Practical Introduction to OpenFOAM on Komondor

OpenFOAM is an open source CFD solver based on Finite Volume Method (FVM) for solving the describing Partial Differential Equations of fluid dynamics. It is widely used both by the academic and industrial community. Fluid dynamics problems are typically very heavy from mathematical i.e. computational point of view. This implies practically the must to use High Performance Computing (HPC) facilities for academical and industrial problems.

For FVM solvers the high performance can be realized by so called domain decomposition technique, where the computational domain is diveded into smaller domains, where the problem is solved for each subdomain separately on a separate CPU core. As flow is flowing among the different subdomains in the solution the separate subdomains need to communicate with eachother. For this reason having access to high number of cpu cores which can communicate “well” with eachother can speed up the simulation, this is provided in our case by Komondor.

For this previously mentioned two reasons the appropriate domain decomposition and IT background of the inter core communication plays an important role in reaching acceleration of the problem solving. In the workshop, practical aspect for the simulation setup and some useful hints to efficiently utilize the Komondor HPC supercomputer will be given and practiced by the audience.

Basically the OpenFOAM simulation workflow will be presented using the Komondor facility.

It will be proposed to install Visual Studio Code editor as Remote-SSH with some hints on further extensions. It will be further proposed to use MobaXterm for terminal emulation. The various OpenFOAM versions and preprocessing tools will be introduced.

A *slurm* script will be prepared to considering important settings of the simulation, including memory, time and core distribution. The use of project and scratch folder will be emphasized. An example will be discussed, starting from a tutorial case how to modify it to be optimal for simulation on Komondor.

The use of gnuplot scripts will be proposed to monitor convergence behavior of simulations, also including iteration time. Furthermore the efficiency of own jobs will be plotted online as an example.

It will be shown how to use the collated filesystem to align with the quota requirements of Komondor. Practical hints will be given on transiting from uncollated to collated filesystem handling.

Simple bash commands will be shown to easily handle big simulation scenarios.

It will be suggested to do visual postprocessing on local desktop using Paraview. The various aspects of appropriate file formats data exporting and data storage options will be discussed.

It will be shown, how to decide on variable storage location (node or cell based) to export only specific regions of the domain
The use of surface LIC for vector-field visualization will be shown, how to highlight core aspects of the flow topology.