Scaling of Molecular Dynamics Simulation of Lignocellulose on ORNL Supercomputer

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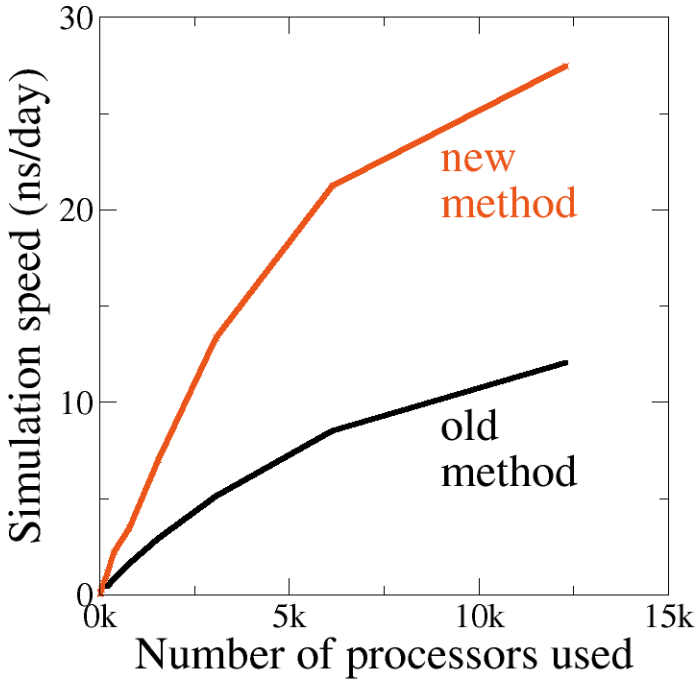
- **Objective: develop technology for multiple-length scale computer simulation of lignocellulose to compliment neutron scattering experiments in understanding structural changes during biomass pretreatment.**
- **Prior to our work the simulation of large biomass-like models was hindered by inefficiency in calculations employing >5k processors in parallel.**
- **ORNL researchers have significantly improved the parallel efficiency of molecular dynamics simulation leading to a 2.5-fold increase in simulation speed.**
- **Impact: increase the time- and length-scales accessible to simulation, enabling interrogation of larger and more complex biomass model systems.**
- **As a result, one of the largest reported biological molecular dynamics simulation was performed at ORNL Jaguar supercomputer. Lignin re-precipitation on cellulose after pretreatment was examined, a process that greatly contributes to recalcitrance of biomass to hydrolysis. Length scales probed vary from 0.1 nm to 100 nm.**



R. Schulz, B. Lindner, L. Petridis, J.C. Smith; Journal of Chemical Theory and Computation ***2009*** *5, 2798-2808*