HemeLB Performance Assessment Summary

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An initial audit examined strong scaling on the Archer Cray XC30 up to 96,000 MPI processes (4,000 compute nodes), and found that the additional time and memory required for grid partitioning with Zoltan+ParMETIS was not productive. A follow-up audit with a higher resolution dataset on the Blue Waters Cray XE up to 239,615 MPI processes (18,432 compute nodes) was found to be less efficient when only thirteen of the sixteen available cores could be exploited due to node memory constraints.

Scaling of the simulate phase is relatively good, with excellent communication efficiency from non-blocking MPI point-to-point communication. Load balance efficiency is somewhat variable, but reasonable for all but the largest configurations: on Blue Waters, unused cores also have a negative impact. Computation efficiency benefits from improved use of data caches until the size of the local grid becomes dominated by its partition borders.

HemeLB is an open-source lattice-Boltzmann code for simulation of large-scale fluid flow in complex geometries, e.g., intracranial blood vessels near aneurysms. It is written in C++ using MPI by UCL and developed within the EU H2020 *CompBioMed* Centre of Excellence.

Archer audit report: https://pop-coe.eu/sites/default/files/pop_files/pop-ar-hemelb-a.pdf
Blue Waters report: https://pop-coe.eu/sites/default/files/pop_files/pop-ar-hemelb-b.pdf
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