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Polymer translocation: some surprising physics learned from Molecular Dynamics Simulations

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Polymer translocation is relevant both in vivo and for nanotechnology applications. Not surprisingly, this apparently simple process has been the subject of intense study over the last 20 years or so. For instance, there have been numerous simulation studies examining aspects of both biased and unbiased translocation. In the first part of this talk, I will review our Molecular Dynamics simulation results for unbiased translocation, and I will focus on the fact that there appears to be no experimentally relevant scaling exponent. I will then present results for translocation driven by unusual system asymmetries. First, I will consider the case of a gradient of solvent viscosity across the membrane: can this drive the translocation, and if so, towards which side? For the second example, I will consider translocation when different obstacle arrangements are present on both sides of the pore. Interestingly, we find that even with uniform concentrations of obstacles, varying arrangement of the obstacles can yield a preferential direction. Finally, I will look at the sources of diffusion in the problem, with a focus on “conformational noise” and ways to control it.

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