

数学与系统科学研究院

计算数学所学术报告

报告人: Prof. Chandrajit Bajaj

**(Department of Computer Sciences, and Institute
of Computational Engineering & Sciences,
Center for Computational Visualization,
University of Texas at Austin)**

报告题目:

**EFFICIENT COMPUTATIONS
FOR DRUG DISCOVERY**

邀请人: 徐国良研究员

报告时间: 2009年12月25日(周五)

上午 10:00—11:00

报告地点: 科技综合楼三层 311

计算数学所报告厅

Abstract:

Human functional processes are mediated through complicated biochemical and biophysical interactions amongst proteins, and other biomolecules. A comprehensive computational model and analysis of these interactions, provide important clues for developing therapeutic interventions related to infections and disease. In this two part talk I shall first describe a combination of geometric algorithms to efficiently construct algebraic spline models of target protein structures, that are culpable in the spread of viral infections. Next, I shall present the use of a fast neighborhood data structure called Dynamic Packing Grids (DPG), and the use of non-uniform fast Fourier estimation methods in the very rapid computation of protein binding energetics, essential for drug screening analysis and discovery.

报告人简介:

Chandrajit L. Bajaj is the director of the Center for Computational Visualization, in the Institute for Computational and Engineering Sciences (ICES) and a Professor of Computer Sciences at the University of Texas at Austin. Bajaj holds the Computational Applied Mathematics Chair in Visualization. He is also an affiliate faculty member of Mathematics, Electrical Engineering, Bio–Medical Engineering, and also a member of the Institutes of Cell and Molecular Biology, and Neurosciences, the Center for Learning and Memory, and the Center for Perceptual Systems. He is an author and editor of over 300 publications, including 225 papers, 30 book chapters, and 1 book and 3 edited volumes. He is on the editorial boards for the International Journal of Computational Geometry and Applications, the ACM Transactions on Graphics, the ACM Computing Surveys, the

SIAM Journal on Imaging Sciences, and the International Journal of Visualization. He is on numerous national and international conference committees, and has served as a scientific consultant to national labs and industry. He is also a fellow of the American Association for the Advancement of Science (AAAS) and the Association of Computing Machinery (ACM).

欢迎大家参加！