Informatik-Kolloquium

Fachgruppe Informatik

Lehrstuhl für Informatik 8

RHEINISCH-WESTFÄLISCHE TECHNISCHE HOCHSCHULE AACHEN

EINLADUNG

Zeit: Donnerstag, 26.07.2012, 10.00 Uhr

Ort: Raum 6317 (Seminarraum Informatik 8), Ahornstr. 55

Referent: Professor Deok-Soo Kim, Ph.D.
Hanyang University, Seoul, Korea

Titel: Understanding molecular geometry

Abstract:

Structure is important for understanding biomolecular functions and geometry is an important aspect of molecular structure. Despite of its importance, the theory for molecular geometry has not been sufficiently developed. In this presentation, we will present a geometric theory for biomolecules and demonstrate how the theory can be used for solving molecular problems.

Voronoi/Delaunay structures are everywhere in nature and useful for understanding the spatial structure of their generators. Being powerful computational tools, their generalization has been made in various directions including the Voronoi diagram of spherical balls (or atoms). The Voronoi diagram of spherical atoms, usually called the additively-weighted Voronoi diagram, nicely defines the proximity among the atoms. Like its counterpart of the ordinary Voronoi diagram of points (or the power diagram), the dual structure (which our group has defined and successfully characterized) is more convenient in both representing and traversing the topology structure of the Voronoi diagram.

This talk will introduce the Voronoi diagram of spherical atoms and its dual structure, the quasi-triangulation, particularly in the three-dimensional space. Based on the quasi-triangulation, we define a new geometric structure called the beta-complex which concisely yet efficiently represents the proximity among all atoms. It turns out that the beta-complex can be used to “precisely,” “efficiently,” and “easily” solve many seemingly unrelated geometry and topology problems for the atom set within a single framework. Among many potential application areas, the structural molecular biology is the most immediate application area.

Application examples include the following: the most efficient/precise computation of van der Waals volume (and area), the volumes within an accessible/Connolly surface; an efficient docking simulation; the recognition of internal voids and their volume computation; the recognition of molecular tunnels, the comparison (or superposition) of the boundary structures of two proteins, shape reasoning such as measuring the sphericity of protein, the efficient computation of the optimal side-chain placement, etc. We anticipate many other important applications will be discovered. In this talk, we will also demonstrate our molecular modeling and analysis software, BetaMol, which is entirely based on the unified, single representation of the beta-complex. Several pieces of application software are freely available at the Voronoi Diagram Research Center (VDRC, http://voronoi.hanyang.ac.kr). The engine software will also be available soon so that researchers can easily create programs for his or her own problem using the functions of this engine.

Es laden ein: Die Dozenten der Informatik

Fachgruppe Informatik

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