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Free Energy from Adaptive Reaction Coordinate Forces: a method for generating well sampled multidimensional free energy surfaces

Free energy has always served as a necessary measure for understanding chemical reactions, particularly knowing whether a reaction will occur spontaneously, but it is also a useful quantity when considering equilibrium systems, revealing qualities such as mean distances and preferred orientations. However adequate sampling of full multidimensional free energy surfaces from molecular dynamic simulations presents several problems the most important of which is that regions of high energy are rarely, if ever, sampled on normal timescales.
The Scientific Computing Research Unit has recently developed a new method [1] to generate complete multidimensional free energy surfaces from MD simulations, based upon umbrella sampling and flat histogram methods. It also integrates the weighted histogram analysis method to allow for multiple simultaneous parallel simulations to run and combine free energy information. Intended to easily integrate into most common MD software packages, this method is capable of utilizing HPC hardware, such as multicluster CPUs running OpenMP, to pot

Presenter Biography

Primary author: BRUCE-CHWATT, Tomas (University of Cape Town)

Co-author: NAIDOO, Kevin J. (University of Cape Town)

Presenter: BRUCE-CHWATT, Tomas (University of Cape Town)

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