Stanford

Vijay Pande

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Vijay Pande, Henry Dreyfus Professor of Chemistry and, by courtesy, of Structural Biology and Computer Science, also currently directs of the Stanford Program in Biophysics and the Folding@home Distribtued Computing project. His research centers on novel cloud computing simulation techniques to address problems in chemical biology. In particular, he has pioneered distributed computing methodology to break fundamental barriers in the simulation of protein and nucleic acid kinetics and thermodynamics. As director of the Folding@home project (http://folding.stanford.edu), Prof. Pande has, for the first time, directly simulated protein folding dynamics, making quantitative comparisons with experimental results, often considered a “holy grail” of computational biology. His current research also includes novel computational methods for drug design, especially in the area of protein misfolding and associated diseases such as Alzheimer’s and Huntington’s Disease.

Professor Pande studied physics at Princeton University (B.A. 1992), where he was first introduced to biophysical questions, especially in undergraduate research with Nobel Laureate P. Anderson. His doctoral research in physics under Profs. T. Tanaka and A. Grosberg at MIT (Ph.D. 1995) centered on statistical mechanical models of protein folding, suggesting new ways to design protein sequences for stability and folding properties. As a Miller Fellow under Prof. D. Rokhsar at UC Berkeley, Prof. Pande extended this methodology to examine atomistic protein models, laying the foundations for his work at Stanford University. Among numerous awards, Prof. Pande has received the Biophysical Society’s Bárány Award for Young Investigators and Protein Society’s Irving Sigal Young Investigator Award, and was named to MIT’s TR100 and elected a Fellow of the American Physical Society.

The Pande research group develops and applies new theoretical methods to understand the physical properties of biological molecules such as proteins, nucleic acids and lipid membranes, using this understanding to design synthetic systems including small-molecule therapeutics. In particular, the group examines the self-assembly properties of biomolecules. For example, how do protein and RNA molecules fold? How do proteins misfold and aggregate? How can we use this understanding to tackle misfolding related degeneration and develop small molecules to inhibit disease processes?

As these phenomena are complex, spanning molecular to mesoscopic lengths and nanosecond to millisecond timescales, the lab employs a variety of methods, including statistical mechanical analytic models, Markov State Models, and statistical and informatic methods. Other tools include Monte Carlo, Langevin dynamics, and molecular dynamics computer simulations on workstations and massively parallel supercomputers, superclusters, and worldwide distributed computing. The group has also done extensive work in the application of machine learning, pioneering traditional and deep learning approaches to cheminformatics, biophysics and drug design.

For example, simulations in all-atom detail on experimentally relevant timescales (milliseconds to seconds) have produced specific predictions of the structural and physical chemical nature of protein aggregation involved in Alzheimer’s and Huntington’s diseases. These results have fed into computational small molecule drug design methods, yielding interesting new chemical entities.

Since such problems are extremely computationally demanding, the group developed a distributed computing project for protein folding dynamics. Since its launch in October 2000, Folding@Home has attracted more than 4,000,000 PCs, and today is recognized as the most powerful supercluster in the world. Such enormous computational resources have allowed simulations of unprecedented folding timescales and statistical precision and accuracy. For more details, please visit http://pande.stanford.edu.