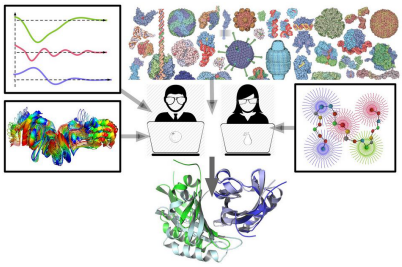

Contribution ID: **1** Type: **Poster**

Studying Protein Structure through Hydrogen Exchange and Coarse-grained Conformational Sampling

Experimentally observing and/or computationally modeling large proteins and macromolecular complexes remain critical challenges for structural biology. Hydrogen-exchange monitoring is cheap and easy to carry out, but cannot produce structural models because of its low resolution. To mitigate this issue, one side of our coupled approach consists of developing computational methods to complement such low-resolution experimental techniques. As these computational methods suffer from the curse of dimensionality when applied to large molecular systems, the other side of our coupled approach consists of guiding them with experimental data.

Here, we present three applications of our coupled approach combining hydrogen exchange on the experimental side and a robotics-inspired method for coarse-grained conformational sampling on the computational side. First, we argue that using coarse-grained conformational sampling of protein structure improves the fit between computationally-generated conformations and experimental hydrogen-exchange data. Second, we show that our approach allows analyzing the variability of a protein's native state described by crystallographic and hydrogen-exchange data. Finally, we explain how to obtain an atomic-resolution structural model of a protein state for which only hydrogen-exchange data is available.

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