

Calculating persistence length

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This example shows how to calculate a persistence length of a duplex DNA. Compile the code and copy it to the PERSISTENCE_LENGTH directory. Then you need to run

```
oxDNA input_persistence
```

Note that for calculation of persistence length, one needs a large number of decorrelated states. The program will produce a trajectory.dat file. To analyze the data, use the python script dspl.py:

```
dspl.py trajectory.dat init.top 10 50
```

This program will produce a table of correlations between helical vectors , $\langle \mathbf{n}_k \cdot \mathbf{n}_0 \rangle$. The persistence length can be obtained from the following equation:

$$\langle \mathbf{n}_k \cdot \mathbf{n}_0 \rangle = \exp(-k \langle l_0 \rangle / L_{ps}). \quad (1)$$

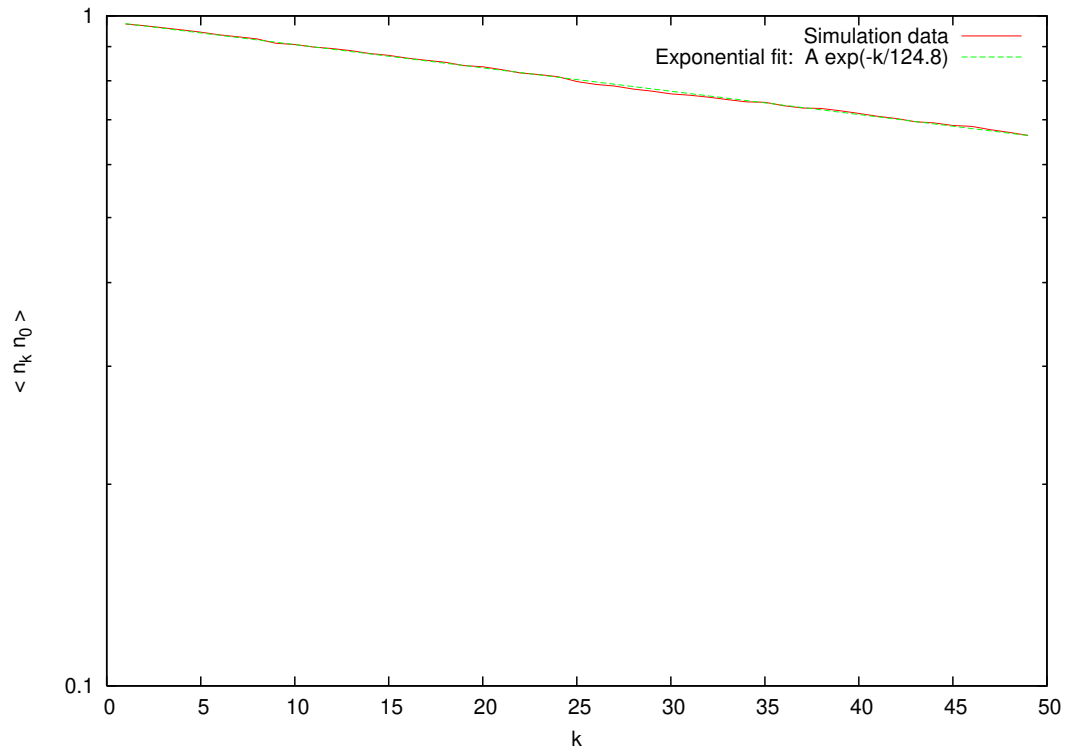


Figure 1: The figure shows an example of an exponential fit to the data obtained from the simulation. In this case, the data show persistence length of 124 base pairs.