Lecture 13, Feb 9, 2023

Unique Properties of Water and Hydrogen Bonds

- Water's hydrogen bond network imposes a minimum volume constraint to drive hydrophobic collapse
  - This forces minimum volume constraints on structures like proteins and drives folding
  - Like how oil forms a sphere in water, but not in hexane
- Hydrogen bonds connect long range forces and makes it flexible so it can flow
- Levinthal's Paradox: Given the astronomical number of permutations, how can proteins find their biological structures?
  - For every amino acid linkage there's 3 degenerate orientations, so even just with that there's 3^{100} permutations or 10^{47}
  - Even sampling one orientation every 10^{-13} seconds (fastest possible) this would take longer than the age of the universe
  - Yet proteins fold on the order of micro to milliseconds
  - Solution: inherent correlations involved in the fluctuations; the assumption that all degrees of freedom are independent is wrong
  - Analogy: What is the optimal strategy to find a parking lot?
    * You instructively try to look further out to see more of the lot at once
    * In this analogy correlated actions are analogous to seeing more of the lot