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

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报告题目：

Scalable Geometric Optimization with Applications to Molecular Interactions

邀请人：　陈冲　博士

报告时间：2018 年 11 月 13 日（周二）

上午 9:00-10:00

报告地点：　　数学院南楼二层

202 教室

Abstract:

Geometric optimization is the computational reduction technique of choice for a wide variety of model selection, ranking and assembly prediction problems. Moreover, optimization occurs naturally for solutions to rigid and flexible geometric shape similarity, complementarity matching problems (e.g. predicting multi-component assemblies, disaster reconstructions etc). The optimization functional is often a multi-dimensional correlation integral while the search space is the product of transformations groups with dimension growth exponential in the number of movable components (e.g. O(3^n) for an n-residue torsionally flexible molecule). In this talk, I shall dwell on solution of geometric optimization methods that combat the curse of high dimensionality, and also achieve adequate tradeoffs between speed and accuracy. Fast approximate estimations to the geometric similarity or complementarity matching optimization problem take advantage of a new scheme of generating low-discrepancy samplings of the n-product configuration spaces, as well as utilization of approximate non-uniform fast Fourier transforms.

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.

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