Combination of a Quantum Mechanics/Molecular Mechanics scheme with Multiple Time Steps with Guided Molecular Dynamics for the calculation of Free Energy Profiles in solution

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The study of reaction mechanisms in condensed phases requires to describe the active site at a quantum mechanical level, and also the inclusion of explicit environment. Because of the high computational cost of ab-initio methods, the entire system can not be treated at quantum level. To solve this, in the past decade, various hybrid schemes (quantum-classical) have been developed, allowing the study of reactions in solution or enzymes to a reasonable computational cost.

This work seeks to implement an efficient method for calculating free energy profiles for these type of reactions, based on the differential requirement of relaxation time of sub-reactive systems, treated at the quantum level, and the environment, treated classical level (multiple time steps).

In this work we show the preliminary results of the implementation of this multiple time steps scheme in the AMBER code. We will show the free energy profiles for a few systems in solution, and the improvement achieved by these new implementacion.