

Abstract Submitted  
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**Biomolecular translocation through nanopores: from an anonymous polymer to realistic DNA** MARIA FYTA, Institute for Computational Physics, University of Stuttgart, SIMONE MELCHIONNA, IPCF - National Research Council, Rome, Italy, SAURO SUCCI, IAC - National Research Council, Rome Italy, EFTHIMIOS KAXIRAS, Physics Department, Harvard University, Cambridge, MA — We have developed an efficient multiscale approach to treat biomolecular motion in a fluid solvent. This scheme has been applied to the problem of polymer translocation through a nanopore, an intensively studied subject due to its variety of applications with ultra-fast DNA sequencing being one of them. Our first results involve an anonymous polymer translocating in pure water. We have obtained important insight into the statistics and dynamics of the process. The translocation time exponent compares well with the experimental values, while we were able to monitor multiconformational translocation, the signatures of which are also relevant to the experimental counterparts. As a next step, we have made our modelling more realistic by including electrokinetic effects, i.e. ions, as well as a realistic quantum-mechanically derived potential for double stranded DNA. We are now able to look more deeply into what happens in the pore. The ionic conductance and DNA blockade can be qualitatively and quantitatively observed and connected to the experiments. Finally, we also investigate the effect of pore geometry in the DNA translocation process.

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