Time-resolved transfer entropy dynamics between particle heading deviations in simulated active matter flocks

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Active-matter research has flourished over the last two decades, as evidenced by the growing number of publications tackling both field and laboratory experiments, as well as mathematical modeling and computer simulations.

One of the many applications that will benefit from an improved understanding of active-matter systems is the control and optimization of smart materials (e.g. micro/nanorobotic swarms) designed to perform collective tasks such as targeted drug delivery, environmental treatment, and optimal space exploration.

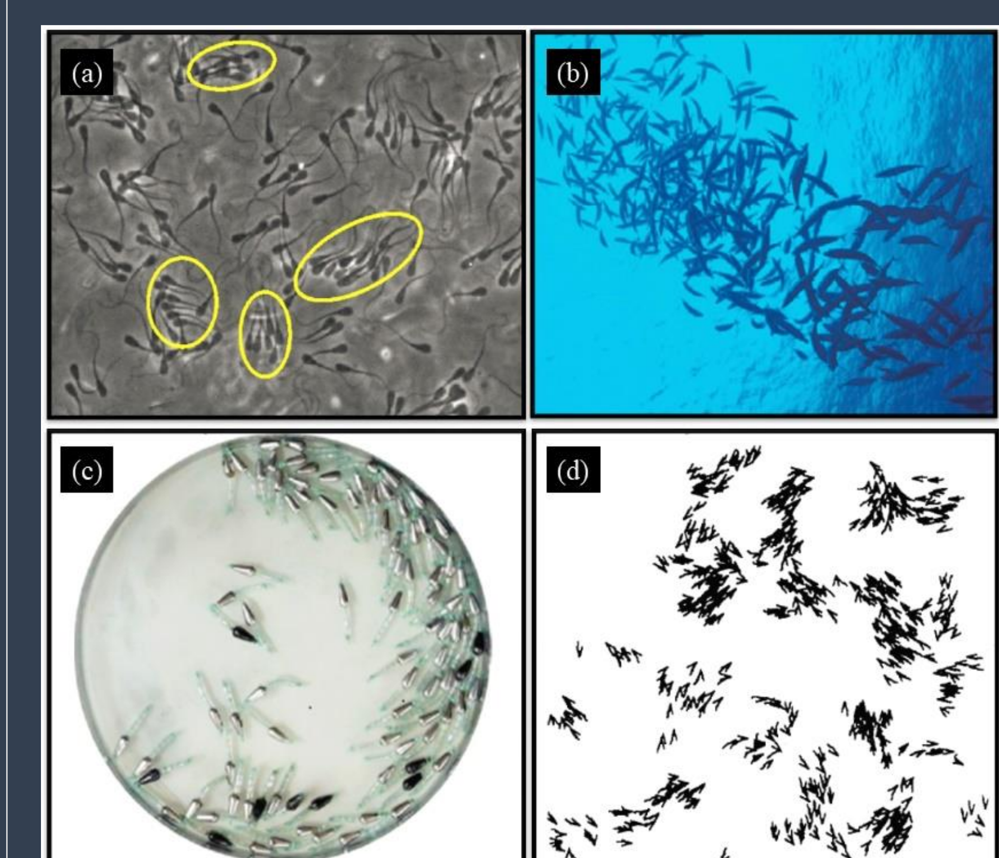

Fig.1. Examples of different active systems with complex behaviors that have been studied in recent years: (a) sperms that swarm collectively and form clusters in Newtonian and viscoelastic fluids, ; (b) poor collective motion patterns in fish schools; (c) experiment snapshot depicting global circulation of bio-inspired active particles,; and (d) Vicsek particles at low-density and noise values, forming small clusters that move coherently in random directions.

In this study, we characterize the time evolution of an active-matter system generated via Standard Vicsek Model (SVM) that is composed by two equations for updating the trajectory and heading of particles as defined below;

$$\vec{\boldsymbol{r}}_i(t+\Delta t) = \vec{r}_i(t) + \bar{v}_i(t)\Delta t$$
$$\theta_i(t+\Delta t) = \bar{\theta}_t(t) + \Delta\theta$$

where $\bar{\mathbf{v}}_i(t)$ is *neighborhood-average velocity* of particle i defined by the equation

$$\bar{\mathbf{v}}_i(t) = |z_i(t)|^{-1}\sum_{j\in z_i(t)}\vec{\mathbf{v}}_j(t)$$

and $\bar{\theta}_t(t)$ as the *average direction* of the particles defined by the equation

$$\bar{\theta}_t(t) = \tan^{-1}\left(\frac{\sin\bar{\theta}_t(t)}{\cos\bar{\theta}_t(t)}\right) = \tan^{-1}\left(\frac{\bar{v}_y(t)}{\bar{v}_x(t)}\right).$$

The $\Delta\theta$ represents the noise or perturbation in the system that is a random number picked with a uniform probability defined from the interval $[-\eta/2, \eta/2]$ with intensity $\eta \in (0, 2\pi)$. The particles in the model interacts by aligning their direction to that of their close neighbors at a radius. To quantify the individual heading deviations of a particle, we have adapted the directional correlation metric used by Attanasi et.al as defined by the equation ,

$$C_i(t) = \frac{\boldsymbol{v}_i(t)}{v_i(t)} \cdot \frac{\boldsymbol{V}(t)}{V(t)}.$$

We used the method of transfer entropy (in terms of joint probabilities), a time asymmetric measure of information transfer defined by the equation

$$T_{A\to B} = \sum_t p(b_{t+1}, b_t, b_t) log \frac{p(b_{t+1}, b_t, a_t)p(b_t)}{p(b_{t+1}, b_t)p(b_t, a_t)}.$$

To measure the strength of asymmetric information flow, we get the net transfer entropy defined by the expression

$$|T_{\text{net}}| = T(C_B \to C_A) - T(C_A \to C_B).$$

We examined a total of 400 independent SVM simulations by keeping the linear size and radius of interaction constant but varying the noise intensity η = {0.1, 0.2, …, 1.0} and number of particles N = {5, 10, …, 200} or equivalently, particle density $\rho \equiv N/L^2$ = {0.0125, 0.025, …, 0.5}. Over the course of 50,000 timesteps, we partition the entire data file into non-overlapping 5000-point epochs, and then estimate the pairwise transfer entropies $T(C_B \to C_A)$ and $T(C_A \to C_B)$, and the net transfer entropy $|T_{\text{net}}| = T(C_B \to C_A) - T(C_A \to C_B)$ for each unique pair of particles A and B. Given that the total number U_{AB} of unique particle pairs in a system is $N!/(2(N-2)!)$, we find the maximum $|T_{\text{net}}|$ for each epoch across varying U_{AB}, e.g., 10 pairs for N = 5 and 19,900 pairs for N = 200.

Rigorous time series analyses shown that the strength of information flow or interactions between particles—as quantified by max $|T_{\text{net}}|$—is influenced by the noise intensity η and density ρ of the flock. In particular, for a given η, we find that the relationship between $|T_{\text{net}}|$ and ρ can be approximated by a power law, i.e., $|T_{\text{net}}| = c\rho^{\alpha}$ where α is the power law exponent and c is a constant.

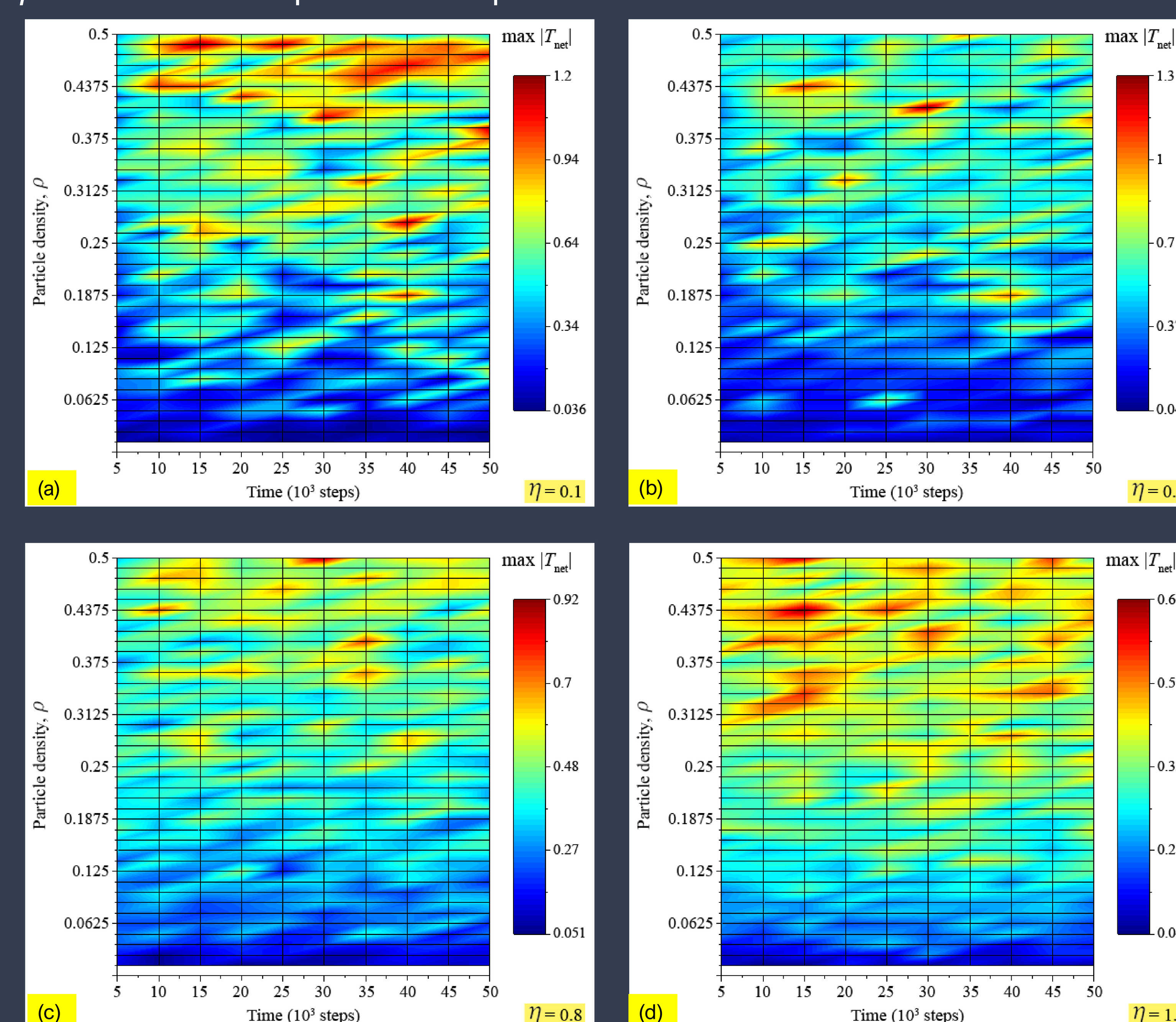

Figure 2. Representative plots in inspecting the time evolution of the net maximum transfer entropy.

Time Window	Noise Intensity									
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
1	0.5023	0.3158	0.3055	0.4163	0.4980	0.3721	0.3300	0.2905	0.3775	0.4298
2	0.6598	0.5206	0.5127	0.5090	0.4688	0.4037	0.5367	0.4565	0.4831	0.5177
3	0.5763	0.4200	0.4869	0.3681	0.5521	0.4505	0.5153	0.4342	0.4276	0.4916
4	0.5235	0.4984	0.3885	0.5517	0.4970	0.3994	0.4981	0.4253	0.4543	0.3553
5	0.7236	0.3983	0.5677	0.4721	0.4870	0.4006	0.4897	0.4748	0.4740	0.4106
6	0.6300	0.4962	0.5401	0.4888	0.4830	0.4354	0.3949	0.4794	0.4034	0.4156
7	0.7257	0.5634	0.4935	0.5009	0.4782	0.4038	0.4229	0.4300	0.3978	0.3434
8	0.5391	0.5395	0.4988	0.5876	0.5480	0.4545	0.4664	0.3366	0.4168	0.4395
9	0.5382	0.6584	0.4447	0.3828	0.4658	0.4816	0.4312	0.3866	0.3482	0.4201
10	0.6612	0.3432	0.5535	0.4496	0.5215	0.4006	0.4071	0.4022	0.4475	0.4385

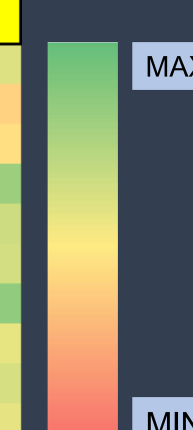

Figure 3. The exponents describing the power law relationship between system particle density and maximum net transfer entropy $|T_{\text{net}}|$.

Time Window	Noise Intensity									
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
1	0.5862	0.4416	0.5090	0.5731	0.7235	0.5886	0.6413	0.6977	0.7140	0.8848
2	0.7052	0.7231	0.6915	0.6175	0.6245	0.6470	0.8322	0.7011	0.7707	0.8798
3	0.6913	0.5953	0.7064	0.5008	0.6962	0.7242	0.7315	0.7850	0.7571	0.8247
4	0.6390	0.6532	0.6168	0.7078	0.6800	0.7238	0.7965	0.6749	0.7046	0.8217
5	0.6670	0.5542	0.6826	0.6424	0.6378	0.6330	0.7950	0.8231	0.7292	0.7573
6	0.5710	0.6856	0.6591	0.5048	0.6624	0.7386	0.7624	0.8024	0.7181	0.7904
7	0.7074	0.7296	0.6672	0.7545	0.6692	0.6907	0.7966	0.7719	0.7453	0.7420
8	0.5971	0.5353	0.6226	0.7041	0.6446	0.6891	0.7381	0.7030	0.6817	0.7543
9	0.5600	0.6679	0.5653	0.5516	0.5382	0.7991	0.6746	0.6988	0.6673	0.8709
10	0.6588	0.3346	0.6180	0.5777	0.6418	0.7603	0.7104	0.7839	0.8094	0.8085

Figure 4. The corresponding R^2 values describing the power law relationship between system particle density and maximum net transfer entropy $|T_{\text{net}}|$ from the configurations in figure 3.

Interestingly, for a given observation window, α decreases while the *coefficient of determination* R^2 (indicating goodness-of-fit to the power-law behavior) increases with increasing noise η. Overall, the estimated mean α is 0.47 $\pm$ 0.08 while the corresponding mean R^2 is 0.69 ± 0.10 for the whole range of η and ρ considered.

It must be noted, however, that there is no significant deviation in the parameters α and R^2 across the ten, consecutive time windows or epochs. That is, while there are observable fluctuations over time in the $|T_{\text{net}}|$ values for a given η and ρ, we cannot distinguish a general trend for $|T_{\text{net}}|$ as a function of observation time.

In future studies, it would be interesting to verify if there will be peaks of the the $|T_{\text{net}}|$ values during collective behavior as observed from biological and artificial active systems. For instance, peaks in information flows for a school of fish making collective U-turns in a spherical tank have been observed [Swarm Intell 12, 283-305 (2018)]. Additionally, by increasing the number of time steps in the simulations and then analyzing the results through the prism of the just recently introduced second law of information dynamics [AIP Advances 12, 075310 (2022)], which requires the information entropy to remain constant or to decrease over time, the time evolution of |Tnet| can be further investigated.