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Towards modelling DNA in biological environments

Thursday 10 July 2025 09:00 (50 minutes)

When aiming for atomic detail, DNA has typically been characterized using short, relaxed fragments (up to 50 base pairs or bp). However, inside cells, DNA is a very long polymer that is supercoiled, subjected to bending and pulling forces, and surrounded by a crowded environment. In our lab, we have developed approaches and protocols for simulating DNA at the atomic level while accounting for these mechanical stresses in order to recreate more realistic conditions. In my presentation, I will show how DNA structure and dynamics respond to supercoiling when combined with pulling and DNA-bending proteins (1-4). Furthermore, I will provide atomistic insights into the non-specific interactions between some of the most abundant proteins in cells and DNA. The aim is to initiate a discussion regarding the potential acceleration of the study of these effects using AI.

1. ALB Pyne *et al.*, *Nat Commun*, **12**, 1053 (2021)
2. S Yoshua *et al.*, *Nuc Acids Res*, **49**, 8684-8698 (2021)
3. GD Watso *et al.*, *Comput Struct Biotech J*, **20**, 5264-5274 (2022)
4. M Burman and A Noy, *Phys Rev Lett*, **134**, 038403 (2025)

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