Mathematics, Methods, and Models for Data-Driven Rheology

by

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While data-driven tools and techniques have revolutionized much of the scientific and engineering landscape, they have yet to make a substantial impact in the field of rheology. Rheological data sets are at once too scarce and too diverse to enable traditional machine learning approaches — their scarcity a reflection of the time- and material-intensive nature of bulk rheometry, and their diversity a product of the many rheometric protocols and tools used to characterize the hereditary behavior of complex fluids. In this thesis, we explore methods and models that combine domain knowledge curated over the nearly century-long history of rheology with modern advancements in data science and machine learning, whose aim is to maximize the utility of the available rheological data and rheometric tools. Essential to each of the methods and models developed in this thesis is a solid mathematical foundation that elucidates the unique nature of rheological data, without which the machine learning techniques could not take firm hold. These Mathematics, Methods, and Models for Data-Driven Rheology promise to advance the field of rheology, and the engineering of complex fluid and soft solid systems, in several ways.

In the first part of this thesis, we derive a new mathematical construction for asymptotic nonlinearities in simple shear flows, called Medium Amplitude Parallel Superposition (MAPS) rheology. Based on a polynomial expansion of the general time-invariant functional relationship between shear stress and strain (or strain rate) in simple shear flows, MAPS reveals a common embedding for many previously disconnected data sets. This asymptotic framework enables direct comparisons of constitutive model predictions with a variety of experimental data, and facilitates data-driven studies throughout the remainder of this thesis.

In the second part of this thesis, we develop a novel data-rich experimental method for weakly nonlinear rheology, which uses three superposed oscillatory tones to obtain high-throughput measurements of a MAPS response function. We present applications of this technique to robust parameter identification within physically motivated constitutive equations, and to data-driven monitoring of rheological transitions within a vitrifying clay dispersion. We next derive an automated method for the analysis of rheological data, based on the longstanding technique of superposing parametrically self-similar data sets. We validate this statistically robust technique, which employs machine learning to automate various types of data superposition tasks, on a broad range of data drawn from the rheological literature.

In the final part of this thesis, we propose a general modeling framework that encapsulates many well-known viscoelastic constitutive equations. This model formulation incorporates an arbitrary tensor-valued function of the stress and rate-ofdeformation tensors into a "generalized nonlinear Maxwell model". The medium amplitude behavior of this model reveals a data-driven framework for constitutive model selection using MAPS rheology, which can accommodate both shear and normal stress data as well as multiple relaxation modes. We then consider a machine learning surrogate for the arbitrary tensor-valued function, and demonstrate that such a machine learning approach can rapidly generate accurate and generalizable models from limited experimental data. By design, these models are highly extensible and directly amenable to three-dimensional simulations of industrially relevant flows, and may therefore facilitate the rapid design and engineering of processes involving complex fluids.

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