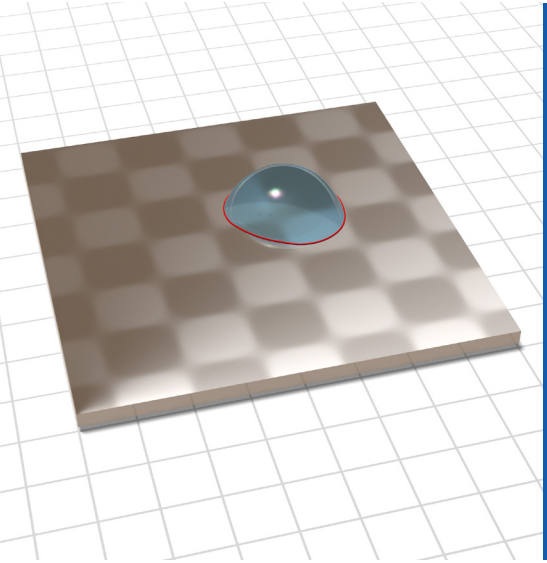
A EuroHPC Success Story: Accelerating the Understanding of Droplet Dynamics



Challange

In CoE RAISE, we have seen that ML can unlock new potential in fields such as high energy physics (HEP), remote sensing, seismic imaging, additive manufacturing, and acoustics. Training Deep Learning (DL) models, however, is no trivial task, especially if the models are large and have many tunable hyperparameters. To tackle this challenge, Hyperparameter Optimization (HPO) can be used to systematically explore the search space of possible hyperparameter configurations. This tends, however, to be a very computationally expensive process as training the target model with a lot of different configurations is usually required.

Solution

This project seeks to address the need for accurate and efficient data generation by adopting deep learning approaches to get high-fidelity simulations. Such efficient data-driven models can be used to inform strategies to control droplet transport. More specifically, by leveraging EuroHPC resources, the project generated datasets for the motion of droplets on surfaces with varied hydrophobic and hydrophilic regions. To achieve this, the team employed the code Basilisk - a powerful, open-source platform for solving partial differential equations on Cartesian grids - to perform direct numerical simulations (DNS).

The adaptive mesh refinement capabilities of the code, which ensure that the fluid interface is accurately captured, in conjunction with an efficient iterative multigrid solver, contributed to the generation of a substantial DNS dataset. This dataset fueled the development of data-driven models based on the Fourier neural operator, to predict droplet trajectories while incorporating insights from reduced-order analytical models.

Impact

The developed workflow is expected to be highly relevant to a broad spectrum of scientific and technological areas:

- Pharma/biomedicine: droplet-based microfluidic devices and lab-on-a-chip devices can batch-process small volumes of chemical/biological samples, without the need of large-scale laboratory equipment. These devices may also be used in high-throughput drug screening. In addition, understanding the behavior of droplets in various pharmaceutical processes is critical for quality control and ensuring consistent product quality.
- Smart materials: self-cleaning surfaces, either with super-hydrophobic or super-hydrophilic coatings, have application on windows, pv panels, etc.
- Energy harvesting: triboelectric energy generators can convert the kinetic energy of rain droplets to electrical energy.
- Printing: droplet-based 3d printing techniques