Stampede Supercomputer Powers Innovations In DNA Sequencing Technologies

June 25, 2014

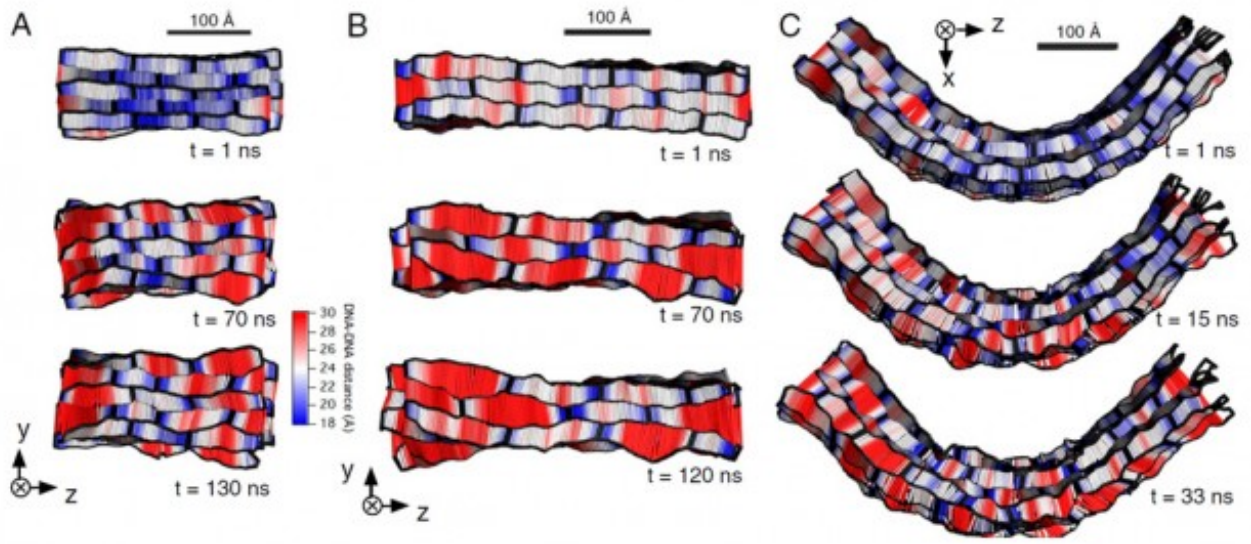

Image Caption: Molecular dynamics of DNA origami. The image shows two stages in the temporal evolution of synthetic DNA nanostructures imaged through all-atom molecular dynamics simulations on Stampede. Scientists believe DNA origami will permit easy fabrication of nanoscale objects. Credit: Jejoong Yoo and Aleksei Aksimentiev, Department of Physics, University of Illinois

Aaron Dubrow, National Science Foundation

Aleksei Aksimentiev, a professor of physics at the University of Illinois-Urbana Champaign, used the National Science Foundation-supported Stampede supercomputer to explore a cutting-edge method of DNA sequencing. The method uses an electric field to drive a strand of DNA through a small hole, or "nanopore," either in silicon or a biological membrane.

By controlling this process precisely and measuring the change in ionic current as the DNA strands move through the pore of the membrane, the sequencer can read each base pair in order.

"Stampede is by far the best computer system my group has used over the past 10 years," Aksimentiev said. "Being

able to routinely obtain 40-80 nanoseconds of molecular dynamic simulations in 24 hours, regardless of the systems' size, has been essential for us to make progress with rapidly evolving projects."

Aksimentiev and his group showed that localized heating can be used to stretch DNA, which significantly increases the accuracy of nanopore DNA sequencing. In addition, he and his team used an all-atom molecular dynamics method to accurately describe DNA origami objects, making it possible to engineer materials for future applications in biosensing, drug delivery and nano-electronics. These results were published in *ACS Nano* and the *Proceedings of the National Academy of Sciences*.

Source: Aaron Dubrow, National Science Foundation