Visions for Quantitative Biology Lecture Series

Is Silico Approach to Protein Folding?

Ulrich Hansmann, Michigan Technological University

Professor, Department of Physics

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Abstract:
Proteins are nanomachines that perform a large number of diverse functions in cells. Despite decades of research we still do not understand in complete detail the mechanism by which they fold into their biologically active form. Computational tools that allow one to evaluate the sequence-structure relationship and the folding process would therefore lead to a deeper insight into the molecular machinery of cells. Unfortunately, computer simulations are extremely difficult for detailed protein models. This is because the energy landscape of all-atom protein models is characterized by a multitude of local minima separated by high energy barriers. Only over the last few years have there been algorithms developed that allow one to overcome this multiple-minima problem. I will discuss some of these techniques, and show applications where they have revealed new folding mechanisms in proteins.

Speaker's Bio:
Dr. Ulrich H.E. Hansmann is an Professor in the Department of Physics at Michigan Technological University, Houghton, MI. During the time of July 2005 till Aug. 2007 he had a joined appointment with the John von Neumann Institute for Computing (Germany's premier supercomputer center) where he was head of the "Computational Biology and Biophysics" group. He received his M.A. degree in philosophy, and his "Diplom" (equivalent to a M.S.) and Ph.D. in physics from the Freie Universität Berlin at Berlin, Germany. Professor Hansmann has an active research program in the areas of biomolecular modeling, complex systems and global optimization techniques. He has published more than 100 papers in various journals and conference proceedings (including prestigious journals such as Physical Review Letters and the Proceedings of the National Academy of Sciences) that received over the last four years between 200-250 citations annually. He has presented numerous invited and contributed talks at international conferences and workshops. His work is sponsored by the National Science Foundation and the National Institutes of Health. Dr. Hansmann advises currently three Ph.D. students. His teaching interests include: Statistical Physics, Computational Physics, Bioinformatics and Biomolecular Modeling, Biophysics; and University Physics for undergraduate students. Dr. Hansmann has taught various short courses on algorithms for simulations of biological molecules. He is also co-author of three widely quoted review articles on that topic. His teaching receives high marks in the student evaluations. Professor Hansmann served in various committees in the Department of Physics including the advisory committee, graduate studies committee and undergraduate committee. He is often asked to write referee-reports for the National Science Foundation, The Wellcome Trust Fund, Petroleum Research Fund, and prestigious journals such as Physical Review Letters and the Journal of the American Chemical Society. He was a recipient of a MTU faculty scholarship award and various fellowships from research institutions such as DFG (Germany), JSPS (Japan), Academia Sinica (Taiwan) and FASP (Brazil).

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2003 Digital Media Center • Telephone: +1 225/578-5890 • Fax: +1 225/578-8957