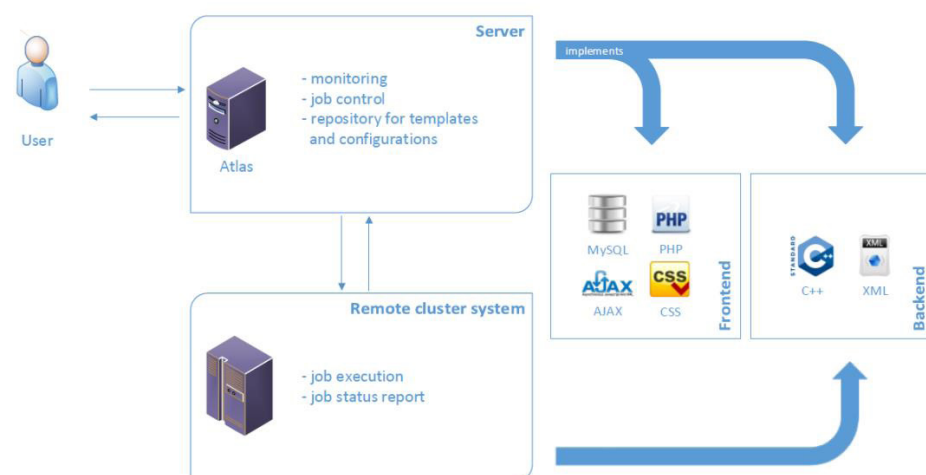# TECHNOLOGY OFFER

PROMETHEUS – PROfessional METhodes to Handle Efficiency Upgrades in Simulations

BACKGROUND

In cases where simulations differ only in the input files but are related logically it is time-consuming and error-prone to set up these simulations one after the other by human interaction. Although the required amount of work necessary to do so differs from one molecular simulations package to another, the GROMOS suite may be used as a representative: an experienced user has to invest up to three hours in the setup process, not to mention the time required to do the analysis afterwards which can be automatized by BASH scripts only in a limited way. In order to establish modern simulation techniques for a wide community and standard applications in e.g. industrial settings there is a need for standardized protocols and automated workflows.

TECHNOLOGY

There are webservers available for running straightforward simulations. However, as far as we know, there is no framework available which meets the flexibility, efficiency and controlling features or PROMETHEUS. For repeated tasks, one may use bash scrips for automatization. Although they are principle quite powerful, it can be difficult to understand them, to keep them up to date, to adapt them, to distribute them and to keep track of the actions performed since they are stateless. Moreover, specific tasks such as IO, blocking statements as well as error handling are not supported to a useful extend in these scripts. Typically such scripts are being redeveloped from scratch for every new simulation project, meaningful sharing and reusage among people is rare.

BENEFITS

- simulate biomolecules and analyze them automatized by computer scripts
- specific tasks such as IO
- webserver available for running straightforward simulations
- simplifies a structured approach and offers detailed progress monitoring and error report

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AVAILABLE FOR:
Investors

KEYWORDS:
- automatization
- hierarchic project management
- easy remote access
- batch job processing

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