Optimization of the extraction of pauses in molecular dynamics

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Single-molecule experiments to study molecular motors once at a time have been developed in recent years. One of the critical points of the data analysis is the identification, characterization and extraction of the effect of the pause states in the motor dynamics [1]. The theoretical model is well-known, but in practice satisfactory results are dificult to attain. We have developed and optimized an algorithm to separate the pause and displacement contributions to the velocity histograms, in order to determine the displacement rate (see Fig. 1).

We simulate a molecular motor (DNA-Polymerase) moving with a displacement rate k_p (replication rate), entering a pause state with rate k_{a1} and exiting from it with rate k_{1a}. We mimic the experimental limitations by assuming the trajectories have a Gaussian random noise in position and measuring the process at given time intervals mimicking the experimental data sampling.

The algorithm has allowed us to identify the optimal speed histogram obtained with our method. We have measured the displacement rate of the motor quite precisely in spite of the experimental limitations simulated in our work.

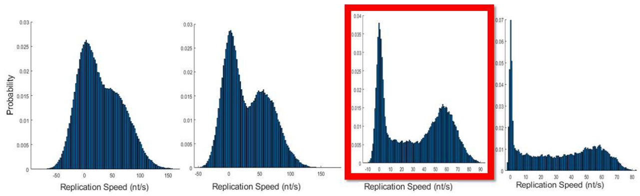

Fig. 1. Replication speed histograms obtained with our algorithm. Histogram for the optimal value indicated with a red box

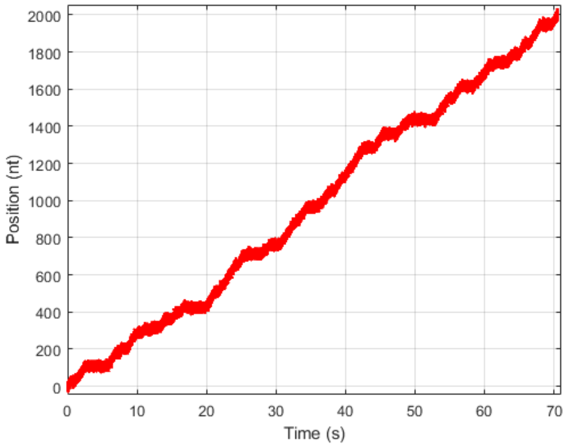

Fig. 2. Synthetic trajectory for DNA-Polymerase during the replication. We include the Gaussian random noise in positions measures.

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[1] J. A. Morin, F. J. Cao, J. M. Lázaro, J. R. Arias-González, J. M. Valpuesta, J. L. Carrascosa, M. Salas, and B. Ibarra, Active DNA unwinding dynamics during processive DNA replication, Proc. Natl. Acad. Sci. USA **109**, 8115-8120 (2012).