A Mesoscopic Method for Simulating Active-Nematics

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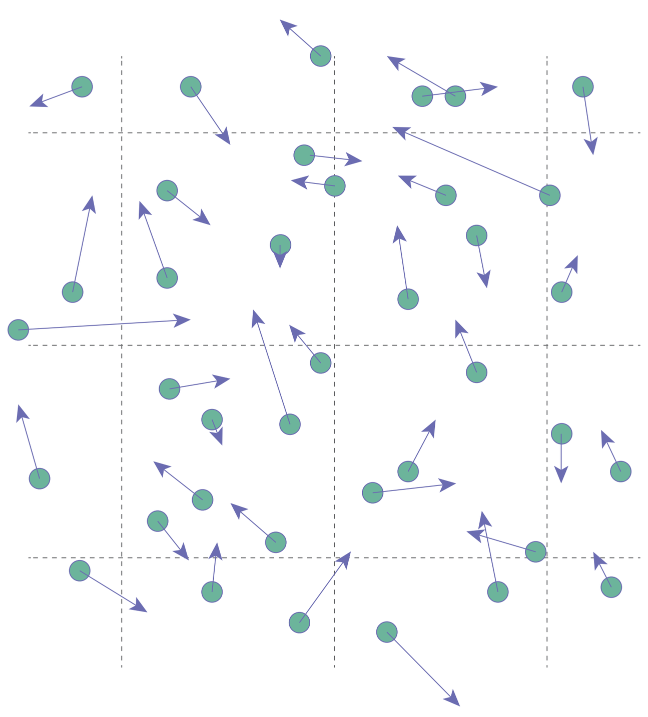
Motivation

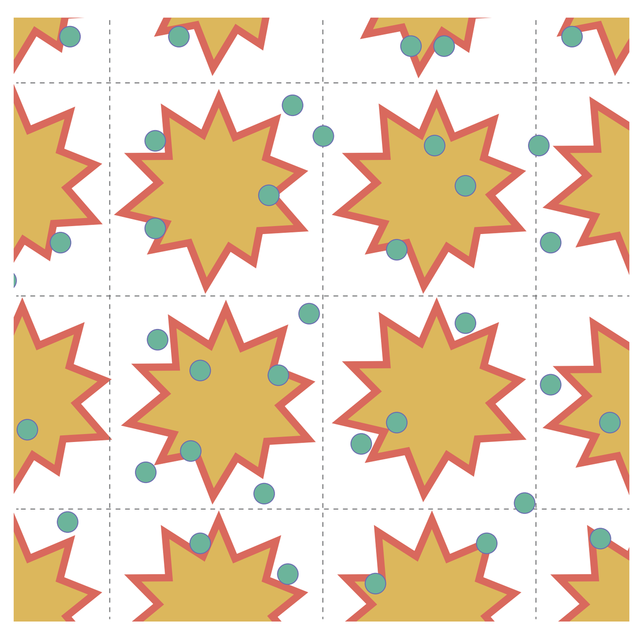
- Mesoscopic algorithms bridge microscopic and continuum, particularly good for fluids with suspensions [1]
- Development of mesoscopic algorithms for active nematic fluids is lacking

Multi-Particle Collision Dynamics

- Particles stream ballistically then binned into grid cells
- Collision operators acting on cells encode dynamics



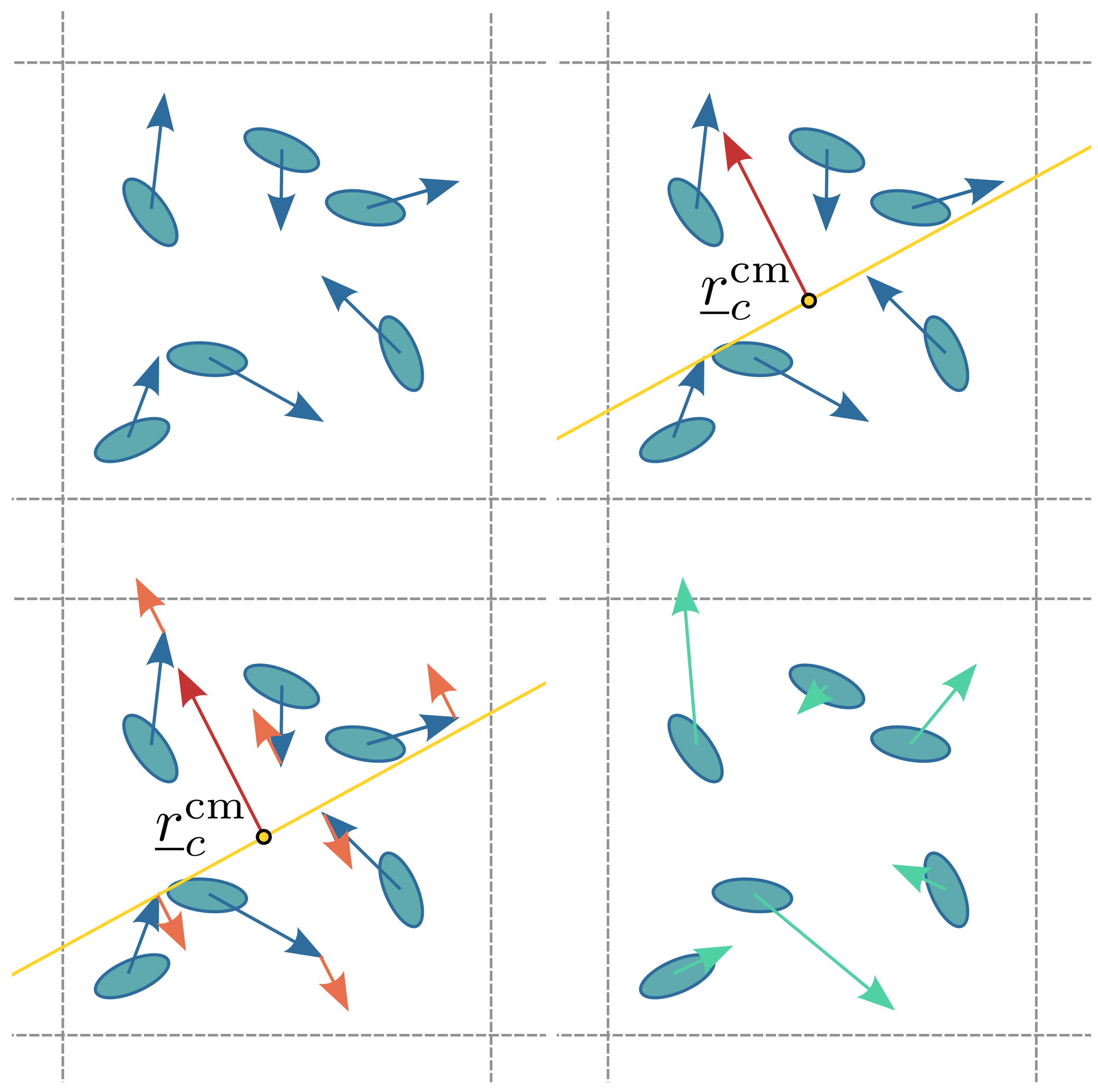
$\underline{r}_i(t+\delta t) = \underline{r}_i(t) + \underline{v}_i(t)\delta t$



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

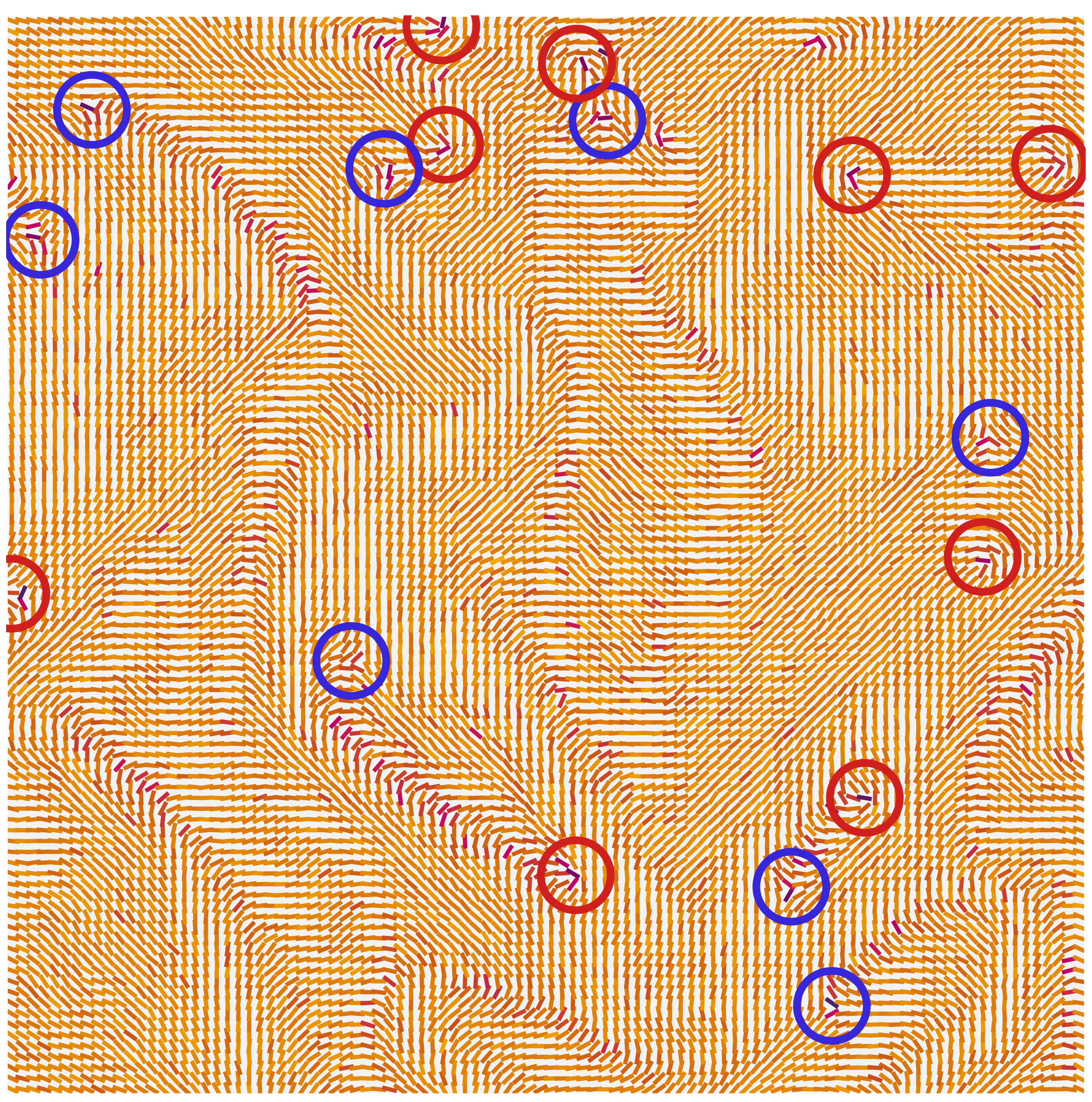
Active-Nematic MPCD

- Start after nematic collision operator by Shendruk and Yeomans [2] is applied, labelled $\Xi^0_{i,c}$
- Force dipole added, producing Active-Nematic MPCD (AN-MPCD)

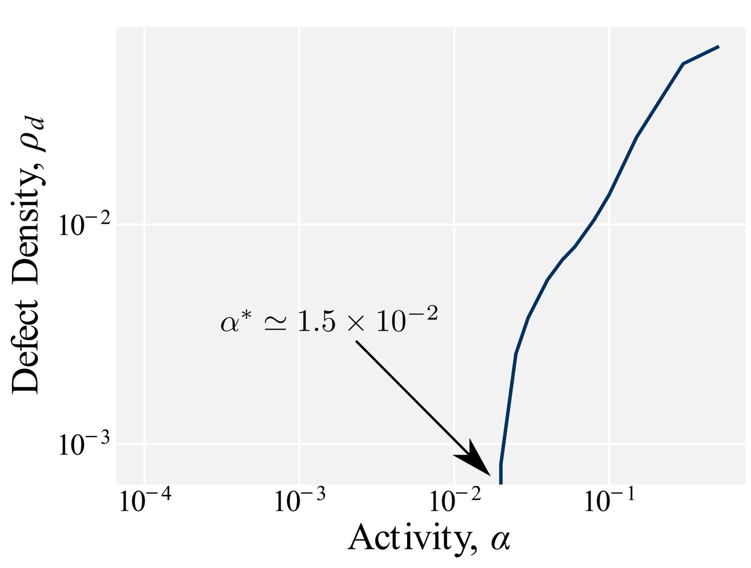


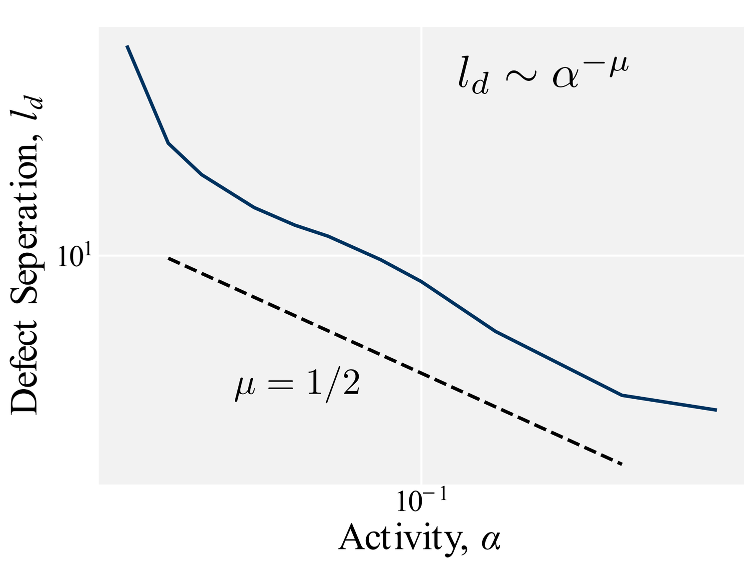
$$\Xi_{i,c} = \Xi^0_{i,c} + \delta t\ \alpha_c \left(\kappa_i - \langle \kappa_j \rangle_c\right) \underline{n}_c$$

Active Turbulence: Defects

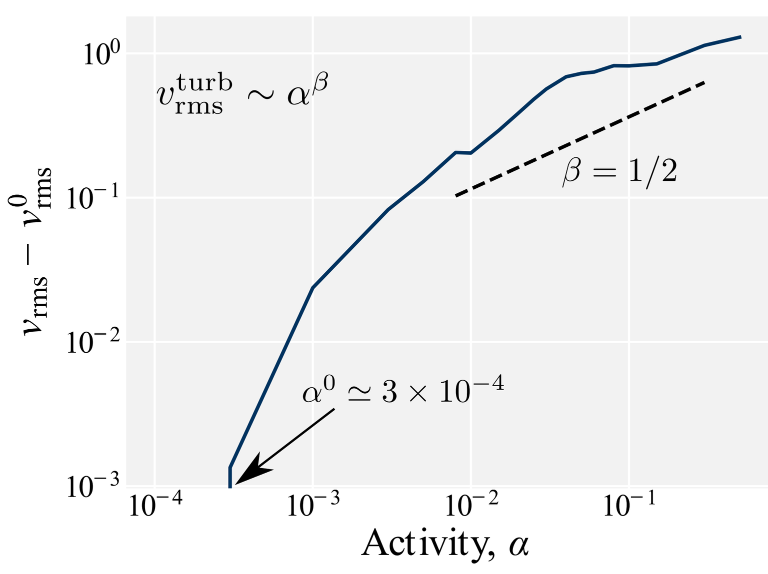


- Continuous pair creation & annihilation of $+1/2$ and $-1/2$ defects is a key feature of active turbulence
- $\alpha^* \lesssim \alpha$: Produces non-zero defect density ρ_d
- In this regime defect the scaling of seperation length scale $l_d = \rho_d^{-1/2}$ agrees with theory





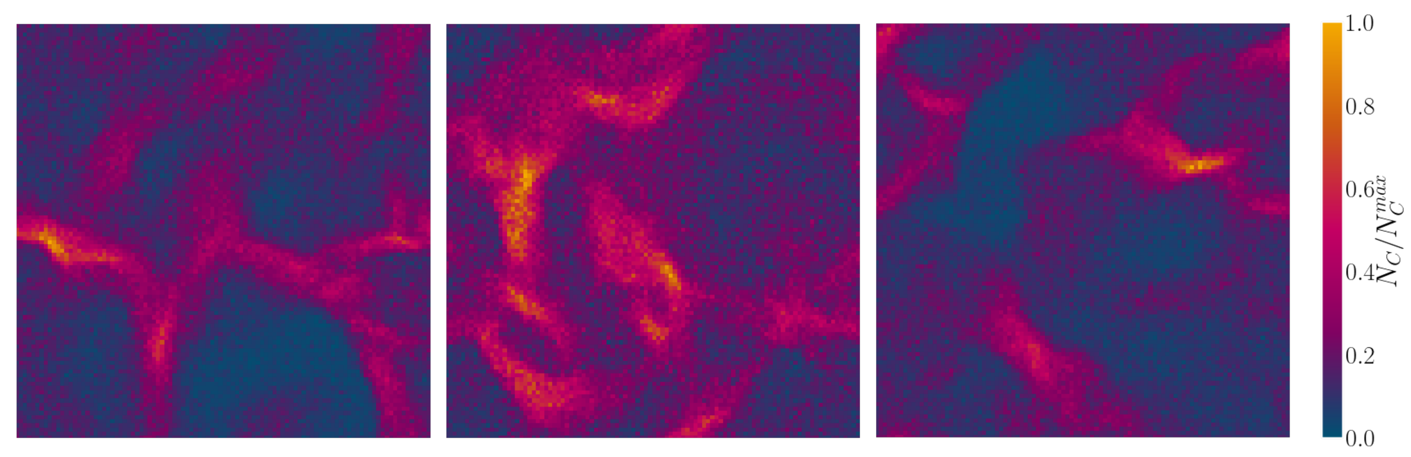
Active Turbulence: Velocity



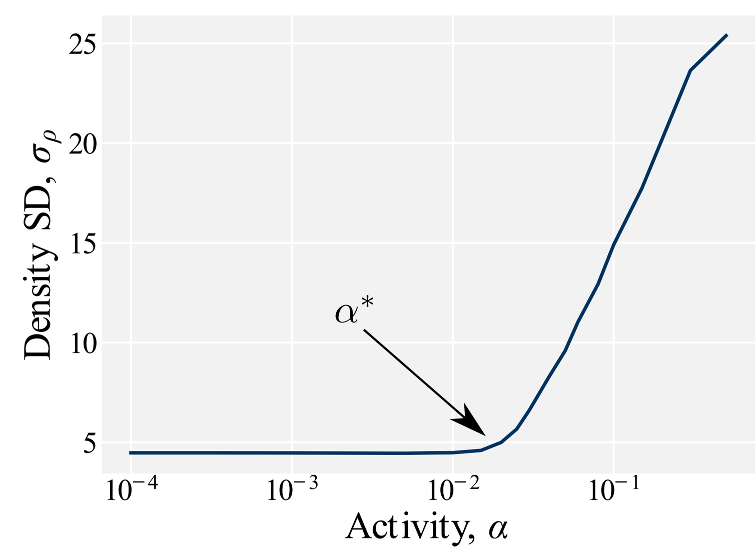
Three regimes:

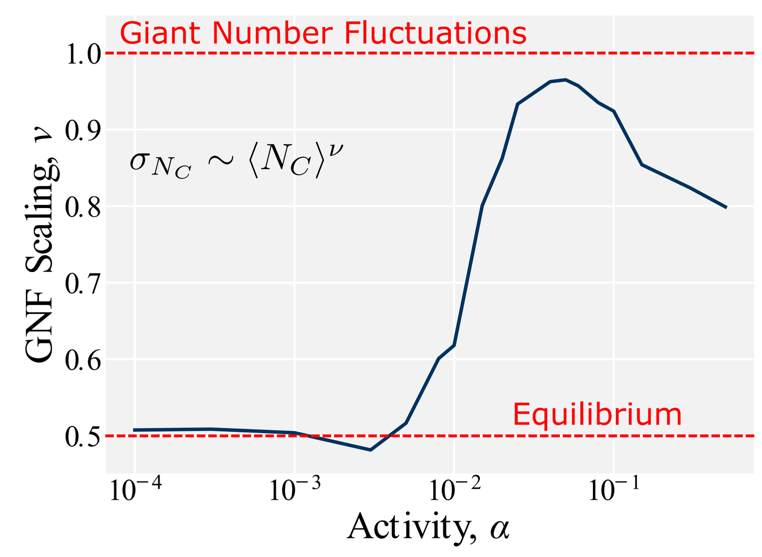
- $\alpha \lesssim \alpha^0$: MPCD absorbs active energy injection
- $\alpha^0 \lesssim \alpha \lesssim \alpha^*$: Scales faster than expected
- $\alpha^* \lesssim \alpha$: Expected scaling for active turbulence

Density Fluctuations



- In AN-MPCD these appear very similar to [3], another particle based algorithm
- Density distribution widens, and giant-number fluctuations at large α





Conclusion & Outlook

- AN-MPCD recreates active turbulence for $\alpha^* \lesssim \alpha$
- AN-MPCD exhibits density fluctuations [4]
- Can be applied to systems with complex solutes

References

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