

# High-Performance Supercomputing for Drug Design

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**Abstract**— High performance supercomputing has become a major focus of attention by government, industry, medical centers and academic institutions. The U.S. government has made this a "top national priority", linking the development of a "data superhighway system" to national competitiveness and national research interest. High performance supercomputing approaches have been used for sequence analysis, gene finding, protein structural prediction, all-atom simulation such as molecular dynamics and quantum calculations, modeling biological networks such as systems biology and more recently drug design and drug discovery. All these approaches are highly computationally demanding, in terms of compute load, communication speed, and memory load. Supercomputing based drug design and drug discovery use high-performance supercomputers and bioinformatics approaches to discover, enhance, and study drugs and related biologically active molecules as well as the sites of protein interactions. Methods include molecular modeling using biophysical approaches such as molecular dynamics, semi-empirical quantum mechanics methods, *ab initio* quantum chemistry methods, density functional theory, receptor - ligand interactions and protein docking and so on. The success of the high-throughput drug design and drug discovery now directly relies on the high-performance supercomputing capabilities. Many research and computational products that were used to be considered impossible now proved to be feasible and effective with the help of today's supercomputing techniques. In particular, the identification of diseases relating to protein structural changes challenges biomedicine as the result of the sophisticated protein interaction networks that demand effective drug design using supercomputing based on mathematical, computational and biophysical models and algorithms for solving the model equations, and the bioinformatics techniques to analyze and validate the results. Those will need our deeper studies of biophysical phenomena and interesting biophysical and algorithmic problems using supercomputing. In this keynote lecture, we follow the scenario of Koshland's "induced-fit" to demonstrate that the identification of intrinsically disordered/unstructured proteins will become increasingly important to the drug design and discovery, because many proteins are folding upon interaction with drugs. The High-performance supercomputing approaches help to reduce the number of targets for a good drug that has to be eventually tested by expensive and time-consuming synthesis and laboratory and toxicology experiments. High-performance supercomputing study of intrinsically unstructured protein related pathways focuses on the discovery and development of novel drugs for the treatment of metabolic and mis-folding related diseases by targeting the metabolic and biological pathways in the protein interaction network. The advances of supercomputing will foster the synergistic relation between biophysical and computational sciences in the future.

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**Bio-** Hamid R. Arabnia received his Ph.D. degree in Computer Science from the University of Kent (Canterbury, England) in 1987. In 1987, he worked as a Consultant for Caplin Cybernetics Corporation (London, England), where he helped in the design of a number of image processing algorithms that were targeted at a particular parallel machine architecture. Prof. Arabnia is currently a Full Professor of Computer Science at University of Georgia (Georgia, USA), where he has been since October 1987. His research interests include Parallel and distributed processing techniques and algorithms, interconnection networks, and applications (in particular, in image processing, computer graphics, medical imaging, and other computational intensive problems). Prof. Arabnia has chaired many national and international conferences and technical sessions in these areas; he is the chair of WORLDCOMP annual research conference (WORLDCOMP attracts 1,800 attendees per year from 78 countries - the event is considered to be the largest research conference in Computer Science). He is Editor-in-Chief of The Journal of Supercomputing (Springer) and is on the editorial boards of 12 other journals and magazines. He is the chair of the world committee of PDPTA (Parallel and Distributed Processing Techniques and Applications research organization: PDPTA is composed of 28 task forces with over 2,800 active participants). Prof. Arabnia is the recipient of William F. Rockwell, Jr. Medal for promotion of multi-disciplinary research (Rockwell Medal is International Technology Institute's highest honor). In 2000, Prof. Arabnia was inducted to the World Level of the Hall of Fame for Engineering, Science and Technology (The World Level is the highest possible level for a living person - there are two higher levels which are posthumous.) He has received a number of awards, including, The Johns Hopkins University National Search (Certificate of Achievement) in recognition of his contributions to the national program for enhancing the quality of life for people with disabilities through the application of computing technology. More recently, Prof. Arabnia received the Distinguished Service Award in recognition and appreciation of his contributions to the profession of computer science and his assistance and support to students and scholars from all over the world; this award was formally presented to him on June 26, 2006 by Professor Barry Vercoe (Massachusetts Institute of Technology / MIT). Prof. Arabnia has published extensively in journals and refereed conference proceedings. He has over 250 research publications (journals, proceedings, editorship) in his area of research. Prof. Arabnia has been a Co-PI/PI on \$7,139,525 externally funded projects/initiatives (includes UGA matching) and on \$103,453 internally funded projects (as of August 2007). He has also contributed projects for justification for equipment purchase (grant proposals worth over \$3 Million - awarded).