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Implementation of a block-based parallelization approach in a fully-differentiable Lattice Boltzmann solver

Master's Thesis, IDP

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Description

Numerical investigation of complex flow phenoma requires highly-resolved simulations to accurately capture all relevant flow physics, see fig. 1 (left). To address this challenge, the efficient parallelization of modern simulation frameworks is essential. Block-based parallelization approaches as sketched in fig. 1 (right) have proven to be immensely efficient and scalable for CFD solvers. They are especially attractive due to their easy extensibility towards adaptive multiresolution schemes [1].

In this work, we will implement a block-based parallelization approach for our in-house fully-differentiable Lattice Boltzmann solver, entirely written in the PyTorch Python package. The implementation will be based on PyTorch's distributed communication package torch.distributed and targets for a multi-GPU parallelization. Ensuring its flawless compatibility with PyTorch's programming paradigm, based on modules and functionals that allow composing complex layer-based architectures, poses several novel and demanding challenges regarding CFD algorithm development.

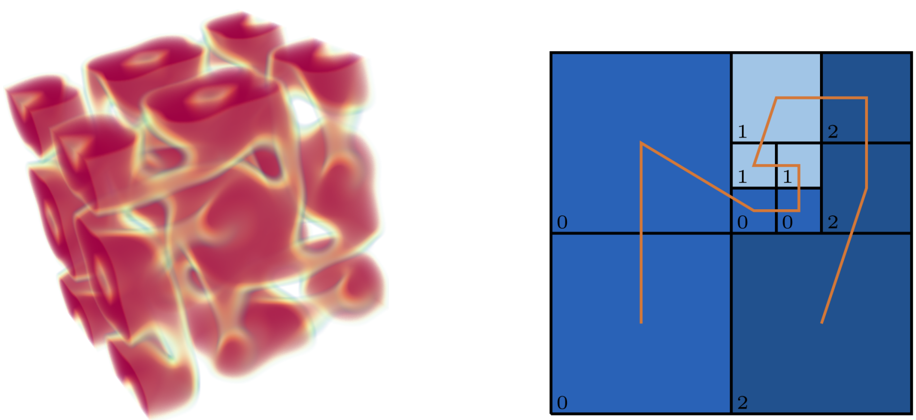

Figure 1: Left: Highly-resolved simulation of a Taylor-Green Vortex. Right: Schematic of a block-based domain decomposition and a space-filling curve used for distributing the computational load. Picture taken from [1].

Tasks

- Familiarize yourself with the in-house Lattice Boltzmann solver.
- Implement a block-based parallelization approach.
- Evaluate the parallel performance based on benchmark test cases and run highly-resolved flow simulations.
- Optional: Extend the implementation towards block-based mesh refinement.

Requirements

- Programming experience in Python.
- Interest in computational fluid dynamics and the Lattice Boltzmann method.
- Benefical: Knowledge of the PyTorch Python package.

References

[1] Hoppe, N., Adami, S., and Adams, N. A. "A parallel modular computing environment for three-dimensional multiresolution simulations of compressible flows". In: *Computer Methods in Applied Mechanics and Engineering* 391 (2022), p. 114486. ISSN: 0045-7825. DOI: https://doi.org/10.1016/j.cma.2021.114486.