



Algorithm for Molecular Simulation and Analysis

Rachel Vincent-Finley

Southern University and A&M College, Department of Mathematics
rachel_finley@subr.edu

The study of protein structure and function is a driving force in research that attempts to identify a relationship between the primary structure of a protein and its three dimensional structure. In this presentation we will discuss a technique for the analysis of molecular simulations. Principal component analysis (PCA) is used to identify the dominant characteristics of molecular dynamics (MD) trajectories and to represent the coordinates with respect to these characteristics.

We apply this method to proteins. With respect to protein dynamics, local motions, such as bond stretching, occur within femtoseconds, while rigid body and large-scale motion, occur within a range of nanoseconds to seconds. To capture motion at all levels, time steps on the order of a femtosecond are used when solving the equations of motion and, it is typically the case that simulations of a few nanoseconds do not provide adequate sampling for the study of large-scale motions. Thus techniques with potential to efficiently extend simulation times can advance the study of protein structure and function. We will discuss issues encountered in the development of this method, explore applications and outline limitations.

Biography

R. Vincent-Finley was born in the New England region and grew up on various military bases throughout the United States. After completing a Bachelor of Arts degree in Mathematics at Bryn Mawr College, R. Vincent-Finley entered the graduate program in Computational and Applied Mathematics at Rice University. Upon completing her doctoral work at Rice University, R. Vincent-Finley served as a postdoctoral fellow in the Institute of Molecular Design at the University of Houston.

Rachel Vincent-Finley joined the faculty of Southern University and A & M College (Fall 2009) as a Louisiana Optical Network Initiative (LONI) Institute Fellow and an Assistant Professor of Computer Science. Her general research interests include numerical linear algebra and numerical analysis with current research applications to molecular biophysics and materials science.

R. Vincent-Finley is a recipient of a 2012 Career Enhancement Fellowship for Junior Faculty (2012 – 2013) administered by the Woodrow Wilson National Fellowship Foundation and funded by the Andrew W. Mellon Foundation.

In the Fall 2013, R. Vincent-Finley will continue service at Southern University as an Assistant Professor of Mathematics.