



Contribution ID: 46

Type: **Talk**

Generating backbone conformational changes with seven league boots

Monday, 12 February 2024 15:50 (25 minutes)

Generating large amplitude conformational changes of complex biomolecules remains a challenge. This talk will review recent work on this problem, based on novel insights on loop closure techniques coupling kinematic models in dihedral angle spaces and MCMC sampling techniques of the Hit-and-Run type. Along the way, I will discuss connections with density of states calculations and thermodynamics.

Refs available from <http://www-sop.inria.fr/teams/abs/publications/frederic-cazals.html>

Enhanced conformational exploration of protein loops using a global parameterization of the backbone geometry

T. O'Donnell, and F. Cazals
J. Comp. Chem., 2023

Geometric constraints within tripeptides and the existence of tripeptide reconstructions

T. O'Donnell, and V. Agashe, and F. Cazals
J. Comp. Chem., 2023

Efficient computation of the the volume of a polytope in high-dimensions using Piecewise Deterministic Markov Processes

A. Chevallier, and F. Cazals, and P. Fearnhead
AISTATS, 2022

Wang-Landau algorithm: an adapted random walk to boost convergence

A. Chevallier, and F. Cazals
J. of Computational Physics, 410 (1), 2020

Submitting to:

Integrative Computational Biology workshop

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Session Classification: Computational Methods and Deep Learning