TOOLs

- Computational simulations via DFT GPL and commercial codes (VASP, Wien2K, QuantumEspresso, ELK, GPAW, ...) as well as APIs, like ASE: ab initio simulations.
- Development and utilization of routines and scripts: use with general-purpose numerical and analytical software (Mathcad, Maple, Mathematica).
- Training in large facilities, such as X-ray synchrotron and neutron sources, and computational infrastructures, as RES and PRACE: large-scale experiments.
- Linux/Unix, Bash Shell scripting, Fortran, batch scheduling and job resource managers (LoadLeveler, Slurm, PBS, LSF), OpenMPI: Access to computational resources.

EQUIPMENT

- Core and paid computing equipment with 8 Xeon Westmere X5650 2.66 GHz 6-core processors, three 500GB HDs and 1 TB extra HD, 24x4GB DDR3 RAM and a 16-port Gigabit switch.
- Core and paid computing equipment with 4 AMD Opteron 6386SE 2.8 GHz 16-core processors, three 900 GB HDs, 24x8GB DDR3 RAM and a 4-port Gigabit switch.
- Core and paid computing equipment AZServer 4G+ Pro with 2 x 4-core Intel Xeon E5-2690v2, 2 x Intel Xeon Phi 7120P 1,24GHz 61 cores, 1TB HD.
- Ab initio licensed software packages installed: VASP, Wien2k, Fireball, Abinit, Quantum Espresso, ELK, GPAW, Octopus, a few MD & kMC GPL codes.

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