

SIAM/APPLIED AND NUMERICAL ANALYSIS SEMINAR

Date: March 17, 2020

Speaker: Alberto Perez

Title: Making sense of macromolecules: Bayesian inference and Markov Models in Structural Biology

We are interested in understanding how proteins and nucleic acids self-assemble and interact with each other. We use computational techniques based on Molecular Dynamics to understand how these macromolecules behave integrating Newtons equations of motion at the femtosecond scale. But, the processes we are interested happen in timescales that are several orders of magnitude longer. To make them feasible, we use advanced sampling techniques such as Bayesian inference on noisy data.

Ultimately, we get conformational ensembles which contain a lot of data that has to be rationalized. To do so we use techniques of data reduction like PCA or tICA. Recently we have started using Markov State Models as a way to rationalize the pathways and kinetics in our systems.