Dynamic Histogram Reweighting

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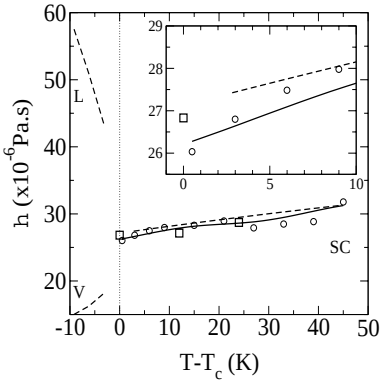
The histogram reweighting (HR) technique[1] is widely used in the determination of thermodynamic equilibrium properties of many-body systems from a reduced amount of Monte Carlo data. In this work [2] we address the problem of how the HR method can be extended to equilibrium dynamic properties, from molecular dynamics simulations. Let $\Gamma[t;\Gamma']$ be the set of all positions and momenta at the time t, as obtained from a set of Molecular Dynamics simulations $\alpha = 1,\ldots,N$ MD at different T_α temperatures. Then correlation functions of two observables A and B as well as transport coefficients at a given, yet arbitrary temperature T, can be obtained as

$$\langle A(t)B(0)\rangle = \int d\Gamma'\, A(\Gamma[t,\Gamma'])B(\Gamma')P_{eq}(\Gamma') \simeq \sum_{\alpha=1}^{N}\sum_{\Gamma'_{i_\alpha}} \left(\frac{A(\Gamma[t,\Gamma'])B(\Gamma')P(\Gamma'_{i_\alpha},T)}{\sum_{\alpha=1}^{N}\Lambda_\alpha P_\alpha(\Gamma'_{i_\alpha},T_\alpha)} \right)$$

In the figure we ploted HR data of the viscosity of Ar near its critical point (solid line) versus independent MD simulations (symbols), and experiments (dashed)



[1] A.M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).

[2] C. Nieto-Draghi, J. Pérez-Pellitero and J. Bonet Avalos, Phys. Rev. Lett. **95**, 040603 (2005).