parvanalysisAmber

August 29, 2014

0.1 Analyzing Amber simulations of Parvalbumin using MDAnalysis and Ptraj

0.1.1 Step 0. File prep

FYI, but not needed for example. (ran as user 'guest' to test)
Use ptraj to generate a concatenated cdf file on DLX, as well as a pdb (ptraj-generated dcd lack header?)
cd ˜/storage/WT_apo_amber_1/

Convert to dcd
catdcd -o WT_holo_1.dcd -s WT_holo_1.pdb -stype pdb -netcdf WT_holo_1.cdf

scp locally from kafka
scp $DLX: /storage/WT_apo_amber_1/WT_holo_1.pdb.scp$DLX:˜/storage/WT_apo_amber_1/WT_holo_1.dcd
.
scp $DLX:˜/Work/WT_apo_amber_1/prmtop .

0.1.2 Step 1. Setting up notebook

Load sources (Must be done prior to opening notebook!)
export MYPATH=/home/AD/pmke226/sources/mypython/ export PYTHONPATH=$PYTHONPATH$:MYPATH/lib/
packages/ python -c "import MDAnalysis"

Launch ipython notebook (see wiki)

0.1.3 Step 2. Reading and analyzing a trajectory with MDAnalysis

```
In [1]: import MDAnalysis
```

```
In [2]: #%cd /net/home/huskeypm/localTemp/parv/amber_holo/
        prefix = "/u1/shared/parvanalysisAmber/WT_holo_1"
        dcdFile = prefix+".dcd"
        pdbFile = prefix+".pdb"
```

Load trajectory

```
In [3]: u = MDAnalysis.Universe(pdbFile, dcdFile)
        print u.trajectory
```

```
< DCDReader '/u1/shared/parvanalysisAmber/WT_holo_1.dcd' with 15601 frames of 1716 atoms (0 fixed) >
```

Define function for analyzing each frame of a trajectory.

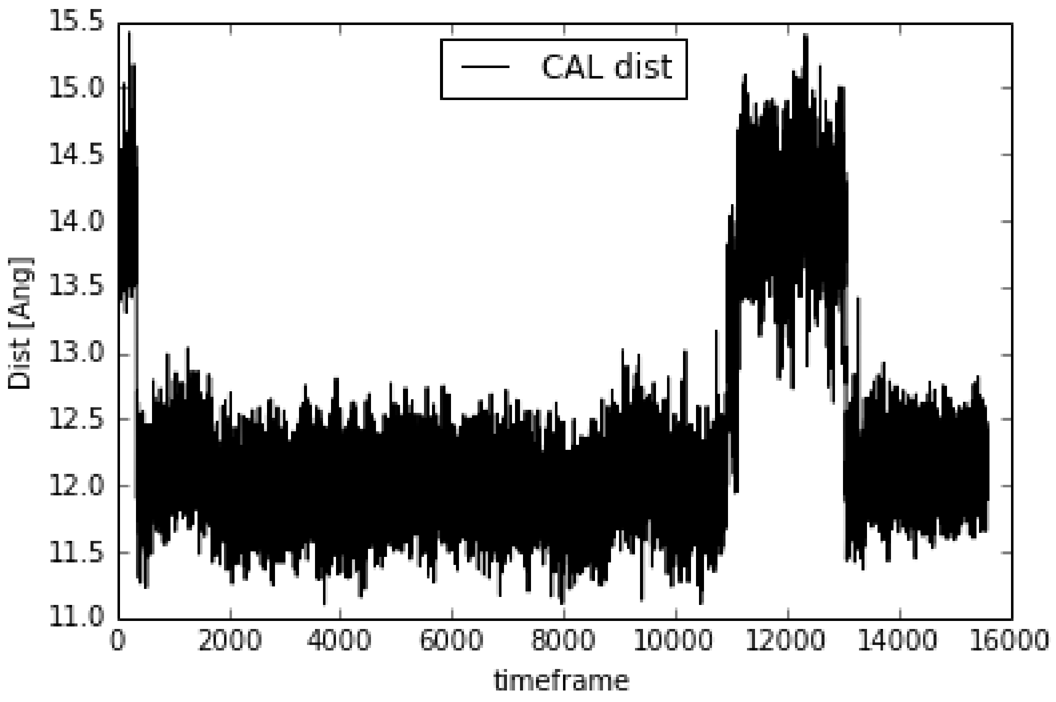
```
In [4]: # u - the universe object
        # bb - an MDAnalysis selection (defined below)
        def trajdist(u,bb):
          ds = np.zeros( u.trajectory.numframes )
          time = np.arange(u.trajectory.numframes )
          for i,ts in enumerate(u.trajectory):
            r = bb[1].pos - bb[0].pos
            d = numpy.linalg.norm(r)
            ds[i]=d
            #print d

          return time,ds
```

Define a selection object for CAL (will have two in this system), then use the previous function to analysis distance over all frames (time slices)

```
In [5]: bb = u.selectAtoms('name CAL')
        time,ds = trajdist(u,bb)
        plot(time,ds,'k',label="CAL dist")
        plt.xlabel("timeframe")
        plt.ylabel("Dist [Ang]")
        plt.legend(loc=0)
```

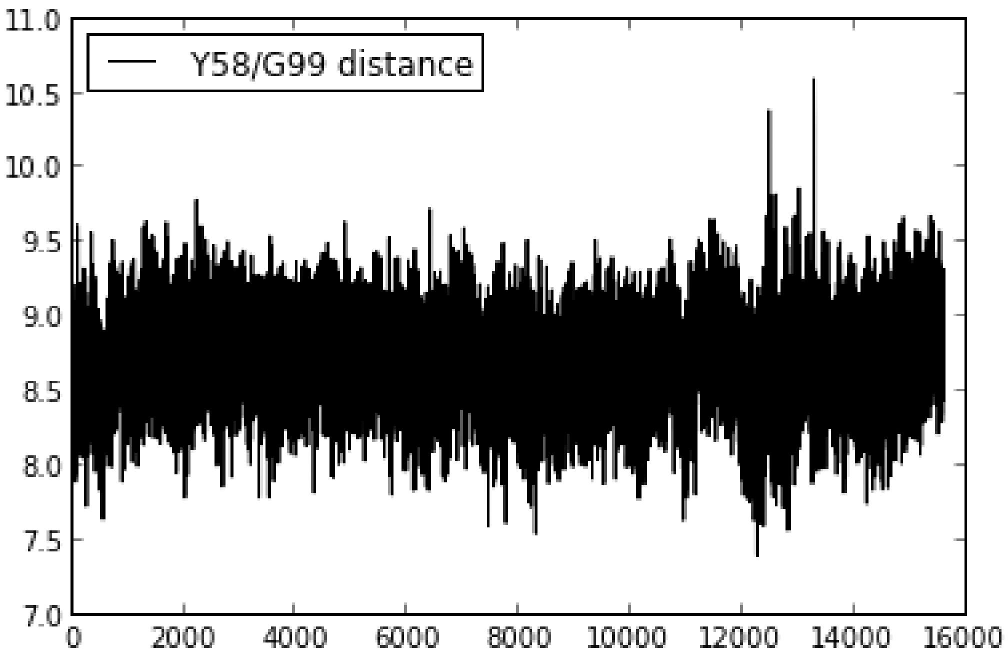
```
Out[5]: <matplotlib.legend.Legend at 0x7f37f404a690>
```



Plot distance between C-alpha atoms of Y58 and G99

```
In [20]: bb = u.selectAtoms('name CA and (resid 58 or resid 99)')
         time,ds = trajdist(u,bb)
         plot(time,ds,'k',label="Y58/G99 distance")
         plt.legend(loc=0)

Out[20]: <matplotlib.legend.Legend at 0x3bbb250>
```



0.1.4 Step 3. Dynamic cross correlation matrix with ptraj

This matrix shows collective motion between residues. Highly correlated residues have correlation values of 1. (red), while uncorrelated have values approaching 0 (blue)

To generate the files needed, I ran the following (but you need not)

Compute cross-correlation matrix using ptraj (also rmsf in the same dccm.in file) source ~/bin/amber.bash PRM=/u1/shared/parvanalysisAmber/WT_holo_1.pdb *AMBERHOME/bin/ptraj*PRM < dccm.in > dccm.out

This command will generate matrix_correl_CA.dat

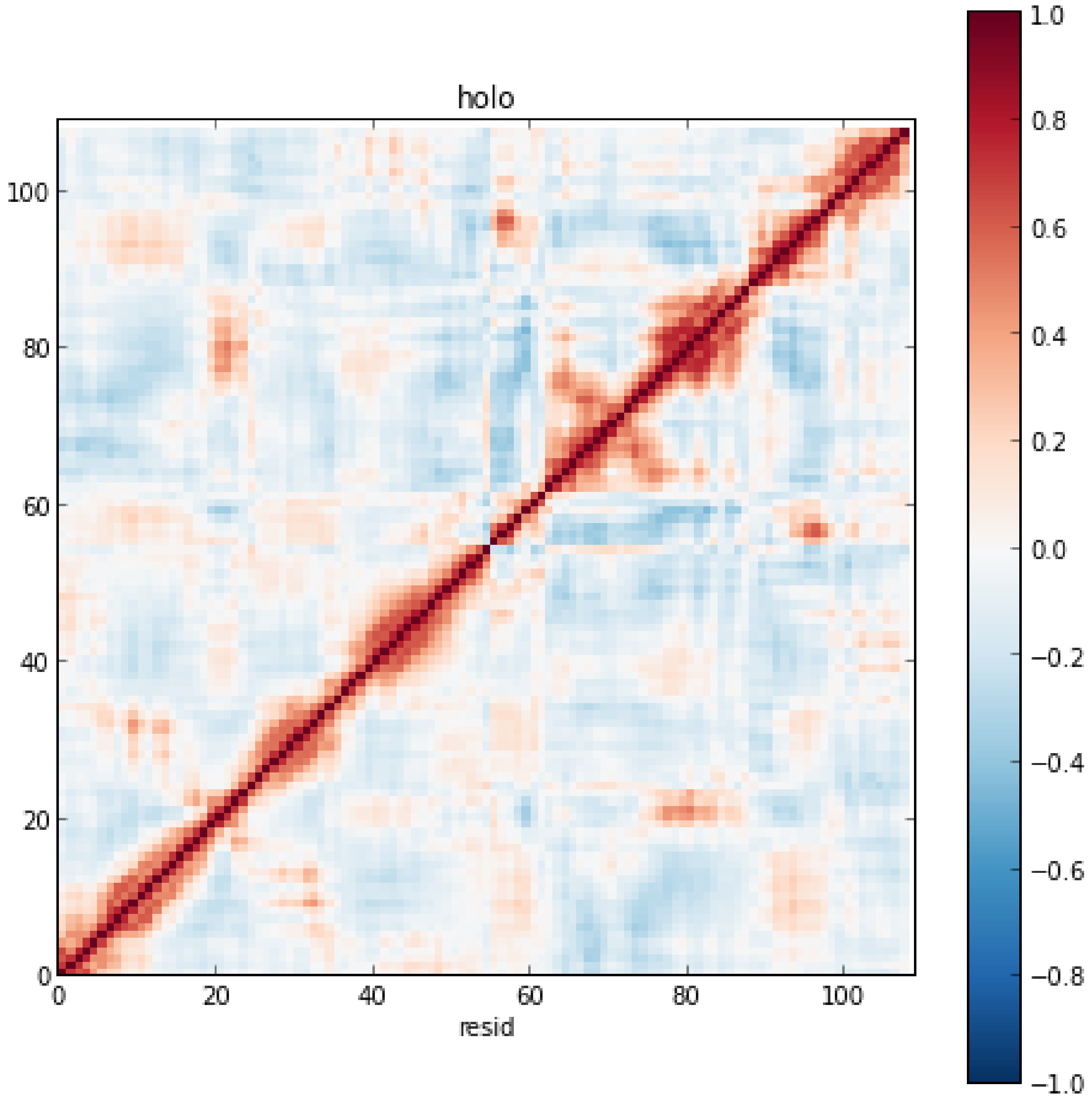
</ul>

Define function

```
In [24]: def plotcorr(dccmName,title=""):
             v=np.loadtxt(dccmName)
             plt.figure(figsize=(8,8))
             #pcolormesh(np.arange(109),np.arange(109),v,cmap="RdBu_r")
             pcolormesh(v,cmap="RdBu_r")
             plt.colorbar()
             plt.xlim([0,109])
```

```
    plt.ylim([0,109])
    plt.clim([-1,1])
    plt.title(title)
    plt.xlabel("resid")
    axes().set_aspect('equal')
    return v
```

```
In [26]: name = "matrix_correl_CA.dat"
         #apoName="/net/home/huskeypm/localTemp/parv/amber_apo/"+name
         holoRoot="/u1/shared/parvanalysisAmber/"
         holoName=holoRoot+name
         #apo=plotcorr(apoName,title="apo")
         holo=plotcorr(holoName,title="holo")
```



Sites I and II (where Ca2+ bind) are located approximately at 52-63 and 92-99. The pairing of Y58-G99 marks the beta sheet formed between sites I and II .

0.1.5 Step 4. RMSF with ptraj

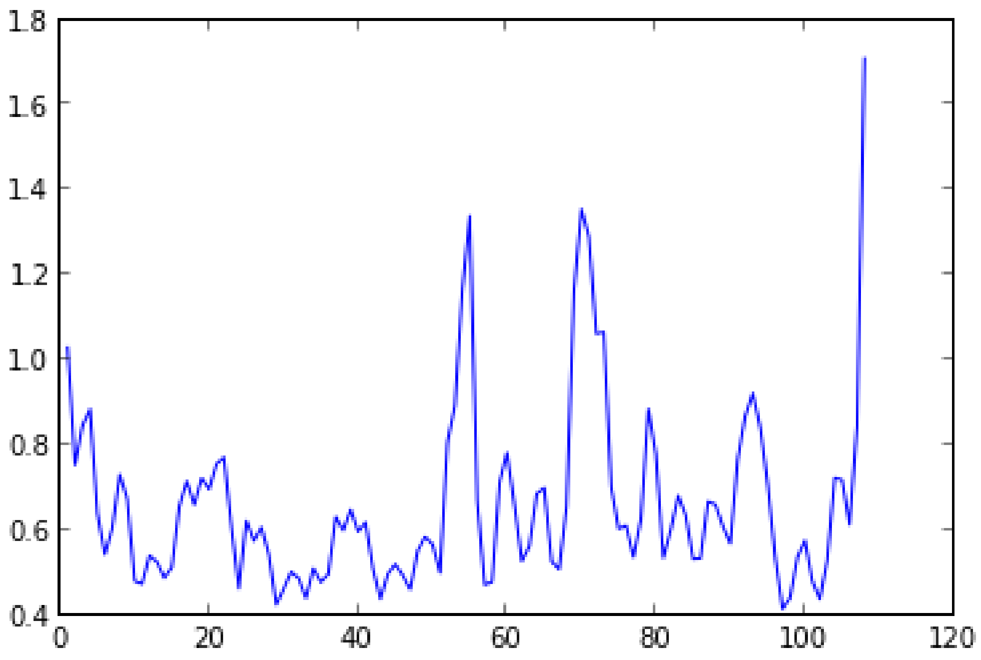
Atomic fluctuations RMSF also computed using ptraj/dccm.in sscript

```
In [32]: def plotrmsf(rmsfName,title="",plot=True):
             v=np.loadtxt(rmsfName)
             if(plot==False):
                   return v
             plt.figure(figsize=(8,8))
             #pcolormesh(np.arange(109),np.arange(109),v,cmap="RdBu_r")
             plt.plot(v[:,0],v[:,1])
             plt.title(title)
             plt.xlabel("resid")
             #axes().set_aspect('equal')
             return v
```

```
In [33]: name = "rmsf.dat"
         #apoName="/net/home/huskeypm/localTemp/parv/amber_apo/"+name
         holoName=holoRoot+name
         #apo=plotrmsf(apoName,title="apo",plot=False)
         holo=plotrmsf(holoName,title="holo",plot=False)
```

```
In [34]: #plot(apo[:,0],apo[:,1],'r',label="apo")
         plot(holo[:,0],holo[:,1],'b',label="holo")
```

```
Out[34]: [<matplotlib.lines.Line2D at 0x44d33d0>]
```



```
In []:
```