Monte Carlo simulations of protein-DNA interactions

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This document shortly describes how the IDL-code can be used to simulate protein-DNA interaction involving binding, dissociation, and linear motion. A theoretical description can be found in "Monte Carlo simulations of protein assembly, disassembly, and linear motion on DNA," by Thijn van der Heijden & Cees Dekker (Biophysical Journal).

The IDL code

The program involves three different files:

- Monte.pro yields a gui for user in- and output.
- Monte_eventcb.pro
- Filamentsingle.pro contains the core of the simulation.

All three files have to be opened in IDL and compiled one after each other as listed above. Running monte.pro shows a gui where the user can set the interaction modes and the rates involved. After pressing the simulate button, the programs yields three different plots: a time-dependent lattice coverage, a kymograph, and a histogram of the bound protein patches. The output of these three curves can be saved into a data file (which you can reopen with e.g. Origin). Finally a log file can be generated to store the parameters which have been used to generate the latest data file.

Examples

The downloaded data set contains also three examples with log files obtained from the program.

Curve fitting

Simulated data sets can be used to extract kinetic parameters from for instance single-molecule time traces as done by Van der Heijden et al. (Nucleic Acids Research, 2007) to study RAD51-DNA interaction. Here, different data sets were generated and fit onto the data set to extract kinetic parameters for binding and dissociation.