VOCE Achievements

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VOCE generic description

- **Virtual Organization for Central Europe**
- **VOCE provides complete grid infrastructure under the EGEE project umbrella**
- **VOCE officially registered as EGEE VO**
  - the first regional, catch-all VO in EGEE
- **VOCE spans the whole Central Europe federation**
  - core services operated by CESNET
  - resources are provided by many institutions across CE region

VOCE generic description

- **Current resource providers**

 **Austria**

 **Croatia**

 **Czech Republic**

 **Hungary**

 **Poland**

 **Slovakia**

- **Potential resource providers (CE region members)**

 **Belarus**

 **Slovenia**

VOCE generic description

- **CPUs statistics** => **8474 cores / 21 CEs ***
- **Storage statistics** => **196,7 TBs / 20 SEs ***
- **End users**

registered so far	642 **
active accounts (2009)	232 **
new accounts (2009)	173
extended accounts	59

* data taken from lcg-infosites tool

** data taken from Perun tool used for user management

VOCE utilization report

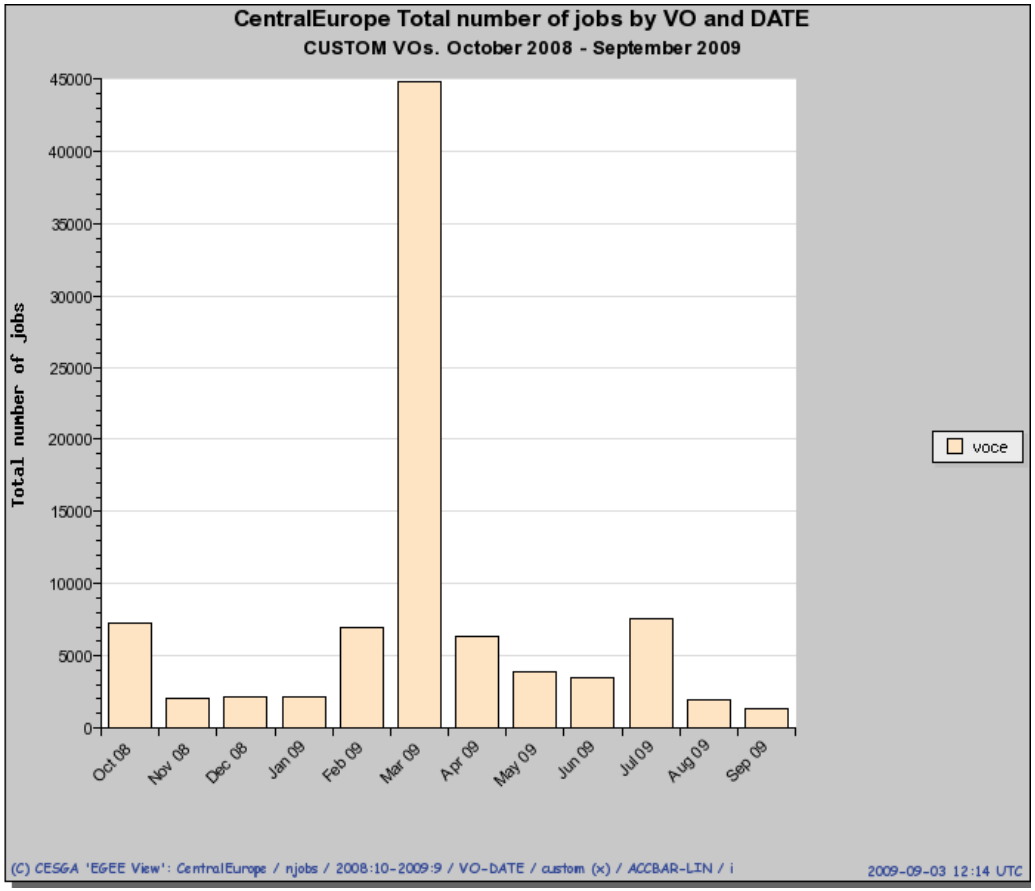
- **Application domains**

  testing jobs (collections, parametric or DAG jobs)
  free energy calculations, docking, MD/QC studies
  development of job submission portlets
  numerical astrophysics simulations
  phylogeny studies, plasma analysis
  porting applications to EGEE infrastructure

  => distinct application areas
  two type of usage (testing & production)

VOCE utilization report

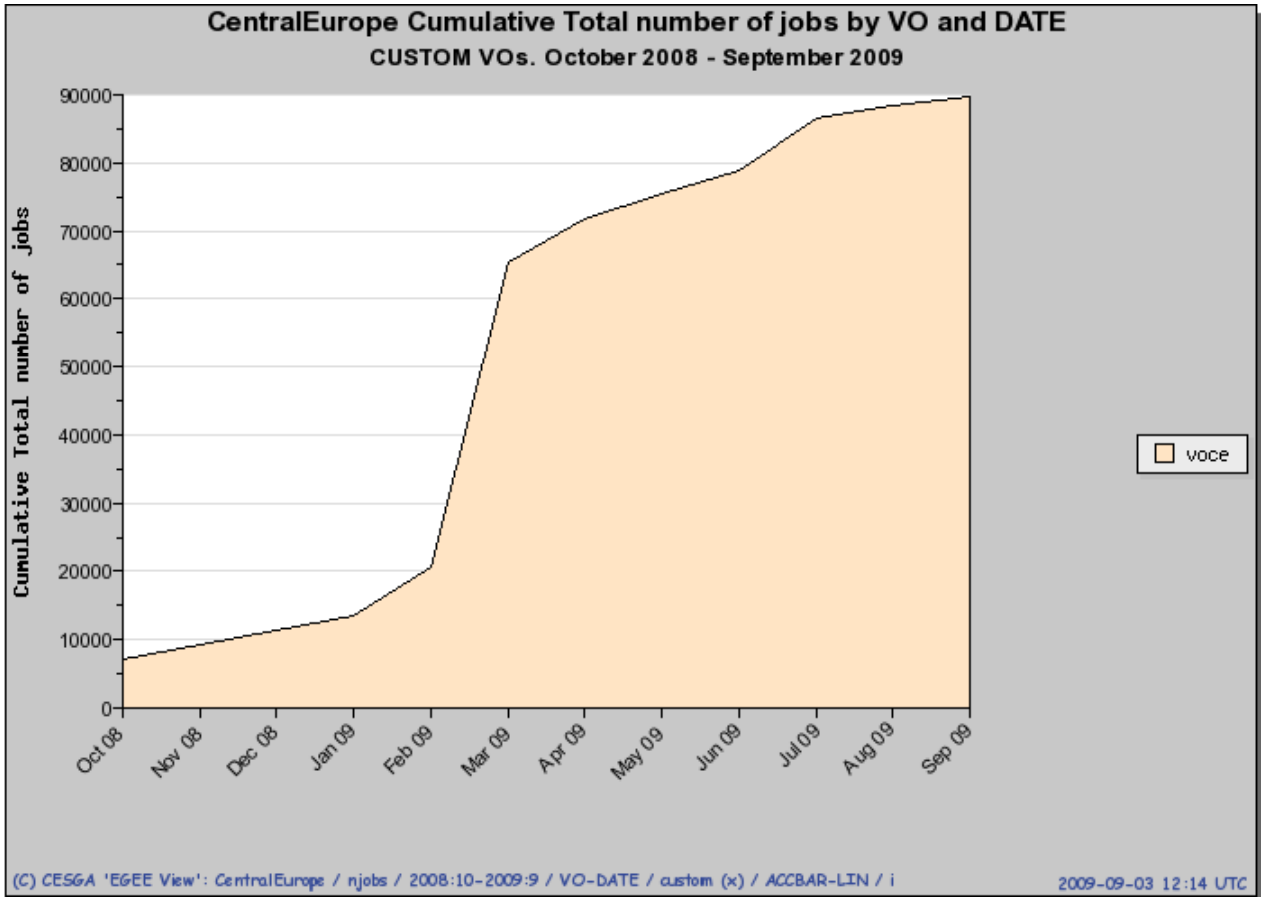
- **EGEE accounting portal ***



*** data from http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html

VOCE utilization report

- **EGEE accounting portal *****



*** data from http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html

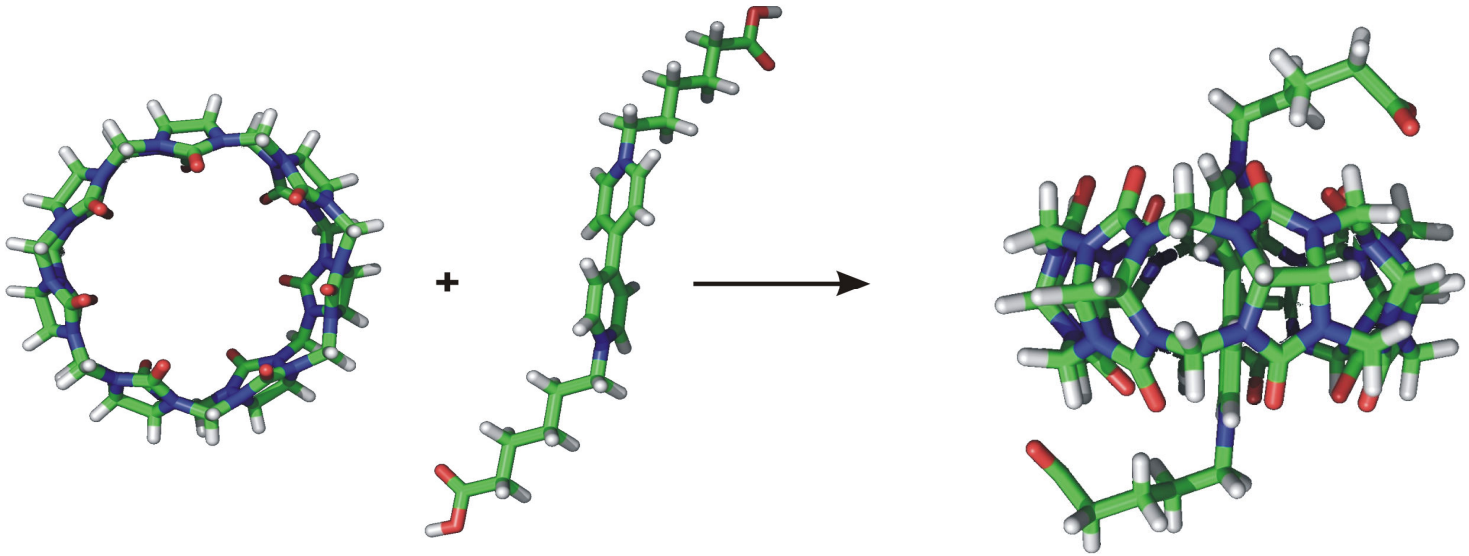
Computational challenges

- **Free energy calculations**
  - basis for the assessment of theoretical models towards experimental data
  - its calculation is still very time consuming task
  - very long simulations are usually necessary to obtain converged and reliable results

- **Accelerating free energy calculations**
  - several techniques were recently suggested and introduced
  - utilization of **Adaptive Biasing Force** (ABF) method accelerated by **Multiple Walkers Approach** (MWA)
    - parallel simulation of several replicas of studied system

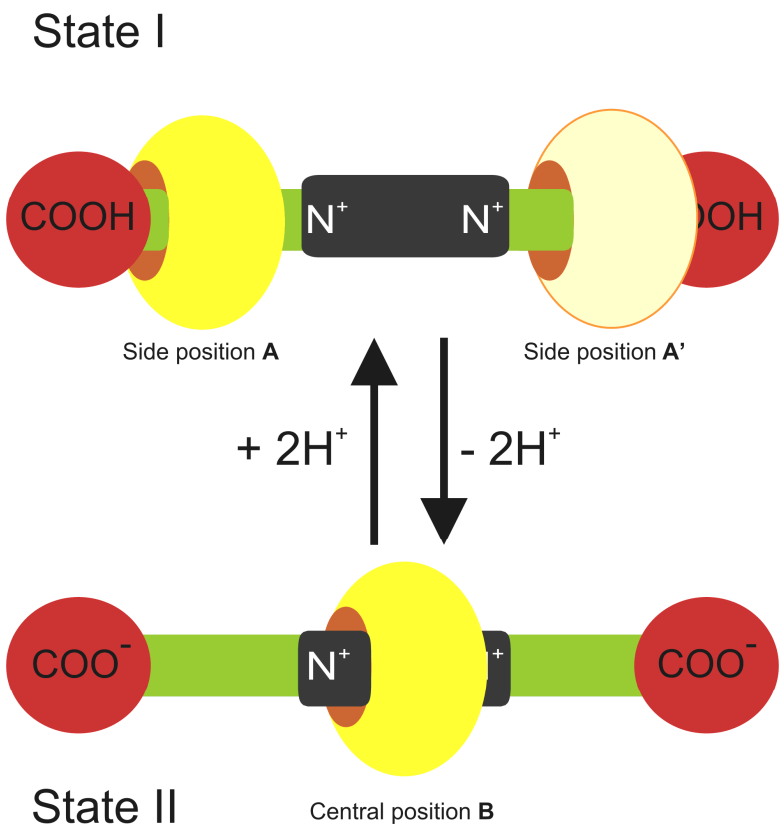
Computational challenges

- **Studied system - supramolecular complexes**
  - pseudorotaxanes - formed by a cyclic molecule (wheel) threaded on a string molecule (axle)
  - limited motion of both components to each other



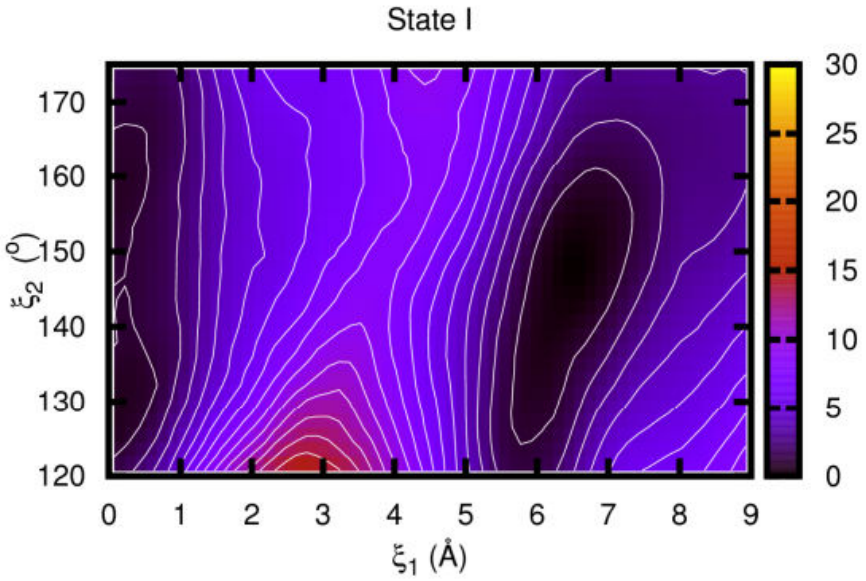
Computational challenges

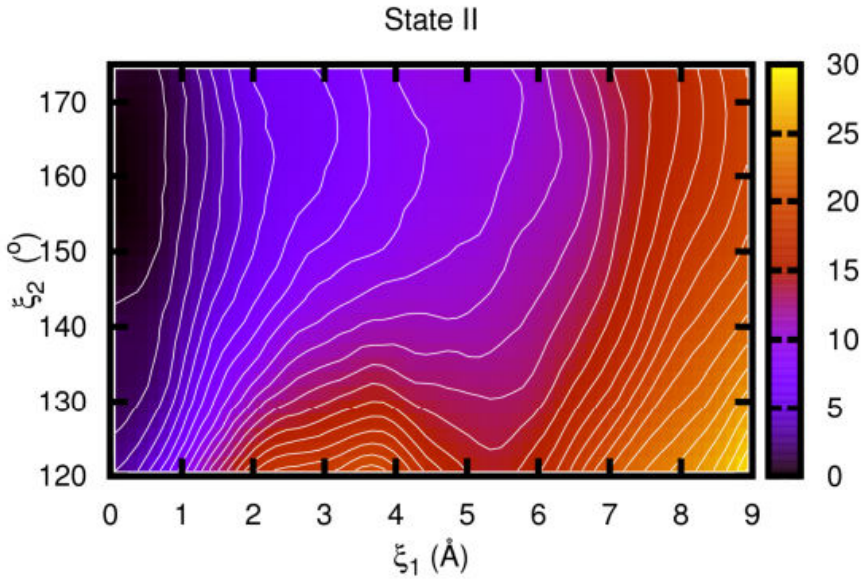
- **Key complex function**
  - protonation states of both axle terminal carboxylic groups can be changed by different pH conditions
  - pseudorotaxane system can be considered as a **molecular switch** which is switched on and off by different pH conditions



Computational challenges

- **Results**
  - detailed free energy profiles of pseudorotaxane complexes in water and ionic solution
  - confirmation of experimental observation (NMR, kinetic studies) concerning molecular shuttle process internals





Large Scale Free Energy Calculations as a Showcase of Worldwide Grid Usability

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Abstract

The free energy forms a basis for the assessment of theoretical models towards experimental data. However, its calculation is still very time consuming task. Recently, an implementation and testing of the multiple walkers approach accelerating such kind of calculations has been performed within the Czech National Grid. The Multiple Walkers Approach (MWA) is based on the exchange of reconstructed free energy potential among nearly independent simulations biased by Adaptive Biasing Force (ABF) method speeding up the whole calculation in almost linear fashion. Due to its nature – a massive set of independent jobs – this task is a suitable target for solution within the production grid environment available worldwide – the Enabling Grid for E-Science (EGEE) infrastructure.

Computational challenges

- **Results**
  - were obtained nearly 40 times faster compared to a conventional run due to employing 40 independent walkers utilized for every single job
  - EGEE worldwide Grid, VOCE in particular, creates a unique medium for performing **large scale, massive computations**
    - due to its nature well suited for execution of huge number of computational jobs
  - currently we are applying this approach to various complexes differed by wheel sizes and axle lengths