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Replica Exchange Molecular Dynamics in the Age of Heterogeneous Architectures

ADRIAN ROITBERG, University of Florida

The rise of GPU-based codes has allowed MD to reach timescales only dreamed of only 5 years ago. Even within this new paradigm there is still need for advanced sampling techniques. Modern supercomputers (e.g. Blue Waters, Titan, Keeneland) have made available to users a significant number of GPUS and CPUS, which in turn translate into amazing opportunities for dream calculations. Replica-exchange based methods can optimally use this combination of codes and architectures to explore conformational variabilities in large systems. I will show our recent work in porting the program Amber to GPUS, and the support for replica exchange methods, where the replicated dimension could be Temperature, pH, Hamiltonian, Umbrella windows and combinations of those schemes.