Minutes: Meeting of the HPC User Representatives, 24th of September 2021

Participants:
Prof. Dr. Caterina Cocchi (agest, ifp), André El-Ama (agmsys, icbm), Dr. rer. nat. Janek Greskowiak (aghydrogeo, ibu), Dr. Stefan Harfst (hrz), Christoph Jüschke (aghumangenetics, dfhm), Prof. Dr. Thorsten Klüner (agtheochem, ifc), Eike Mayland-Quellhorst (agplantbiodiv, ibu), Robert Röhse (agtheochem, ifc), Holger-Dietrich Saßnick (agest, ifp), Erik Marc Schetzke (agnumerics, ifm), Matthias Schröder (agcomplexsys, icbm), Fynn Schwietzer (hrz), Sven Stephan (agnanoopt, ifp), Wilke Trei (agtwist, windlab), Felix Thole (hrz),

Start / End
10 AM – 11 AM
Moderation
Dr. Stefan Harfst
Protocol
Stefan Harfst, Fynn Schwietzer

Meeting was held in English

1. Status HPC clusters (CARL/EDDY)
   a. Nodes
      • everything on track except from a few failed nodes
      • workload soaring again after quiet summer season
   b. Storage/GPFS
      • $WORK nearly full again
        → Mail to users with highest consumption will be sent again
   c. SLURM
      • no news
   d. Software Installation
      • no news

2. Next HPC Cluster
   a. DFG proposal for CARL-II
      • proposal has been submitted
      • reviewers already responded with minor technical questions
      • we expect to receive more scientific questions
   b. Hardware & Benchmarks
      • benchmarks are needed especially to choose the right CPU & GPU types
        → VASP, NAMD, etc.
      • machine learning group specifically important for choosing the right GPU
      • benchmarks will be performed on current system (1.5h – 2h target) & on new potential systems (0.5h target)
      • question: It can be very hard to find the right compilers & dependencies to reach the best performance depending on the system. Is it likely for the vendors to accomplish this task?
SH: We will have to supply instructions for what is probably best ways to compile the packages way.
• we also must be careful about the test results being accurate
  → Questions about these issues will be discussed with the vendors prior to the benchmarking phase
• time frame for the benchmarks: January
• EDDY successor: a BMWi proposal was put on hold due to lack of funding, as an alternative EFRE-funding was requested, no decision yet (same as for the DFG proposal), a revised BMWi proposal may add funds
• users may also be encouraged to apply for computing time at NHR project
• question/remark: additional funding available in agest, can be added to the call or used later with conditions from the call

c. Server Room Improvements
• ongoing, and will be finished until end of this <yeas

d. Planning the Vendor Interviews
• up to ~5 user representatives are welcome to join the vendor meetings (limited due to corona safety regulations)

3. Miscellaneous
• tutor for C++ wanted!
• Stefan on vacation: 27.09.-08.10.

Next Meeting: 10.12.2021 (suggestion)