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Molecular Dynamics and Docking Simulations Using Parameter Sweep Workflows

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Carbohydrate recognition is a phenomenon critical to a number of biological functions in humans. Computer programs which can provide insight into such biological recognition processes have significant potential to contribute to biomedical research if the results of the simulation can prove consistent with the outcome of conventional wet laboratory experiments. In order to validate these simulation tools and support their wider take-up by the bio-scientist research community high-level easy to use integrated environments are required to run massively parallel simulation workflows.

Detailed analysis

Modelling the interaction between receptors and ligands includes several steps where numerous scripts and simulation programs are utilized and the data is fed from one component to another. Working through such a complex scenario manually is a tedious process. Moreover, some of the steps require massive computing resources and the analysis of several parallel scenarios. First the receptor and the ligand file are selected, checked, energy minimized and validated. Next the docking parameters and the target grid-space are defined, followed by the actual docking simulations. The simulations are run on a predefined number of parallel branches (typically around 10 parallel simulations are executed) each of which perform a genetic algorithm of a set number of evolutions (typically around 100). The best results of these simulations are then selected and energy minimization and molecular dynamics is performed, again in a number of parallel branches, on every selected docking result. The above scenario has been implemented using the WS P-GRADE portal and its workflow engine, and the execution of components has been mapped to resources of EGEE and the UK National Grid Service.

Conclusions and Future Work

The implemented solution efficiently automates the process of executing and visualising complex molecular docking and molecular dynamics simulations in a grid environment, and providing a rich and easy to use interface for the biologist end-users. Future work includes the creation of more customized workflow scenarios using the already developed and also new workflow components as building blocks. While the first stage workflow was created with significant support from the technical team, it is envisaged that future development will be based more on specialist end-user involvement.

Impact

In order to increase the uptake of current e-Infrastructures new user communities with no Grid related knowledge have to be targeted. These researchers are reluctant to use this infrastructure due to its complexity and the very steep learning curve required. The aim of the above described work was to illustrate how high level Grid development and execution environments can be used to produce easy to use solutions with no or very minimal software engineering. These high level environments allow a small number of specifically trained researchers with more affinity towards software tools to serve the needs of larger user communities. The

created workflow allowed researchers at the University of Westminster UK to validate and fine tune their wet laboratory experiments and to provide useful feedback for the developers of the software tools regarding the appropriateness and usability of the products. Moreover, the developed environment can be efficiently used in teaching to allow students without specific grid related knowledge to utilise docking and molecular dynamics packages and to support the in-vitro experiments.

Keywords

Grid portal, grid workflow, molecular docking, molecular dynamics, simulation

URL for further information

https://engage.cpc.wmin.ac.uk

Justification for delivering demo and/or technical requirements (for demos)

The demonstration will show how the simulation workflows can be parameterized, customized, executed and visualized using the extended WS-P-GRADE portal. The demonstration requires internet connection

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