d=loaddat

Loads data files `amino12.in`, `aminoct12.in`, and `aminont12.in` that contain information about each amino acid. These data files and the code define a "force field" – they define the forces between the atoms. The force field used for this class is Amber (see `http://ambermd.org/`). See `http://ambermd.org/doc/prep.html` for more details about the file format.

Each section of the file describes one amino acid. 3 dummy atoms are first defined, then all else is defined in relation to them. For example, let us look at the description of Alanine. Each row describe one atom in the amino acid, here we look at atom 9. Here is what each column signifies:

9	index
HB1	name (not important)
HC	atom type (which the force field is defined in terms of)
E	not important (if M, atom is in backbone)
8	the next three fields define indices of reference atoms (see below)
6	
4	
1.090	distance to atom 8
109.500	angle between atoms 9, 8, and 6
60.000	dihedral angle between atoms 9, 8, 6, and 4
0.060300	charge

The state described in the table is what the amino acid will initial look like when the simulation starts. The charge of each atom is the *only* factor which affects long-range forces in proteins (see our energy equation, specifically the last term).

p=loadphys

Loads the data file `parm10mod12sb.dat`, which is separated into 6 sections. See `http://ambermd.org/formats.html#parm.dat` for more details on the file format. These parameters ultimately all define components of the energy function:

$$E = \sum_{\text{bonds}} K_r(r - r_{\text{eq}})^2 + \sum_{\text{angles}} K_\theta(\theta - \theta_{\text{eq}})^2 + \sum_{\text{dihedrals}} \frac{V_n}{2}[1 + \cos(n\phi - \gamma)] + \sum_{i<j} \left[\frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^6} + \frac{q_i q_j}{\epsilon R_{ij}} \right]$$

1st section

C	12.01	0.616
atom types	mass of atom	("polarizability"; not used)

2nd section: bonds

```
    C -C              310                1.525
pair of atoms    spring constant    preferred length
```

3rd section: angles

```
 C -C -O           80.0                120.0
3 atoms      spring constant    preferred angle
```

4th section: dihedral angles

```
 X -C -C -X                        4    14.5                 180.0   2.
   4 atoms       strength of interaction is V_n/2 = 14.5/4    γ      n
```

If ϕ is the dihedral angle, this line will correspond to a term in the energy function of $\frac{14.5}{4}[1 + \cos(2\phi - 180)]$. If you see negative n, this is an indicator that there are more lines that contribute to the *same* dihedral term – the energy contribution of this dihedral angle will be the sum of many cosine terms with different orders n. The atom identifier "X" matches *any* atom, so thus this line will match all four-tuples of atoms (any atom) - (Carbon atom of type "C") - (Carbon atom of type "C") - (any atom) unless a more specific match is found elsewhere in the file.

5th section: improper dihedral angles

A dihedral angle is called "improper" if the 3 bonds involved share a vertex. The edge around which the dihedral angle is measured is found between the *last* two listed atoms in this case, and not the middle two (C and O below). Despite the structural difference, improper dihedral angles are processed by the force field with the regular dihedral angles. The format is the same as above except the second column that the interaction strength was divided by above is omitted.

```
 X -X -C -O                10.5              180.   2.
   4 atoms      interaction strength V_n/2    γ     n
```

6th section: Lennard-Jones potential

This potential is what keeps atoms from overlapping. It is accounted for in the first two parts of the last term in our energy equation. Instead of thinking of this potential as $\frac{A}{R^{12}} - \frac{B}{R^6}$ as it appears in the energy equation, it is more intuitive to (equivalently) parameterize it via an interaction strength c and an effective radius ρ to yield

$$c\left(\frac{1}{(\frac{R}{\rho})^{12}} - \frac{2}{(\frac{R}{\rho})^6}\right)$$

(The 2 in the numerator is omitted in some definitions, which would give a slightly different meaning for c and ρ.) To define c and ρ for the interaction of a pair of atoms, the data files define an individual c_i and ρ_i for each atom, where the Lennard-Jones radius for the interaction of atoms i and j is just the sum $\rho = \rho_i + \rho + j$ (intuitively, each atom has a certain radius, and this potential starts penalizing pairs of atoms that "overlap"), and the interaction strength is the geometric mean of the interaction strengths, $c = \sqrt{c_i c_j}$.

```
   H              0.6000                     0.0157
 atom     characteristic radius (ρ_i)   interaction strength (c_i)
```

Center of Mass

Why is the center of mass important? Because the total force acting on a body acts as though it is just a force on the center of mass. Take Newton's second law, applied to each atom i, $F_i = m_i a_i$ and sum it up over all the atoms and divide by the total mass $\sum_i m_i$:

$$\frac{\sum_i F_i}{\sum_i m_i} = \frac{\sum_i m_i a_i}{\sum_i m_i}.$$

The left hand side is the acceleration of a hypothetical particle that has all the mass of the system $\left(\sum_i m_i\right)$ and all the force of the system $\left(\sum_i F_i\right)$ acting on it. The right hand side is the second derivative of $\frac{\sum_i m_i p_i}{\sum_i m_i}$, which is the formula for the center of mass of the system. Thus the equality says that the acceleration of the center of mass of the system equals the acceleration of a hypothetical particle with all the mass of the system and all the forces of the system acting on it. If you have not seen this before, it is something useful (and trivial!) to keep in mind.