

## Goals

CERIT-SC provides highly flexible computation environment and primary data storage capacities for the national e-Infrastructure.

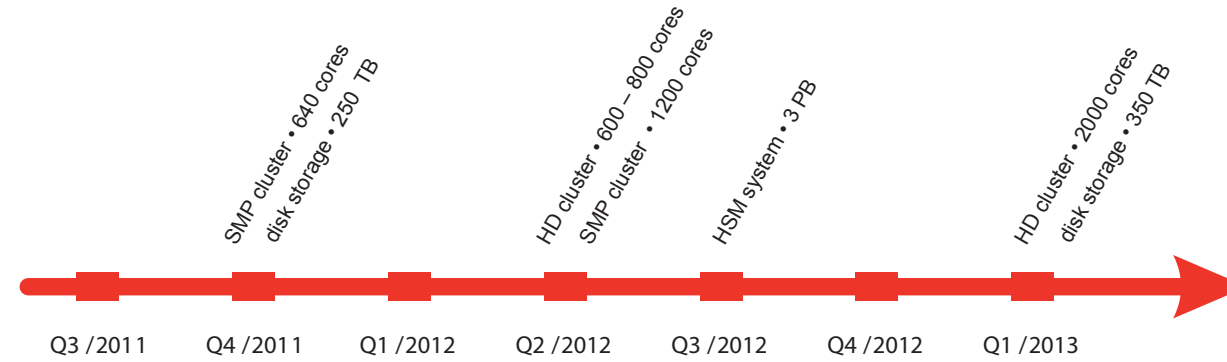
Research and development in CERIT-SC is focused on:

- work with users on tools and means for efficient use of the e-Infrastructure by applications
- cooperation with the users in development, deployment, and operation of new and modified systems and programs running in flexible computation environment

- systems for storing, archiving, and retrieval of data
- tools and protocols for data storage facilities interconnection, ...

The research work evolves in a doctoral school with student participation from both IT and application areas.

CERIT-SC is becoming an important node of the national e-Infrastructure as well as the European Grid Infrastructure. The integration will be achieved by tight cooperation with CESNET on development and adoption of appropriate standards.

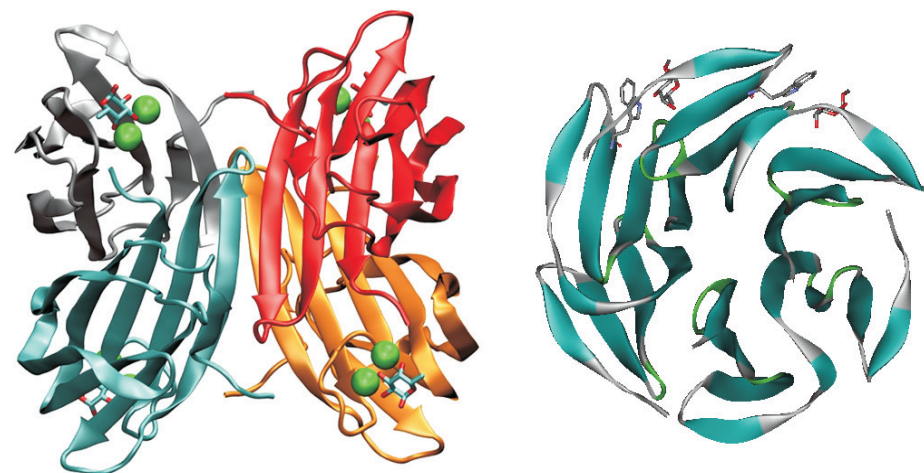


Numbers of cores and data capacities are in current price/capacity ratios (last update: November 1, 2011)

## Equipment

The project plans to purchase the following resources:

- SMP – Symmetric MultiProcessing clusters, with more than 64 cores and 128 GB memory per node (min. 1800 cores total)
- HD – High Density clusters with higher number of nodes with 8-16 cores and 16-32 GB memory (min. 3200 cores total)
- HSM – Hierarchical Storage Management system (min. 3 PB)
- disk storage (min. 600 TB)
- development tools and application software



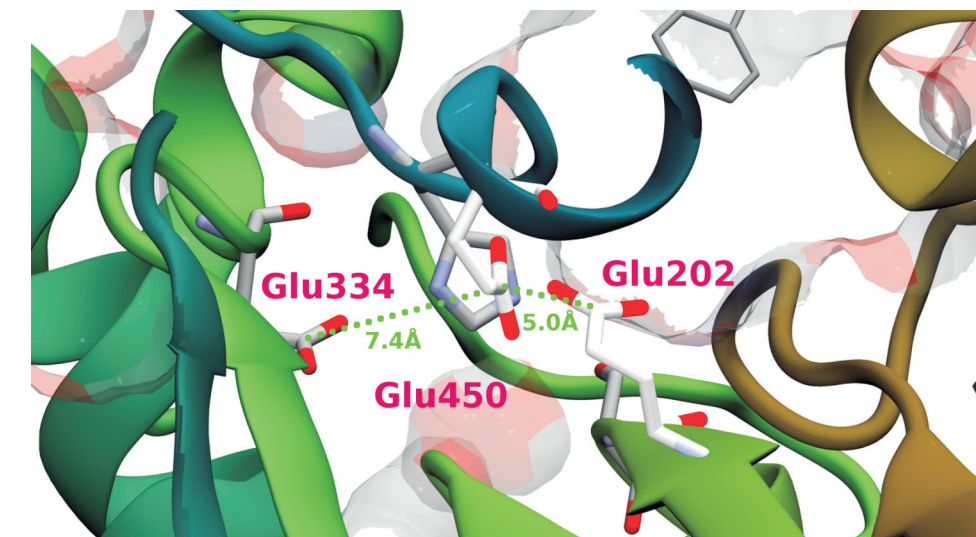
Lectin PA-IIL and RSL, CEITEC, National Centre for Biomolecular Research

## Flexible resources

Provision of the resources ranges from traditional batch queues, through interactive access upto the cloud paradigm. The resources are provided free of charge. Prioritisation of the users is based on their scientific results; resource allocation is achieved by technical means, combining advanced resource scheduling, virtualization, and the cloud paradigm; no complex administrative process is required.

By careful balancing the scheduling strategies, successful users get better share while new users, students etc. are not prevented from using the resources. CERIT-SC computational resources are mostly intended to serve unexpected and unplanned requirements of the users.

Data resources serve to store and share data semipermanently and permanently. They are tightly integrated with the computational resources.



Acetylcholinesterase, CEITEC, National Centre for Biomolecular Research



A cluster in a CERIT-SC server room

## Cooperation with users

This work results in common publications. Targeted projects are also expected.

Formal agreements on future collaboration (LoI):

- R&D: AdMaS, BIOCEV, CEITEC, CzechGlobe, RECAMO
- cooperating institutions: IBA, MZK, Loschmidt Labs., RECETOX
- ESFRI projects (in negotiation): LINDAT-CLARIN, Euro-Biolmaging

Deluge of experimental data is expected in near future. Many existing computational methods will break or stop scaling, new developments will be required. User communities will come up with interesting problems, CERIT-SC will provide the necessary IT expertise.

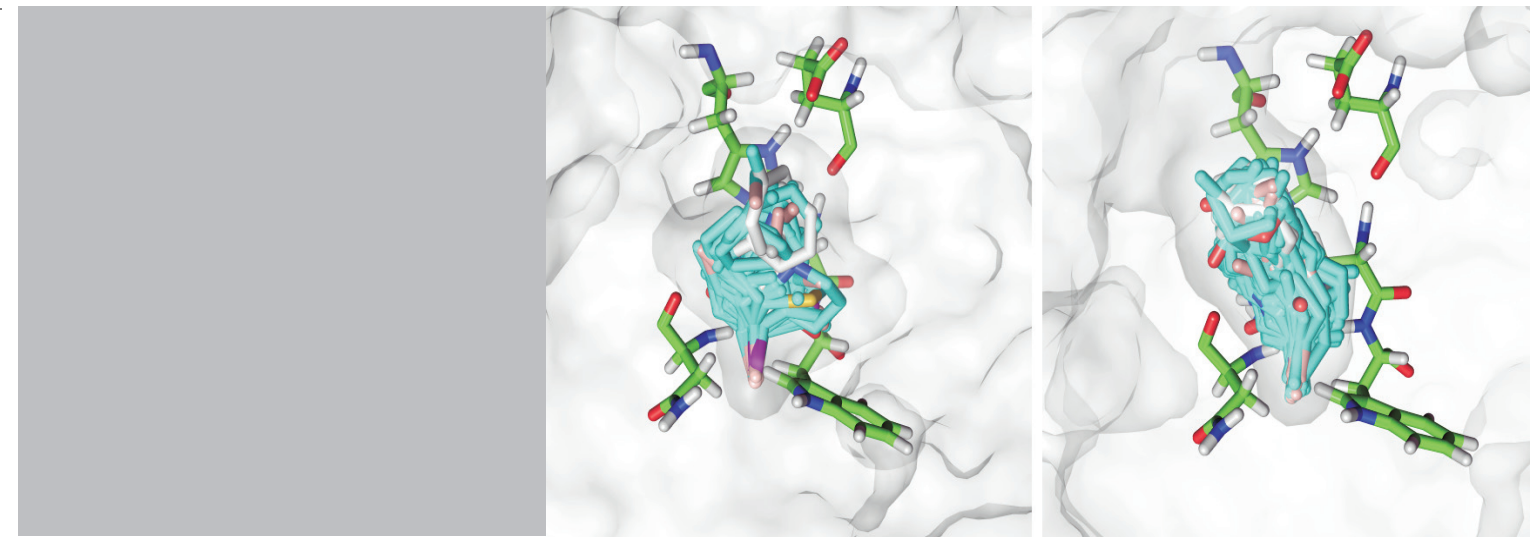
Joint teams are being formed:

- consisting of experts from both IT and user communities
- addressing specific research areas – both ad-hoc and long term work
- involving students (undergraduate and PhD)

## History

Supercomputing Centre Brno (SCB) is a part of Institute of Computer Science, Masaryk University. SCB was founded in 1994 as one of big supercomputing centres in the Czech Republic of that time. Similar cooperating centres were founded by other universities (Prague, Pilsen, Brno, Ostrava).

SCB has been working with Faculty of Informatics, Masaryk University, for a long time. The cooperation is both personal and factual, formally expressed, e.g., in a common research intent "Highly parallel and distributed computation systems".



Top 50 potential substrates of HLDs identified by virtual screening, Loschmidt Laboratories

### Mission

CERIT Scientific Cloud centre, the successor of Supercomputing Centre Brno at the Masaryk University, is a national centre providing flexible computational and storage capacities. Provision of these resources is complemented with extensive research activities, carried both in cooperation with user communities and in the e-Infrastructure area itself.

### Funding

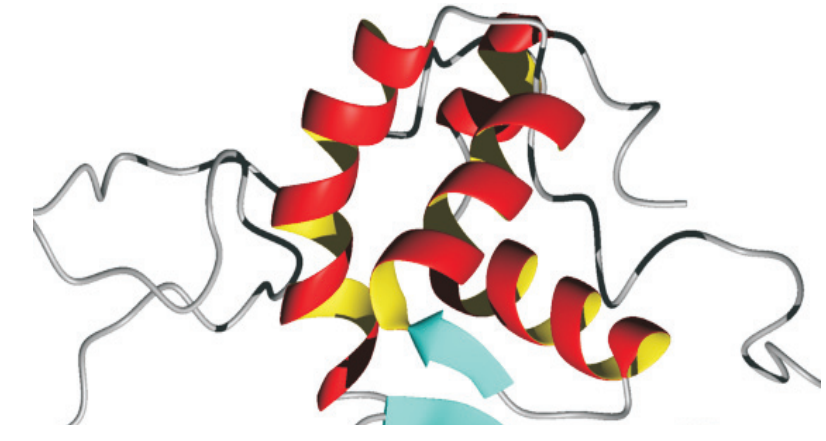
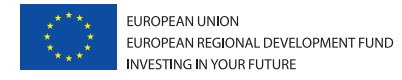
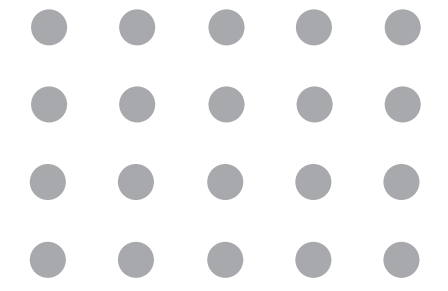
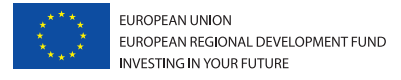
Transformation of SCB into CERIT-SC will be supported by a project of the 3rd axis of the RD&I Operational Programme. The project is being realised from May 2011 to October 2013. Its overall budget is 5 MEur. CERIT-SC is included in the Roadmap for Large Research, Development and Innovation Infrastructures in the Czech Republic.

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Molecule visualisation, CEITEC, National Centre for Biomolecular Research

