Machine Learning for Soft Matter Flows (JH220054)

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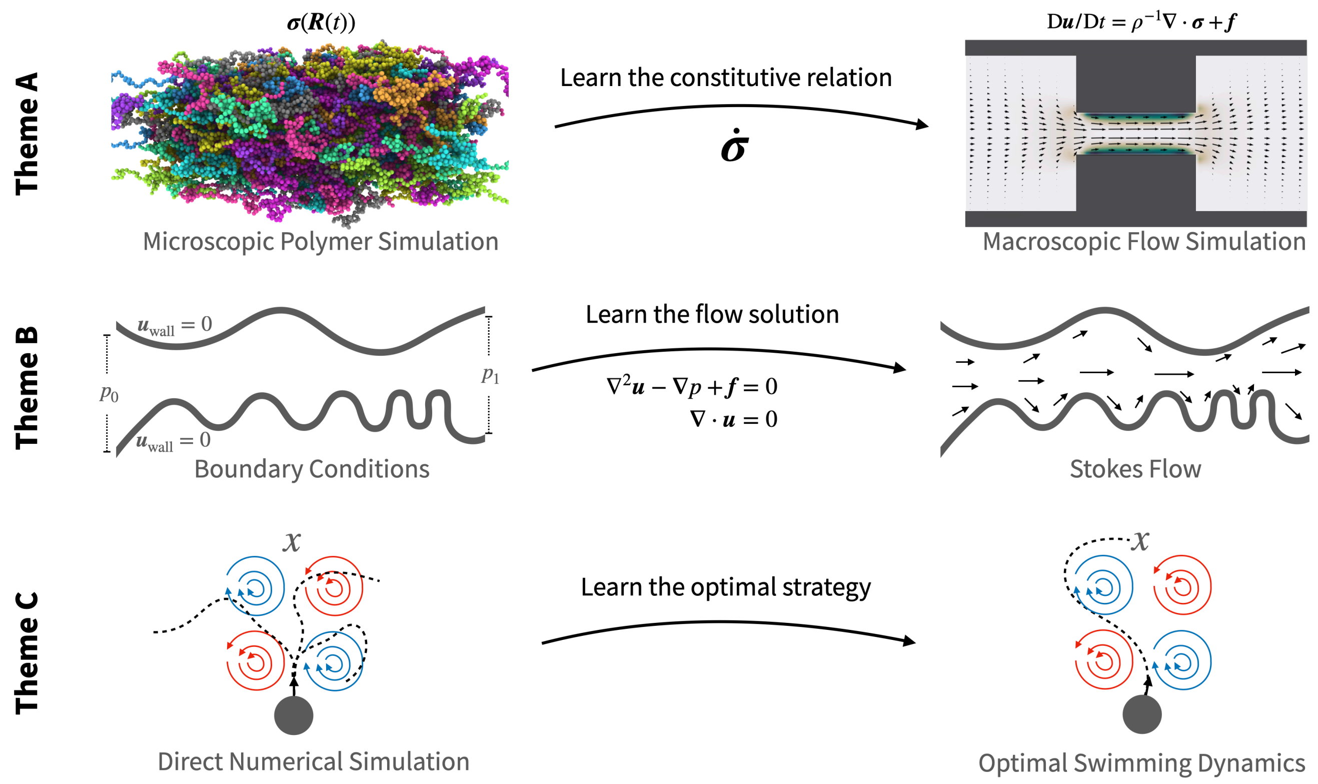

Fig. 1. Schematic representation of the three different flow problems (themes) and learning we will consider. (A) Learning constitutive relations of entangled polymer flows for accelerated Multi-Scale-Simulations, (B) learning the solutions to the Stokes flow problem, and (C) learning optimal control strategies for microswimmers.

Abstract

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 dispolymeric materials, colloidal dispersions, and cellular tissues, among others. Our goal is to develop **physics informed Machine Learning** (ML) methods to solve several characteristic flow problems encountered in Soft Matter: (A) Learning the constitutive relation of entangled polymer melts, (B) learning solutions to the Stokes flow equation, and (C) learning efficient swimming strategies for active particles navigating complex flows.

Theme A is focused on learning constitutive relations to accelerate multi-scale simulation methods, with the hope of better understanding and optimizing polymer processing flows used in industry. Theme B is focused on developing a general Stokes flow solver, to be used for systems with complex fluids and boundaries, as well as noisy/missing data, where traditional methods fail. Theme C is focused on understanding how the collective dynamics of hydrodynamically interacting particles emerges from low-level individual behaviours.

Principal Models & Methods

Gaussian Process (GP) Regression

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 the probability of observing both f_1 and f_2 is[1]

$$\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} K_{11} & K_{12} \\ & K_{22} \end{bmatrix}\right)$$

with $\boldsymbol{\mu}$ the average, and $\boldsymbol{K}$ the covariance matrices. If f_2 is known, we can use this information to update our conditional distribution for f_1. This conditional distribution is another GP.

$$f_1 \,\big|\, f_2 \sim \mathcal{N}\left(\mu_1 + K_{12}K_{22}^{-1}(f_2 - \mu_2), K_{11} - K_{12}K_{22}^{-1}K_{21}\right)$$

Since GP are closed under linear operations, we can incorporate knowledge of the physics of our problem in the structure of the GP. For Stokes flow, this gives rise to the following GP

$$\boldsymbol{g} \equiv \nabla^2 \boldsymbol{u} - \nabla p + \boldsymbol{f} = 0 \qquad \nabla \cdot \boldsymbol{u} = 0$$

$$\begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \\ \boldsymbol{g} \\ \nabla \cdot \boldsymbol{u} \end{bmatrix} \sim \mathcal{N}\left(\boldsymbol{0}, \begin{bmatrix} K_{uu} & K_{up} & K_{ug} & K_{u\nabla\cdot u} \\ & K_{pp} & K_{pg} & K_{p\nabla\cdot u} \\ & & K_{gg} & K_{\nabla\cdot u\nabla\cdot u} \end{bmatrix}\right)$$

from which we can compute the posterior distribution for the velocity $\boldsymbol{u}_d$ and pressure $\boldsymbol{p}_d$ fields inside the domain, conditioned on the velocity $\boldsymbol{u}_b$ (pressure $\boldsymbol{p}_b$) at the boundaries, together with the enforcement of the Stokes ($\boldsymbol{g} = 0$) and incompressibility ($\nabla \cdot \boldsymbol{u} = 0$) conditions. All correlation matrices can be expressed in terms of K_{uu}, K_{up}, and K_{pp}.

$$\boldsymbol{u}_d, \boldsymbol{p}_d \,\big|\, \boldsymbol{u}_b, \boldsymbol{p}_b, \boldsymbol{g}, \nabla \cdot \boldsymbol{u} \sim \mathcal{N}(\boldsymbol{\nu}, \boldsymbol{\Sigma})$$

Macroscopic Flows

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

$$\rho_i \frac{\partial \boldsymbol{v}_i}{\partial t} = \nabla \cdot \left[\boldsymbol{\sigma}_i - P_i \mathbf{I}\right] + \boldsymbol{F}_i \qquad \nabla \cdot \boldsymbol{u} = 0$$

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

For the coupled particle-fluid simulations (C) we use the Smooth Profile Method[2] to solve the full Navier-Stokes equation

$$\partial_t \boldsymbol{u} = -\rho^{-1}\nabla p + \rho^{-1}\eta \nabla^2 \boldsymbol{u} + \phi_p \boldsymbol{f}$$

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

with ρ and η the density and viscosity of the host fluid, respectively, and $\phi_p \boldsymbol{f}$ a constraint force to enforce particle rigidity.

Microscopic Polymer Dynamics

We will learn the constitutive relations of non-isothermal and isothermal flows. While special focus will be given to the Doi-Takimoto (DT) dual-slip link model, the canonical polymer entanglement model, we will also consider Dumbbell/Rouse and Kremer-Grest models. In the DT model, the 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 several different relaxation mechanisms and has shown excellent predictive capabilities[3].

Research Plan

(A) **Learning constitutive relations of entangled polymers**: Extend our learning method to entangled polymer melt[4]. Parallelize / Optimize our MSS code to to scale up to $\simeq 10^5$ fluid particles in 3D, to validate our learning. To allow for exact inference of 3D constitutive relations, with $10^3 - 10^6$ training points, we will implement GPyTorch's Black-Box Matrix Matrix multiplication (BBMM) algorithm into our custom GP+JAX code.

(B) **Learning solutions to the Stokes equation**: Use Physics Informed GP to perform one-shot learning of Stokes flow problems. The underlying GP covariance matrix, specifying correlations between velocities, pressures and forces contains fourth-order kernel derivatives, for which we will use JAX's automatic differentiation + JIT capabilities. Perform exact inference of 3D flows again requires the use of BBMM (A).

(C) **Learning optimal swimming strategies**: Use a combined deep Q-Learning + hydrodynamics solver to learn the optimal control strategies for swimmers in complex flows. This requires that we implement force (torque) free actions that the swimmer can take in response to covariant measurements of physically meaningful local variables.

Preliminary Results

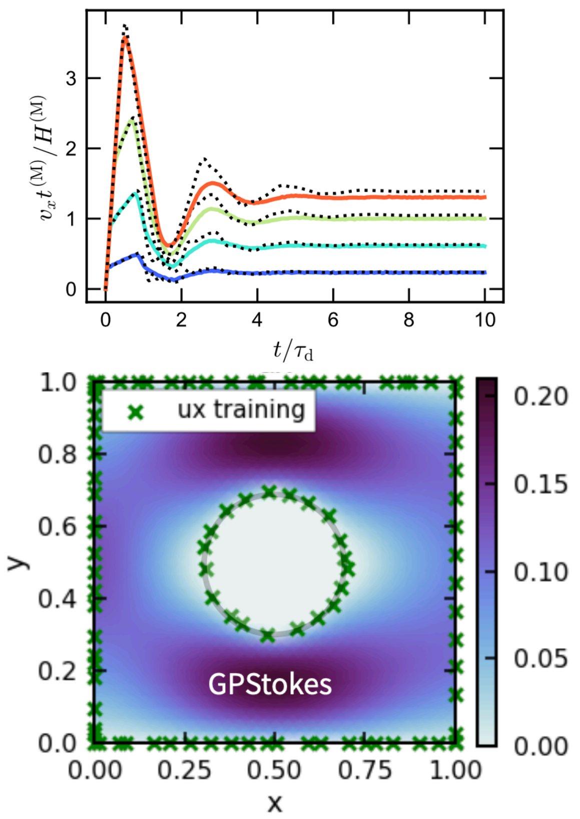

Fig. 2. (top) Poiseuille flow through a channel using full MSS (dotted) and GPMSS (solid) for different positions. (bottom) GPStokes prediction for 2D pressure driven flow past a cylinder.

Acknowledgements

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