PROSIM: PROTEIN MOLECULE SIMULATION ON THE GRID

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Partners

- Centre for Parallel Computing, University of Westminster, UK
- School of Life Science, University of Westminster, UK
- Department of Life Sciences, Imperial College London, UK

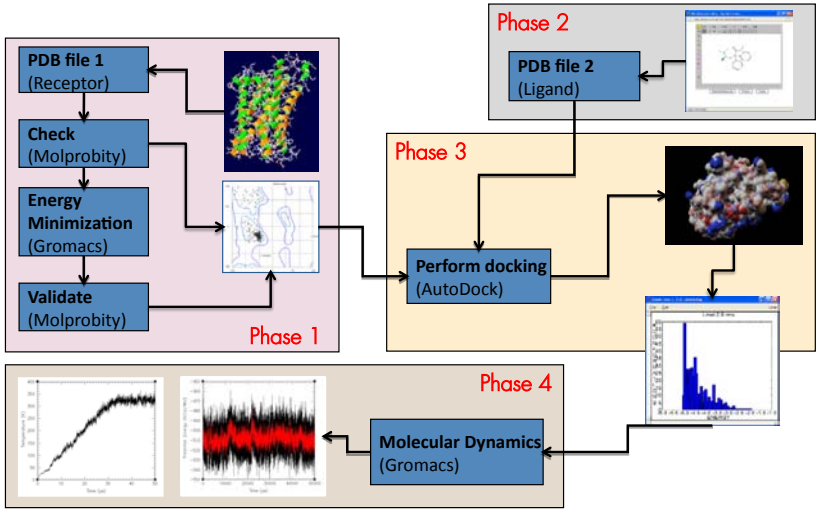
Website

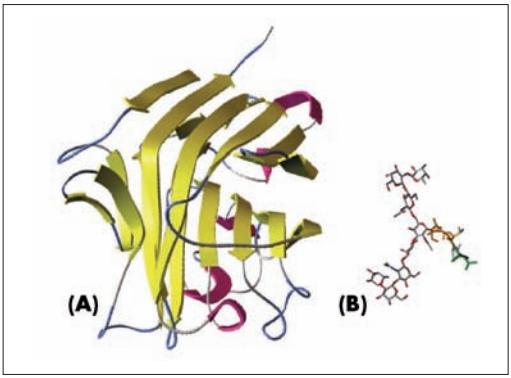
https://sites.google.com/a/staff.westminster.ac.uk/engage/Home

Synopsis

Protein molecule research is an area of great interest in bio-science but it requires many resources to run wet lab experimentation. Substrates are expensive and "wet" methodologies require access to sophisticated machinery. Introduction and validation of in silico tools would enable researchers to focus their resources and better plan experiments by allowing them to visualise potential interactions and determine the best molecules to investigate in the wet laboratory. This reduces time and cost but also increases the numbers of molecules screened.

In silico experiments are time consuming. They can take up to a few weeks or even a few months to be completed on a single computer. To speed up these experiments the ProSim projects ports these experiments to and runs them on the Grid. Considering that bio-scientists are not Grid experts, the computer scientists will provide seamless access to computer and data resources available on the UK National Grid Service (NGS) using a Grid portal to run simulations. The project will also exploit the Grid portal's ability to access





additional resources scattered amongst various other Grids, such as the EU Enabling Grid for E-SciencE (EGEE), the US Open Science Grid (OSG) and the US TeraGrid (TG), which also support international co-operation between researchers.

The project is a cross-domain one including a bio scientist and a computer scientist team. Computer scientists migrate the protein molecule simulation application as legacy code to the Grid creating Grid services. They also create workflow templates representing different low-level user scenarios and/or applications portlets corresponding to high-level user scenarios. The bio-scientists are able to select among these two options to run protein molecule simulations on the Grid. Workflow templates allow bio-scientists to modify these templates or create their own workflows, parametrise and run them. Application specific portlets hide even the workflow-level details. These enable users to very easily define their input parameters, run and monitor their experiments, and capture and visualise the results.

Developing the application portlets the ProSim project creates a simulation environment where bio-scientists even with a basic IT skills can run their simulations.

Brief USP

Proving that real scientists can easily use and benefit from DCI's using the P-GRADE portal.

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