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Multi scale

"Understanding how processes at these different scales interact is therefore an important computational challenge"

01 Introducing myself

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My name is Khush Bakhat Rana, and I am a postdoctoral researcher at the Laboratory for Molecular Modeling at the National Institute of Chemistry in Ljubljana. I obtained my PhD in Mechanical Engineering, and my research interests include computational fluid dynamics, numerical methods, and hybrid multiphysics and multiscale simulations.

02 My role in the MultiXscale project

Within the MultiXScale project, my work focuses on coupling two simulation frameworks: waLBerla, which describes fluid behaviour at a larger scale using the lattice Boltzmann method, and LAMMPS, which models fluids at the particle level. In simple terms, we are developing an interface that enables microscopic and macroscopic scales to communicate within one computational domain. This work includes development and testing of multiscale fluid-flow models. One of our current test cases involves the propagation of ultrasound waves through particle-based and continuum regions.

03 Impact of my work

Developing this hybrid multiscale coupling requires not only understanding the underlying physics but also implementing the numerical methods correctly, testing the software, and ensuring that it can run efficiently on different high-performance computing systems. Therefore, we collaborate with researchers who have expertise in different numerical methods, simulation software, and high-performance computing.
The main advantage of multiscale modeling is that computationally expensive particle-based simulations can be used only in regions where this level of detail is necessary, while less computationally expensive continuum models can be used elsewhere. This can make it possible to investigate much larger and more complex physical systems without losing important microscopic information. Such approaches are relevant to researchers working in molecular dynamics, computational fluid dynamics, multiscale modeling and high-performance computing.

04 Looking ahead

Many natural physical phenomena involve processes at different time and length scales. Understanding how processes at these different scales interact is therefore an important computational challenge. Looking ahead, we are interested in exploring how machine-learning models and physics-informed neural networks can support the prediction, analysis and interpretation of complex multiphysics simulations. These methods will not replace physics-based modelling, but they may provide useful new tools for analysing and understanding increasingly complex simulations.