In my thesis I am going to do research on the three-dimensional polycrystalline models of FCC crystals with the log-normal grain size distribution. This structure is constructed by constrained Voronoi tessellation and by using Voro++ library for C++ programming language. For achieving needed distribution of grain sizes and grain orientation we used Genetic Algorithm with Least Square. Molecular-dynamics method in LAMMPS software is used to obtain the relaxed polycrystalline structure. For the relaxation process and for the simulation we used multibody potential.

For obtaining some scientific meaningful results I need to do generation and simulation for at least 1000 of particles for Voronoi tessellation and tens of thousands of atoms. These operations are very demanding for the resources and processor time.

For the simulation by using molecular dynamics I am going to apply LAMMPS software with a multibody potential that is much more demanding for the resources.

It is also known that all work will be needed in very big data storing and data transferring because for the analysis it is necessary to do many hundreds of runs for many particles and store obtained data for the further averaging or making some conclusion.

The reasons mentioned above are showing my need in LAN connection to the supercomputer servers to be able to perform my computations.