

## All-atom modelling of nucleosome positioning

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The mechanical properties of DNA are now recognized as playing a significant role in the specificity of protein-DNA interactions, even if the "code" linking sequence and mechanics is far from being fully understood. The importance of heterogeneous mechanics is particularly important in the case of nucleosome binding, where little specificity can be attributed to direct protein-base contacts and DNA deformability plays a major role. This is however an important problem to solve, since nucleosome positions are known to be an important factor in gene expression.

While most theoretical approaches to understanding nucleosome positioning have adopted simplified models of DNA based on elastic rod approaches, with sequence effects represented via parameters for each unique dinucleotide or trinucleotide step, we are attempting to solve this problem using all-atom models and appropriate force fields, which allow DNA deformation and DNA-protein interactions to be taken into account simultaneously and do not require any assumptions about the underlying mechanism of DNA mechanics.

This approach, which already yields some encouraging results, required the development of a new methodological approach and the extensive use of grid computing facilities. I will describe the development of this methodology and allow discuss how the results can be used in larger scale models of multiple nucleosome binding on long fragments of genomic DNA.

### References

[1] C. Deremble, R. Lavery, K. Zakrzewska (2008) *Comput. Phys. Comm.* **179**, 112-119.