535a Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA

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We report a multi-scale modeling of transport and orientation properties of single strand DNA molecules in a nanoscale channel. A novel nanotechnology concept has been proposed which offers the possibility of unprecedented rapidity in the detection of DNA sequences. The proposed device consists of a detection gate of approximately two to five nanometers in width placed between two nonconductive plates. The DNA molecules in aqueous solution contained between the plates will be driven by an electric field through the detection gate. Individual base pairs within the DNA sequence are determined experimentally by examining the variations in the tunneling conductance of the gate. We are conducting large scale molecular dynamics simulations to study the transport and orientation of the DNA segment and the orientation of each base pair when they pass through the nanogate. Electric fields are applied along both vertical and horizontal directions to control the motion of DNA segments and the orientations of the base pairs. Molecular dynamics is used to determine ideal gate widths, optimal electric fields to be applied, and ideal solvent environment. Preliminary results from these molecular dynamics simulations are presented. In the broader project, the molecular dynamics simulations are combined with ab initio calculations of differences in electron transport across the nanoscale gap as different amino acids pass through the gap; these calculations are combined with experimental fabrication of the actual device. Both the computational and experimental projects are supported by complementary NIH grants.