Scaling of Multimillion-Atom MD Simulation on a Petascale Supercomputer

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Poster Abstract

This poster outlines a strategy for all-atom molecular dynamics (MD) simulation of multimillion-atom biological systems, using lignocellulosic biomass as test system. In the era of petaflop supercomputers, such simulation is limited by the parallel efficiency of the MD algorithms. The bottleneck for highly-parallel all-atom simulations is the computation of the electrostatic interactions. To overcome the limitations of the commonly-used Particle Mesh Ewald we present the performance and accuracy of the reaction field (RF) method for electrostatics. Comparison of RF and PME simulations of cellulose and water show very good agreement. The RF method enables simulation to be performed of a 3.3 million atom system yielding 27.5ns/day