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Molecular mechanics of DNA stretching, electrophoresis and condensation

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Without a doubt, DNA is the most celebrated macromolecule as it carries the genetic blueprint of a living organism. In addition to its fundament role in biology, DNA exhibits a variety of unusual physical properties. For example, the force-extension dependence of double-stranded DNA has a well-defined plasticity plateau that is associated with melting of its two strands. Being highly negatively charged, DNA molecules can attract one another and form a condensed state. The direction of the DNA motion in free electrophoresis can reverse upon changing the concentration of the surrounding electrolyte. Despite a number of theoretical and experimental studies, the nature of the microscopic processes that give rise to the above phenomena remain highly debated. With the advent of massively parallel supercomputers it became possible to characterize these processes directly, through all-atom molecular dynamics simulations. In this talk I will describe the results of multiple sub-microsecond simulations of various DNA systems that provide insights into the microscopic origin of the plasticity plateau in stretched DNA and into the mechanisms of DNA-DNA attraction and electrophoresis.