1 Solving stationarity conditions for the cgDNA model with parameter continuation

Parameter Continuation with cgDNAeq

You can download from `http://lcvmwww.epfl.ch/teaching/modelling_dna/public_files/ParamCont_cgDNAeq.zip` the script implementing the parameter continuation that start from the ground state of a given sequence (solution at $\epsilon = 0$) and perform pulling and pushing numerical experiment by moving the last base pair position of along the z axis. Hereafter we show the obtained result for the two considered sequences.

i) The moments and the forces as a function of the displacement along the z axis for the two sequences are shown in Figures (1) and (2). One can observe the significant difference in the value of the z component of the Force between the two sequences. Moreover once can remark that for the pushing numerical experiment for the sequence poly$(AT)_{79}$ we reduced the displacement step due to issue in the convergence of computation. In fact for poly(AT_{79}) the convergence of solver `fsolve` depend upon the chosen (negative) displacement even when the starting configuration is close to the ground state. Here we can do a brief analogy with the compression of an isotropic rod. Imagine to push vertically an isotropic rod, the solution to this problem is in fact a family of solutions around the vertical axis. This problem is known as buckling problem. We stress here that we are not saying that poly$(AT)_{79}$ is isotropic but that some behaviour of this sequence are close to some behaviour of isotropic material. [Remark: In Figure (1 and 2) if you want the unit to be pNÅ for the moment and pN for the forces, multiplies all the entries of the vector lambda by 42.

ii) We show here the 3D reconstruction of the result of the pulling and twisting numerical experiment performed on CAP (Figure 3) and poly$(AT)_{79}$ (Figure 4).

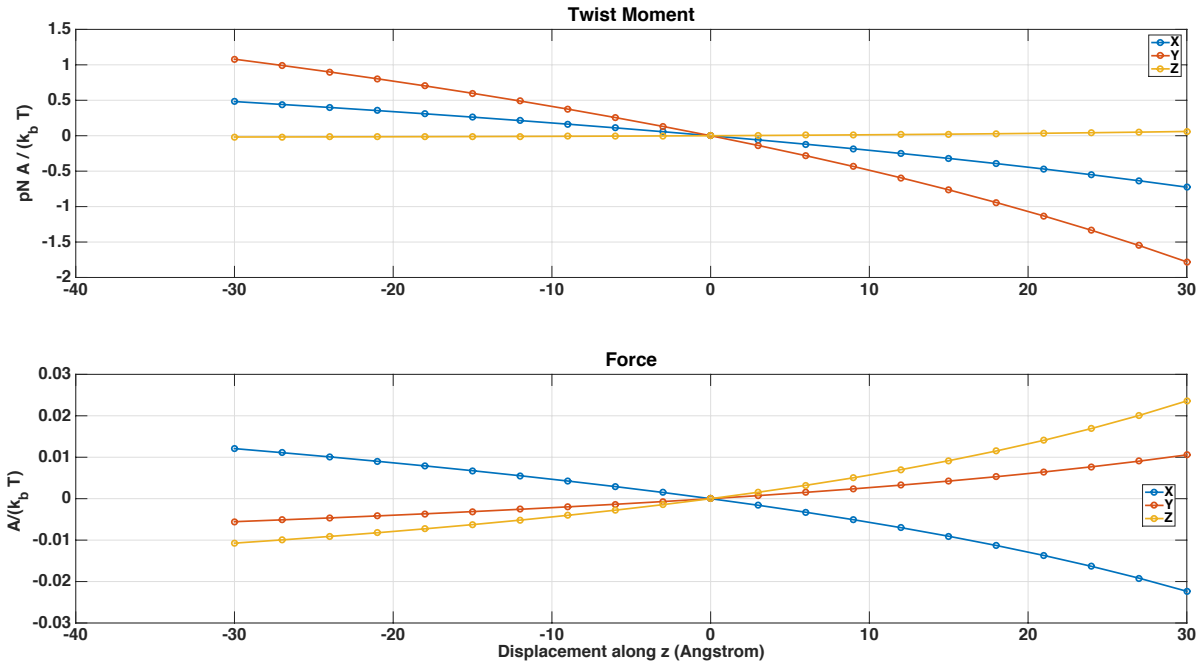

Figure 1: Value of the components of the Lagrange multiplier $\boldsymbol{\lambda}$ versus the displacement for the sequence CAP. The Twist Moment are the first three components of $\boldsymbol{\lambda}$ while the forces are the last three components.

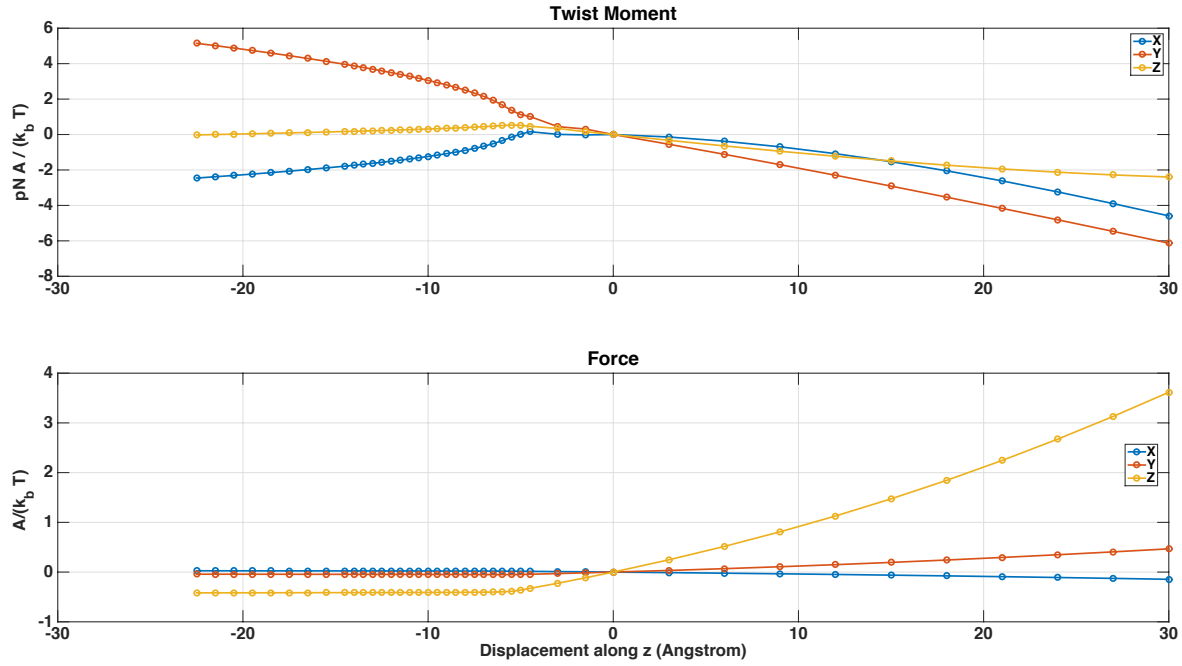

Figure 2: Value of the components of the Lagrange multiplier $\boldsymbol{\lambda}$ versus the displacement for the sequence poly$(AT)_{79}$. The Twist Moment are the first three components of $\boldsymbol{\lambda}$ while the forces are the last three components.

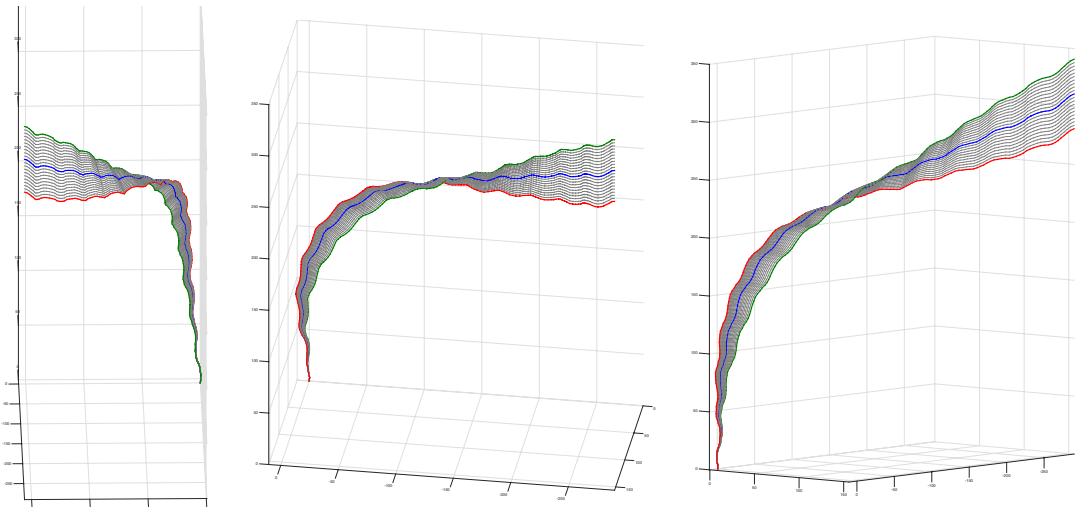

Figure 3: Three different views of all the 3D reconstructions of the computed solution for CAP. The ground state is shown in blue, the most pulled configuration in green and the most pushed one in red

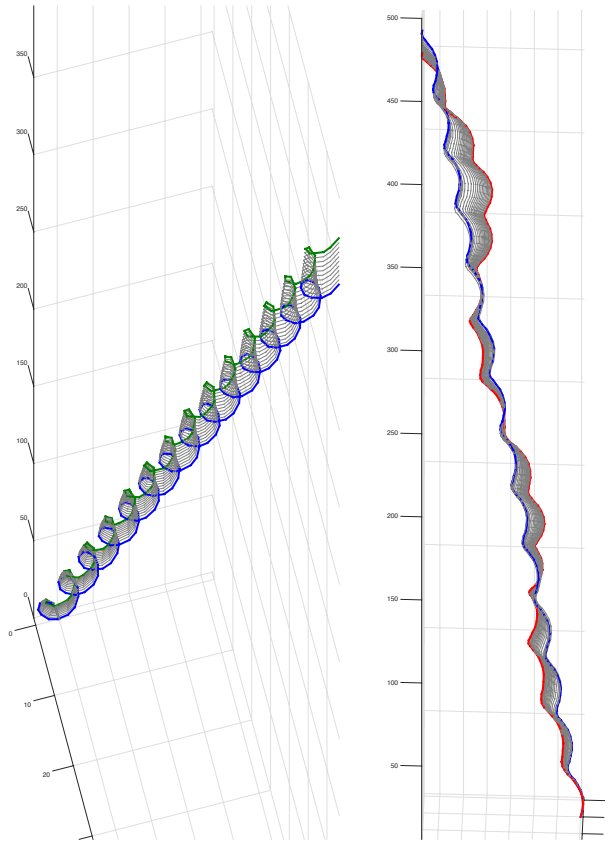

Figure 4: On the right the pulling experiment for poly$(AT)_{79}$, starting from the ground state (blue) until the condifuration in green. On the left the pushing expriment for poly$(AT)_{79}$, starting from the ground state (blue) until the condifuration in red.