Physics-Based Framework for Determining Transferable Potentials from a Databank of Structures for Different Proteins

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Low resolution coarse-grained (CG) models have played a central role in many areas of computational protein science. Since the seminal work by Tanaka and Scheraga, many groups have employed structural correlations within the protein databank (PDB) to parameterize a "knowledge-based" potential function for CG protein models. However, it has proven challenging to provide a first principles theory for knowledge-based potentials determined from the protein databank. It is well established that conventional knowledge-based approaches do not correctly treat either the many-body structural correlations present within compact folded proteins. Furthermore, it has not been clear how conventional statistical thermodynamics can be applied to analyze structural correlations for different proteins. The present talk will discuss our recent work addressing these two challenges. We have recently derived the first generalization of the famous Yvon-Born-Green theory for complex molecules with flexible internal degrees of freedom. This generalized-Yvon-Born-Green theory determines a variationally optimal potential function directly from structures. In addition, we have developed an extended ensemble formalism for developing transferable potentials from structural correlations for multiple proteins. In combination, these two advances provide a physics-based framework for determining transferable potentials from a databank of structures for multiple proteins.

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