Knowing *How* to Fold Them

Sequencing the human genome was a tremendously significant accomplishment, but now comes the hard part: Understanding the structure and function of proteins. The 100,000 proteins in our bodies initiate, control, or perform every one of our biological functions through shapes (called *folds*) and communication with other proteins. Misfolded or mistargeted proteins can cause diseases such as cancer, mad cow, and cystic fibrosis. Computational biologists are using geometry, probability, and knot theory to begin to describe the intricate folding of proteins. Once it is known just exactly how a malfunctioning protein goes awry, drugs can be designed that address the problem, thereby restoring affected cells.

Proteins assemble and re-assemble in an infinitesimal space and, most often, time span, yet the simulations of their functions are enormous, involving millions of calculations at each of billions of tiny time intervals. Almost every subject in mathematics—including integrals, partial differential equations, linear algebra, and numerical analysis—goes into simulating protein behavior, which, even for the simplest proteins, requires parallel computation to solve. It may seem unusual to concentrate such massive effort on such a small scale, but it is productive: Some strains of HIV had been resistant to treatment, but models of an HIV protein, *integrase*, revealed a nanoscale-sized trench that researchers can fill with a compound to overcome the resistance.

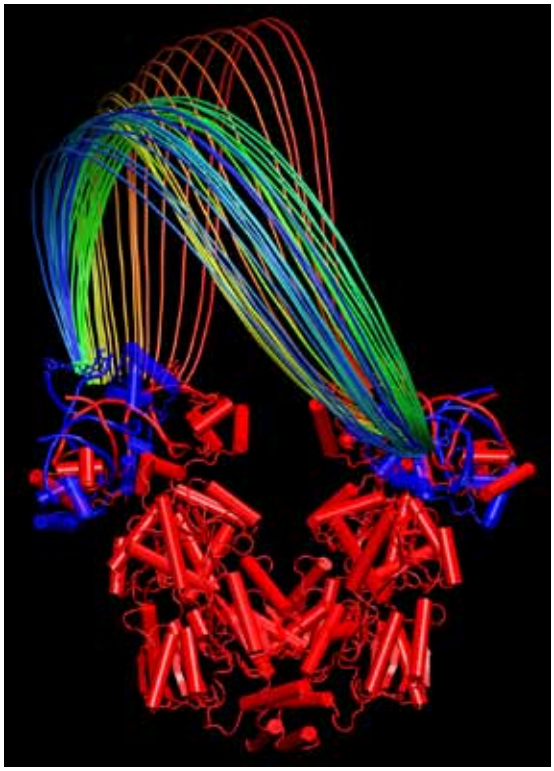

Image courtesy of Theoretical & Computational Biophysics Group, University of Illinois.

For More Information: *From Protein Structure to Function with Bioinformatics*, Daniel John Rigden, Editor.

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