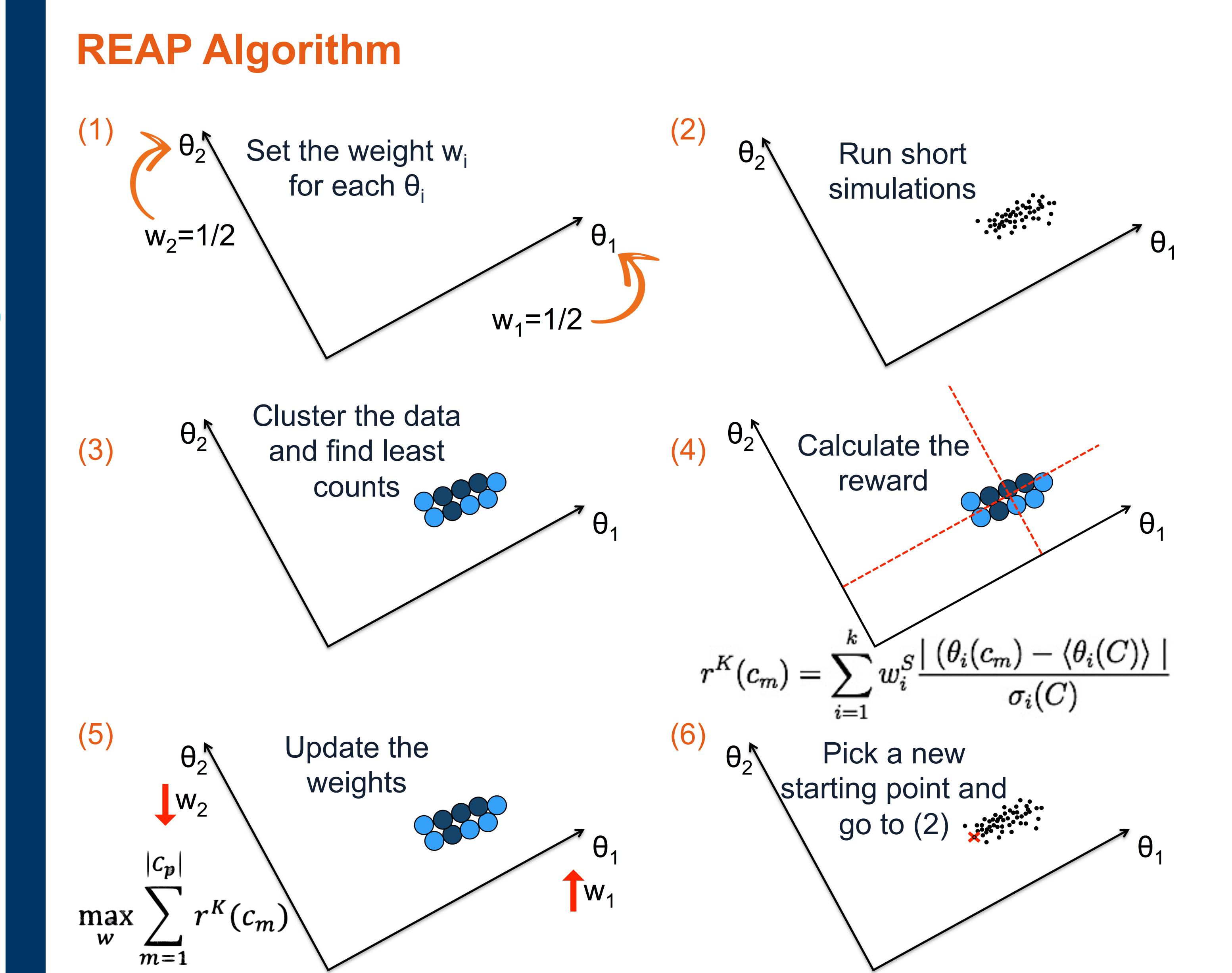
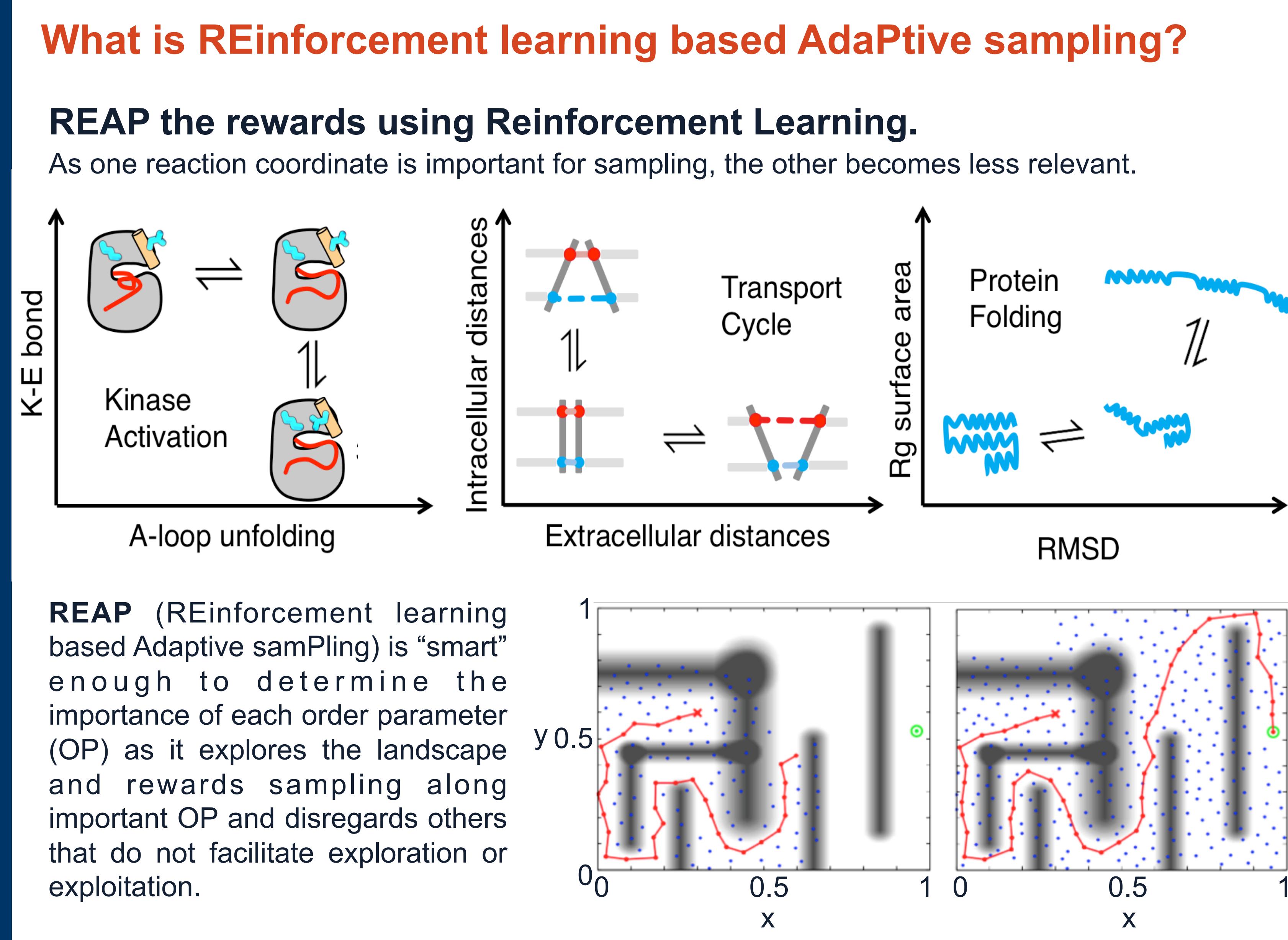
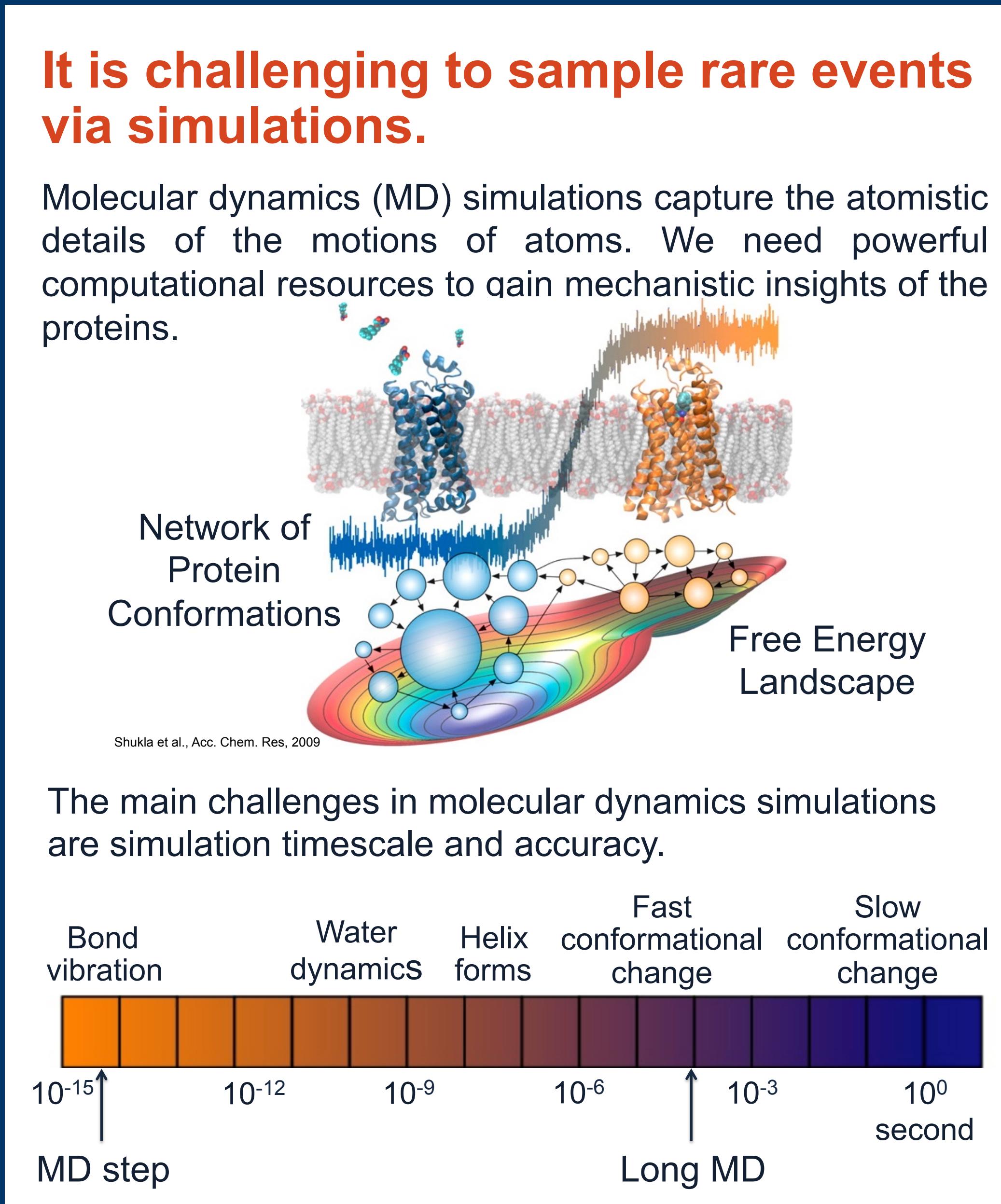


Efficient unbiased sampling of protein dynamics using reinforcement learning

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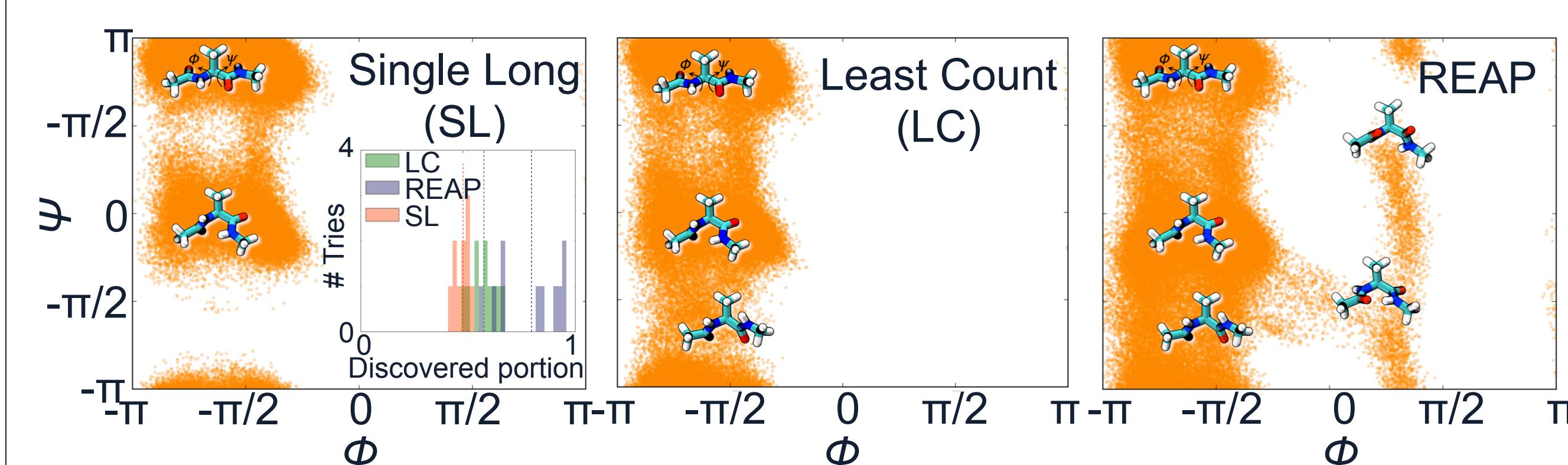
¹Department of Chemical and Biomolecular Engineering, ²Center for Biophysics and Quantitative Biology, University of Illinois at Urbana-Champaign
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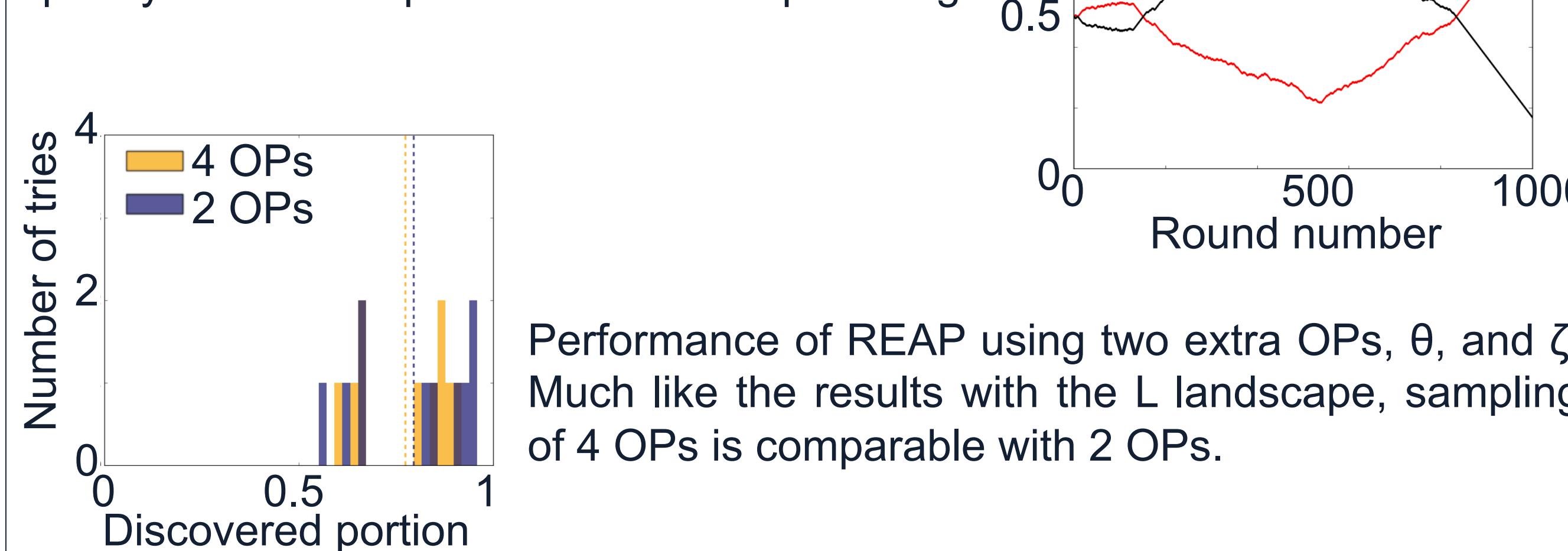
How effective is REAP?

Conformational sampling: Alanine dipeptide

Total of 2 ns MD simulation of Alanine dipeptide using SL, LC, and REAP were performed. REAP samples the dihedral angle landscape more effectively in the same amount of simulation time.

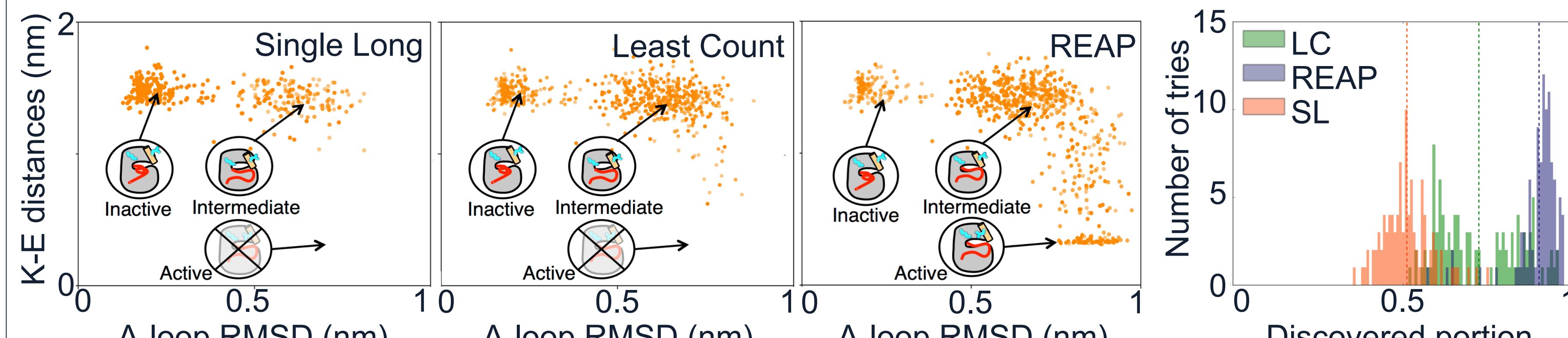


The algorithm initially starts from ϕ direction, but quickly learns that ψ is the best to sample along

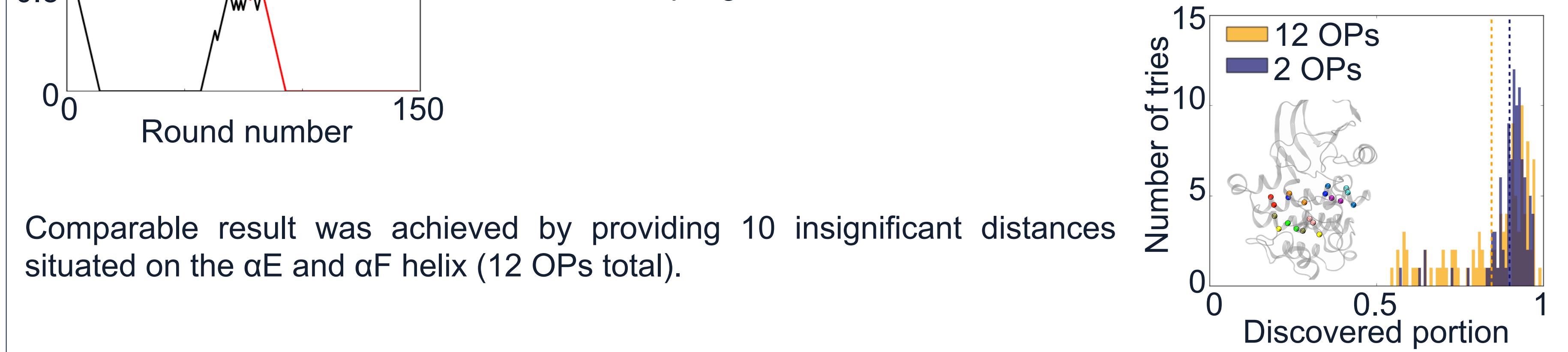


Enzyme activity: Src kinase activation

We furthermore demonstrated that the REAP algorithm's effectiveness in a protein system that has implications in cancer drug discovery. Total of 15 μ s Monte Carlo simulations on MSM of Src kinase using SL, LC, and REAP were performed.



REAP initially finds sampling along the A-loop RMSD more important than K-E distance. Afterwards, the weights fluctuate until the K-E distance then becomes relevant for sampling.



Conclusion

The proposed algorithm, REAP, has been shown to efficiently sample landscapes. It achieves this by identifying which RCs maximizes a reward function that encourages exploratory behavior. In all systems that were studied, REAP consistently outperformed the traditional simulation approach and least count based sampling when examining the distribution landscape discovered for the same simulation time.

Shamsi, Z., Cheng, J. K., & Shukla, D. REinforcement learning based Adaptive samPling: REAPing Rewards by Exploring Protein Conformational Landscapes, arXiv: 1710.00495, 2017.

Acknowledgements

