PHYSIKALISCHES KOLLOQUIUM

des Fachbereichs Physik
der Johann Wolfgang Goethe-Universität Frankfurt

Mittwoch, den 04.05.2022, 16 Uhr c.t.
Großer Hörsaal, Raum _0.111,
Max-von-Laue-Str. 1

Dr. Jürgen Köfinger

Max Planck Institut für Biophysik
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ANTRITTSVORLESUNG

"Integration of experimental data and molecular simulations"

To understand life on the molecular level, we apply molecular dynamics simulations to increasingly larger and more complex biomolecular systems over longer times. We aim to maximize the predictive power of these simulations by choosing an appropriate molecular model or force field to trade off sampling errors and systematic force field errors. We further alleviate these intrinsic limitations by integrating additional experimental information. After introducing some basic concepts, capabilities, and goals of biomolecular simulations, I will discuss the use of Bayes theorem to refine molecular simulations by integrating ensemble averaged experimental data. The Bayesian inference of ensembles (BioEn) method [Hummer and Köfinger, J. Chem. Phys. (2015)] preserves the character of the simulation ensemble while it improves the agreement with the data. The resulting refined ensemble is a better representation of the true ensemble underlying the data. On this basis, I will introduce the Bayesian inference of force fields (BioFF) method [Köfinger and Hummer, N. J. Phys. B (2021)] to refine force field parameters using various data. BioFF systematically resolves force field issues and encodes learned information directly in the force field. These refined force fields are transferable and can be applied to diverse biomolecular systems. Such formalized, systematic, and (semi)automatic machine-learning efforts to ensemble refinement and force field optimization are set to play an indispensable role in the promising future of biomolecular simulations.

Die Dozenten der Physik

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