JASMAC Conference of the Japan Society of Microgravity Application

PS22

動的濡れに対するPhysics-informed neural networkの適用
Application of Physics-informed neural network to dynamic wetting

田實 健人[1], 星山 敬利[1], 白鳥 英[2]
Kento TAJITSU[1], Keito HOSHIYAMA[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

In microgravity environments, surface tension becomes the dominant force governing fluid behavior, making wetting phenomena prominent. Therefore, the understanding and modeling of wetting are crucial for the control of liquid films in space applications. However, a complete physical model has not yet been established, especially for dynamic wetting, which is the focus of this study. It is known that at the microscale, an extremely thin liquid film, known as a precursor film 1), forms beyond the apparent edge of the visible liquid film. Within this film, a local force called disjoining pressure acts to maintain a constant film thickness, thereby determining the stability of the liquid film.

As a method for predicting such thin film flows, Physics-Informed Neural Networks (PINNs) 2), a machine learning technique constrained by physical laws, have garnered attention. However, the application of PINNs has thus far been limited to reproducing global physical phenomena, and there are no reports of their use in incorporating local physics, such as disjoining pressure. Therefore, the objective of this study is to verify whether a PINN can learn the local force term by applying it to the governing equation of thin film flow that includes disjoining pressure.

2. Approach

In this study, we applied a PINN to the governing equation of thin film flow including disjoining pressure to investigate its ability to learn local physics. As the problem setup, anticipating the future use of observational data for model acquisition, we considered the process of a liquid droplet flowing and relaxing on an inclined substrate, which is governed by

$$\frac{\partial h}{\partial t} = -\nabla \cdot \left[\frac{h^3}{3\mu} \left(\sigma \nabla \nabla^2 h - \rho g \nabla h \cos\beta + \rho g \sin\beta + \nabla \Pi \right) \right], \tag{1}$$

$$\Pi = \sigma \theta_e^2 \frac{(n-1)(m-1)}{2h_*(n-m)} \left[\left(\frac{h_*}{h} \right)^n - \left(\frac{h_*}{h} \right)^m \right], \tag{2}$$

where $\Pi, h(x,t), h_*, \sigma, \theta_e^2$ are the disjoining pressure, film thickness, precursor film thickness, surface tension, and equilibrium contact angle, respectively. For the disjoining pressure, we adopted an Lennard-Jones type model with the empirical exponents $n = 3$ and $m = 2$. The initial condition was a numerically given equilibrium droplet shape on a non-inclined substrate, and periodic boundary conditions were set.

Since the non-uniqueness of the solution to the governing equation complicates the learning process, we incorporated a volume conservation constraint into the overall loss function—in addition to the governing equation, initial, and boundary conditions common to PINNs—to guide the network towards a physically plausible solution. Furthermore, given that the influence of disjoining pressure is highly localized, we introduced an exponential exp activation function to enhance the model's sensitivity to sharp changes in film thickness, preventing this critical feature from being lost during training.

3. Results

The validity of the learning results was verified by comparing them with a numerical solution obtained via the Finite Difference Method (FDM). **Figure 1** shows selected snapshots (at time instants $t = 0, 2, 5, 10$)

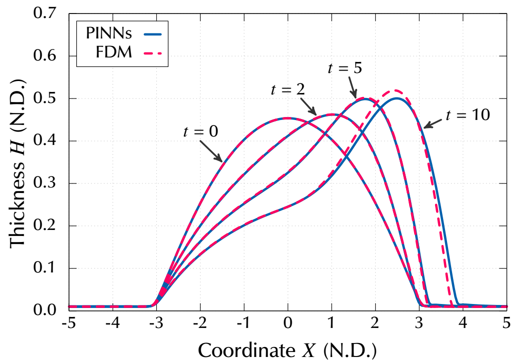

Figure 1. Selected snapshots of thickness distribution calculated by FDM (red dashed lines) and PINN (blue solid lines).

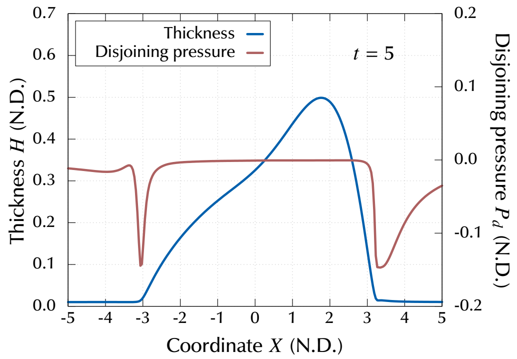

Figure 2. Spatial distribution of disjoining pressure predicted by disjoining pressure (red line) and thickness (bule point) at the $t = 5.0$

of the thiskness distribution calculated by the PINN and FDM. In the range of t =0.0–5.0, the PINN shows almost complete agreement with the FDM, successfully reproducing the contact line motion and the asymmetric deformation of the droplet. Figure 2 shows the film thickness and disjoining pressure distributions predicted by the PINN at $t = 5.0$. It is clear that the disjoining pressure value is large at points where the droplet's film thickness changes sharply. This indicates that the PINN is capable of properly predicting the local force of disjoining pressure.

Acknowledgments

This work was supported by JSPS KAKENHI Grant Number JP23KK0262. This research was conducted using the Supermicro ARS-111GL-DNHR-LCC and FUJITSU Server PRIMERGY CX2550 M7 (Miyabi) at Joint Center for Advanced High Performance Computing (JCAHPC).

References

1) L. W. Schwartz *et al.*: *Journal of Colloid and Interface Science*, Vol. 234, No. 2, pp. 363–374, 2001.
2) M. Raissi *et al.*: *J Comp Phys.* **378**, *686–707, 2019.*