F. Schmid
friederike.schmid@uni-mainz.de

P. Virnau
virnau@uni-mainz.de

L. Stelzl
lstelzl@uni-mainz.de

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Seminar über Theorie der kondensierten Materie / TRR146 Seminar

June 21, 2023 at 2:30 p.m.
Minkowski Room, 05-119, Staudingerweg 7

Abhishek Singharoy
Arizona State University

Biophysics at the Dawn of Exascale Computer – The Age of Molecular Simulation Bots

Molecular modeling of biomolecular assemblies exemplifies a disruptive area holding both promises and contentions. We will start with a brief story of simulating the first ever cell organelle in molecular details to find how nature has chosen survival fitness over efficiency of energy transfer as an evolutionary design (Cell, 2020). Despite such advances in exascale computing, biophysical simulation continues to grapple with handling molecular diversity. So, we will employ deep learning approaches often used in Google searches, called the inception network, to marry interaction signatures from Alphafold models and proteomics analysis with predictable patient outcomes (Cell Sys, 2022). An application will highlight how molecular modeling is used at an industrial scale to de-risk vector-based vaccines for distribution across 194 countries (Sci Adv 2021). We will conclude by seeing how transient interactions are difficult to predict, and path integrals with reinforcement learning offer a possible way to track diversity of dynamics (NeurIPS, 2022).

Contact:
Lukas Stelzl
lstelzl@uni-mainz.de

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