**September 10, 2014**

**Biocomputing Lab, via San Giacomo 9/2**

**2pm-6pm**

**Lecture 1: Coarse-Grained Molecular Simulation Techniques**

In this lecture difficulties inherited from protein structure prediction techniques will be discussed for nicotinic acethylcholine receptor family of ligand gated ion channels along with enhanced molecular dynamics simulations (MD) and normal mode analysis (NMA). MD and NMA allow for atomistic characterization of biomolecular processes associated with protein function, however their computational demands have prevented simulations from reaching realistic timescales or atomistic resolutions on which these events often occur. A novel coarse-grained MD tecnique based on rigid-body Newtonian propagation scheme will be discussed respectively. Last but not least, advanteges and disadvantages of coarse grained NMA techniques will be explored.

**Lecture 2: Advanced Homology Modeling via Including Structural Features of Proteins**

The accuracy of comparative models derived from homologous proteins in the low sequence similarity range is limited substantially by inaccuracies in the alignment. In spite of recent advances in profile-profile, profile-sequence, and other alignment methods, the accuracy of the alignments remains a primary factor in the accuracy of the final model. In this lecture various different alternative techniques based on iterative approaches of model building and model assesment will be discussed along with standard protein structure modeling techniques. Moreover structural features of membrane proteins that distinguish them from water-soluble proteins will be explained in addition to discussing their functional roles via their dynamic nature and conformational changes caused by external perturbations to the cell. Finally membrane transport systems and ion channel proteins, and their mechanism of action will be explored.

**Short-bio:**

Prior to joining the faculty at Kadir Has University, Sebnem Essiz Gokhan held post-doctoral scholar positions at Lawrence Livermore National Lab and Prof. Andrej Sali’s Lab at Univ. of California, San Francisco. She received her PhD in Computational Biophysics from Univ. of Pittsburgh, PA following her BS degree in Chemistry from Koc University, Turkey. Her main research interests are coarse-grained simulation techniques for the study of long time scale conformational dynamics of proteins, ion channel proteins, ligand-induced conformational changes, and enhanced sampling algorithms for homology-based structure prediction tools.