

BioSimGrid: a distributed environment for archiving and analysis of biomolecular simulations

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The comparison of simulations carried out by different packages or in different labs is logistically difficult due to high volumes of data, proprietary data formats, variety of tools available to analyse the data, and lack of sharing of the data. The Biosimgrid project is developing a software environment to address these issues. With Biosimgrid we provide not only a distributed repository in which we store these large trajectories but also a common environment where they may be analysed with a range of system-supplied or user-supplied tools. The trajectories may be queried by other workers on the basis of their associated metadata. We have developed routines to automate deposition of trajectories from NAMD, Charmm, GROMACS and Amber and demonstrate the strength of the Biosimgrid environment by analysing different biosimulation trajectories using our standard toolkit. The results may be displayed in a variety of different formats to allow their easiest possible interpretation.