

# Modified PSD Code Documentation

- Why modification in the first place?

We believe the code is designed for surfaces which are perfectly planar, however, in membrane systems, there is a high chance that a monomer end can come out resulting in increment in box dimension in that direction, which induce bogus pore sizes while calculating PSD at the surface.

- What to do?

Open PDB in vmd and run the commands in Tk console

```
pbcbbox -center bb
pbcbbox get
```

Your output will be [a b c  $\alpha$   $\beta$   $\gamma$ ]

- Implementation

```
psdM < xyz-file > < test particle radius(Å) > < bin-size(Å) > < a > < b > < c >
```

- Optimal bin-size is 0.25 Å