We offer computing time

We offer lease computing time on peak supercomputers of cluster type in operating system Linux Debian with simulation programmes, installation of other software is also possible.

Computing time is available on following instruments:

- Cluster Melian for computing with big memory demands
    - Server + 18 nodes Intel E5550 2,67 GHz and 6 nodes Intel E5430 2,66 GHz
    - altogether 216 cores
    - 24x 1 TB HDD, 32/16/8 GB RAM
- Cluster Ingwe with high speed processors and large discs
    - Server + 17 nodes Intel E5420 2,5 GHz
    - altogether 272 cores
    - 17x 2 TB HDD, 4 GB RAM
- Cluster Elwe with graphic cards NVidia for speeding up massively parallel calculations
    - Server + 35 nodes Intel Q6600 2,4 GHz, from which 15 nodes with GPU NVidia GTX 480
    - altogether 140 CPU cores and 7200 GPU cores supporting CUDA technology
    - 35x 2 TB HDD, 4 GB RAM
- Cluster Olwe with high number of cores per board
    - Server + 20 nodes AMD Opteron 6168 1,9 GHz
    - altogether 960 cores
    - 20x 4 TB HDD, 16 GB RAM

We offer carrying out molecular simulation studies

We also offer expertise and carrying out of molecular modelling and its application in following regions:

- Studies of biomolecular and nanomaterial systems
- *In silico* testing of medicaments and bioinformatic analyses
- Studying of chemical reactivity and quantum calculations of reaction mechanisms
- Calculations of electronic and also mechanic properties of materials
- Spectral molecule properties

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