

Electronic Supplementary Information: Transport of probe particles in polymer network: effects of probe size, network rigidity and probe-polymer interaction

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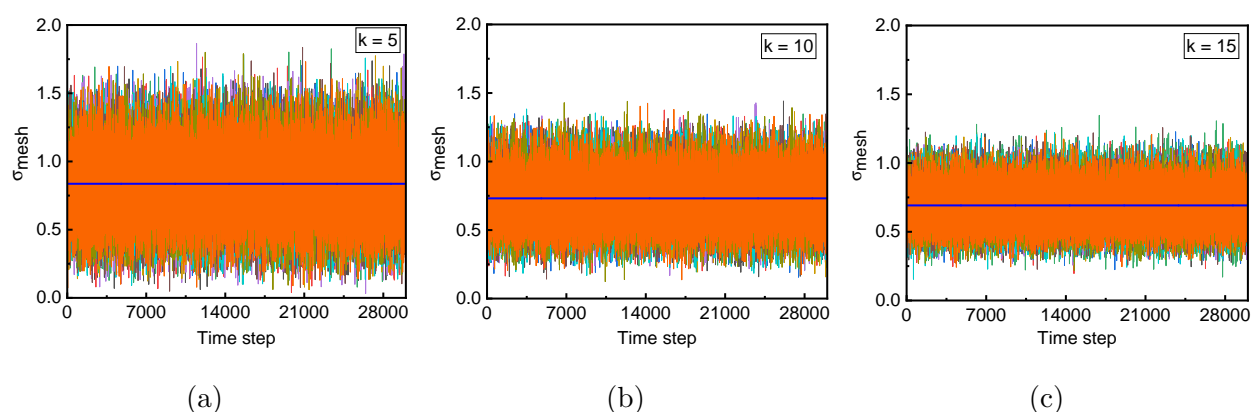


FIG. S1: Plots of the mesh size (σ_{mesh}) vs time step for different stiffness $k = 5, 10, 15$.
The blue line represents the average mesh size.

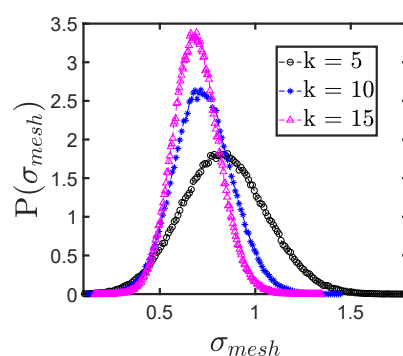


FIG. S2: Distribution $P(\sigma_{\text{mesh}})$ of the mesh size for different stiffness $k = 5, 10, 15$.

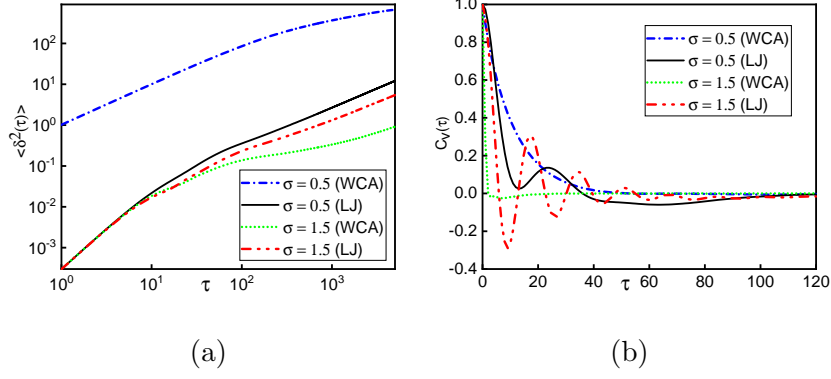


FIG. S3: Plots of $\langle \delta^2(\tau) \rangle$ (a) and VACF ($C_v(\tau)$) (b) vs lag-time τ for WCA and LJ ($\epsilon = 2$) with different size of the tracer particle $\sigma = 0.5, 1.5$ for stiffness $k = 5$.

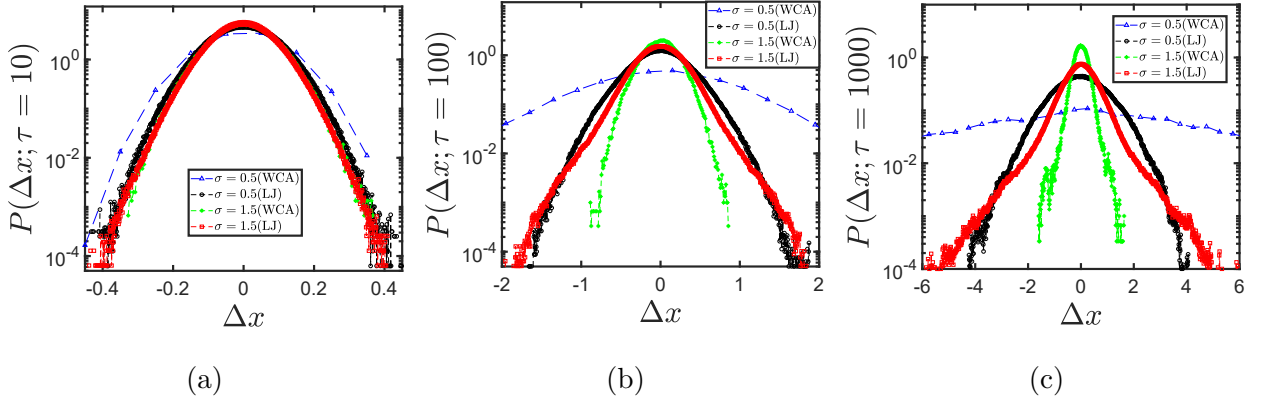


FIG. S4: Plots of the self part of the van-Hove functions in x , $P(\Delta x; \tau)$ for three chosen lag-times τ (100, 1000, 10000) for WCA and LJ ($\epsilon = 2$) with different size of the tracer particle $\sigma = 0.5, 1.5$ for stiffness $k = 5$.

File Name: Supplementary Movie 1

Description: Molecular dynamics simulation of probe particles with binding affinity ($\epsilon = 2$) in polymer network (blue) of stiffness $k = 5$. The dynamics of the bigger tracer (red) with size $\sigma = 1.5$ becomes slower than the relatively smaller tracer (green) with size $\sigma = 0.5$.

File Name: Supplementary Movie 2

Description: Molecular dynamics simulation of probe particles with size $\sigma = 0.5$ in polymer network (blue) of stiffness $k = 5$. The probe particle (red) with higher binding affinity ($\epsilon = 5$) moves slowly as compared to the probe particle (green) with lower binding affinity ($\epsilon = 2$).

File Name: Supplementary Movie 3

Description: Molecular dynamics simulation of probe particle (green) with binding affinity $\epsilon = 2$ and $\sigma = 0.5$ in polymer network (blue) of stiffness $k = 5$. Here the tracer is less caged as compared to the case for $k = 15$.

File Name: Supplementary Movie 4

Description: Molecular dynamics simulation of probe particle (green) with binding affinity $\epsilon = 2$ and $\sigma = 0.5$ in polymer network (silver) of stiffness $k = 15$. Here the tracer is caged.