

Two Protein Folding Problems

- (1) **Simulating an actual folding pathway** across the energy surface – **very difficult and expensive**. Limited by large number of possible conformations, folding being a rare event on MD timescale (in real world approx 10^{-3} – 1 sec).
- (2) **Protein structure prediction** – care only about final answer and can use knowledge of sequence-structure relationships amongst known proteins. Generally less difficult, unless the protein has a very novel structure that's not been seen before.

Protein Folding Problems

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