

Reply to Comment on “Length Scale Dependence of DNA Mechanical Properties”

Agnes Noy and Ramin Golestanian

Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 3NP, UK

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In a Comment [1] on our recent study of the length scale dependence of DNA elasticity [2], Mazur brings up a number of technical points about the analysis of the MD trajectories used in our simulations, broadly categorized as concerns about equilibration and interpretation of the observed results. In Ref. [2], we compare the results we obtain for the segment with 4 DNA turns to that with 2 DNA turns, and interpret their agreement as a sign of equilibration. The shorter segment (2 DNA turns), which we simulated and analyzed for 130 ns, safely falls within the time scale of equilibration, and so does most of the analysis for the longer segment (4 turns), with the possible exception of the bending mode which might be marginal. We have been careful to avoid drawing conclusions only based on the information at the longest length scale. For instance, twist or contour-length elastic profiles from both fragments present the plateau at lengths shorter than a DNA turn, and bend modulations are uniformly distributed at all studied lengths. The only long-scale effect reported in our paper was the end-stretching mode, which is already present for the shorter segment, and does not directly involve bending. The choice of wa-

ter model should not affect the overall equilibrium properties [3], but will affect relaxation times and could also incur quantitative differences [4].

We have performed new simulations and produced 300 ns trajectories using both water models, to further probe the issue of equilibration (see Fig. 1). Figure 1 shows that the 36mer fragment is clearly equilibrated, and that the two water models lead to the same qualitative features, although with a quantitative difference in the rate of bending decay (i.e. value of persistence length). The 56mer fragment with the TIP3P model is equilibrated, and so is the twist and stretch response of the SPC/E case, while the bending shows small differences between 100 ns, 200 ns, and 300 ns trajectories [7].

When we start from an atomistic resolution, the definition of the DNA axis on the bp-level can be somewhat arbitrary. However, with the exception of rise, the influence of either the choice of the reference frame or the mathematical algorithm is shown to be negligible [8]. Similar bending periodicity to what we report has been observed using FREEHELIX [9], CURVES [10] and Monte Carlo coarse-grained simulations over long molecules of DNA [11]. Moreover, Dickerson and coworkers described the same helical periodicity analyzing entirely experimental structures [9]. This effect is due entirely to the static structure of DNA, namely its spontaneous curvature. Because DNA is a twisted polymer, this periodicity emerges when a regular DNA with a systematic positive roll is built (blue line of Fig. 3c [2]). Due to this residual average static (helical) structure, orientation correlation function will have a periodic shape even at zero temperature and without any fluctuations. If one artificially uses an axis that averages over this static structure, one can eliminate the periodicity. What we point out about definitions of persistence length from the decay of this function is aimed at alerting to the fact that using a local slope, as has been used in interpreting some experimental data, might give erroneous results due to this residual structure.

For the reasons given above, we do not believe the Comment by Mazur provides any evidence against our work.

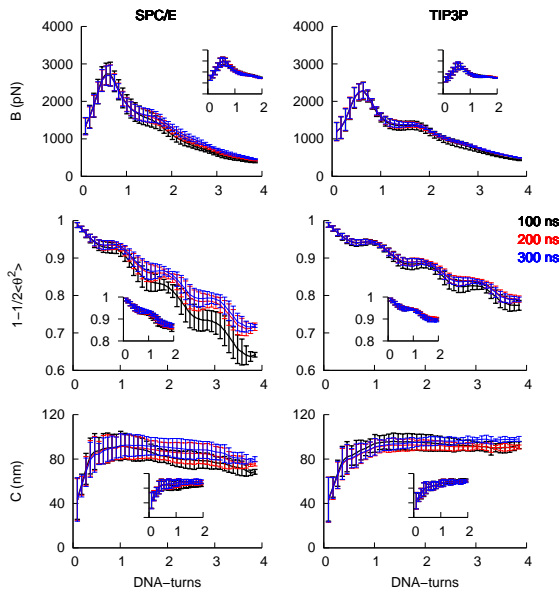


FIG. 1. Length scale dependence of stretch modulus B (Top), directional decay (Middle) and Torsional persistence length C (bottom) evaluated from different trajectories lengths using the 56mer (inset 36mer) fragment

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