Protokoll: Treffen der HPC Nutzervertreter, 13.12.2019

Teilnehmer:
Stefan Harfst (Wiss. Rechnen), Felix Thole (IT-Dienste), Jürgen Weiß (IT-Dienste), Nils Krüger (Physik), Robert Röhse (Chemie), Thorsten Klüner (Chemie), Caterina Cocchi (Physik), Karsten Lettmann (ICBM), Matthias Schröder (ICBM), Jörn Anemüller (Medi. Physik), Ana Valencia (Physik), André El-Ama (ICBM), Eike Mayland-Quellhorst (Biologie), Fabian Schuhmann (Physik), Michele Guerrini (Physik), Sven Stephan (Physik), Wilke Trei (ForWind)

Beginn / Ende
10:00 Uhr – 11:00 Uhr

Moderation
Dr. Stefan Harfst
Protokoll
Stefan Harfst

Meeting was held in English, new record for number of participants. 😊

1. Status HPC Cluster (CARL/EDDY)
   a. Cluster continues to run stable at high load, Infiniband cards have been replaced on some nodes, the computing nodes in the cluster are no longer under maintenance, necessary repairs with spare parts are still possible
   b. Storage: GPFS ($WORK) is nearly full (>90%), users should remove any data that is not actively used on the cluster (e.g. move to $DATA or $OFFSITE). WT has already talked to some users at Forwind
   c. As already mentioned in the Newsletter, a number of nodes in the partition carl.p and also 1 GPU node have reservations to make sure that resources for testing are available always, should also improve the scheduling for jobs requiring complete nodes.
   d. Software: we started installing new software in hpc-env/8.3, where more recent compilers are available

2. Next HPC-Cluster
   a. Report for CARL was sent to the DFG, report is available upon request
   b. Timeline: proposal to DFG is work in progress (group leaders have been asked to provide description of research plans with HPC needs), submission of proposal is planned for September, decision from the DFG can be expected for Q2 in 2021, procurement in late 2021, installation after that
   c. Important input from the research groups are the requirements on hardware, discussions with vendors will take place after the proposal was submitted, TK and CC will be part of the discussion, others are welcome to join
   d. TK points out, that an I/O solution has to be discussed in addition to decisions about CPUs and RAM, SH mentions the NVMe server which will be ready for benchmarking soon
   e. The server room will be made ready for the new HPC cluster which will use direct water cooling, IT services and Dezernat 4 have started the planning
3. Other topics:
   a. The block-course Introduction to HPC was held online end of March, the next course is planned for September, date will be announced in the next Newsletter
   b. Some new HPC groups have started at UOL: Prof. Frühbis-Krüger in Mathematics, research topic Computer Algebra, Prof. Cocchi in Physics, research topic Electronic Structure Theory, and Prof. Solov'yo in Physics, research topic Quantum Biology
   c. Question about security incidents at several HPC sites, is an additional security measure like 2factor authentication planned? JW: IT services have currently no plans to change the working security concept, SH: 2-factor authentication might not be practical and is also not 100% bulletproof, best protection are sensible users

4. Nächster Termin:
   Friday, September 18th, 10:00 Uhr, most likely online again