

Code modernization of DL_MESO LBE to achieve good performance on the Intel Xeon Phi.

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DL_MESO LBE [1] is a general purpose mesoscopic simulation package which can simulate multi component lattice-gas systems using the Lattice Boltzmann Equation (LBE). It is used to model systems with multiple fluids and/or phases coupled to solute diffusion and heat transfer, as well as apply geometrically complex boundaries comparatively easily.

The main version of this code implements a SWAP algorithm [2], where data dependencies are circumvented by a strict processing order of the lattice nodes. The SWAP algorithm performs well using multiple low core count processors with MPI, however, performance in a modern architecture like the Intel Xeon Phi was disappointing. To solve that, several incremental approaches have been tried, but the improvements were moderate and the execution time was still behind those in regular Xeon processors.

In this work we have re-implemented the Lattice Boltzmann solver within DL_MESO using a double-buffered and computationally simpler algorithm. This implementation utilises twice as much memory but it eliminates all of the data-dependencies due to processing order. Therefore, standard parallelisation and optimization techniques such as loop tiling, loop fusion, threading and vectorization can be implemented in the code easily. Figure 1 shows how by applying all the mentioned optimization techniques, the performance on the Intel Xeon Phi was improved by more than five times, making it capable of executing a simulation 30% faster than in a 2 by 12 core Xeon node. Also, this new implementation has the advantage of being ready to use the features of other modern and future hardware architectures to come.

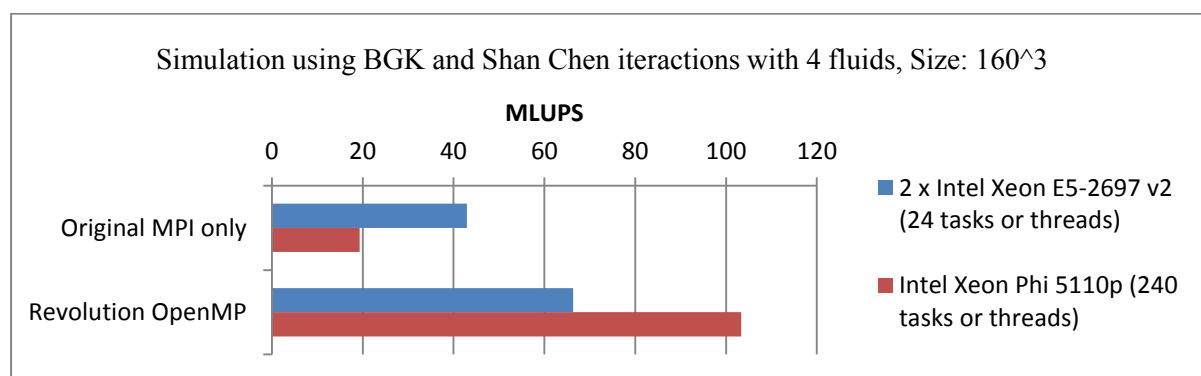


Figure 1. Performance comparison of the new and the original version of DL_MESO Lattice Boltzmann on the Xeon and the Xeon Phi platforms.

References:

- [1] M. A. Seaton, R. L. Anderson, S. Metz and W. Smith, DL_MESO: highly scalable mesoscale simulations, *Mol. Sim.* **39** (10), 796–821 (2013)
- [2] K. Mattilaa, J. Hyväluomaa, T. Rossia, M. Aspö and J. Westerholme, An efficient swap algorithm for the lattice Boltzmann method, *Computer Physics Communications*. February 2007