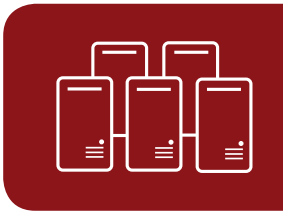
8th Blue Gene Extreme Scaling Workshop



From 23 to 25 January 2017, Jülich Supercomputing Centre (JSC) organized its eighth IBM Blue Gene Extreme Scaling Workshop. The entire 28-rack JUQUEEN Blue Gene/Q was reserved for over 50 hours to allow six selected code teams to investigate and improve the scalability of their applications. Ultimately, all six codes managed to run using the full complement of 458,752 cores (most with over 1.8 million threads), qualifying two new codes for the High-Q Club [1,2].

The MPAS-A multi-scale non-hydrostatic atmospheric model (from KIT & NCAR) and "pe" physics engine rigid body simulation framework (from FAU Erlangen-Nürnberg) were both able to display good strong scalability and thereby qualify for High-Q Club membership. Both exclusively used MPI parallelization, with the latter demonstrating strong and weak scalability to over 1.8 million processes in total. Available compute node memory and the lack of support for nested OpenMP parallel regions limited MPAS-A to a single MPI task per core, however, substantial code improvements in the two years since its first workshop participation (particularly the use of SIONlib for massively-parallel file reading and writing), combined with a larger 2km cell-size global mesh (147 million grid cells), were key success factors.

ParFlow (developed by the University of Bonn and FZJ-IGB) is an integrated hydrology model simulating saturated and variably saturated subsurface flow in heterogeneous porous media that had recently demonstrated how improvements to its solver, coupling with the p4est parallel mesh manager, allowed it to scale to the 458,752 cores of JUQUEEN to qualify for High-Q Club membership. During the workshop the focus was investigating the performance of the writing of output files with its SILO library, which was requiring prohibitive amounts of time for larger numbers of MPI processes.

KKRnano is a Korringa-Kohn-Rostocker DFT/Green's function simulation of quantum nano-materials from FZJ-IAS which is being extended to support a million atoms. While solver components were found to perform acceptably, Fortran direct access file I/O impeded overall scalability. The performance of the latest version of the CPMD (Car-Parrinello Molecular Dynamics) code with a large 1500-atom organic-inorganic hybrid perovskite system was also investigated by a team from RWTH-GHI and FZJ-IAS/INM.

The final code was a prototype multi-compartment neuronal network simulator designed for massively-parallel and heterogeneous architectures, NestMC (JSC SimLab Neuroscience). Implementations using 64 OpenMP or C++ threads per MPI process were compared and weak-scaling limitations identified.

Detailed workshop reports provided by each code-team, and additional comparative analysis to the 28 High-Q Club member codes, are available in a technical report [3]. The participants greatly appreciated the opportunity to have dedicated access to the entire JUQUEEN

system over the three day period to investigate their applications' performance and scalability. The workshop was immediately followed by the second "Big Blue Gene Week" dedicated to exploiting JUQUEEN for capability computing jobs, including extreme-scale atmospheric science, materials science and neuroscience simulations by High-Q member codes and prior scaling workshop participants.

References

[1] **The High-Q Club:**
http://www.fz-juelich.de/ias/jsc/high-q-club

[2] **Brömmel, D., Frings, W., Wylie, B.J.N:**
Extreme-scaling applications en route to exascale, Proc. Exascale Applications and Software Conference 2016, ACM, 2016
http://dx.doi.org/10.1145/2938615.2938616

[3] **Brömmel, D., Frings, W., Wylie, B.J.N. (eds.):**
JUQUEEN Extreme Scaling Workshop 2017, Tech. Report FZJ-JSC-IB-2017-01
https://juser.fz-juelich.de/record/828084

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