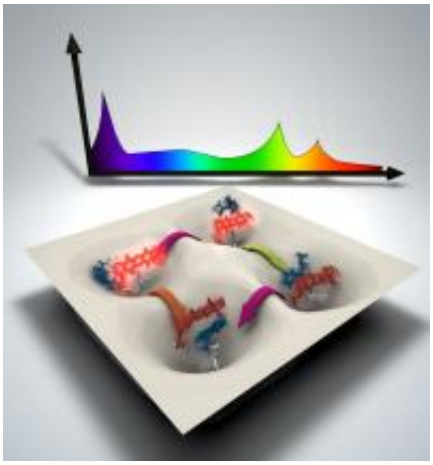
'Fingerprints' match molecular simulations with reality

February 22 2011



As a molecule jumps between structural states (below), it creates "dynamical fingerprints" (top spectra) that can tie together high-performance simulation and experiments.

A theoretical technique developed at the Department of Energy's Oak Ridge National Laboratory is bringing supercomputer simulations and experimental results closer together by identifying common "fingerprints."

ORNL's Jeremy Smith collaborated on devising a method -- dynamical fingerprints -- that reconciles the different signals between experiments and computer simulations to strengthen analyses of molecules in motion. The research will be published in the Proceedings of the National

Academy of Sciences.

"Experiments tend to produce relatively simple and smooth-looking signals, as they only 'see' a molecule's motions at low resolution," said Smith, who directs ORNL's Center for Molecular Biophysics and holds a Governor's Chair at the University of Tennessee. "In contrast, data from a supercomputer simulation are complex and difficult to analyze, as the atoms move around in the simulation in a multitude of jumps, wiggles and jiggles. How to reconcile these different views of the same phenomenon has been a long-standing problem."

The new method solves the problem by calculating peaks within the simulated and experimental data, creating distinct "dynamical fingerprints." The technique, conceived by Smith's former graduate student Frank Noe, now at the Free University of Berlin, can then link the two datasets.

Supercomputer simulations and modeling capabilities can add a layer of complexity missing from many types of molecular experiments.

"When we started the research, we had hoped to find a way to use computer simulation to tell us which molecular motions the experiment actually sees," Smith said. "When we were finished we got much more -- a method that could also tell us which other experiments should be done to see all the other motions present in the simulation. This method should allow major facilities like the ORNL's Spallation Neutron Source to be used more efficiently."

Combining the power of simulations and experiments will help researchers tackle scientific challenges in areas like biofuels, drug development, materials design and fundamental biological processes, which require a thorough understanding of how molecules move and interact.

"Many important things in science depend on atoms and molecules moving," Smith said. "We want to create movies of molecules in motion and check experimentally if these motions are actually happening."

View a supercomputer simulation of a protein in motion here: www.ornl.gov/ornlhome/hg_mer.htm

"The aim is to seamlessly integrate supercomputing with the Spallation Neutron Source so as to make full use of the major facilities we have here at ORNL for bioenergy and materials science development," Smith said.

Provided by Oak Ridge National Laboratory