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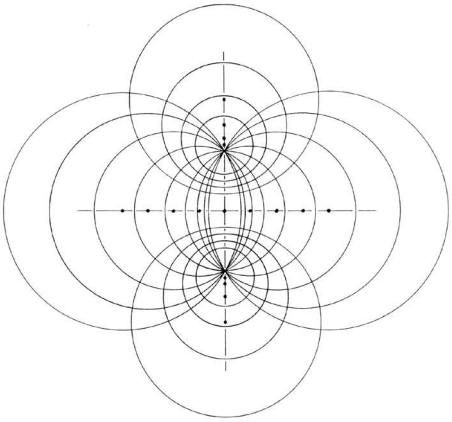
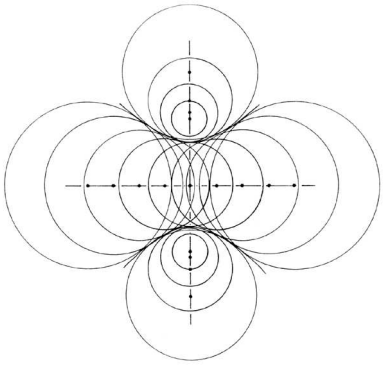
Computational Biology Seminar Series





Complex Geometry for Modeling Biomolecules

Herbert Edelsbrunner
University of Illinois, Urbana-Champaign

The use of geometric models for molecular conformations dates back at least to Lee and Richards who in the 70s defined the solvent accessible (SA) model as the union of spherical balls representing atoms. Soon after, Richards and Greer introduced the molecular surface (MS) model as a smooth and possibly more realistic variant of the SA model. We will introduce the new molecular skin (SK) similar to the MS model that has an additional symmetry relevant in studying questions of complementarity.

This talk introduces the alpha complex as the dual of the Voronoi decomposition of an SA model. The complex is a combinatorial object that leads to fast and robust algorithms for visualizing and analyzing geometric models of molecules. As an example we will see that the alpha complex can be used to compute the precise volume and surface area of an SA model without constructing it. The alpha complex offers a direct method to defining and computing cavities of molecules. Recent biological studies provide evidence for the physical relevance of this cavity definition.

Friday, March 20th, 3pm
Refreshments 2.30pm
Beckman Institute Auditorium