

Protein-DNA Interactions and DNA Conformation: Simplified Modeling Studies

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Abstract:

For DNA-binding proteins such as transcription factors to work properly, they should first search their targets on DNA strings. Hence, efficient searching mechanisms are crucial. Indeed, it was shown that the searching time is much shorter than that is expected for simple 3D diffusion; which could be attained by the combination of 1D and 3D diffusional searching, so-called facilitated diffusion.

In the cell, moreover, DNA is not a simple, randomly folded polymer. Brackley et al. discussed the effects of DNA conformation on the facilitated diffusion process by using simple coarse-grained Brownian dynamics simulations. Particularly, they focused on local structures such as loops [1,2]. They also considered effects of other proteins acting as crowders and blockers [3]. Recently, the same group also discussed how such structures could be formed, by just simple physical interactions between DNA and proteins [4,5,6].

In this seminar, I will overview these works and discuss possible directions that could be further explored by similar, simplified models.

References:

1. C. A. Brackley et al., Phys. Rev. Lett. 109, 168103 (2012).
2. C. A. Brackley et al., Biochem. Soc. Trans. 41, 582-588 (2013).
3. C. A. Brackley et al., Phys. Rev. Lett. 111, 108101 (2013).
4. C. A. Brackley et al., Proc. Natl. Acad. Sci. USA 110, E3605-E3611 (2013).
5. J. Johnson et al., J. Phys. Cond. Matt. 27, 064119 (2015).
6. C. A. Brackley et al., Nucl. Acids Res., in press, doi:10.1093/nar/gkw135 (2016).