1139-92-587 **Marcio Gameiro***, gameiro@math.rutgers.edu, and **Konstantin Mischaikow**, mischaik@math.rutgers.edu. *Analysis of Protein Structure via Persistent Homology.*

Though tremendous progress has been made over the years, it is still not possible to predict with sufficient certainty the geometric structure of a protein from its defining amino acid sequence. The Protein Data Bank (PDB) provides a database for the experimentally determined three-dimensional structures of well over 100,000 proteins and thus provides a baseline against which predictions can be tested. There are a variety of reasons why current techniques for predicting protein folding may fail, including uncertainties and the existence of local minima in the energy functional used to optimize the protein structure. Our work focuses on the question of whether there are particular global geometric structures that give rise to a significant portion of the error. With this in mind, we are applying persistent homology to search for correlations between global geometric structures and the failure to predict the desired folding. Our hope is that this technique could help guide the energy minimization techniques to the correct minimum corresponding to the correctly folded protein. (Received February 20, 2018)