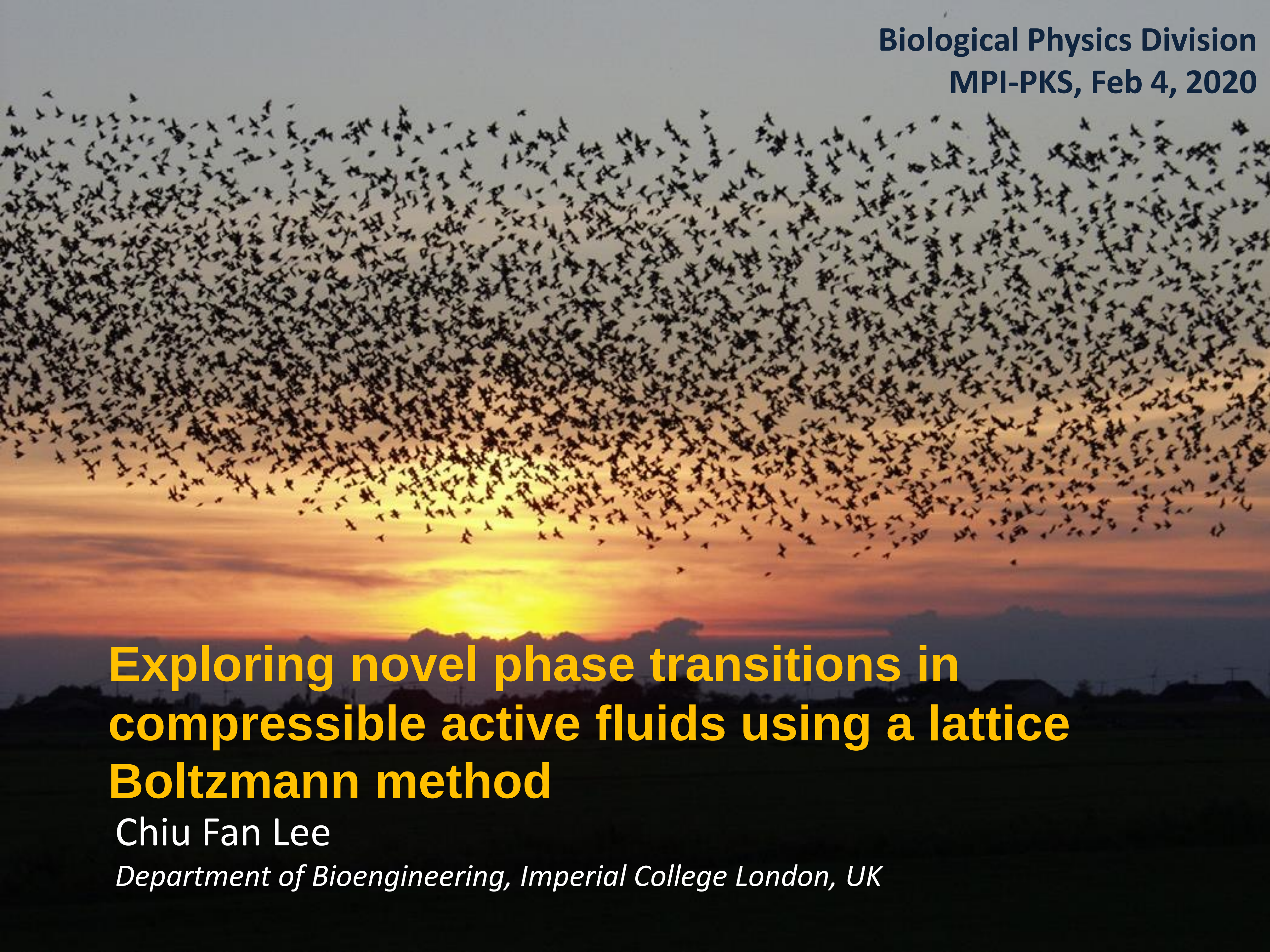
Biological Physics Division
MPI-PKS, Feb 4, 2020



Exploring novel phase transitions in compressible active fluids using a lattice Boltzmann method

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Plan

1. Active fluids – Vicsek model as an example
2. Symmetry-based hydrodynamic theory – Toner-Tu equations
3. Simulating active fluids – A Lattice Boltzmann method
4. Novel phase behaviour – Active systems with contact inhibition of locomotion
5. Summary

1. ACTIVE FLUIDS – VICSEK MODEL AS AN EXAMPLE

The Vicsek model - algorithm

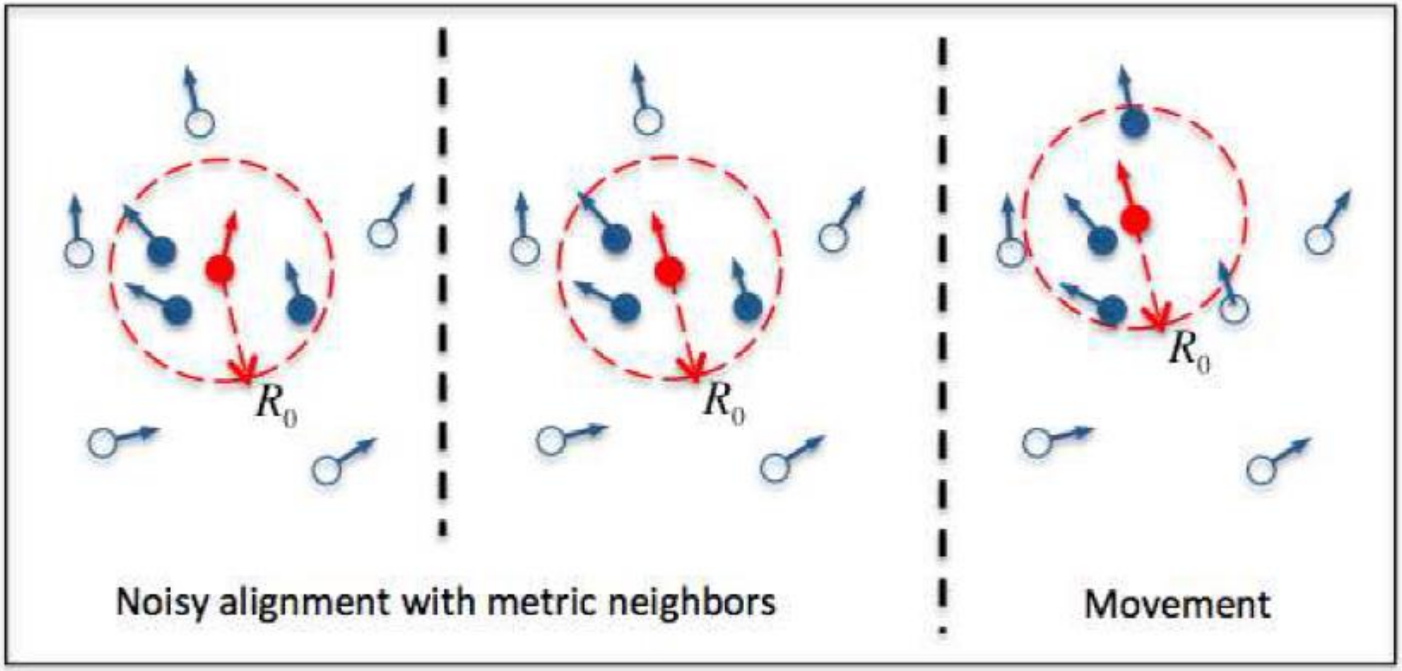
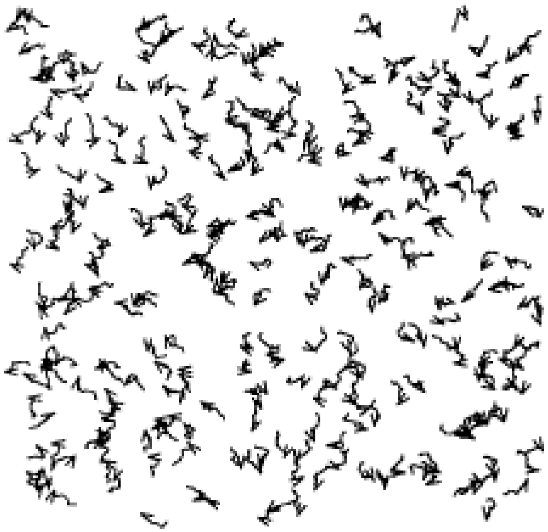


Figure from F. Ginelli, arXiv:1511.01451

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 (HD)



Homogeneous ordered (HO)

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. SYMMETRY-BASED HYDRODYNAMIC THEORY – TONER-TU EQUATIONS

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

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

- 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)

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

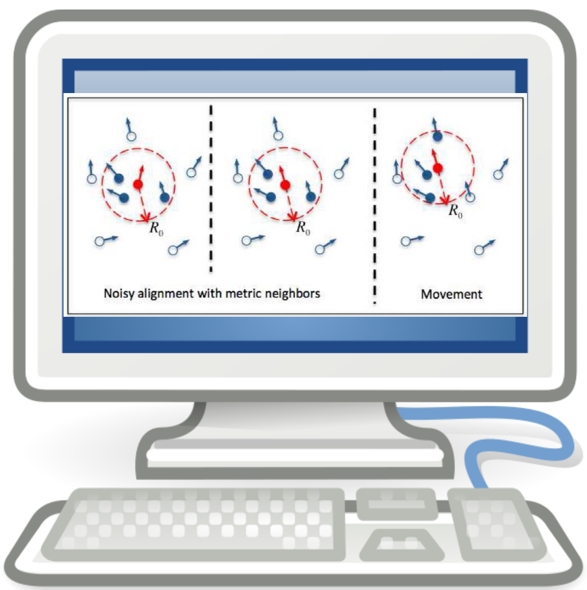
$$\partial_t \mathbf{g} + \lambda_1 (\mathbf{g} \cdot \nabla)\mathbf{g} + \lambda_2 (\nabla \cdot \mathbf{g})\mathbf{g} + \lambda_3 \nabla g^2 \; = \; U(\rho, \mathbf{g})\mathbf{g} - \kappa_1 \nabla \rho - \kappa_2 \mathbf{g}(\mathbf{g} \cdot \nabla \rho) + \mu \nabla^2 \mathbf{g} + \mathbf{f} + \cdots$$

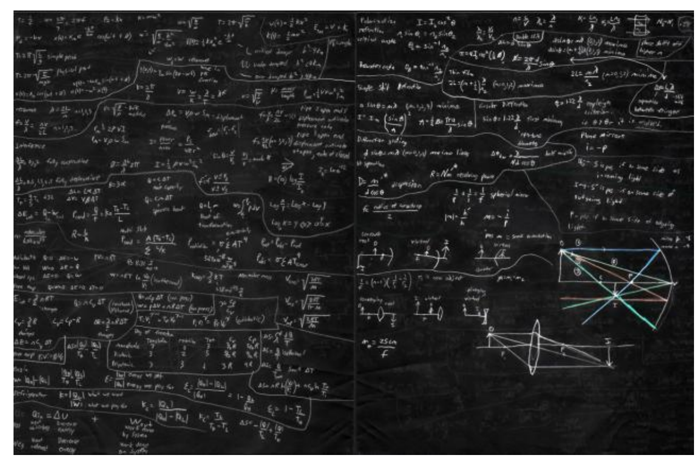
[Toner & Tu (1995) PRL; Toner & Tu (1998) PRE; Toner (2012) PRE]

Gaussian noise terms

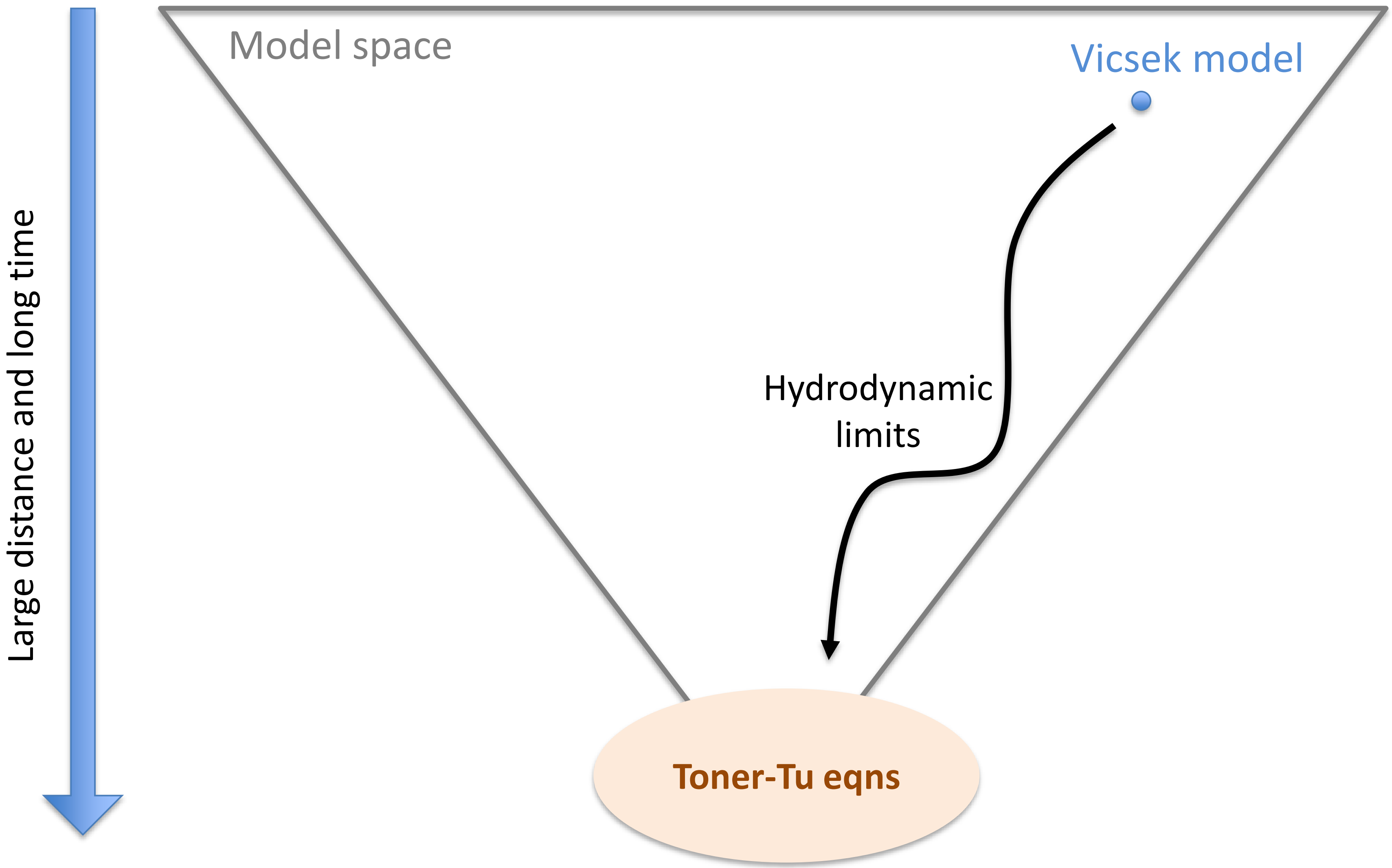
$$\langle f(\mathbf{r}, t) \rangle = 0$$

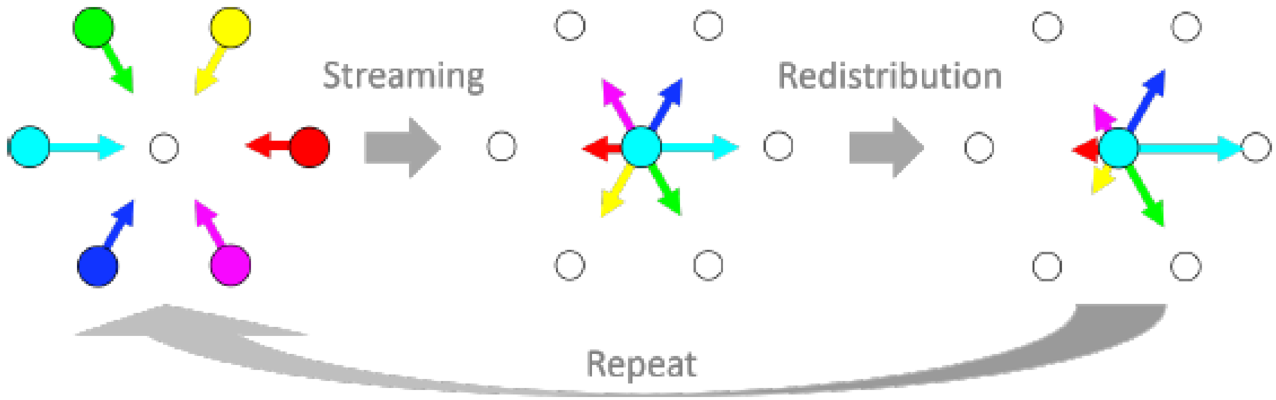
$$\langle f(\mathbf{r}, t) f(\mathbf{r}', t') \rangle = 2D\delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$$





A class of active fluid models





3. SIMULATING ACTIVE FLUIDS – A LATTICE BOLTZMANN METHOD

A naïve question

- Can we not just do analytical calculations now that we have the hydrodynamic equations?
- Think good old fluid mechanics, most research is computational

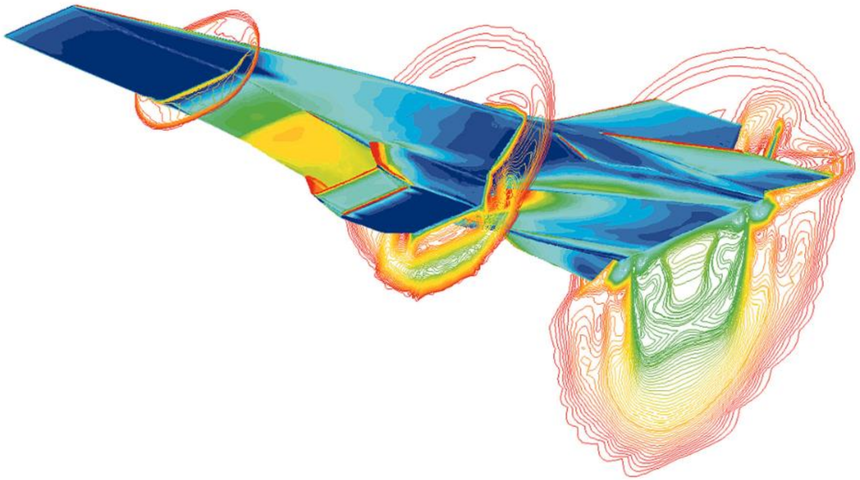


Figure from Wikipedia

What can we learn from good old fluid mechanics?

- (Practically) no one does molecular dynamics simulation
- Computational fluid dynamics (CFD)
  - Numerically solve Navier-Stokes equation (2^{nd} order PDE)
- Lattice Boltzmann methods (LBM)
  - Forget about Navier-Stokes and get to the hydrodynamic behaviour from scratch

LBM over CFD

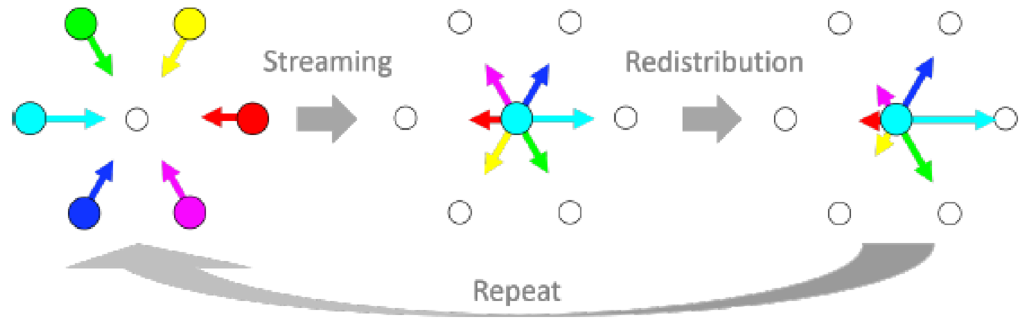
- Advantages
  - Easy to parallelise
  - Can handle complex geometries
- Disadvantages
  - Hard to deal with high Mach numbers
  - No consistent thermo-hydrodynamic scheme

LBM over CFD

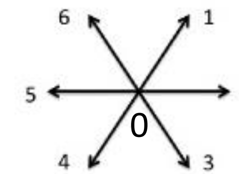
- Advantages
  - Easy to parallelise
  - Can handle complex geometries
- Disadvantages
  - Hard to deal with high Mach numbers
  - ~~No consistent thermo-hydrodynamic scheme~~

No need for such a scheme in active fluids

LBM – algorithm



Each node has a collection of mass density distribution:



$f_i(\vec{r},t), i = 0, \ldots, 6$, with orientation $\vec{e_i}$

1. Streaming: $f_i(\vec{r},t)$ are passed along their orientation $\vec{e_i}$
2. Hydrodynamic variables are calculated:

$$\rho = \sum_{i=0}^{6} f_i \quad ; \quad \rho\vec{u} = \sum_{i=0}^{6} f_i c\vec{e_i}$$

3. Equilibrium mass distribution is calculated:

$$f_i^{eq} = w_i \left[1 + 4\frac{\vec{e_i}\cdot\vec{u}}{c} + 8\frac{(\vec{e_i}\cdot\vec{u})^2}{c^2} - 2\frac{|\vec{u}|^2}{c^2} \right]$$

4. Redistribute f_i as $f_i \longleftarrow f_i + \frac{1}{\tau}\left(f_i^{eq} - f_i\right)$
5. Repeat from Step 1.

LBM for active fluids with contact inhibition of locomotion

Identical algorithm to LBM for passive fluids, BUT instead of using the equilibrium mass distribution

$$f_i^{eq} = w_i \left[1 + 4\,\frac{\vec{e_i}\cdot\vec{u}}{c} + 8\,\frac{(\vec{e_i}\cdot\vec{u})^2}{c^2} - 2\,\frac{|\vec{u}|^2}{c^2} \right],$$

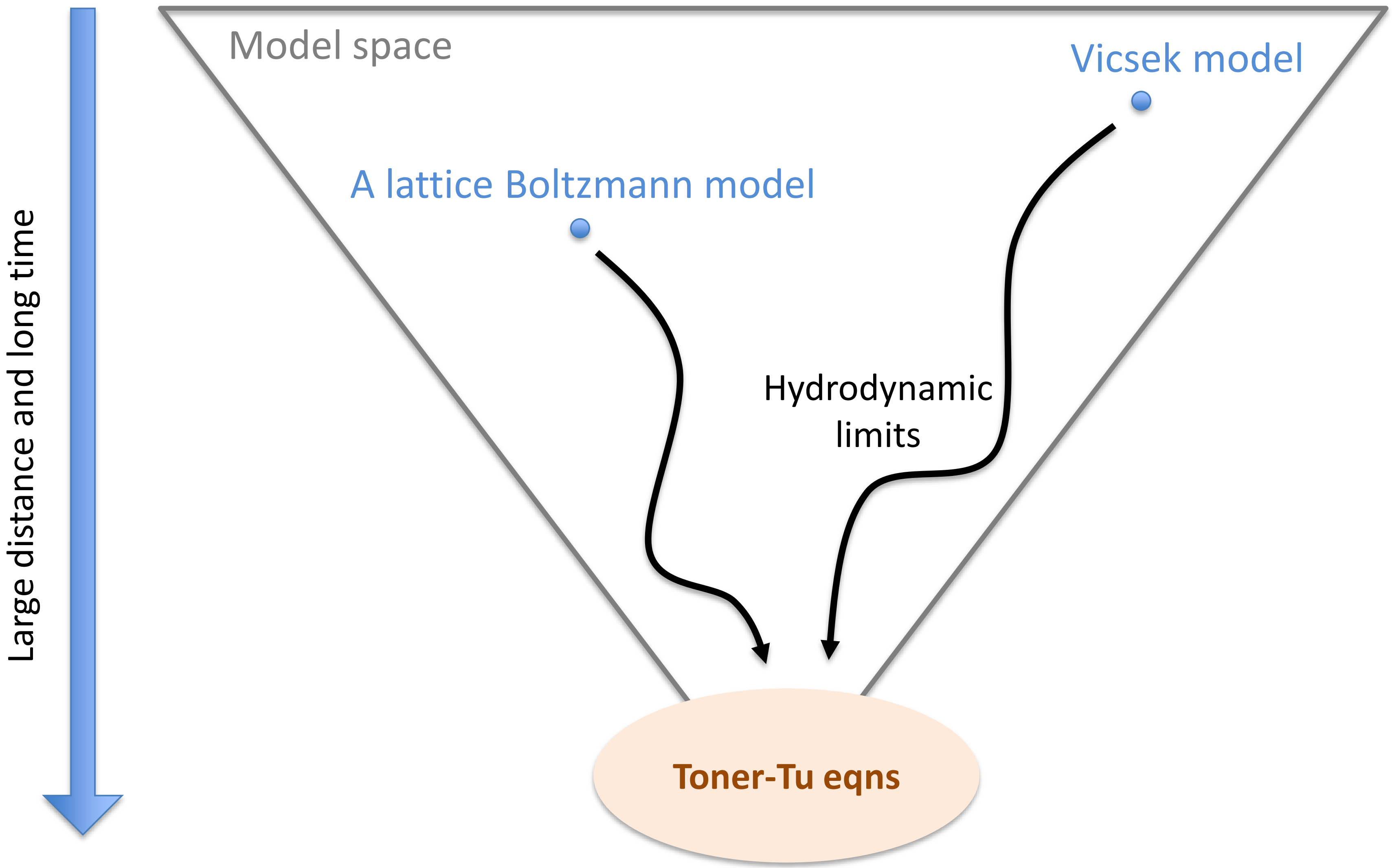
we use the non-equilibrium steady-state distribution

$$f_i^{ss} = w_i \left[1 + 4\,\frac{\vec{e_i}\cdot\vec{u*}}{c} + 8\,\frac{(\vec{e_i}\cdot\vec{u*})^2}{c^2} - 2\,\frac{|\vec{u*}|^2}{c^2} \right],$$

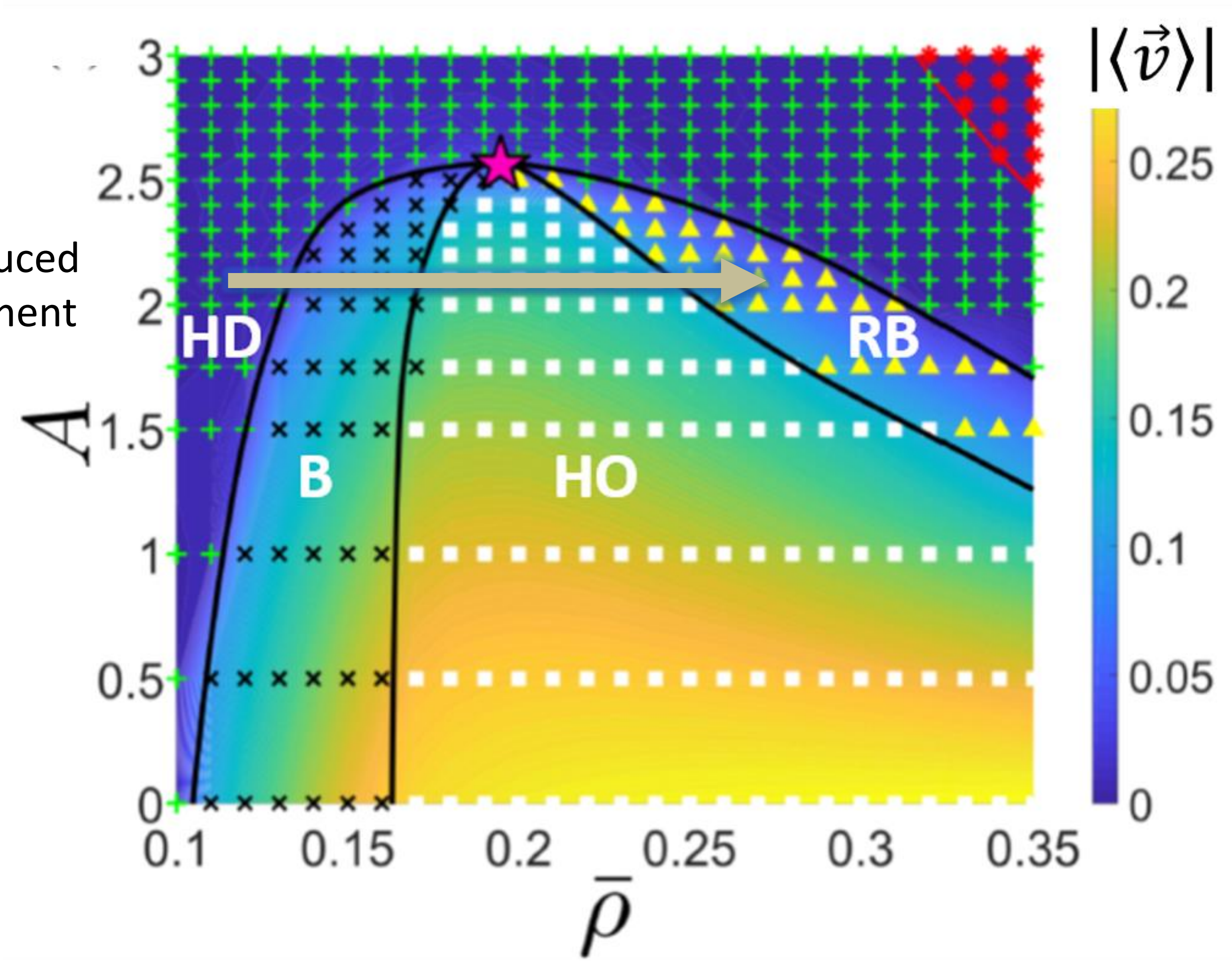
where $\mathbf{u}^* = U_0(\rho)\frac{\mathbf{u}}{|\mathbf{u}|}$ and $U_0(\rho) = \begin{cases} -A\rho^2 + B & \text{if } B \geq A\rho^2 \\ 0 & \text{otherwise} \end{cases}$

A corresponds to the level of density-induced slowing down

Why is the LBM an active fluid model?



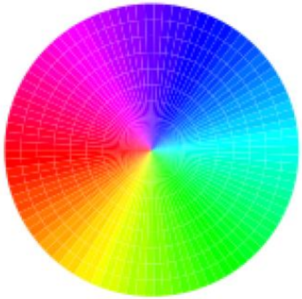
Level of density-induced locomotion impediment

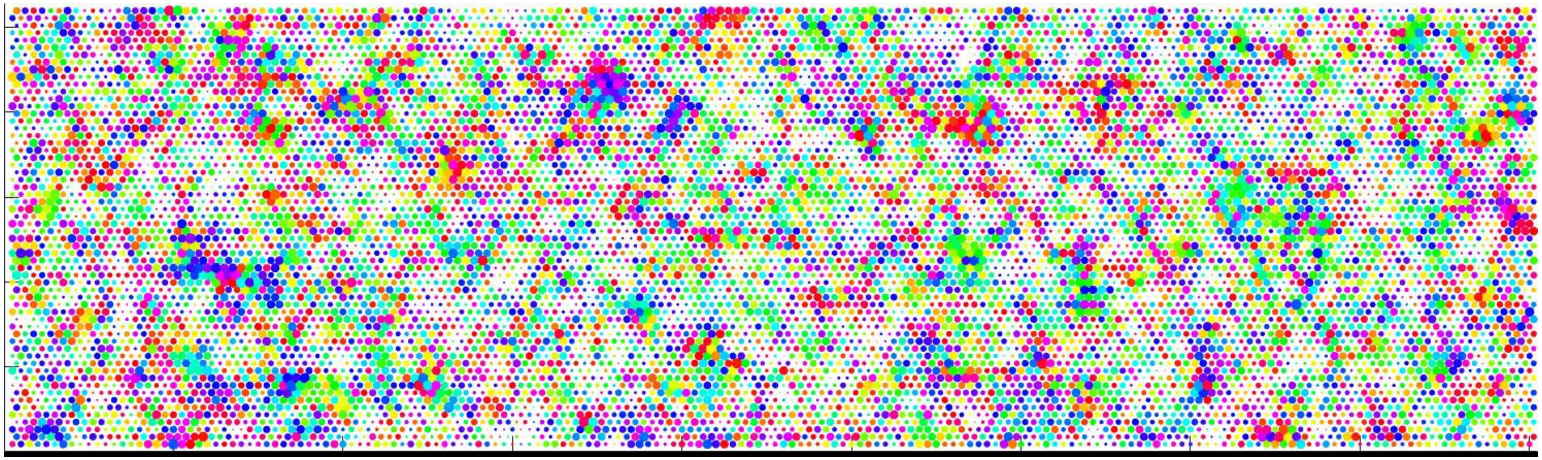


4. NOVEL PHASE BEHAVIOUR – ACTIVE SYSTEMS WITH CONTACT INHIBITION OF LOCOMOTION

Homogeneous disordered (HD) phase

Colour wheel used to determine direction of velocity

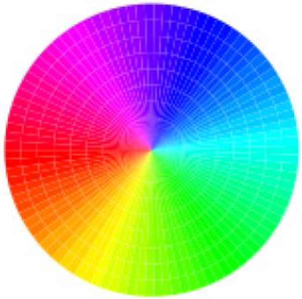


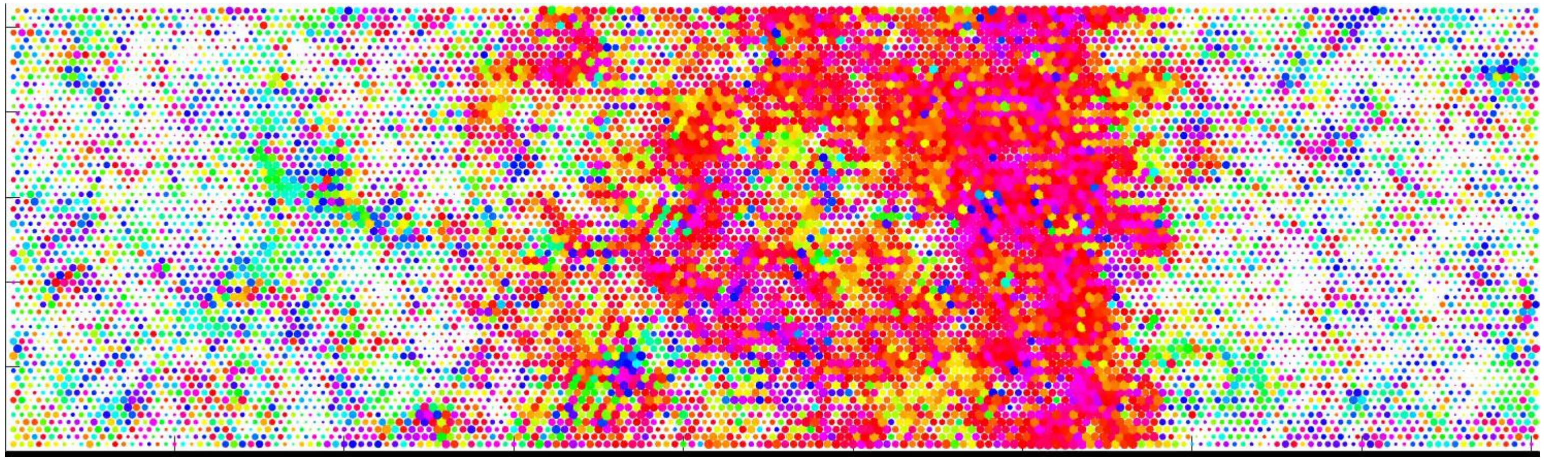


D Nesbitt, G Pruessner & CFL
Uncovering novel phase transitions in dry polar active fluids using a lattice Boltzmann method. E-print: arXiv:1902.00530

Banding (B) regime

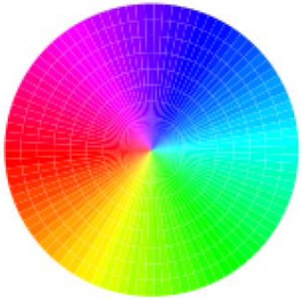
Colour wheel used to determine direction of velocity

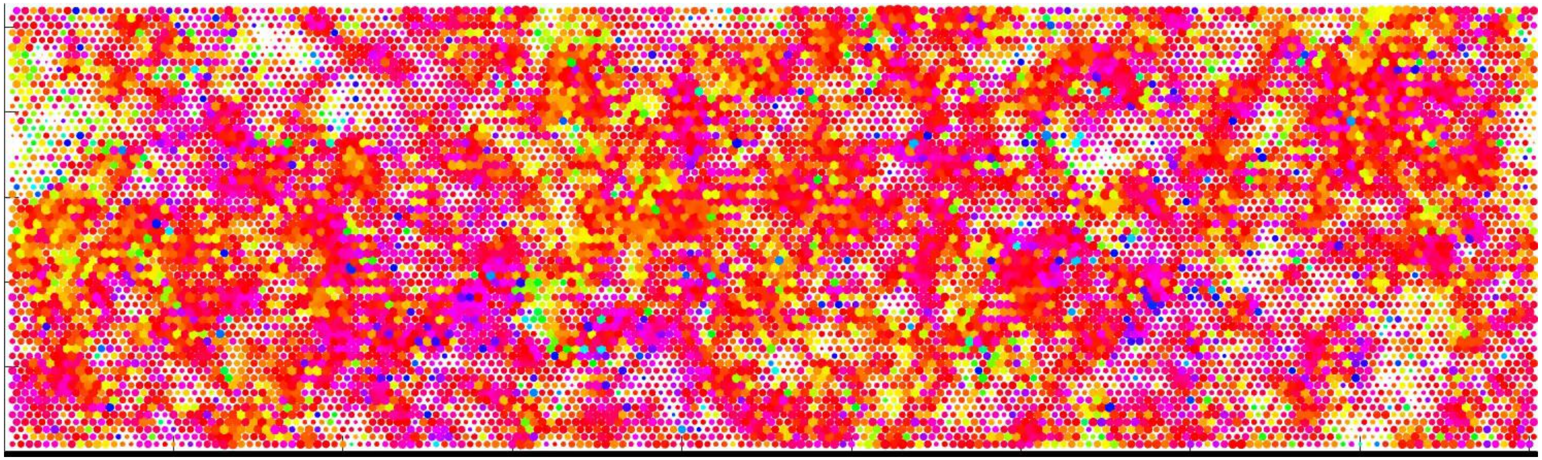




Homogeneous ordered (HO) phase

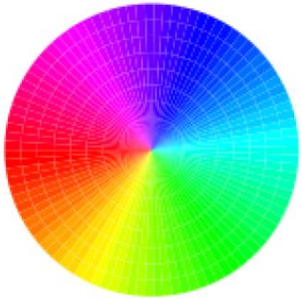
Colour wheel used to determine direction of velocity

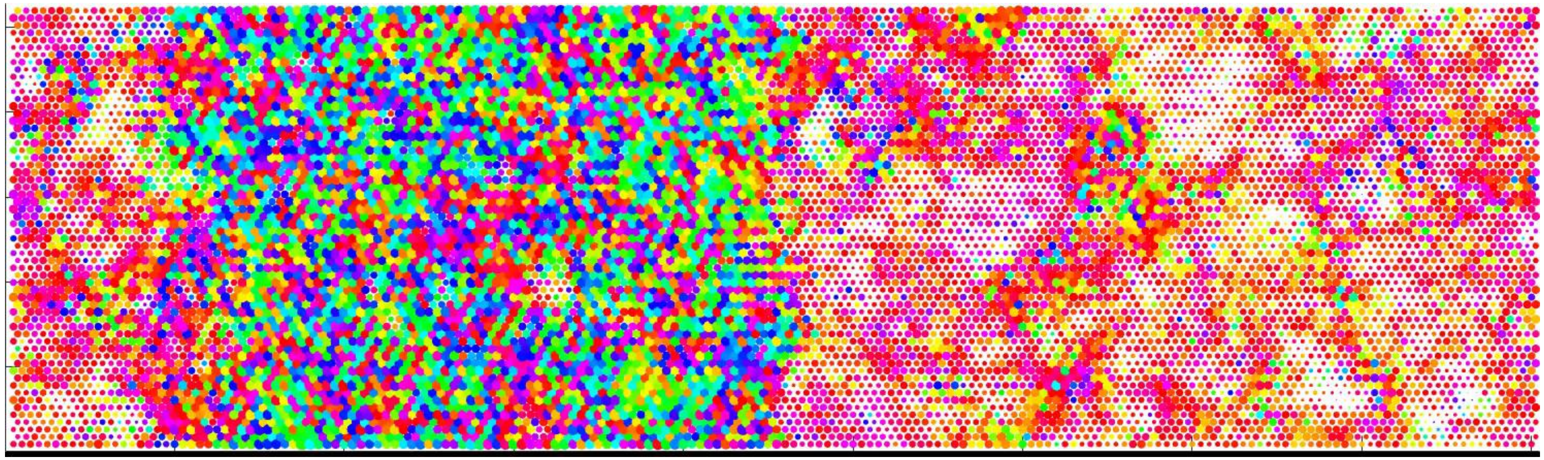




Contact inhibition -> Reverse banding

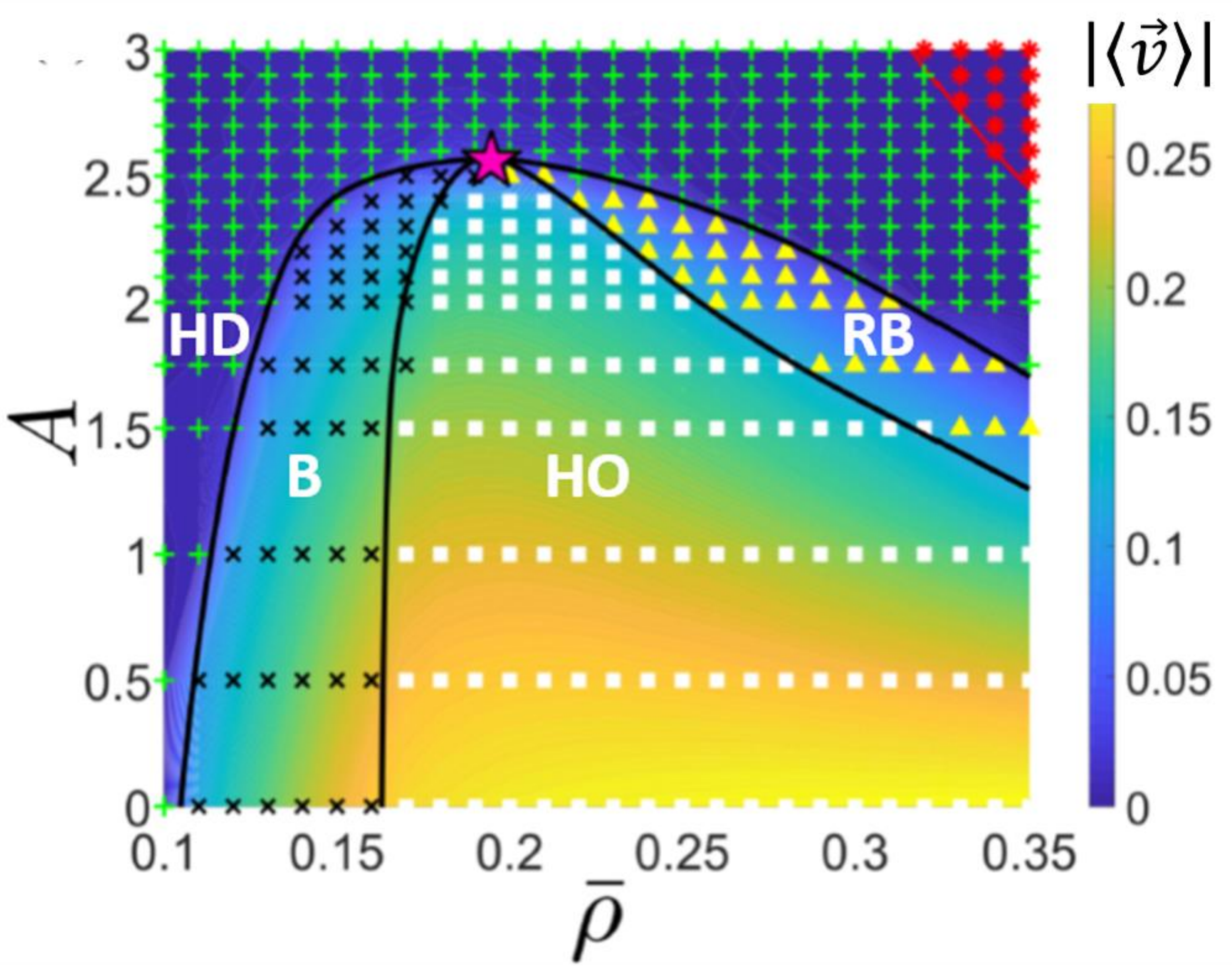
Colour wheel used to determine direction of velocity





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

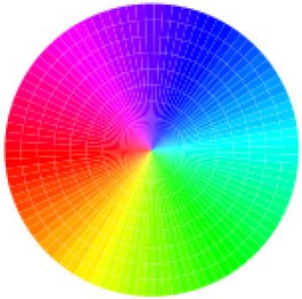
Potential critical behaviour by fine-tuning two parameters

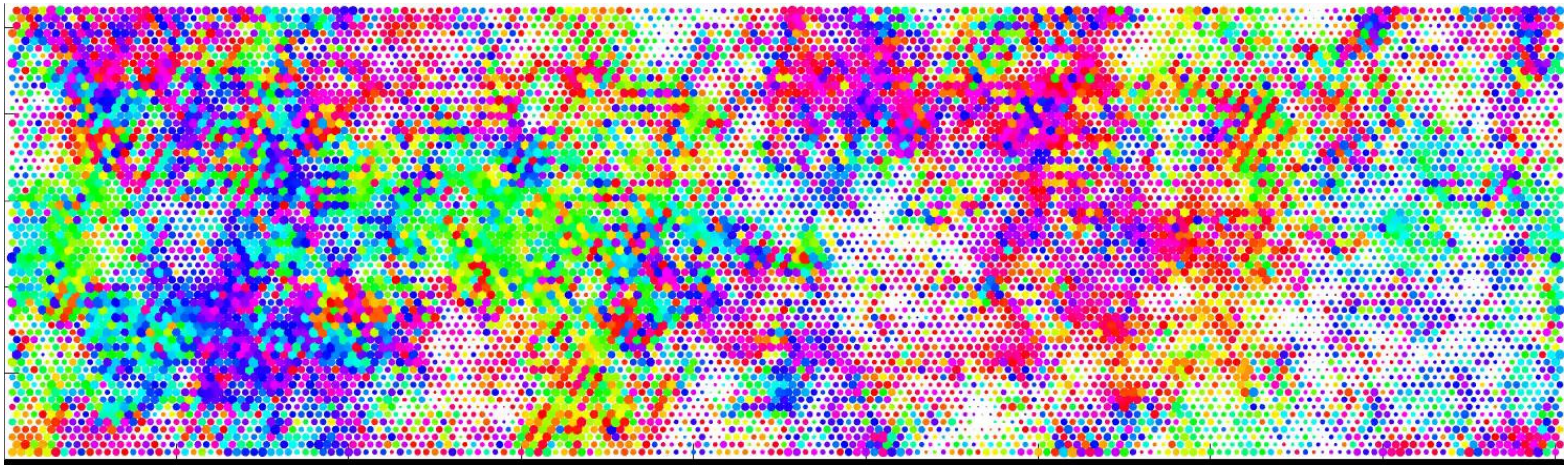


Surprising because critical order-disorder transition is not typically expected from compressible active fluids!

Around the critical point

Colour wheel used to determine direction of velocity





Known critical phenomena in polar active matter

1. Self-propelled particles with long-ranged metric alignment interactions [Ginelli & Chaté (2010) PRL]
2. Incompressible active fluids [Chen, Lee & Toner (2015)]
3. Active Lévy matter [Cairoli & Lee, arXiv:1904.08326]
4. Critical motility-induced phase separation [Partridge & Lee (2019) PRL; Siebert, et al. (2018) PRE; Caballero, Nardini & Cates (2018) J Stat Mech]
5. Self-propelled particles with velocity reversals and alignment interactions [Mahault, et al. (2018) PRL]

Our critical behaviour is different because

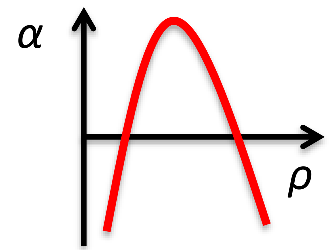
1. Self-propelled particles with long-r… metric alignment interactions [Gi… (2010) PRL]
2. Incompressible … fluids [Chen, Lee & Toner (2015)]
3. Activ… matter [Cairoli & Lee, arXiv:1904.08326]
4. Critical motility-induced ph… n [Partri… …t, et al. (2018) PRE; Caballero, Na… (2018) J Stat Mech]
5. Self-propelled particles with … … [Mahault, et al. (2018) PRL]

Our model does not have long-range interactions

Our order parameter is continuous, not discrete

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

Can we understand the transitions analytically?



- 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

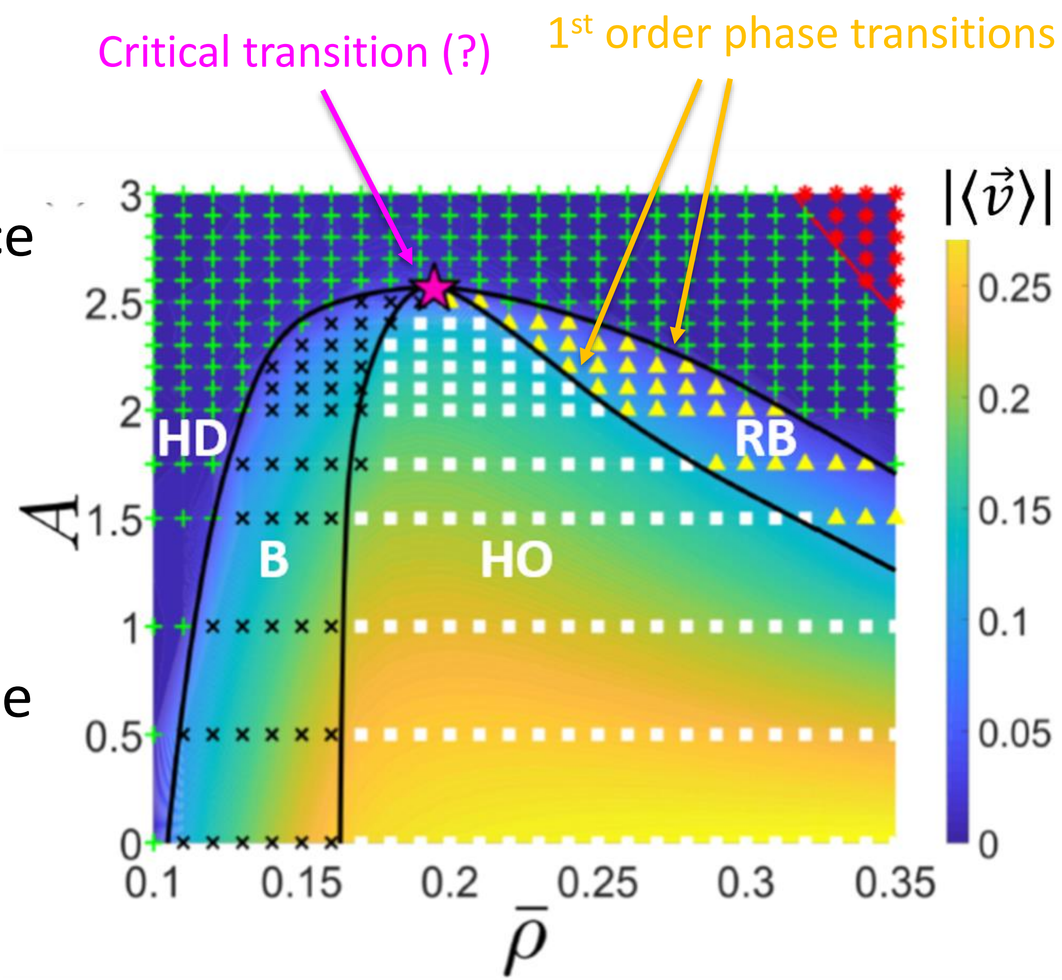
$$\frac{\alpha_1^2}{\beta} - 2\alpha_0 \left(2\kappa + \frac{\alpha_1 \lambda}{\beta}\right) > 0$$

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

Summary

- We developed a Lattice Boltzmann model of active fluids with contact inhibition of locomotion
- We obtained the phase diagram with novel phase transitions



Ref: D Nesbitt, G Pruessner & CFL. Uncovering novel phase transitions in dry polar active fluids using a lattice Boltzmann method. E-print: arXiv:1902.00530

The Team at Imperial College

Ben Partridge | Jean David Wurtz | **David Nesbitt** | Andrea Cairoli | Alice Spenlauhauer

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Collaborator: Gunnar Pruessner (Mathematics, Imperial College)