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Machine Learning for Soft Matter Flows

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Abstract

We aim to develop Physics Informed Machine Learning (ML) methods capable of accelerating and/or complementing standard simulation methods for Soft Matter flows. We have identified three characteristic problems, (A) simulating entangled polymer melt flows, (B) inferring flow solutions, and (C) navigating non-uniform flows, and developed ML techniques to solve each of them. (A) We used ML to learn the constitutive relation of entangled polymers within the Doi-Takimoto model, and then employed these relations to perform flow simulations that are an order of magnitude faster than state-of-the-art Multi-Scale Simulations (MSS), with no significant loss of accuracy. (B) We developed a probabilistic Stokes flow inference framework that is capable of inferring the flow solution given partial and/or noisy data, and which exactly satisfies the physics of the problem. (C) Finally, we also developed a learning protocol for swimmers in non-uniform flows, and showed that it is possible to achieve near-optimal performance using only local hydrodynamic signals.

1 Basic information

1.1 Collaborating JHPCN centers

The University of Tokyo

1.2 Theme area

- Large-scale computational science

1.3 Research area

- Very large-scale numerical computation
- Very large-scale data processing

1.4 Project members and their roles

- J.J Molina: ML for Soft Matter.
- H. Shiba: Support for code optimization.
- T. Shimokawabe: Support for code optimization.
- R. Yamamoto: Soft Matter theory.
- T. Taniguchi: MSS for polymer flows, GPU coding.
- M.S. Turner: Intelligent/active Soft Matter theory.
- T. Sato: MSS for polymer flows.
- D. Mayank: Microscopic polymer modeling.
- S. Miyamoto: ML and MSS for polymer flows.
- Y. Xu: Microscopic polymer modeling.
- K. Ogawa: ML for flow inference.
- S. Schnyder: Simulation/optimal control of active matter.
- K. Sankaewtong: Simulation/optimal control of active matter.
- H.L. Devereux: Simulation/optimal control of active matter.
- M.P. Lynch: ML for optimal control.
- A.C. Meneses: Simulation/optimal control of active matter.

2 Purpose and Significance of the Research

Soft Matter systems are ubiquitous in our daily lives. Understanding, predicting, and/or con-

trolling their properties is a crucial but incredibly challenging task. The difficulty comes from the coupling between the microscopic and macroscopic degrees of freedom. Computer simulations have become the method of choice, but they remain incredibly expensive. Thus, the goal of this work is to develop ML techniques to replace and/or enhance existing methods. In particular, we have focused on three basic Soft Matter problems: (A) entangled polymer melt flows, (B) low-Reynolds number flows, and (C) navigating non-uniform flows.

(A) We propose to accelerate the state-of-the-art Multi-Scale simulations, which directly couple micro/macro degrees of freedom, by using a machine-learned constitutive relation. This will allow us to optimize for polymer processing flows and lead to the establishment of a bottom-up design framework for polymer products. For this FY, we have extended our learning to incorporate the principle of objectivity, and obtained drastically improved flow predictions.

(B) Stokes flows, characteristic of flows at small scales or large molecular weight polymeric fluids, are fundamental to biology and industry. However, existing numerical methods are not suited for solving under-determined or inverse problems (e.g., unknown boundary conditions). We propose a probabilistic Stokes flow solver that is applicable to arbitrarily complex geometries, and which allows for mixed boundary conditions and missing and/or noisy data. This will allow us to provide experimental colleagues with a robust tool to analyze their experiments (e.g., particle-image velocimetry data on biological flows). For this FY, we have extended the method to allow for flow inference from sparse measurements typical of such experiments.

(C) Active Soft Matter, composed of agents that consume energy to perform work, are ubiquitous in biology, and have immense technological applications (e.g., targeted drug delivery). However, understanding how they react to their environment remains an open question. To investigate how biological swimmers behave, we have proposed a Machine-Learning/Direct Numerical Simulation approach to design optimal navigation strategies in complex flows. This will allow us to design "intelligent" artificial agents capable of performing useful work. For this FY, we have demonstrated how to teach agents to swim efficiently in non-uniform flow fields using only local hydrodynamic signals.

3 Significance as JHPCN Joint Research Project

The goal of this project is to develop Physics Informed Machine-Learning methods to simulate/analyze characteristic flow problems encountered in Soft Matter. For this FY, we focused on three particular flow problems: (A) simulating entangled polymer melts, (B) inferring Stokes flow solutions from partial data, and (C) learning optimal control strategies for swimming in complex flows. The training, learning, and validation for each of these problems requires considerable computing resources. For example, (A) the full MSS of entangled polymers, needed to validate our ML solution, requires simulations with $\mathcal{O}(10^8)$ polymer chains; (B) the Stokes flow inference for 3D flows requires a GP regression with $\mathcal{O}(10^6)$ training points, which can only be performed on high-performance GPU clusters. Likewise, the Reinforcement Learning used to train a swimmer to navigate a complex flow requires accurate hydrodynamic simulations, which are notoriously expensive. Where possible, we have used specialized GPU and/or Python/JAX code, in order to take full advantage of Tokyo's Wisteria-BDEC cluster.

4 Outline of Research Achievements up to FY2021 (Only for continuous projects)

During FY2021 we were mainly working on the precursors for Themes (A) and (B) of the current project. For theme (A), we developed and implemented a ML method to learn the constitutive relation of polymeric materials with memory, allowing us to drastically reduce the calculation cost of MSS. The method was extended to entangled polymers within the Doi-Takimoto model, but due to the simple training protocol used, the flow predictions were only in semi-quantitative agreement with MSS. Furthermore, we also extended and validated the Doi-Takimoto model, to include the stretch/orientation induced reduction of friction, which is required to correctly reproduce the strain hardening observed under fast elongational flows. Finally, we also ported the non-interacting polymer models to GPU using OpenACC and CUDA. Our results were incredibly encouraging, with a single GPU running $\mathcal{O}(10^3)$ times faster than a single CPU, and $\mathcal{O}(10)$ times faster than a 25 core CPU/MPI computation. For theme (B), we established the proof-of-concept for the probabilistic Stokes flow solver, and demonstrated that it was capable of inferring the solution to a flow problem given the full set of boundary conditions.

5 Details of FY2022 Research Achievements

5.1 Learning the constitutive relation of entangled polymer melts

We have extended and improved our ML accelerated MSS method, which uses a Gaussian Process (GP) regression scheme to learn the constitutive relation for the Doi-Takimoto (DT) polymer entanglement model. We successfully used these relations to perform polymer melt flow simulations in simple geometries (i.e., pressure driven flow between parallel plates). For the training, we used a microscopic DT system, with 10^4 chains, and measured the stress response under steady and oscillatory shear, using $\simeq 50$ different shear rates. From this, we obtain a training dataset of $\simeq 3 \times 10^3$ points $(\boldsymbol{\kappa}, \boldsymbol{\sigma}, \dot{\boldsymbol{\sigma}})$, consisting of velocity gradients $\boldsymbol{\kappa}$, stresses $\boldsymbol{\sigma}$, and their time-derivatives $\dot{\boldsymbol{\sigma}}$. The GP regression was performed using the Python/GPyTorch package, in order to learn the constitutive relation $\dot{\boldsymbol{\sigma}}(\boldsymbol{\kappa}, \dot{\boldsymbol{\sigma}})$. For the $2D$ flows we have considered here, the generation and learning can be performed in a relatively short time ($\simeq 0.1$ hours on a single GPU). However, this is expected to dramatically increase when simulating complex 3D flows/deformation modes.

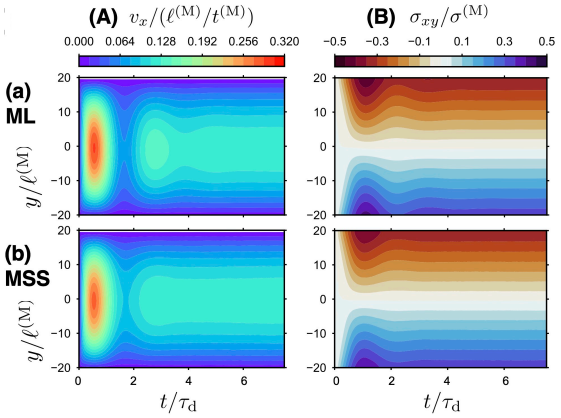

Fig. 1 Simulation results for pressure driven flow of an entangled polymer melt between flat parallel plates. Shown are the normalized (A) velocity v_x and (B) shear stress σ_{xy} profiles, as a function of the scaled height y and time t, obtained from (a) ML constitutive relations and (b) full MSS (Miyamoto et al., under review at *Physics of Fluids*).

The machine-learned constitutive relation was then used to simulate the pressure-gap-driven flow between parallel plates. For the flow solver, we used the Smoothed Particle Hydrodynamics

(SPH) method, as implemented in the *Framework for Developing Particle Simulators* code (Iwasa et al., Publ. Astron. Soc. Jpn. 68, 54, 2016), which has MPI capabilities. The ML constitutive relation, instantiated via GPyTorch, was called from this C++ SPH code using Torchscript. The number of SPH particle was set to 800. The flow prediction was assessed by comparing against a full Multi-Scale Simulation (MSS), using embedded microscopic simulators (10^4 chains per SPH particle), in which the macroscopic fluid particle and microscopic simulators are fully distributed among CPU cores using MPI. Fig. 1 shows the comparison of the velocity profiles v_x and shear stresses σ_{xy}, as a function of the channel height and time. The ML model provides excellent predictions, within $\lesssim 10\%$ relative error, but with an order of magnitude increase in efficiency, both in compute time and memory requirements. As an example, running on a single 40-core CPU, the ML accelerated MSS took $\simeq 2$ hours, using $\simeq 2$GB of memory, whereas the full MSS required $\simeq 1$ day, and used $\simeq 12$GB of memory. This efficacy is expected to increase for complex 2D or 3D systems, as the MSS will require considerably more compute time.

Finally, we have also investigated the use of more detailed polymer models, e.g., coarse-grained and all-atom models (using GROMACS and LAMMPS), in order to provide more quantitative predictions (e.g., to study the difference between natural and synthetic rubber).

5.2 Learning the Stokes equation

We have extended our Gaussian Process (GP) based Stokes flow solver to allow for missing boundary conditions and/or sparse training data, as required for analyzing experiments. We refer to this probabilistic framework as a Stokesian Process (SP). In particular, we use known values of the velocity $\boldsymbol{v}$ and/or pressure p, and require that the governing equations, here the Stokes/force-balance equation $\boldsymbol{f} \equiv \boldsymbol{\nabla} p - \mu \nabla^2 \boldsymbol{u} = 0$, and the continuity equation $s \equiv \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$, be satisfied at arbitrarily chosen training

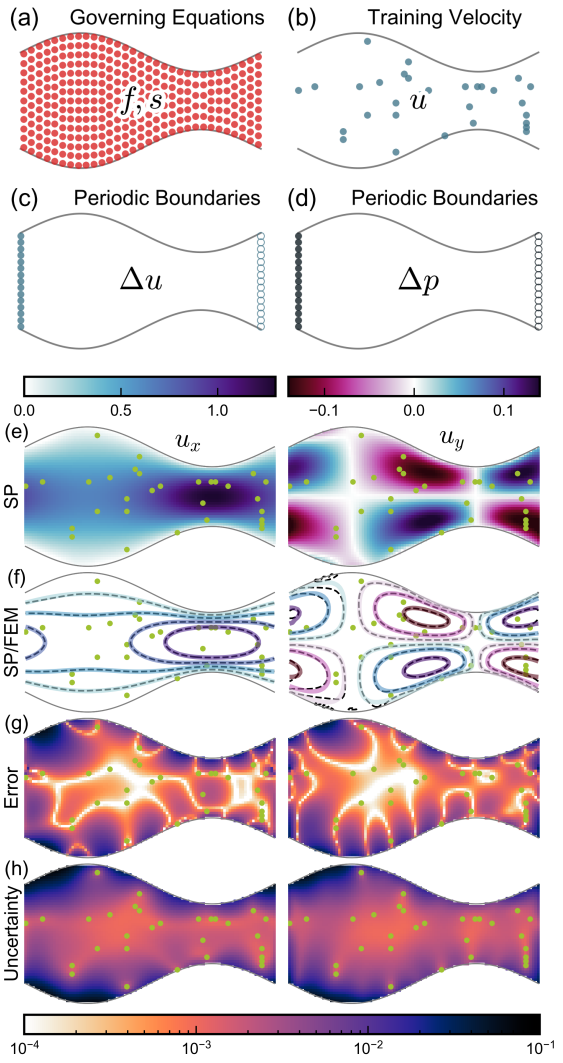

Fig. 2 SP inference for a pressure driven flow through a sinusoidal channel. (a-d) Location of the training points for the governing equations (i.e., Stokes $\boldsymbol{f} = 0$ and continuity $s = 0$), the training FEM velocities, and the periodic boundary conditions for the velocity and pressure fields; (e) SP predicted velocities, (f) SP and FEM velocity contours, (g) error between SP and FEM results, and (h) SP prediction uncertainties (Molina et al., unpublished).

points. Furthermore, the correlations between these fields, $\boldsymbol{u}, p, \boldsymbol{f}$ and s are directly encoded into the GP correlation matrices, ensuring that the physics of the problem is satisfied (on average). This is only possible thanks to the linearity of the Stokes equations, and the fact that GPs are closed under linear operators. Our SP framework is implemented using Python/JAX, which allows us to leverage the built-in automatic differentiation capabilities to define the custom physics-informed kernels, which can contain up to fourth-order derivatives.

As an example, we have tested our method on a pressure driven flow problem through a sinusoidal channel. As expected, given the full set of boundary conditions (e.g., zero velocity at the walls, constant pressure gap between inlet/outlet) we can accurately infer the flow. However, a more interesting/challenging task is to reconstruct the flow given sparse measurements, and without knowledge of the boundaries. For this, we used a reference FEM solution (generated using the FEniCSx computing platform), and randomly selected 30 points within the domain, to use the corresponding velocities as training points for the GP inference. We introduced additional training points to enforce the governing equations, i.e., the Stokes $\boldsymbol{f} = 0$ (337×2 points) and continuity $s = 0$ (337 points) equations, as well as the periodic boundary conditions (15×2 points for the velocity and 15 for the pressure), but no other information was required. Our SP solver was able to accurately infer the flow, as shown in Fig. 2 for 5184×2 test/prediction points. Furthermore, the prediction uncertainties, which come for free with the GP (in contrast to Neural-Networks), are in good agreement with the actual error (computed using the FEM solution), showing the robustness of this ML approach. We have confirmed that the error decreases upon increasing the number of training points, likewise, the prediction error increases with the distance to the training points. While a single calculation (training+prediction) for such a simple 2D flow problem is relatively inexpensive ($\simeq$ 5 minutes on a single GPU), it relies on the ability to run Python+JAX on high-performance GPUs ($\gtrsim$ 20GB memory). Finally, we note that while our method is more expensive than FEM for this sample problem (almost 8 times slower), it will become much more competitive when we consider 3D flows in the presence of moving boundaries, where remeshing becomes a serious bottleneck to FEM.

5.3 Machine Learning optimal control

We have established a combined ML/Direct Numerical Simulation approach to tackle the optimal control problem of a swimmer navigating complex flows. In particular, we have used Deep Q-Learning, trained on detailed hydrodynamic simulations of swimming particles in a non-uniform zig-zag shear flow. The Deep Q-Learning is implemented using the PyTorch package, while the direct numerical simulations are computed using the Smoothed Profile method, as implemented in the KAPSEL simulator. The swimmer, here modeled as a rigid spherical squirmer, is endowed with surface sensors that allow it to measure hydrodynamic forces, which it uses to select an optimal strategy (here a body rotation) for the particular task at hand (e.g., swimming in the flow, shear-gradient, or vorticity directions). The actions of the swimmer are encoded in a neural-network with three hidden layers, each with 100 neurons, and an output layer with 27 neurons (each specifying a different axis of rotation). We have shown that the swimmer can achieve near-optimal performance using only local information. However, we did notice a reduced performance when tasked with navigating in the flow direction, as the swimmer was not able

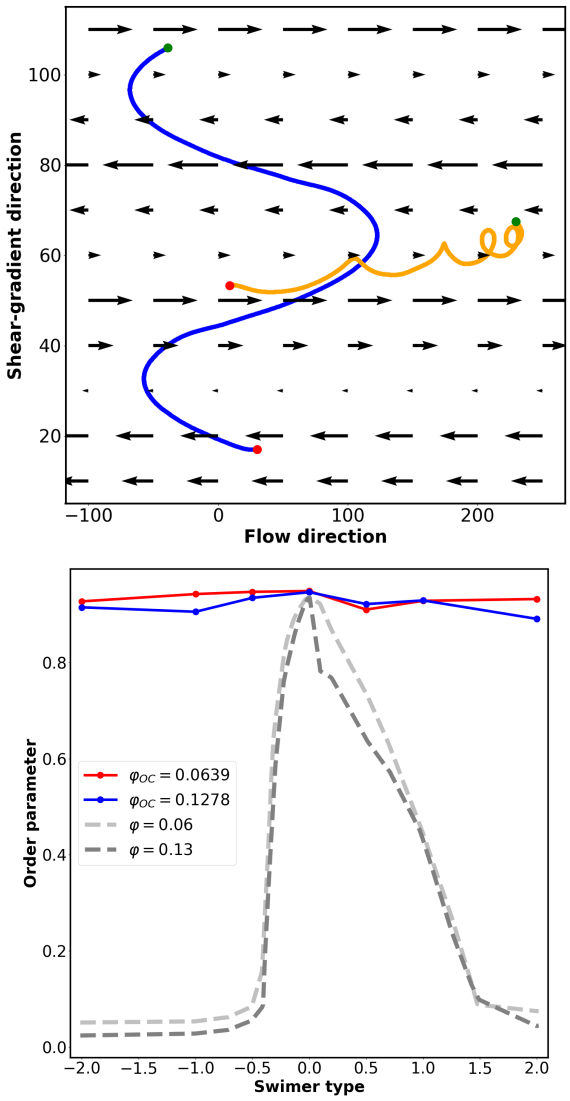

Fig. 3 (top) Trajectories of a "smart" or optimally controlled (OC) swimmer, trained to travel in the shear gradient direction, compared to a "naive" swimmer. (bottom) Polar order parameter for a dispersion of swimmers, as a function of volume fraction φ. For a dispersion of "naive" swimmers, ordered motion is only seen for relatively weak swimming parameters. However, a dispersion of "smart" swimmers is able to achieve polar ordering, regardless of swimming type or concentration (K. Sankawtong et al, unpublished).

to consistently maintain itself in the shear-plane. Finally, we have shown that it is possible to train a collection of swimmers to show ordered collective motion (see Fig.3), although the training cost increases dramatically with the concentration of swimmers.

6 Self-review of Current Progress and Future Prospects

Our original plan was divided into the three themes of, (A) learning the constitutive relation of entangled polymer melts, (B) learning the Stokes equation, and (C) learning efficient swimming strategies. For theme (A), we have successfully improved our learning method, to the point where we are now able to perform 2D flow simulations in complex geometries that are in good quantitative agreement with full MSS. For theme (B), we have successfully extended our probabilistic flow solver to 2D. We have tested our method on a non-trivial problem for which no exact solution is known, and shown that we can accurately reproduce the flow given incomplete information (e.g., sparse sampling of the velocity only). For theme (C), we have successfully developed a Reinforcement Learning method to teach swimmers to navigate non-homogeneous flows using only local hydrodynamic signals. Furthermore, we have also considered suspensions of such swimmers, training them to exhibit targeted collective motion. Finally, we have also explored how to apply these ML methods to other active systems, in particular, crawling/proliferating cells.

Our research plan for FY2023 will continue to develop these themes. For theme (A), we will learn constitutive relations applicable to complex 3D flows of entangled polymer melts (e.g., non-isothermal flows). Furthermore, we will focus on porting our full code-base (microscopic polymer models as well as SPH fluid solvers) to GPUs, as this is required to simulate large scale systems. We will also optimize our learning pro-

tocol (e.g., active learning) and implement the method on GPUs, to allow us to perform exact inference using millions of training points (also required for 3D flows). In this way, we will be able to perform simulations for complex processing flows relevant to industrial applications. For theme (B), we need to optimize our code to handle large scale 3D systems and moving boundaries. This requires replacing the basic Cholesky decomposition approach with the Black-Box-Matrix-Matrix algorithm introduced by GPyTorch. Unfortunately, given the complexity of our custom physics-informed kernels, we are not able to use GPyTorch, and must instead implement these methods in a JAX-friendly (functional) way. With this, we will be able to analyze real-world flow experiments. Finally, for theme (C) we will continue to investigate how to control the collective motion of dense swimmer dispersions. For this, we will aim to minimize the overhead of interfacing the C++ hydrodynamic code with the GPU learning code.

7 List of publications and presentations

Journal Papers (Refereed)

- K. Sankaewtong, J.J. Molina, M.S. Turner(+), R. Yamamoto, "Learning to swim efficiently in a nonuniform flow field", *Physical Review E*, in press, 2023.
- S. Miyamoto, T. Sato, T. Taniguchi, "Stretch-orientation-induced reduction of friction in well-entangled bidisperse blends: a dual slip-link simulation study", *Rheologica Acta* **62**, pp.57 - 70, 2022.
- M. Dixit, T. Taniguchi, "Substantial effect of terminal groups in *cis*-Polyisoprene: A multiscale molecular dynamics simulation study", *Macromolecules* **55**, pp.9650-9662, 2022.
- J. Li, S.K. Schnyder, M.S. Turner(+), R. Yamamoto, "Competition between cell types under cell cycle regulation with apoptosis", *Physical Review Research* **4**, 033156, 2022.

Proceedings of International Conference Papers (Refereed)

Presentations at International conference (Non-refereed)

- T. Taniguchi, M. Dixit, "Role of terminal groups of cis-1,4-polyisoprene in the formation of physical cross-linking in NR–All-atom simulation study", American Physical Society March Meeting, 5-10 March, 2022.
- S. Miyamoto, T. Sato, T. Taniguchi, "Friction reduction in well-entangled bidisperse blends under fast flows: A dual slip-link study", 16th International Workshop for East Asian Young Rheologists, 18-21 February, 2023. –Best Presentation Award–
- S. Miyamoto, J.J. Molina, T. Taniguchi, "Machine-learned constitutive relations for simulating well-entangled polymer melt flows for their history-dependent flows", Society of Rheology 93rd Annual Meeting, 9-13 October, 2022.
- K. Sankawtong, J.J. Molina, M.S. Turner(+), R. Yamamoto, "Learning to swim efficiently in a nonuniform flow field", 6th International Soft Matter, 19-23 September, 2022.
- S. Miyamoto, J.J. Molina, T. Taniguchi, "Applications of machine-learned constitutive relation to simulate well-entangled polymer melt flows", 37th International Conference of the Polymer Processing Society, 11-15 April, 2022.
- K. Ogawa, J.J. Molina, T. Taniguchi, "Flow problems as inference problems", 37th International Conference of the Polymer Processing Society, 11-15 April, 2022.

Presentations at domestic conference (Non-refereed)

- S. Miyamoto, T. Sato, T. Taniguchi,“摩擦低減効果を考慮したスリップリンクモデルによる二様分子量分布高分子溶融体の粘弾性予測”, 日本レオロジー学会　2022 年通常総会および第 49 年会, 12-13 May, 2022.
- M. Dixit, T. Taniguchi, “The substantial effect of terminal groups in NR: A multiscale molecular dynamics simulation study”, 70th Autumn Meeting of the Rheological Society, Japan, 13-14 October, 2022.

Published open software library and so on

Other (patents, press releases, books and so on)

- S. Miyamoto, J.J. Molina, T. Taniguchi, “からみ合い高分子溶融体の流動解析手法の進展－マルチスケールシミュレーション法と機械学習の融合－”, 化学工学会誌 **87**, pp.111-113, 2023.