ORNL TITAN supercomputer used to determine molecular mechanism of lignin’s adverse effect in biofuel production

Objective:
• Elucidate mechanism by which lignin hinders cellulases in converting biomass into biofuels and bioproducts.

Approach:
• Molecular dynamics (MD) simulations performed of a biomass system containing lignin, cellulose fibers of different degrees of crystallinity and the cellulase Cel7A.
• One of the largest MD simulations ever performed, run using 20% of the ORNL TITAN supercomputer under an INCITE award.

Results:
• Lignin binds preferentially both to the elements of cellulose to which the cellulases also preferentially bind (the hydrophobic faces) and also to the specific residues on the cellulose-binding module of the cellulase that are critical for cellulose binding.
• Lignin thus binds exactly where for industrial purposes it is least desired, providing a simple explanation of why hydrolysis yields increase with lignin removal.

Significance:
• This molecular-level description may be used to rationally optimize biofuel production processes which minimize lignin interference, for example, by devising pretreatments that lead to noncrystalline cellulose, which associates less with lignin than the crystalline form.

Part of the BER Biofuels SFA at ORNL


Models obtained from MD simulation of cellulose (green), lignin (brown) and cellulase Cel7A (orange). The overall system size is 20M atoms. This research is funded by the Genomic Science Program, Office of Biological and Environmental Research, U.S. Department of Energy. An award of computer time was provided by the INCITE program under Contract DE-AC05-00OR22725.