Sally R. Ellingson
Graduate Research Assistant
Center for Molecular Biophysics
University of Tennessee

Virtual High-Throughput Molecular Docking

Abstract

Many pharmaceuticals act by selectively binding to a specific protein and thus inhibiting a specific process relevant to a disease or illness. Because of this, the early stage of drug discovery consists of identifying potential compounds that bind to a protein of interest with a high affinity and specificity. Experimentally testing a very large number of these compounds is both costly and time consuming. Virtual high-throughput screening is an equivalent computational process that can reduce the time and cost of discovering new drugs. After a potential lead compound is identified in the drug discovery process further tests must be done in order to determine toxicity and side effects. Computational tools, such as the ability to virtually screen a lead compound against a very large number of different proteins at once, to help predict these effects earlier in the drug discovery pipeline would be valuable.

In this talk, I will discuss an MPI (Message Passing Interface) version of Autodock4, an open source docking program, that was developed to run on high-performance computers. This software facilitates high-throughput virtual screens, docking large libraries of chemical compounds into a target protein on up to thousands of processors. Recently we ran a virtual screen of one million chemical compounds in just under 24 hours on the Jaguar Supercomputer. I will discuss the limitations of this program when examining multiple proteins and steps that need to be taken in order to facilitate this new technique.

Biosketch

After receiving her B.S. in Computer Science and Mathematical Sciences at the Florida Institute of Technology, Sally joined the Department of Genome Science and Technology (GST) at the University of Tennessee through the SCALE-IT program. SCALE-IT (Scalable Computing and Leading Edge Innovative Technologies) is an NSF-IGERT funded program which aims to integrate the fields of computer science and quantitative biology in order to reach new insights on biological questions of high societal value. In addition to her training through GST and SCALE-IT, Sally is also enrolled in the IGMCS (Interdisciplinary Graduate Minor in Computational Science) program at the University of Tennessee. While pursuing her PhD, she is working at the Center for Molecular Biophysics at Oak Ridge National Laboratory under the supervision of Dr. Jerome Baudry. Her research interests include the development of virtual drug screening tools that run on high-performance computers that reduce the time and cost for novel pharmaceutical discovery.