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M&S Colloquium

Modeling and Simulation of Proteins

V. Sundararajan

Scientific & Engineering Computing Group,
Centre for Development of Advanced Computing

Wednesday, 26 October 2005, 3:00–5:00 PM
Sir C. V. Raman Auditorium, Department of Physics

• colloquium duration includes a tea break •

Protein structure prediction is one of the challenging tasks in molecular biology due to its complexity and hence can play an important role of bridging the gap between the rate at which sequences are made known and the rate of finding their native structures. Till date, there is no single method, which can make ab initio prediction. This talk briefly reviews protein folding problem and the various methodologies followed to make protein structure predictions using Genetic Algorithms. Genetic Algorithms has been in use for about few decades now. Though it works for smaller peptides, there are severe problems faced as the size of the protein approaches the larger and real ones. There is a lot of work that needs to be done to predict real protein structures in order to emphasize the importance of ab initio methods so that, a protein without any sequence similarity and unknown folds could be modelled.

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Dr. Vijayraghavan Sundararajan was born in Bangalore, India in 1960. Had his basic education in Chennai (Madras). Did his Ph.D. in Physics from Anna University, Chennai in 1989. After a brief stint of post-doctoral work at University of Pune, he worked as a lecturer there till March 1994. During this tenure, he visited International Centre for Theoretical Physics, Trieste, Italy for about 14 months during 1992-93. Since April 1994 he has been working at Centre for Development of Advanced Computing, (C-DAC), Pune. Currently, he is the coordinator of the scientific and Engineering Computing Group which spearheads the high performance computing applications on the PARAM machine developed by C-DAC. He was visiting associate professor at Institute of Materials Research and Centre for inter-disciplinary studies, at Sendai, Japan, for about five months during 2000-01 and later as a guest scientist at the German Cancer Research Centre, Heidelberg for about 15 months. His major areas of research interest are protein structure prediction multiscale modeling and simulations, applied Evolutionary computing and high performance computing. He has about 40 published research articles to his credit.