Scientific Computing at IST Austria

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In 2016, the cluster for scientific computing at IST Austria has been used by 56 individual users from different disciplines in the area of biology, neuroscience, computer science, mathematics and physics. Most noteable developments are: the cluster was extended by another 28 nodes, the costs for these nodes were below 75.2 Euro / (GHz * CPUcore), where each node has 128 GB RAM and Mellanox EDR 100 Gb/s InfiniBand. These nodes provide 13.2 TFLOPS according to Linpack. We plan to report performance and scalability results on several selected projects. In particular we'll focus on Infiniband and MPI performance, storage access, and software applications (e.g. OpenPipeFlop [1] and Relion [2]).

As a general trend, we have noticed among our heterogeneous user base that there is a constantly growing interest and demand for GPU acceleration, most noteable in the area of Cryo-EM software, Relion2 can now be run on GPU machines. First tentatitve results show large performance improvements [2]. For getting this GPU-accelerated version of Relion2 to run on our compute nodes based on Debian Linux, a bug had to be tracked down.

Moreover, we had also the need for a large shared memory machine with up to 1.7 TB RAM. These computations have been performed on the Mach Computer from UIBK. Simulations of a real-size hippocampal CA3 network model with up to N=660k neuronal elements [3] were carried out. In order to generate a connectivity matrix with a certain probability distribution of four different motives (convergent, divergent, chain, reciprocal) we have adapted the SONET algorithm of Zhao and Nykamp, and applied the following changes to their algorithm: (i) minimized cache misses by using a block-based partitioning, (ii) reduced the memory requirements by using single precision, (iii) fixed the indexing such that it goes beyond the $2\hat{3}2$ matrix elements, (iv) and the resulting output matrix is now stored as a sparse binary array in CSR format. Overall, this resulted in a speed-up of over 100 (an estimated runtime of 80 days could be reduced to 18 hours).

References

[1] Willis, A.P., and Kerswell, R.R., J Fluid Mechanics **619**, 213 (2009).

[2] Kimanius, D., Forsberg, B.O., Scheres, S., and Lindahl, E., bioRxiv, (2016).

[3] Guzman, G., Schlögl. A., Frotscher, M., and Jonas, P., Science **353**, 1117 (2016).