

Biomedical Computation Review

Simbios AN NIH NATIONAL CENTER FOR BIOMEDICAL COMPUTING

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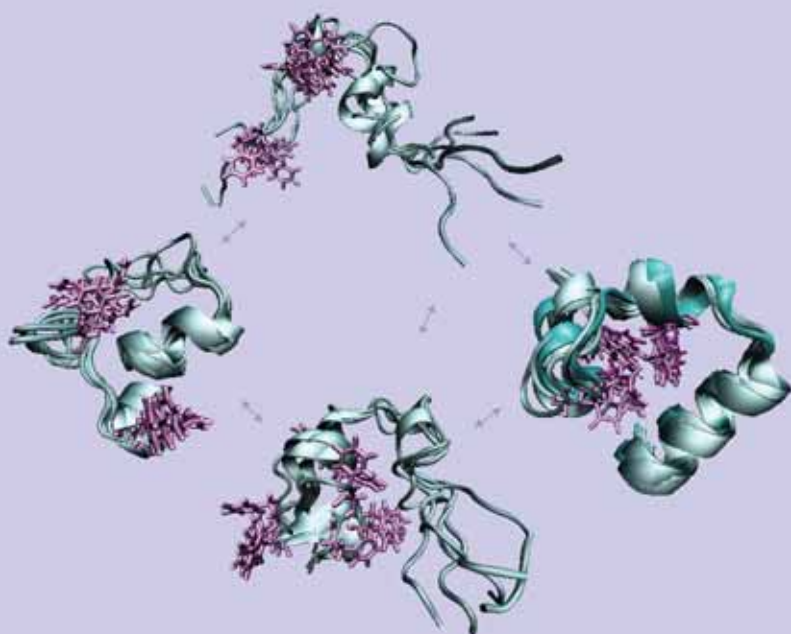
BY JOY KU, PhD

Dealing With a Flood of Conformations Using MSMBuilder

In the world of molecular dynamics (MD), researchers often need to analyze and extract meaningful results from millions of conformations. Existing software for accomplishing this task focuses on geometric metrics—organizing the data only by the structural information. But **Greg Bowman**, a graduate student in biophysics at Stanford University, and his colleagues saw the need to also incorporate dynamic behavior—as a way to access

important kinetic properties of the system. Their solution, MSMBuilder, automatically divides an MD trajectory data set into groups, or states, based on similarities in their kinetic behavior. It then identifies relationships between these states, resulting in a Markov state model (MSM). It is now freely available for download from <http://simtk.org/home/msmbuilder>.

“MSMBuilder is the first available software for kinetic clustering,” says **Xuhui Huang, PhD**, a research associate with Simbios at Stanford University and a co-developer of MSMBuilder. Moreover, Bowman says, MSMBuilder ensures the analysis is done on a representative sampling of the conformations’ true distribution. “Without a tool like MSMBuilder that helps provide good sampling, you can spend lots of limited computing resources doing the same thing over and over again and not get any more information.” □



Bowman and his colleagues’ first test of MSMBuilder’s predictive capabilities sought to automatically identify the native state of the villin protein from an MD data set with nearly 8 million conformations. Shown here are 4 clusters of conformations automatically identified by MSMBuilder. Each cluster represents a state of the villin protein. Arrows indicate transitions between states, also identified by MSMBuilder. The group or cluster representing the native state (right-most) was accurately identified. Its members match the crystal structure (shown in darker blue and magenta) with an average root mean square deviation (RMSD) of 1.8 Angstroms. MSMBuilder is freely available for download from <http://simtk.org/home/msmbuilder>.