

18.417 : Introduction to Computational Molecular Biology

Foundations of Computational Structural Biology

Computational structural biology aims to model and predict the structure of biomolecules (e.g., proteins, DNA, RNA). The topics covered will range from the classic techniques in the field (e.g. molecular dynamics, Monte Carlo, dynamic programming) to more recent advances in analyzing and predicting RNA and protein structure, ranging from Hidden Markov Models and 3D lattice models to attribute Grammars and tree Grammars.

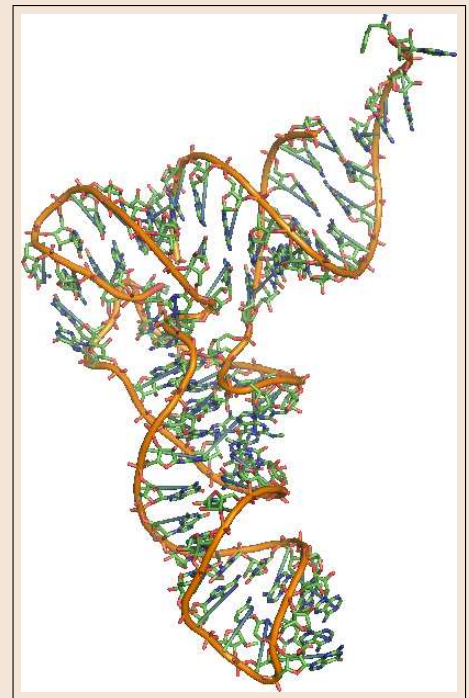
The class is intended for grad students and senior undergrads interested in the application of mathematical and computational methods to structural biology and also for biologists and biochemists interested in the algorithmic foundations of the approaches used in this field. Prerequisites : Basic understanding of algorithms. No biological background required. The class will provide background for any advanced methods discussed.

RNAs :

- Secondary structure with and without pseudo-knots,
- Multiple alignment,
- Equilibrium statistical mechanics,
- RNA hybridization, RNA mutants, saturated structures, RNA shapes.

Proteins :

- Secondary structure prediction,
- Threading, side-chain packing.
- Molecular mechanics, motion planning.
- 3D lattice models for protein folding,
- Structural template based methods,
- NMR related algorithms.



Transfer RNA of *E. Coli*

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