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Multi-architecture implementation of Adaptive Mesh Refinement for Lattice-Boltzmann Method

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The research work presented herein proposes an implementation of a Lattice Boltzmann Method [1] (LBM), coupled with an Adaptive Mesh Refinement (AMR) algorithm, with main focus on the portability and the optimisation of the code on different high performance computing (HPC) architectures. To preserve the efficiency of LBM for HPC when using the adaptive grid, as well as to optimally exploit the available HPC resources and keep up-to-date with their progress, the developed computational tool is built atop of Kokkos [2] C++ library for scientific computing. Kokkos handles automatically the adaptation and optimisation of a single piece of software on different computer architectures, such as CPUs, GPUs, shared and distributed memory systems alike.

The proposed method uses the BGK collision operator but alters the streaming step. Instead of using multiple time-steps [3], a single time-step with a Lax-Wendroff [4] spatial discretisation scheme is employed, which accommodates computational cells of different sizes, while sub-iterations per computation step and variable scaling between different grids are avoided, and data sweeps and exchanges are minimised. The computational domain is discretised by a cell-centred mesh, which is organised in a block-based octree structure. Computations, as well as refinement and coarsening operations, are performed on each block separately. Block communication and boundary condition imposition are realised through layers of ghost cells filled by quadratic polynomial interpolations. Preliminary assessment and validation tests, on transport problems of a Gaussian distribution profile, for which analytical solutions exist, show that the AMR approach with respect to a fully refined uniform mesh simulation, can reduce the total number of computational cells, and therefore the mean time of a single computational iteration, 5 times, without loss of accuracy. In addition, hard disk I/O processes get accelerated. The normalised gradient of the concentration was used as a refinement criterion and coarsening occurred automatically on neighbouring blocks that did not require refinement.

These encouraging results, indicate the great potential of the method's application on more complex physical problems, such as porous media or multiphase flows and dissolution modelling, coupled with Navier-Stokes equations.

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