Evaluating Molecular Dynamics Simulations by Comparison with NMR Experiments

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Molecular dynamics simulations and NMR spectroscopy provide complementary approaches to the study of protein structure and dynamics. We have carried out several long molecular dynamics simulations of globular proteins and compared the results to a range of NMR experiments that probe the structure and dynamics of these proteins. Such comparisons allow for the evaluation of the quality of the simulations and at the same time provide an atomistic interpretation of the NMR experiments. Comparison of the results obtained using different commonly used molecular mechanics force fields show that recent modifications of these force fields significantly improve the agreement between simulation and experiments. We have also used such comparisons to validate molecular dynamics integration algorithms both on commodity hardware and on Anton, a massively parallel special-purpose supercomputer.