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Energy parameterization of protein coarse-grained models MARCOS BETANCOURT, Indiana Univ. Purdue Univ. Indianapolis — Protein coarse-grained models are simplified representation of proteins that in principle can be used to perform long time scale simulations of protein folding dynamics, thermodynamics, and native structures. The main challenge in realizing these models is to find a physically accurate energy parameterization. Here two approaches are considered for this purpose. The first is the popular knowledge based potential approach, where the energies are extracted from the sequence and structure of known proteins. The advantages and limitations of this approach are examined from the perspective of minimal lattice models. It is concluded that this approach is less accurate in the determination of non-bonded interactions. The other approach involves the straightforward coarse-graining of individual residue pairs by performing molecular dynamics simulations. This approach does not suffer from the approximations involved in knowledge-based potentials and have the advantage that their quality can be controlled. The final energy model is built from a balanced combination of knowledge based potentials and coarse-grained interactions from molecular dynamics. Applications of this model to protein structure prediction are described.

Marcos Betancourt
Indiana Univ. Purdue Univ. Indianapolis

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