LCPQ Facilities Equipment Resources available for PIRE

Computer Codes and Computational Resources

The simulations will be achieved with the deMonNano code, a free program hosted and developed in the laboratory (http://irssv2.ups-tlse.fr/codes/pages/demon_nano.html). The deMonNano code can be compiled and used easily on a variety of machines. All the molecular dynamics simulations and electronic structure calculations for the PIRE project will be achieved with this code, which the researchers involved in the present project are very familiar with.

The LCPQ owns a local cluster, maintained by a computer engineer (David Sanchez), constituted from several nodes that are characterized by different configurations which match the needs of the different teams. Here is a brief description of the cluster, totalizing 117 nodes, i.e. 1460 cores/2232 threads and more than 7.7 TB of RAM. For the PIRE project, the following nodes, dedicated to parallel computing, will be available :

- 7 intel ivy bridge nodes : 20 cores and 64 GB of RAM per node.
- 9 intel haswell nodes : 24 cores and 128 GB of RAM per node.
- 1 intel broadwell node : 28 cores and 128 GB of RAM.

Besides, we will run simulations on the national supercomputing center (GENCI) and on the regional computing mesocenter CALMIP. We already have 3 million hours (monoprocessor) allocated in total in both centers, that we can dedicate partially to the project.