

# Abstracts book

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# CoPS - The Complex Comparison of Protein Structures supported by grid

## Overview :

The presentation shows results and benefits from a gridification of a data- and compute-intensive application CoPS, a system designed for complex comparison of protein structures using the Evolutionary Secondary Structures Matching (ESSM) algorithm. The CoPS is developed and used by the Baltic States research communities. Usage of the BalticGrid-II infrastructure significantly improve the outcome of the research. The CoPS is run within the Migrating Desktop -intuitive interface to Grid resources

## Analysis :

The CoPS application offers a method applied for exploration of potential evolutionary relationships between the CATCH protein domains and their characteristics and uses the so-called 3D graphs approach. This is a convenient tool which allows easy detection not only structural similarity but also possible fold mutations between these proteins. This method consists of two stages: 1) All-against-all comparison of CATCH domains by the ESSM software; 2) Construction of fold space graphs on the basis of the output of the 1st stage. This approach, useful in the exploration of basic tendencies in evolution of the protein structures and functions, is based on the assumption that protein structures, similarly to sequences, have evolved by a stepwise process, each step involving a small change in protein fold. The application gridified within BalticGrid-II is using the Protein DataBase (PDB) and comparing several proteins independently or in parallel.

## Impact :

The CoPS application uses BalticGrid-II computing infrastructure to compare protein structures. It can automatically identify different types of protein structure mutations between a pair of proteins. It should be noted, that for exploration of protein structures all-against-all comparison have to be done. Grid infrastructure is providing a possibility to process the whole protein database, for example the CATH database, where the number of pairwise comparisons is few billions. Due to the need of powerful computing resources and large network bandwidth, the CoPS is a good example of application which benefits from the usage of the BalticGrid-II infrastructure.

## Conclusions :

Development and implementation of this application will provide significant benefits and a clear starting point for other biologists, who are working with similar protein applications. The CoPS application is conspicuous for the large data amount (Protein database ~ 8GB), which is being used in every parallel job. The specific requirements of the CoPS application is a good motivation to create a separate VO, which would be later used by other biologists as well.

## URL :

<http://www.balticgrid.org>

## Keywords :

protein structures, grid computing, ESSM, Migrating Desktop, BalticGrid-II

## Demo details :

We intend to show a live-demo of the CoPS life cycle, starting from defining the input parameters, submitting the job to the BalticGrid-II testbed, job monitoring, and ending with visualization of the results. The application is run within the "Migrating Desktop" - advanced GUI that hides the complexity of the grid and makes access to the resources easy and transparent. We believe that the interesting scientific content combined with intuitive interface will attract the audience's attention.

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Track classification : Scientific results obtained using grid technology

Contribution type : Demo

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Submitted on Tuesday 09 December 2008

Last modified on : Friday 12 December 2008

Comments :