The Fortieth AAAI Conference on Artificial Intelligence (AAAI-26)

Learning Droplet Dynamics on Rough Unstructured Surfaces Using Physics-Informed Neural Networks (Student Abstract)

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Abstract

This study develops a physics-informed neural network (PINN) framework to predict droplet spreading dynamics on unstructured rough surfaces. The trained model effectively captures temporal evolution of the droplet shape, contact line motion, and interfacial deformation. This integration of multiphase physics with neural networks provides a mesh-free and computationally efficient alternative to numerical solvers, enabling rapid analysis and design of wettability-controlled surfaces, microfluidic devices.

Introduction

Droplet dynamics, especially on rough surfaces (Chamakos et al., 2016) is a crucial phenomenon in various medical, scientific, and engineering applications which includes microfluidic systems for lab-on-a-chip, inkjet printing, spray cooling, self-cleaning surfaces, anti-icing coating, etc. The droplet spreading, recoiling, and pinning depends on a balance of surface tension, viscous forces, inertial effects, and interaction with the underlying surface morphology and wettability characteristics. On rough or heterogeneous surfaces, the complexity increases as a result of additional factors such as contact line pinning, dynamic contact angle hysteresis, and microscale topography effects. The numerical approaches require high computational cost, especially for high-resolution simulations over unstructured domains with rough geometries. Moreover, conducting parametric or inverse studies using these solvers becomes computationally prohibitive, and their performance often sensitive to meshing, boundary conditions, and time-step constraints. To mitigate these limitations, PINNs have emerged as a novel paradigm in computational science and machine learning.

PINN integrate governing physical laws typically represented as partial differential equations into the loss function of a neural network, enabling the model to learn the solutions that adhere to physical constraints without requiring dense labeled data (Sun et al., 2020). This makes PINN particularly attractive surrogate modelling, especially when data is difficult to generate. Karniadakis et. al. has demonstrated the successful application of this approach across broad spectrum of CFD, including complex multiphase flows systems (Karniadakis et al., 2021).

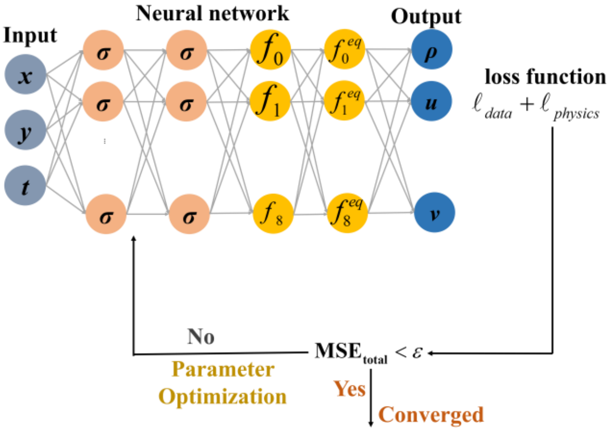

Figure 1: The model architecture of PINN based on the physics of Shan-Chen multiphase lattice Boltzmann method.

Physics-informed Neural Networks Approach

The PINN framework (Raissi et al., 2019) is designed to predict the droplet dynamics on rough surfaces using the data extracted from Shan-Chen multiphase LBM. The neural network is provided with the spatio-temporal coordinates (x, y, t) as inputs and it tasked with reconstructing the fluid density distribution as well as velocity components u, and v across the domain. The model is trained using a composite loss function that combines supervised loss from sparsely sampled LBM data with unsupervised physics-based loss derived from the residuals of the governing equations. The

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pressure is calculated using the Peng-Robinson equation of state and is used to compute the pseudopotential ψ , which accounts for interfacial tension. The gradients of ρ , u, and v are automatically computed using the auto-differentiation capabilities of TensorFlow, enabling the enforcement of continuity and momentum equations. These physical constraints are built into the loss functions, ensuring the network adheres to the underlying multiphase flow physics. The model is optimized using the Adam optimizer on mini-batches of data, and it learns to generalize well to unseen spatiotemporal domains.

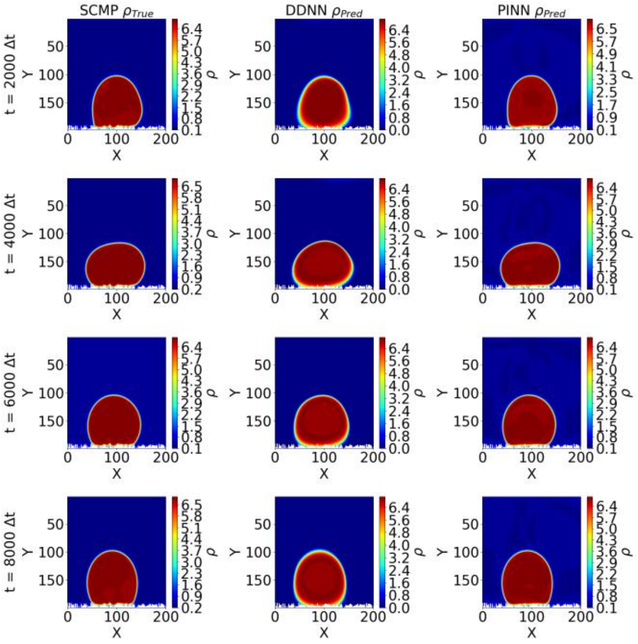

Figure 2: Prediction of phase fields using PINN and compared with Shan-Chen multiphase (SCMP) lattice Boltzmann model and data-driven neural network (DDNN).

Preliminary Results

To model the droplet spreading dynamics over unstructured surfaces, we implement a physics-informed neural network trained on high-fidelity data generated using the Shan-Chen pseudo-potential based multiphase lattice Boltzmann method. We provide (*x,y,t*) as inputs and train for the corresponding phase fields and fluid flow variables, represented by conservation of mass and momentum. The training process employs a composite loss function that combines supervised losses from sparsely sampled LBM data with unsupervised physical-based losses enforcing the residuals of the governing equations derived from the LBM formulation, coupled with interfacial force terms specific to the Shan-Chen model. Boundary conditions, including periodicity and no-slip walls, are encoded directly within the PINN architecture to maintain the physical consistency. with an attention in gradient computation to ensure numerical stability Once trained, the PINN generalizes to predict the dynamics of spatiotemporal evolution of the droplet on rough substrates, with requiring dense simulation data at every time step.

LR	Total	Data	Physics	BC
1 x 10^{-3}	**0.00132**	**0.00114**	**0.00003**	**0.00015**
1 x 10^{-4}	0.00229	0.00189	0.00023	0.00017
1 x 10^{-5}	0.00382	0.00333	0.00032	0.00019
1 x 10^{-6}	0.00540	0.00505	0.00018	0.00021

Table 1: Effect of learning rate on training loss.

Figure 2 illustrates the spatiotemporal evolution of the spreading of the droplets on a rough surface, comparing predictions from a purely DDNN and PINN. The DDNN model was trained solely on a supervised data while the PINN incorporated governing physical laws based the Shan-Chen multiphase lattice Boltzmann model. Both models capture the two-phase interfacial dynamics of a water droplet, but PINN shows superior accuracy in reconstructing the droplet morphology and wetting behavior, particularly near the rough wall and the curved interface region. Table 1 shows that the learning rate strongly affects convergence. The model trained with learning rate of 1×10^{-3} achieves the lowest total loss of 0.00132, with data loss 0.00114, physics loss 0.00003, and boundary loss 0.00015, indicating stable and balanced learning. As the learning rate decreases to 1×10^{-4} and 1×10^{-5} , the total loss rises to 0.00229 and 0.00382, reflecting slower optimization. At 1×10^{-6} , the model shows highest loss of 0.00540 and reflects overall poorer accuracy. The PINN with learning rate of 0.001 and Adam optimizer achieves the lowest total loss of 0.00132 but DDNN model only could achieve the total loss up to 0.01565. The result highlights the ability of the PINN to simulate multiphase wetting phenomena with high spatial accuracy, offering a mesh-free, data-efficient alternative to numerical CFD solvers and experimental approaches.

Conclusion

In this study, a PINN model was developed to study the droplet spreading on unstructured rough surfaces using Shan-Chen multiphase LBM data. The network captured the spatiotemporal evolution of density and velocity fields while enforcing the underlying physics through PDE residuals. This approach shows the ability for the reconstruction of phase fields of droplets on complex rough surfaces and thus helps in design optimization, and analysis of wettability-flow driven flows in complex geometries.

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