Simulations of active polymer translocations

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This presentation concerns the translocation of a polymer through narrow pores where a time dependent force is acting.

Translocation of long biochemical structures through channels is a normal process in biology. Drug absorption, protein and DNA/RNA passage through cell membranes and nuclear pores, DNA injection by phage viruses are only few examples of a broad biological phenomenology.

Following the seminal paper by Kasianowick in 1996, both theoretical and experimental investigations have been developed in order understand the basic physics involved in this process.

In the recent years technological advances have permitted to manipulate single molecules, and to observe translocation under time dependent driving. In fact, beside the fluctuating opening/closing gate of the pore channels due to ligands or the reaction of the pore walls, the translocation can be driven by molecular protein motors.

Because of the high number of particles involved in molecular kinetics, the theoretical computational study of translocation of real molecules presents the inconvenience to be extremely time consuming when using full atom simulations. For this reason, many gross grain polymer models have been developed not only to describe the translocation process in affordable conditions, but also to better control the specific contribution of the different parameters involved in the dynamics.

In this contribution, some recent results using Rouse-based models will be presented, in order to describe the active translocation of a polymer through a narrow pore, i.e. the translocation assisted by time dependent forces, from sinusoxidal to random dichotomous. Moreover, the most recent results of translocation of a polymer enriched with the flexibility degree of freedom under the specific force provided by the action of a molecular motor, will be presented. This kind of motors are characterized by an actuation triggered by the bonding of an ATP molecule (the fuel) to the protein motor. The bonding is modeled as a Poisson process and the overall motor actuation presents a paradigmatic dichotomous driving for ATP-based motors that provide a Michaelis-Menten kinetics outcome.

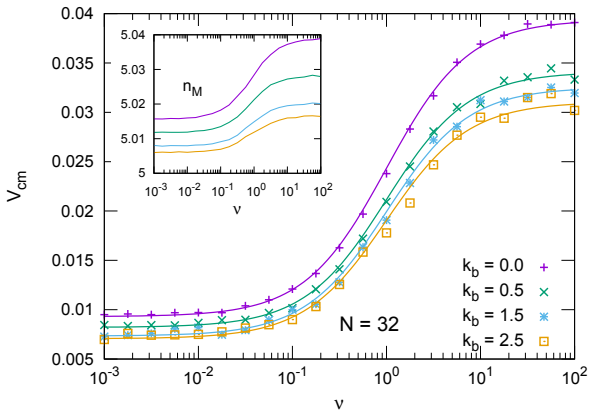

Figure 1: Michaelis-Menten velocity of the centre of mass of the polymer which translocates under a dichotomous ATP-fueled molecular motor.

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