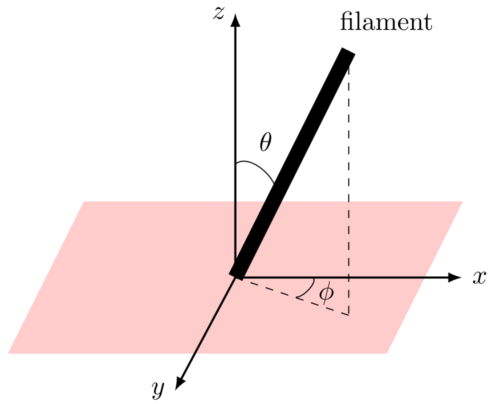
1 Filament attachment rates

Consider a filament with a tip attached at the membrane and making some orientation (θ, ϕ) with respect to the membrane normal. Here is a picture:



We will assume that the filament is attached at one end and otherwise performs a rotational diffusion, with the probability $P(\Omega)$ of observing a certain orientation $\Omega(\theta, \phi)$ satisfying:

$$\partial_t P = D\left[\frac{1}{\sin^2\theta}\,\partial_\phi^2 P + \frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta P)\right]. \tag{1}$$

The way the units are set up here is that D has units of inverse time. So, it is a "rotation rate". The ϕ direction is symmetric, so we just need to solve the θ portion, which reads:

$$\partial_t P = D\partial_x\left[(1-x^2)\partial_x P\right], \tag{2}$$

with $x = \cos\theta$. To find first-passage to the plane, we require the boundary condition: $P(x=0,t) = 0$, as we have an absorbing boundary when $\theta = \pi/2$. The general expansion is as follows:

$$P(\theta, t) = \sum_\nu A_\nu P_\nu(\cos\theta)\exp\left[-\nu(\nu+1)Dt\right]. \tag{3}$$

The boundary condition that $P(\theta = \frac{\pi}{2}, t) = 0$ forces $\nu = 1, 3, 5, \ldots$. Thus:

$$P(\theta, t) = \sum_{n=0}^{\infty} A_n P_{2n+1}(\cos\theta)\exp\left[-(2n+1)(2n+2)Dt\right] \tag{4}$$

We now need the coefficients A_n. These come from the initial condition, which is:

$$P(\theta, 0) = \sum_{n=0}^{\infty} A_n P_{2n+1}(\cos\theta) = \frac{1}{2\pi}, \tag{5}$$

for C a constant. We also have the condition:

$$\int_0^1 P_n(z)P_m(z)\,\mathrm{d}z = \frac{\delta_{mn}}{2n+1}. \tag{6}$$

Therefore:

$$\frac{A_m}{2(2m+1)+1} = \frac{1}{2\pi}\int_0^1 P_{2m+1}(z)\,\mathrm{d}z = \frac{1}{2\pi}\left[\frac{P_{2m}(0) - P_{2m+2}(0)}{4m+3}\right]. \tag{7}$$

These evaluated Legendre polynomials have explicit forms. It's also useful to know the generating function:

$$\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x)\,t^n \quad \text{so that} \quad \frac{1}{\sqrt{1+t^2}} = \sum_{n=0}^{\infty} P_{2n}(0)t^{2n}. \tag{8}$$

The explicit form of the coefficients (from the binomial expansion of the square root) are:

$$P_{2m}(0) = \frac{(-1)^m (2m)!}{(2^m m!)^2} \tag{9}$$

This lets us evaluate explicitly:

$$\int_0^1 \mathrm{d}z\, P_{2n+1}(z) = \frac{(-1)^n\,(2n-1)!}{4^n (n+1)!(n-1)!}. \tag{10}$$

So, our coefficients are:

$$A_m = \frac{1}{2\pi}[P_{2m}(0) - P_{2m+2}(0)] = \frac{(-1)^m (3+4m)\Gamma(m+1/2)}{4\pi^{3/2}\Gamma(m+2)} \tag{11}$$

The solution is thus:

$$P(\theta, t) = \sum_{n=0}^{\infty} \frac{(-1)^n (3+4n)\Gamma(n+1/2)}{4\pi^{3/2}\Gamma(n+2)} P_{2n+1}(\cos\theta) e^{-(2n+1)(2n+2)Dt} \tag{12}$$

This should be the probability that a filament that initially attached at orientation θ has still not reacted. Integrating, we get the survival probability:

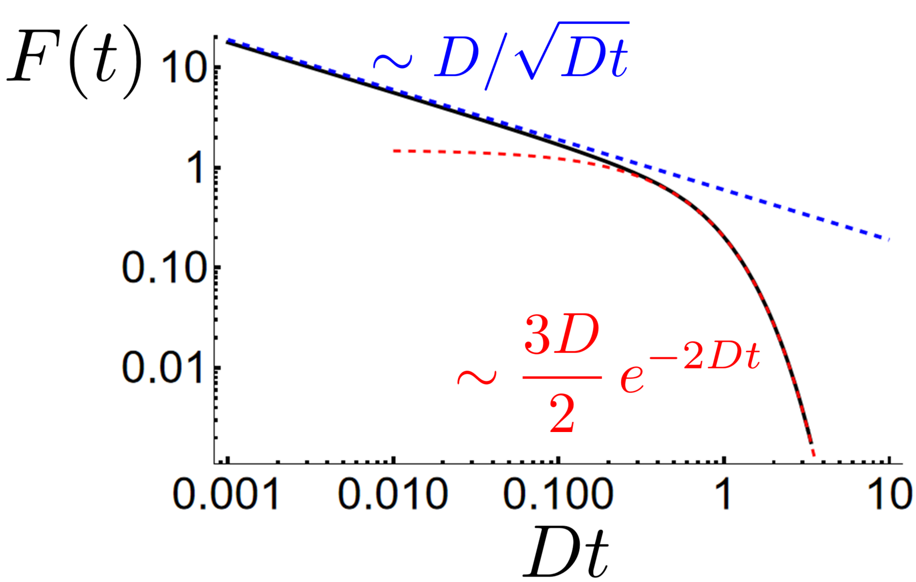
$$\begin{aligned} S(t) &= 2\pi \sum_{n=0}^{\infty} \frac{(-1)^n (3+4n)\Gamma(n+1/2)}{4\pi^{3/2}\Gamma(n+2)} \left[\frac{(-1)^n\, n(n+1)\Gamma(2n)}{4^n \Gamma(n+2)^2}\right] e^{-(2n+1)(2n+2)Dt} \\ &= \boxed{2\pi \sum_{n=0}^{\infty} \frac{(4n+3)\Gamma\left(n+\frac{1}{2}\right)^2}{8\pi^2 [(n+1)!]^2}\, e^{-(2n+1)(2n+2)Dt}.} \end{aligned} \tag{13}$$

This could be used to get a first passage distribution, although for a situation where we have an initially uniform distribution of orientations θ when the filament first attaches. In this case, the probability distribution of the survival times t is:

$$F(t) = -\frac{dS}{dt} = \frac{D}{2\pi} \sum_{n=0}^{\infty} \frac{(4n+3)(n+1)(2n+1)\Gamma\left(n+\frac{1}{2}\right)^2 e^{-(2n+1)(2n+2)Dt}}{[(n+1)!]^2} \tag{14}$$

$$\approx \begin{cases} 0.6\sqrt{\frac{D}{t}} & Dt \ll 1 \\ \frac{3D}{2} e^{-2Dt} & Dt \gg 1 \end{cases} \tag{15}$$

For small times $Dt \ll 1$, this function decays as $F(t) \sim \sqrt{D/t}$ and for long times $Dt \gg 1$, the exponential decay dominates, with $F(t) \sim 3De^{-2Dt}/2$. It is easy enough to plot this:



One way to approximate a reaction rate would be to look at the mean first passage time, which actually has a closed form solution in terms of hypergeometric functions, but evaluates to:

$$\langle t\rangle = \int \mathrm{d}t\, t\, F(t) \approx \frac{0.386294}{D} \text{ so that } k = \frac{1}{\langle t\rangle} \approx \boxed{2.5887D} \tag{16}$$

Now suppose we fix an initial angle θ_0 at which the filament first attaches. Then the initial condition is a bit different:

$$P(z,0) = \sum_{n=0}^{\infty} A_n P_{2n+1}(z) = \delta(z - z_0) \tag{17}$$

$$\frac{A_n}{4n+3} = P_{2n+1}(z_0) \qquad A_n = (4n+3)P_{2n+1}(z_0) \tag{18}$$

So, the probability distribution is:

$$P(\theta,t) = \sum_{n=0}^{\infty}(4n+3)P_{2n+1}(\cos\theta_0)P_{2n+1}(\cos\theta)e^{-(2n+1)(2n+2)Dt}. \tag{19}$$

The survival probability is:

$$S(\theta_0,t) = \int_0^1 \mathrm{d}z P(z,t) = \sum_{n=0}^{\infty} P_{2n+1}(\cos\theta_0)\frac{(4n+3)\,(-1)^n\,(2n-1)!}{4^n(n+1)!(n-1)!}e^{-(2n+1)(2n+2)Dt} \tag{20}$$

And the corresponding first passage probability is:

$$\begin{aligned} F(\theta_0,t) = -\frac{dS}{dt} &= D\sum_{n=0}^{\infty} P_{2n+1}(\cos\theta_0)\frac{(4n+3)\,(-1)^n\,(2n-1)!(2n+1)(2n+2)}{4^n(n+1)!(n-1)!}e^{-(2n+1)(2n+2)Dt} \\ &= \boxed{2D\sum_{n=0}^{\infty}\frac{(-1)^n\,(4n+3)\Gamma(n+\frac{3}{2})}{\sqrt{\pi}\,n!}P_{2n+1}(\cos\theta_0)e^{-(2n+1)(2n+2)Dt}} \end{aligned} \tag{21}$$

Computationally, this sum is a little bit annoying to compute beyond $n = 150$ or so. Most computational libraries will not allow you to evaluate gamma functions for such large arguments. There is actually an asymptotic formula that can be used beyond the first couple of n values:

$$\frac{\Gamma(n+\frac{3}{2})}{n!} \approx \sqrt{n} + \frac{3}{8\sqrt{n}} + \mathcal{O}(n^{-3/2}). \tag{22}$$

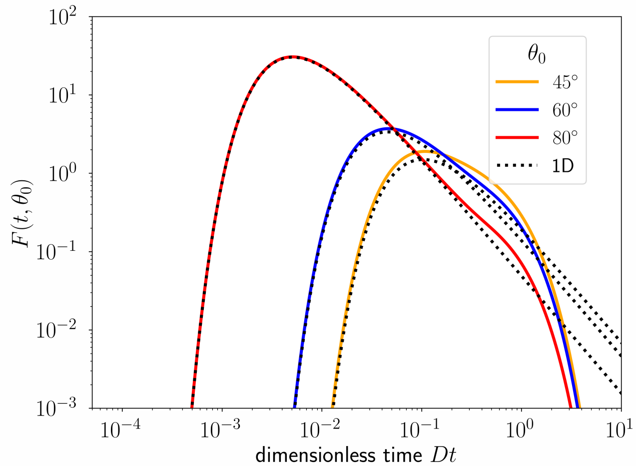
Thus, to an extremely good approximation:

$$\begin{aligned} F(\theta_0,t) \approx\ & 2D\sum_{n=0}^{99}\frac{(-1)^n\,(4n+3)\Gamma(n+\frac{3}{2})}{\sqrt{\pi}\,n!}P_{2n+1}(\cos\theta_0)e^{-(2n+1)(2n+2)Dt} \\ &+ 2D\sum_{n=100}^{\infty}\frac{(-1)^n\,(4n+3)\left[\sqrt{n}+\frac{3}{8\sqrt{n}}\right]}{\sqrt{\pi}}P_{2n+1}(\cos\theta_0)e^{-(2n+1)(2n+2)Dt} \end{aligned} \tag{23}$$

You can plot this distribution for various θ_0, or average over a distribution of possible attachment angles. Again, this is the first passage probability given an initial orientation θ_0 for the filament. When θ_0 is close to $\pi/2$, then we have a 2D diffusion with an *absorbing line.* In this case, to a good approximation, the first passage distribution should look like a 1D diffusion with an absorbing point. The angular distance to the absorbing "line" is always $\frac{\pi}{2} - \theta_0$, so we would expect:

$$F(\theta_0,t) = 2D\sum_{n=0}^{\infty}\frac{(-1)^n\,(3n+4)\Gamma(n+\frac{3}{2})}{\sqrt{\pi}\,n!}P_{2n+1}(\cos\theta_0)e^{-(2n+1)(2n+2)Dt} \approx \frac{\left[\frac{\pi}{2}-\theta_0\right]}{\sqrt{4\pi Dt^3}}\,e^{-\left[\frac{\pi}{2}-\theta_0\right]^2/4Dt}. \tag{24}$$

One can check that these functions do indeed look pretty similar for a decent range of angles. Some comparisons are shown below with the solid lines representing the computed first passage, and the black dashed lines corresponding to the 1D approximation formula (for the $D = 1$ case).



It's also interesting to look at these without the logarithmic scales. We can check for small angles that the approximation formula does not do so well, where we now color the corresponding 1D approximation with the same color. You can see that the match is not so good, with 45° being unsurprisingly the closest one.