Cellulosomes in Action: Peta-Scale Atomistic Bioenergy Simulations

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Abstract.
Cellulosic ethanol has the potential to satisfy 30% of our transportation fuel demand, unlike corn-based ethanol, which is expected to be insufficient. A key step in the production of ethanol is the degradation of cellulose, the tough material in plant cell walls that exists in the form of two-dimensional crystalline sheets. Bacteria have evolved an efficient mechanism to degrade cellulose, employing a suite of nanomachines called cellulosomes. These are essentially designed to degrade of the two-dimensional crystalline sheets of cellulose; however, they must also work in the midst of the degradation products when the sheets have disintegrated into more amorphous structures. Once degradation has commenced, the changes in the morphology of the cellulose interfere with effective degradation. RoadRunner will be used to simulate the process of cellulosome migration through partially processed cellulose, shedding light on one of the key bottlenecks in cellulosic ethanol production. We will address the question, (1) What parts of the cellulosome machine interact with what parts of cellulose?, and (2) How do these interactions differ between the crystal-like phase, the partially degraded phase and the amorphous phase of degradation? (3) How does the presence of several cellulosomes affect this process?