

Development of physics informed machine learning for soft matter : polymer flows and beyond



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Abstract

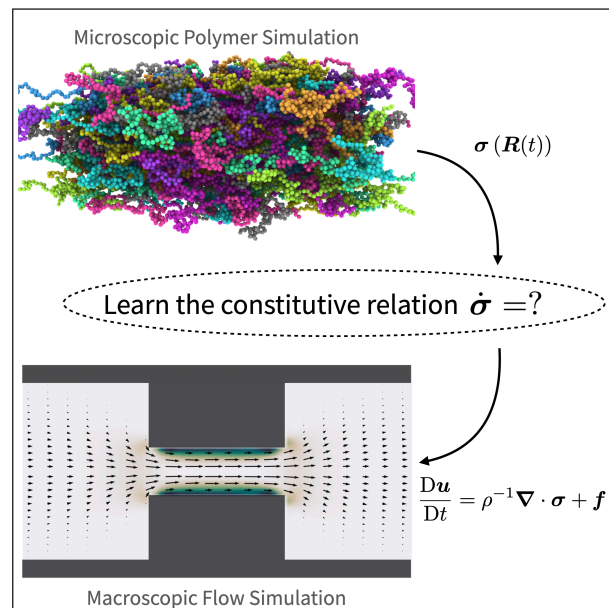


Fig. 1. Schematic representation of proposed learning. Given a microscopic model, we wish to infer the appropriate constitutive relation.

Soft Matter systems are characterized by a **hierarchy of length- and time-scales**, in which the dynamics of the **microscopic constituents** are intricately coupled to the **macroscopic dynamics**. Examples include colloidal dispersions, cellular tissues, and polymeric materials, among others. Due to their significance for material science, we focus here on polymer melt flows, although the methods we develop can be extended to other systems.

The **traditional approaches** used to tackle such problems are : (1) a **Multi-Scale Simulation (MSS)** [1,2], in which the micro/macro coupling is added explicitly, or (2) a fully **macroscopic description** using a specific constitutive relation. The former is incredibly expensive, while the latter often lacks a theoretical foundation.

Our goal is to **develop physics informed Machine Learning (ML)** methods to **learn the constitutive relation** for the stress of **polymeric flows with memory**[3,4]. This will allow us to drastically reduce the calculation time compared to state-of-the-art Multi-Scale Simulations, while still maintaining their superior accuracy. We have used a Gaussian Process regression scheme, which allows us to account for missing and/or noisy data, and naturally fits within a principled Bayesian framework.

Model

Macroscopic Flow

We use a Smoothed Particle Hydrodynamics (SPH) description to model the flow[5]. The fluid is discretized into fluid particles carrying mass, momentum, energy, etc. The momentum equation for the i -th particle is

$$\rho_i \frac{\partial v_i}{\partial t} = \nabla \cdot [\sigma_i - P_i \mathbf{I}] + \mathbf{F}_i$$

$$\nabla \cdot \mathbf{u} = 0$$

ρ : density
 \mathbf{v} : velocity
 $\boldsymbol{\sigma}$: stress-tensor
 \mathbf{F} : body-force
 P : pressure

Microscopic Polymer Dynamics

We use the dual-slip link model originally developed by Doi and Takimoto[6], which accounts for polymer entanglement. The

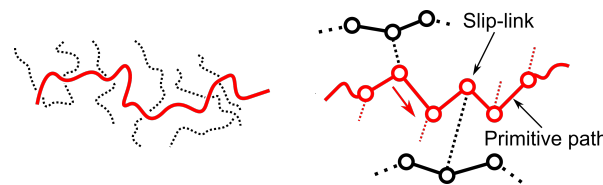


Fig. 2. Representation of the Doi-Takimoto dual slip-link model.

entangled polymer chain is represented as a primitive path with slip-links. The primitive path corresponds to the limited motion area of the chain, whereas a slip-link is the entanglement point that couples with a slip-link on another chain. The model includes three different relaxation mechanisms of polymer melts

- Contour Length Fluctuations
- Reptation
- Constraint Renewal (of slip-links)

The polymer chain length L relaxes according to

$$\frac{dL}{dt} = -\frac{1}{\tau_R} (L - L_{eq}) + \left(\frac{dL}{dt} \right)_{\text{affine}} + g(t)$$

and the stress is derived from the entropy elasticity

$$\sigma^{\alpha\beta} = \sigma_e \left\langle f_{\text{FENE}} \frac{r^\alpha r^\beta}{a|r|} \right\rangle, \alpha, \beta \in \{x, y, z\}$$

Gaussian Process (GP) Regression

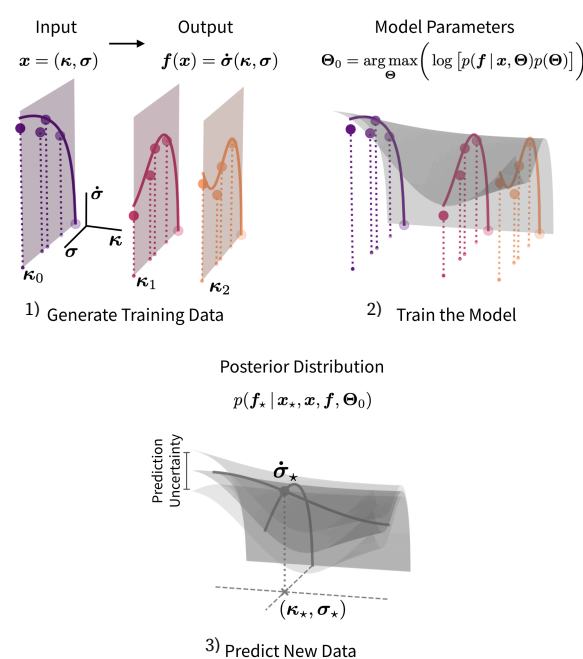


Fig. 3. Scheme used to learn the constitutive relations for the stress of polymer melt flows[4].

Let f_1 and f_2 denote two arbitrary functions. Without loss of generality, we can place a GP prior on the joint distribution, such that[7]

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \right)$$

$$f_1 | f_2 \sim \mathcal{N} \left(\boldsymbol{\mu}_1 + \mathbf{K}_{12} \mathbf{K}_{22}^{-1} (f_2 - \boldsymbol{\mu}_2), \mathbf{K}_{11} - \mathbf{K}_{12} \mathbf{K}_{22}^{-1} \mathbf{K}_{21} \right)$$

with $\boldsymbol{\mu}$ the average, and \mathbf{K} the covariance matrices. If f_2 is known, we use this information to update our conditional distribution for f_1 . This conditional distribution is yet another GP. Here, f_1 and f_2 correspond to the training and test stresses, respectively

Research Plan

Our research is divided into four themes / components:

- MSS validation** : Parallelize / Optimize our current MSS code to scale up to $\approx 10^5$ fluid particles in 3D. This is necessary to validate our ML approach.
- Constitutive Equation Learning** : Learn the Doi-Takimoto constitutive relation to simulation entangled polymer melts.
- Polymer Processing Flows** : Used the learned constitutive relations (B) to simulate processing flows used in industry. Results will be validated against full MSS (A).
- Soft Matter Extensions** : Extend our study to learn the constitutive relation of colloidal dispersion / cellular tissues.

The goal of this JHPCN project is to accelerate / optimize each of these components, where possible by moving most of the calculations to GPUs.

Preliminary Results

Doi-Takimoto model + Planar Poiseuille Flow

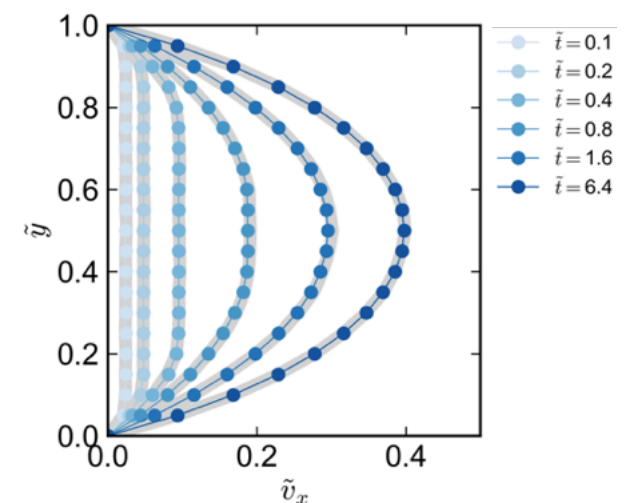


Fig. 4. MSS (solid) vs GP-MSS results (symbols).

MSS Parallelization & Optimization

Original Code	Memory Optimization	OMP/ACC Parallelization
1.0	0.54	<i>in progress</i>

(smaller is better)

Acknowledgements

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