Institut Européen de Chimie et Biologie

I E C B

Simulating molecular motions with robotics-inspired algorithms. Control of enzyme selectivity by engineering the substrate binding site and access channel

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The development of methods to compute feasible motions for a system in a physical workspace is an active field of research in robotics since the 70s. Sampling-based algorithms developed in this field during the last decade are efficient and general techniques for exploring constrained high-dimensional spaces. Such algorithms have been successfully applied to challenging problems in diverse domains beyond robotics, including computational structural biology. In this talk, I will give an overview of recent works carried out at LAAS-CNRS in this domain. In particular, I will present robotics-inspired algorithms for simulating protein conformational transitions, and protein-ligand access/exit pathways. The presentation will also show encouraging results on interesting systems such as enzymes and transmembrane proteins. Finally, I will talk about a novel approach to rational enzyme engineering that we are currently investigating in collaboration with LISP-INSA.