

Michigan Math Club

Thursday at 4pm in the Commons

Free Pizza and Pop



Modeling Biological Interactions

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Abstract for 1 April 2010

Computational medicine blends the fields of mathematics and medical research to fight disease. One goal of computational medicine is to provide tools for researchers to analyze the functions of biological molecules. The strength of the biological interactions among proteins is in part determined by how well such molecules fit together at their binding sites. Hex, designed by Dave Ritchie of the LORIA in France, is a software program to evaluate the degree of fit on binding sites of proteins. The degree of fit is computed using a mathematical algorithm that attempts to match two molecules together. One feature of this algorithm is that it accounts for rotational movement by virtual simulation with spherical harmonics (similar to Fourier transforms).

