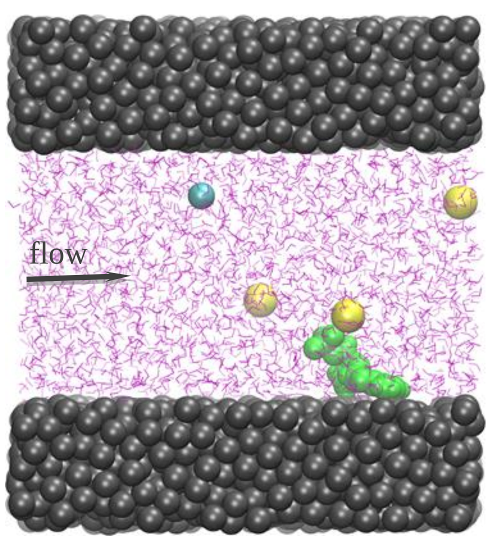
Atomistic Simulations Show Proof of Concept for a Novel DNA Sequencing Technology

Outcome: Louisiana State University Professors Dorel Moldovan, Dimitris Nikitopoulos, and Steven Soper, together with their postdoctoral researcher Brian Novak and graduate student Kai Xia, have demonstrated, using atomic scale simulations, the feasibility of a novel DNA sequencing technology based on cutting a DNA strand into single units (nucleotides) and then measuring their times of passage ("times of flight") as they move through a 3 nanometer wide slit, a few microns long. Their NSF LA-SiGMA funded studies of flow of nucleotides through nanochannels with carbon walls indicate that the optimization of the wall-nucleotide interactions may further reduce the required channel length below a micron.

Impact/ benefits: A faster and less expensive DNA/RNA/protein sequencing technology would greatly impact the development of personalized medicine and expand its availability. Forensic science would benefit from a faster analysis of DNA samples. The ability to sequence a large number of samples for a reasonable cost would also allow more extensive genetic studies of human and non-human populations.

***Background/ Explanation*:** Sequencing the entire genomes of a large number of individuals is cost and time prohibitive with the current technologies. Recently, a large effort has been undertaken to develop new sequencing technologies that use nanometer scale devices and sequence intact strands or strands that are cut up unit by unit. These new technologies could greatly reduce the time and cost of sequencing.

The simulation study shows that the specific interactions of the different DNA nucleotides with the walls of a nanometer scale channel cause multiple adsorptions and desorptions of the nucleotides and can be used to determine their identities based on their times of passage through the channel. Given that the strength of these interactions can be varied, by modifying the chemical composition of the surface of the channel walls, one can optimize the device and obtain the desired channel length and amount of time that the nucleotides spend in contact with the walls.



Side view snapshot depicting the flow of: a nucleotide (green), ions (yellow and blue), and water (purple) through a carbon nanochannel (gray). The nucleotide interacts and adsorbs and desorbs multiple times to the walls as it moves through the channel.