Thomas E. Cheatham, III

Associate Professor of Medicinal Chemistry

College of Pharmacy, University of Utah

Channeling XSEDE computational resources for assessing and validating RNA simulations

Abstract

Molecules of RNA have diverse biological roles ranging from protein synthesis and catalyzing chemistry to gene regulation and biomolecular sensing. The functions of RNA are intimately related to the molecular structure, and often the interesting activities relate not only to non-canonical structural features like bulges and loops but to their dynamics. Atomistic molecular dynamics simulations provide one means to characterize RNA structure and dynamics. However, until fairly recently, the common "force fields" that describe nucleic acid structure tended to do a poor job of modeling non-canonical RNA structure. We will highlight our efforts to improve nucleic acid force fields and to validate and assess MD simulation of RNA molecules across a large range of structures and interactions. This has been made possible by access to significant computational resources, including GPU-aware versions of AMBER. These resources push us to our limits in terms of workflow, data handling and process management.

Biosketch

Thomas Cheatham, Associate Professor of Medicinal Chemistry in the College of Pharmacy at the University of Utah, received his B.A. degrees in Chemistry and in Mathematics and Computer Science from Middlebury College in 1988, worked as a Programmer/Analyst at the Aiken Computational Lab at Harvard, then in 1990 joined the Pharmaceutical Chemistry PhD Program at the University of California San Francisco working with the late Peter Kollman. After receiving his PhD in 1997, Cheatham was a NRC postdoctoral fellow with Bernie Brooks at the National Institutes of Health before moving to Utah in 2000 where he managed the mine fields of multiple departments and research track professor positions to ultimately get tenure.

Cheatham's research centers on the development, application and validation of biomolecular simulation methods to provide insight into biomolecular structure, dynamics, energetics and interactions. He is one of the core AMBER developers and primary author of the "ptraj" molecular dynamics trajectory analysis software. Current resources supporting the Cheatham lab include funding from three NIH grants (R01 GM-081411, GM-098102 and GM-074249), a NSF PRAC travel award (OCI-1036208), and a large allocation of computational resources from the NSF XSEDE (MCA-01S027). For more information, see http://www.chpc.utah.edu/~cheatham