Effect of Vicsek-like Activity on the Dynamics of a Flexible Polymer

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CQT Computational Quantum Field Theory

Motivation and aim

- Bacteria mostly move using conformational changes of their flexible flagella.
- Transport in many biological systems is performed by collective behavior of molecular motors distributed along the polymer length [1].
- A passive polymer undergoes coil-globule transition while quenched from good to poor solvent [2].
- Here, we apply the Vicsek-like alignment interactions [3] among the beads of a flexible polymer to see the effect of activity on its collapse transition.

Model and methods

Flexible homopolymer using bead spring model in poor solvent [2]:

$U_{LJ}(r) = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]$ → Non-bonded interaction

$U_{FENE}(r) = -\frac{K}{2}R^2 \ln[1-(\frac{r-r_0}{R})^2]$ → Bonded interaction

$T_f = 0.5$

Equation of motion has been solved via molecular dynamics using Langevin equation [4,5]:

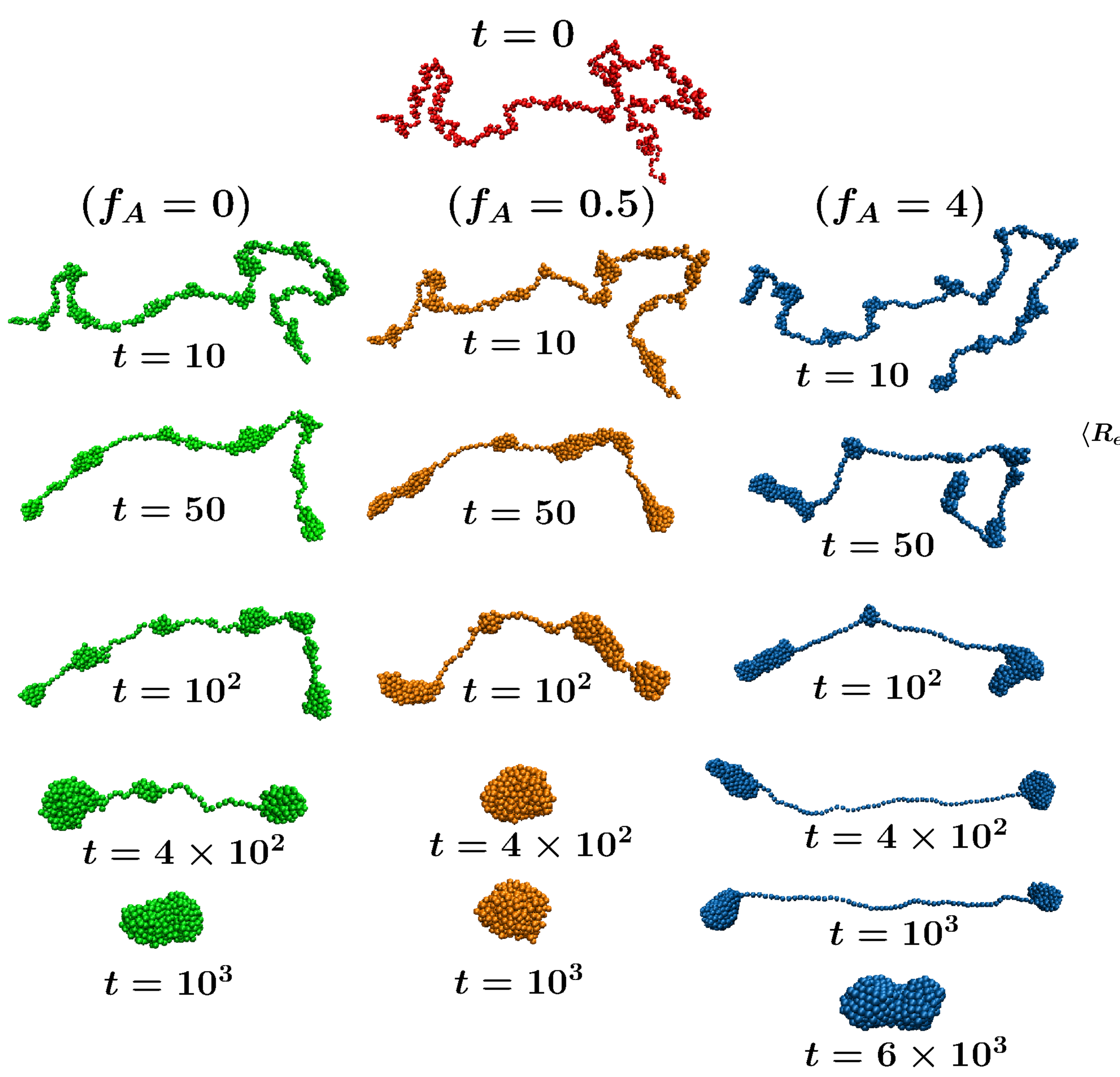
$$m_i \frac{d^2\vec{r}_i}{dt^2} = -\vec{\nabla}U - \gamma m_i \frac{d\vec{r}_i}{dt} + \sqrt{2\gamma m_i k_B T}\,\vec{N}_i(t) + \vec{f}_i$$

$\vec{N}_i(t)$ = Random noise; $\vec{f}_i$ = Active force;

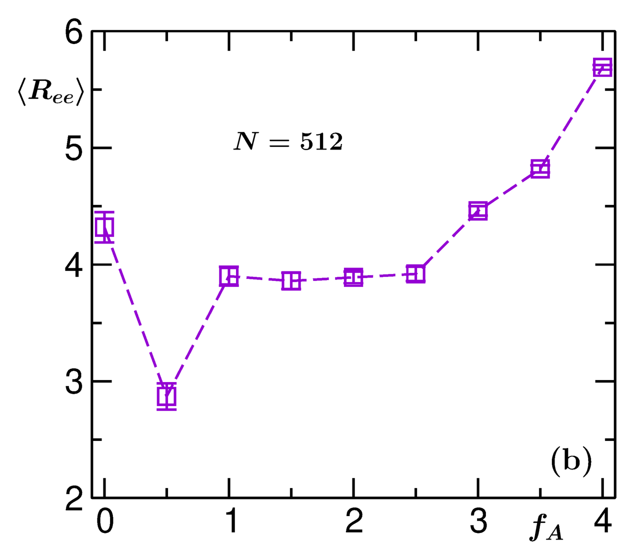
$\vec{f}_i = f_A \frac{\langle \vec{v}_j \rangle_{r_v}}{\langle |\vec{v}_j| \rangle_{r_v}}$; Here, we choose $r_v = 2.5\sigma$; $\delta t = 5 \times 10^{-4}$

Parameters: $\sigma, \gamma = 1$; Time is measured in units of $\sqrt{m\sigma^2/\epsilon}$

Results [5,6]

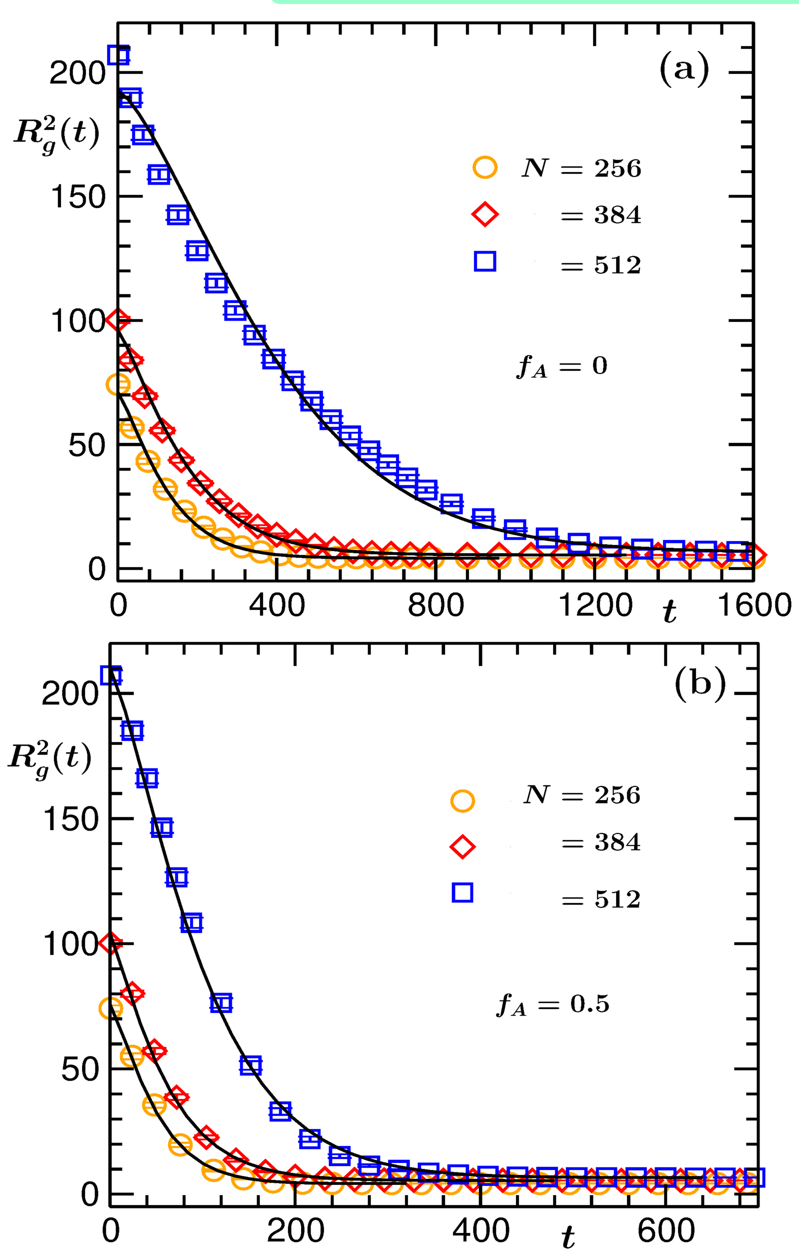


$\vec{r}_{ee} = \vec{r}_1 - \vec{r}_N$

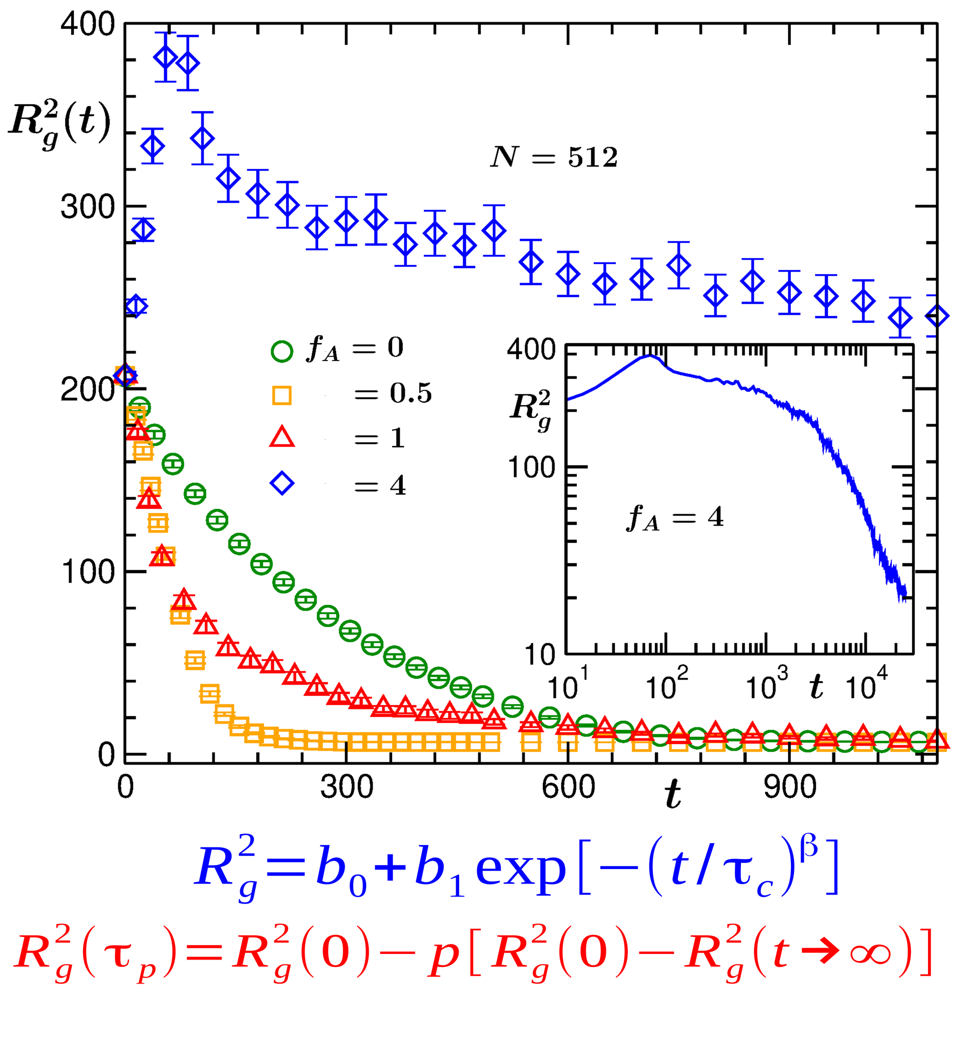


Coarsening occurs via formation of pearl-necklace like structures

Radius of gyration



$$R_g^2 = \frac{1}{2N^2}\sum_{i,j}(r_i - r_j)^2$$



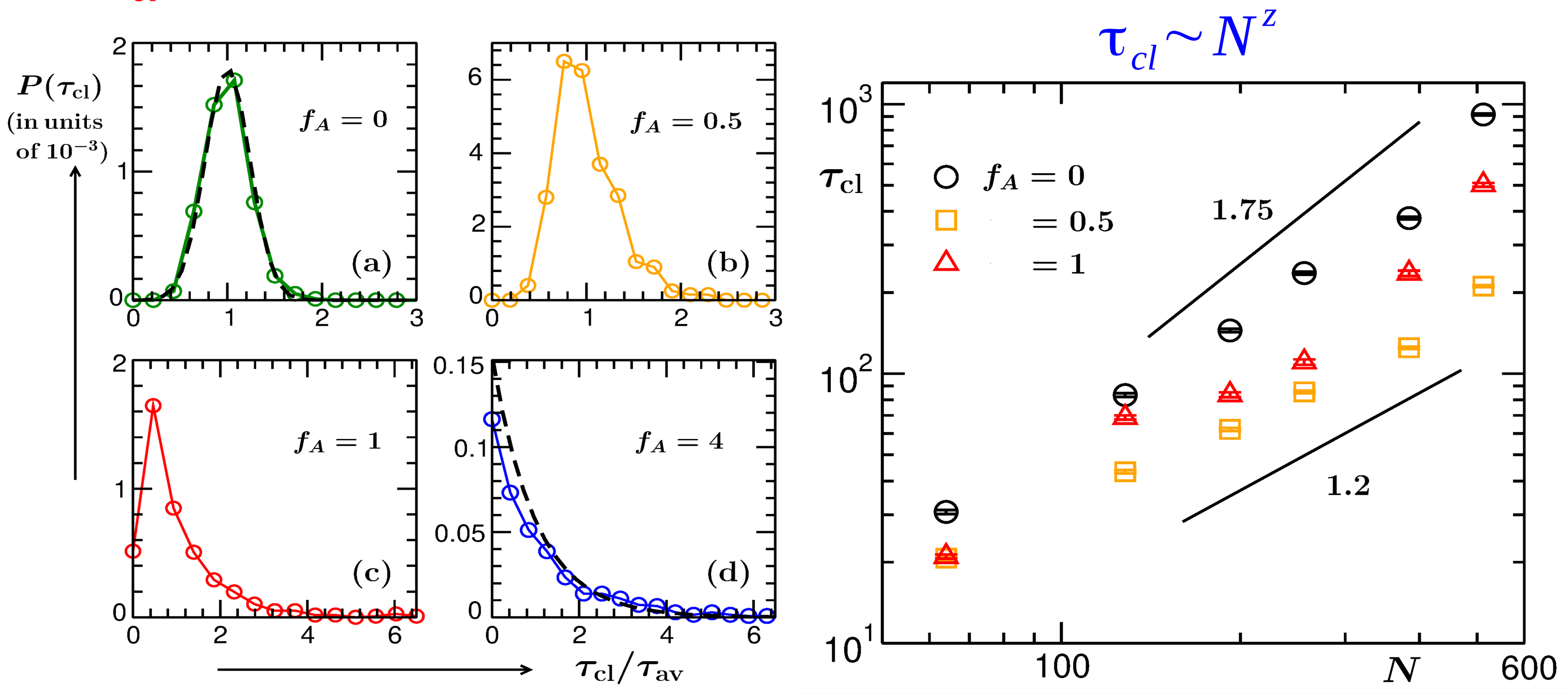
$$R_g^2 = b_0 + b_1 \exp[-(t/\tau_c)^\beta]$$

$$R_g^2(\tau_p) = R_g^2(0) - p[R_g^2(0) - R_g^2(t\to\infty)]$$

Relaxation dynamics

τ_{cl} is the time when number of clusters becomes 1.

$\tau_{cl} \sim N^z$

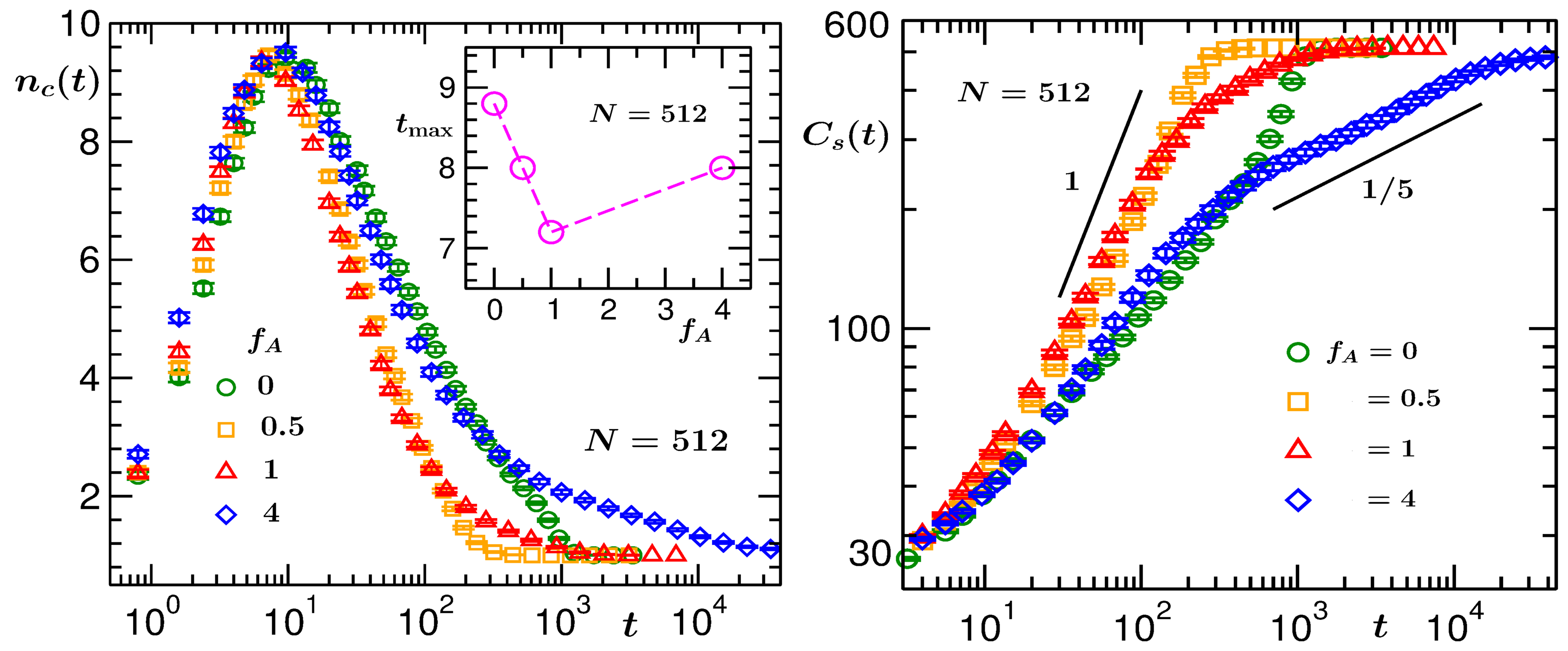


Growth of clusters

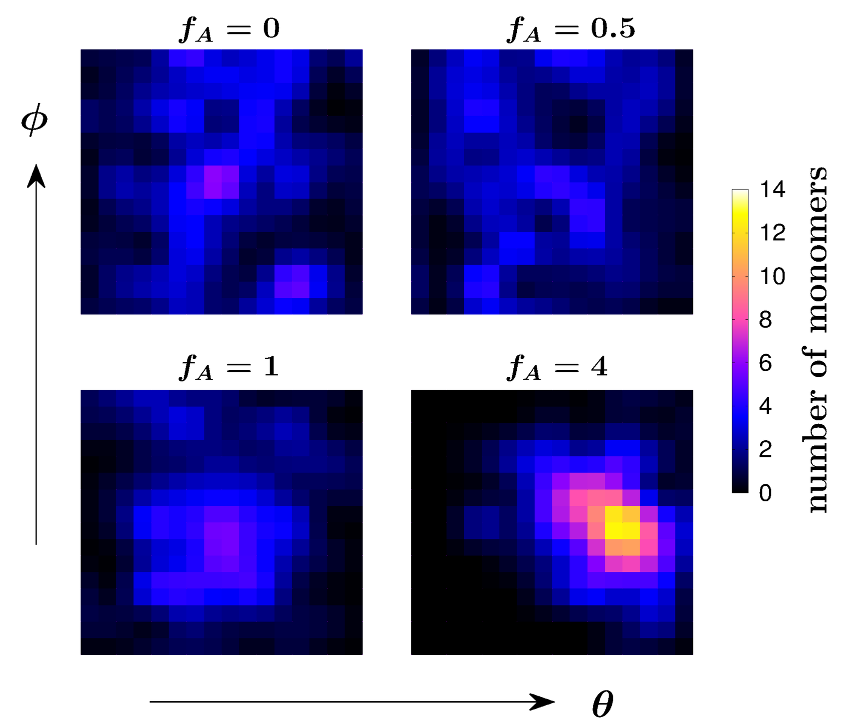
Cluster identification $n_i = \Sigma_{j=1}^{N}\Theta(r_c - r_{ij})$

if $n_i \geq n_{min}$, $i, j \in C_s$

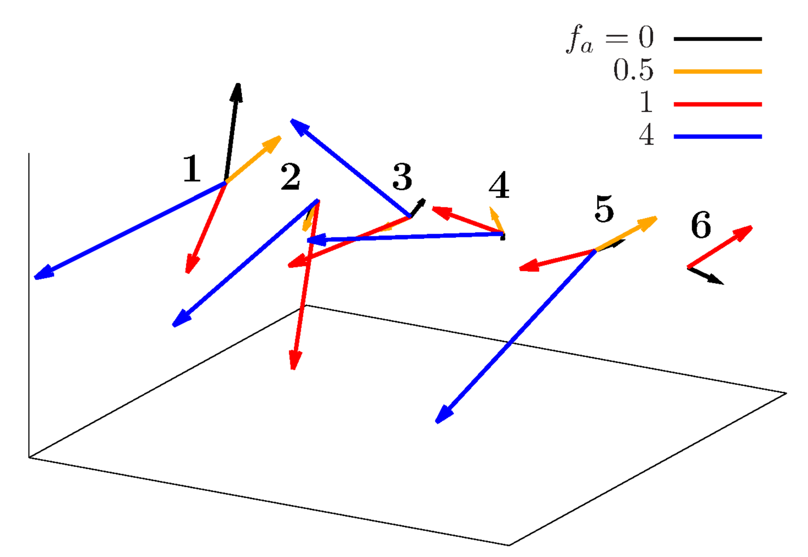
$C_s(t) \sim t^{\alpha_c}$



$\theta_j = \cos^{-1}(v_j^z/v_j)$; $\phi_j = \tan^{-1}(v_j^y/v_j^x)$



Velocity-alignment of clusters

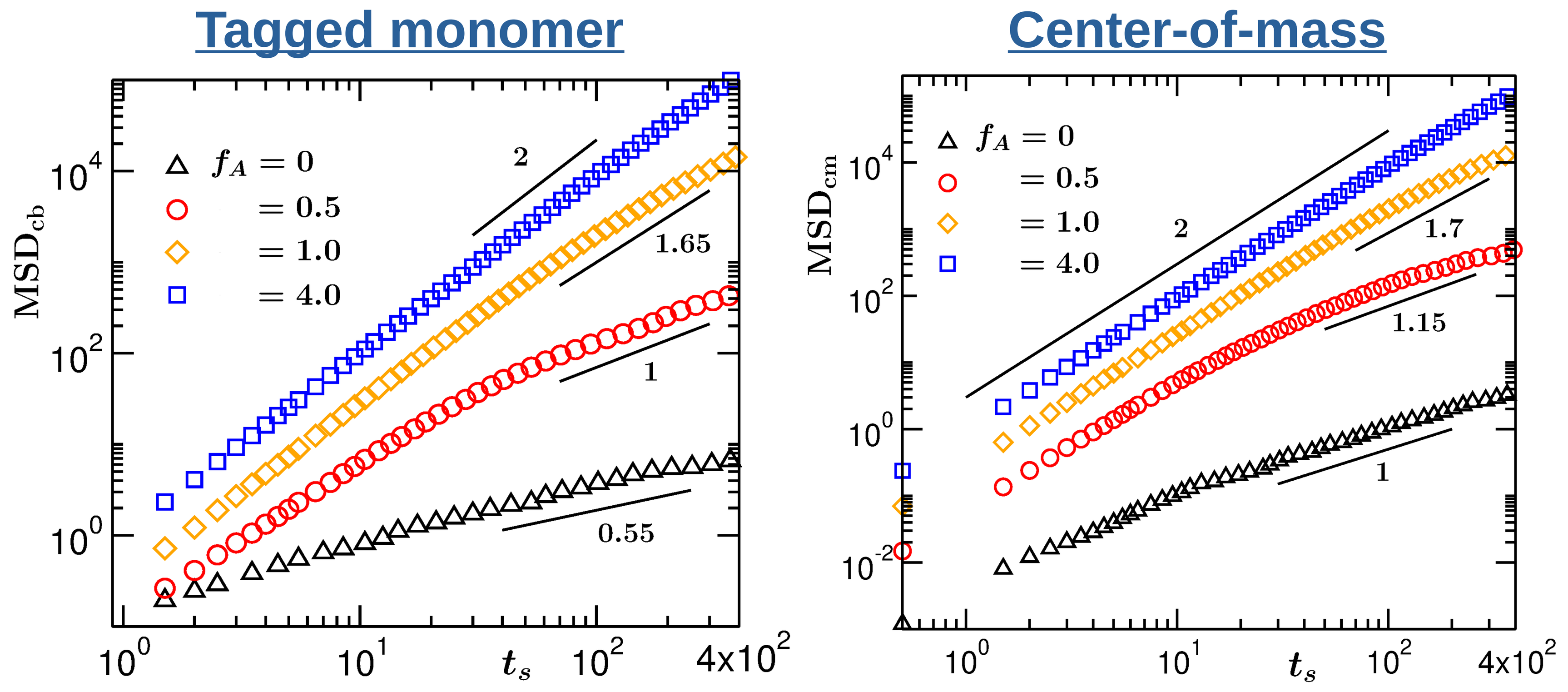


Steady state dynamics:

$MSD(t) = \langle [\vec{r}(t) - \vec{r}(t_0)]^2 \rangle$; $MSD \sim t^\alpha$

Tagged monomer

Center-of-mass



Conclusion

1. Various stages of collapse kinetics have been studied for an active polymer and compared with the corresponding passive scenario.
2. While lower activity makes the coarsening faster, larger activity delays it by making the polymer chain effectively a 'stiffer' one.
3. The MSD for the polymer changes from super-diffusive to ballistic behavior under the influence of activity in contrast to the diffusive motion for the passive polymer.

References

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[6] S. Paul, S. Majumder, S. K. Das and W. Janke, Leipzig preprint (2021).