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InSilicoLab – grid environment for supporting numerical experiment in chemistry

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Overview

Although the capacity and technical advancement of computiational resources offered by the European computing centres is constantly improving, the progress in development of high-level tools facilitating access to those resources is still slow. In this paper, we present our approach to such high-level, customized environment, called InSilicoLab - designed especially for chemists who want to use Grid Infrastructure.

Impact

Computational Chemistry is one of the three science domains that utilise grid resources most - along with High Energy Physics and Biology. While many computing centres offer a variety of scientific packages for chemists, the use of these software suites is hindered by the lack of intuitive interfaces to them.
InSilicoLab, not only provides the users from the Computational Chemistry domain with easy access to Grid by the means of job management, but, more importantly, supports scientific experiment planning and evolution. While the first functionality is already offered by grid portals [1], and some aspects of the latter are covered by specialised tools invented for Computational Chemistry (like WebMO [2] or ECCE [3]), only expensive commercial User Interfaces (like Accelrys Material Studio [4]) join these features. Still, these proprietary tools are mostly desktop applications - what makes them inaccessible from outside a local computer and hinders collaboration.

Description of the work

InSilicoLab is a Web portal for the scientists from the Computational Chemistry domain who want to take advantage of Grid Resources. The portal allows them to create and manage scientific experiments and their results using terms specific to their domain of science.
The multi-layer architecture of InSilicoLab supports this domain-specific interaction by introducing a “scientific”layer, responsible for communication with the users, while a separate layer is reserved for communication with computational and storage resources. These two layers are

interconnected via a third - intermediate - layer, which processes and translates the objects and methods defined by the user to parallel grid jobs and/or calls to other services and tools required by the user. This separation of the domain- and grid-specific layers and concepts related to them makes the InSilicoLab portal more intuitive to users, enabling them to focus on their work instead of on the technical details of configuring the computation, and, thus, making their work more efficient.

URL

https://insilicolab.grid.cyfronet.pl

Conclusions

The InSilicoLab portal facilitates in-silico experiments performed with help of the most popular Computational Chemistry packages - Gaussian [5], GAMESS [6] and Turbomole [7]. The tool is available to any user with a valid Grid certificate registered in Gaussian VO [8] or vo.plgrid.pl (a Virtual Organization maintained by the Polish NGI - PL-Grid [9]). It can be accessed at http://insilicolab.grid.cyfronet.pl.

References:
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