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CDISE Advanced Multiscale Simulations Lab Seminar
CHARACTERIZING SINGLE PARTICLE DIFFUSION USING BAYESIAN ANALYSIS

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November 25, 2019, 14.00 - 15.00

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ABSTRACT

Particle diffusion in heterogeneous systems poses the following question: Can a single model describe the entire dynamics of a particle in complex biological, soft matter systems? Indeed, often several different physical mechanisms are at work and it is more insightful to rank them based on the likelihood of them explaining the dynamics. This talk will discuss — within the Bayesian framework — (a) how maximum-likelihood model selection can be done by assigning probabilities to each feasible model and (b) how to estimate the parameters of each model. In particular, the implementation of this powerful statistical tool using the Nested Sampling algorithm to compare — at the single trajectory level — models of Brownian motion, viscoelastic anomalous diffusion and normal yet non-Gaussian diffusion will be discussed. Finally, the application of this method to experimental data of tracer diffusion in polymer-based hydrogels (mucin) will be presented. Viscoelastic anomalous diffusion is often found to be most probable, followed by Brownian motion, while the model with a diffusing diffusion coefficient is only realised rarely. Also, diffusion of tracers in the mucin gels is found to be mostly non-Gaussian and non-ergodic at low pH that corresponds to the most heterogeneous networks.

Short BIO

Samudrajit Thapa is a Ph.D. student in the Theoretical Physics group of Prof. Ralf Metzler at the University of Potsdam, Potsdam, Germany. Samudrajit received his B.Sc. degree in Physics in 2012 and the M. Sc. degree in Physics in 2014 from the University of Delhi, New Delhi, India. Currently, his research focuses on the studies of stochastic processes which can explain the normal and/or anomalous diffusion observed in different biological and soft matter systems. For such studies he uses different tools of Statistical Physics such as Bayesian inference and machine learning. Samudrajit's Ph. D. is funded by a Deutscher Akademischer Austauschdienst (DAAD) scholarship.

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