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Molecular dynamics of proteins in the cloud

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A key computational technique in Structural Biology is Molecular Dynamics (MD), a computer simulation of the motion of atoms and molecules as a function of time. MD simulations capture the behavior of biological macromolecules in full atomic detail using statistical thermodynamics laws. Such simulations serve as a computational microscope, revealing biomolecular mechanisms at various spatial and temporal scales.

In our work, we have implemented and tested a variety of approaches to the use of grid and cloud computational infrastructures for MD simulations. Previously, we implemented a web interface to setup MD simulations that were then executed on the European Grid Infrastructure [1]. We then exploited the technologies developed by the INDIGO-Datacloud project to expand both the types of computational infrastructures that can be used and the portfolio of services. For this we implemented the AmberTools suite [2] as a container for Docker. Next, we implemented the use of cloud storage resources to save trajectories and perform their analysis and comparison with experimental data, such as NMR order parameters. Cloud storage uses the Onedata solution, which can work with large files such as those typically output by MD simulations. Cloud computing can also be exploited for specific applications. The setup of simulations and analysis are still performed via web interfaces, so that the user does not need to know which kind of infrastructure is used. For this use the FutureGateway, a programmable interface of a RESTful API Server developed within INDIGO-Datacloud. The availability of these new solutions to support MD simulations allows non-expert users to get access to standardized protocols for state-of-the-art calculations and analysis that enable the successful application of MD with a low learning barrier. The solutions are available also through the West-Life Virtual Research Environment for Structural Biology [3].

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[1] A Grid-enabled web portal for NMR structure refinement with AMBER. Bertini I, Case DA, Ferella L, Giachetti A, Rosato A.
[2] http://ambermd.org/
[3] http://about.west-life.eu/

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