Adam Mickiewicz University
Faculty of Mathematics and Computer Science

Geometry and Topology Seminar

10:15 am, Tuesday, November 6, 2017
B1-38, Collegium Mathematicum

Speaker: Maria Marchwicka (Adam Mickiewicz University)

Title: Generic trace of proteins

Abstract:

Amino acids linked by peptide bonds form a polypeptide chain. This chain is folded. Its unites, amino-acids, that are far from each other in the linear sequence can be placed in close neighborhood (be in contact). Information about it is represented as a protein contact map. Based on this map we construct a fatgraph model. Polypeptides can by classified by genus of this fatgraphs. Moreover, genus can be thought of as function of polypeptide length. Changes in genus correspond with structure motifs along the chain.

In my talk I will introduce main ideas of a project I was involved in. I will show how to get information about protein structure from Protein Data Base and how to establish a reasonable contact map. Then, I will discuss how to compute genus for a given contact map — I will sketch some algorithms and their implementations (Python). Finally, I will briefly talk about results of my work.