CSCE 769 Computational Structural Biology
Fall 2012 **Location/Time: SWGN 2A24** **T, Th 11:00-12:15**

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Course Description:
This course is intended to familiarize interested investigators with theoretical concepts and some subset of the algorithmic tools currently utilized in the field of protein folding such as ROSETTA and I-TASSER. Other software packages such as Xplor-NIH and NAMD that are extensively used by the community of experimental/computational biologists will also be introduced . Upon the completion of this course, participants are expected to be able to embark in competitive research in the area of protein folding.

Course Prerequisite:
Due to the multidisciplinary nature of this course, a variety of topics will be explored. Introductory material will be presented before the start of every new area. Therefore, the only prerequisite requirement for this course is graduate standing in any of the Engineering and Sciences disciplines. During the past five years students from engineering, biology, chemistry, biochemistry, physics, mathematics and school of medicine have been participants of this course.

Required Text:
Although there are no text requirements, the following text books are recommended for the enthusiastic students:

- Structural Bioinformatics, Bourne & Weissig, Wiley-Liss, ISBN 0-471-20199-5
- Protein Structure Prediction, Tramontano, Wiley-VCH, ISBN 3-527-31167-X
- Protein Bioinformatics, Eidhammer, Jonassen, Taylor, Wiley, ISBN 0-470-84839-1

Objective:
Recent assessment of the first phase of the structural genomics initiative (PSI) project by the NIH revealed significant advances in both experimental methods of structure determination and protein expression/purification. However based on this assessment, current state of computational protein folding has advanced little since the late 1990's. The main objective of this course is to enhance participants' understanding of techniques and challenges in the field of protein folding. Participants will have an opportunity to report their findings in the form of a journal paper as their midterm and propose future research in the form of an NIH grant as their final project.

Topics:
The general outline of this course will consist of a brief introduction to main concepts of molecular biology, introduction to experimental methods of protein structure determination (mostly NMR) and, introduction to general classes of protein folding approaches (Ab Initio versus threading). Various visualization, evaluation and computation tools will be introduced along the way. The following includes some example topics:

- Topics in structural biology
- Topics in protein structure characterization and classification.
- Topics in experimental data (NOE and RDC data from NMR)
- Computational protein folding by force field minimization and constrained optimization.
- Protein folding based on threading algorithms.
- Topics in molecular modeling, molecular mechanics and quantum mechanics.

Attendance Policy:
To be announced in class.

Grading & assignment:
Approximately four assignments, one midterm and a final project will determine the final grade in this course. The following table shows the individual percentage contribution of each assignment:

Assignment 1	5%	Assignment 2	10%
Assignment 3	10%	Assignment 4	15%
Midterm	25%	Final	35%

Weekly Schedule:
The following table lists the schedule of topics that will be presented in this class. Please note that this list is still under development and is very likely to be changed.

Week	Topics
1	• Introduction/discussion • Introduction to Cell Biology, Central Dogma of Molecular Biology • Last day for drop/add
2	• MLK • Introduction to Biochemistry
3	• Amino Acids, peptide planes and Proteins • Peptide geometry, Energetics of Secondary Structural Elements • Molecular Visualization Tools (MolMol)
4	• Protein Structure • Experimental means of protein structure determination
5	• Energetics of protein structure • Ab Initio structure determination
6	• XPLOR-NIH, Restrained optimization • Euler rotations
7	• Molecular Dynamics Simulation • Structure Validation
8	• Era of Bioinformatics, Sequence alignment • Sequence homology, Secondary Structure Prediction
9	• Spring break @ USC
10	• Introduction to Multivariate Statistics • Artificial Neural Networks, Structrual homology assessment
11	• Protein folding based on threading techniques
12	• Protein folding based on threading techniques
13	• Other experimentally-assisted protein folding
14	• TBA
15	• Session ends