ACTIVITY MODULATION MITIGATES DENSITY FLUCTUATIONS IN ACTIVE SIMULATIONS

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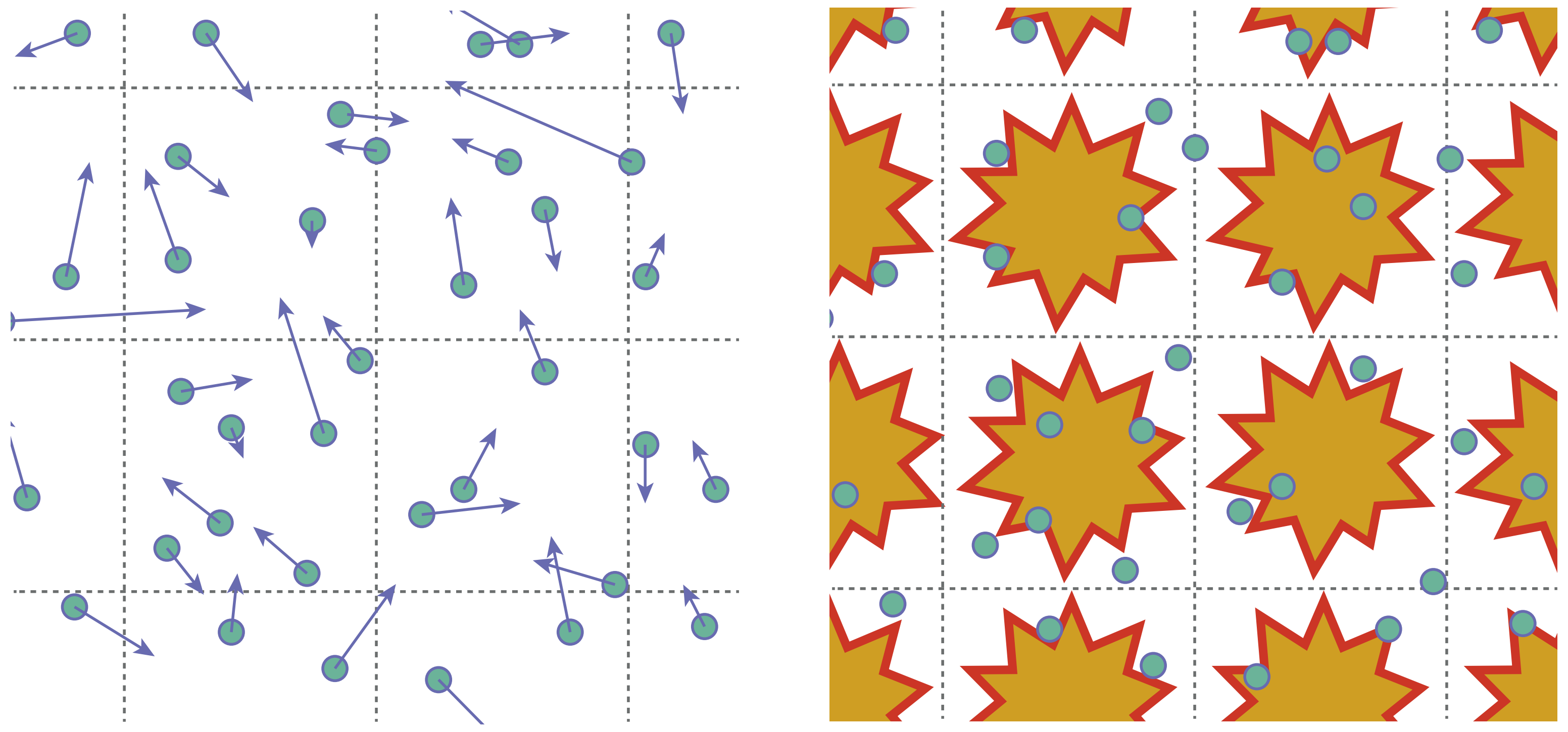
Motivation

- Self-propelled particles exhibit flocking and motility-induced density fluctuations
- Hydrodynamic solvers reproduce active turbulence and defect dynamics
- Mesoscopic algorithms bridge microscopic and continuum
- Useful for simulating suspensions [1]
- Mitigation of density fluctuations in mesoscale models can expand their scope

Multi-Particle Collision Dynamics (MPCD)

- Particles i stream ballistically, then are binned into grid cells
- Collision operators act on cells c, encoding system dynamics



Streaming

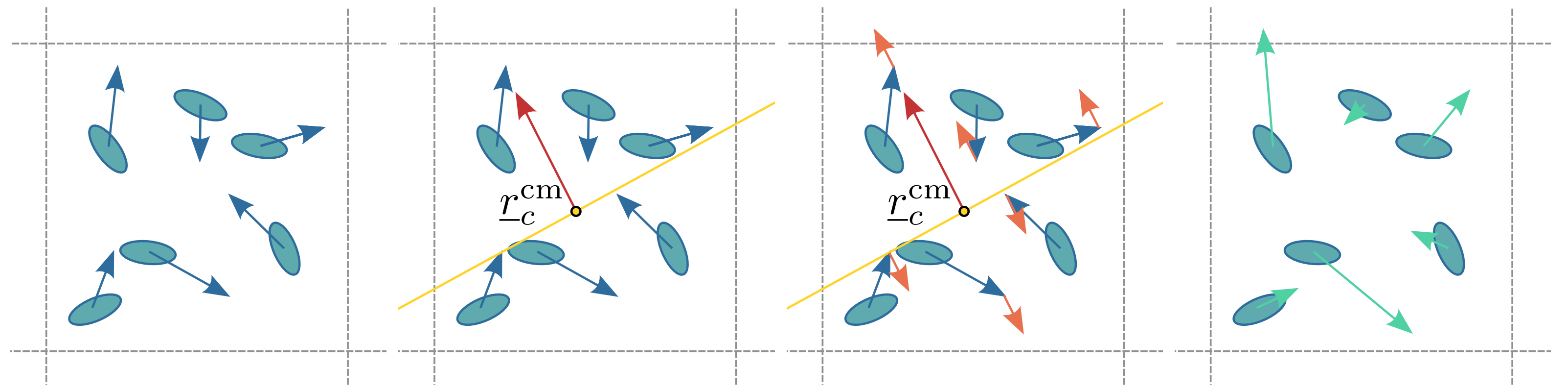
$$\underline{r}_i(t+\delta t) = \underline{r}_i(t) + \underline{v}_i(t)\delta t$$

Collision

$$\underline{v}_i(t+\delta t) = \underline{v}_c^{\mathrm{cm}}(t) + \underline{\Xi}_{i,c}$$

Active-Nematic MPCD (AN-MPCD)

- Utilises nematic collision operator $\Xi^0_{i,c}$ [2]
- Applies local force dipoles, with cellular strength α_c due to particle activity α_i
- Locally injects energy but conserves momentum
- Sufficient for **both** active nematic turbulence and density fluctuations [3]



$$\Xi_{i,c} = \Xi^0_{i,c} + \delta t\ \alpha_c \left(\frac{\kappa_i}{m_i} - \left\langle \frac{\kappa_j}{m_j} \right\rangle_c \right) \underline{n}_c \quad ; \qquad \alpha_c = \sum_{i=1}^{\rho_c} \alpha_i \overset{\text{const.act.}}{=} \rho_c \alpha$$

References

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4. Kozhukhov, Loewe & Shendruk. *In Prep.* (2023).
5. Ramaswamy, Simha & Toner. *EPL* **62,** 196–202 (2003).

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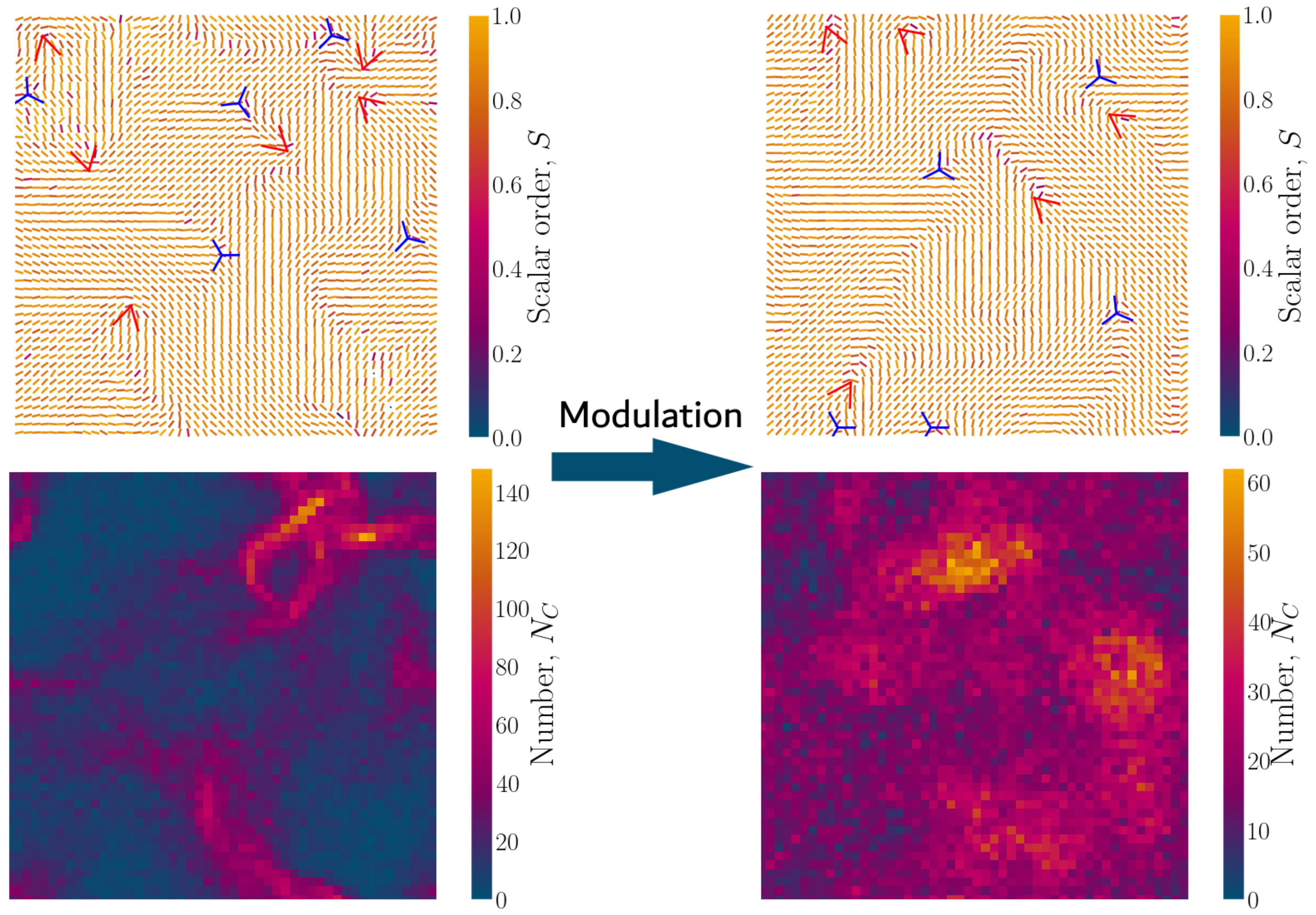
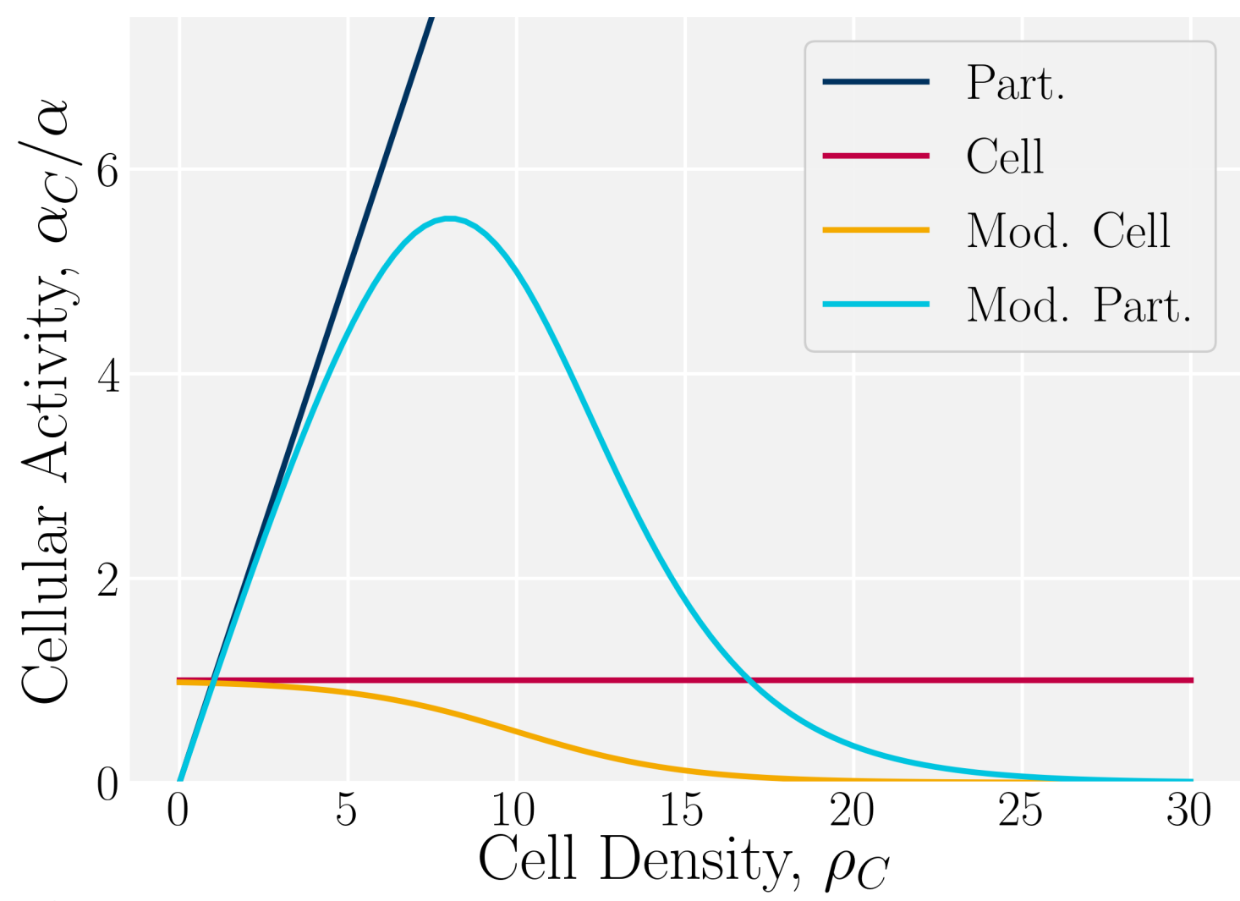


Density control through activity modulation

Modulate activity through dipole strength α_c to reduce density variations [4]:

- Denote original **linearly increasing** formulation as *particle-carried* activity, α_c^{P}
- Averaging by local density gives **constant** *cell-carried activity*, α_c^{C}
- Modulate α_c^{P} and α_c^{C} smoothly **down to zero**, giving *modulated particle-carried* activity α_c^{MP} and *modulated cell-carried* activity α_c^{MC}



$\langle\rho_C\rangle = 5.0,\ \sigma_p = 1.0,\ \sigma_w = 1.0$

- Part.: $\alpha_c^{\mathrm{P}} = \sum_{i=1}^{\rho_c} \alpha_i$
- Cell: $\alpha_c^{\mathrm{C}} = \frac{1}{\rho_c}\alpha_c^{\mathrm{P}}$
- Sigmoidal modulation:

$$\mathcal{S}_c(\rho_c; \sigma_{\mathrm{w}}, \sigma_{\mathrm{p}}) = \frac{1}{2}\left(1 - \tanh\left(\frac{\rho_c - \langle\rho_c\rangle(1+\sigma_{\mathrm{p}})}{\langle\rho_c\rangle\,\sigma_{\mathrm{w}}}\right)\right)$$

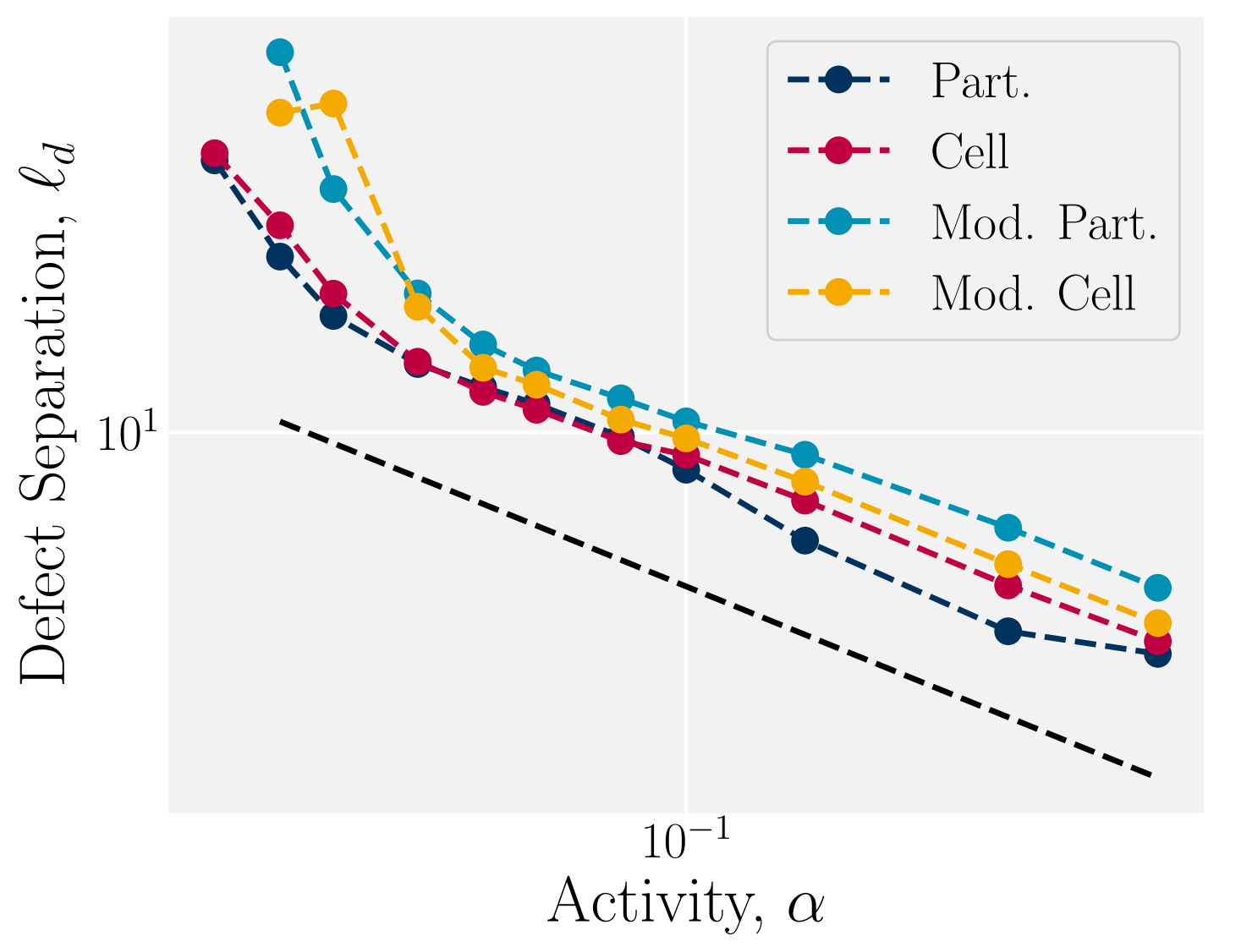
giving:

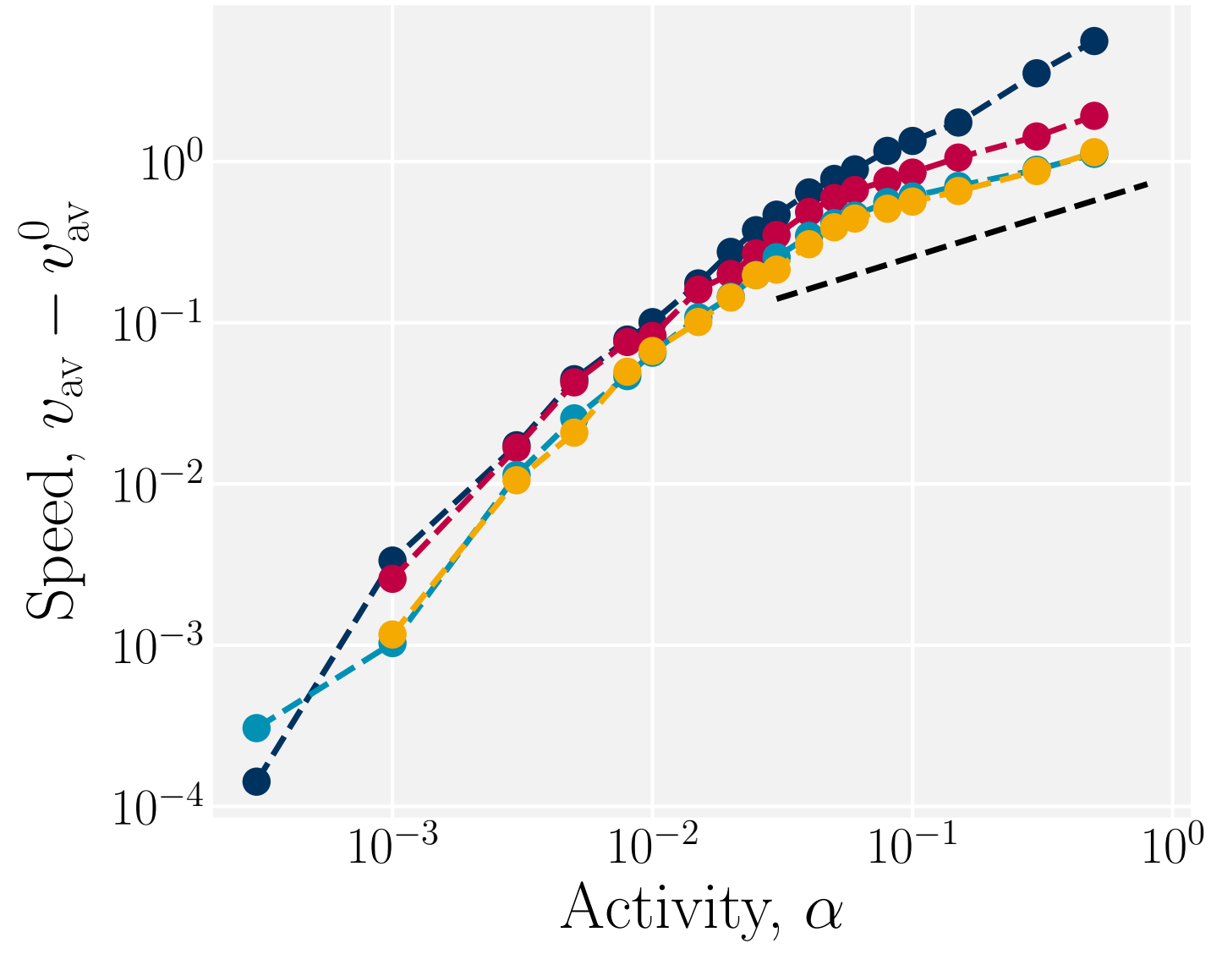
- Mod. Cell: $\alpha_c^{\mathrm{MC}} = \alpha_c^{\mathrm{C}}\mathcal{S}_c(\rho_c)$
- Mod. Part.: $\alpha_c^{\mathrm{MP}} = \alpha_c^{\mathrm{P}}\mathcal{S}_c(\rho_c)$

Active turbulence in AN-MPCD

AN-MPCD reproduces active turbulence [3] for suitable activities:

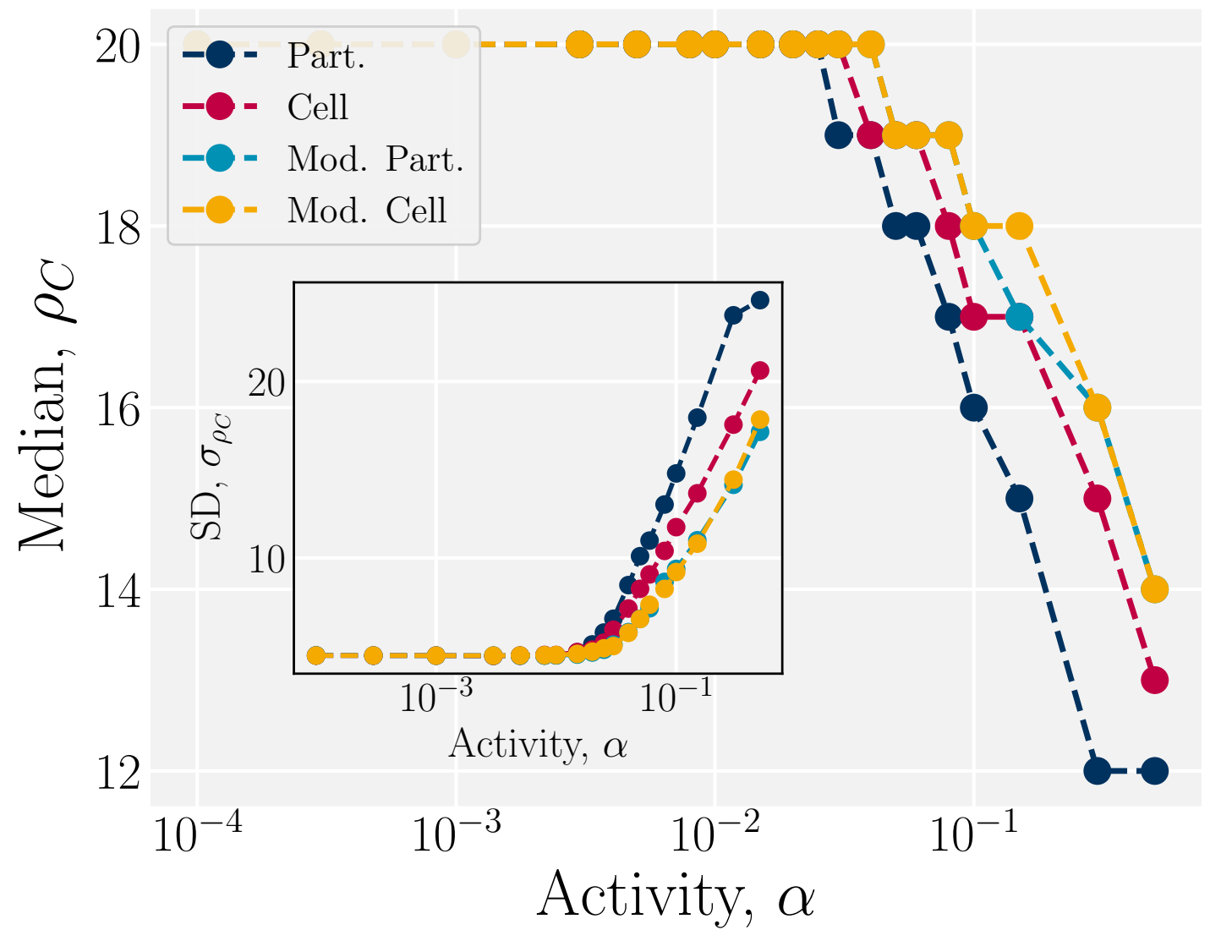
- Defect separation scales as $\ell_{\mathrm{d}} \sim \alpha^{-1/2}$
- Speed scales as $v_{\mathrm{av}} \sim \alpha^{1/2}$

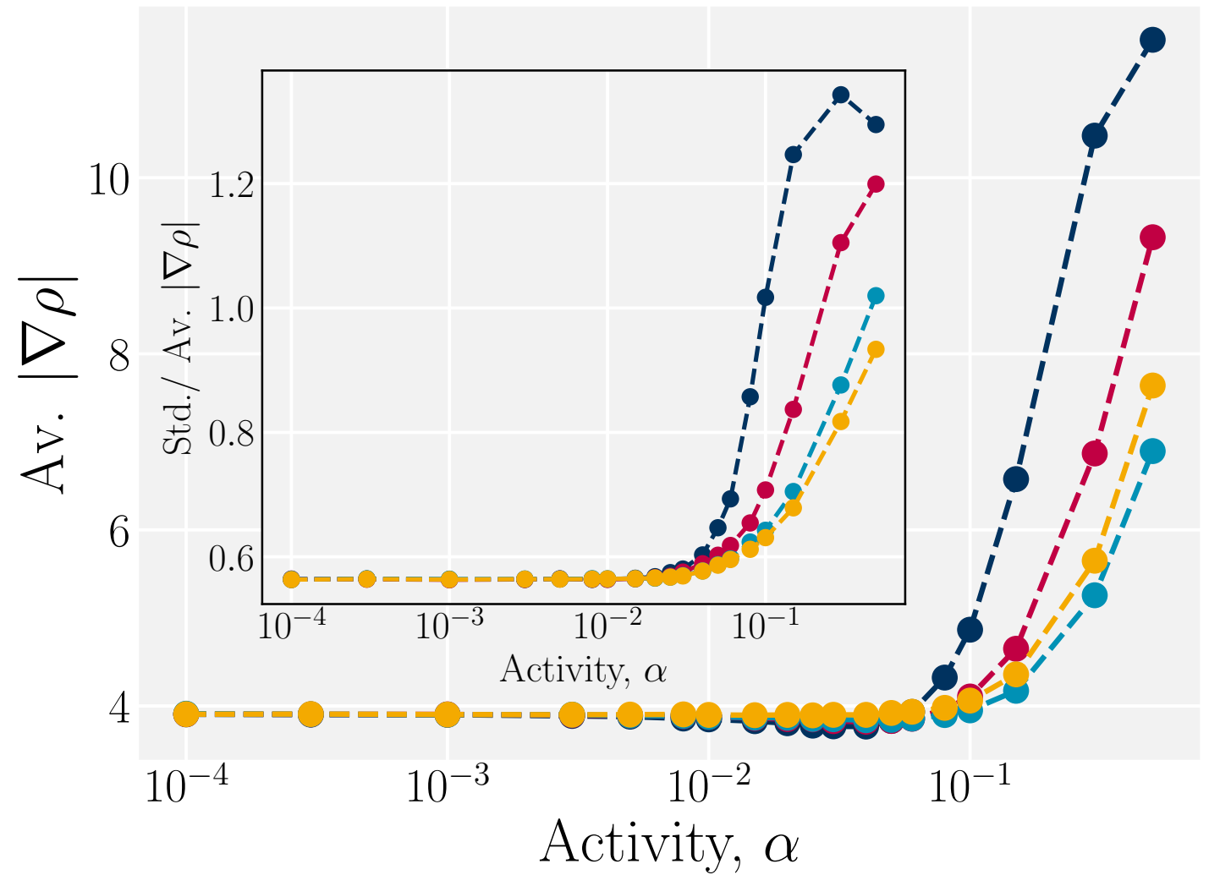




Modulation decreases density fluctuations

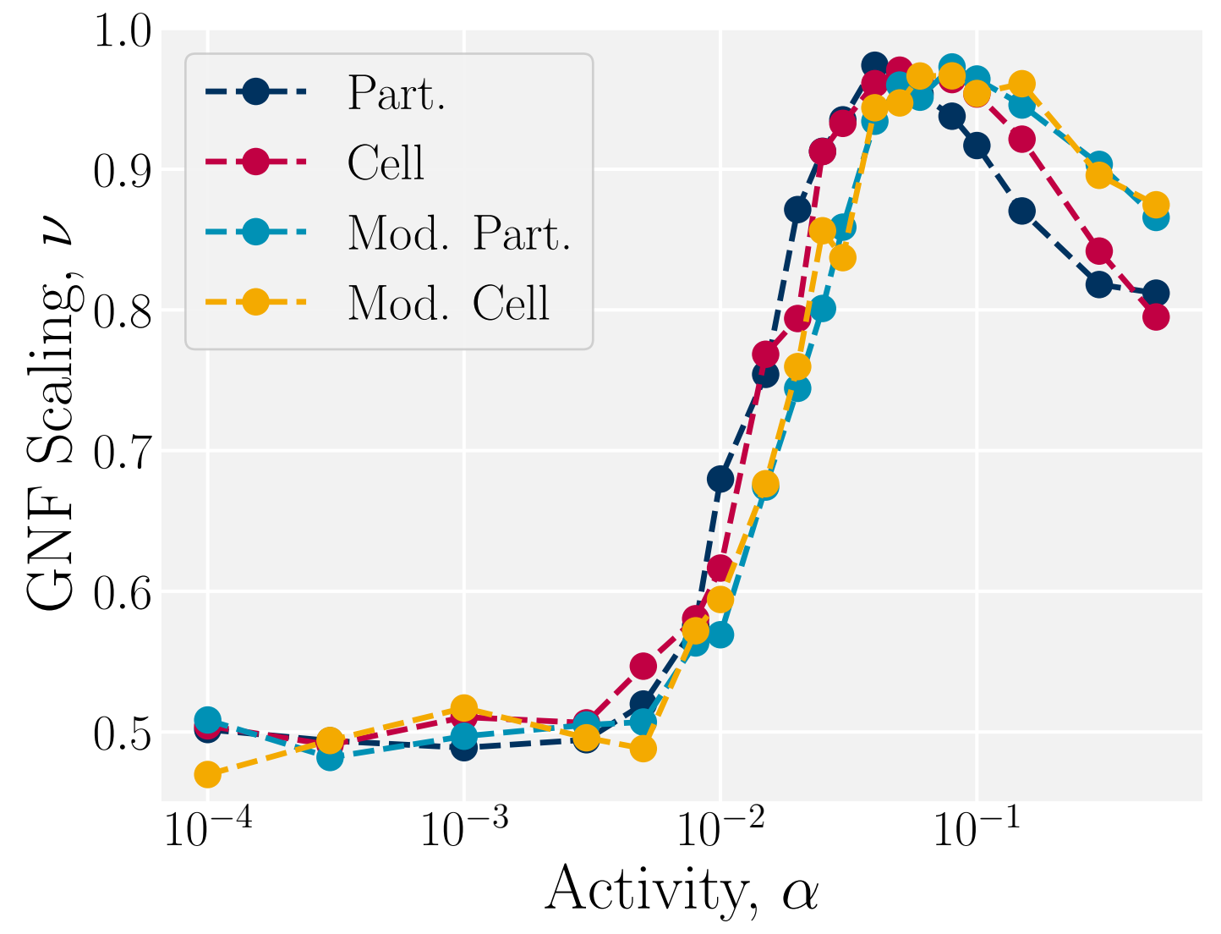
- Density fluctuations decrease with modulation
- $\sigma_{\mathrm{w}} = 0.5$, $\sigma_{\mathrm{p}} = 0.4$ are particularly effective:
  - While systems get more dilute, standard deviations of density remain at the passive limit for larger activities
  - Fickian diffusive flux ($\sim \nabla\rho$), remains constant for larger activities

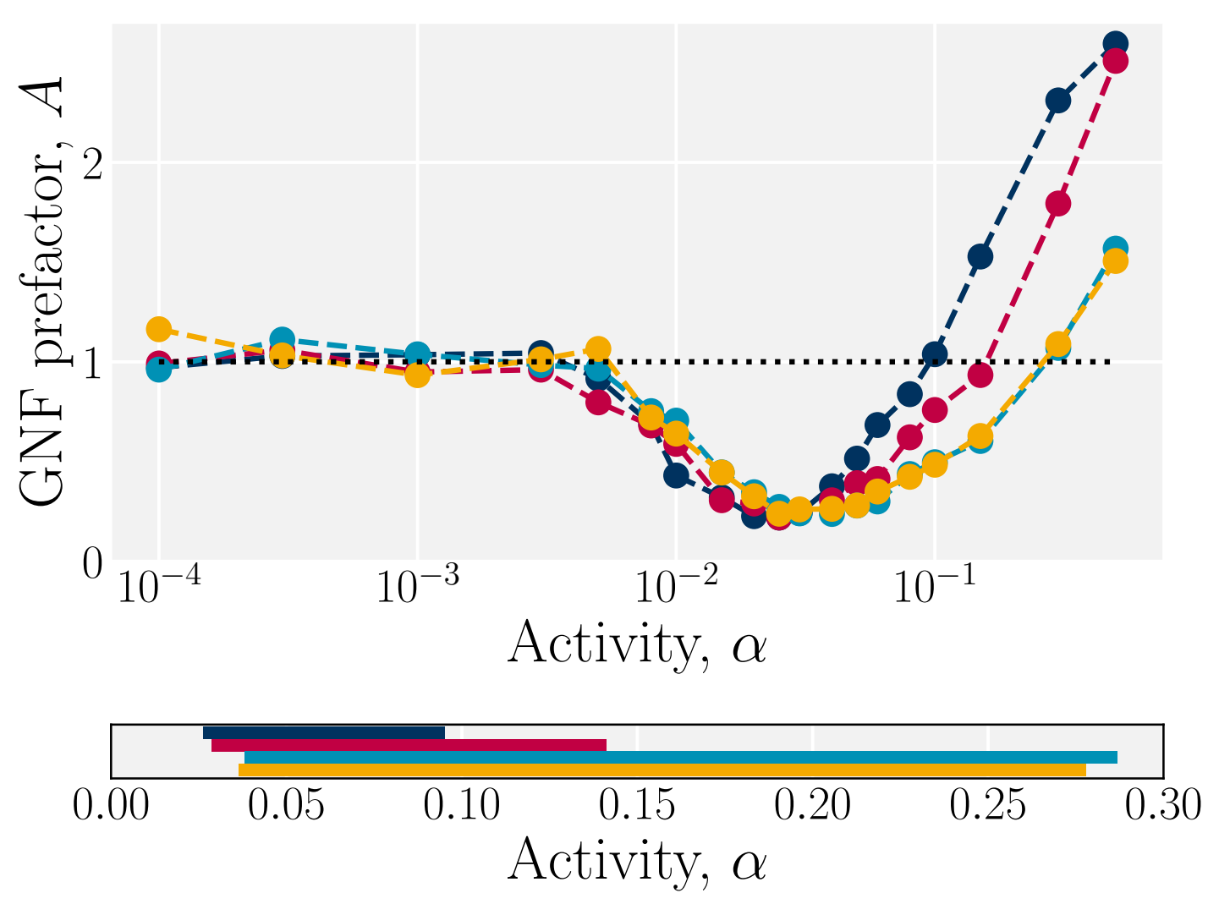




Number fluctuations reveal algorithm regimes

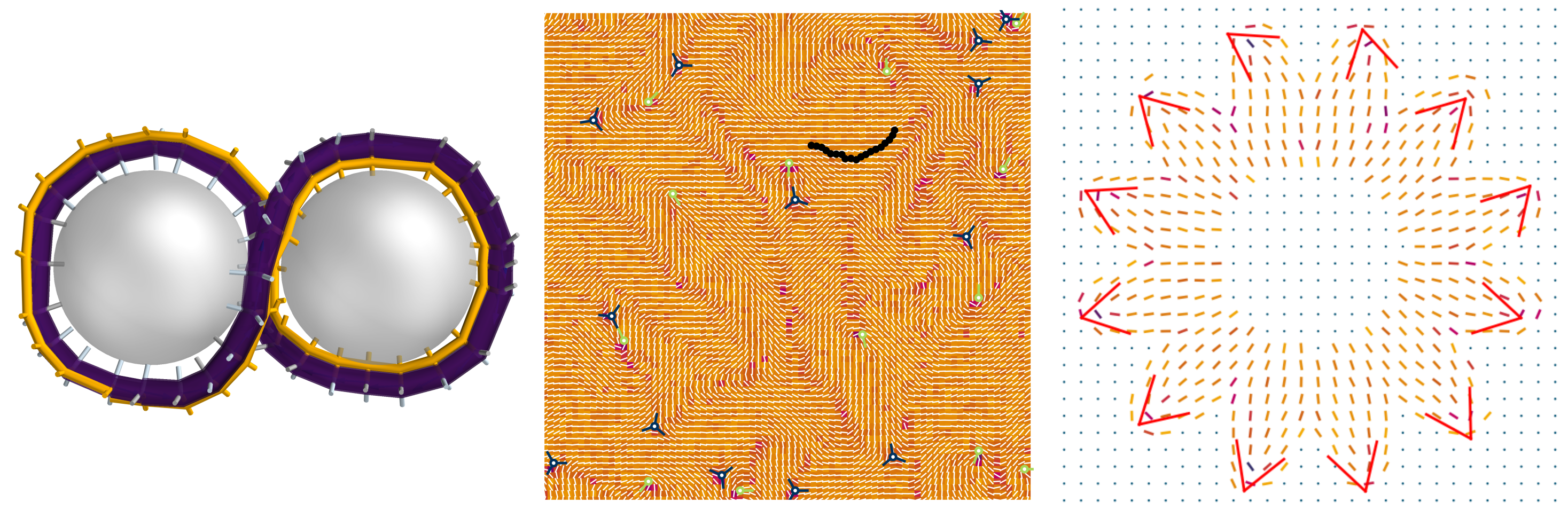
- As a particle-based method, “giant number-fluctuations” must remain [5]
- Scaling of fluctuations $\sigma_\rho(\rho) = A\alpha^\nu$, shows no change
- The prefactor A reveals extended turbulence regimes for new formulations





Conclusions and outlook

- AN-MPCD proves to be an exciting method to study active nematics with
  - complex solutes*
  - confined geometries*



* Figures courtesy of L. Head, Z. Valei, B. Loewe