

Mission

Within the context of the national e-Infrastructure, Center CERIT-SC focuses on highly flexible real time computing and storage resources provisioning. Virtualized computing and storage resources, available through novel interfaces combining grid and cloud environment, represent unique installation in the Czech Republic and even in the Central Europe and eventually even larger region.

Provision of these resources is complemented with extensive research activities, carried both in cooperation with user communities and in the e-Infrastructure area itself.

Joint research projects are run, targeted at ICT-assisted solutions of specific scientific problems, as well as novel infrastructure architecture and its configuration, and resulting also in publications with both-sides authorship.

Center CERIT-SC works closely with the Faculty of Informatics and other parts of the Masaryk University. The research work evolves in a doctoral school with student participation from both ICT and application areas.

Funding

Transformation of SCB into CERIT-SC is supported by a project of the 3rd axis of the RD&I Operational Programme. Its overall budget is 5 MEUR. CERIT-SC is included in the Roadmap for Large Research, Development and Innovation Infrastructures in the Czech Republic.

Selected Collaborations

Computational Chemistry

- **Reconstruction of RNA geometry from NMR measurements** (CEITEC). Existing software package CYANA was considerably extended to include molecular-dynamics simulation of the reconstructed system while favouring constraints which reflect the NMR inputs. The result is far more realistic geometry of the reconstructed macromolecule. Parallel processing on both multiple CPU cores and GP-GPU is deployed.
- **Empiric methods of atomic charge calculation** (CEITEC). Atomic charges are an essential property leveraged in bioinformatics and molecular modeling. Two existing software packages EMP and TRON were re-engineered into a more universal NEEMP, while improving both stability and quality of the generated results by addressing numerical instability issues, and achieving significantly higher performance by various optimizations and multi-core implementation.
- **Speedup of molecular metadynamics** (VŠChT). Modified Plumed + Gromacs implementation was deeply analyzed and due to rewriting critical code sections significant speedup was achieved. Opportunities for parallel processing are also opened.

Astronomy

- **Exo-planet photometry** (Faculty of Science MUNI). Data of the WASP archive (more than 3 TB) were rearranged and indexed for efficient search and retrieval.

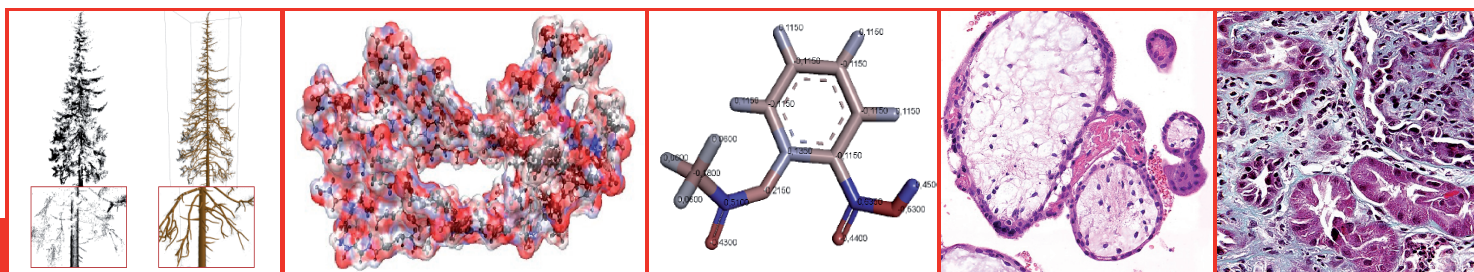
- **Photometric Archive of Astronomical Images** (Faculty of Science MUNI). The service collects unsorted CCD images from various astronomical telescopes (both professional and non-professional), adds systematic annotations and provides appropriate indices. Identification of objects in the images and development of a standardised interface to Virtual Observatory.

Environmental Sciences

- **Three-dimensional Tree Reconstructions from LiDAR Scans** (CzechGlobe). A unique fully-automated method for tree reconstructions from laser scan measure was developed. The algorithm is very general, it can deal with sparse and non-uniform 3D points cloud. Unlike previous methods no manual intervention is required. Results can be used for reliable computation and branch statistics.

Medical and Health Sciences

- **Web-based Virtual Microscopy Using JPEG2000** (University Hospital MUNI). A new version of our web based virtual microscopy application was developed. On the server side, the application uses JPEG2000 format that is suitable for storing large images that are accessed as small tiles in various resolutions. It was possible to reduce required storage space for a single image by half using JPEG2000 while preserving image quality. On the client side, the application supports arbitrary zoom level, rotation, annotations, and shared sessions.





■ Equipment

Storage

- volumes of spinning disks (260 and 375 TB) for immediate usage mainly for data being processed
- HSM (hierarchical storage management) system (4 PB) built on MAID (massive array of idle disks), intended for archival storage or large data volumes

Computing

- HD (High Density) – 3 clusters of 48, 112, and 32 nodes of 8-16 CPU cores and 96-128 GB RAM each, suitable for high-throughput and coarse-grain distributed applications with moderate memory requirements
- SMP (Symmetric MultiProcessing) – 20 nodes of 80 CPU cores and 512 GB RAM each, suitable for fine-grain parallel applications and higher memory requirements
- NUMA (Non-Uniform Memory Architecture) server (SGI UV2) – a single server with 288 CPU cores and 6 TB RAM, suitable for highly-parallel applications with enormous memory requirements

High-speed networking

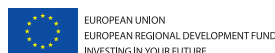
- 10 Gbit/s uplinks of all the clusters and storage resources to the NREN backbone
- 40 Gbit/s low-latency InfiniBand local interconnect in both CERIT-SC sites

■ Contact

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■ Center CERIT-SC

The national Center CERIT-SC (CERIT Scientific Cloud) continues the tradition of the Supercomputing Centre at the Masaryk University in Brno, providing flexible storage and computing resources and related services, for both production and experimental use. Provision of these resources is complemented with extensive research activities, carried both in cooperation with the user communities and in the e-Infrastructure area itself.