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Diversity of phase transitions and phase separations in active fluids

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Fluids

Many-body systems that can readily rearrange internal configurations

Passive fluids:
Flow under shearing and/or pressure gradients

Active fluids:
Flow under self-generated stresses + external forces

https://twitter.com/i/status/1408878326370930690

Plan

1. Active fluids – Vicsek model as an example
2. Setting up the Equation of Motion (EOM)
   - Hydrodynamic variable, conservation laws, & symmetries
3. Phase behaviour from mean-field analysis
4. Refining phase diagram with linear stability analysis
5. Further refining phase diagram with numerical methods

1. ACTIVE FLUIDS – VICSEK MODEL AS AN EXAMPLE

The Vicsek model - algorithm

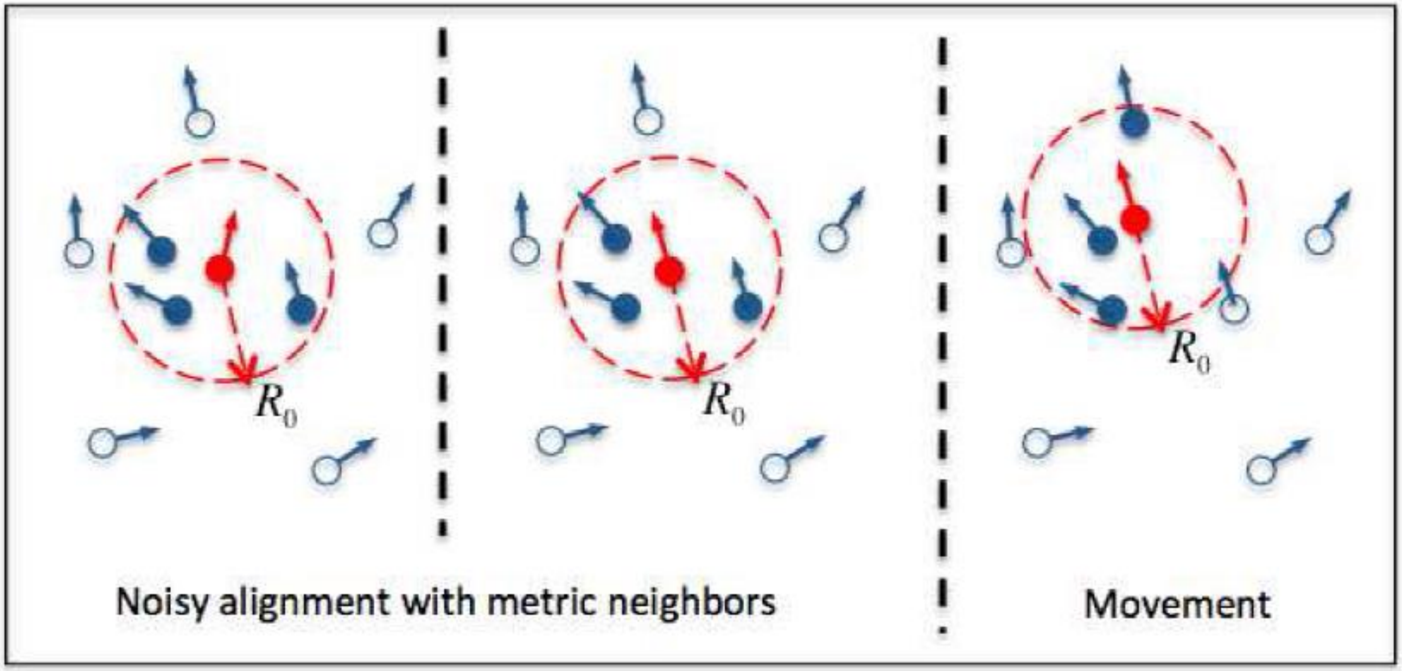
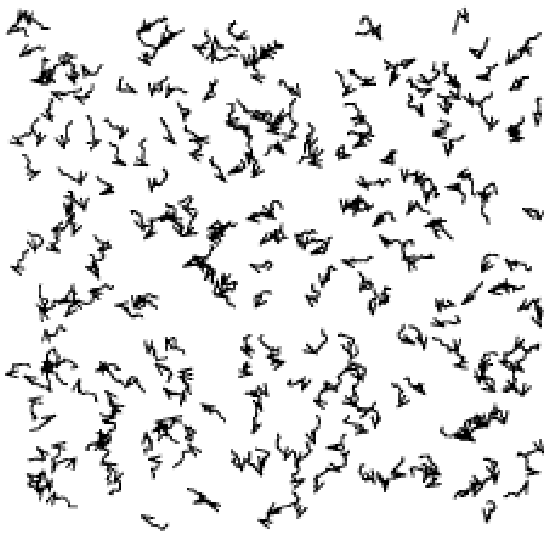


Figure from F. Ginelli, arXiv:1511.01451

T Vicsek, A Czirók, E Ben-Jacob, I Cohen & O Shochet (1995) Novel Type of Phase Transition in a System of Self-Driven Particles *Phys. Rev. Lett.* 75 1226–9

The Vicsek model – observations

Homogeneous disordered (D)



Homogeneous ordered (O)

Noise level

T Vicsek, A Czirók, E Ben-Jacob, I Cohen & O Shochet (1995) Novel Type of Phase Transition in a System of Self-Driven Particles *Phys. Rev. Lett.* 75 1226–9

What’s the big deal?

1. A continuous symmetry (rotational symmetry) seems to be broken in 2D!
   – A violation of the Mermin-Wagner-Hohenberg theorem at thermal equilibrium

2. Non-equilibrium dynamics is a crucial ingredient

3. It could be a new state of matter

   [Toner & Tu (1995) PRL; Toner & Tu (1998) PRE; Toner (2012) PRE; Mahault, Ginelli & Chaté (2019) PRL]

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Need to understand the physics!

2. SETTING UP THE EQUATION OF MOTION (EOM)

Hydrodynamic variables and conservation laws?

- Hydrodynamic variables: density ρ and momentum $\vec{g}$

- Conservation law: Mass conservation

$$\boxed{\begin{aligned} \partial_t \rho + \nabla \cdot \mathbf{g} &= 0 \\ \partial_t \mathbf{g} &= \mathbf{F} \end{aligned}}$$

Symmetries

$$\begin{aligned} \partial_t \rho + \nabla \cdot \mathbf{g} &= 0 \\ \partial_t \mathbf{g} &= \mathbf{F} \end{aligned}$$

- What is the force **F**?

- Starting with symmetries:
  - Temporal invariance: **F** does not depend on time
  - Translational invariance: **F** does not depend on position **r**
  - Rotational invariance: **F** does not depend on a particular direction
  - Chiral (parity) invariance: **F** is not right-handed or left handed

Toner-Tu Equations of Motion (EOM)

$$\partial_t \rho + \nabla \cdot \mathbf{g} = 0$$

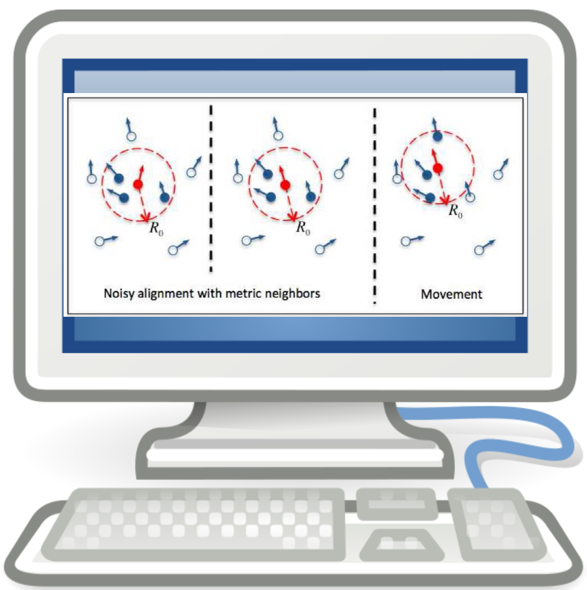
$$\partial_t \mathbf{g} + \lambda_1(\mathbf{g}\cdot\nabla)\mathbf{g} + \lambda_2(\nabla\cdot\mathbf{g})\mathbf{g} + \lambda_3\nabla g^2 = U(\rho,\mathbf{g})\mathbf{g} - \kappa_1\nabla\rho - \kappa_2\mathbf{g}(\mathbf{g}\cdot\nabla\rho) + \mu\nabla^2\mathbf{g} + \mathbf{f} + \cdots$$

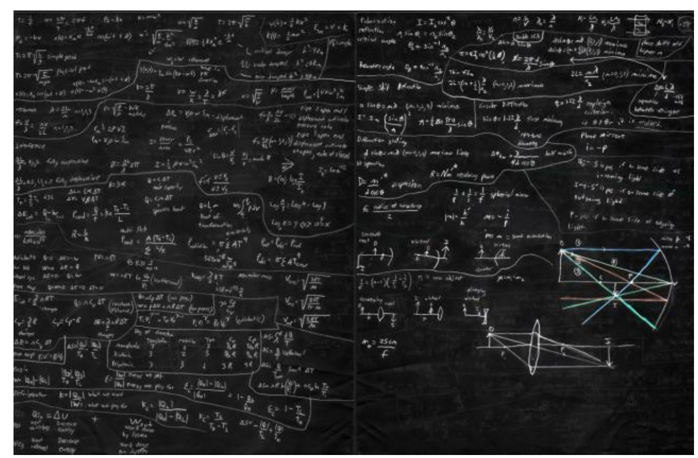
[Toner & Tu (1995) PRL; Toner & Tu (1998) PRE; Toner (2012) PRE]

Gaussian noise terms

$$\langle f(\mathbf{r},t)\rangle = 0$$

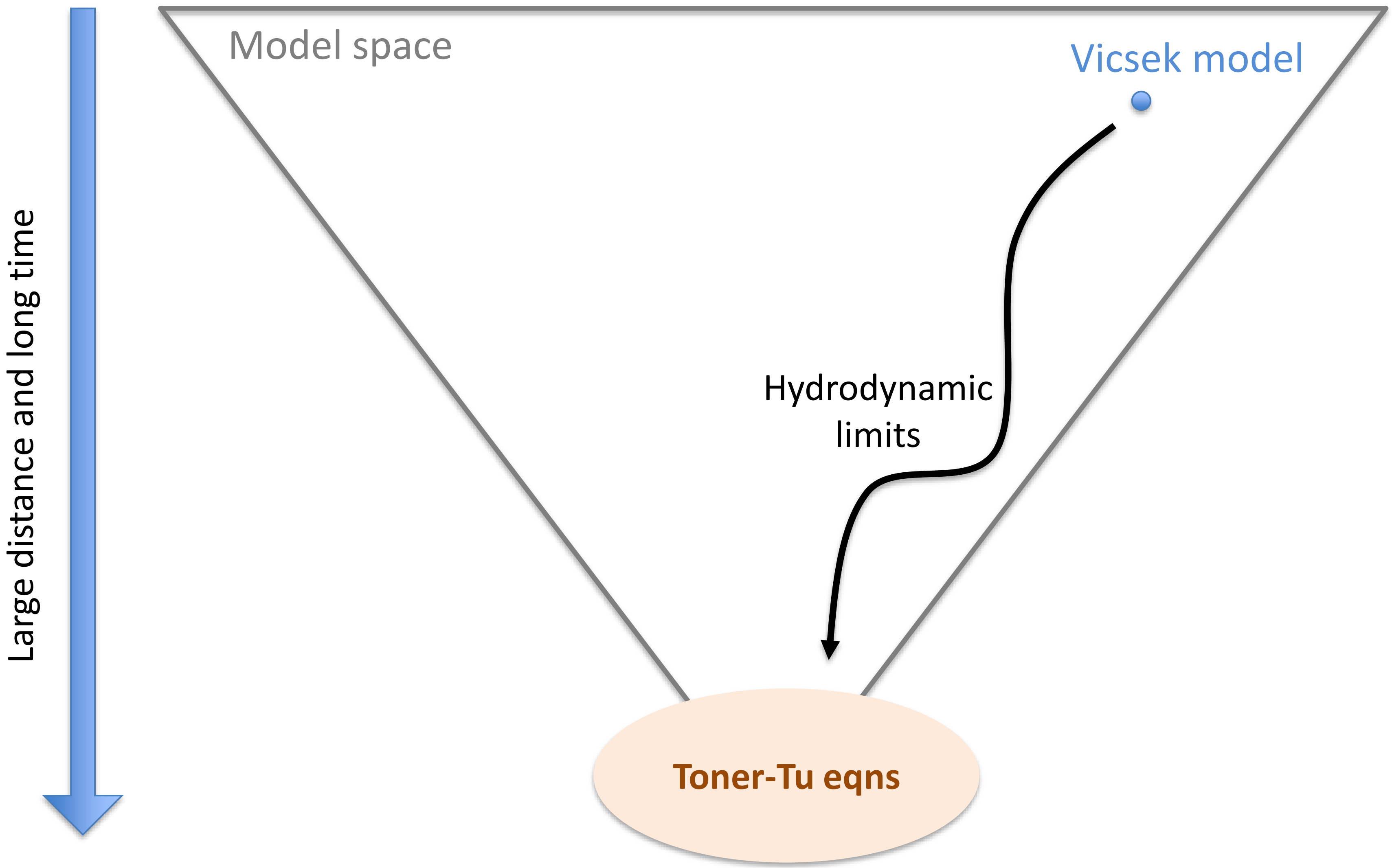
$$\langle f(\mathbf{r},t) f(\mathbf{r}',t')\rangle = 2D\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$



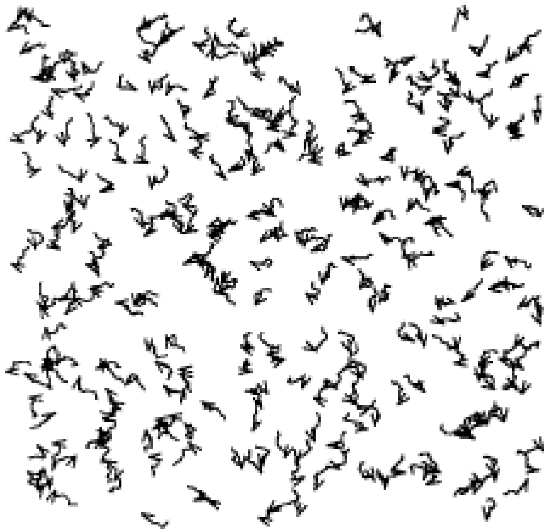


Active fluids

A class of non-equilibrium systems



Homogeneous disordered (D)



Homogeneous ordered (O)

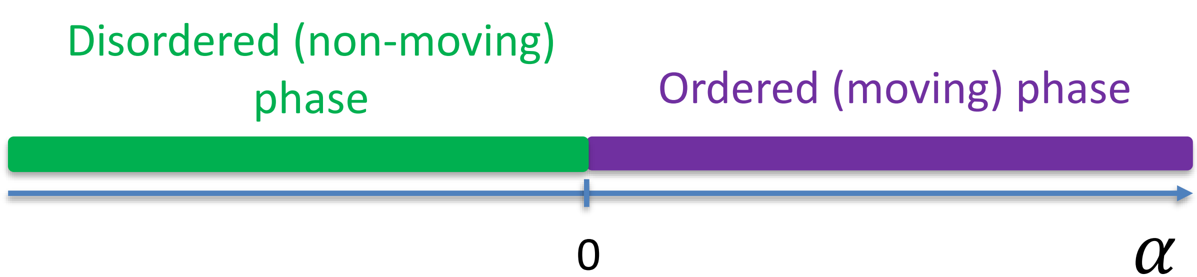
3. PHASE BEHAVIOUR FROM MEAN-FIELD ANALYSIS

Mean field picture
Ignoring spatial variations & Noise

$$\partial_t \rho + \cancel{\nabla\cdot\mathbf{g}} = 0$$

$$\partial_t \mathbf{g} + \cancel{\lambda_1(\mathbf{g}\cdot\nabla)\mathbf{g}} + \cancel{\lambda_2(\nabla\cdot\mathbf{g})\mathbf{g}} + \cancel{\lambda_3\nabla g^2} = U(\rho,\mathbf{g})\mathbf{g} - \cancel{\kappa_1\nabla\rho} - \kappa_2\cancel{\mathbf{g}(\mathbf{g}\cdot\nabla\rho)} + \cancel{\mu\nabla^2\mathbf{g}} + \cancel{\mathbf{f}} + \cdots$$

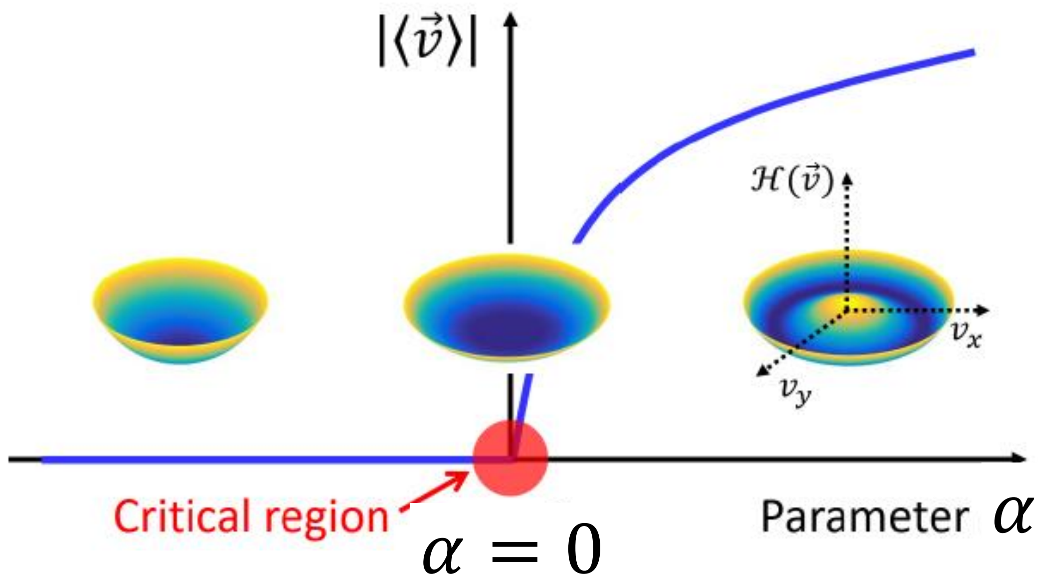
For example, $$\partial_t \mathbf{g} = (\alpha - \beta g^2)\mathbf{g} + \mathcal{O}(g^4)$$

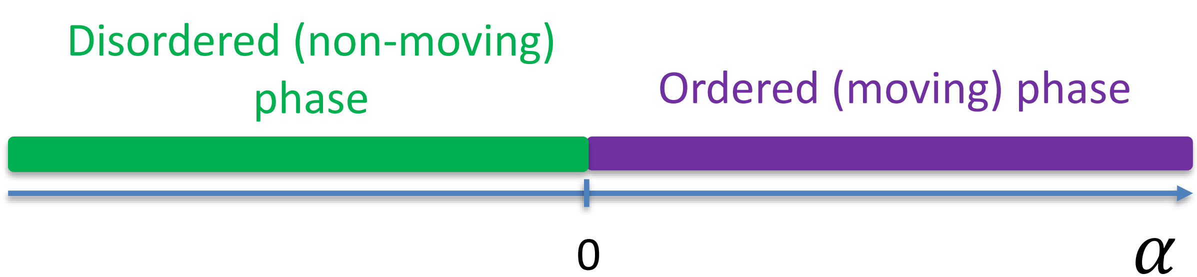


Mean field picture
Ignoring spatial variations & Noise

$$\partial_t \mathbf{g} + \cancel{\lambda_1 (\mathbf{g} \cdot \nabla)\mathbf{g}} + \qquad + \cancel{D\nabla^2 \mathbf{g}} + \cancel{\mathbf{f}} + \cdots$$

For example,





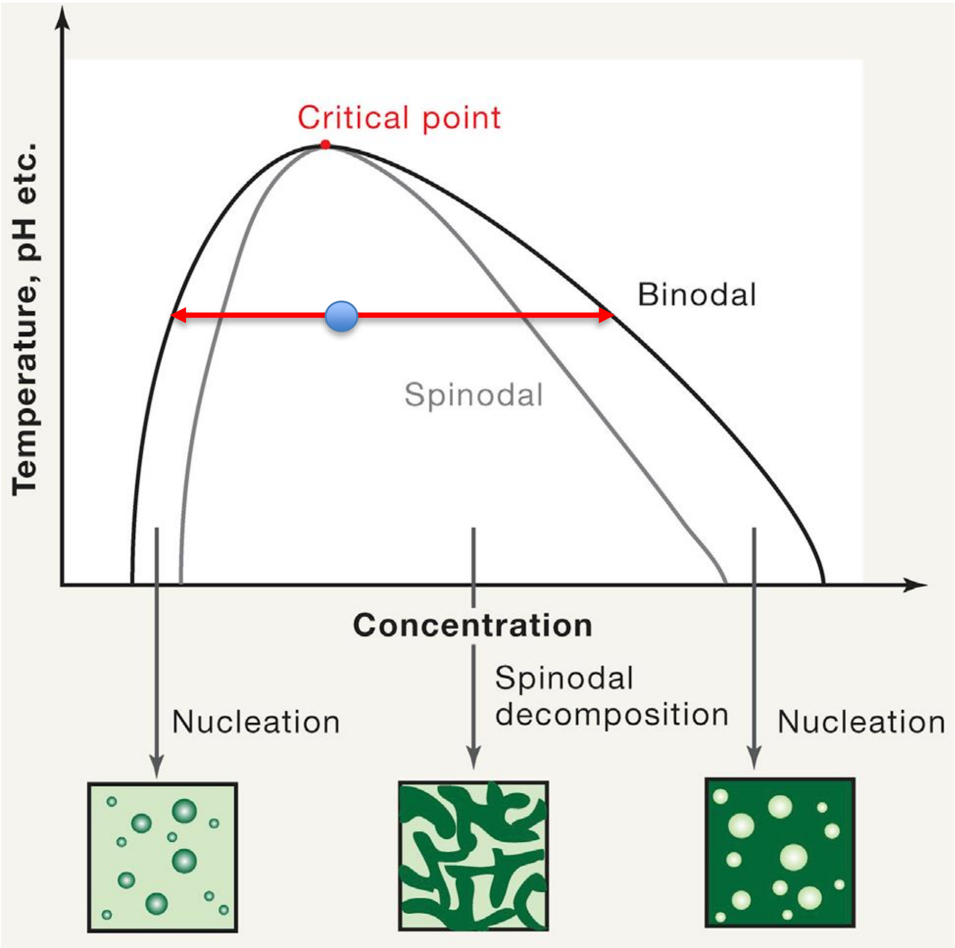
3. REFINING PHASE DIAGRAM WITH LINEAR STABILITY ANALYSIS

Think about gas-liquid phase separation

- High temp. -> Gas
- Low temp. -> Liquid

Think about gas-liquid phase separation

- High temp. -> Gas
- Low temp. -> Liquid
- But in a closed system (i.e., with mass conservation), phase separation can occur



Alberti, Gladfelter & Mittag (2019) Cell

Phase diagram from dynamics

- Perform stability analysis on the EOM, e.g., Cahn-Hilliard equation

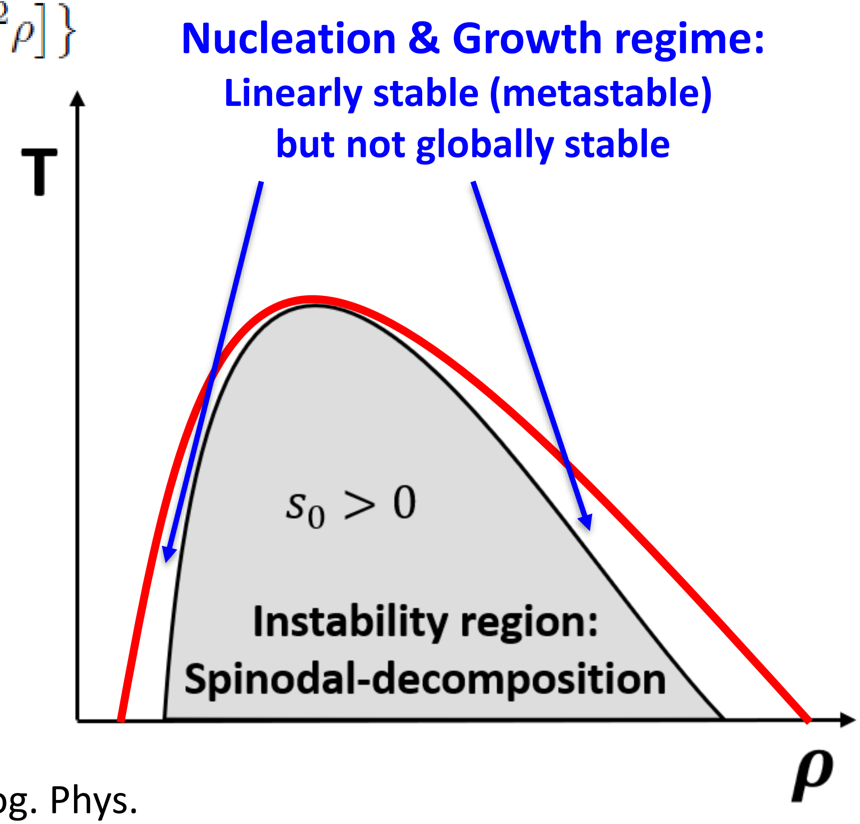
$$\partial_t \rho = \nabla \cdot \{\Lambda \left[a(\rho - \rho_c)^3 - b(\rho - \rho_c) - \kappa \nabla^2 \rho\right]\}$$

$$\rho(\mathbf{r}, t) = \bar{\rho} + \epsilon \exp\left(st + \mathrm{i}\mathbf{q} \cdot \mathbf{r}\right)$$

$$s(\mathbf{q}) = -q^2 \Lambda \left[3a(\bar{\rho} - \rho_c)^2 - b + \kappa q^2\right]$$

$$s_0 = \lim_{q \to 0} s(\mathbf{q})$$

- But SD is not everything



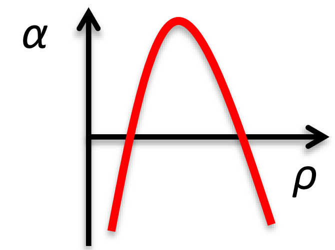
Review: Weber, Zwicker, Jülicher, Lee (2019) Rep. Prog. Phys.

Back to active fluids

In passive fluids, there is one phase (fluid) and one conserved quantity (total concentration)

In polar active fluids, there are two phases (Ordered & Disordered) and one conserved quantity (total concentration)

Linear stability in active fluids



- At the linear level, our EOM are

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot \mathbf{g} &= 0 \\
\partial_t \mathbf{g} + \lambda \mathbf{g} \cdot \nabla \mathbf{g} &= \mu \nabla^2 \mathbf{g} - \kappa \nabla \rho + \alpha(\rho)\mathbf{g} - \beta g^2 \mathbf{g}
\end{aligned}
$$

- Around the moving phase, the system is unstable if

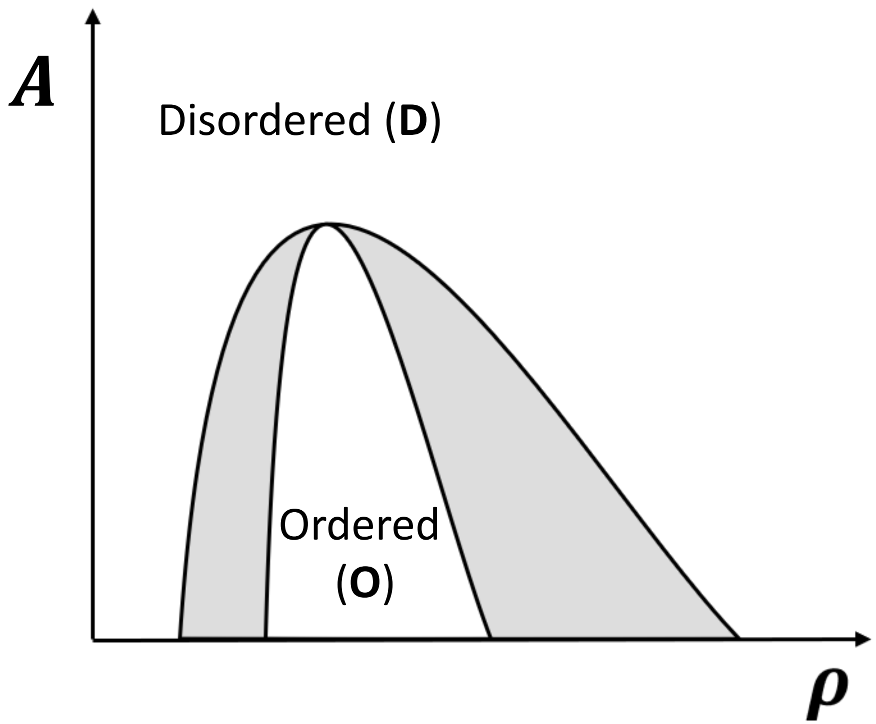
$$
\frac{\alpha_1^2}{\beta} - 2\alpha_0 \left(2\kappa + \frac{\alpha_1 \lambda}{\beta}\right) > 0
$$

where $\alpha(\rho_0 + \delta\rho) = \alpha_0 + \alpha_1 \delta\rho + \mathcal{O}(\delta\rho^2)$

E Bertin, M Droz & G Grégoire (2006) PRE
D Nesbitt, G Pruessner & CFL (2021) NJP

Phase diagram from linear stability

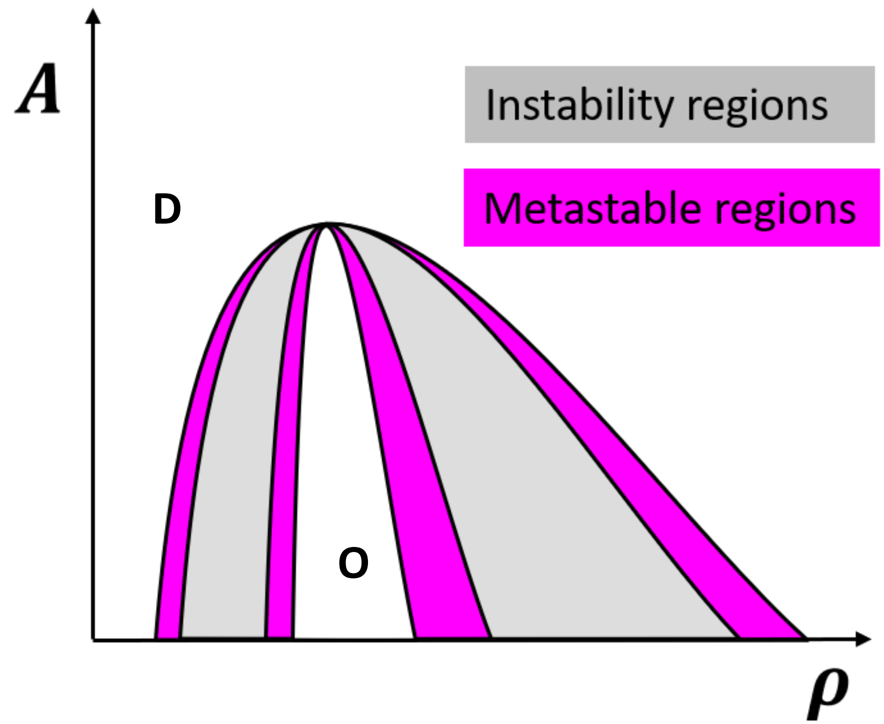
Ex: $\alpha(\rho) = -A + \rho - \rho^2$



Phase diagram from linear stability

Ex: $\alpha(\rho) = -A + \rho - \rho^2$

Expect that instability regions are flanked by nucleation & growth (metastable) regions

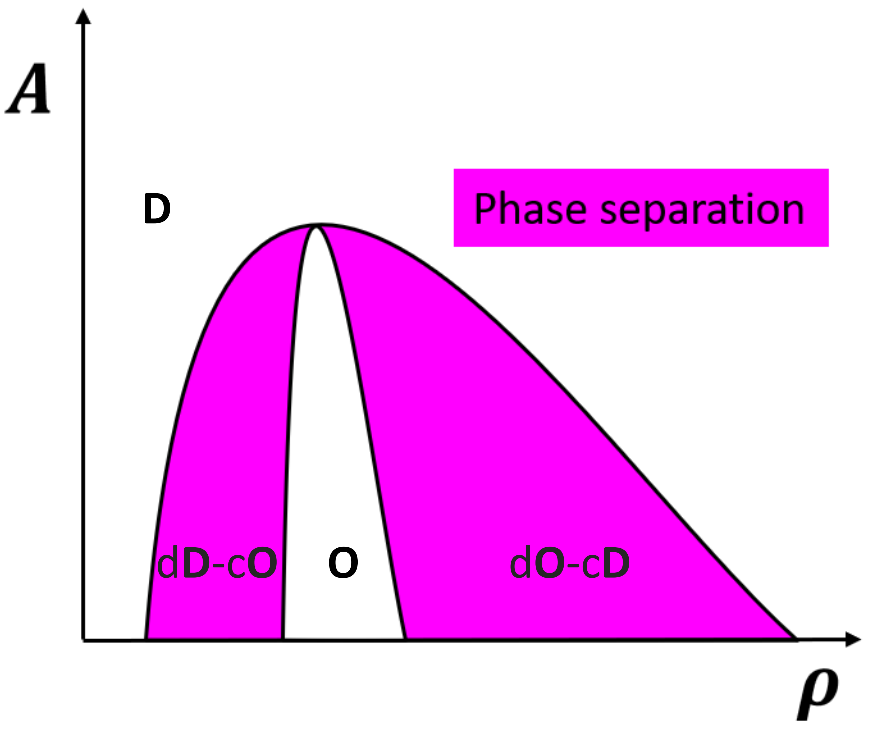


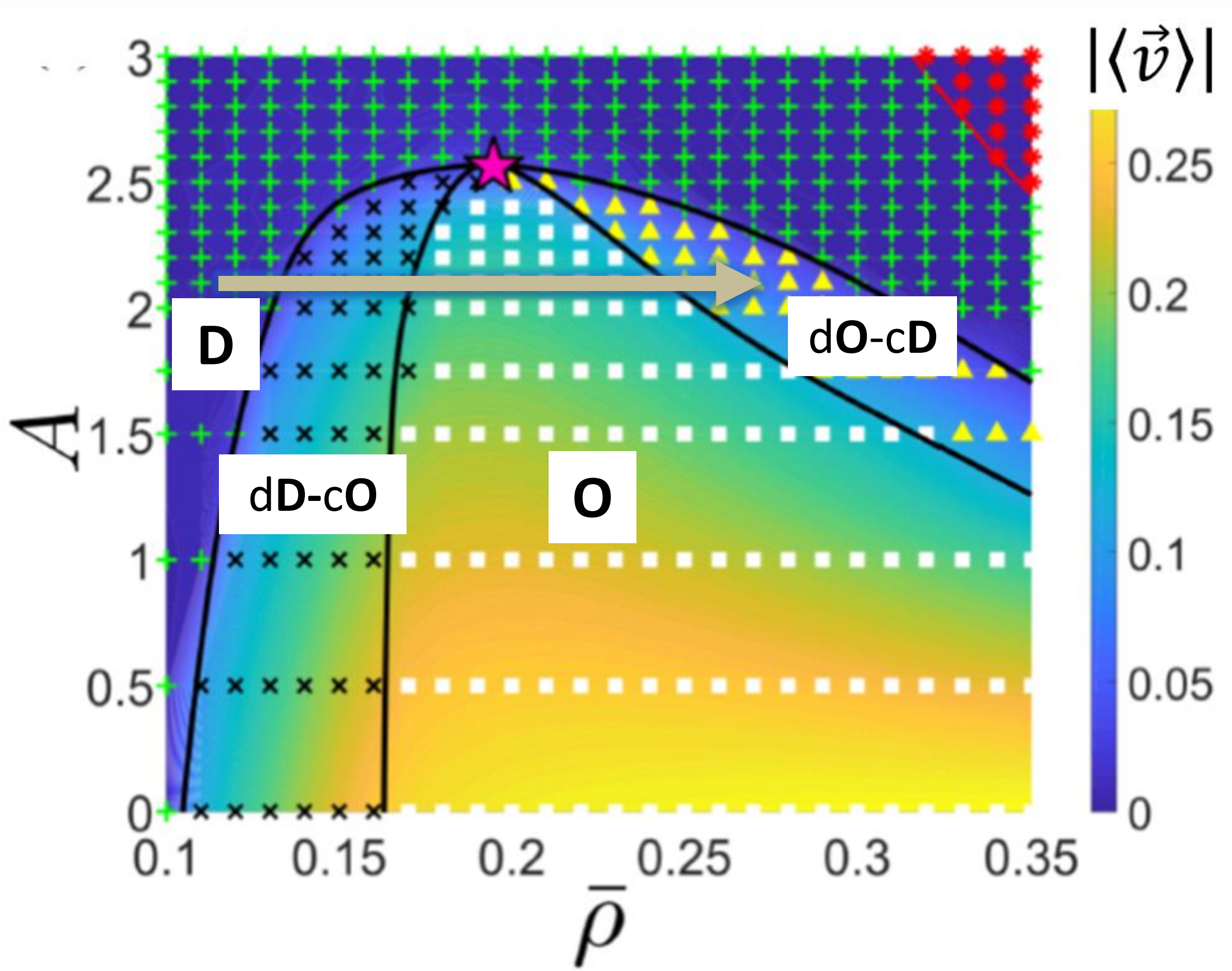
Phase separations

Ex: $\alpha(\rho) = -A + \rho - \rho^2$

Two distinct phase separation regimes:

1) dilute-disordered phase coexisting with condensed-ordered phase (d**D**-c**O**)
2) dilute-ordered phase coexisting with condensed-disordered phase (d**O**-c**D**)

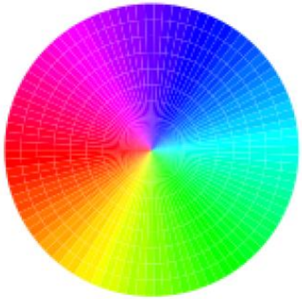


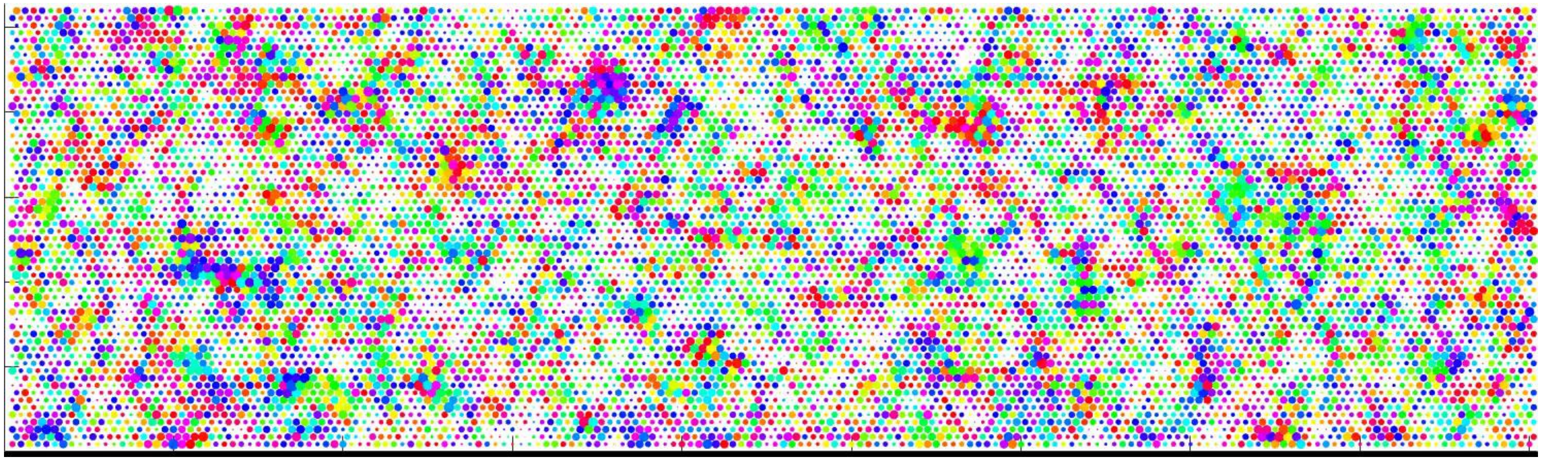


5. FURTHER REFINING PHASE DIAGRAM WITH NUMERICAL METHODS (LATTICE-BOLTZMANN)

Disordered (O) phase

Colour wheel used to determine direction of velocity

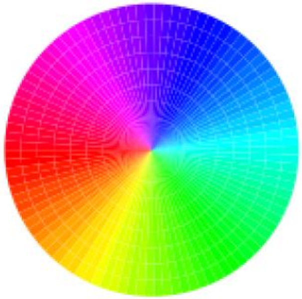


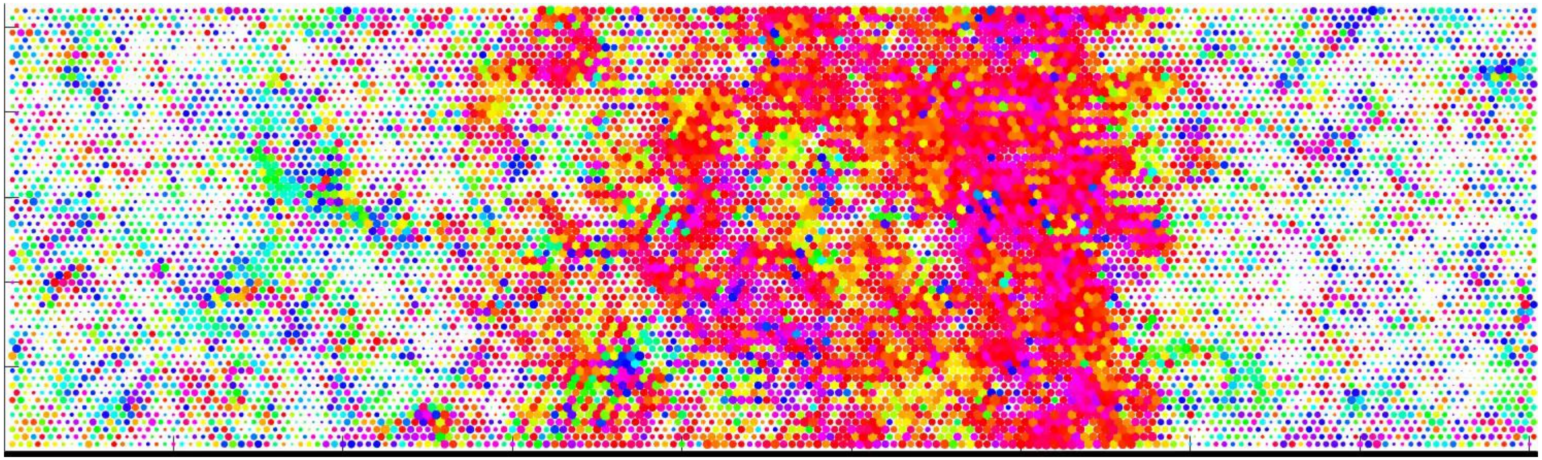


D Nesbitt, G Pruessner & CFL (2021) NJP 23, 043047

dD-cO co-existence regime

Colour wheel used to determine direction of velocity





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Ordered (O) phase

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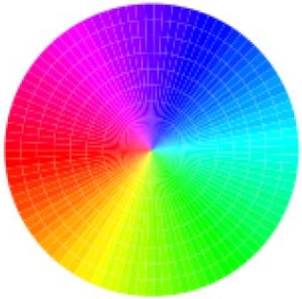

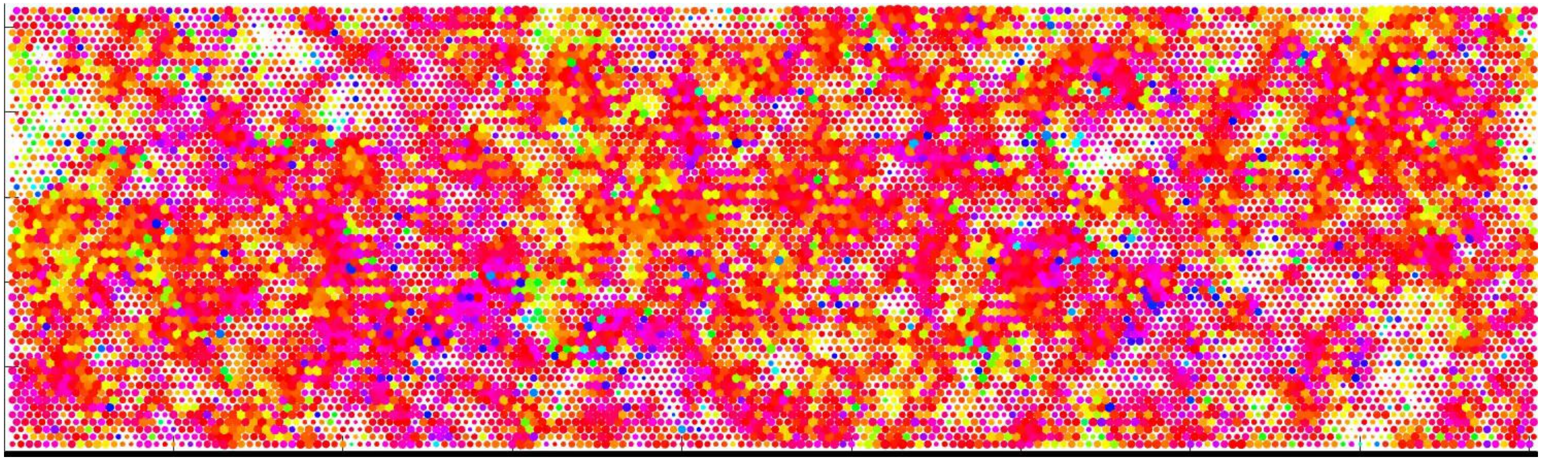

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dO-cD co-existence phase

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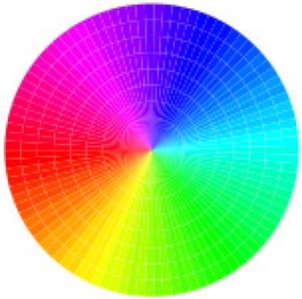
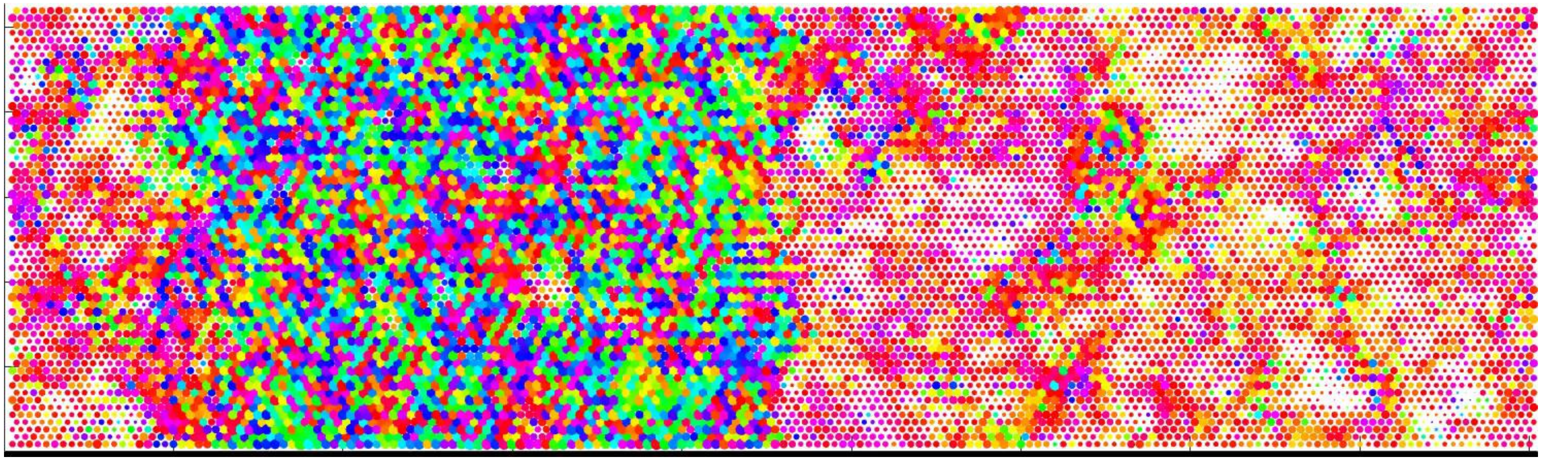
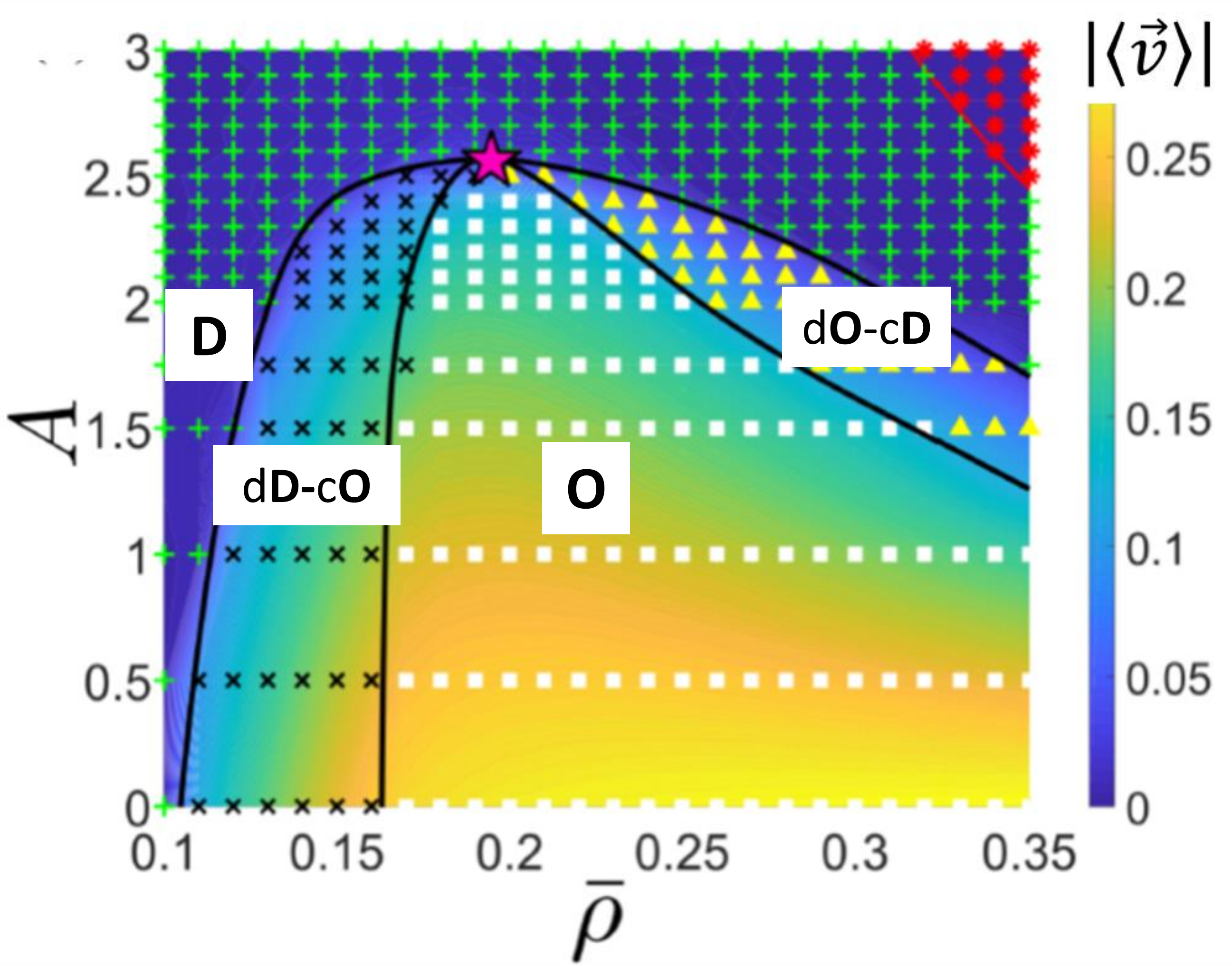




See also: S Schnyder et al. (2017) *Collective motion of cells crawling on a substrate: roles of cell shape and contact inhibition*. Sci. Rep.; Geyer, David Martin, Julien Tailleur, and Denis Bartolo (2019) Freezing a Flock: Motility-Induced Phase Separation in Polar Active Liquids. PRX

D Nesbitt, G Pruessner & CFL (2021) NJP 23, 043047

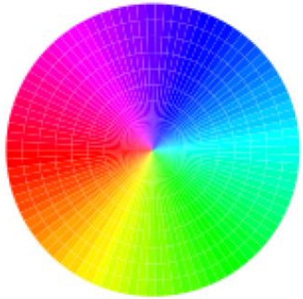
Critical behaviour by fine-tuning two parameters

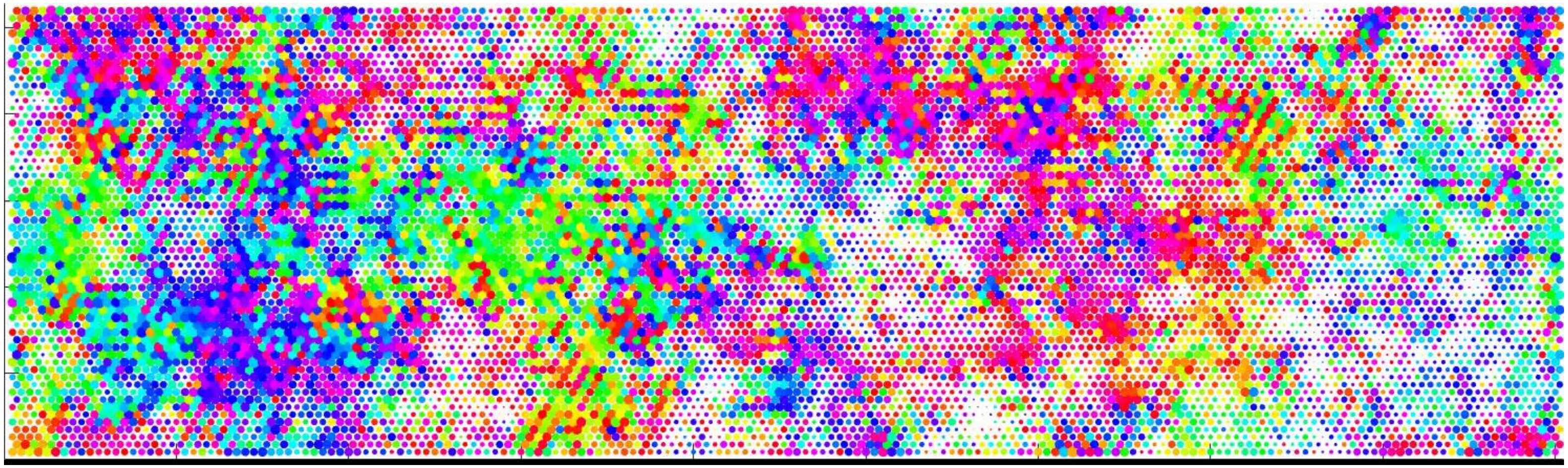


Surprising because critical order-disorder transition is not typically expected from compressible active fluids!

Around the critical point

Colour wheel used to determine direction of velocity





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Known critical phenomena in polar active matter

1. Incompressible active fluids [Chen, Lee & Toner (2015)]
2. Active Lévy matter [Cairoli & Lee, arXiv:1904.08326]
3. Critical motility-induced phase separation [Partridge & Lee (2019) PRL; Siebert, et al. (2018) PRE; Caballero, Nardini & Cates (2018) J Stat Mech]
4. Self-propelled particles with velocity reversals and alignment interactions [Mahault, et al. (2018) PRL]

Known critical phenomena in polar active matter

1. Incompressible acti… s [Chen, Lee & Toner (2015)]

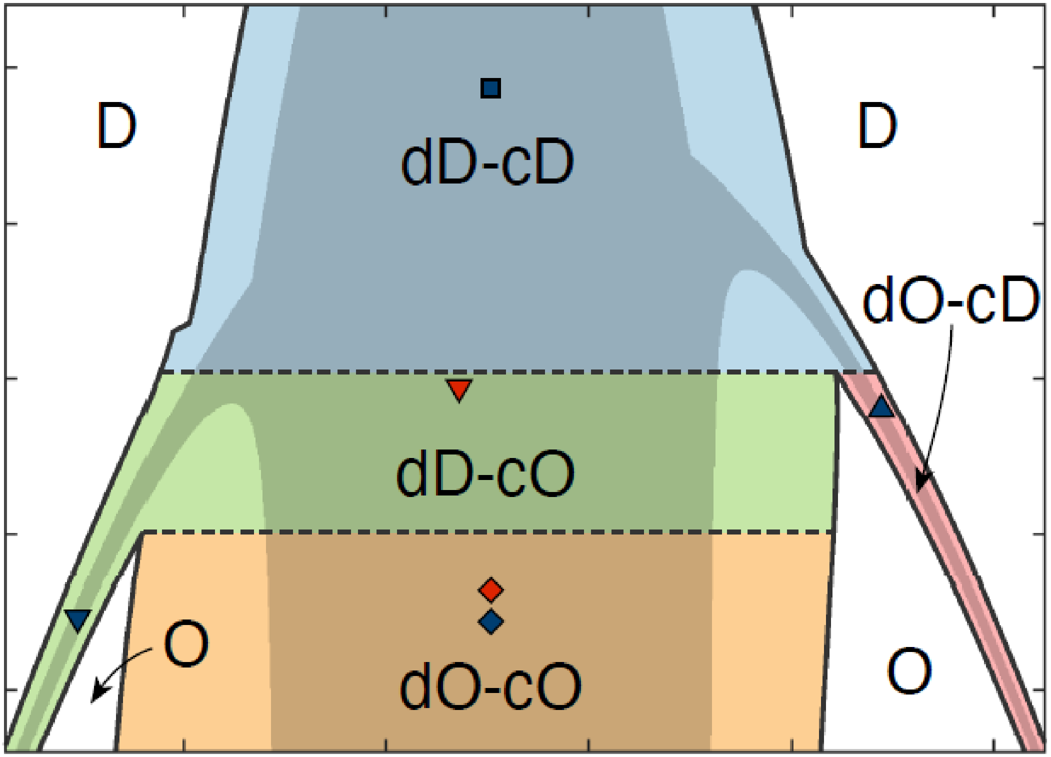
Our model does not have long-range interactions

2. Ac… Levy matter [Cairoli & Lee, arXiv:1904.08326]
3. Critical motility-induced phase s… on [Partridge & L… et al. (2018) PRE; Cab… & Cates (2018) J Stat Mech]

Our order parameter is continuous, not discrete

4. Self-propelled particles with velo… rever… t interactions [Mahault, … al. (2018) PRL]

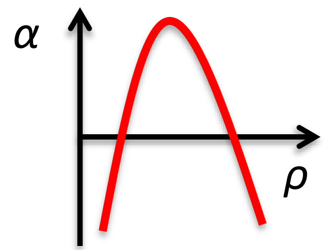
Our ordered state has long-range order, not quasi-long-range order



THERE ARE MORE CO-EXISTENCE PHASES

Back to EOM

- At the linear level, our EOM are



$$\partial_t \rho + \nabla \cdot \mathbf{g} = 0$$

$$\partial_t \mathbf{g} + \lambda(\mathbf{g} \cdot \nabla)\mathbf{g} = \mu \nabla^2 \mathbf{g} - \kappa(\rho)\nabla\rho + \alpha(\rho)\mathbf{g} - \beta g^2 \mathbf{g}$$

B Partridge & CFL (2019) PRL 123, 068002
T Bertrand & CFL (2021) arXiv:2012.05866

Back to EOM

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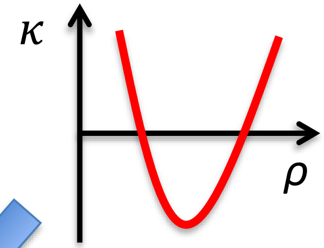


$$\partial_t \rho + \nabla \cdot \mathbf{g} = 0$$

$$\partial_t \mathbf{g} + \lambda(\mathbf{g} \cdot \nabla)\mathbf{g} = \mu \nabla^2 \mathbf{g} - \kappa(\rho)\nabla\rho + \alpha(\rho)\mathbf{g} - \beta g^2 \mathbf{g}$$

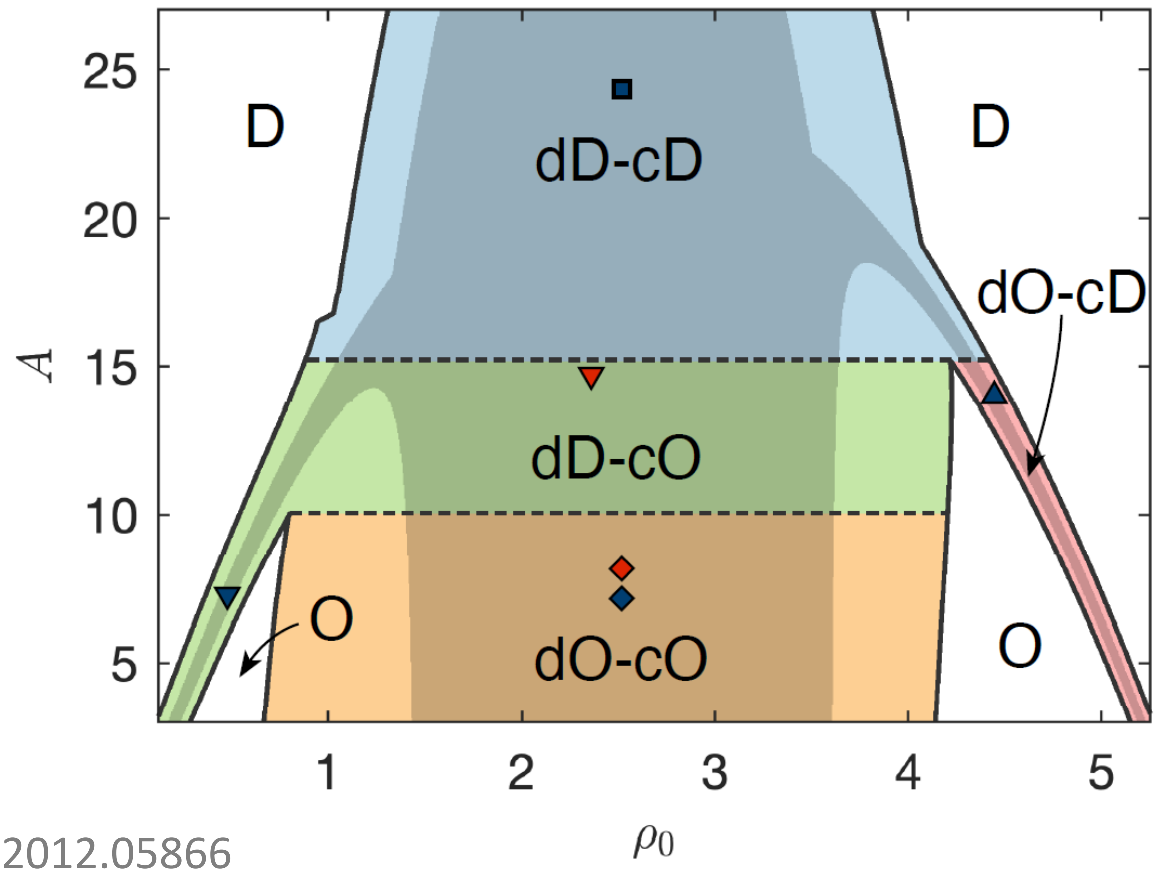
- Form of $\kappa(\rho)$ can also induce phase separation
  - A manifestation of motility-induced phase separation

B Partridge & CFL (2019) PRL 123, 068002
T Bertrand & CFL (2021) arXiv:2012.05866

Phase diagram from linear stability

Ex: $\alpha(\rho) = -A + 18\rho - 10/3\rho^2$

$\kappa(\rho) = 140 - 145\rho + 30\rho^2$,



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Phase diagram from linear stability

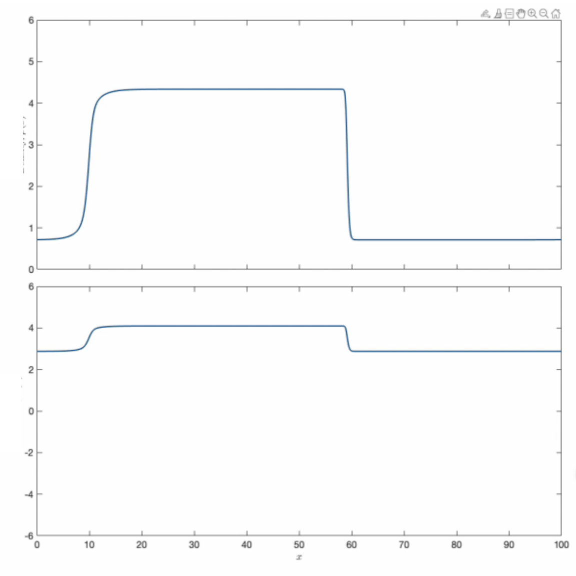
Ex: $\alpha(\rho) = -A + 18\rho - 10/3\rho^2$

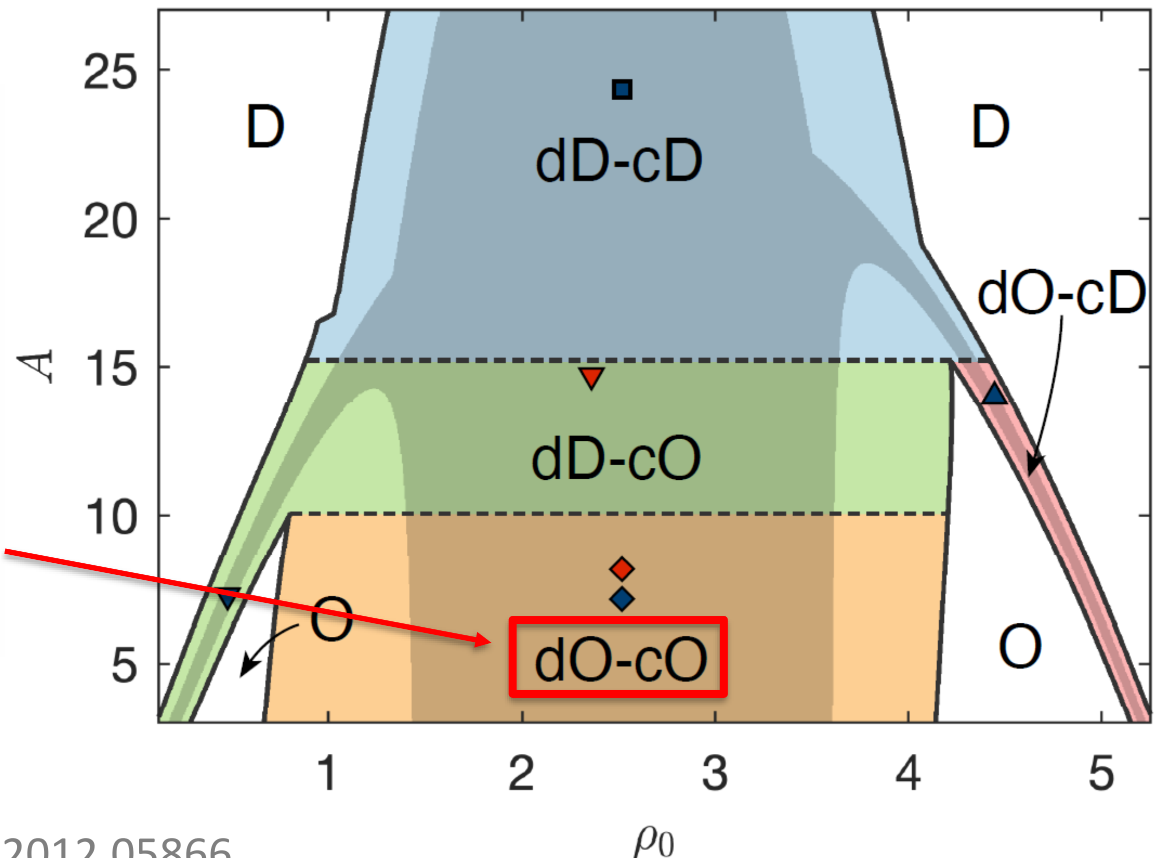
$\kappa(\rho) = 140 - 145\rho + 30\rho^2$,

New co-existence regime

ρ

g

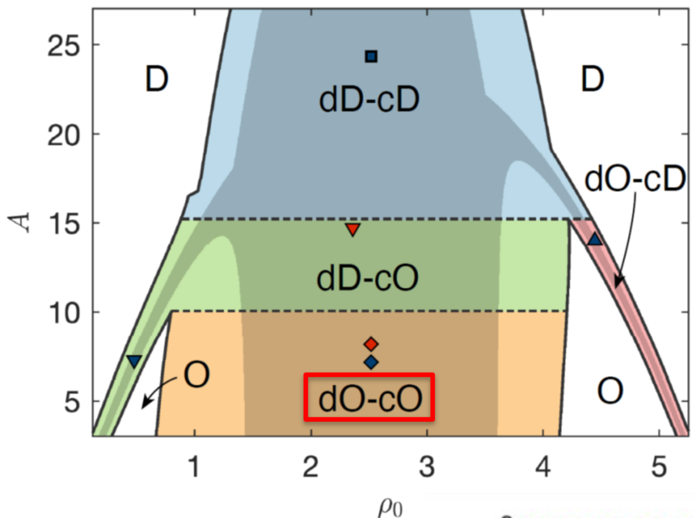


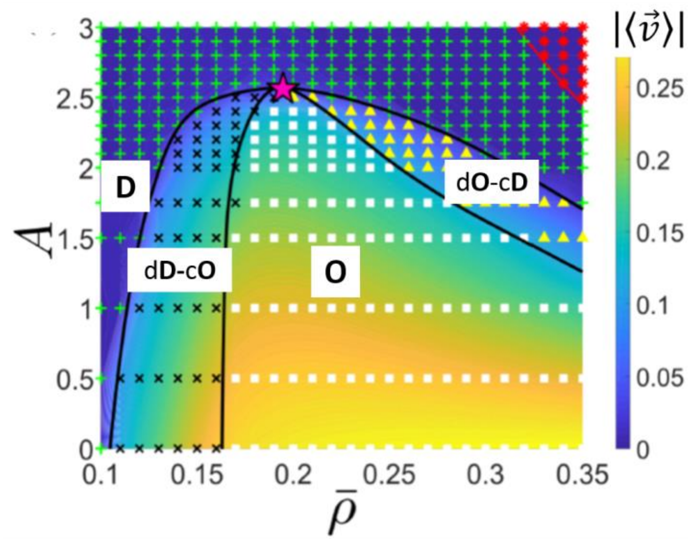


T Bertrand & CFL (2021) arXiv:2012.05866

Summary

- Two distinct phases (D/O) & four distinct co-existence phases dD-cD, dD-cO, dO-cD, dO-cO
- One novel co-existence phase: dO-cO, and one novel critical point





References:

1. T. Bertrand and CFL. Diversity of phase transitions and phase co-existences in active fluids. E-print: arXiv:2012.05866.

2. D. Nesbitt, G. Pruessner & CFL (2021) Uncovering novel phase transitions in dense dry polar active fluids using a lattice Boltzmann method. New Journal of Physics 23 043047.

Acknowledgement

Thank you for your Attention!

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