PI-GC-AdResS Sims

Application of Adaptive Resolution simulations and related schemes on Path-Integral Molecular Dynamics Simulations of fullerene in water

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In Short

- Multiscale Simulations
- Path Integral Simulatinos
- GC-AdResS
- PI-GC-AdResS

In our E-CAM project (CECAM-DE-MMS), our goals are to optimize (performance-wise) and generalize an established GROMACS based Adaptive resolution simulation (GC-AdresS) algorithm. Currently, we have a simplified and faster version of GC-AdResS available which has been tested on small water systems.

We want to use our new implementation and apply it to Path-Integral molecular dynamics (PIMD) simulations of water systems. There are two reasons for this, one is performance/accuracy data point for the new code. The other, more essential part, is a scientific one. Studies of 2 fullerene in water with SPC/FW 1 water models show that water-mediated processes can be captured and reproduced. SPC/FW is a very simple model, we want to expand those previous studies to more complex flexible, quantum/path-integral water models with PI-GC-AdResS (PIMD in GC-AdResS). Using those models we want to simulate 2 fullerene in water, and study their aggregation. A systematic study of this process with respect to the used models via PI-GC-AdResS is absolutely innovative and at the same time possible because GC-AdResS is very efficient computationally. We estimate a speed-up with respect to a full PI-MD Simulations of up to a factor 10.

All the simulations will be performed by high-performance molecular dynamics simulation package GROMACS with some slight modifications, which have the requirement to not effect the overall efficiency of GROMACS. The purpose of our current implementation is to even increase the performance of the existing one.

WWW

http://userpage.fu-berlin.de/dellesite/acti_new.html

More Information

[1] A. Agarwal, L. Delle Site, J. Chem. Phys. 143, 094102 (2015); A. Agarwal, L. Delle Site, Comp. Phys. Comm., 206, 26-34 (2016); A. Agarwal, L. Delle Site, Phys. Chem. Chem. Phys. 19, 13030-13037 (2017).