



Meiji University Global COE Program

49th Mathematical Sciences based on



Modeling, Analysis and Simulation seminar

Date: January 27, 2012, 16:30~18:00

Location: Meiji Univ. Ikuta Campus, Build 2 Annex A, Room A306.

Deok-Soo Kim (Hanyang University, Korea)

Title : Biogeometry based on the Voronoi diagram
and the Beta-complex.

Abstract: The Voronoi/Delaunay structures are everywhere in nature and are useful for understanding the spatial structure of a point set. Being powerful computational tools, their generalization has been made in various directions. One of the generalizations, the Voronoi diagram of spherical balls nicely defines the proximity among the balls. Like its counterpart of the ordinary Voronoi diagram of points or the power diagram, the dual structure can be more convenient in both representing and traversing the topology structure of the Voronoi diagram.

This talk will introduce the concept of "biogeometry" using the Voronoi diagram of balls 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 spherical balls within the boundary of the input ball set, where its boundary is appropriately defined. It turns out that the beta-complex can be used to efficiently solve many geometry and topology problems for the ball set. Among many potential application areas, the structural molecular biology is the utmost application area because the beta-complex immediately and efficiently solves many geometry problems related to important structural molecular biology problems.

Application examples include the computation of the molecular surface, the extraction of pockets on the boundary of molecule, the computation of areas of various types of surfaces defined on a molecule, the computation of various kinds of volumes defined on a molecule, the docking simulation, etc. We will also demonstrate our molecular modeling and analysis software, BetaMol, which is entirely based on the unified, single representation of the quasi-triangulation and the beta-complex.:

Everyone is welcome to attend the MAS seminar.

Meiji institute for Advanced Study of Mathematical Science (<http://www.mims.meiji.ac.jp>)

(Organizers: M. Mimura, D. Ueyama, Y. Wakano, K. Ikeda and S.Kinoshita)

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Access: 10 minutes on foot from Ikuta St. Odakyu line,
Or 10 minutes by bus No. 13「明治大学正門前」, get off at the last stop.
See http://www.meiji.ac.jp/koho/campus_guide/ for details.