The Problem

- Given two sets of coordinates for a protein structure produce intermediate frames.

- Merely doing linear interpolation between the corresponding atoms will not produce acceptable results.
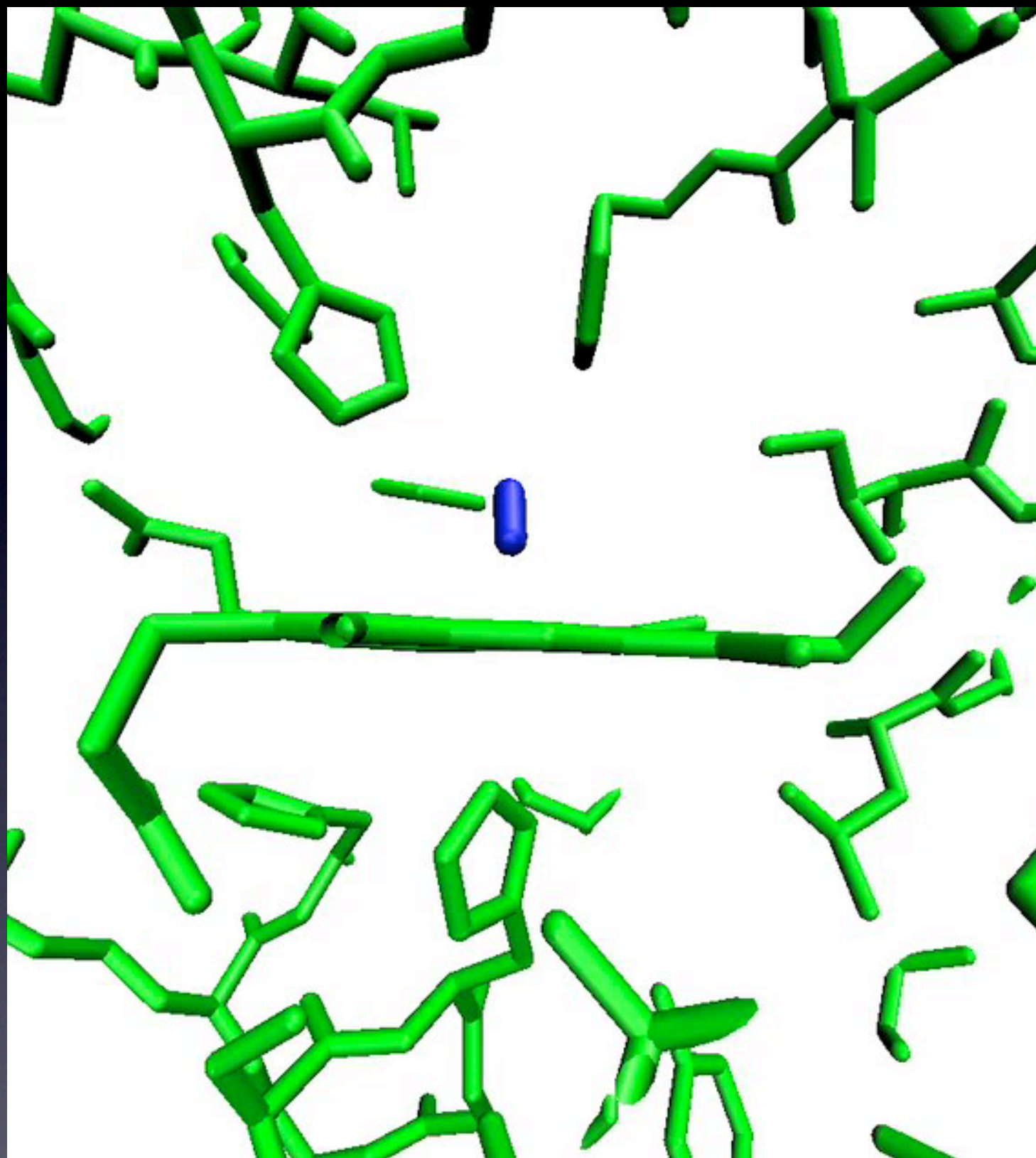
*Frames courtesy of Phillips lab

Possible Approaches

- For small scale animations, require the user to specify how various pieces should be interpolated

- Use knowledge of the physical and chemical properties of the protein to constrain how the various pieces can move

- To go yet a step further use normal mode analysis techniques to determine which directions a molecule can move in without going to a higher energy state

My Approach

- A simplified view of the second approach, that is to attempt to constrain the interpolation within the bounds of physical reality.

Constrained Interpolation

- Create a linear system of equations defining all of the constraints on how you want your system of particles to move.

- Add constraints specifying the velocities of the particles that must move from one place to another

- This has the problem that not all constraints can be satisfied.

Constraints I Used

- Distance Constraint - the original distance between each set of particles should be maintained.

- Other useful constraints include general collision avoidance between atoms and allowing movement only in backbone torsion angles and rotamer chi angles.

Dealing with Impossible sets of Constraints

- Instead of demanding an exact solution to the system of equations attempt to minimize squared error of the system

- Using the linear least squares allows the system to be under or over determined and deals well with ill-conditioned systems

Toy Version of the Problem

- Limited number of points on a two-dimensional plane

- Specify how many points are going to move or move one interactively.

- Apply user specified distance constraints

- Observe how the system reacts

Current Status

- Having trouble getting constraints to perform as expected using LSQR

- Presumably this will be fixed and I will have moved beyond the toy version of the problem by the final deadline