

Optimisation of CFD simulation for Komondor

OpenFOAM is one of the CFD softwares commonly used at Komondor. In the first level course (workshop) some tools for data transfer, configuration and postprocessing were presented and discussed. In this second level workshop the content of the first level workshop will be reviewed but it is not intended to redo the exercises.

Short simple overview about the hardware architecture of Komondor (with main focus on CPU partition) will be given. Some insight will be given how to influence hardware/software usage properties using Slurm to facilitate the discussion of the next topics.

To compile OpenFOAM for Komondor is not a trivial task, the organiser of the workshop is aiming to provide a precompiled version of latest OpenFOAM version for various number representations (float and integer) and compilers (AOCC vs GCC) and MPI (Cray MPI vs OpenMPI) implementation. It is important to be able to compile various third-party packages. The organizers' experiences and experiences from the participants will be collected together.

To optimally use a supercomputer for CFD is far from being a trivial task, especially since decisions need to be done case by case. Simulation cases can vary based on number of cells, elongation of the simulation domain, number of equations solved (also type of physics involved) and if the simulation is steady or unsteady.

The topic of parallel efficiency applied to actual CPU partition composed of nodes having 128 cores will be presented in an example, where the participants should run the various configurations and the complete efficiency curve will be developed as a team work exercise.

Various goal functions for parallel efficiency optimization will be compared. Depending on application, simulation price, or simulation time could be more important, the optimal solution can be chosen by a well prepared parallel efficiency study.

In this section beside generic concept and question of parallel efficiency, various methods (scotch, zoltan, metis) available for OpenFOAM domain decomposition will be shown. Furthermore experiences from the participants will be collected.

Further simulation settings influencing efficiency of the simulation will be discussed. One important topic is appropriate selection of time-step size and accuracy of time resolved simulation. The multigrid solver also contains parameters which could be tuned.

The topic of available/required memory will be also mentioned and discussed.

It will be proposed to generate an e-mailing list to share questions and experiences among OpenFOAM (and/or perhaps CFD) users.