A New Era in Computational Biology

Klaus Schulten

A Q&A with Klaus Schulten, professor of physics, The University of Illinois at Urbana-Champaign

Tell us about your early user experience on Stampede?

We are extremely excited about the strong computational power of Stampede. It is the fastest machine we have experienced right away, and we have performed a lot of interesting scientific computational experiments on the machine.

What types of problems are you using Stampede to solve?

With the advanced computational power of Stampede, we performed molecular dynamics simulations on biomolecules as a "computational microscope." We aim to not only unravel fundamental problems such as how a "newborn" protein folds, but also solve today's pressing questions, like designing enzymes to produce second-generation biofuels.

Texas Unleashes Stampede

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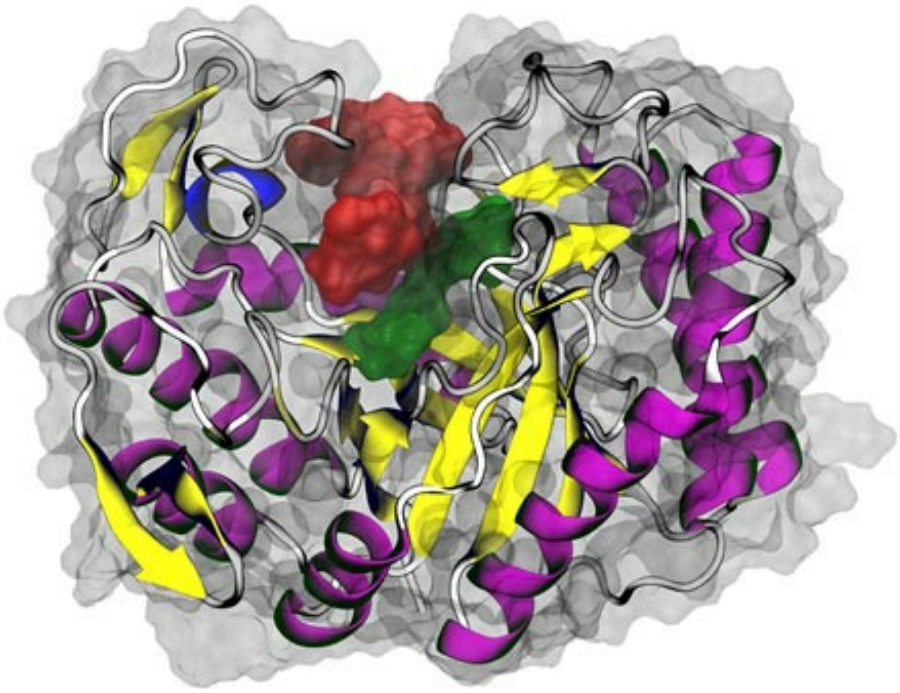
What science questions can a nearly 10-petaflop system like Stampede help answer in your field?

With such an advanced computational system, a new era in computational biology starts. We can now use biomolecular simulations as a computational microscope to observe long biological events that were hard to access before, and to relate molecular structures and interactions with their biological functionalities.



Biofuels are among the most studied alternative sources of fossil-derived fuels, particularly due to their smaller effect on greenhouse gas accumulation. Interest in the so-called second-generation biofuels has increased recently because they can be produced using the waste of agricultural production. Enzymatic hydrolysis to release carbohydrates units from plant cell wall polysaccharides has been one of the most promising strategies to produce these new renewable biofuels, but the natural resistance of the plant biomass makes the industrial process not cost-effective. To address this problem, Schulten and his research team are performing a joint computational and experimental study to unravel the mechanism of biomass degradation by cellulases, the enzymes found in some microbes that can digest plant fibers.