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Coupling of atomistic and mesoscopic scales: visualizing the translocation of biopolymers through nanopores MARIA FYTA, Department of Physics, Harvard University, SIMONE MELCHIONNA, INFM-SOFT, Department of Physics, Universita di Roma La Sapienza, P.le A. Moro 2, 00185 Rome, Italy, MASSIMO BERNASCHI, Istituto Applicazioni Calcolo, CNR, Viale del Policlinico 137, 00161, Roma, Italy, EFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA, SAURO SUCCI, Istituto Applicazioni Calcolo, CNR, Viale del Policlinico 137, 00161, Roma, Italy — We investigate the process of biopolymer translocation through a narrow pore using a multiscale approach, which combines Langevin Molecular-Dynamics with a mesoscopic Lattice-Boltzmann method for the solvent dynamics. We analyze the statistical features of the translocation process through extensive simulations over various polymer conformations and lengths. The translocation time obeys a power law dependence to the polymer length with an exponent 1.28 ± 0.01 in very good agreement with experiments of DNA translocation through solid state pores. We focus on the morphological aspects of the translocation dynamics, the folding behavior of the translocating molecule and the associated cooperation of the surrounding solvent, and report the first computational evidence of quantized current blockades.

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