High performance computing at IST Austria: modelling the human hippocampus

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Current state: The scientific computing cluster at IST Austria consists currently of about 70 compute nodes mostly from Supermicro. This includes 1 GPGPU node, three nodes with 512 GB RAM, as well as a few NFS storage servers with a capacity of about 150 TB. All nodes are connected through QDR 40 GB Infiniband. Just recently, all compute nodes have been upgraded to Debian 8. For job scheduling, GridEngine is currently used.

In the last 12 month, the cluster has been used by about 50 users from various disciplines, including biology, neuroscience, physics, and computer sciences. The requirements vary greatly. There are jobs which require more than 50 GB RAM per CPU core, OpenMP jobs (e.g. gromacs), as well as OpenMPI jobs, and hybrid (MPI/OpenMP) jobs.

Currently, more than 35 different software packages are installed, and managed through the "Lmod: Environmental Modules System". Because many packages have more than one version installed, over 70 different packages are currently available. In addition, numerous scientific software packages from Debian 8 are available.

Future plans: A cooperation with VSC has been started, and a number of selected users have test accounts since autumn 2015. The selection has been done based on the criteria of high CPU usage with an efficient RAM/CPU core ratio, and to have software requirements that are already fullfilled on VSC-3. Users that have more demanding requirements like very high storage volume or require more than 16 GB RAM per CPUcore, have a need of proprietary licenses (e.g. Matlab, Mathematica), or have a very difficult software setup, are currently not included in that program. A status update of the user experience will be presented.

Modelling the human hippocampus: The hippocampus is a brain structure that seems to be important for learning. For estimating the storage capacity, a model based on pattern storage and pattern retrieval has been proposed. Based on physiological evidence, the structure of neurons seems to be quite regular and there are estimates that the hippocampus contains about 330 000 neuronal cells. These cells have on average about 20 000 dentrites, connected to other cells in the hippocampus. A number of parameters as well as the question whether a random structure or a more regular structure has a higher storage capacity is addressed. A model has been implemented on a realistic scale containing all 330 000 neurons and its possible connections between all neurons.