Conference of the Japan Society of Microgravity Application

PS07

データ同化による塗膜物性値の複数同時推定

Simultaneous estimation of multiple coating film properties by data assimilation

小山翔太郎[1], 茂木 涼[2], 石澤 翔[1], 白鳥 英[2]
Syoutarou KOYAMA[1], Ryou MOTEGI[2], Kakeru ISHIZAWA[1], and Suguru SHIRATORI[2]

[1] 東京都市大学大学院, Graduate School, Tokyo City University
[2] 東京都市大学, Tokyo City University

1. Introduction

With the advancement of science and technology in the space environment, material and life sciences under microgravity are becoming increasingly important. In microgravity environments such as the International Space Station and on the lunar surface, surface tension-driven phenomena are more apparent than on the ground. Therefore, measuring surface tension is extremely important for understanding and controlling such phenomena. In addition to surface tension, fluid behavior is strongly affected by several physical properties like viscosity, density, and the diffusion coefficient. Although it is necessary to obtain a complete set of these physical properties, conventional measurement methods require individual equipment and advanced measurement techniques for each property, resulting in huge cost and effort.

This study proposes a new method for estimating physical properties by combining a Physics-Informed Neural Network (PINN)1), a machine learning approach based on physical laws, with data assimilation. PINN enables the easy prediction of liquid behavior and the calculation of physical property gradients necessary for data assimilation. In this study, we developed a system that uses PINN and data assimilation to estimate multiple physical properties, such as surface tension and viscosity, from a single type of measurement data—specifically, the spatiotemporal variation of a liquid film. We then report on the measurement accuracy of this system.

2. Approach

This study proposes a method to estimate the physical properties of the liquid from measured data by combining PINN and data assimilation. Although the concept and basic validation have been carried out in our previous study 2), their validation was limited to the twin experiment using synthetic data. This study aims to validate our proposed method for the real experimental data. The key to estimating physical properties with data assimilation is to accurately capture changes in film thickness from the spatiotemporal variations of the liquid film. To do this, we utilize thin-film interferometry with a hyperspectral camera as a fast, non-contact, optical 3D measurement technique suitable for liquid films.

In the experiment, silicone oil with known physical properties is coated onto a silicon wafer, and the relaxation process of the liquid film's shape is observed after a droplet is dispensed onto the wafer. This is a dynamic phenomenon where the influence of physical properties is noticeable, and we can measure these dynamics with high accuracy, non-contact, and over a wide spatial range in a short time. Using a hyperspectral camera and a halogen light source, the thickness distribution of the liquid film can be recovered as a time series from the interference fringes of the reflected light, based on the principle of thin-film interference.

The measured film thickness, along with its corresponding position and time information, is then used as observation data for data assimilation. Specifically, the trained PINN predicts film thickness using time, space, and physical property values such as surface tension and viscosity coefficient as input parameters. The physical properties are updated via data assimilation to minimize the loss function, which is defined by the error between the film thickness predicted by the PINN and the film thickness values from the measured data. The automatic differentiation of the PINN enables efficient gradient calculation for this loss function, thereby allowing for the simultaneous estimation of surface tension and the viscosity coefficient. This makes it possible to easily and accurately identify multiple physical properties of a liquid from a single measurement system.

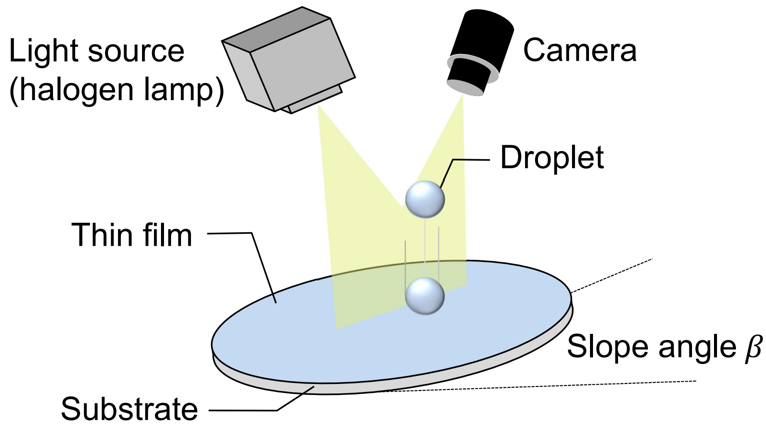

Figure 1. Experimentation image. Film thickness fluctuations are photographed when droplets dropped to the thin film.

In this study, the following two-dimensional and three-dimensional gradient-extended governing equations for liquid film flow are used to train the PINN as a predictor of film thickness h.

$$\frac{\partial H}{\partial T} = -\frac{\partial}{\partial X}\left[H^3\frac{\partial^3 H}{\partial X^3} - BoH^3\frac{\partial H}{\partial X}\right], \tag{1}$$

$$\frac{\partial H}{\partial T} = -\hat{\mu}_{inv}\bar{\nabla}\cdot\left[\hat{\sigma}H^3\bar{\nabla}\bar{\nabla}^2 H - BoH^3\bar{\nabla}H + Bo_h H^3\boldsymbol{e_x}\right] \tag{2}$$

Equations (1) and (2) are partial differential equations that represent the time evolution of the film thickness distribution under the influence of Laplace pressure and gravity. Equation (2) represents a three-dimensional state to allow the physical model to reproduce the actual phenomenon. In Eq. (2), the gravity term is decomposed into two components: one in the direction of inclination and the other in the direction of film thickness, because the measured data is acquired from a droplet dropped on an inclined surface with an angle β, as shown in **Fig. 1**. H, T, and X are non-dimensionalized film thickness, time, and coordinates, respectively, and Bo is the Bond number. Here, $H = h/h_0$, $T = t/t^*$, $X = x/L$, $t^* = 3\mu L^4/\rho g h_0^3$, and, σ, μ, ρ and g are surface tension, viscosity, density, gravitational acceleration, respectively. In addition, L, h_0, and t^* are non-dimensionalized as the coefficients of representative length, length in the thickness direction, and time, respectively. If the coefficients are in the denominator when fitting the coefficients during learning using PINN, the learning may fail because the solution diverges when the coefficients reach 0. This is why $\hat{\mu}$ is defined as the reciprocal $\hat{\mu}_{inv}$.

3. Results

Figure 2 shows a graph of the spatiotemporal variation of the liquid film's thickness, as acquired from the hyperspectral camera. As time progresses, the maximum film thickness relaxes to about half. Some observational data points are missing due to the effect of light reflection in areas where the liquid film's gradient is large.

Figure 3 shows the results of physical property estimation during PINN training, using the measured data in **Fig. 2** as the training data. The figure shows the relative physical properties of surface tension ($\hat{\sigma}$) and viscosity ($\hat{\mu}_{inv}$) after 5 million learning epochs, relative to their initial true values.

4. Conclusion

In order to establish a new method for estimating physical properties by combining learned PINN and data assimilation, we constructed a measurement system that can measure the spatiotemporal variation of film thickness and investigated the measurement accuracy. The viscosity tended to converge to the true value, but the surface tension tended to be slightly higher than the true value. Future tasks include clarifying the

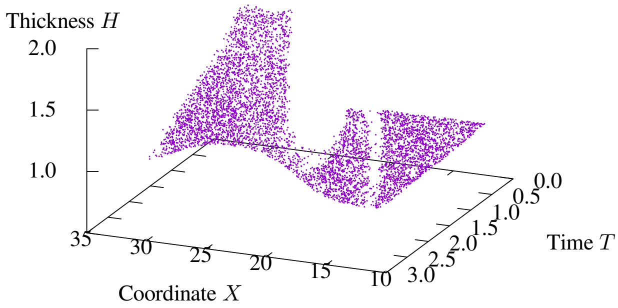

Figure 2. Observation point for actual measurement data.

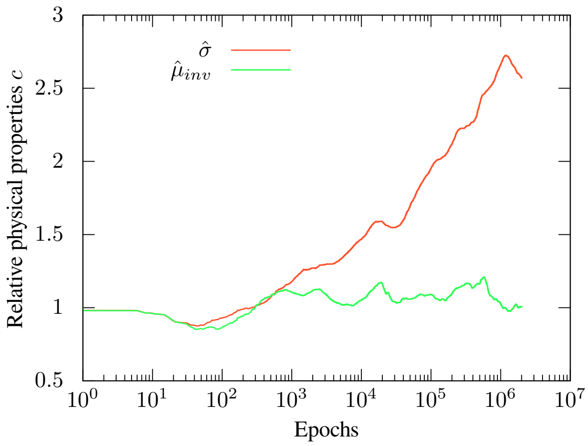

Figure 3. The History of physical properties after 5,000,000 learning cycles.

cause of data loss due to the influence of light reflection, based on the light's wavelength and the amount of reflected light. We also aim to improve estimation accuracy by refining the droplet shape and acquiring a more comprehensive picture of the relaxation behavior.

Acknowledgments

This work was supported by JSPS KAKENHI Grant Number JP22K03909 and JP23KK0262.

References

1) M. Raissi, P. Perdikaris and G. Karniadakis: Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, **378** (2019) 686, DOI: 10.1016/j.jcp.2018.10.045.
2) K. Ishizawa, S. Yamashita, S. Shiratori, H. Nagano and K. Shimano: Data assimilation based on pretrained physics-informed neural networks, Modelling, Data Analytics and AI in Engineering (MadeAI 2024) (2024).