A pinch of salt on your DNA ?

Sam Meyer[1,2,3], Richard Lavery[4], Ralf Everaers[2,3]
[1] LIRIS, INSA de Lyon, Université de Lyon
[2] Laboratoire de physique, ENS de Lyon, Université de Lyon
[3] Centre Blaise Pascal, ENS de Lyon
[4] Institut de biologie et de chimie des protéines, Univ. Lyon I, Univ. de Lyon

Our genetic sequence is encoded as a succession of bases inside the negatively charged DNA double-helix. All genetic transactions (replication, transcription...) involve the interaction of DNA with positively charged proteins; many of these transactions are sequence-specific and can involve an indirect recognition of the bases. In these processes, electrostatics plays a major role, crucially affected by the mobile ions present in the physiological solution (salt). At a large scale of 10-100 nanometers, these ions screen out the charges between the macromolecules and determine their unspecific interaction. At the nm-scale where the proteins sample the DNA sequence, they distribute around the DNA, and modify the electrostatic properties of the molecule in a sequence-dependent way. We study these distributions by numerical simulations at two different resolutions and lengthscales: Molecular Dynamics of short DNA oligomers and continuous approaches based on the Poisson-Boltzmann description, and particularly a recent derivate (Dipolar Poisson-Boltzmann Langevin) which takes into account the finite size of ions and water molecules. The studies suggest that the sequence-dependent charge distribution in the solvent could be a major determinant of sequence recognition by DNA-binding proteins.