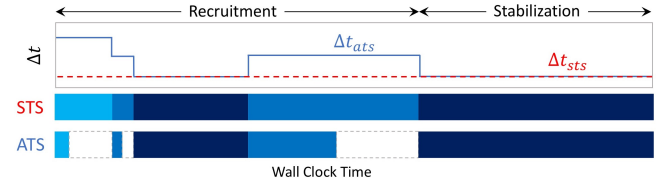


Figure 5: Speed comparison in wall clock time.

Table 1: Time stepsizes comparison

State	1	2	3	4	5
Time Stepsize					
ATS ($\times 10^{-4}$)	4	2	1	2	1
STS ($\times 10^{-4}$)	1	1	1	1	1
Speedup	4.0	2.0	1.0	1.9	1.0

including platelet flipping, margination, recruitment, aggregation, adhesion and formation of thrombosis. Today's computing power, though is increasing at a high speed, is not fast enough to solve such complex systems at multiple scales. Our ATS algorithm is novel at making more efficient use of these computing powers and offered a promising insight for solving massive particle-based multiscale problems efficiently.

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