Learning the constitutive relation of non-newtonian fluids with memory

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【はじめに】**Describing the dynamics of polymeric flows is a challenging problem due to the separation of length- and time-scales between the microscopic dynamics of the polymer chains and the macroscopic dynamics of the flow. The current state-of-the-art techniques resort to Multi-Scale Simulation Methods in which both degrees of freedom are coupled to each other. However, this requires incredible computational costs. In this study, we extend a recently developed learning strategy to polymeric systems with memory. We use training data obtained at the microscopic scale to learn the corresponding constitutive relation. This allows us to solve for the (fast) macroscopic model, while still maintaining the necessary microscopic information.`**

【結果と考察】

The current standard approach for studying polymeric flows is to use a Multi-Scale Simulation Method (MSS) to directly couple the microscopic and macroscopic degrees of freedom through the stress and strain rate fields. This can be achieved, for example, by employing Lagrangian fluid particles containing polymer chains(1). Instead, we propose to use the microscopic model to "learn" the corresponding constitutive relation. This constitutive relation can then be used to perform macroscopic flow simulations, without having to consider the microscopic degrees of freedom explicitly, but still maintaining the appropriate information about the stress/strain relationship.

This learning strategy was first proposed by Zhao et al.(2) to consider Non-Newtonian flows, but memory effects were not taken into account. In this work, we show how to extend this procedure to include memory effects and thus consider more realistic polymeric flows. Using a suitable microscopic model of the polymer chains, simulations at fixed strain-rate ($\dot{\gamma}$) are performed to generate training data consisting of stresses (σ) and their time-derivatives ($\dot{\sigma}$). This training data ($\dot{\gamma}$, σ, $\dot{\sigma}$) is then used within a Gaussian-Process Regression (GPR) to infer the constitutive relation, i.e., $\dot{\sigma}(\dot{\gamma}, \sigma)$. This constitutive relation can then be used to predict how the stresses in the fluid are changing in time. We note that (a) no assumptions are made regarding the functional form of the constitutive relations, and (b) at the end of the training we cannot say what the functional form is, but we can predict the value of $\dot{\sigma}$ given the values of $\dot{\gamma}$ and σ. To validate the method, we used Hookean dumbbells as our microscopic polymer chain model, and considered the case of simple-shear flow between flat parallel plates, which is effectively a 1D problem, for which analytic solutions are known. We obtained very good quantitative agreement with the MSS results at a fraction of the cost (3). Current work is underway to consider more complicated flows (e.g. contraction-expansion), for which all components of the stress-tensor are required.

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【参考文献】

(1) T. Sato, K. Takase, and T. Taniguchi. J. Soc. Rheol. Jpn. 44, 265 (2016)
(2) L. Zhao, Z. Li, B. Caswell et al., J. Comp. Phys. 363, 116 (2018).
(3) N. Seryo, T. Sato, J. J. Molina, T. Taniguchi, in preparation.