Project ideas

CS/BioE/CME/Biophys/BMI 279
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Project Ideas

- You are welcome (and encouraged) to pick something that is not on this list.
  - It should involve structure or spatial organization at a molecular or cellular level
- See project assignment sheet on website for details on project writeup and other information

Molecular dynamics simulation

- Write your own code
- Or use existing software
  - GROMACS, Desmond, NAMD, AMBER (PMEMD module): designed for performance. GROMACS, Desmond, and NAMD are free (for academic use); AMBER is not
  - Tinker—slow, but designed to be easy to work with the code
  - Most of these are designed for Linux, but Windows and Mac executables are available for Tinker
- Don't reuse BMI/BIOE/GENE 214/CS 274 code, but can build on it
- Either focus on simulation of a particular protein, or on methods (e.g., molecular dynamics vs. Monte Carlo)

Protein structure prediction

- Further exploration of PyRosetta/Rosetta
- Other approaches:
  - Phyre2 (web server)
  - I-Tasser (web server or download code)
  - Modeller (web server called ModWeb, or download code)
  - SWISS-MODEL (web server)

Protein Design

- Rosetta software is free for academic use
- Rosetta Design server: http://rosettadesign.med.unc.edu/

Docking

- Established, free codes and web servers:
  - Autodock Vina
  - SwissDock
- Rosetta Dock (newer; can use in PyRosetta framework)
- Not recommended:
  - GLIDE and GOLD are powerful but not free.
  - UCSF DOCK is free and powerful, but is reputedly difficult to install and learn.

- ZINC ligand database: http://zinc.docking.org/

Image analysis

- Useful software:
  - Matlab (general-purpose)
  - ImageJ (free, widely used for biological image processing)
  - CellProfiler (free, includes machine learning applications)
- Sample image sets:
  - CellProfiler site: http://www.cellprofiler.org/
  - Cellular images at http://biomedicalimaging.org/2014/program/challenges/

Reaction-diffusion simulation

- Use existing codes:
  - MCell, Smoldyn, Simmune
  - For MCell, consider using CellOrganizer or CellBlender to make models or renderings
- Write your own code
- Build a model of a cellular process, or consider methodological issues

Single-particle electron microscopy

- Software packages:
  - XMIPP: has a graphical user interface, somewhat easier to use
  - Relion: more mathematically sophisticated (Bayesian methods)
- Most use MPI, which complicates installation.
- Alternative: implement something yourself
  - Work in two dimensions for simplicity

Crystallography

- Structure factors (i.e., primary crystallographic data) are often available in PDB. See http://www.rcsb.org/pdb/101/static101.do?p=education_discussion/Looking-at-Structures/structurefactors.html
- CNS software (http://cns-online.org/v1.3/)

Other topics

- CellPack (http://www.autopack.org/): packing proteins into a cell
- EVFold (http://evfold.org/): protein structure prediction based on covariation across sequences