Effective potentials from complex simulations: a potential matching algorithm and its application on Reverse Monte Carlo data

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The projection of complex interactions onto simple distance or angle-dependent classical mechanical functions is a long-standing theoretical challenge. One can find several theoretical attempts mostly in the field of colloid science concerning bio-molecules, aggregates and simple cases as the asymmetric binary hard-sphere models. The construction of an effective potential may base on theoretical assumptions, on the application of fitting procedures or inverse methods on experimental data, and on the simplification of complex molecular simulations. Recently, a force-matching method was elaborated to project the data of Car-Parrinello *ab initio* molecular dynamics simulations onto two particle classical interactions[1]. The method was successfully applied on different systems.
We developed a potential matching algorithm as a practical analogue of this force-matching algorithm. The algorithm requires a large number of configurations (particle positions) and a value of potential energy for each configuration. We show the details of the algorithm and test calculations on simple systems.
The application of the algorithm on reverse Monte Carlo configurations is also discussed. We present some possibilities to define fictive energies to the reverse Monte Carlo configurations on the basis of statistical analysis of different quantities obtained from Metropolis and reverse Monte Carlo simulations.

[1] S. Izvekov, M. Parrinello, C. J. Burnham, G. A. Voth, J. Chem. Phys. 120, 10896 (2004).