Tailoring molecular potentials for dynamics using quasi-elastic neutron scattering

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As experimental techniques are used to probe increasingly complex systems, subtle emergent behaviour can lead to significant difficulties when interpreting the data. This is particularly evident in quasi-elastic neutron scattering (QENS), where simple analytical models may be unrepresentative of the underlying dynamics. By augmenting QENS with molecular dynamics (MD) or other simulation techniques, it is possible to observe this complex behaviour. However achieving agreement between scattering and simulation is frequently challenging; a significant source of the disparity is because intermolecular potentials are commonly established using structural rather than dynamical data, and often only at ambient conditions. In order to address this problem, we are in the process of developing an algorithm which can be viewed as a dynamical hybrid of the highly regarded EPSR and RMC methods. This approach uses Monte Carlo methods to minimize the difference between MD and neutron observables (both dynamical and structural) by optimizing the intermolecular potential parameters. Here we describe the underlying algorithm and present our initial results on water.