Principles of protein folding, interaction and evolution from intermediate resolution coarse-grained simulations

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ABSTRACT: Protein research is increasingly emphasizing the role of global conformational changes for how proteins carry out their biological functions. An important example is so-called intrinsically disordered proteins (IDPs) which do not spontaneously fold into a stable native structure but yet are fully functional. Highly dynamic proteins pose new challenges to both experiments and biomolecular simulations. In this presentation, I will introduce a coarse-grained approach to protein simulations that extend the reach of detailed molecular simulations to larger time scales and system sizes while maintaining sufficient realism and generality. The approach is characterized by an intermediate level of geometric detail and a procedure for determining effective model parameters based on properties of the global free energy landscape of proteins. I will highlight applications of this approach in the folding, interaction and evolution of proteins. In particular, I will discuss the role of conformational disorder-order transitions for the function of IDPs and conformational switching for the evolution of new protein folds.

Dr. Wallin is a candidate for an appointment to the Department of Physics and Physical Oceanography.

ALL ARE WELCOME!!!