DY 1: Statistical physics of biological systems (joint session BP/DY)

Time: Monday 10:00–11:15 Location: H1

Invited Talk DY 1.1 Mon 10:00 H1

Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth — •Robert Endres[1], Henry Cavanagh[1], Rob Lind[2], Andreas Mosbach[3], and Gabriel Scalliet[3] — [1]Imperial College London, UK — [2]Syngenta International Research Centre, UK — [3]Syngenta Crop Protection AG, Switzerland

The morphodynamical analysis of cells can be a powerful and cost-effective way of understanding the phenotypic effects of perturbations, but current techniques often only work for stationary cell behaviour. Here, we introduce a novel framework that extends the morphodynamic analysis to nonstationary dynamics during early-stage growth of the soybean rust P. pachyrhizi. At its core, our approach learns the 2-dimensional feature space of cell shape using variational autoencoders from deep learning, and subsequently models how populations of cells develop over this space using two simple differential equations, each capturing complementary aspects of the dynamics with parameters depending on the perturbations. First, a Fokker-Planck model to describe the diffusive development on a Waddington-type energy landscape, providing a global perspective on the dynamics, and second, a cell-mechanical model describing local growth as a persistent random walk. Informative perturbation-dependent parameters are found by fitting simulations to the shape-space embeddings, representing a powerful tool for linking machine-learning and biophysical modelling.

DY 1.2 Mon 10:30 H1

Collisions increase self-diffusion in odd-diffusive systems — •Erik Kalz[1,2], Iman Abdoli[1], Hidde Derk Vuijk[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere, 01069 Dresden — [2]Technische Universität Dresden, Institut für Theoretische Physik 01069 Dresden

It is generally believed that collisions of particles reduce the self-diffusion coefficient. We show that in odd-diffusive systems, which are characterized by diffusion tensors with anti-symmetric elements, collisions surprisingly can enhance the self-diffusion. In these systems, due to an inherent curving effect, the motion of particles is facilitated, instead of hindered by collisions. We refer to this as an overdamped swing-by effect. Consistent with this we find that the collective diffusion remains unaffected. We demonstrate this counterintuitive behavior in a system of Brownian particles under Lorentz force. Using a geometric model, we theoretically predict a magnetic-field governed crossover from a reduced to an enhanced self-diffusion. The physical interpretation is quantitatively supported by the force-autocorrelation function, which turns negative with increasing magnetic field. Using Brownian dynamic simulations, we show that the predictions are also valid for active chiral particles as another odd-diffusive system.

DY 1.3 Mon 10:45 H1

How is anomalous diffusion compatible with thermodynamics in biophysical systems? — •David Hartich and Aljaz Godec — Mathematical bioPhysics Group, MPI-BPC, Göttingen, Germany

In a finite system driven out of equilibrium by a constant external force the thermodynamic uncertainty relation (TUR) bounds the variance of the conjugate current variable by the thermodynamic cost of maintaining the non-equilibrium stationary state. Here we highlight a new facet of the TUR by showing that it also bounds the time-scale on which a finite system can exhibit anomalous kinetics. In particular, we demonstrate that the TUR bounds subdiffusion in a single file confined to a ring as well as a dragged Gaussian polymer chain even when detailed balance is satisfied. Conversely, the TUR bounds the onset of superdiffusion in the active comb model. Remarkably, the fluctuations in a comb model evolving from a steady state behave anomalously as soon as detailed balance is broken. Our work establishes a link between stochastic thermodynamics and the field of anomalous dynamics that will fertilize further investigations of thermodynamic consistency of anomalous diffusion models.

[1] DH, A. Godec, Phys Rev. Lett. (in press), arXiv:2102.06678.

DY 1.4 Mon 11:00 H1

Maximum likelihood estimates of diffusion coefficients from single-particle tracking experiments — •Jakob Tómas Bullerjahn[1] and Gerhard Hummer[1,2] — [1]Department of Theoretical Biophysics, MPI of Biophysics, Frankfurt am Main, Germany — [2]Institute of Biophysics, Goethe University, Frankfurt am Main, Germany

Single-molecule localization microscopy allows practitioners to locate and track labeled molecules in biological systems. When extracting diffusion coefficients from the resulting trajectories, it is common practice to perform a linear fit on mean-squared-displacement curves. However, this strategy is suboptimal and prone to errors. Recently, it was shown that the increments between the observed positions provide a good estimate for the diffusion coefficient, and their statistics are well-suited for likelihood-based analysis methods. Here, we revisit the problem of extracting diffusion coefficients from single-particle tracking experiments subject to static noise and dynamic motion blur using the principle of maximum likelihood. Taking advantage of an efficient real-space formulation, we extend the model to mixtures of subpopulations differing in their diffusion coefficients, which we estimate with the help of the expectation-maximization algorithm. This formulation naturally leads to a probabilistic assignment of trajectories to subpopulations. We employ the theory to analyze experimental tracking data that cannot be explained with a single diffusion coefficient, and test how well the data conform to the model assumptions. https://doi.org/10.1063/5.0038174