# Learning local dominant force balances in active particle flows

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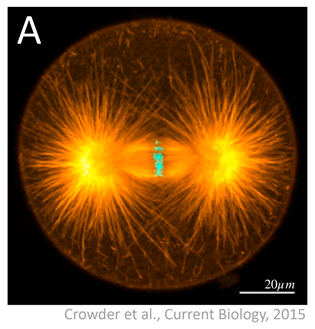
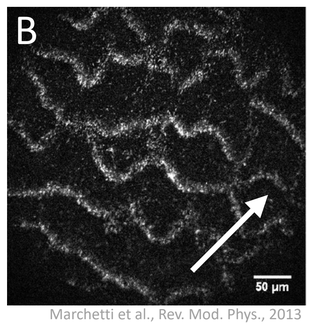
## Abstract

Systems of self-propelled particles exhibit self-organized collective behavior that leads to the formation of complex spatio-temporal patterns that can be observed all over nature (see i.e. Fig. below). Because of their abundance the question of *how* they form these rich macroscopic structures remains of central interest in cell biology. While there exist several hydrodynamic theories that are able to describe the observed dynamics, it is often hard to determine the local interactions that shape and regulate the structures. On the other hand, we also know that most systems can be locally well approximated by the balance of just a few dominant physical processes. The goal of this work is to extract such dominant balance models in a data-driven fashion and use them to understand which forces are locally driving the emergence of macroscopic patterns.




Crowder et al., Current Biology, 2015

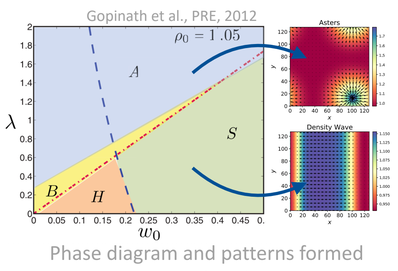



Marchetti et al., Rev. Mod. Phys., 2013

*In vivo* observations of patterns that can be reproduced by the hydrodynamic models considered here. **A**) Formation of asters during the assembly of the cellular mitotic spindle in the embryo of *C. marginatus.* **B**) Moving density waves in dense actin motility essays. Arrow denotes direction of movement.

## Macroscopic Model of Self-Propelled Particles

Hydrodynamic equations that describe the emergence of macroscopic motion from the microscopic interactions of self-propelled particles can be derived for various systems. Here we consider particles that move by a constant speed $w_0$ that can be modeled by the following coupled PDEs based on the density $\rho$ and polarity $\boldsymbol{W}$ of the particles.




Phase diagram and patterns formed by model ($\lambda = \lambda_{\{1,2,3\}}$).

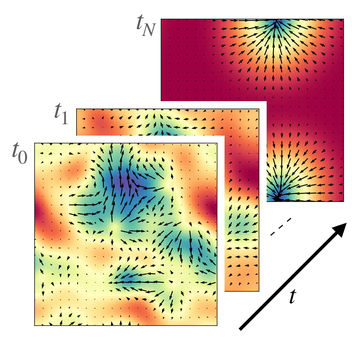
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (w_0 \boldsymbol{W} - D \nabla \rho)$$

$$\frac{\partial \boldsymbol{W}}{\partial t} + \lambda_1 (\boldsymbol{W} \cdot \nabla)\boldsymbol{W} = -(a_2(\rho) + a_4(\rho)|W|^2)\boldsymbol{W} + K\Delta \boldsymbol{W} - w_0 \nabla \rho + \frac{\lambda_3}{2}\nabla |W|^2 + \lambda_2 \boldsymbol{W}(\nabla \cdot \boldsymbol{W})$$

self-advection — spontaneous polarization — pressure — splay-induced pressure — polarity-compressibility feedback

## Method: Data-Driven Dominant Balance Models

### 1. Data Aquisition



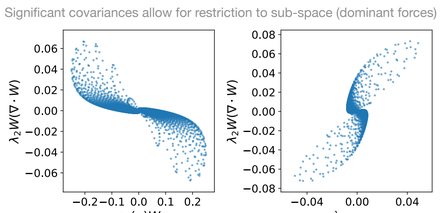

### 2.Dictionary & Equation Space

$$\frac{\partial \boldsymbol{W}}{\partial t} + \mathcal{N}(\boldsymbol{W}, \boldsymbol{x}, t; \boldsymbol{\xi}) = 0, \ \boldsymbol{\xi} = \{\lambda_1, \lambda_2, \dots\}$$

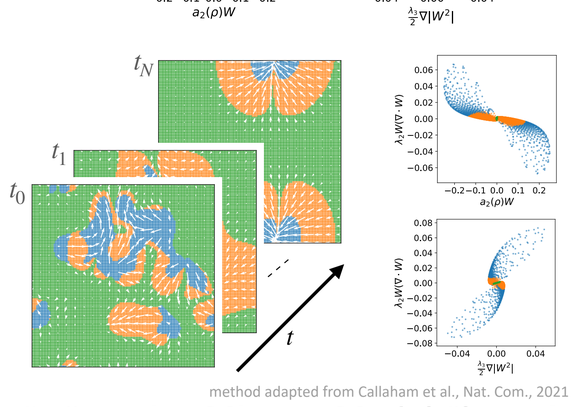
$$\Theta = \begin{bmatrix} \partial_t \boldsymbol{W}(\boldsymbol{x}_0) & \cdots & \boldsymbol{\xi}_F \mathcal{N}_F(\boldsymbol{x}_0) & \vdots \\ \vdots & \vdots & \ddots & \\ \partial_t \boldsymbol{W}(\boldsymbol{x}_N) & \cdots & \boldsymbol{\xi}_F \mathcal{N}_F(\boldsymbol{x}_N) & \end{bmatrix}$$

Dict. from Model terms

Significant covariances allow for restriction to sub-space (dominant forces)



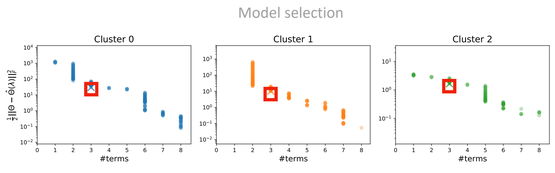

### 3. Gaussian Mixture Model Clustering




method adapted from Callaham et al., Nat. Com., 2021

### 4. Sparse PCA & Model Selection

Model selection

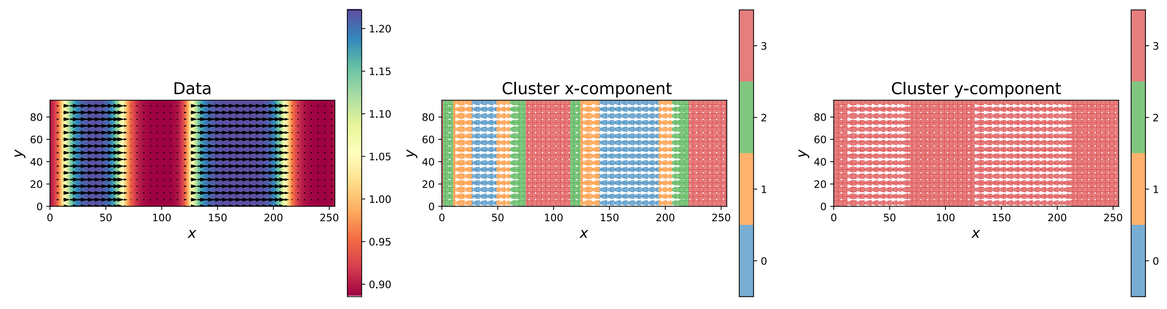



Dominant Forces

- $a_2, a_4, \lambda_2$ (Spon. Polarization, neg. Compressibility)
- $a_2, a_4, \lambda_3$ (Spon. Polarization, Splay-induced Pressure)
- $a_2, a_4, \lambda_3$ (Spon. Polarization, Splay-induced Pressure)

## Results

### Formation of Moving Density Waves



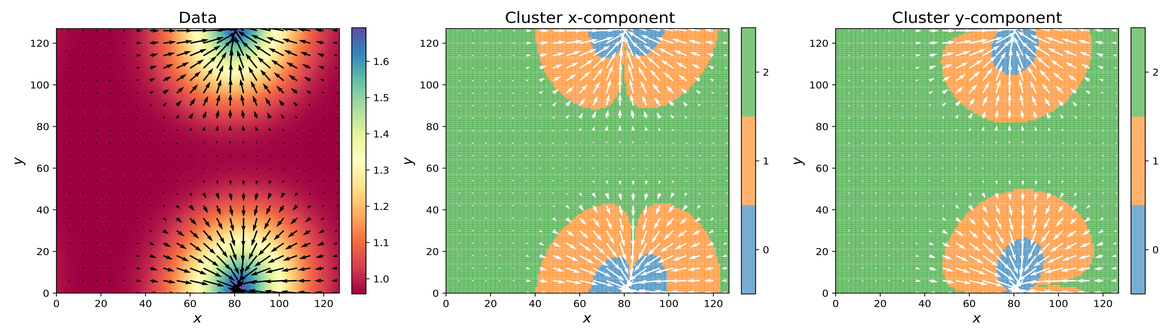

- $a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}$
- $\partial_t \boldsymbol{W}, a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}, w_0\nabla\rho$
- $\partial_t \boldsymbol{W}, a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}, w_0\nabla\rho$
- $a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}, K\Delta\boldsymbol{W}, w_0\nabla\rho$

GMM clustering and inferred local forces for the case of moving density waves.

In the high density region we infer a steady state equation based on the spontaneous polarization terms. This means, in the vicinity of a characteristic density $\rho_c$ the system will yield a stable polarized state with $\boldsymbol{W} = \sqrt{-a_2(\rho)/a_4(\rho)}\boldsymbol{e}_\theta$ due to local alignment interactions as predicted by the hydrodynamic theory. The emerging density gradient between the band and the background results in the stable convection of the high density region. Such mechanisms are in alignment with a separately derived description of moving density waves in (Gopinath et al., PRE, 2012) as

$$\frac{\partial \boldsymbol{W}}{\partial t} = -(a_2(\rho) + a_4(\rho)\frac{|W|^2}{\rho^2})\boldsymbol{W} - w_0 \frac{\partial \rho}{\partial x}$$

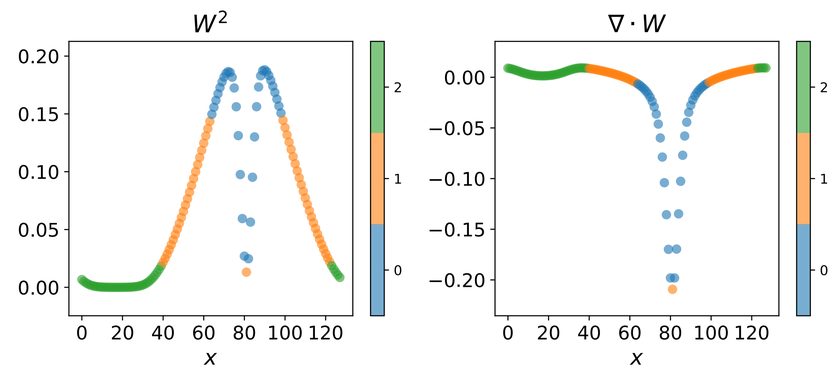
### Splay-Induced Negative Compressibility and Asters




- $a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}, \lambda_2\boldsymbol{W}(\nabla\cdot\boldsymbol{W})$
- $a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}, \frac{\lambda_3}{2}\nabla|W|^2$
- $a_2(\rho)\boldsymbol{W}, a_4(\rho)|W|^2\boldsymbol{W}, \frac{\lambda_3}{2}\nabla|W|^2$

GMM clustering and inferred local dominant forces for the case of the asters formation.

Similar to (Gopinath et al., PRE, 2012) we find that strong particle interactions leading to splay-induced pressure gradients and the negative compressibility near the center of the structures are the driving mechanism of asters formation.




Magnitude of local order parameter (left) and divergence of the polarity field (right). This shows the effect of arising negative compressibility due to strong particle interactions in the high density region.

## Conclusions and Outlook

We have shown that data driven methods can be used to extract local dominant forces that lead to pattern formation in active matter systems. Moreover, in alignment to previous work we identified two distinct processes: 1) density waves are formed by alignment interactions and driven by density gradients; 2) asters are shaped through effects of negative compressibility due to strong particle interactions. We envision this framework to be used to gain more insight on dominant force balances in living systems, i.e. the assembly of cell structures like spindles or the organization of tissues.

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