HemeLB Performance Assessment Summary

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This audit examined strong scaling of HemeLB on the SuperMUC-NG Lenovo ThinkSystem with up to 309,696 MPI processes (on 6,452 compute nodes) using a 21.15 GiB testcase. Although the code always ran correctly, several compute nodes with notably inferior memory performance were identified and needed to be explicitly avoided. Compared to the smallest configuration that could be run using 864 processes (on 18 'fat' compute nodes each with 768 GiB), 190x speed-up was delivered with 80% scaling efficiency maintained to over 100,000 processes for the simulation phase.

Non-blocking MPI point-to-point message-passing ensures excellent communication efficiency, whereas load balance is somewhat variable but remains relatively good. Computation scaling is excellent to over 50,000 processes before progressively deteriorating due to extra instruction overhead from local grid block surface to volume issues which are only partially compensated by improving IPC scaling.

HemeLB is an open-source lattice-Boltzmann code for simulation of large-scale fluid flow in complex sparse geometries such as those found in vascular networks. It is written in C++ using MPI by UCL and developed within the EU H2020 *CompBioMed* Centre of Excellence for computational biomedicine.

The assessment can be found at
https://pop-coe.eu/sites/default/files/pop_files/pop2-ar-hemelb.pdf

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Notices: *The research leading to these results has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 676553 & 824080.*