# Simultaneous Mean First Encounter Time for 3 beads of the Rouse chain

April 27, 2015

Given a Rouse chain, composed of $N$ beads, let the position of any bead be $R_i(t)$ , $i = 1..N$. We wish to calculate the mean first simultaneous encounter time (MFET) of 3 beads $1, N', N$, with $1 < N' < N$

$$\tau = inf\{t; |R_1(t) - R_N(t)| < \epsilon, |R_1(2) - R_{N'}(t)| < \epsilon\} \tag{1}$$

Given the harmonic potential induced by the springs in the Rouse chain

$$\phi(R_1, R_2, ..., R_N)_{Rouse} = \frac{2}{\kappa}\sum_{n=1}^{N}(R_n - R_{n-1})^2 \tag{2}$$

with $\kappa$ the spring constant, the Rouse system is defined as

$$\dot{R}_n(t) = -D\nabla_{R_n}\phi_{Rouse} + \sqrt{2D}\dot{w}_n(t) \tag{3}$$

We transform the Rouse system (3) and the condition 1 to their normal coordinates representation.

$$u_p(t) = \sum_{n=1}^{N}\alpha_p^n R_n(t) \tag{4}$$

where

$$\alpha_p^n = \begin{cases} \sqrt{\frac{1}{N}}, & p = 0 \\ \sqrt{\frac{2}{N}}\cos((n-1/2)\frac{p\pi}{N}) & otherwise \end{cases} \tag{5}$$

the backward transformation is defined as

$$R_n(t) = \sum_{p=0}^{N-1}\alpha_p^n u_p(t) \tag{6}$$

The rouse system (3) is now represented as

$$\dot{u}_p(t) = -D_p\kappa_p u_p(t) + \sqrt{2D_p}\dot{w}_p(t) \tag{7}$$

with $D_p = D, \kappa_p = 4\kappa\sin^2(p\pi/2N), p = 1, 2, .., N-1$

The simultaneous encounter condition (1) can now be defined in terms of $u_p$. The conditions $|R_1(t) - R_N(t)| < \epsilon$, and $|R_1(t) - R_{N'}(t)| < \epsilon$

$$|\sum_{p=0}^{N-1}\alpha_p^1 u_p(t) - \alpha_p^N u_p(t)| = |\sum_{p=0}^{N-1}(\alpha_p^1 - \alpha_p^N)u_p(t)| = 0 \tag{8}$$

$$|\sum_{p=0}^{N-1}\alpha_p^1 u_p(t) - \alpha_p^{N'} u_p(t)| = |\sum_{p=0}^{N-1}(\alpha_p^1 - \alpha_p^{N'})u_p(t)| = 0 \tag{9}$$

substituting (5) into (8), and (9) we find

$$\sum_{p=0}^{N-1}\sqrt{\frac{2}{N}}(\cos(0.5p\pi/N) - \cos((N'-0.5)p\pi/N))u_p(t) = 0 \tag{10}$$