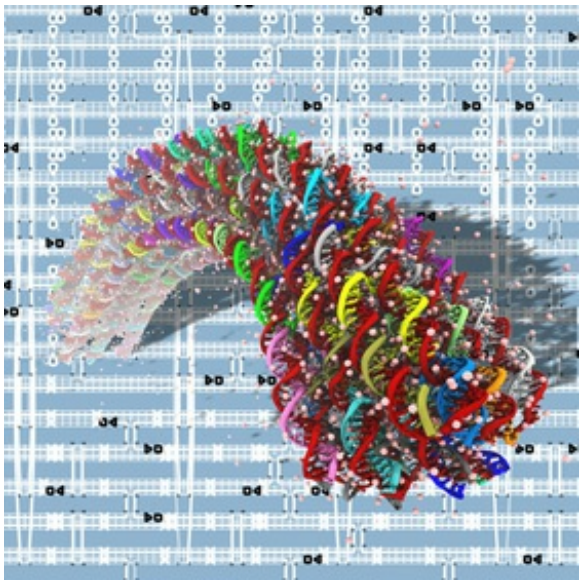
Aksimentiev's team demonstrates DNA origami bends and twists in solution

By Siv Schwink
November 27, 2013

Associate Professor Aleksei Aksimentiev

DNA has been used as a nanoscale construction material in scientific experiments since the early 1980s. The invention of DNA origami—the deliberate folding of long viral DNA strands into two or three dimensional shapes using several smaller DNA segments as "staples"—opened up new potential for nanoscale applications, such as advanced drug delivery vehicles and enzyme immobilization; at the same time, it provided experimental physicists with greater design control over nanoscale DNA structures, which are frequently used as scaffolding material to support other molecules.

Scientists have successfully imaged DNA origami structures, but until now, no one had ever seen how the structures behave in the aqueous environment used to make them.



Pictured is an atomic-scale model of DNA origami consisting of a long scaffold strand (red), stapled together by short fragments of DNA (various colors). The background image shows the blueprint of the structure. Yoo and Aksimentiev used a large supercomputer system to describe behavior of such DNA nanostructures in solution, elucidating their intrinsically dynamic nature. Image courtesy of Aleksei Aksimentiev

Now, University of Illinois physicists at the Center for the Physics of Living Cells have for the first time uncovered the atomic structure and dynamics of DNA origami within an aqueous solution. Associate Professor Aleksei Aksimentiev, working with postdoctoral researcher Jejoong Yoo, designed a simulation modeling and analysis program and ran it on the Stampede supercomputer at the Texas Advanced Computing Center (TACC) in Austin, TX. Aksimentiev accessed Stampede through the Extreme Science and Engineering Discovery Environment (XSEDE) project, an NSF-funded digital research services ecosystem that allows researchers free access to some of the world's most powerful supercomputers and expert help staff.

The team's findings are reported in *Proceedings of the National Academy of Sciences,* "In situ structure and dynamics of DNA origami determined through molecular dynamics simulations," published online ahead of print on November 25, 2013.

"DNA origami permits easy fabrication of nanoscale objects with a high level of resolution and reproducibility," explains Aksimentiev. "Experimentally, people just mix the stuff and it falls into whatever shape they want."

“The custom program we wrote took the design of a DNA origami structure and converted it to an all–atom representation, then placed it in an aqueous environment. Our simulations show how a structure that was at first a static geometrical design is actually quite dynamic and undergoes structural fluctuations. These conformational fluctuations reveal the local mechanical properties of DNA origami in solution: its propensity for bending and twisting at the nanoscale.”

DNA origami structures are designed using computer modeling programs, so the team’s findings are a game changer—this new understanding of dynamics will improve the structural integrity it’s possible to achieve within DNA origami. Aksimentiev and his team will use the new atomic-modeling method to further their studies of nanopore sequencing of DNA and proteins.

“Understanding the local mechanical properties of DNA origami structures will help us to design new structures, including scaffolds for nanoelectronic applications or advanced drug delivery vehicles,” said Aksimentiev.

This research was funded in part by grants from the National Science Foundation (DMR-0955959, PHY-0822613, and ECC-1227034) and the National Institutes of Health (R01-HG005115). The conclusions presented are those of the scientists and not necessarily those of the funding agency.

If you have questions about the Department of Physics or ideas for other stories, contact Siv Schwink, 217.300.2201