論文の内容の要旨

Data-driven approach and numerical simulation for reproduction and measurement of complex fluids

（データ駆動的アプローチと数値計算による複雑流体の再現と計測）

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In this thesis, we perform the analyses related to the reproduction and measurements of various fluids classified as a complex fluid having interesting properties, solid-like behavior, and nonlinear viscosity, e.g., sauces, creams, and pastes from the perspective of micro or macro, by effective use of the data-driven approach and the numerical simulation.

A wide variety of fluids can be seen around us in various fields and regions, such as food production, daily commodities, biological body, and natural landscape. We make use of these in our daily lives by measuring, reproducing, and understanding their physical property. There are simple fluids with constant viscosity in the fluids around us, e.g., water and honey. However, some fluids have more interesting properties. For example, viscosity nonlinearly changed depending on the shear rate related to the flowing velocity (e.g., sauce, lubricant) and behaving like a solid (e.g., cream, form). These characteristic phenomena, which are nonlinear viscosity and solid-like behavior, are known to be due to some inclusion of internal elements such as colloids and polymers in the fluid, and these fluids are categorized as complex fluids. We will focus on the nonlinear viscosity and solid-like properties as the characteristic properties of complex fluids to be analyzed and investigate the reproducing and measurements for these properties.

In analyzing the complex fluids, the parts that can be simplified and coarse-grained are modeled and then reproduced using numerical simulation. On the other hand, when the internal structure or mechanism is an unknown or a black box, a data-driven fitting approach is used. In this thesis, these two approaches, the numerical simulation and the data-driven approach, are smartly used for the target to be analyzed, we thus would like to obtain new knowledge and methods for handling more complex fluids. It also aims to investigate the knowledge and methodologies that can be applied to as broad a class of complex fluids as possible, rather than limiting the class of fluids with certain internal elements, structures, and properties.

In the context of reproducing the solid-like behavior, we explored the limits of reproducing the solid-like behavior of complex fluids and the uncleared physical behavior occurring around them. It is well known that the existence of solid-like behavior, in a form and paste, is due to the jamming transition phenomenon, which depends on the density of particles as internal elements in the fluid. The Reversible-Irreversible (RI) transition, which is related to the reversibility of particle trajectories in the oscillatory sheared system, has been reported to be qualitatively different in the high-density and low-density regions, implying a connection with the jamming phenomenon. In this thesis, a numerical simulation of a simple particle system as an athermal colloidal suspension was performed under various density conditions around the jamming transition density and shear amplitude to obtain exhaustive data. We obtained a phase diagram covering the intermediate density region for the RI transition and the relationship between the RI transition and solid-like behavior from these data. We also observed the existence of nontrivial RI transitions and nonlinear elastic behavior in the region below the jamming density, indicating the existence of a richer physical property. In addition, we found that the RI transition and solid-like behavior are related and can be described by the contact number reflecting the mesoscopic structure of the particle system.

In the context of reproducing the nonlinear viscosity, we aim to find a method for reproducing and estimating the nonlinear viscosity of the complex fluid mixture, including various classes of fluids mixture as possible, irrespective of the internal elements and the structure. From a macroscopic perspective, we can consider the complex fluid with disorder internal elements as a homogeneous fluid with a (nonlinear) flow curve representing the physical property of flowing. We observed that the Harshall-Bulkley model could represent the flow curves of various pure fluids and their mixtures. Hence, as a blending model that reproduces the physical properties of mixtures, we considered a new model that reproduces the physical properties of mixtures from the physical properties of individual pure fluids and the mixing ratio, which is closed by the parameters of the Harshall-Bulkley model. In order to consider the blending model, we introduced the laws of blending and a general blending model satisfying these laws. Using a data-driven approach, we chose the proposed model. We showed that the model exists that can qualitatively reproduce the characteristic behavior of a mixture of various fluids combinations within the general blending model. In addition, macroscopic simulations of mixtures were performed using our proposed model and compared with real experiments to verify the effectiveness of our model.

In the context of measuring the complex fluid, we proposed a video-based measurement method for conveniently measuring the flowing behavior of complex fluids that non-specialists can use. Although fluids with various and rich properties are very familiar to us, the method to measure with accurate them is not common because it requires a mechanical experimental device called a rheometer, which is expensive and needs expert knowledge. A physical property measurement corresponds to the inverse problem of the forward problem of reproducing a certain physical property. We interpret the existing video-based viscosity measuring method for Newtonian as a method based on the numerical solution of the inverse problem by combining a fluid simulation and optimization. Extending it to the complex fluids as the Herschel-Bulkley model, we proposed a method for estimating and measuring the flow curve of various classes of complex fluids from the experimental videos. In addition, we proposed a method to evaluate effective experimental setups to capture the fluid video for estimation and to select new setups. We validated the effectiveness of our method by using the artificial data and real data.