Nonequilibrium Organization and Fluctuations in Active Interfaces and Polymers

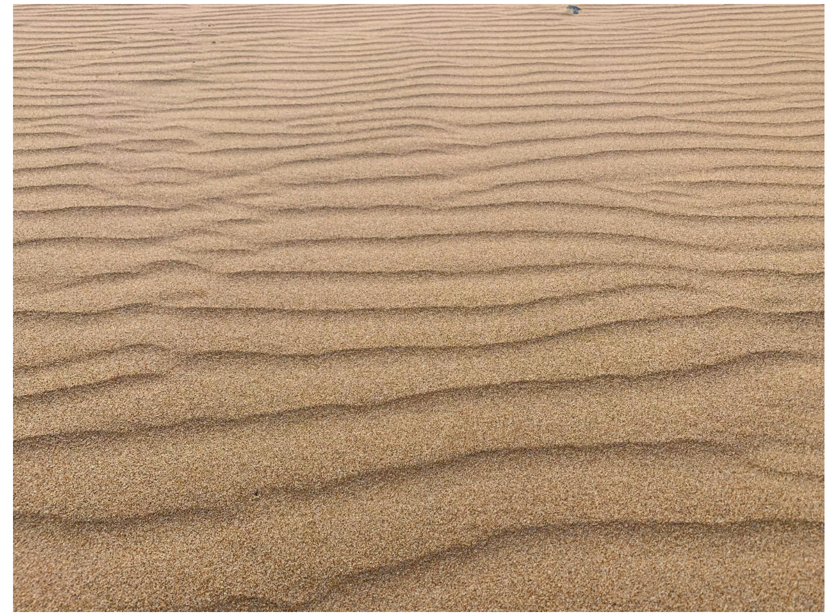
Love Grover

Pre-PhD Seminar

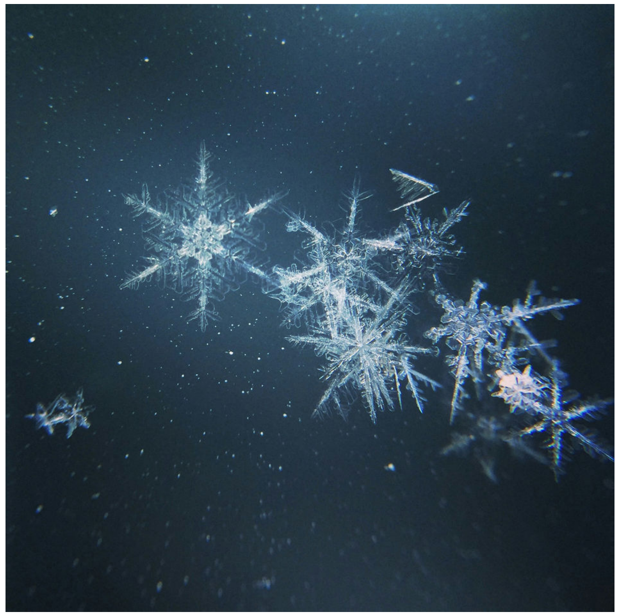
Indian Institute of Science Education and Research Mohali, India

Non-equilibrium Organization and Fluctuations

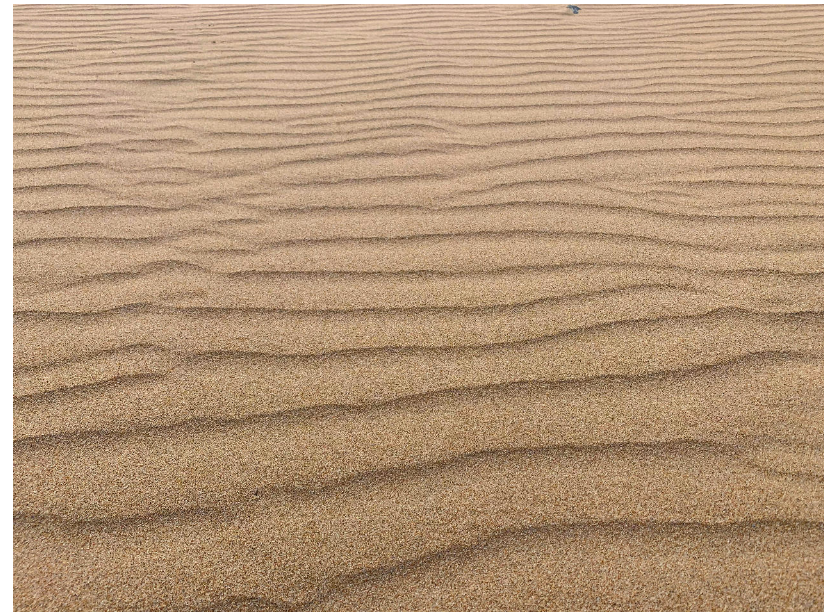
Non-equilibrium Organization and Fluctuations

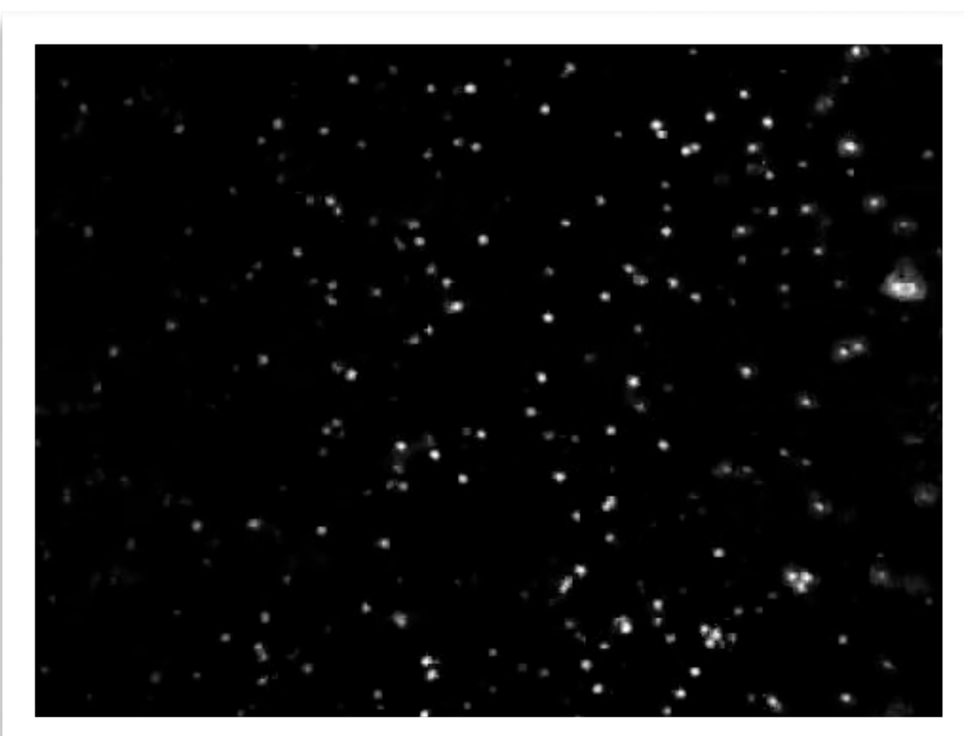


Non-equilibrium Organization and Fluctuations



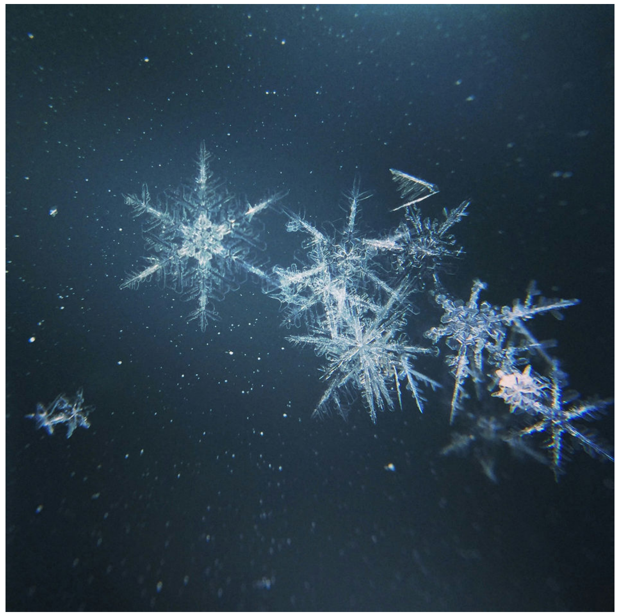
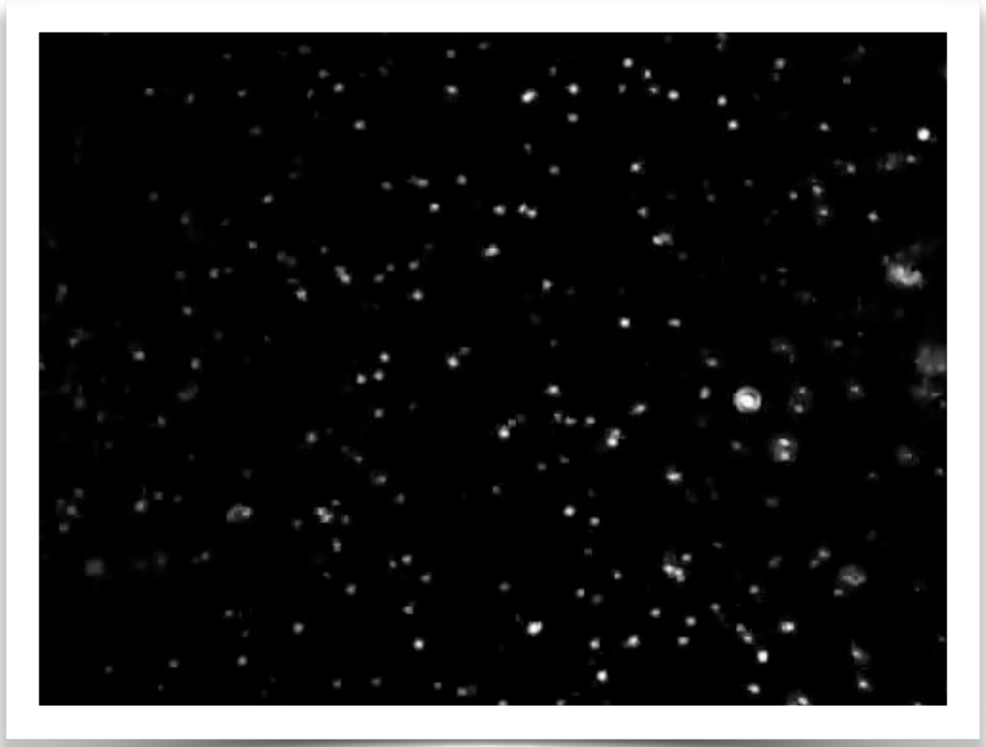
Non-equilibrium Organization and Fluctuations



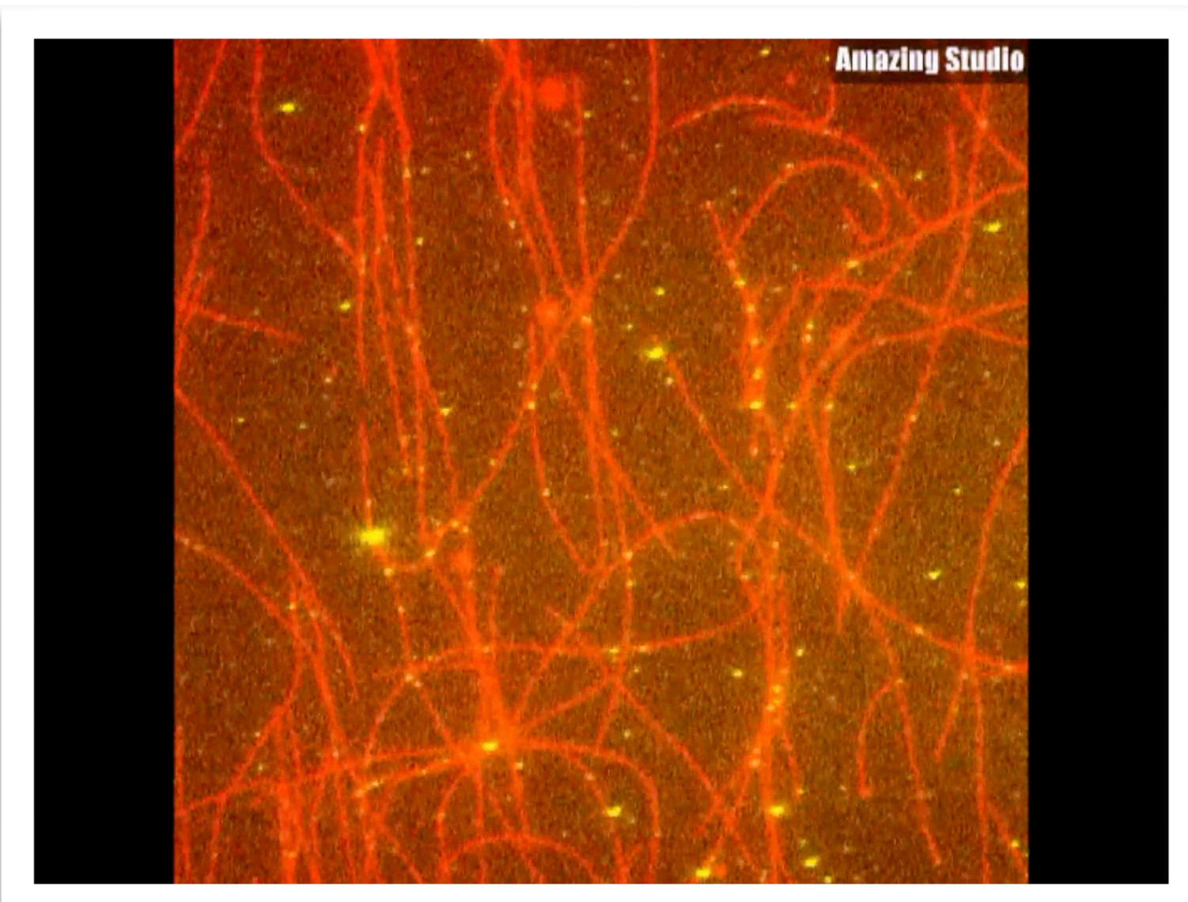


Non-equilibrium Organization and Fluctuations



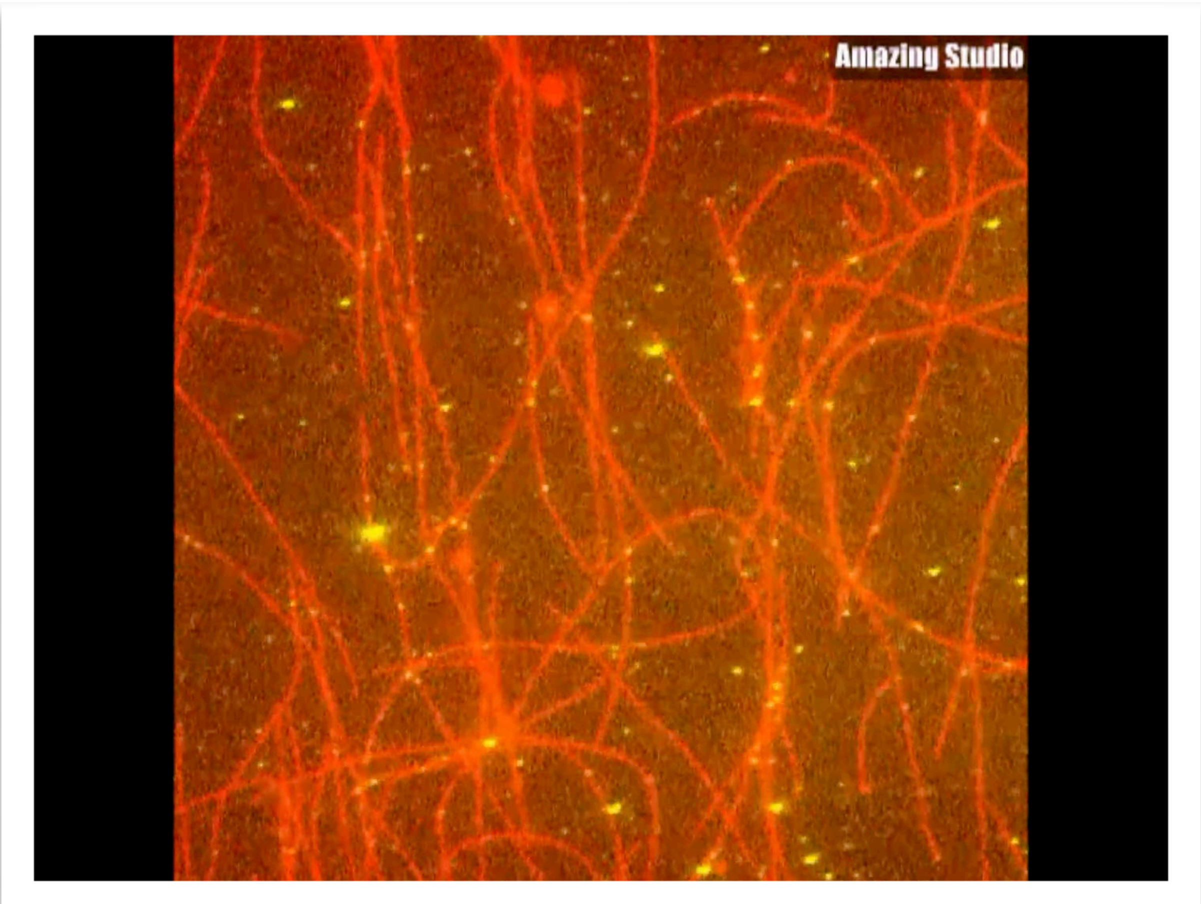

Active Systems as Non-equilibrium systems



GFP tagged Kinesin walking on TRITC labled microtubules.

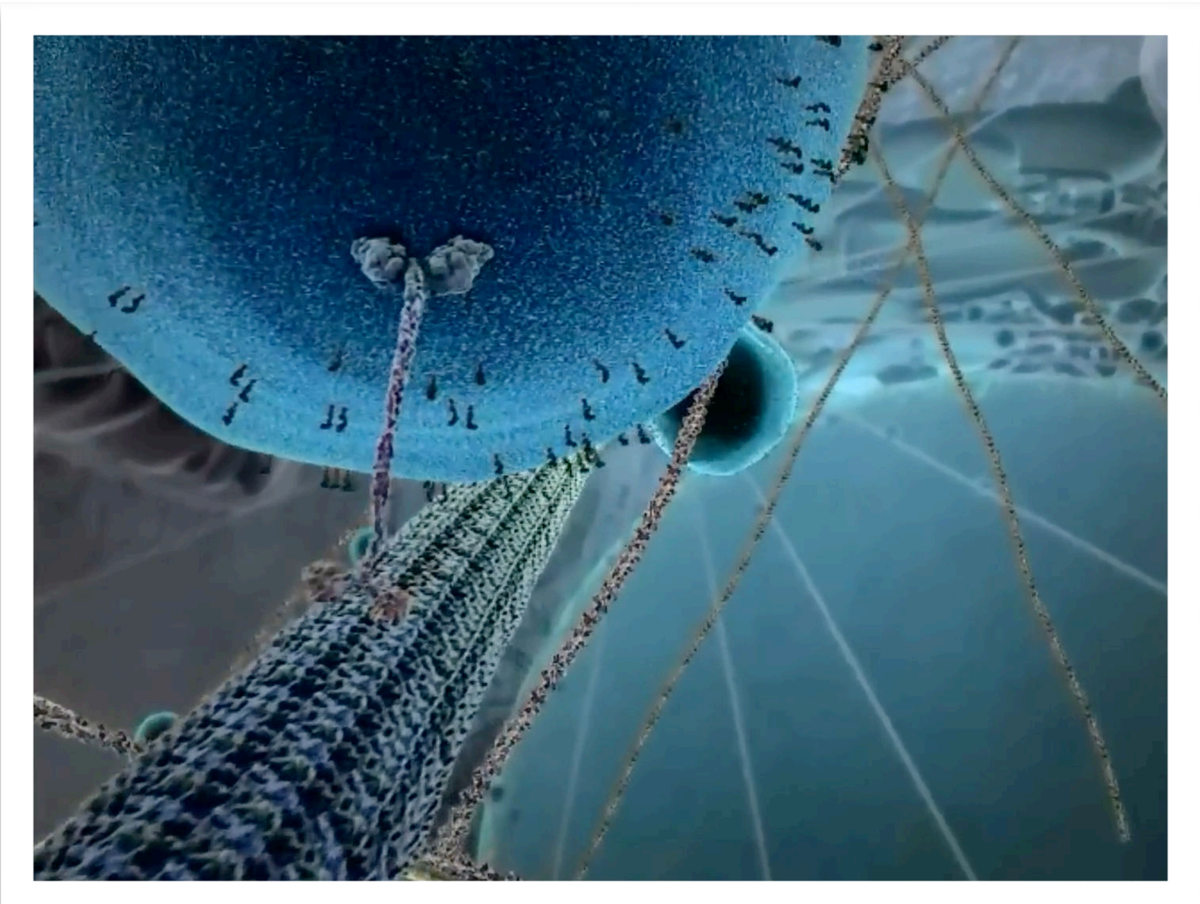
(Video courtesy of Cytopirate Labs, an educational community biolab).

Active Systems as Non-equilibrium systems



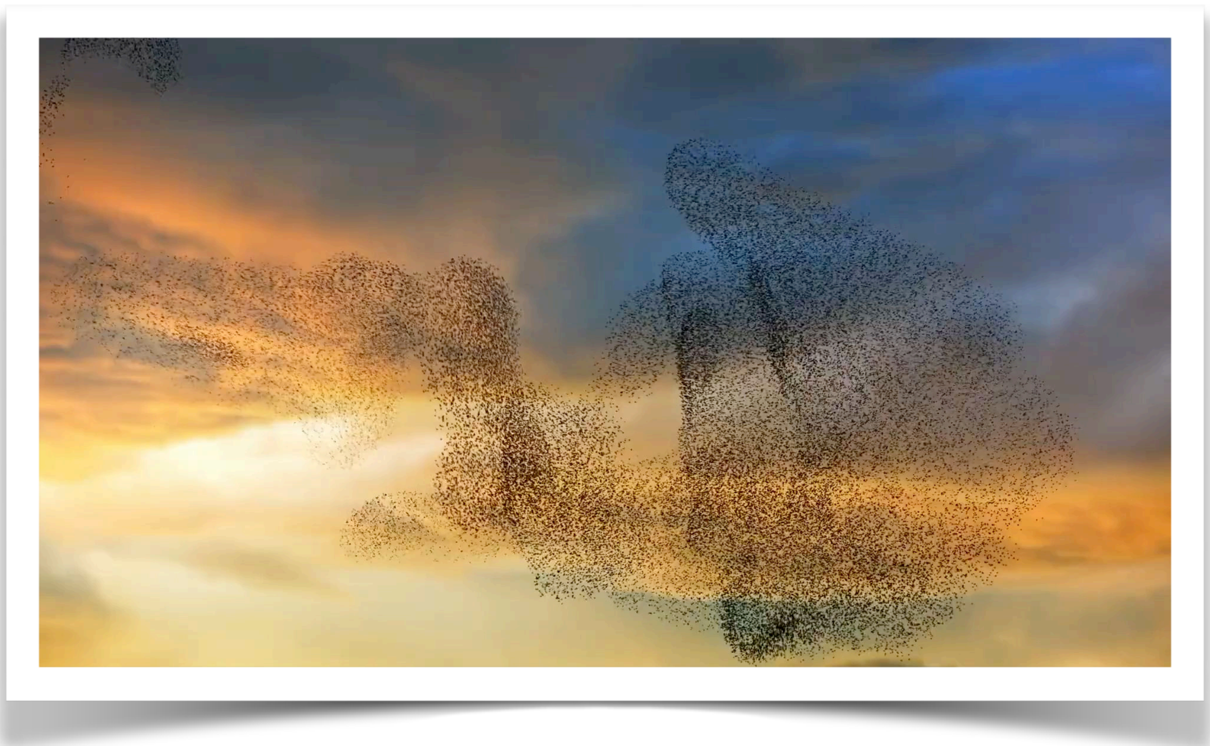
GFP tagged Kinesin walking on TRITC labled microtubules.

(Video courtesy of Cytopirate Labs, an educational community biolab).



Kinesin protein walking on a microtubule in a cell

Collective behaviour in active matter



A flock of birds

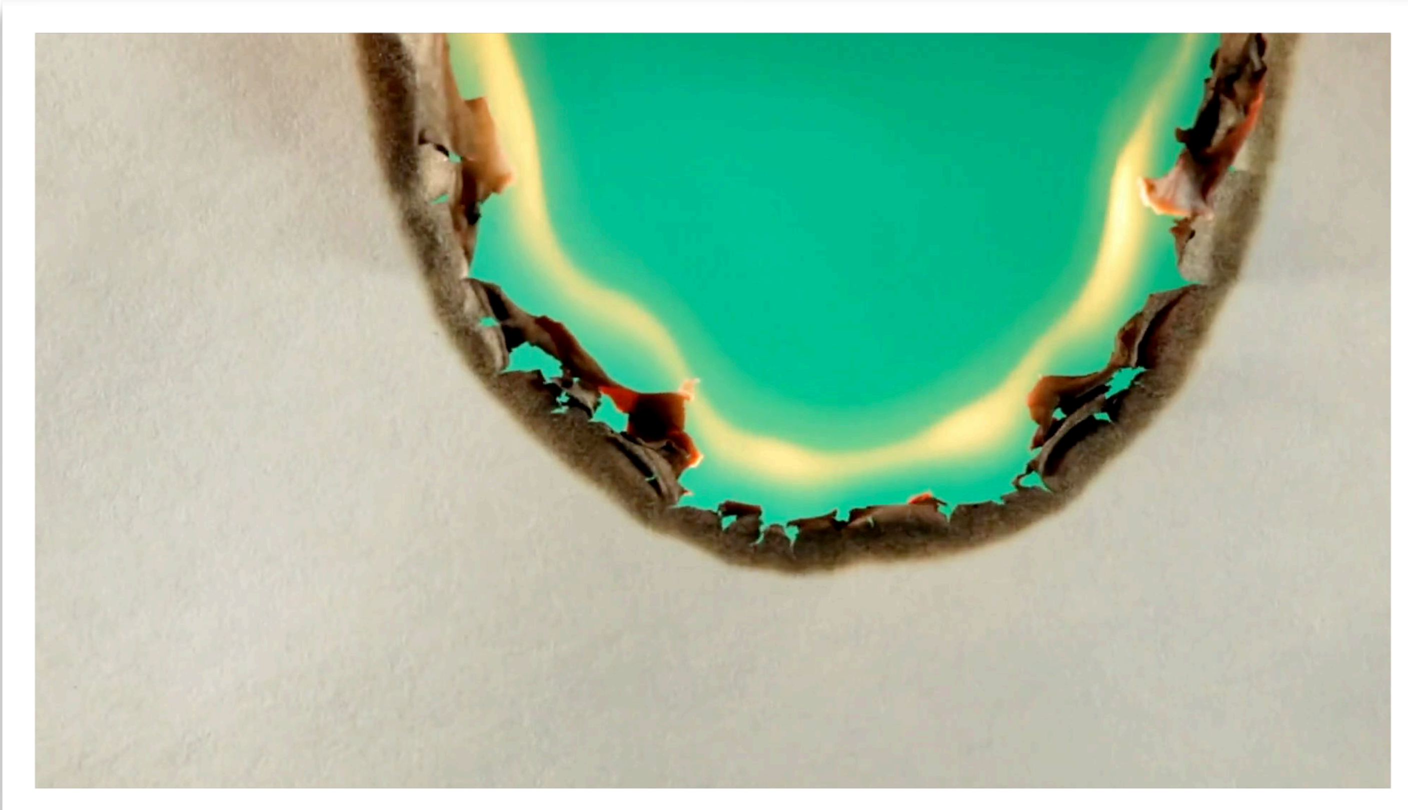
Collective behaviour in active matter

A flock of birds

Jeremie Palacci et al. ,Living Crystals of Light-Activated Colloidal Surfers.Science339,936-940(2013).DOI:10.1126/science.1230020

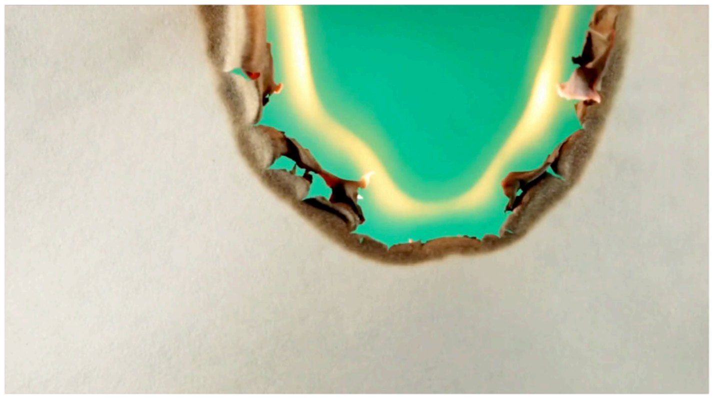
Living Crystals of Light-Activated Colloidal Surfers

Growth Vis-à-Vis: The Non-Active vs. Active



A non-living KPZ interface.

Growth Vis-à-Vis: The Non-Active vs. Active



A non-living KPZ interface.

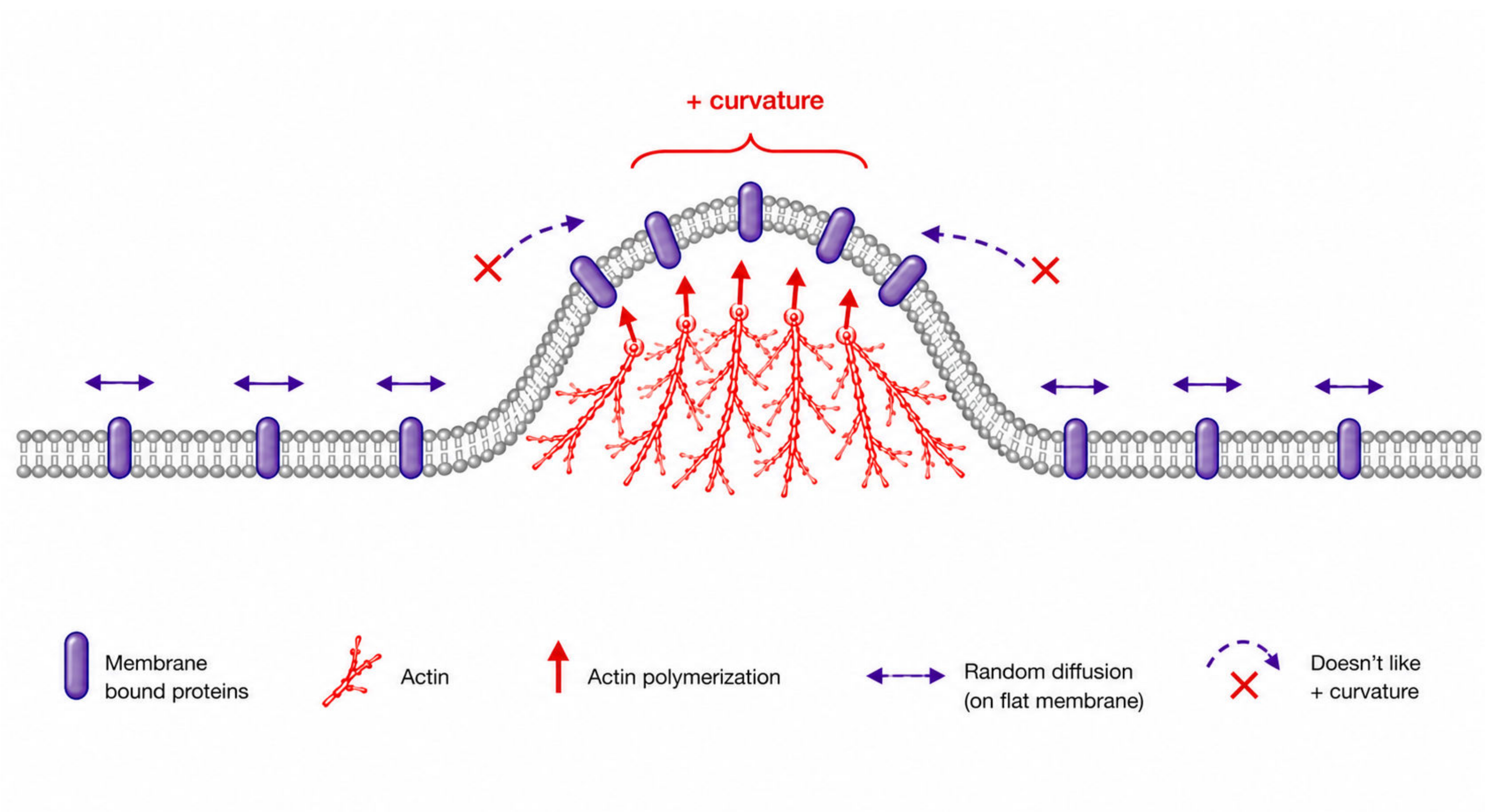
Time-lapse video of flower-like patterns that emerge when E. coli and A. baylyi grow over a 24-hr. period.

Xiong et al. elife 2020;9: e48885

Part A

Active particles interacting with an interface

A model for an active interface



A model for an active interface

Model Setup

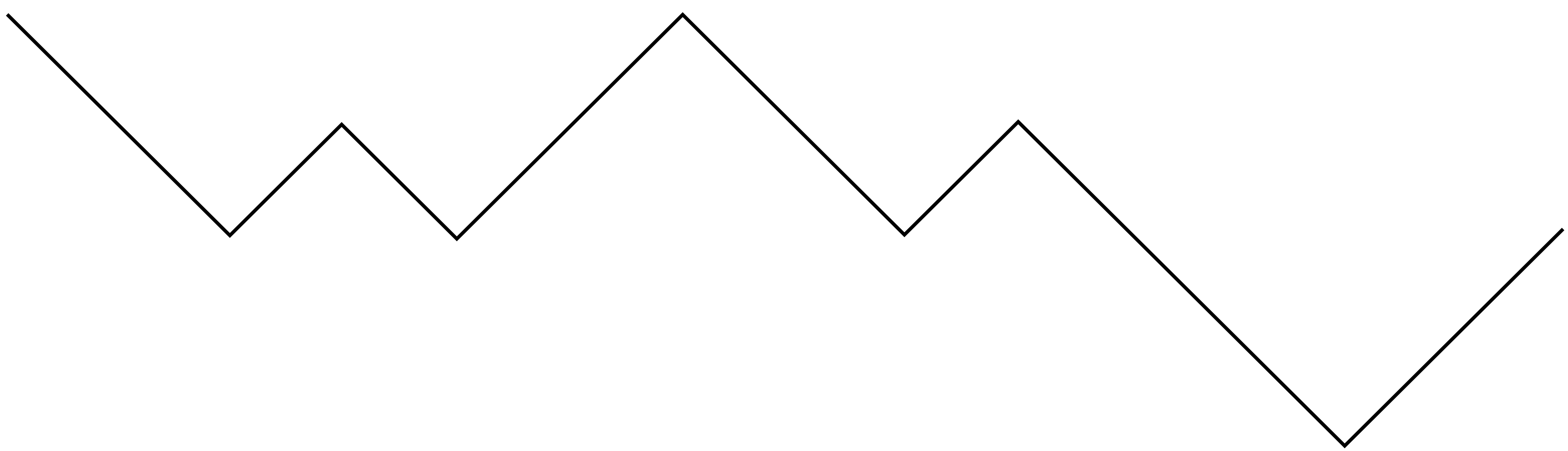
- **The Single-Step Model:** We model the interface as a 1D lattice where the local height difference between adjacent sites is strictly restricted to slopes of $\tau = \pm 1$ (a zig-zag membrane).

Love Grover, Rajeev Kapri and Abhishek Chaudhuri. "Spatial organization of multiple species of active particles interacting with an interface." Phys. Rev. E, 111, 045412, 2025.

A model for an active interface

Model Setup

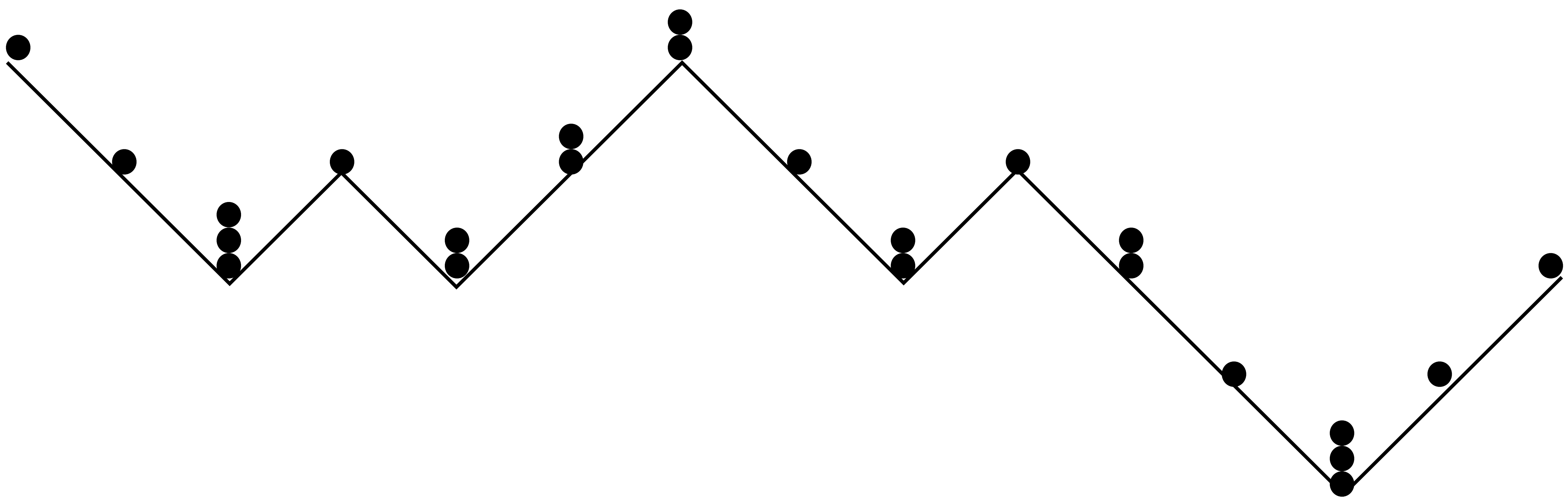
- **The Single-Step Model:** We model the interface as a 1D lattice where the local height difference between adjacent sites is strictly restricted to slopes of $\tau = \pm 1$ (a zig-zag membrane).



A model for an active interface

Model Setup

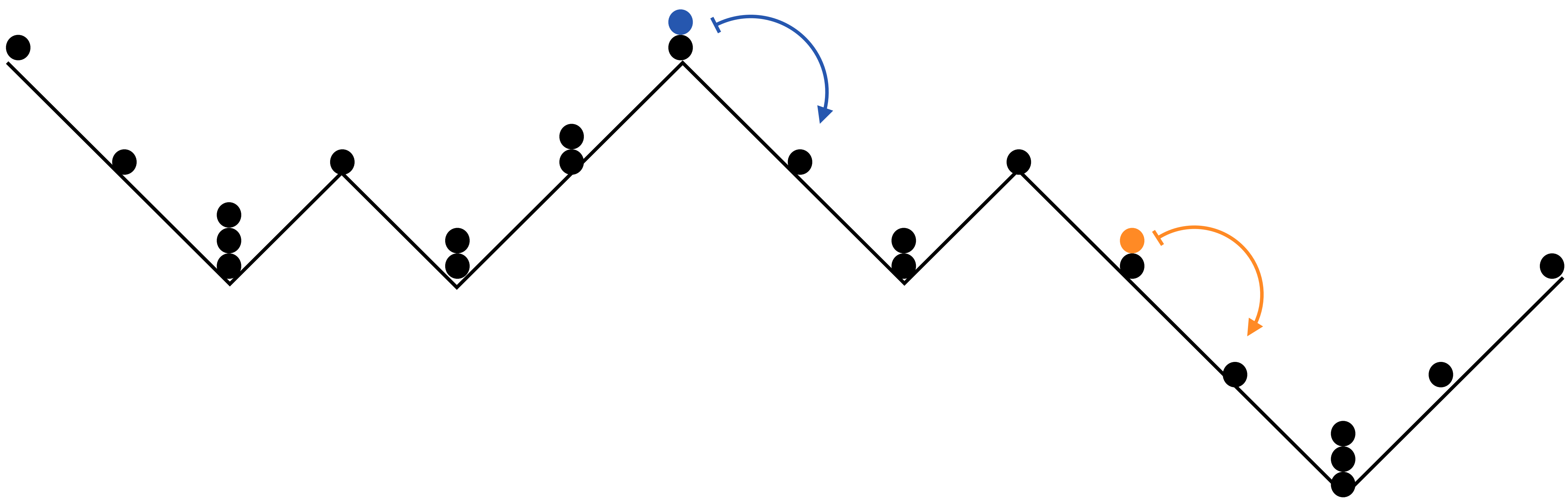
- **Particles Residing on Membrane:** We introduce particles into this environment. These particles occupy the nodes (the joints between the slopes) along the membrane.



Particle Kinetics

Moving on the Lattice

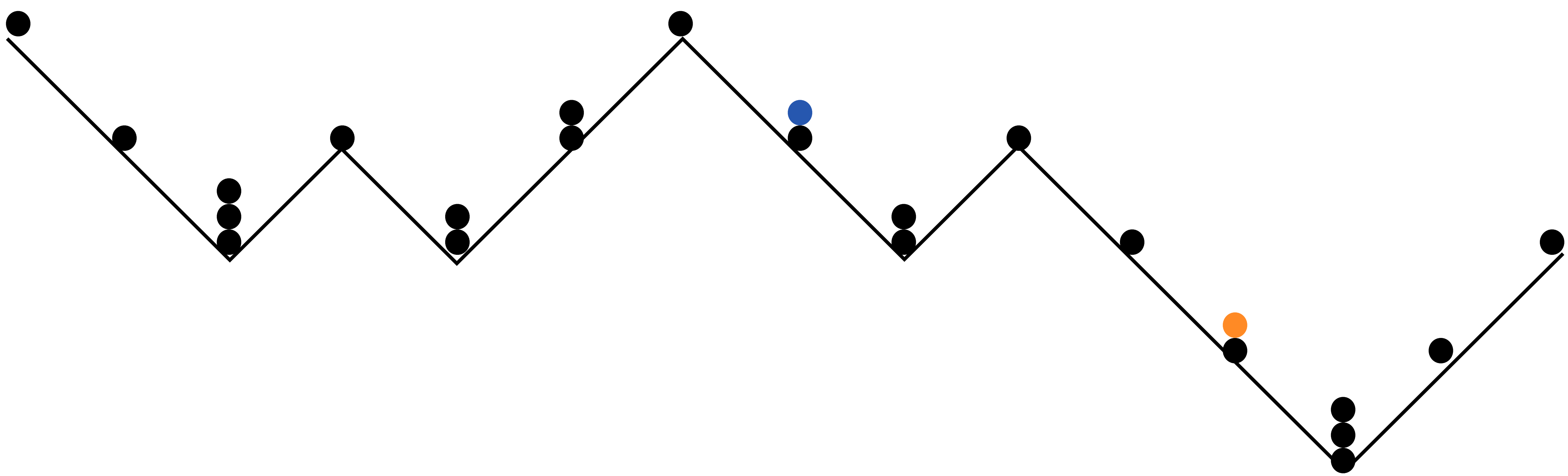
- **Topology-Dependent Hopping:** Particles do not just move blindly; they sense the local slopes. They hop to right adjacent nodes with a base rate $q^R \equiv q^-$(and $q^L \equiv q^+$), but preferentially slide down slopes due to local "gravity".



Particle Kinetics

Moving on the Lattice

- **Topology-Dependent Hopping:** Particles do not just move blindly; they sense the local slopes. They hop to right adjacent nodes with a base rate $q^R \equiv q^-$(and $q^L \equiv q^+$), but preferentially slide down slopes due to local "gravity".

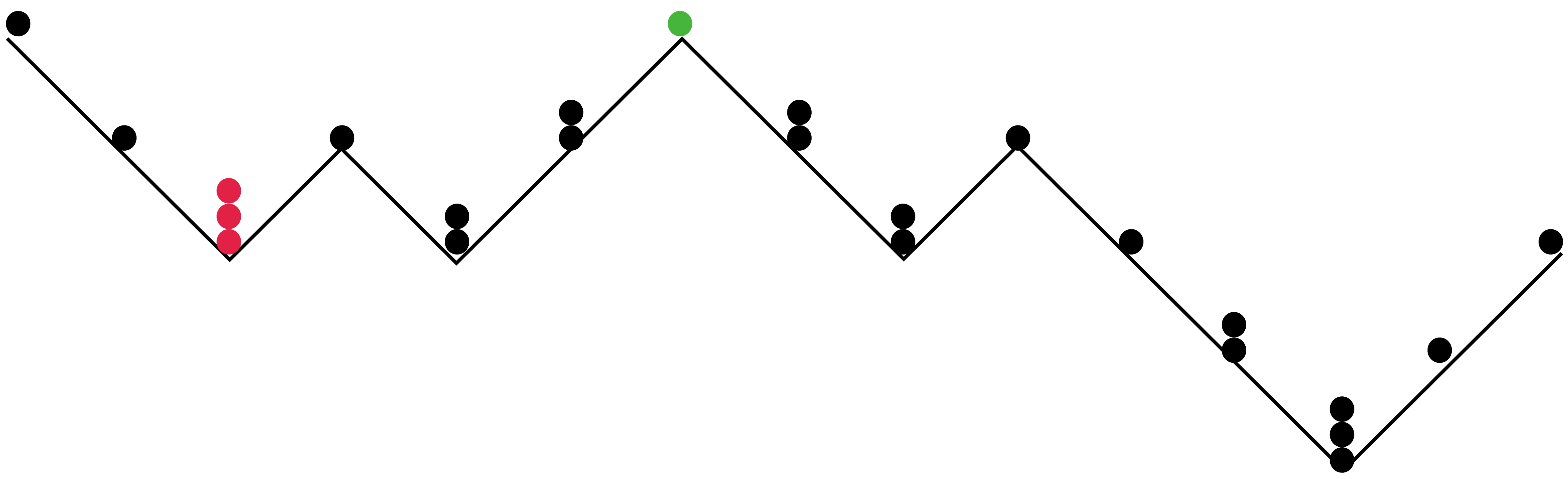


$$q^{\pm} = q_0(1 \pm \frac{\gamma}{2} \nabla h)$$

Membrane Kinetics

EW vs KPZ vs Active

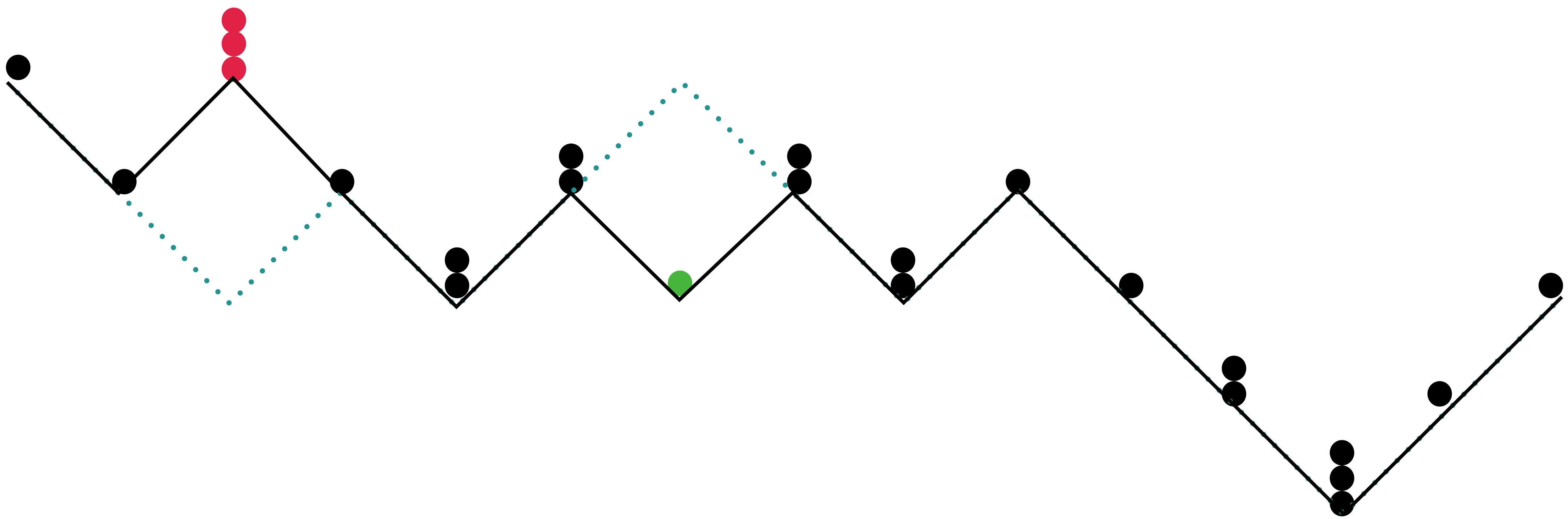
- **The Local Flips:** The membrane evolves through localized inversions. A valley ($\vee$) can invert into a peak ($\wedge$) with probability p^+, and a peak can invert into a valley with probability p^-.



Membrane Kinetics

EW vs KPZ vs Active

- **The Local Flips:** The membrane evolves through localized inversions. A valley ($\vee$) can invert into a peak ($\wedge$) with probability p^+, and a peak can invert into a valley with probability p^-.



Membrane Kinetics

EW vs KPZ vs Active

- **EW:** $p^+ = p^-$
- **KPZ:** $p^+ \neq p^-$
- **Active:** $p_n^\pm = f(n, \nabla^2 h)$

p^+ is the rate at which the $\vee$ is converted to a $\wedge$.

Membrane Kinetics

EW vs KPZ vs Active

- **EW:** $p^+ = p^-$
- **KPZ:** $p^+ \neq p^-$
- **Active:** $p_n^\pm = f(n, \nabla^2 h)$

p^+ is the rate at which the $\vee$ is converted to a $\wedge$.

$$p_n^\pm = u \frac{e^{\pm n\beta}}{e^{n\beta} + e^{-n\beta}}$$

Membrane Kinetics

EW vs KPZ vs Active

- **EW:** $p^+ = p^-$
- **KPZ:** $p^+ \neq p^-$
- **Active:** $p_n^\pm = f(n, \nabla^2 h)$

p^+ is the rate at which the $\vee$ is converted to a $\wedge$.

$$p_n^\pm = u\frac{e^{\pm n\beta}}{e^{n\beta} + e^{-n\beta}}$$

$$p_{\{n_1,n_2\}}^\pm = u\frac{e^{\pm(n_1\beta_1+n_2\beta_2)}}{e^{(n_1\beta_1+n_2\beta_2)} + e^{-(n_1\beta_1+n_2\beta_2)}}$$

Single Species Organization

Competition of parameters

- **The Two parameters:** β and γ are the two parameters in active membrane.
  - β defines the activity generated by particles on membrane:
    $$p_n^{\pm} = u\frac{e^{\pm n\beta}}{e^{n\beta} + e^{-n\beta}}$$
  - γ defines the gravity in the system for the particles:
    $$q^{\pm} = q_0(1 \pm \frac{\gamma}{2}\nabla h)$$

Single Species Organization

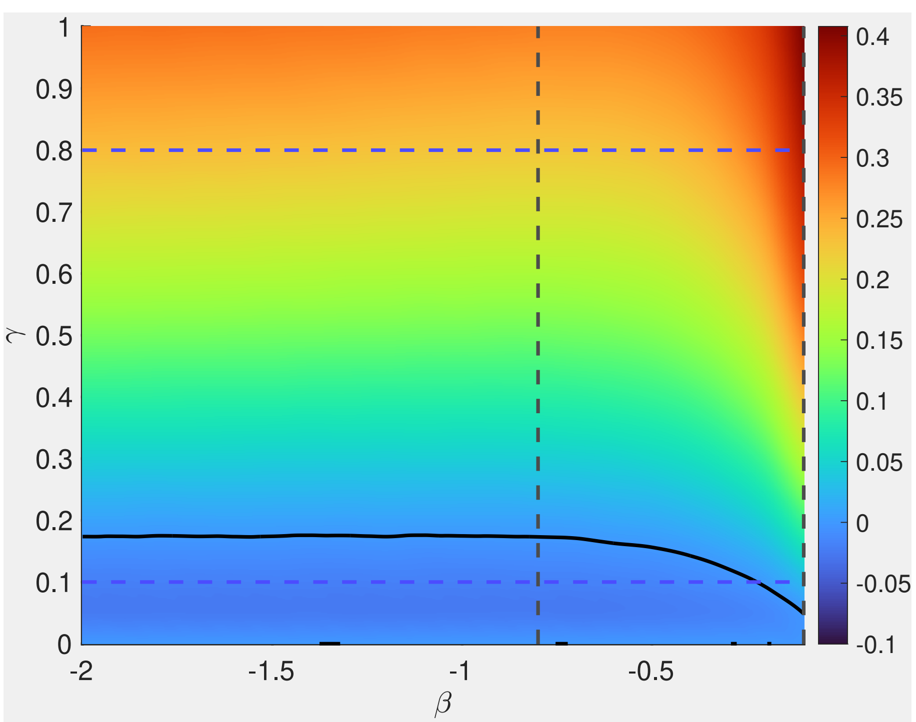
Competition of parameters

- $\beta < 0$ **: Pulls up the membrane**
- $\gamma > 0$ **: particle falls in gravity downwards**
  - Particles gets collected due to gravity
  - As particles gets collected more and more the valley becomes more and more unstable due to activity and eventually converted to hill.
  - Particles collected found themselves on hill which is an unstable situation due to gravity and local microcluster breaks as the particle moves to find a new valley.

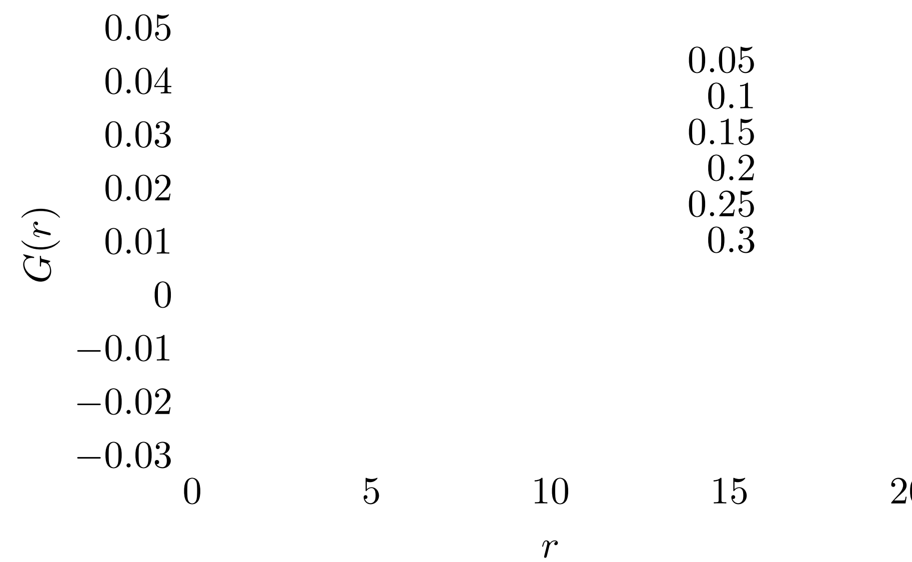
Competition

Anticorrelation, Zero-Correlation and Correlation Regime

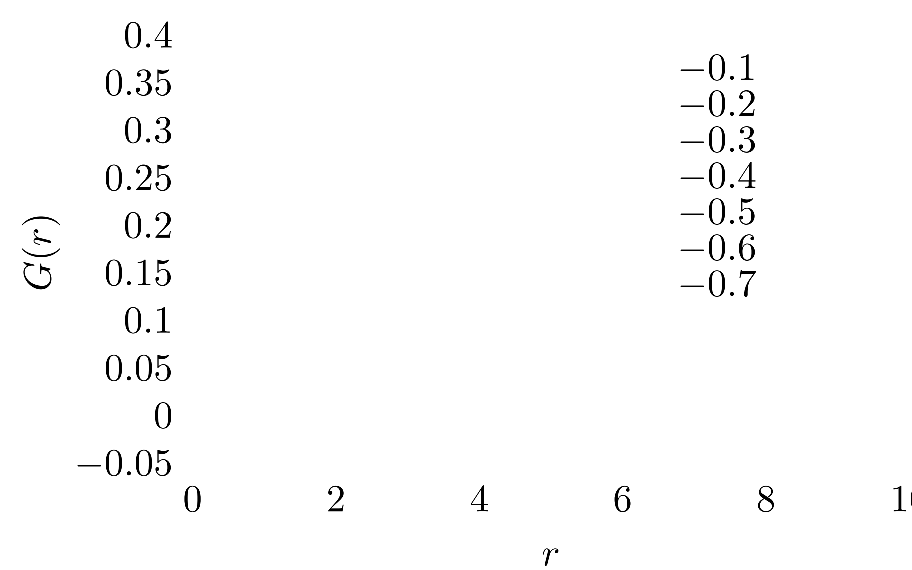
- $$G(r) = \frac{\langle s_i s_{i+r} \rangle - \langle s_i \rangle^2}{\langle s_i^2 \rangle - \langle s_i \rangle^2}$$



- $G(1)$ in β and γ phase-space



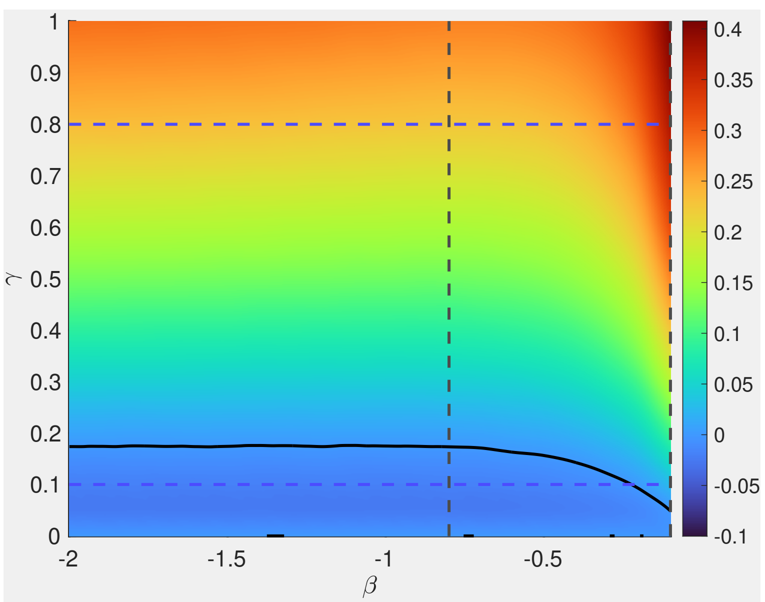
$\beta = -0.8$ and varying γ

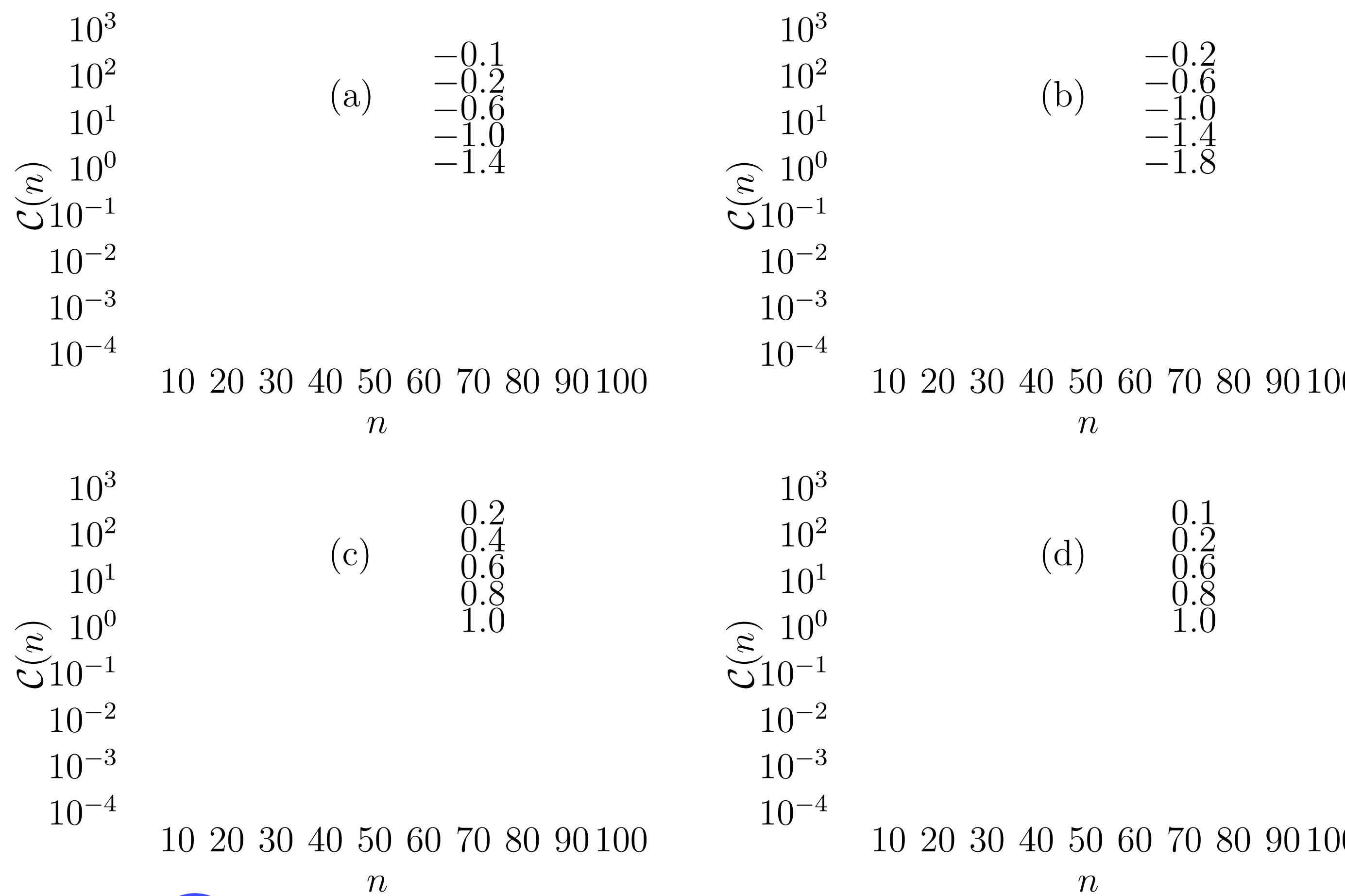


$\gamma = 0.8$ and varying β

Cluster Distribution Function

- A cluster is defined as a contiguous group of particles such that empty sites on both ends bound the group.





- △ is for zero-gravity case; ◯ is for passive case (zero activity).
- [(a) $\gamma = 0.1$; (b) $\gamma = 0.8$] (β variable);
- [(c) $\beta = -0.1$; (d) $\beta = -0.8$](γ variable)

Two types of active species

4 Cases

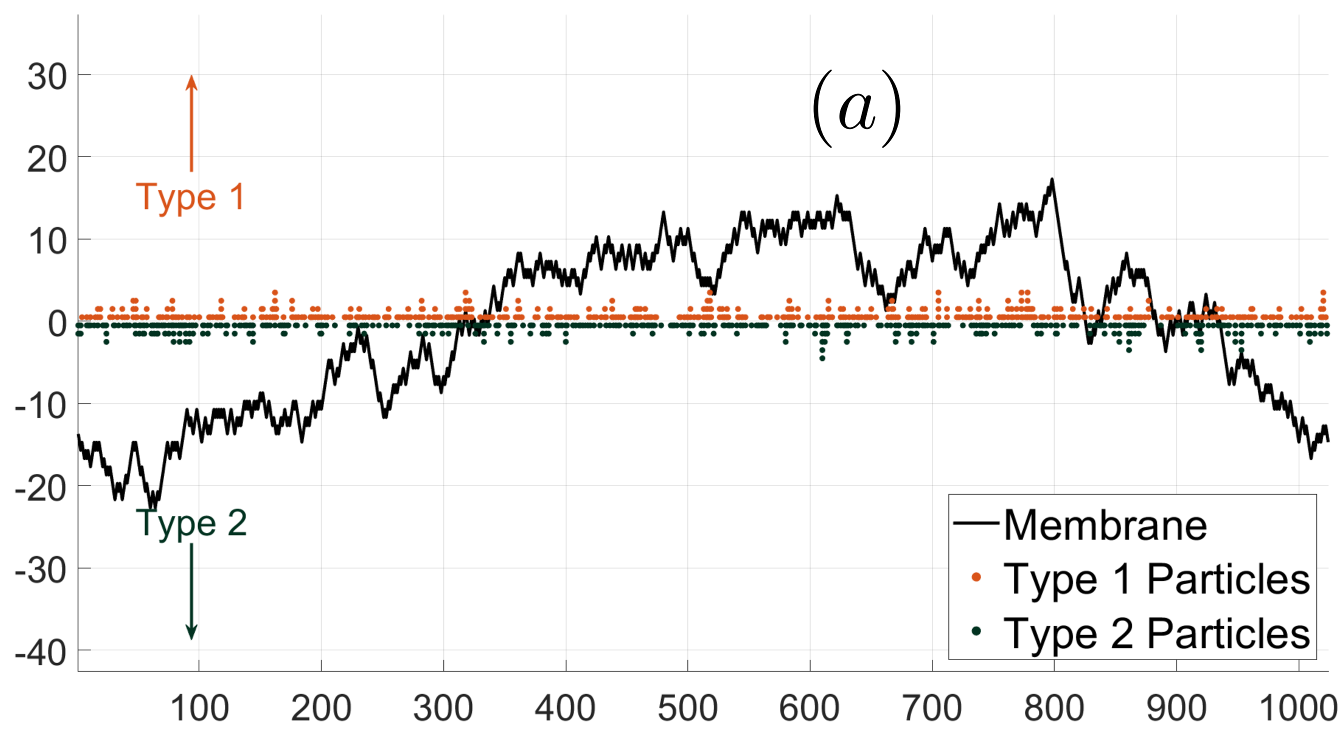
- **Sign Convention:** Gravity and activity acting in downward direction is positive.

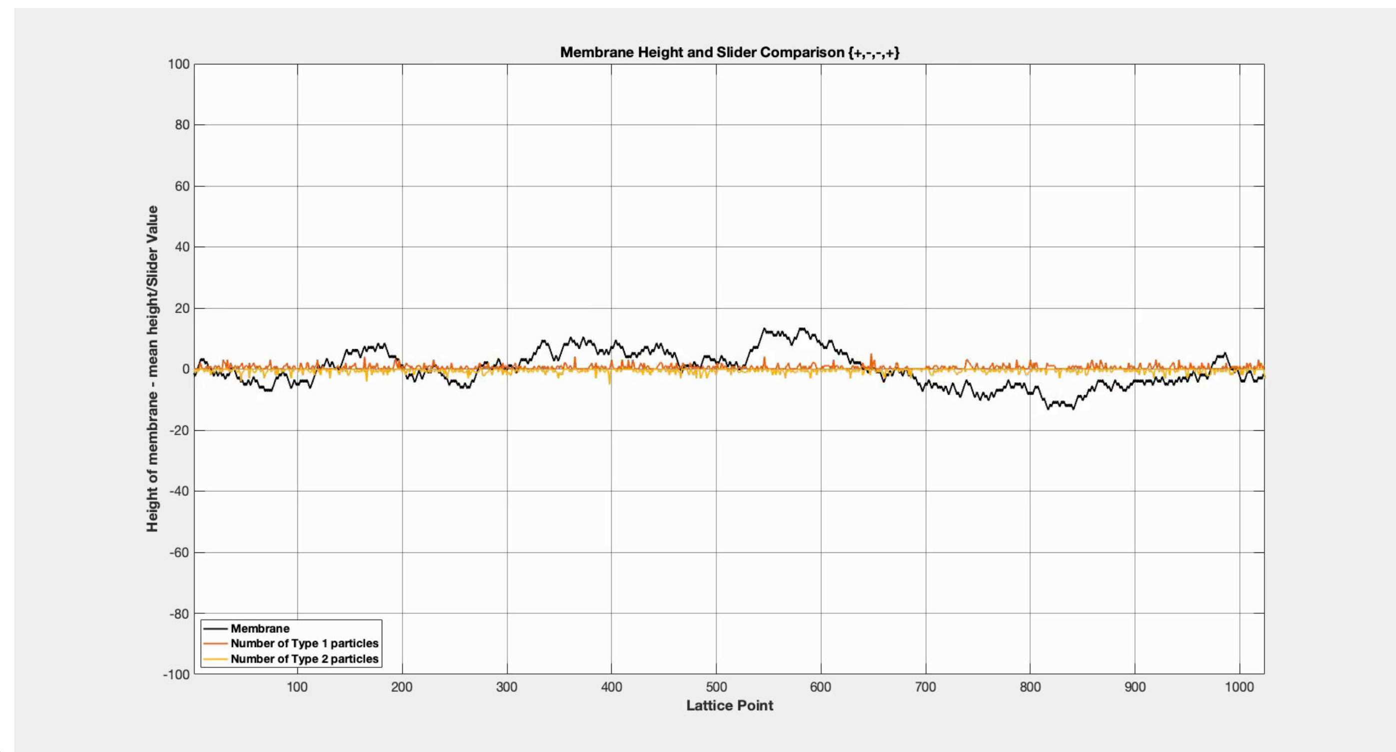
Cases\Symmetries	Reversal	Exchange	Both
{+,+,-,+}	{-,-,+,-}	{-,+,+,+}	{+,-,-,-}
{+,+,-,-}	{-,-,+,+}	C(2)	C(1)
{+,-,-,+}	{-,+,+,-}	C(2)	C(1)
{-,-,-,+}	{+,+,+,-}	{-,+,-,-}	{+,-,+,+}
Trivial cases			
{-,-,-,-}	{+,+,+,+}	C(1)	C(2)
{+,-,+,-}	{-,+,-,+}	C(1)	C(2)

Signs of $\{\beta_1, \gamma_1, \beta_2, \gamma_2\}$, whereas we kept $\left|\beta_i\right| = 2$ & $\left|\gamma_i\right| = 1$

Two types of particles

{+,-,-,+}



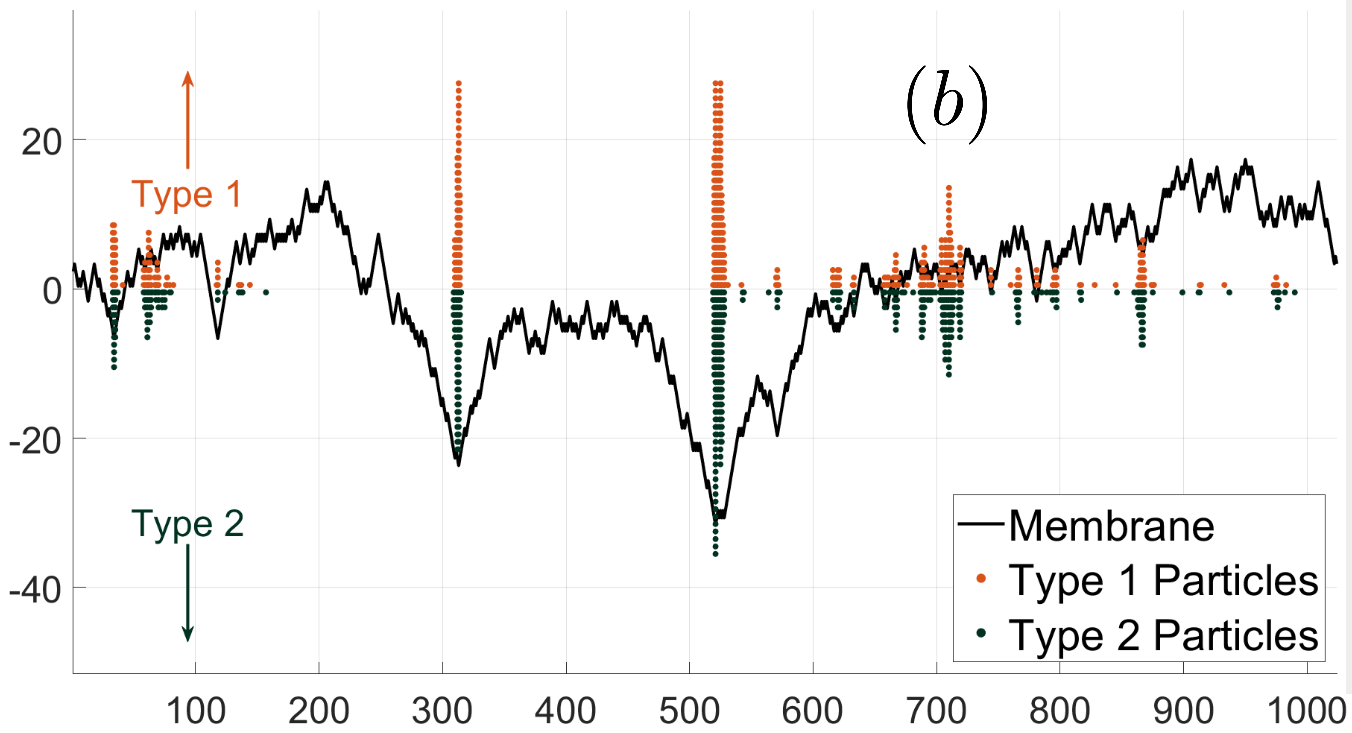


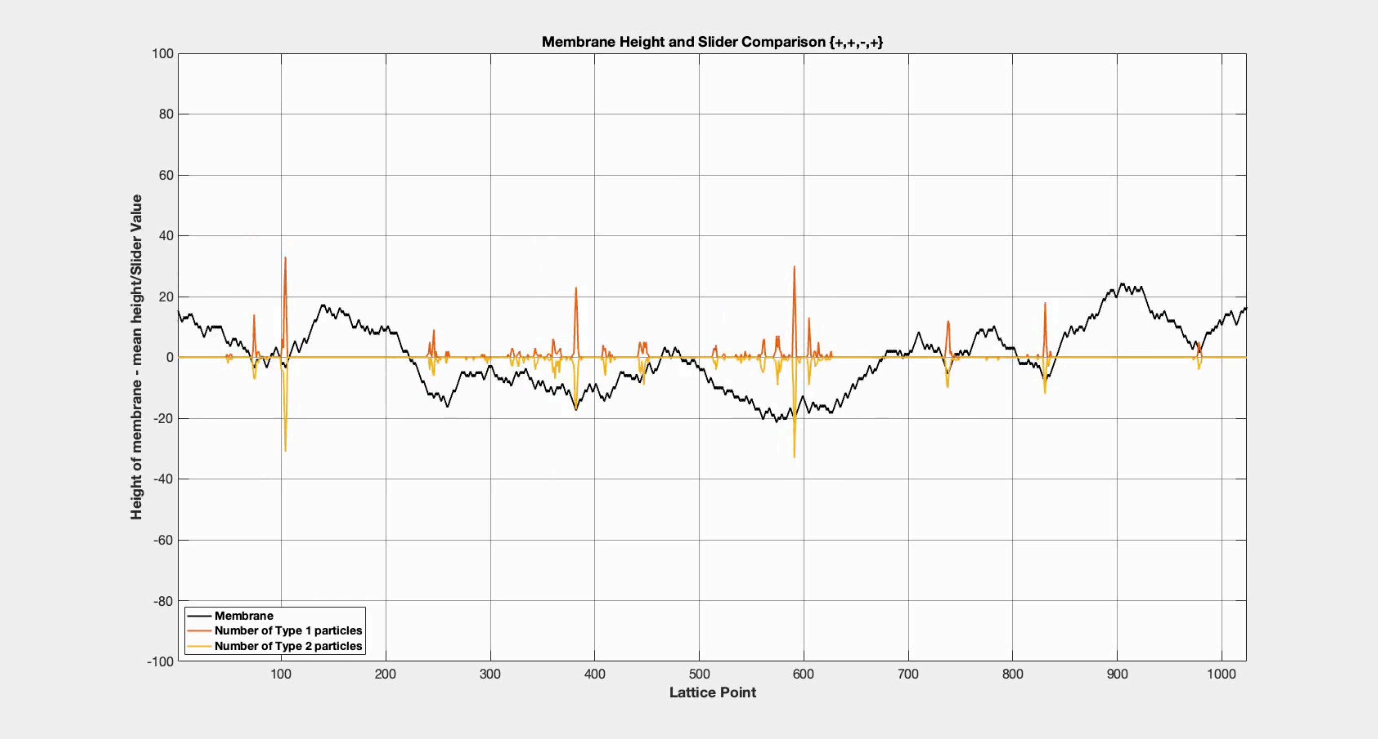
Type 1: Pulling membrane up and like valleys
Type 2: Pushing membrane down and like hills

Becomes like a single type of particle picture.

Two types of particles

{+,+,-,+}



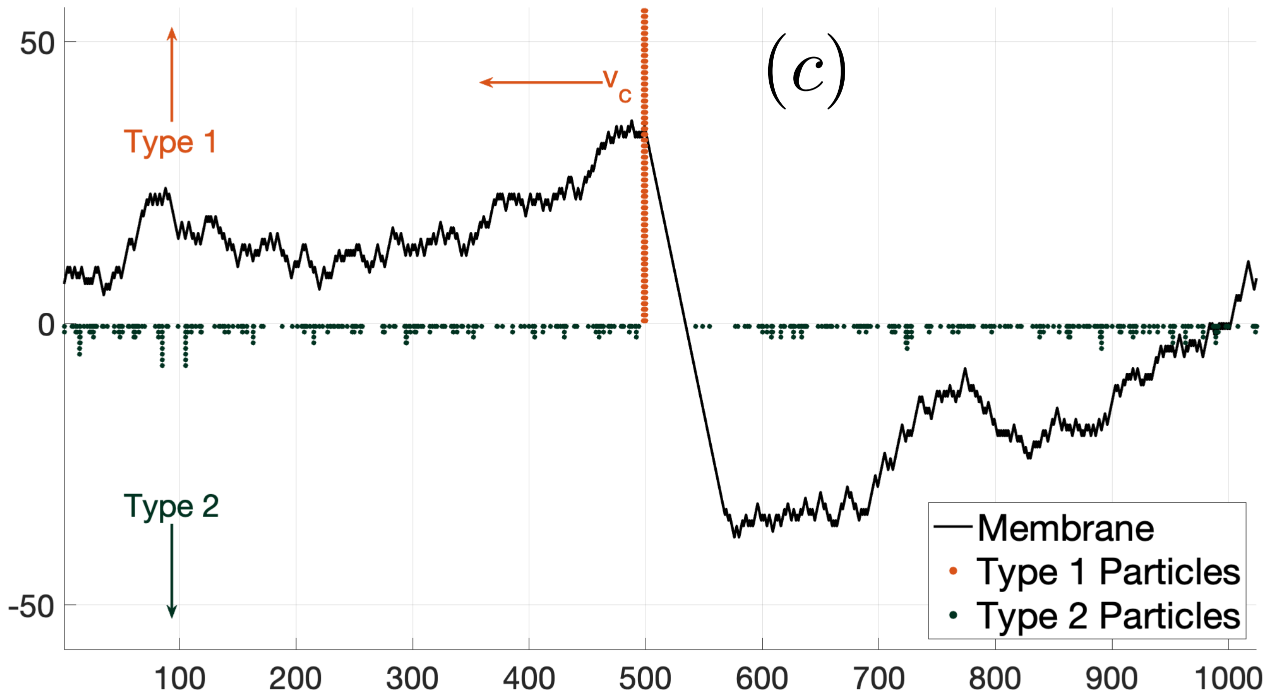


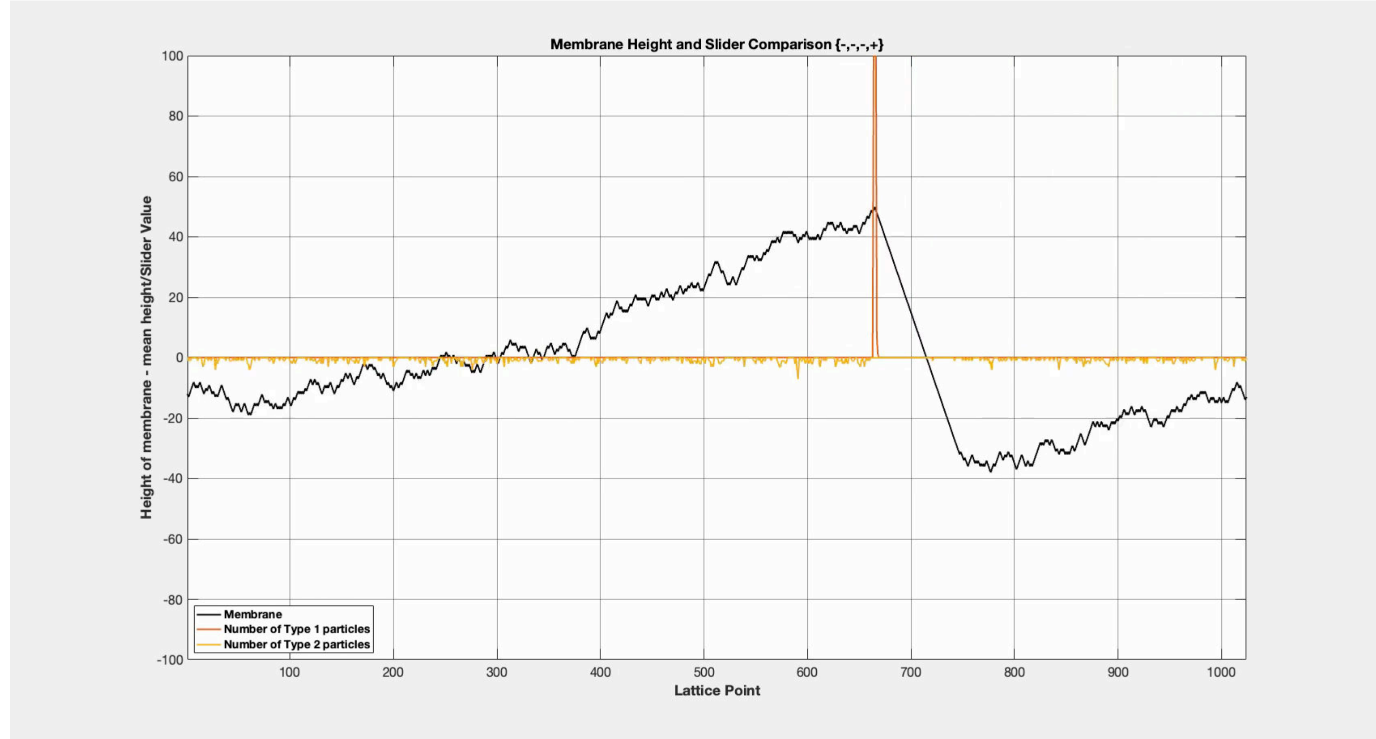
Type 1: Pulling membrane up and like hills
Type 2: Pushing membrane down and like hills

Becomes like a passive slider case, particles always stays balanced

Two types of particles

{-,-,-,+}



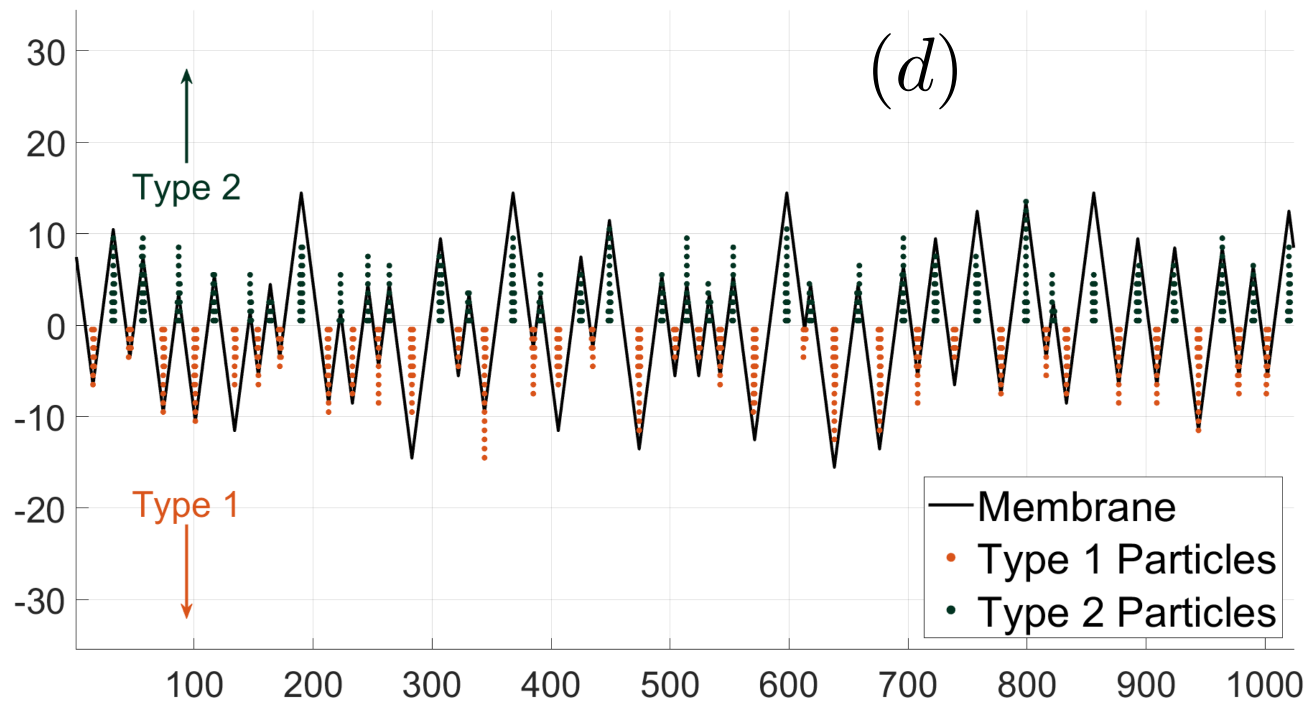


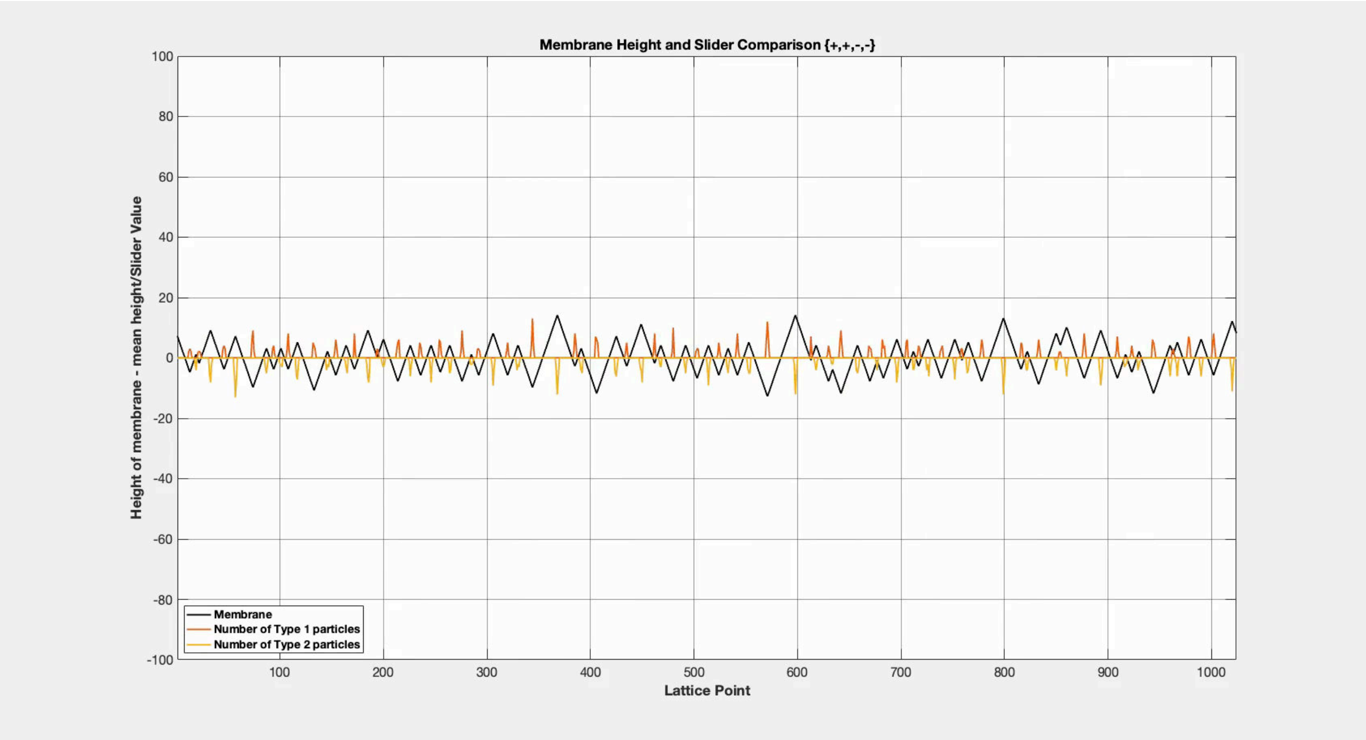
Type 1: Pushing membrane down and like valleys
Type 2: Pushing membrane down and like hills

CMAM like motion but with a memory. Non-Markovian motion of clusters.

Two types of particles

{+,+,-,-}





Type 1: Pulling membrane up and like hills
Type 2: Pushing membrane down and like valleys

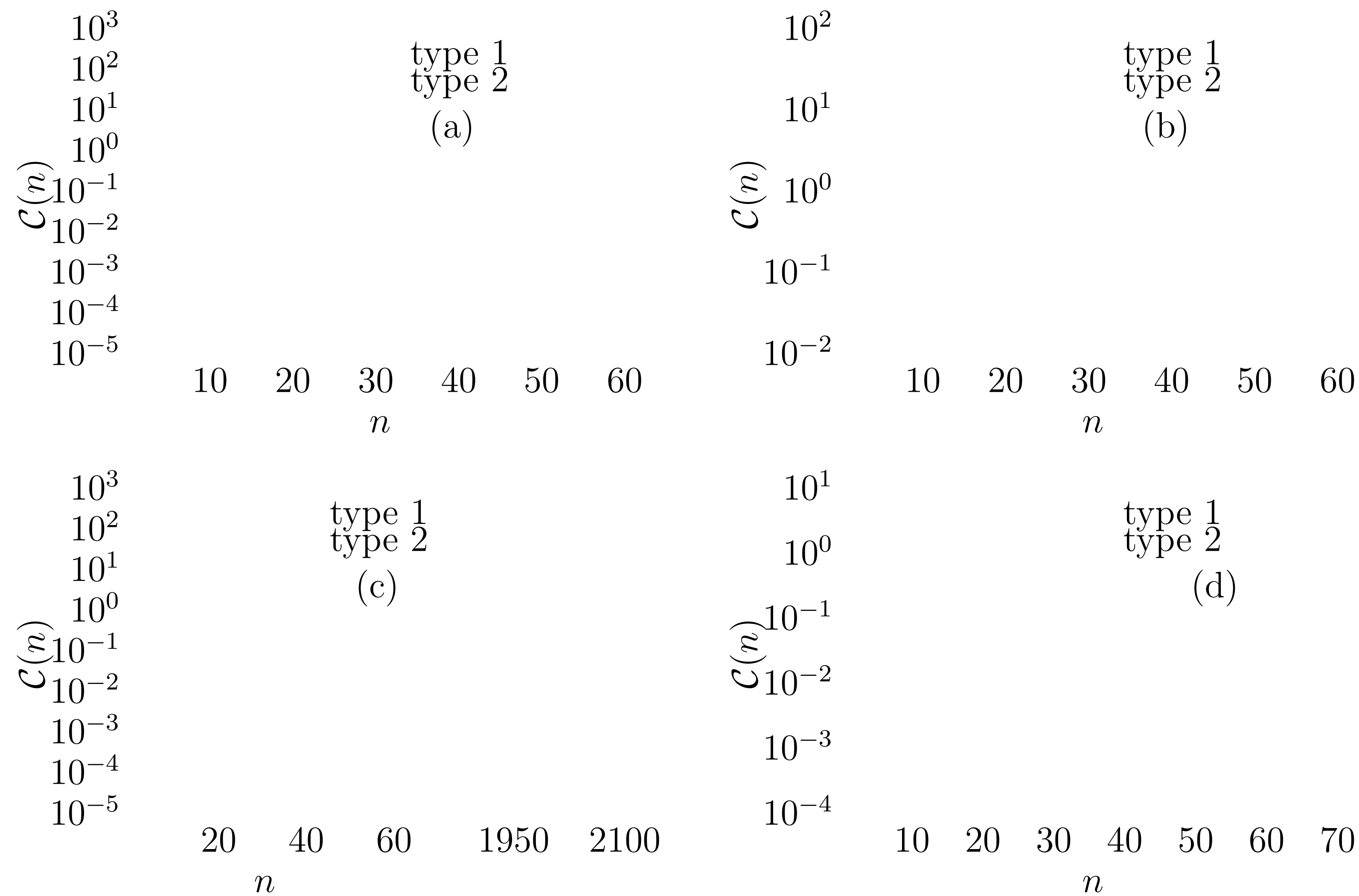
CMAM like motion but with a memory. Non-Markovian motion of clusters.

Cluster Distribution function

Two types of particles

Reference: $\{\beta_1, \gamma_1, \beta_2, \gamma_2\}$

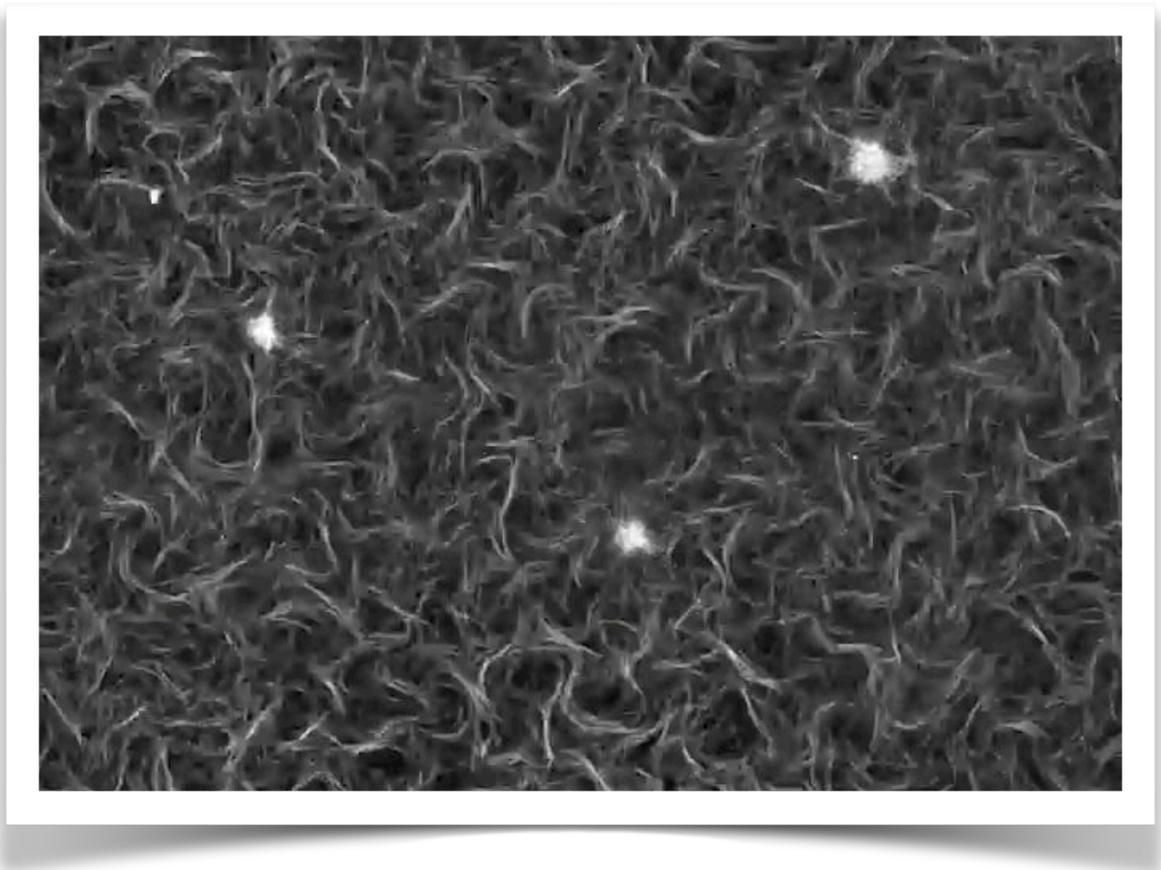
- (a) {+,-,-,+}
- (b) {+,+,-,+}
- (c) {-,-,-,+}
- (d) {+,+,-,-}

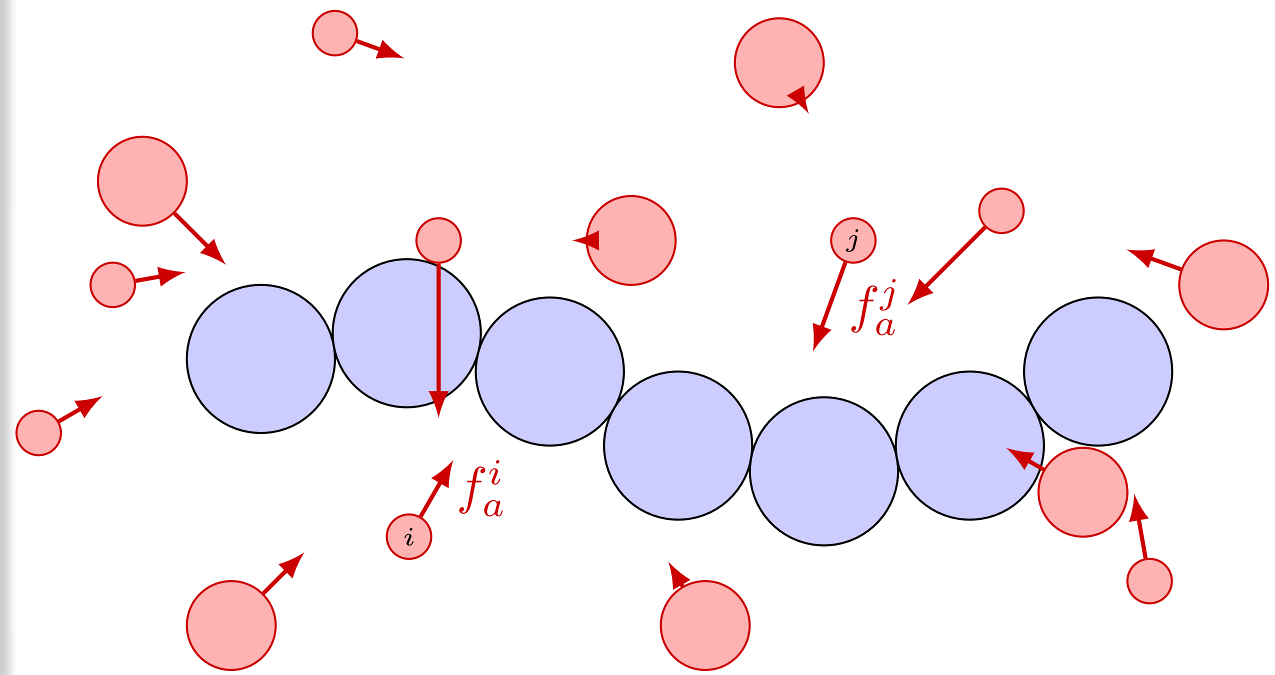


Part B

Polymer in active bath

Polymer in an active environment





Active collection of microtubules and kinesin motors.

A single polymer immersed in an active environment.

"Percolating Active Network of Microtubules." YouTube, uploaded by Dogic Lab, 9 Jan. 2014, https://www.youtube.com/watch?v=NuFMIoTVTsg.

Model

Semiflexible Polymer

- Harmonic bonds.

$$V_b = \frac{k_s}{2} \sum_{i=2}^{N} (\,|\,\mathbf{r}_i - \mathbf{r}_{i-1}\,| - r_0)^2$$

- Rigidity: Semiflexibility.

$$V_a = \kappa \sum_{i=2}^{N-1} (1 - \cos\theta_i)$$

- Excluded volume interactions.

$$V_{WCA}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \epsilon\,;\ \text{for } r \leq 2^{1/6}\sigma\,;\, 0 \text{ otherwise}$$

- Equations of motion of monomers:

$$m\frac{d\mathbf{v}_i}{dt} = -\,\gamma_t\,\mathbf{v}_i + \mathbf{F}_i^{c} + \sqrt{2\gamma_t k_B T}\,\boldsymbol{\xi}_i(t),$$

Model

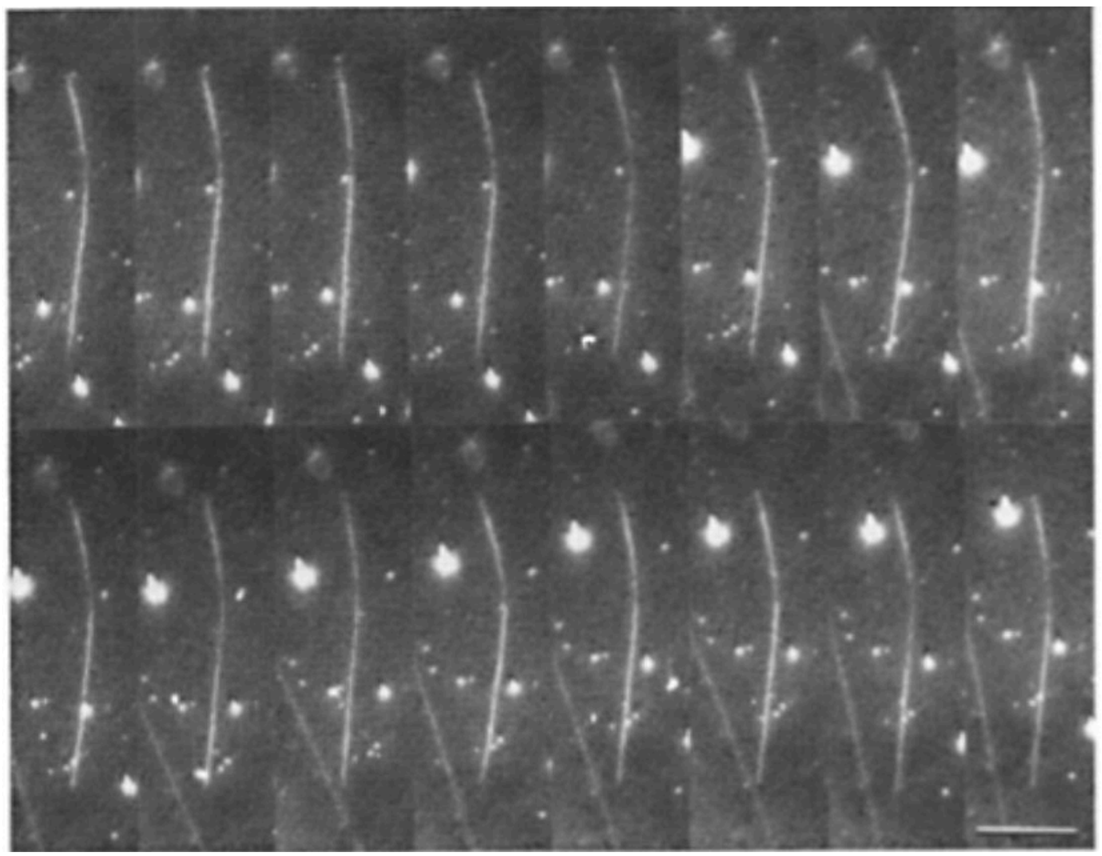
Active particles

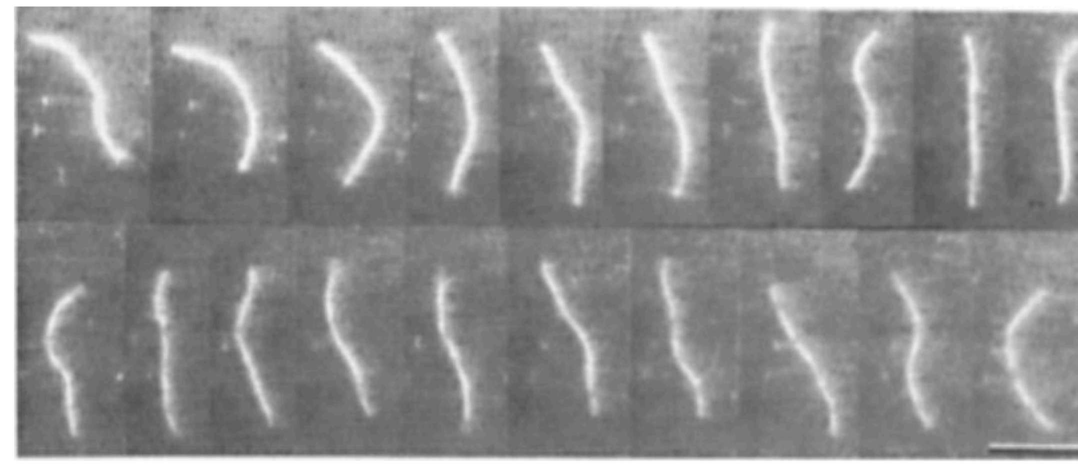
- Active forcing: f_a
- Persistence time: $\tau = 1/D_r$
- Excluded volume interactions.
- **Equations of motion:**

$$m_a \frac{d\mathbf{V}_j}{dt} = -\gamma_t \mathbf{V}_j + \mathbf{F}_j^{\mathrm{c}} + f_a \hat{\mathbf{n}}_j + \sqrt{2\gamma_t k_B T}\, \boldsymbol{\Xi}_j(t),$$

$$I \frac{d^2\theta_j}{dt^2} = -\gamma_r \frac{d\theta_j}{dt} + \sqrt{2D_r}\, \eta_j(t),$$

Mode Amplitude





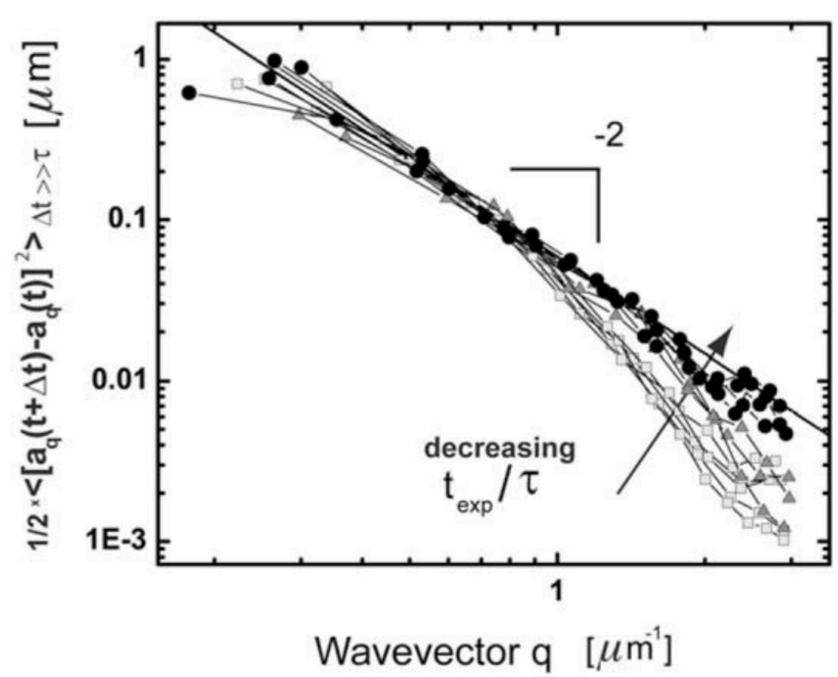
Actin filaments undergoing thermal fluctuations

Microtubule undergoing thermal fluctuations

Gittes, Frederick, et al. "Flexural rigidity of microtubules and actin filaments measured from thermal fluctuations in shape." *The Journal of cell biology* 120.4 (1993): 923-934.

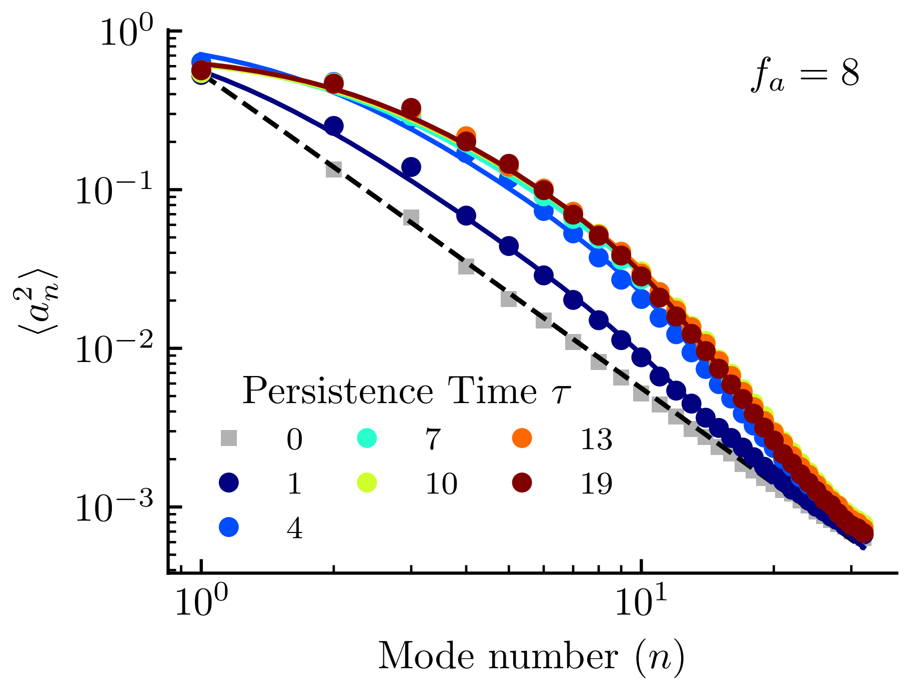
Mode Amplitude

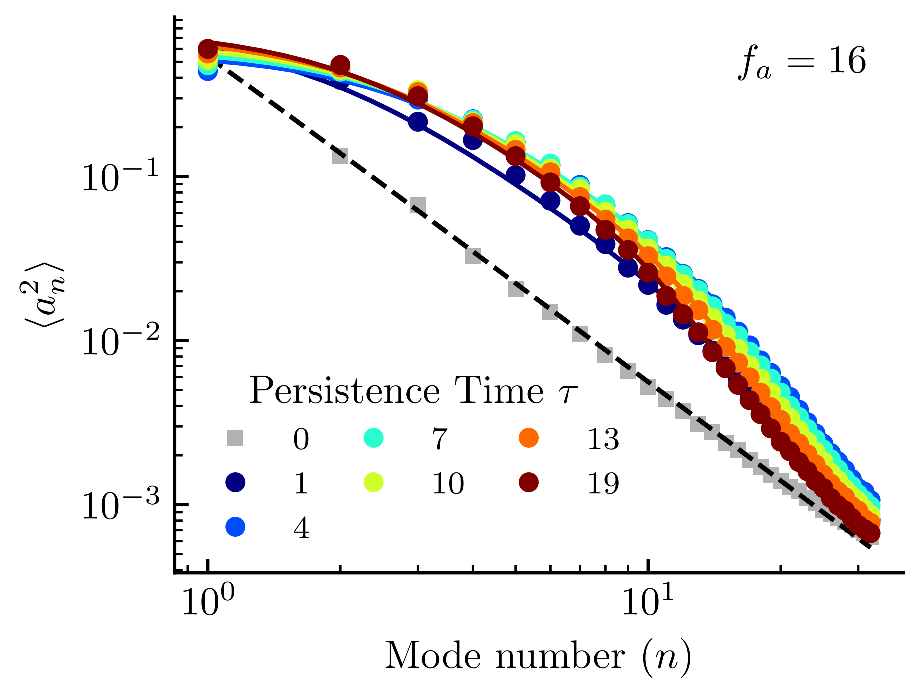
- Bond vectors: $\Delta\mathbf{r}_k = \mathbf{r}_{k+1} - \mathbf{r}_k$
- We decompose the bending modes:
$$\mathbf{b}_n = \sqrt{\frac{2}{N}} \sum_{k=1}^{N-1} \Delta\mathbf{r}_k \cos\left[\frac{n\pi}{N}\left(k + \frac{1}{2}\right)\right]$$
- Then we calculated the variance of these modes:
$\langle |a_n|^2 \rangle = \langle |\mathbf{b}_n|^2 \rangle$
- What do we expect in purely thermal bath:
$$\langle a_n^2 \rangle = \frac{k_B T}{\kappa q_n^2}$$



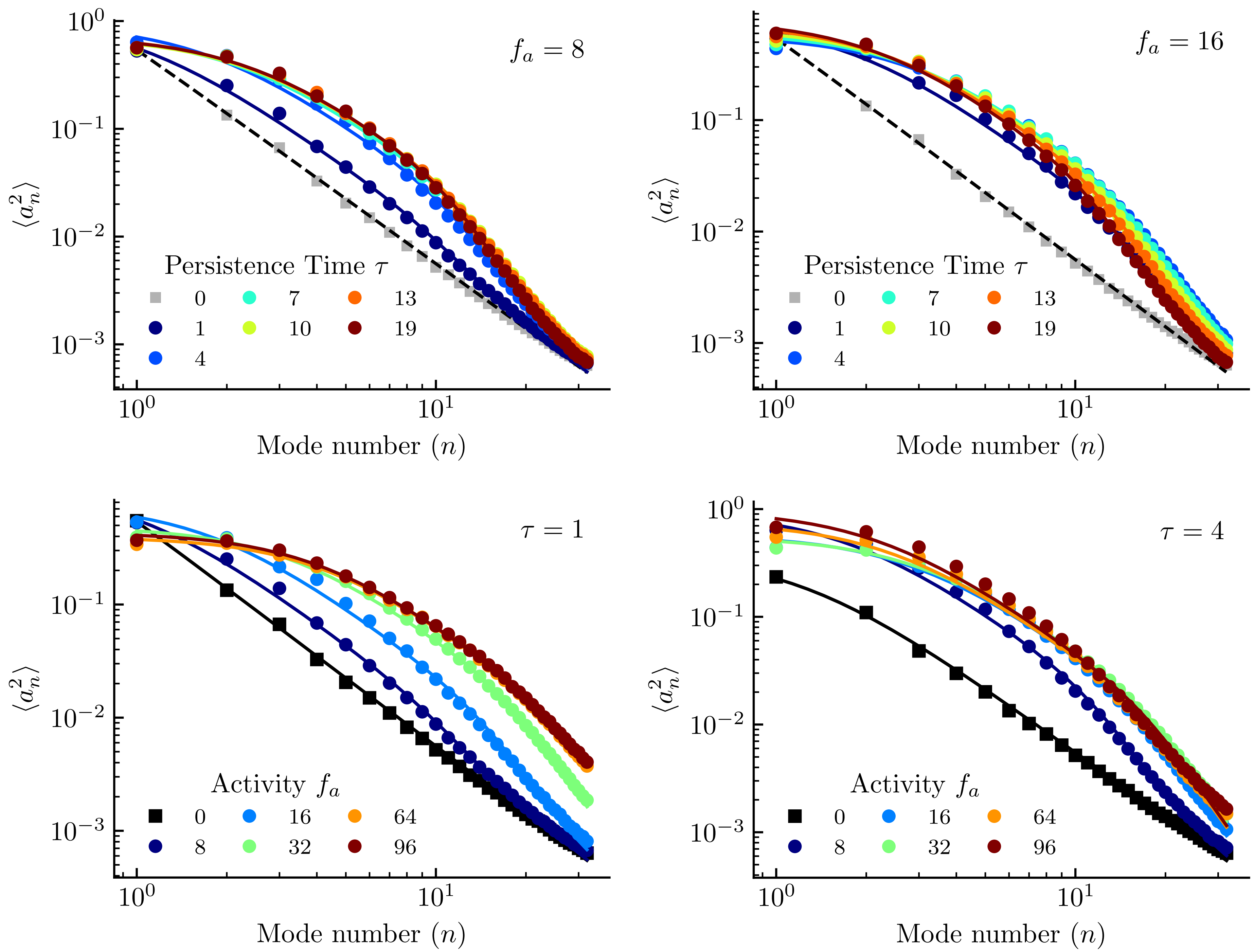
Brangwynne, Clifford P., et al. "Bending dynamics of fluctuating biopolymers probed by automated high-resolution filament tracking." *Biophysical journal* 93.1 (2007): 346-359.

Semiflexible polymer in active bath





Semiflexible polymer in active bath



Theoretical framework

- **Semiflexible polymer in weak bending limit**

$$\zeta \partial_t u_\perp = -\kappa \partial_s^4 u_\perp + \eta_u^{th} + \eta_u^{act}$$

- **Decompose in cosine modes:**

$$u_\perp(s,t) = \sum_{n\geq 1} a_n(t)\, \phi_n(s)$$

- **We can immediately write the equation of motion of** a_n

$$\zeta\, \dot{a}_n(t) + \kappa q_n^4 a_n(t) = \xi_n^{\text{th}}(t) + \xi_n^{\text{act}}(t),$$

- **Fourier transform leads to the form of** $\langle a_n^2 \rangle$

$$\langle |a_n|^2 \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} |H_n(\omega)|^2 \left[S_n^{\text{th}}(\omega) + S_n^{\text{act}}(\omega) \right]$$

- **If we can calculate the active force-force correlations we will be able to get a form of variance of tangent mode amplitude.**

Theoretical framework

- From microscopic picture of active particles

$$C_{\alpha\beta}(\Delta\mathbf{r},\Delta t) = \rho_0 V_0^2 \sigma^{2d} \left(\frac{\pi}{A(\Delta t)}\right)^{d/2} \left[\frac{\delta_{\alpha\beta}}{2A(\Delta t)} - \frac{\Delta r_\alpha \Delta r_\beta}{4A(\Delta t)^2}\right] \exp\left[-\frac{|\Delta\mathbf{r}|^2}{4A(\Delta t)}\right],$$

- With some further approximations

$$\left\langle \xi_n^{u,\mathrm{act}}(t)\, \xi_m^{u,\mathrm{act}}(t')\right\rangle = \delta_{nm}\, q_n^2 D_0\, e^{-q_n^2\sigma^2}\, e^{-|\Delta t|/\tau_{\mathrm{eff}}}.$$

- And therefore
- $S_n^{\mathrm{act}}(\omega) = q_n^2 D_0 e^{-q_n^2\sigma^2} \dfrac{2\tau_{\mathrm{eff}}}{1+\omega^2\tau_{\mathrm{eff}}^2}.$

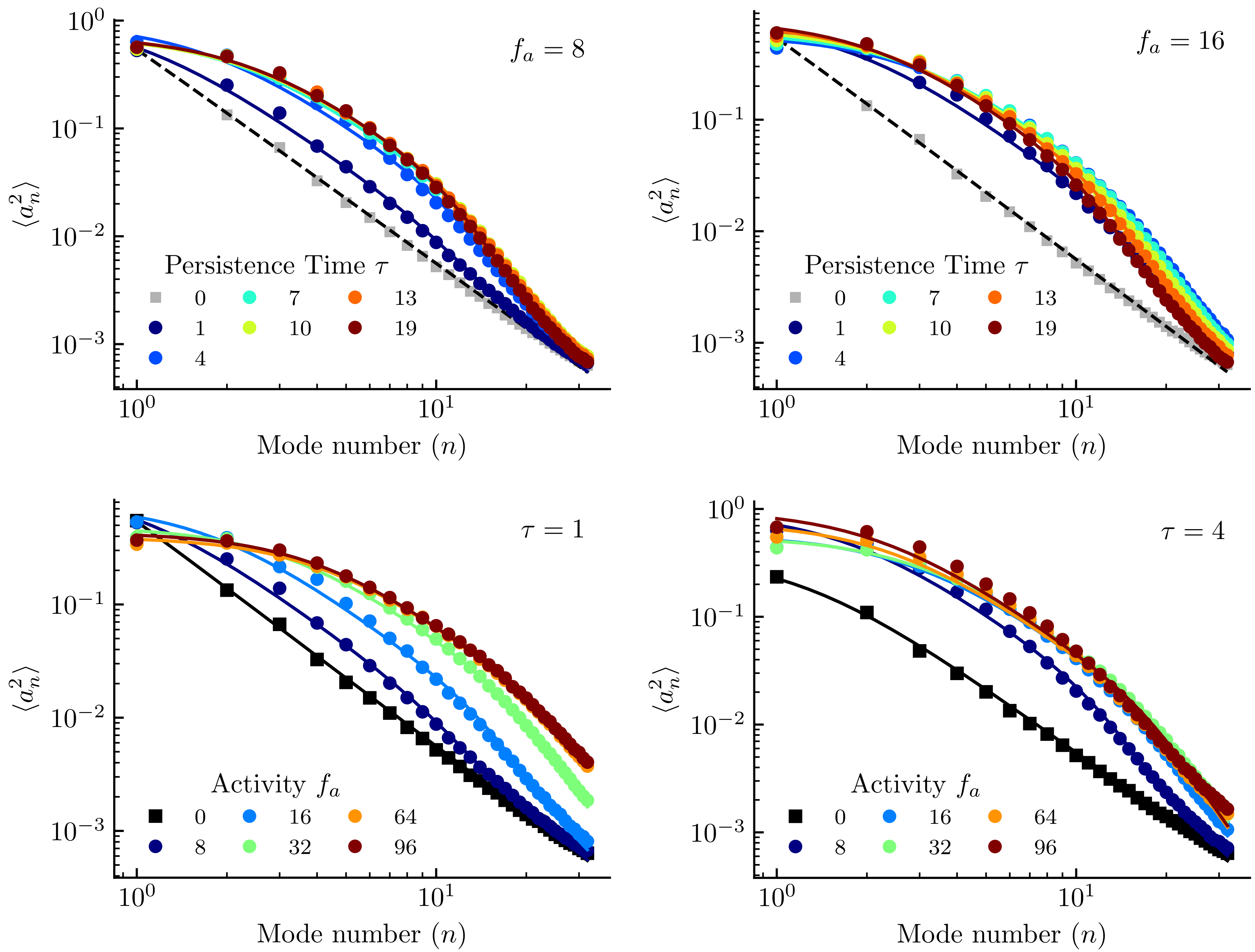
- The variance is finally:

$$\langle |a_n|^2\rangle = \frac{1}{\kappa q_n^2}\left[k_B T + \frac{D_0\tau_{\mathrm{eff}}}{\zeta\,[1+\tau_{\mathrm{eff}}\omega_n]} e^{-q_n^2\sigma^2}\right]$$

Further a mode dependent temperature can also be defined here:

$$T_n^{\mathrm{eff}} = T + \frac{D_0\tau_{\mathrm{eff}}}{k_B\zeta\,[1+\tau_{\mathrm{eff}}\kappa q_n^4/\zeta]} e^{-q_n^2\sigma^2}.$$

Semiflexible polymer in active bath

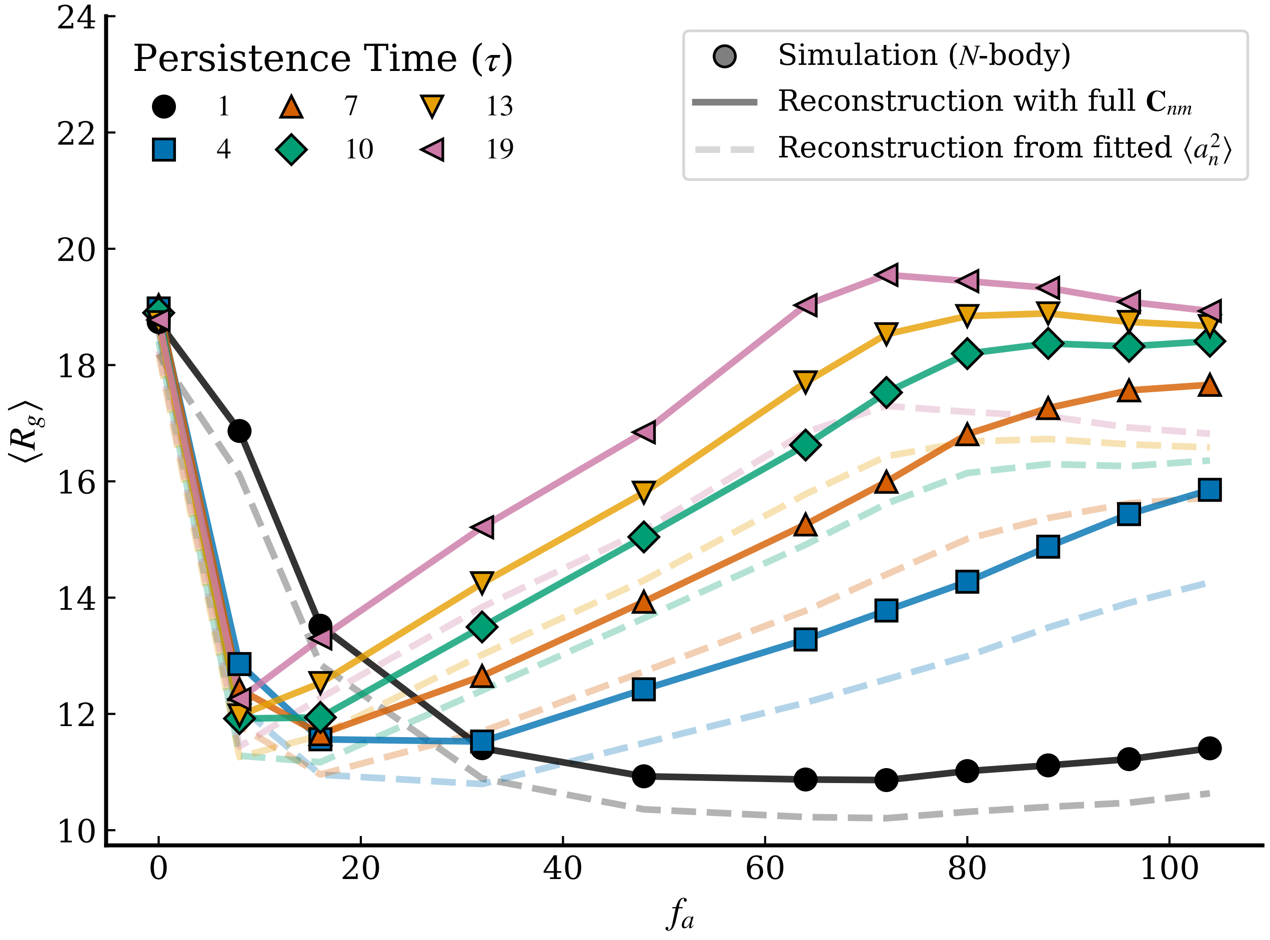


$$\langle |a_n|^2 \rangle = \frac{1}{\kappa q_n^2 + \mathcal{T}} \left[k_B T + \frac{D_0 \tau_{\text{eff}}}{\zeta \left[1 + \tau_{\text{eff}} \omega_n(\mathcal{T}) \right]} e^{-q_n^2 \sigma^2} \right]$$

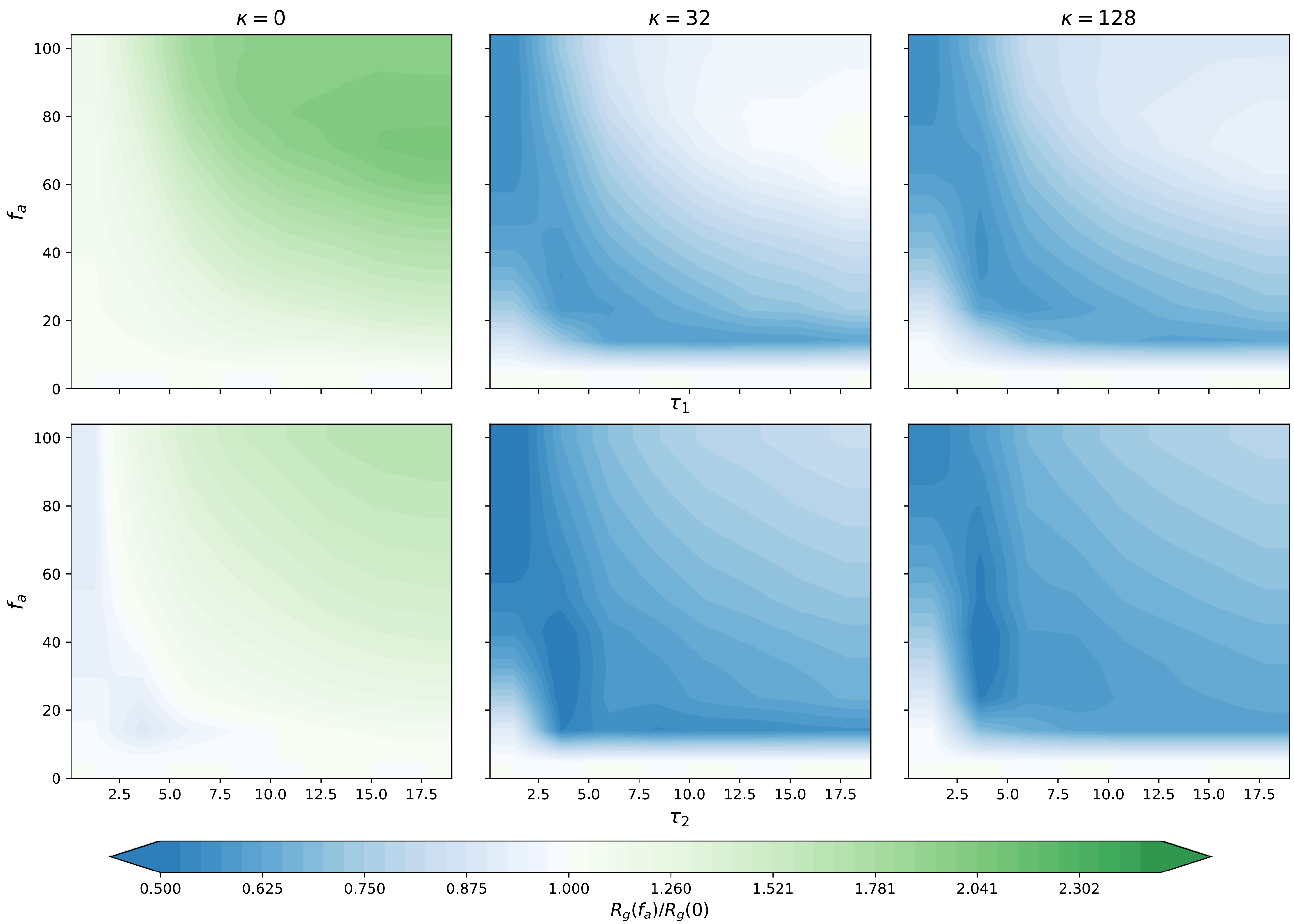
R_g reconstruction using mode variance

- Radius of gyration of polymer can be written as:
  $$R_g^2 = \frac{1}{(N+1)^2} \sum_{i=0}^{N} \sum_{j=i+1}^{N} \left\langle |\mathbf{r}_j - \mathbf{r}_i|^2 \right\rangle .$$
- We can expand the bond vector in discrete cosine basis
  $$\Delta \mathbf{r}_k = \frac{1}{2}\mathbf{b}_0 + \sum_{n=1}^{N-1} \mathbf{b}_n \cos\left[\frac{n\pi}{N}\left(k+\frac{1}{2}\right)\right]$$
- $$R_g^2 = W_{00}\langle \mathbf{b}_0 \cdot \mathbf{b}_0 \rangle + \sum_{n \geq 1} W_{nn} \langle \mathbf{b}_n \cdot \mathbf{b}_n \rangle + \sum_{n \geq 1} W_{0n} \langle \mathbf{b}_0 \cdot \mathbf{b}_n \rangle + \sum_{n<m} W_{nm} \langle \mathbf{b}_n \cdot \mathbf{b}_m \rangle .$$

R_g reconstruction using mode variance



R_g comparison of explicit vs implicit bath



Limitations & Caveats

- Due to high active force and long persistent time the bond angle stretched is a factor that needed to be accounted further.
- The spatial correlations are not considered completely.
- With our theory which is with weak bending limit the reconstruction of R_g is systematically lesser than the actual R_g.
- Assumption that the different modes decouple.

Acknowledgement

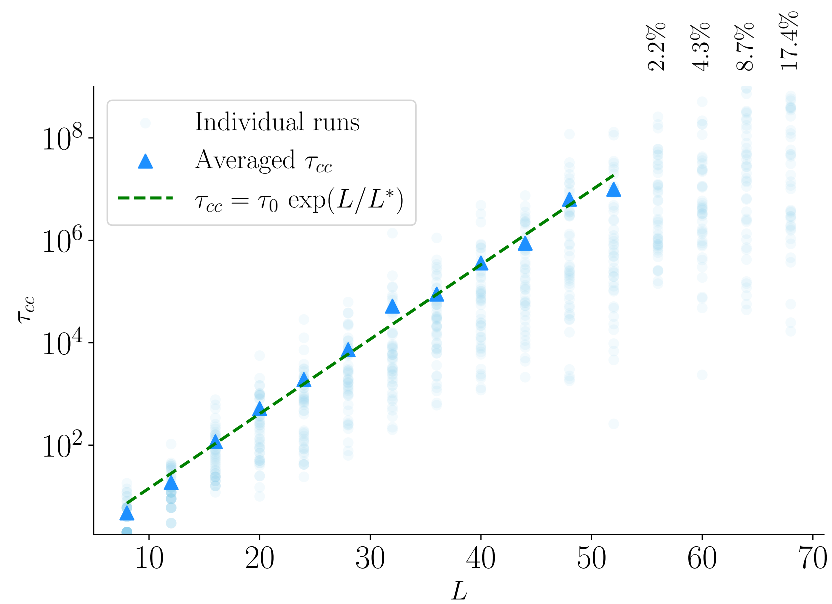
- I would like to express my sincere gratitude to all my teachers for their guidance and support throughout my academic journey. I am especially thankful to my supervisor **Prof. Abhishek Chaudhuri** and **Prof. Rajeev Kapri**, & **Dr. Anil Kumar Dasanna** for their invaluable mentorship and insights.
- I am deeply grateful to my parents for their unwavering belief in me and constant encouragement.
- I would also like to thank my wife for her support, patience, and understanding.
- I would also like to thank my Brother Kush Grover for supporting me throughout.
- Finally, I thank all my group members for their collaboration, discussions, and support, especially **B K, Dr. Sandip Roy, and Joydeep**.

Thank you :)

Questions?

Slow Coarsening and Large Cluster movements

- {+,+,-,-}



- {-,-,-,+}