Topological Loss Factor

Dr. Joseph presented a method of coarse-graining polypeptides as amino acid beads with force field parameters that depend on pairwise amino acid coupling parameters, MPIPI. However, by modeling each residue as a bead, some interactions dependent on R-group geometry may be lost (entanglement of long side chains, MET-aromatic interaction, etc.). As such, I would be interested in calculating a “loss factor”, the energy difference between the MPIPI model, where each bead contains an entire amino acid, and a model with an explicit side chain.

This could be done by running identical simulations between the MPIPI coarse-grained model and another with a coarse-grained backbone and atomistic-resolution side chain. The energy of each interaction would then be subtracted.