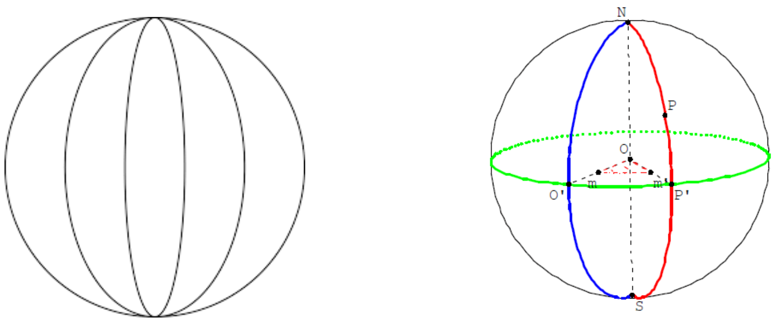
Strategy for Total Integration calculation

Debasis Das

The total probability is given by

$$P_{total} = \int_0^{2\pi} \int_0^{\pi} \rho(\theta, \phi)\, sin\,\theta\; d\theta\; d\phi \tag{1}$$

From the FiPy meshing, we get the cartesian coordinates of the cellcenters. As our state space is an unit sphere so the probability is calculated in spherical polar coordinate system as can be seen from Eq. 1. So first, we need to convert the cellcenters from cartesian(x, y, z) to spherical polar(r, θ, ϕ) coordinate. As we are dealing with an unit vector$(\hat{m})$, so our r coordinate would be 1 and the variables would be θ and ϕ.



(a) (b)

Figure 1: (a) Longitudes around a unit sphere; (b) Two consecutive longitudes of an unit sphere.

If we want to create the meshing of an unit sphere surface with θ and ϕ, we would expect, for every value of ϕ, there would be a set of θ values ranging from 0 to π. The range of ϕ is from 0 to 2π. This schemetacially shown in Fig. 1(a), where each longitudinal line is for a particular value of ϕ and the θ values vary along the longitudinal line. This means that there would be repetative value of ϕ in the $\theta - \phi$ table.
In our simulation, we have not found any repetative value of ϕ. For example, we have values like 0.003, 0.0032, but not 0. So we approximate those values which are nearly equal to zero as 0. For the integration we have taken the following strategy:

1. Fix a small value of δ.
2. take $\phi = 0$.
3. Find the indices of ϕ_{actual} which lies between $\phi \leq \phi_{actual} < \phi + \delta$.
4. Take out the values of θ for the corresponding indices and dump it in θ_ϕ. This represents, all the possible values of $\theta(0 \leq \theta_\phi \leq \pi)$ for a particular value of ϕ.
5. Do $\int_0^{\pi} \rho(\theta, \phi)\, sin\,\theta\; d\theta$ and store the result in I_ϕ.
6. Then $\phi = \phi + \delta$, and repeat the process from step 3 to 6, until ϕ reaches $2\pi - \delta$.
7. Do $\int_0^{2\pi} I_\phi\; d\phi$ to get the total probability P.