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Physics-informed neural network を用いたガスジェット浮遊液滴周りの気流計算法

Prediction of flow around aerodynamically levitated droplets based on physics-informed neural networks

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1. Introduction

Sustainable human activities on the lunar surface are planned in the near future, and metal manufacturing technology using lunar regolith will be of significant importance. Preliminary numerical simulation must be efficient for saving resources and energy. Thus, it is essential to accurately measure the thermophysical properties of molten metal oxides, which are major components of lunar regolith. Although the aerodynamic levitation (ADL) method is considered potentially applicable, its reliability as a measurement method has not been fully established due to the lack of a mathematical model that can quantitatively describe the effect of surface deformation and droplet internal flow due to the aerodynamic pressure and shear force from external gas flow. To solve these problems, the authors' research group is trying to develop a mathematical model for time-averaged fields and disturbance fields deviated therefrom. The analysis of the latter oscillatory flows has been conducted in our previous study[1)]. This study is aiming to develop an efficient prediction procedure for the time-averaged flow fields.

In the ADL method, the location of the droplet is determined so that the total upward aerodynamic force is balanced with the droplet weight. The levitation force can be controlled by changing the gas flow rate. Even for the constant gas flow rate, the levitation force may change depending on the vertical location of droplets. Thus, there are multiple combinations for location and flow rate that satisfy the force balance. To find such balanced conditions by numerical simulation, a volume-of-fluid (VOF) can be considered as an appropriate method. However, finding many possible conditions of droplet location and gas flow rate requires huge computational time. To solve this problem, we apply physics-informed neural networks (PINNs), as recently proposed by Raissi et al.[2)]. The PINNs learn the solutions of a partial differential equation (PDE) for a given dataset. In the training process for a PINN, a loss function is defined as the mean square error of the predicted solutions of the PDE. To evaluate the loss function, the temporal and spatial derivatives of the unknowns are calculated by automatic differentiation (AD), which is implemented in the neural network (NN) framework. Once a PINN has been trained, the solutions for any time instance can be calculated directly without time integration by forward computation by the NN. In addition, the gradient of the solution with respect to the input variable can be calculated using AD. The methodologies of the PINN are based on supervised learning; nevertheless, it does not require supervisor data, because the supervisor is assigned to the governing equation which must equate to zero. Therefore, the PINN is expected to perform well with limited training data. The research group of this work applied the PINNs to the liquid film flow problem. The PDE under long-wave approximation contains 4th-order spatial derivative and 4th-order nonlinear term with respect to the Laplace pressure. Due to this term, some improvements are needed in the training of the PINNs[3)].

2. Problem formulation

Governing equations

We consider two-phase flows of incompressible Newtonian fluids of densities ρ_L, ρ_G and viscosities μ_L, μ_G. The subscripts L and G stand for liquid and gas, respectively. The surface tension of the liquid is defined as σ. The flow is governed by the conservation of mass and momentum

$$\frac{1}{r}\frac{\partial(ru)}{\partial r} + \frac{\partial w}{\partial z} = 0, \tag{1a}$$

$$\rho\left(u\frac{\partial u}{\partial r} + w\frac{\partial u}{\partial z}\right) = -\frac{\partial p}{\partial r} + \mu\left[\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial(ru)}{\partial r}\right) + \frac{\partial^2 u}{\partial z^2}\right] + \sigma\kappa n_r\delta_s, \tag{1b}$$

$$\rho\left(u\frac{\partial w}{\partial r} + w\frac{\partial w}{\partial z}\right) = -\frac{\partial p}{\partial z} + \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial w}{\partial r}\right) + \frac{\partial^2 w}{\partial z^2}\right] + \sigma\kappa n_z\delta_s - \rho g, \tag{1c}$$

$$u\frac{\partial \alpha}{\partial r} + w\frac{\partial \alpha}{\partial z} = 0, \tag{1d}$$

$$|\nabla\psi| - 1 = 0, \tag{1e}$$

where u and w are radial and axial components of the velocity. p, α, and ψ are pressure, liquid volume fraction, and level-set function, respectively. n_r, n_z,are radial and axial components of interface normal vector and κ is a curvature of the interface. δ_s is the smoothed delta function, which has a nonzero value only near the interface. ρ and μ are density and viscosity of mixture phase defined as follows:

$$\begin{aligned} \rho &= \alpha\rho_L + (1-\alpha)\rho_G, \\ \mu &= \alpha\mu_L + (1-\alpha)\mu_G. \end{aligned} \tag{2}$$

Physics-informed neural networks

In this study, we have been using simple deep feed-forward NN architectures, as shown in **Figure 1**. All the hidden layers are fully connected dense layers, and all the activation functions are hyperbolic tangents. The outputs of the network are selected as velocities u, w, pressure p, and level-set function ψ. From the predicted ψ, the liquid fraction α is calculated as

$$\alpha = \frac{1}{2}\left[1 - \tanh\left(\frac{\psi}{\epsilon}\right)\right], \tag{3}$$

where ϵ is small constant.

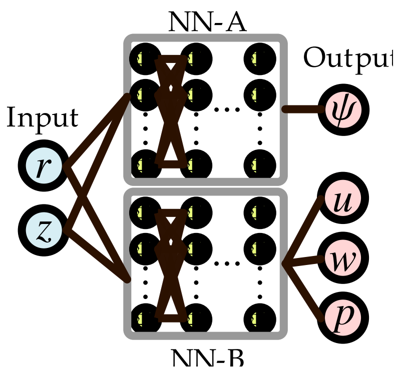

Fig.1 Structure of physics-informed neural network used in this study.

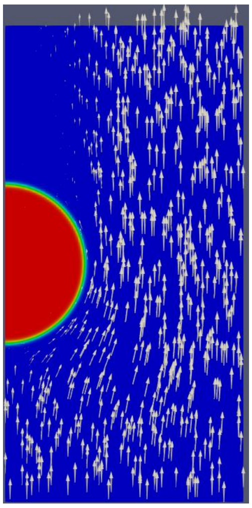

Fig.2 Calculated two-phase flow fields.

The loss function for the training is defined as follows:

$$\begin{aligned} J &= J_{\mathrm{GE}} + J_{\mathrm{BC}} + J_{\mathrm{VOL}}, \\ J_{\mathrm{GE}} &= \frac{1}{N_f}\sum_{i=1}^{N_f}\sum_{k=1}^{N_k}\left[F_k\left(r_f^i, z_f^i\right)\right]^2, \\ J_{\mathrm{BC}} &= \frac{1}{N_b}\sum_{i=1}^{N_b}\left(\mathcal{B}\left(r_b^i, z_b^i\right) - b^i\right)^2, \end{aligned} \tag{4}$$

where J_{GE} is the mean squared error (MSE) of the governing equations $F_k(r, z)$. The component J_{BC} is the MSE of the boundary conditions. The component J_{VOL} is the loss for the constraint of volume of liquid droplet. The NN is trained to minimize the loss function J by L-BFGS-B method, which is a quasi-Newton, full-batch gradient-based optimization algorithm.

3. Results

Figure 2 shows the flow field predicted by the trained PINN. The color contour indicates the volume fraction of liquid, whereas the vectors stand for the velocity. Validity and efficiency of the prediction was confirmed by comparison with the solution obtained by the finite volume method.

Acknowledgments

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References

1) S. Shiratori, Y. Yoshino, S. Koike, S. Ozawa, Y. Seimiya, Y. Takahashi, S. Kato, H. Kobatake, K. Kawamoto, K. Sugioka, and T. Ishikawa, 38th Space Utilization Symposium (2024).
2) M. Raissi, P. Perdikaris, G. Karniadakis, J. Comput. Phys. 378 (2019) 686-707, DOI: 10.1016/j.jcp.2018.10.045
3) Y. Nakamura, S. Shiratori, R. Takagi, M. Sutoh, I. Sugihara, H. Nagano, and K. Shimano:, Int. J. Numer. Meth. Fluids.94 (2022) 1359-1378, DOI: 10.1002/fld.5093