Advanced techniques to simulate turbulent flow in boiling liquid

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The inherent complexity of physical systems presents a significant challenge for computational modeling. Direct Numerical Simulation (DNS), even for relatively simplified representations of real-world phenomena, often exceeds the capabilities of current computing resources. Physically based machine learning (PbML), also referred to as Scientific Machine Learning (SciML), has emerged as a promising paradigm to address this challenge, aiming to create fast and inexpensive models that realistically simulate complex phenomena [1].

This computational bottleneck motivated the development of efficient and accurate surrogate models capable of capturing the underlying physics without the big cost of traditional numerical methods. They can be useful, for example, in simulating the weather on the global scale. In spite of significant progress having been made in that domain, certain physical systems, particularly those involving phase change phenomena like boiling, continue to present challenges for mainstream machine learning architectures such as CNNs, GNNs, FNOs and U-Nets. These architectures often struggle to capture the whole complexity of dynamics and sharp gradients inherent in boiling processes, leaving considerable room for improvement.

In our project, we focus on addressing these limitations, leveraging as a data source the BubbleML dataset [2], a comprehensive collection of high-fidelity simulations providing accurate ground truth information for various boiling regimes, including nucleate pool boiling, flow boiling, and sub-cooled boiling. Specifically, our aim is to address the open problems identified by Brandstetter et al. [2], namely the difficulty of accurately capturing the turbulent dynamics of bubbles and maintaining simulation stability during long-term roll-outs. We hypothesize that accurately representing the complex spatio-temporal dynamics inherent in boiling is crucial for achieving stable and reliable long-term simulations.

To overcome these challenges, we identified two relatively unexplored directions in SciML architecture design: Wavelet Neural Operators (WNOs) [3] and Reservoir Computing (RC)[4]. WNOs offer a compelling approach to learning mappings between infinite-dimensional function spaces, enabling them to efficiently represent and evolve complex physical fields. The use of wavelets provides a natural framework for capturing multiscale features and localized phenomena crucial for boiling simulation. Reservoir computing, a type of Recurrent Neural Network (RNN), provides an efficient way to model the temporal evolution of complex systems. Its ability to efficiently approximate dynamical systems makes it a strong candidate to capture time-dependent boiling behavior [3].

In our project we set the goal to design a novel architecture to accurately simulate boiling phenomena using either WNOs or RC, or a combination of both, leveraging the BubbleML dataset for training and benchmarking. We are expecting to see that those models will outperform state-of-the-art deep learning methods in terms of accuracy, stability, and computational efficiency. For WNOs, we investigate various architectural designs and wavelet bases, comparing their accuracy against baseline models. The results will demonstrate the potential of WNOs advancing the state-of-the-art in turbulent quasi-chaotic simulation and contribute to the broader field of SciML.

References

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