数学与系统科学研究院

计算数学所系列学术报告

报告人： **Prof. Chandrajit Bajaj**

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

报告题目：

Learning to Dock and Predict Assemblies

邀请人： 陈冲 博士

报告时间：2018 年 11 月 13 日（周二）

上午 **10:00-11:00**

报告地点： 数学院南楼二层

202 教室

Abstract：

I shall present a multi-stage machine learning approach to automatically choosing weighting and threshold filter parameters, in a multi-term scoring functions and ☐filters. Such scoring functions are often used in molecular docking software. In particular we have applied and compared the improvement of docking results achieved by using our Fast Fourier based docking and re-ranking software called F2Dock. I shall then describe TilerGen which generates which generates almost congruent polyhdedral tilings and layouts. The governing rules yields tile arrangements with maximal vertex, edge and face symmetries. The family of all such congruently tiled cages create a new generative class of polyhedra, beyond the well-studied regular, semi-regular and quasi-regular classes, and their duals (platonic, Catalan and Johnson). Our construction thus further enables the prediction of generative tiled assemblies. This is joint work with Dr. Muhibur Rasheed.

报告人简介：

Chandrajit Bajaj is a Professor in the Department of Computer Science, and Institute of Computational Engineering and Sciences, and Center for Computational Visualization at The University of Texas at Austin, USA. He received his B.Tech. in Electrical Engineering (1980) from Indian Institute of Technology, New Delhi, India; and his M.S. and Ph.D. in Computer Sciences (1983, 1984) from the Cornell University, Ithaca, USA. He is the Fellow of AAAS, Fellow of ACM, Fellow of IEEE, and Fellow of SIAM.

欢迎大家参加！