Seminar über Fragen der Mechanik

zu folgendem Vortrag wird herzlich eingeladen

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https://fau.zoom-x.de/j/64561316157

Understanding an artificial motor protein Using Langevin equations

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Motor proteins are essential for the existence of cellular life. They help to overcome the diffusive nature of the nanoscale world and facilitate directed movements. Famous cases are the myosin or kinesin motor families, responsible for transport processes. While the results of protein-motor stepping can generally be experimentally observed, it is difficult to understand what the actual microscopic behavior patterns are that result in these steps, due to having to resolve the Å-nm structures in time steps of ns or ps. It is expected that diffusion is an integral part of the movement of these motors.

One way to help understand the details of e.g. a step of a myosin V motor protein is to simulate the movement with a coarse grained model taking into account its structure and the effects of the thermal environment [1].

In our study, we analyse a concept for an artificial motor [2] of two (modified) tryptophan repressor (TrpR) proteins being linked together with a glycine-serine chain, walking along a specific DNA track. This motor concept utilizes its inherent asymmetry by exploiting a chemical cycle akin to ATP-ADP to only allow the 'back' positioned TrpR to unbind, which then can bind in front of the still bound TrpR, reversing their roles and thus facilitating processive, autonomous movement.

We use (overdamped) Langevin dynamics describing translational and rotational degrees of freedom [1,3] of these motors. We further model the motor by employing a coarse grained approach not from first principles but using plausible models for the involved parts. We analyze what makes the motor perform the autonomous processive movement, which constraints are needed on the motor parameters to allow for moving, and the efficiency with which it can move. This coarse grained analysis allows us to both understand better the fundamental movement of biological motors, but also help in the direct design process of the actual artificial motors.

[1] Craig, Linke: PNAS 106, 43 (2009)

[2] Linke et al., Biophysical Reviews volume 12, pages 1041–1054 (2020)

[3] Naess, Elgsaeter, Macromol. Theory Simul. 2004, 13 (2004)

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