A Multi-Scale Approach to the Simulation of Lignocellulosic Biomass

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In concert with the imminent increase in the Department of Energy’s (DOE) leadership supercomputing power to the petaflop range, the objective of this project is to develop multiscale methods for extending the time- and length-scales accessible to biomolecular simulation on massively parallel supercomputers. This project also aims to apply the developed multiscale approaches to obtain an understanding of the structure, dynamics and degradation pathways of extended cellulosic and lignocellulosic materials. Information from multiscale simulation, when closely integrated with experiment, will provide fundamental understanding needed to overcome biomass recalcitrance to hydrolysis. In this poster, we will describe the development of multiscale simulation methods and their application to solve critical problems needed for understanding the bottleneck in cellulosic ethanol production: the recalcitrance to hydrolysis of lignocellulosic biomass. The multiscale methodologies span from accurate quantum-chemical techniques, needed to understand critical local interactions in biomass, to atomistic and coarse-grained simulations, needed to approach systems-level phenomena.