DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE
UNIVERSITY OF SOUTHERN DENMARK, ODENSE

Mathematics colloquium

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Tuesday 16 December 2014, 14:15-15:00, IMADAs seminar room

A New Method for Evaluation of the Fourier Coefficient Vectors in Protein-Protein Docking Problem

Abstract:
We present a new computational method for computing the Fourier coefficient vectors in docking problem by using orthonormal spherical polar radial basis functions. This computational technique arises from the modeling of the molecule. Representing the molecules as three-dimensional functions in terms of orthonormal spherical polar radial expansion provides a straightforward way of computing the correlation between pairs of these functions. After rotating and translating the original functions, the correlation has the form of scalar products of suitably rotated and translated coefficient vectors. In this work we also explain our algorithms for computing these coefficients.

Host: Achim Schroll