LAUFER CENTER
FOR PHYSICAL AND QUANTITATIVE BIOLOGY

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Seminar

Linearization of Protein Loop Motion

Proteins are the machinery of life. They operate by interacting with their environment and this interaction largely depends on structure. However, structure is not a static property. Especially loop segments extending outward from a protein demonstrate dynamic behavior and span a large conformational space. Understanding loop behavior is therefore important to understand protein function. Existing methods either rely on molecular dynamics simulations, which provide a lot of insight but are computationally expensive, or extensive sampling of possible loop conformations, which is a powerful tool for protein design (as in the Rosetta software suite), but gives limited insight into the mechanics of loop behavior. In this talk an alternative approach is introduced that lies midway these extremes, which relies on a linearization technique originally developed for robotics analysis. Vector algebra is used to obtain a first-order approximation of the inverse kinematics, an unsolved problem in protein analysis. This first-order model is subsequently coupled to an energy function to analyze local loop motion at low computational cost.

Wednesday, February 12, 2020

2:00 PM

Laufer Center Lecture Hall 101

Host: Vageli Coutsias

Refreshments following the seminar Laufer Hub 110

For a disability related accommodation, call 631-632-5400