PROTEIN VISUALIZATION AND SIMULATION IN 3D

STUDENT POSTER PRESENTATION

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The function of a protein is primarily determined by its three-dimensional geometry, which is, in turn, determined by its one-dimensional amino acid sequence. It is not practical to replicate this process, called protein folding, with brute-force algorithms and today’s computer technology. Instead, biological scientists and pharmacologists can utilize protein visualization software, which allows them to view and explore known protein structures in 3D on personal computers. In this way, researchers apply human intuition to the folding problem and can develop drugs that interact with proteins without directly solving the folding problem.

Most protein visualization software parses Protein Databank (PDB) or like files in order to form rigid, 3D protein models. However, a protein is not a wholly rigid construct. Proteins naturally move and deform—sometimes a lot—and this movement is also related to the protein’s function. So we have developed a scalable 3D model for a protein that accounts for all degrees of freedom along a protein’s carbon backbone. We have utilized this model to great effect in our new protein visualization software.

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