1056-52-51 **Adnan Sljoka** (adnanslj@yorku.ca), Mathematics and Statistics, 4700 Keele Street, York University, Toronto, Ontario M3J 1P3, Canada, and **Walter Whiteley*** (whiteley@mathstat.yorku.ca), Mathematics and Statistics, York University, 4700 Keele Street, Toronto, Ontario M3J 1P3, Canada. *Predicting Flexibility and Motions of Proteins Using Rigidity.*

Given the 3-D structure of a biomolecule such as a protein, understanding how it functions depends in critical ways on predicting which parts are rigid, and which are flexible. Some biological data (NMR ensembles, multiple configurations, HD exchange) can provide experimental insight. We can model the molecule like an engineered structure of fixed units (atoms with their bond angles as rigid units, bonds as potential hinges) plus biochemical constraints coming from the geometry (hydrogen bonds, hydrophobic interactions). This generates a 'molecular graph' in the theory of combinatorial rigidity. Drawing on graph-theoretic algorithmic methods for bar-body frameworks (the $6|V|-6$ pebble game), as well as the 25 year old molecular conjecture, a basic algorithm on the molecular graph makes flexibility/rigidity predictions for the molecular structure. The predictive algorithm is embedded in an online FIRST server at flexweb.asu.edu, along with an extension FRODA to model the initial motions of the molecule.

Our recent work has extended this basic model to predict hinge motions of proteins, as well as some preliminary predictions for 'allostery' – where binding on one portion of a large molecule changes the shape or binding at a distance 'active site' of the molecule. (Received July 13, 2009)