

MSRI
**Introductory Workshop on Computational
Applications of Algebraic Topology**
September 5 – September 8, 2006

Schedule

Tuesday, September 5

9:30 – 10:30 Robert Ghrist
10:30 – 11:00 Morning Break
11:00 – 12:00 Günter Ziegler
12:00 – 1:30 Lunch
1:30 – 2:30 Sergio Rajsbaum
2:30 – 3:30 Konstantin Mischaikow
3:30 – 4:00 Afternoon Break
4:00 – 5:00 Shmuel Weinberger
5:00 – 6:00 Reception

Wednesday, September 6

9:30 – 10:30 Robert Ghrist
10:30 – 11:00 Morning Break
11:00 – 12:00 Rade Zivaljevic
12:00 – 2:30 Lunch
2:30 – 3:30 Konstantin Mischaikow
3:30 – 4:00 Afternoon Break
4:00 – 5:00 Susan Holmes

Thursday, September 7

9:30 – 10:30 Gunnar Carlsson
10:30 – 11:00 Morning Break
11:00 – 12:00 Eric Babson
12:00 – 1:30 Lunch
1:30 – 2:30 Bob MacPherson
2:30 – 3:30 Persi Diaconis
3:30 – 4:00 Afternoon Break
4:00 – 5:00 Contributed Talk: Rima Izem

Friday, September 8

9:30 – 10:30 Gunnar Carlsson
10:30 – 11:00 Morning Break
11:00 – 12:00 Yuliy Baryshnikov
12:00 – 1:30 Lunch
1:30 – 2:30 Persi Diaconis
2:30 – 3:15 Contributed Talk: Christian Laing
3:15 – 4:00 Contributed Talk: Steven Ellis

Contributed Talks

Rima Izem

Christian Laing

Talk Title: Writhe invariants as RNA shape descriptors

Keywords: writhe, RNA, classification

Abstract: Given a polygonal curve (not necessarily closed or connected), geometric measures involving combinations of writhe and average crossing numbers of subcurves can be computed to obtain a set of features for the purpose of shape characterization. The function of nucleic acids and proteins are determined to a very large degree by the 3-dimensional shape of the biomolecule. We apply these writhe-based shape descriptors to RNA tertiary structures based on the polygonal carbon-phosphate backbone of the RNA. These geometric measures have been previously used by Peter Rogen and Boris Fain to correctly classify protein domains, by using the protein backbone of alpha-carbons, and producing a 98.5% success rate. In aims to find an optimal projection of the feature space into a plane that maximizes the variance among RNA classes, principal component analysis methods are applied. Also clustering techniques such as multiple discriminant and principal component analysis methods are used in the RNA shape classification.

Among tRNA structures a differentiation between thermophilic and non-thermophilic species is obtained, and also, a clear distinction between tRNA and diverse Ribozymes is produced.

Steven Ellis