MonteCarlo Implementation

Siwei Zhang(Daniel)

I use MonteCarlo method to calculate volume and superficial area of a protein structure
shell command:

$ python MonteCarlo.py test.pdb

volume results:

N	10	100	1000	10000	100000
volume	108171.343	17307.415	32018.718	35047.515	35590.535
SD	34206.782	5869.23	2429.366	797.116	253.635

N is the number of points I dropped in the “box”. As the result showing, as N increases, the volume become stable and the standard deviation become small which means that the results become more accurate.

superficial areas:

N	5	10	20	50	100
srf_area	37586.418	36425.108	36583.493	36707.647	36499.14

In this case N stands for the number of points I dropped on surface of each of atom.
As N increases, the results become more stable.

The regular spherical coordinates is not suitable to this project, because points picked will be "bunched" near the poles, which leads to an inaccurate result.

I use the following algorithm to generate points on the surface of an atom[1] :

$$x = \sqrt{1 - u^2}\,\cos\theta$$
$$y = \sqrt{1 - u^2}\,\sin\theta$$
$$z = u,$$

Reference

[1] Sphere Point Picking: http://mathworld.wolfram.com/SpherePointPicking.html