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Role of Nucleoid Associated Proteins in Stabilizing Supercoils[1]
KATELYN DAHLKE, CHARLES SING, Univ of Illinois - Urbana — Nucleoid associated proteins (NAPs) play an important role in prokaryotic cells by manipulating the shape and structure of the DNA. These NAPs act by bending or twisting DNA, and there are indications that NAPs bind preferentially to DNA that is already bent or twisted. We hypothesize that these binding behaviors strongly impact the stability and structure of DNA. We use coarse-grained simulation of NAPs and DNA that allow us to achieve the time and length scales where DNA supercoiling occurs. Supercoils are twist-induced structures that are the result of relaxing highly-twisted DNA by inducing higher degrees of bending and writhe. We are able to reproduce experimental observations, such as the extension of a DNA molecule as a function of force, linking number, and NAP concentration. Building upon these test cases, we allow the binding and unbinding energy of the simulated NAPs to be a function of the bending angle of the DNA at the site of binding ($\Delta E_B(\theta)$). Consequently, NAPs localize along the contour of the supercoil, and this binding preference is capable of stabilizing supercoils that form within the nucleoid.

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