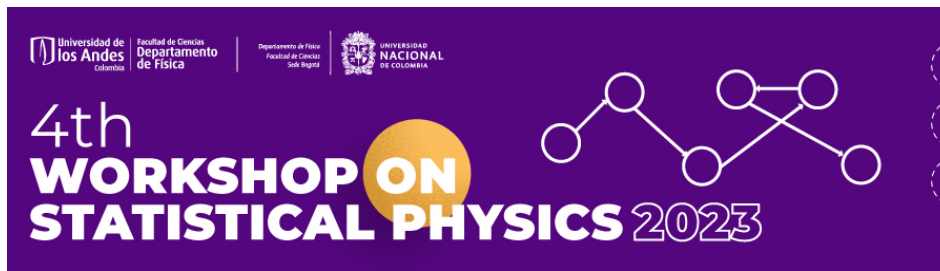


## 4th Workshop on Statistical Physics



Contribution ID: 53

Tipo: **Invited talk**

# Bayesian analysis of free energies using Cryo-EM particle images

*viernes, 6 de octubre de 2023 16:20 (20 minutos)*

Cryo-electron microscopy (cryo-EM) has recently become a leading method for obtaining high-resolution structures of biological macromolecules. However, cryo-EM is limited to biomolecular samples with low conformational heterogeneity, where most conformations can be well-sampled at various projection angles. While cryo-EM provides single-molecule data for heterogeneous molecules, most existing reconstruction tools cannot retrieve the ensemble distribution of possible molecular conformations from these data. To overcome these limitations, we build on a previous Bayesian approach and develop an ensemble refinement framework that estimates the ensemble density from a set of cryo-EM particle images by reweighting a prior conformational ensemble, e.g., from molecular dynamics simulations or structure prediction tools. Our work provides a general approach to recovering the equilibrium probability density of the biomolecule directly in conformational space from single-molecule data. To validate the framework, we study the extraction of state populations and free energies for a simple toy model and from synthetic cryo-EM particle images of a simulated protein that explores multiple folded and unfolded conformations.

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