CS 150: Assignment 2
(100 pts)
Due date: TBD

Purpose:
Learn to compute solvent accessible surface area (SASA)

Reference:
[1] Internal cavities and buried waters in globular proteins, Biochemistry 25:3619-25, 1986.

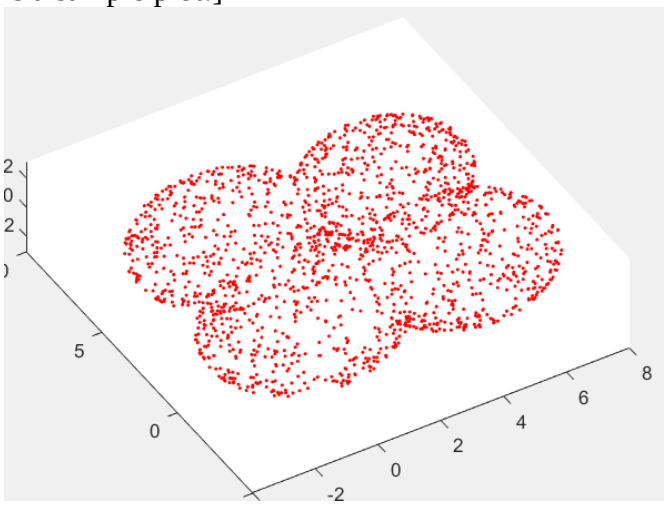
Assignment Description:

In this assignment, you are to construct the solvent accessible surface of a protein (2GB1.pdb) and compute solvent accessible surface area (SASA) for each atom in the protein. You may use the same algorithm as described in [1] to approximate the surface by **500 uniformly distributed points**. Choose a probe sphere of size **1.4** Angstrom. Use Bondi's van der Waals radii for the sizes of atoms (H: 1.20, C: 1.70, O: 1.52, N: 1.55, S: 1.80, etc.).

[Note: I am attaching a MATLAB program called quaternionSample.m that samples N random points on the surface of a sphere. Feel free to use it or borrow the idea from it.]

Compute the solvent accessible surface area for each atom (this is estimated by counting how many of its 500 surface points are exposed, i.e., not inside other atoms). Sum these numbers up to get the total surface areas of the protein. Output the results in a text file called 2GB1-SASA.txt.

[Note: I am attached another MATLAB program called accessibleSurfaceExample.m that shows how to compute and plot the solvent accessible surface areas of four atoms. Below is a sample plot.]



(Optional) Save the points that represent the protein surface. Is there a way to triangulate these points to form a surface mesh? (one such method is called ball-pivoting.)

(Optional) Question to ponder: is there an analytical solution to SASA?

Submission:
when you have finished and are ready to submit, put your program and the output files into a folder called hw2*yourLastName*. Zip up the folder into hw2*yourLastName*.zip. *Don't use other archivers than zip.*, and then upload it to the HW2 assignment on Canvas.

For this assignment, you can either work alone or form teams of 2. If so, only one submission per team is needed.