

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

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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  $1 < N' < N$

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

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

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

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

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

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

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

where

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

the backward transformation is defined as

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

The rouse system (3) is now represented as

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

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

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

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

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