

Probabilistic sampling for physics: finding needles in a field of high-dimensional haystacks

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Type: **Non spécifié**

Sampling protein structure

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Setting aside the problem of designing force fields, sampling protein conformations to estimate their thermodynamic and kinetic properties remains a challenge. In this talk, I will review recent work on two connected problems in this realm.

The first one is the calculation of high dimensional volumes of polytopes, using random walks (hit-and-run, HMC, PDMP).

The second one is the sampling of protein conformations in internal coordinates, using the same kind of random walks.

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Classification de Session: Challenge and Perspective