

Special LASSP Seminar



**Wednesday
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**416 Physical Sciences
Building**

2 P.M.

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From kB to kB: Entropy evaluation made easy

Entropy and free-energy estimation are key in thermodynamic characterization of simulated systems ranging from spin models through polymers, colloids, protein structure, and drug-design. Current techniques suffer from being model specific, requiring abundant computation resources and simulation at conditions far from the studied realization. In this talk, I will present a novel universal scheme to calculate entropy using lossless compression algorithms and validate it on simulated systems of increasing complexity. Our results show accurate entropy values compared to benchmark calculations while being computationally effective. In molecular-dynamics simulations of protein folding, we exhibit unmatched detection capability of the folded states by measuring previously undetectable entropy fluctuations along the simulation timeline. Such entropy evaluation opens a new window onto the dynamics of complex systems and allows efficient free-energy calculations.

Hosted by Itai Cohen