Bachelor Thesis:  
Quantifying Uncertainties in Coarse-Grain DNA Models

Course of Study: Mathematics, Computer Science, Physics or similar

Topic
Deoxyribonucleic acid, or DNA, is undoubtedly one of the most important molecules in all known life forms on earth. Correctly modeling its shape and mechanical properties is key to understanding numerous biological processes, and to paving the way towards personalized medicine. Consequently, investigating the properties of DNA is one of the central endeavors in modern Biophysics. A major challenge in theoretical and computational studies of DNA is the molecule’s sheer size. This makes it difficult, if not impossible, to model by standard molecular dynamics (MD) techniques.

As an alternative, various levels of coarse-graining are being employed as a compromise between physical accuracy and computational speed. One particularly promising coarse-graining paradigm relies on a so-called rigid-base simplification. However, as with any other coarse-graining technique, the rigid-base approach leads to loss of information, leading to uncertainties in the model prediction. In our group, we develop a Bayesian uncertainty quantification (UQ) framework to model the predictions of rigid-base DNA models and its errors in a probabilistic sense. This thesis project aims at improving theory and implementation of the framework, as well as its evaluation based on MD data.

Tasks
- Implementation of enhancements in the coarse-grain DNA framework
- Extension of the software towards fully differentiable models
- Implementation of Markov chain Monte Carlo (MCMC) methods for high dimensional state spaces
- Information-theoretical comparison of different MD designs

What we can offer
You will work on a research topic of current interest, and have the opportunity to bring in your own ideas and strengths. We are a relatively small group and place value on close supervision of and collaboration with our thesis workers. In particular, we will introduce you to modern tools and techniques in applied mathematics, software development, and high performance computing.

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