Project Title:

Large scale cerebral haemodynamics

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subtitle:

LB3D Lattice Boltzmann code evaluation

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This quick access project aims for evaluation of deployability and performance of the multi-component lattice Boltzmann code LB3D on the K-Computer. The code exhibits excellent scaling on e. g. Intel Nehalem and IBM Blue Gene(/P) architectures.

The source code of the GPL released version 7 of LB3D was copied to the Riken testing environment. Compilation tests utilising the cross-compiler were performed. After initial problems with linking parallel libraries, the core code compiles. Minor issues still exist with the compilation of the parallel i/o library HDF5 against the parallelisation environment.

Further progress in deployment was hindered due to delays in work on optimisation of the code. Current efforts focus on redesign of the memory layout.
Changing the current 'array of structs' layout into a 'struct of arrays' promises easier vectorisation and optimal hybrid parallelisation results. Important in context of the latter is furthermore a reimplementation of the lattice decomposition strategies, currently centered around MPI.
Change of the memory layout is however affecting the whole of the function layout of the program as well as all lattice accessing algorithms. Paying great attention to the correctness of introduced changes, the redesign process takes up significantly more time than first anticipated.

The overall progress in the redesign process makes us optimistic to be able to run full benchmark tests on the K-computer as well as integrate machine specific optimisations to make optimal use of the vectorisation capabilities of the machine in the near future. Thus we would like to kindly ask for an extension of our quick access project.