1. Download Code folder from Teams

This contains a subdirectory (Analysis) containing python codes for performing some basic analysis of the simulation

traj\_brush\_prof.py: calculate density profiles for peptoid brushes

traj\_orientation-group.py: calculate orientation of group within protein (relative to surface)

traj\_residue-z.py: calculate residue-surface separations

These use the MDAnalysis library (<https://www.mdanalysis.org/>). You can look in the source of these programs.

1. Download Data folder from Teams

This contains data from a simulation of a fibronectin fragment (FnIII-9 domain) adsorbing onto a surface coated with a peptoid brush (specifically composed of polysarcosine – this was studied in a previous paper Langmuir, 35, 1483).

1. Go to the bottom of this directory tree

cd Data/PeptoidBrush/PS20/Fibronectin

1. There will be tar file (fnIII-9\_PS20\_Nchain6\_run1.tar.gz) containing the simulation data. Untar this using

tar xzvf fnIII-9\_PS20\_Nchain6\_run1.tar.gz

1. Change into this. This contains a number of files. For now the most important are

fnIII-9\_ps20\_Nchain6\_T298\_nw.gro and fnIII-9\_ps20\_Nchain6\_T298\_nw.xtc. These are gromacs gro (coordinates) and xtc (trajectory) files (with the water removed). You can visualise these using VMD

1. First we can calculate the between the protein centre-of-mass and residue centre-of-mass z-coordinates. To do this use the traj\_residue-z.py program

python <PATH TO CODE FOLDER>/traj\_residue-z.py -g fnIII-9\_ps20\_Nchain6\_T298\_nw.gro -x fnIII-9\_ps20\_Nchain6\_T298\_nw.xtc -o1 fnIII-9\_ps20\_Nchain6\_run1.protein\_z -o2 fnIII-9\_ps20\_Nchain6\_run1.res\_z --nres 89

The -g option gives the gro file, -x xtc file, -o1 is the file that contains the protein centre-of-mass position, -o2 the centre-of-mass position for each residues, and --nres gives the number of residues in the protein (not the double dash in front of nres).

1. Then use the traj\_brush\_prof.py code to calculate the density profile of the peptoid chains. Use

python <PATH TO CODE FOLDER>/traj\_brush\_prof.py -g fnIII-9\_ps20\_Nchain6\_T298\_nw.gro -x fnIII-9\_ps20\_Nchain6\_T298\_nw.xtc -o fnIII-9\_ps20\_Nchain6\_run1.brush\_prof --brush\_res\_start 90 -- brush\_res\_stop 244 --nbin 1400 --deltaz 0.1 --tskip 100000

Here -o gives the file containing the density profile for the peptoid brushes, brush\_res\_start and brush\_res\_stop give the first and last residues in the brushes, nbin is the number of bins used in the calculation of the density profiles, deltaz the bin width, and tskip the time (in ps) after which to calculate the density profiles (we neglect the first 100 ns for this calculation).

1. Now use traj\_orientation\_group.py to calculate the orientation of the PHRSN group (this is the so-called synergy region involved in integrin binding). Use

python <PATH TO CODE FOLDER>/traj\_brush\_prof.py -g fnIII-9\_ps20\_Nchain6\_T298\_nw.gro -x fnIII-9\_ps20\_Nchain6\_T298\_nw.xtc -o fnIII-9\_ps20\_Nchain6\_run1.phrsn-orientation --protein\_res\_start 1 --protein\_res\_stop 89 –group 51 52 53 54 55

Here protein\_res\_start and protein\_res\_stop give the first and last residues in the protein and group give the residues involved in the group of interest (in this case residues 51-55)