

Technical requirements for a high performance computing station.

A) Minimum hardware configuration requirements:

- 1) Number of processors: 66 or more (preferred Intel® Xeon® Platinum 9222 Processor 2.30 GHz)
- 2) Speed of computation: 9 TerraFlop or more
- 3) RAM: DDR4-2933 (384 GB per node, 768 GB in total)
- 4) Storage at least 900 GB (preferred 2 x 480GB M.2 SATA)
- 4) Samsung 34" LC34J791 Monitor

B) Minimum software requirements:

- 1) Operating System: Centos 7.x or Ubuntu
- 2) Compilers, Libraries and MPI: GNU, BLAS, OepnMPI, MPICH
- 3) Job Scheduler: PBS Pro OpenSource
- 4) Applications: OpenFoam dev pack (CFD), LBSolver, WRF, MOM, Gromacs, NWChem, ABINIT