Web-based MD Simulations using MoSGrid

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1 Introduction

Molecular simulations play an increasingly important role in the fields of chemistry, biology, physics and life sciences. Despite their importance most tool suites and applications are lacking a user-friendly interface and direct connection to high-performance or high-throughput compute resources (HPC/HTC). The molecular simulation grid (MosGrid; www.mosgrid.de) is a web-based science gateway bridging this gap and enabling easy access to molecular simulations [1].

2 MoSGrid

The gateway represents a multi-layered stack of different services needed to compose, submit, monitor and analyse simulations belonging to the domains of quantum chemistry, molecular dynamics or docking. The only component visible for users is the Liferay-based webpage, hiding the complexity beneath. In brief, MoSGrid relies on WSPGRADE/gUSE for workflow and job management, connected via the UNICORE middleware to HPC and HTC resources [2], using a federated storage solution based on XtreemFS. The authentication relies on personal X.509 certificates and trust delegation based on them. Currently access is possible for all researchers with an affiliation to a German research institution.

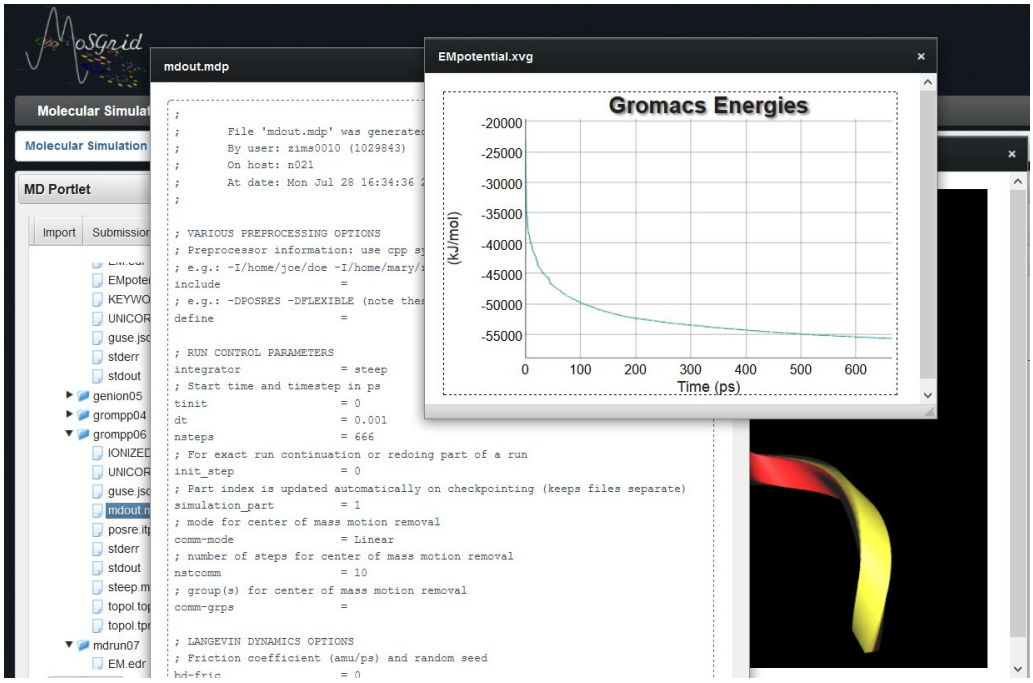

Figure 1: The MD portlet of the MoSGrid portal and some of its functionality are shown. In addition to monitoring and navigation capabilities, the visualization of molecules, numerical data and textual information is possible.

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3 Molecular Dynamics

The focus of the presentation will be on molecular dynamics (MD) simulations, while MoSGrid is able to support a variety of other simulation types. MD simulations in particular with GROMACS, follow a distinct pattern: a molecular input structure is pre-processed using multiple small applications, a job description is compiled, the actual simulation is carried out, the raw data is processed and analyzed [3]. Such a simulation protocol can be conveniently represented as workflow. The presentation will highlight all essential steps for such a typical MD workflow, from the simulation system preparation, over equilibration steps to the analysis of a production run.

In order to ensure full metadata annotation and storage of provenance information consequently ensuring full reproducibility a molecular simulation markup language (MSML) template is associated to each workflow. Furthermore this documents serves as basis to dynamically create the graphical user interface (see Figure 1). Workflows for different kinds of MD simulations are provided aiming at different scientific use cases and different levels of user expertise.

4 Outlook

The maintenance and extension of the MoSGrid is ongoing work. Depending on the needs of the community modifications, additions and extensions are planned and implemented. In the past auxiliary applications such as a direct UNICORE connection for the Cm2 MembraneEditor or APL@Voro were developed [4]. Current endeavour focuses on the connection to PRACE resources via UNICORE and the implementation of an US version of MoSGrid, enabling convenient access to XSEDE resources.

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