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Virtual Organisation for Central Europe (VOCE) achievements

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Abstract

One of the crucial concepts allowing seamless utilization of any advanced research e-infrastructure - the worldwide EGEE Grid in particular - is the so-called "catch-all" virtual organization (VO) approach. Nowadays, the catch-all virtual organizations represent an effective way for end users to fully exploit the potential of e-infrastructures. Catch-all VOs are provided as a service to users communities as part of user support activities of several projects. Catch-all VOs bind together resource providers and different end user communities creating a worldwide grid platform easily available to users. Decreasing the entrance barrier is especially important for various regions with high heterogeneity and different grid knowledge of involved parties. Here we describe Virtual Organization for Central Europe (VOCE) - the catch-all VO service offered to all researchers from Central Europe region. VOCE proved the usability of the concept through its several years of existence by supporting general applications ranging from molecular modeling through phylogeny studies, plasma analysis up to astrophysics. Apart from individual routine utilization for daily research production it also supports challenging computational campaigns of various kinds.

One of such important areas is the application and implementation of novel methods for the free energy calculations. The free energy is an important thermodynamical quality used in biochemical and chemical disciplines. It forms an essential connection between theoretical models and experimentally observed data. Unfortunately, its calculation requires very long simulations to obtain converged and reliable results. Several method were suggested and developed to overcome this well-known sampling problem. One of them is Multiple Walkers Approach [1] (MWA) connected with Adaptive Biasing Force (ABF) method [2]. Both implemented methods were applied in the study of supramolecular complexes. The study resulted into large-scale free energy calculations allowing to obtain detailed insight into interactions taking place in supramolecular structures.

References

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