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Machine Learning for Soft-Matter Flows

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Abstract

We have developed (Physics Informed) Machine Learning (ML) methods capable of replacing and/or complementing simulation methods for Soft Matter flows. We focus on three characteristic problems: (A) simulating entangled polymer melts, (B) inferring flow solutions, and (C) navigating non-uniform flows. (A) We used ML to infer the constitutive equation of entangled polymers within the Doi-Takimoto and Kremer-Grest models, and used these learned equations to perform macroscopic flow simulations. These simulations can be orders of magnitude faster than state-of-the-art Multi-Scale Simulations (MSS), without sacrificing accuracy. (B) We developed a (Bayesian) probabilistic flow inference framework capable of inferring the solution to arbitrary Stokes flow problems given partial and/or noisy data. In contrast to alternative ML approaches, we guarantee that the underlying physical equations are satisfied exactly (on average). (C) Finally, we have developed a learning protocol to enable swimmers to navigate complex flows using only local hydrodynamic signals.

1 Basic information

1.1 Collaborating JHPCN centers

- The University of Tokyo
- Osaka University

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: HPC support
- T. Shimokawabe: HPC support
- R. Yamamoto: Soft Matter theory
- T. Taniguchi: MSS for polymers
- M S. Turner: Soft Matter Theory
- T. Sato: MSS for polymer flows
- D. Mayank: Polymer simulations
- S. Miyamoto: ML/MSS for polymers
- X. Yuan: Polymer simulations
- T. Ueno: ML for polymers
- M. Ohta: MSS for polymers
- K. Ogawa: ML for flow inference
- S. K. Schnyder: Optimal control for active matter
- K. Sankaewtong: Optimal ML for active matter
- M. Lynch: ML for optimal control
- A. C. Meneses: Active matter simulations

2 Purpose and Significance of the Research

Soft Matter systems are crucial for modern technologies. To create better, more energy-efficient, and robust materials requires that we be able to understand and control their properties. However, Soft Matter materials are particularly complicated, as they are characterized by a hierarchy of length- and time-scales, which severely limits any theoretical descriptions. This leaves computer simulations as the preferred way to study/probe these systems. For this, multi-scale / coarse-grained descriptions have shown great promise, but they remain incredibly expensive. Thus, the goal of this project is to develop (physics-informed) machine-learning methods that can enhance and/or supplement current simulation methods. We focus on flowing soft matter, along 3 themes (A, B, C).

(Theme A) The purpose is to understand the flow of entangled polymer melts, which is crucial to develop more efficient and environmentally friendly materials. For this, we should understand the micro/macro coupling. To avoid Multi-Scale Simulation (MSS) that directly couple these degrees of freedom, we aim to learn the constitutive relations. This year we worked to improve the robustness of the learning and apply it to complex flows.

(Theme B) The purpose is to understand Stokes flows, inherent to small length-scales (e.g., biological flows) and/or high viscosity fluids (e.g., high-molecular weight polymers). To replace traditional methods, which cannot be directly applied to experimental settings, we developed a probabilistic Stokes Flow framework. This year, we worked to extend the method to 3D, in order to analyze experimental data, e.g., particle-image velocimetry (PIV) measurements.

(Theme C) Active systems, composed of agents capable of consuming energy to perform work, are ubiquitous in biology and engineering. The goal of this project is to understand how swimming particles can learn to use local hydrodynamic signal to perform useful work. This year we focused on achieving robust flocking behavior.

3 Significance as JHPCN Joint Research Project

The goal of this project is to develop Machine-Learning methods to simulate flowing Soft Matter. We have focused on three such problems: (A) entangled polymer melts, (B) inferring Stokes flows, and (C) learning navigation strategies 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 O(10^8) polymer chains; (B) the Stokes flow inference of 3D flows requires a GP regression with O(10^6) training points, which is only possible on high-performance GPU clusters. Likewise, the Reinforcement Learning used to train a swimmer to navigate complex flows requires expensive fluid/particle simulations.

4 Outline of Research Achievements up to FY2022 (Only for continuous projects)

For theme (A), we developed and implemented a ML method to learn the constitutive relation of polymer melts with memory, first using a non-entanglement model, then learning the Doi-Takimoto entanglement model. We also included the stretch/orientation induced reduction of friction in the Doi-Takimoto model, needed to account for the strain hardening under fast elongational flows. Finally, we ported the non-interacting polymer models to GPU using OpenACC and CUDA. For theme (B), we established the proof-of-concept of our probabilistic Stokes flow solver for simple 2D flows. For theme (C) we developed a reinforcement-learning (RL) protocol, coupled with direct numerical simulations, to teach a single swimmer to navigate a non-uniform flow using local signals coupled with externally applied torques/rotations.

5 Details of FY2023 Research Achievements

5.1 Learning Constitutive Relations of Entangled Polymer Melts

We have extended our Gaussian-Process (GP) learning method to predict general/complex flows of well-entangled polymer melts [4,6,7]. In particular, we have extended the method to allow for multi-deformation modes and satisfy the principle of material objectivity. For this, the constitutive relation for the stress is now assumed to be a function of the stress $\boldsymbol{\sigma}$ and the strain rate $\boldsymbol{D} = (\boldsymbol{\kappa} + \boldsymbol{\kappa}^T)/2$ ($\boldsymbol{\kappa} = \boldsymbol{\nabla u}$ the velocity gradient), i.e., $\dot{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}}(\boldsymbol{\sigma}, \boldsymbol{D})$. Simulations for constant strain-rate shear (rate $\dot{\gamma}$) and planar elongational (rate $\dot{\epsilon}$) deformations are performed to generate the time-series of the stress for the training data. From this, we estimate the time-derivative of the stress $\boldsymbol{\sigma}$, and learn the appropriate constitutive relation by placing a GP prior on $\dot{\boldsymbol{\sigma}} \sim \mathcal{N}(\mu, K)$ and conditioning on the training data. This learned constitutive relation can then be used within macroscopic Smooth-Particle Hydrodynamics (SPH) flow simulations. In contrast to previous work, the numerical integration of the constitutive relations is performed in the material frame of the Lagrangian SPH particles. For this, the $\boldsymbol{\sigma}$ and $\boldsymbol{D}$ tensors are rotated from lab coordinates into material coordinates, as dictated by the rotational strain-rate $\boldsymbol{W} = (\boldsymbol{\kappa} - \boldsymbol{\kappa}^T)/2$.

This extended method has been used to perform flow simulations for a $4 : 1 : 4$ contraction expansion channel using the coarse-grained Doi-Takimoto polymer entanglement model. To generate the training data we performed 40 independent pure-shear and elongational deformation simulations with 10^4 chains, and randomly chose 3×10^3 points in the $(\boldsymbol{\sigma}, \boldsymbol{D})$ constitutive equation space for the GP learning. SPH simulation results using the ML constitutive relation are shown in Fig. 1 and compared to full-MSS (using microscopic simulators with 10^4 chains inside each SPH particle). We obtain very good overall agreement, with the benefit that the ML results are considerably smoother.

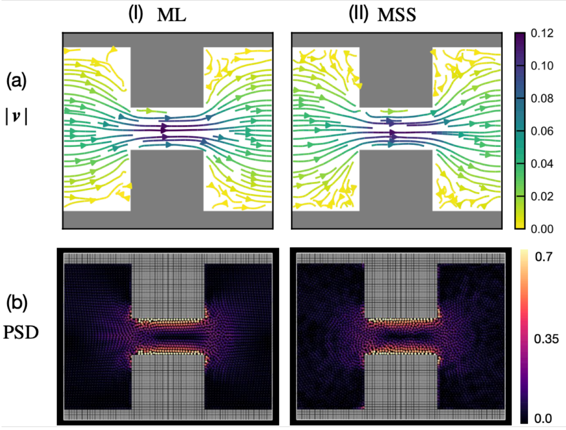

Fig. 1 SPH simulation snapshots for polymer flow through a contraction expansion channel, using (I) ML constitutive relations and (II) full-MSS with Doi-Takimoto simulators. (a) Velocity stream-lines and (b) principle stress differences PSD= $\left(4\sigma_{xy}^2 + (\sigma_{xx} - \sigma_{yy})^2\right)^{1/2}$, color-coded by their respective magnitudes.

We have shown that it is possible to learn the constitutive relation for the Kremer-Grest Coarse-Grained (KGCG) model, which includes the chain-chain interactions and correlations absent in the Doi-Takimoto model [4]. For this, we considered only uniaxial elongational deformations (e.g., modeling melt-spinning processes). Compared to standard MSS, our machine-learned constitutive relation resulted in a speed-up of three orders of magnitude. To improve our microscopic understanding, and hopefully explain the superior properties of natural rubber compared to synthetic rubber, we have also performed extensive simulations for the formation of physical junction points between peptides/proteins and terminal groups [2,5].

5.2 Learning the Stokes Equation

We have extended our physics-informed probabilistic/Gaussian Process (GP) Stokes framework to generic 2D/3D flows. Our method allows for missing and/or partial information, making it an ideal candidate to analyze PIV measurements. We refer to this method as Stokesian Processes (SP). Briefly, we use all known information, including velocity $\boldsymbol{v}$ and pressure p measurements, together with knowledge of the underlying physics, i.e., the Stokes $\boldsymbol{f} \equiv \boldsymbol{\nabla} p - \mu \nabla^2 \boldsymbol{u} = 0$ and continuity equation $s \equiv \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$, to compute the posterior probability distribution for the unknown variables (e.g., velocity). This is done by expressing the correlations between the fields of interest, $\boldsymbol{u}, p, \boldsymbol{f}$ and s, in terms of only $\boldsymbol{u}$ and p, and incorporating them into the GP correlation matrices. In this way, we ensure that the physics is exactly satisfied (on average). Furthermore, we note that we do not require knowledge of the absolute pressure field p, information on pressure differences is enough, in fact, the method also works without pressure information. We have implemented our SP framework in a Python/JAX module, which allows us to easily extend and customize our code, without sacrificing speed/accuracy, as we benefit from JAX's builtin automatic-differentiation and JIT compilation support.

This work has been published in Ref.[3], where we tested the method on a benchmark flow problem: 2D pressure driven flow past a sinusoidal channel. We obtain excellent agreement with respect to the “exact”

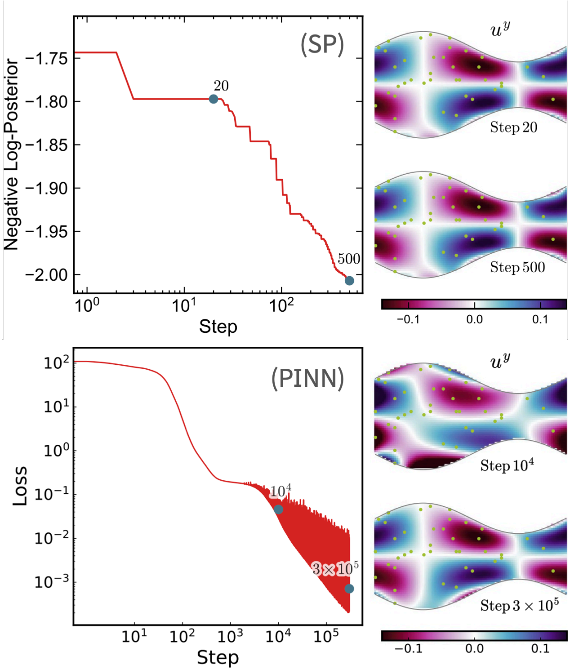

Fig. 2 Evolution of training loss and velocity predictions for (top) SP and (bottom) PINN, for pressure driven flow in a sinusoudal channel. Insets show the v_y predictions (symbols are the randomly sampled training data). Adapted from J.J. Molina et al., Mach. learn.: sci. technol. **4**, 045013, 2023 (CC BY 4.0) [3].

Finite-Element Method calculations (using the FEniCSx computing platform). In particular, our method is able to infer physically meaningful solutions from sparse/noisy measurements, as required for analyzing PIV data. Compared to alternative ML methods, i.e., Physics-Informed Neural Networks (PINN), ours provides more robust predictions and is faster to train (see Fig.2). To illustrate this, consider that for the sample 2D problem of Ref.[3], on a single NVIDIA A100 GPU (Wisteria/BDEC-01), using $N_{\text{train}} \simeq 10^3$ training points, $N_{\text{test}} \simeq 10^5$ test points, the SP calculations require ∼ 1 min, whereas the PINN needed ∼ 6 hours to achieve a similar level of accuracy! Furthermore, the SP is guaranteed to exactly reproduce the training points, but no such guarantee is possible for PINNs. This shows the promise of our approach.

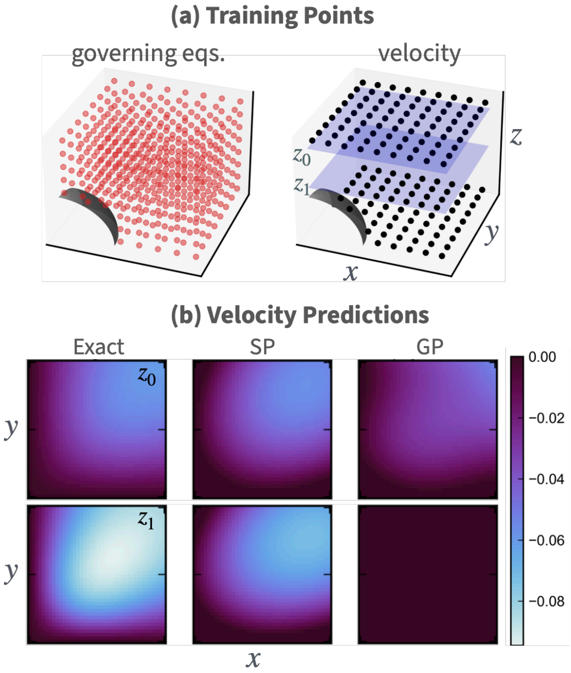

Fig. 3 Reconstruction of the 3D velocity field for flow past a fixed particle. (a) SP training points for the governing equations (489 × 4 points) and the velocity (151 points), red and black symbols, respectively. (b) v_y as a function of (x, y) from the exact solution, SP prediction, and naive GP prediction, for $x-y$ planes at two different heights z_0 and z_1. Adapted from K. Ogawa, Master Thesis, Kyoto University (2024).

We have extended our method to 3D systems and validated the results. For this, we considered flow past a fixed sphere, for which analytical solutions are available. To limit the calculation time, we considered training/test data in one octant around the sphere. To mimic PIV experiments the velocity training data is taken from two x/y planes, whereas the training data for the governing equations is uniformly sampled (see Fig. 3). Our method is able to provide robust predictions/interpolations of the full 3D velocity field. This is in contrast to naive (non physics-informed) GP regression, which only provides reliable predictions very close to the training points.

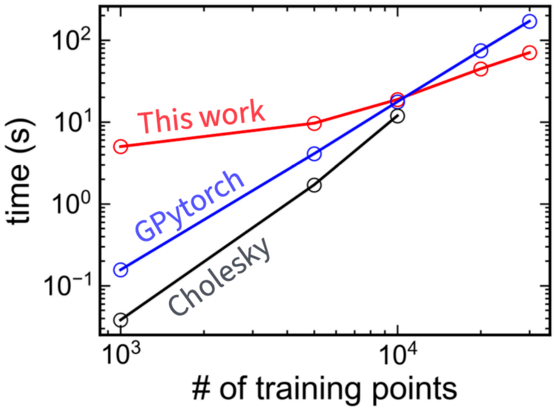

Fig. 4 Compute time for GP inference as a function of the number of training points. Results of our BBMM implementation, GPytorch (BBMM), and a Cholesky decomposition. Choleksy results are not available for $N > 10^4$ due to memory constraints. K. Ogawa, Master Thesis, Kyoto University (2024).

To allow for large-scale 3D flows, we have implemented the Black-Box Matrix-Matrix (BBMM) algorithm pioneered by GPyTorch, which allows for exact GP inference on millions of training points, and parallelizes to muli-GPU architectures (J. R. Gardner et al., arXiv:1809.11165, 2018). This posed significant difficulties, as it required us to rewrite the algorithm in terms of pure/stateless functions, to be JAX-compatible. We tested our implementation on a simple GP regression problem: learning a 1D sinusoidal function. We validated our BBMM implementation against GPytorch's BBMM, as well as a standard Cholesky decomposition. As shown in Fig. 4, running on a single NVIDIA A100 GPU (Wisteria/BDEC-01), our JAX implementation can be faster than GPyTorch, at least for large problems.

5.3 Learning Efficient Swimming Strategies

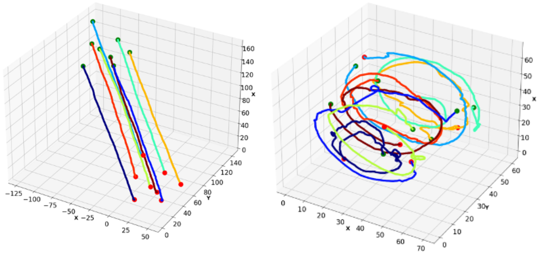

Fig. 5 Simulation snapshots for "smart" microswimmers tasked with maximizing (left) polar order and (right) vortex order.

We have extended and improved upon our combined RL/Direct Numerical Simulation approach to solve for the optimal control of swimmers navigating complex flows [1]. For this, we have used Deep Q-Learning (as implemented in Pytorch), coupled to direct numerical simulations of spherical swimming particles, within the canonical squirmer model (as implemented in Kapsel). We train the swimmers to navigate non-uniform flows using local hydrodynamic signals. As in our previous work, the swimmers possess surface sensors that measure hydrodynamic force signals, which they use to select an optimal strategy (i.e., rotation). However, in contrast to our previous model, we now include the torque free constraint on the swimmers by using a squirmer that is capable of autonomous rotations around its body axes (no longer requiring an external torque). We have trained a collection of swimmers to maximize various order parameters, targeting different types of collective motion. In this way, we are able to obtain non-trivial collective behavior (see Fig. 5), for different types of swimmers.

6 Self-review of Current Progress and Future Prospects

For theme (A), we have successfully improved upon our learning method by incorporating the principal of material objectivity. This allows us to achieve good quantitative performance on complex 2D flow simulations, as compared against full MSS. For theme (B), we have extended our probabilistic Stokes flow framework to 2D/3D, incorporating stress and force inferences. Furthermore, we have shown that our method outperforms alternative ML approaches, i.e., Physics-Informed Neural Networks. We have also implemented the BBMM algorithm used by GPytorch for large-scale GP inference, but the performance is still sub-optimal. For theme (C), we have successfully developed a Reinforcement Learning protocol capable of teaching force/torque free swimmers to collectively navigate non-homogeneous flows using only local hydrodynamic signals.

Our research plan for FY2024 will continue to develop these themes. For theme (A), we will improve our learning method to provide fast and quantitative predictions for complex 3D flows of entangled polymer melts. Furthermore, we will continue with our effort to port the code entirely to GPUs. This will allow us to perform simulations of the complex processing flows used in industry. For theme (B), will investigate why the BBMM method does not provide any significant speedup on our specific physics-informed GP regression (it's currently slower than a Cholesky based calculation). Our goal is to allow for large scale 3D systems with moving boundaries to analyze PIV data. Finally, for theme (C) we will continue to investigate how ML can be used to solve complex Optimal Control problems.

7 List of publications and presentations

Journal Papers (Refereed)

[1] K. Sankaewtong, J. J. Molina, R. Yamamoto, "Autonomous navigation of smart microswimmers in non-uniform flow fields", *Physics of Fluids*, **36**, 041902 (2024)

[2] M. Dixit, T. Taniguchi, "Effect of Impurities on the Formation of End-Group Clusters in Natural Rubber: Phenylalanine Dipeptide as an Impurity Protein", *Macromolecules*, **57**, 2588–2608 (2024)

[3] J. J. Molina, K. Ogawa, T. Taniguchi, "Stokesian Processes : inferring Stokes flows using physics-informed Gaussian Processes", *Machine Learning: Science and Technology*, **4**, 045013 (2023).

[4] X. Yan, S. Miyamoto, T. Taniguchi, "Machine-learning based multi-scale simulation for polymer melt-spinning process", *Nihon Reoroji Gakkaishi* (Journal of the Soci-

ety of Rheology, Japan), **51**, 281-294 (2023)

[5] M. Dixit, T. Taniguchi, “ Role of Terminal Groups of cis-1,4-Polyisoprene Chains in the Formation of Physical Junction Points in Natural Rubber”, *Biomacromolecules*, **24**, 3589-3602 (2023)

[6] S. Miyamoto, J. J. Molina, T. Taniguchi, “Machine-Learned constitutive relations for multi-scale simulations of well-entangled polymer melts”, *Phys. Fluids*, **35**, 063113 (2023) -Editor’s Pick-.

Proceedings of International Conference Papers (Refereed)

[7] S. Miyamoto, “Short Review on Machine Learning-Based Multi-Scale Simulation in Rheology”, *Nihon Reoroji Gakkaishi*, **52**, 15-19 (2024)

Presentations at International conference (Non-refereed)

[8] S. Miyamoto, Y. Ueno, T. Taniguchi, J. J. Molina(*), “Bayesian Machine Learning for Multi-Scale Simulations of Polymer Flows”, International Congress on Rheology (ICR2023), 2023

[9] J. J. Molina(*), S. Miyamoto, Y. Ueno, T. Taniguchi, “Machine Learning for accelerated Multi-Scale Polymer Flow Simulations”, 10th Ingernational Congress on Industrial and Applied Mathematics (ICIAM2023), 2023

[10] J. J. Molina(*), K. Ogawa, T. Taniguchi, “Stokesian Processes: Physics Informed Machine Learning for Soft Matter Flows”, The 7th International Soft Matter Conference (ISMC2023), 2023

Presentations at domestic conference (Non-refereed)

[11] S. Miyamoto(*), J. J. Molina, T. Taniguchi, “構成関係の機械学習回帰モデルを用いた高分子溶融体の流動予測シミュレーション”, 日本流体力学会年会 2023, 2023

[12] S. Miyamoto(*), J. J. Molina, T. Taniguchi, “Flow simulations of well-entangled polymer melts using machine-learned constitutive relations”, 第 71 回レオロジー討論会, 2023

[13] K. Ogawa(*), J. J. Molina, T. Taniguchi, “Inferring Stokes Flows using Physics-Informed Gaussian Processes”, 第 71 回レオロジー討論会, 2023

[14] J. J. Molina(*), K. Ogawa, T. Taniguchi, “Physics Informed Machine Learning for Soft Matter Flows” アクティブマター研究会 2024, 2024

Published open software library and so on

None.

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

None.