Phase transition in polar active fluids

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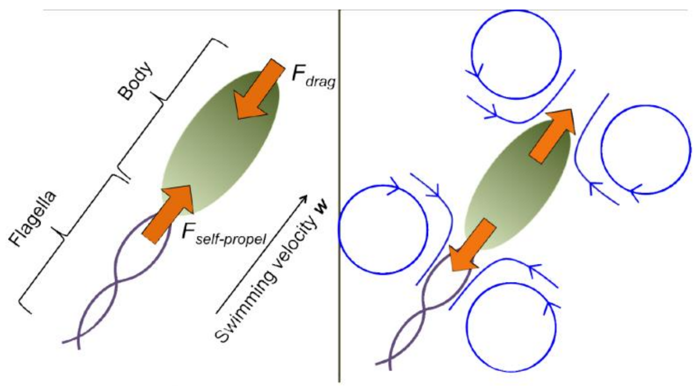
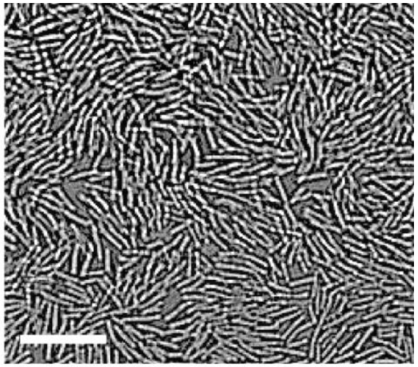
ACTIVE FLUIDS

Forces acting on a bacterium

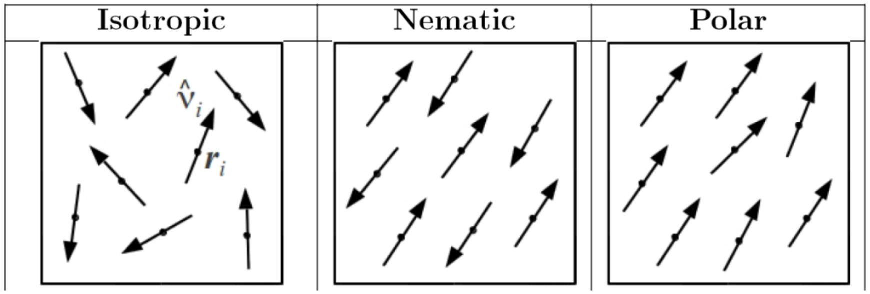
Forces acting on the surrounding fluid by the bacterium



Schematic of a single bacterium suspended in a fluid solvent



Bacterial suspension;
Wensinka et al. PNAS, 4, 2012, 109, 36



Orientational order in a suspension of active particles

polar order in a sardine school

1. Elsen Tjhung, Phenomenology and Simulations of Active Fluids, PhD thesis, 2013

CONTINUUM MODEL

Two dynamical fields: velocity **u,** polarization **P**

$$\begin{cases} \frac{\partial \mathbf{P}}{\partial t} + (\mathbf{u} + w\mathbf{P}) \cdot \nabla \mathbf{P} = -\underline{\underline{\Omega}} \cdot \mathbf{P} + \xi \underline{\underline{v}} \cdot \mathbf{P} - \frac{1}{\Gamma} \frac{\delta F}{\delta \mathbf{P}} \\ \rho \left\{ \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right\} \mathbf{u} = -\nabla P + \nabla \cdot \left(\underline{\underline{\sigma}}^{passive} + \underline{\underline{\sigma}}^{active} \right) \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

Leslie–Ericksen theory of nematic liquid crystals

Incompressible Navier-Stokes equations

$$\underline{\underline{\sigma}}^{passive} = \underline{\underline{\sigma}}^{viscous} + \underline{\underline{\sigma}}^{elastic}$$

$\underline{\underline{\sigma}}^{active} = -\zeta \mathbf{PP}$ active stress due to the permanent force dipole in each particle.

$F[\mathbf{P}] = \int dV \left\{ -\frac{a}{2} |\mathbf{P}|^2 + \frac{b}{4} |\mathbf{P}|^4 + \frac{\kappa}{2} (\nabla \mathbf{P})^2 \right\}$ free energy functional

$\mathbf{h} = -\frac{\delta F}{\delta \mathbf{P}}$ tends to relax the system towards the free energy minimum

$\underline{\underline{v}}$ and $\underline{\underline{\Omega}}$ are the symmetric and anti-symmetric part of the velocity gradient tensor, Γ is a relaxational constant related to the rotational viscosity of the liquid crystalline fluid and ξ is related to the geometry of the swimmers, i.e. $\xi > 0$ for rod-like molecules and $\xi < 0$ for oblate molecules

2.P. G. de Gennes and J. Prost. The Physics of Liquid Crystals. Clarendon Press,1993.

3. Y. Hatwalne, S. Ramaswamy, M. Rao and R. A. Simha, Phys. Rev. Lett., 2004, 92, 118101.

RESULTS

non-slip walls are defined at z=0 and z=L with strong anchoring conditions for the polarization field $\mathbf{P} = \hat{y}$, whereas periodic boundaries are defined at y=0 and y=L

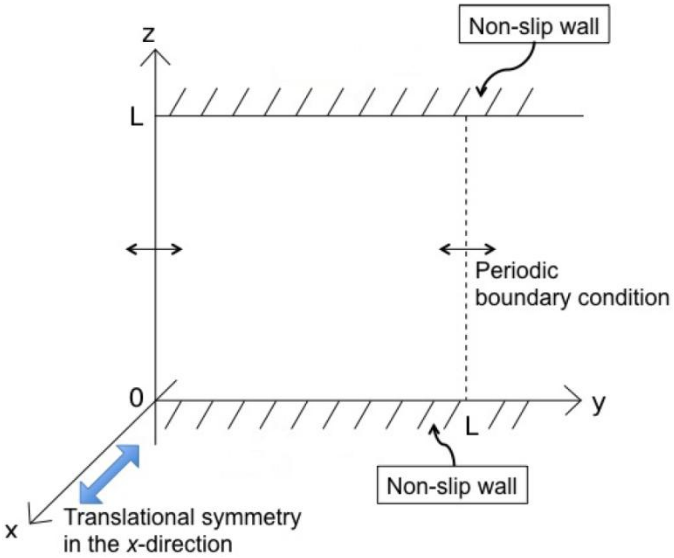
parameters values:

$\Gamma = 1 \quad \xi = 1.1 \quad a = b = 0.1 \quad \kappa = 0.04 \quad \tau = 2.5$

$w = 0$ shakers

$\zeta > 0$ extensile

system size=30x30



quasi two-dimensional geometry [4]

4. E. Tjhung, M. E. Cates and D. Marenduzzo Nonequilibrium steady states in polar active fluids. Soft Matter, 2011, 7, 7453

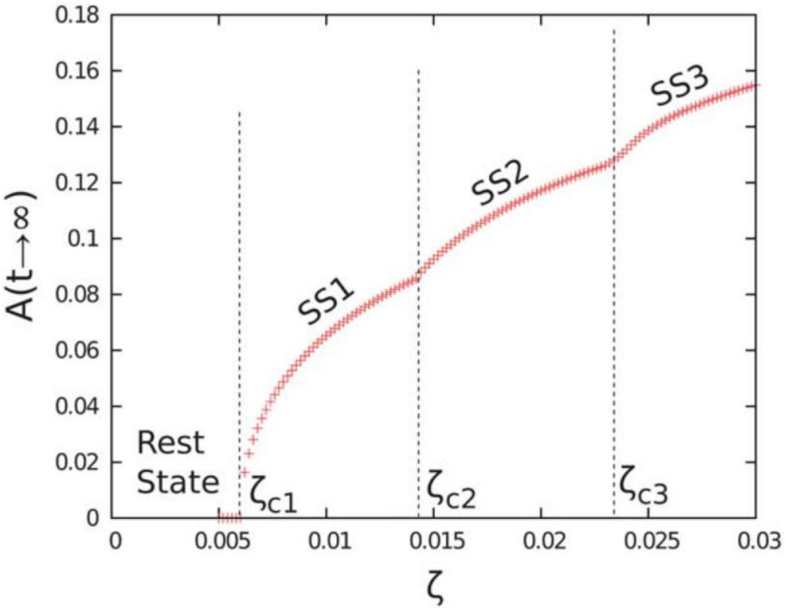
RESULTS

One obvious solution of the governing equations is the no-flow or rest state

$$\mathbf{P}(\mathbf{r},t) = \hat{y} \qquad \mathbf{u}(\mathbf{r},t) = 0$$

However, at higher activities (above some critical value) the rest state becomes linearly unstable and the system undergoes a spontaneous flow transition

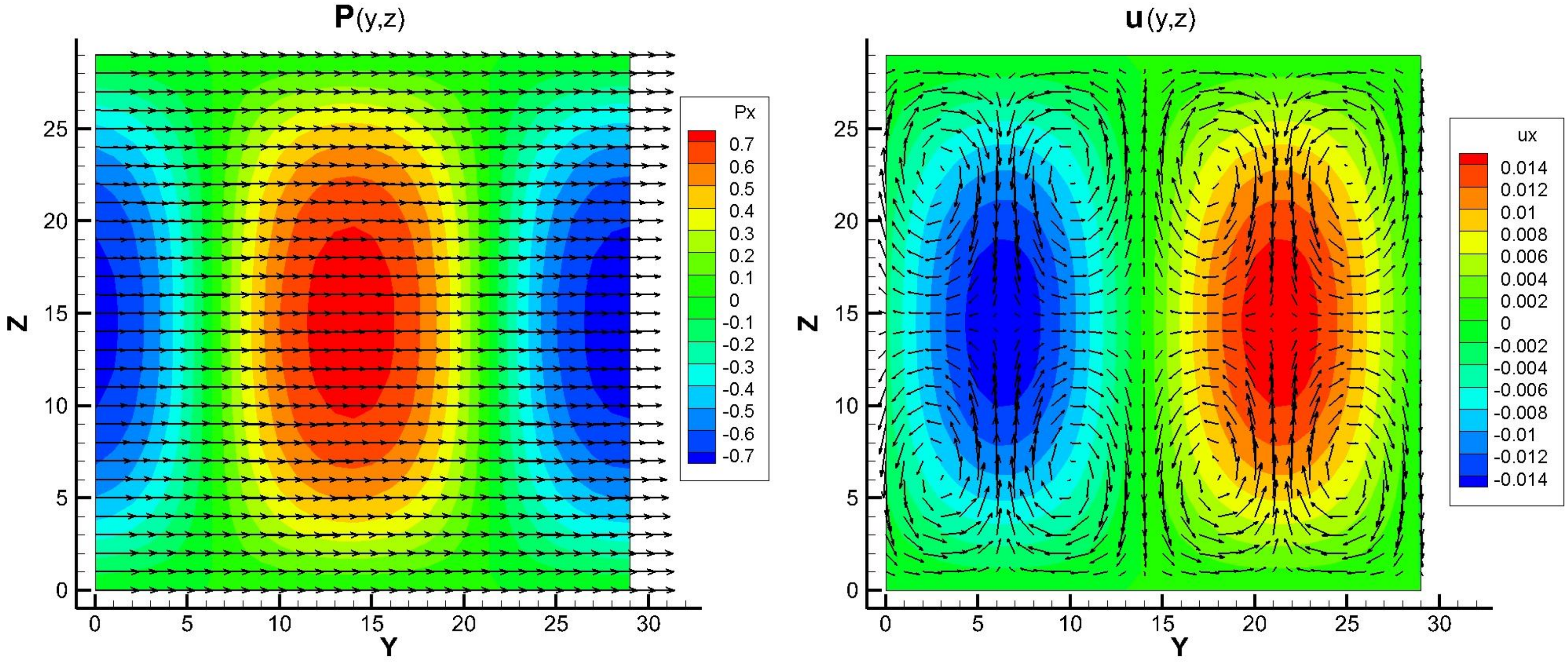
$$A(t) = \left(\frac{1}{V} \int dV (\nabla \mathbf{P})^2 \right)^{\frac{1}{2}}$$ amplitude of deformation which characterizes the spontaneous flow transition



Amplitude of deformation as a function of the activity. The plot shows three distinct steady states separated by three critical points. Below the first critical point, the rest state is stable. However past this threshold there is a flow transition and three different steady state (SS) can be identified.
For higher activity, the unstable system becomes oscillatory or even chaotic

4. E. Tjhung, M. E. Cates and D. Marenduzzo, Nonequilibrium steady states in polar active fluids. Soft Matter, 2011, 7, 7453

SS1



Steady state polarization field (left) and fluid velocity (right). The out-of planes components may dominate the in-plane ones. For instance, typically the out-of-plane velocity is 2-3 orders of magnitude larger then the in-plane ones.

RESULTS WITH A NEW PHENOMENOLOGICAL TERM

In order to force the alignment between polarization and velocity vector a new phenomenological term, proportional to **u**, was introduced in the evolution equation of the polar vector, which becomes

$$\frac{\partial \mathbf{P}}{\partial t} + (\mathbf{u} + w\mathbf{P}) \cdot \nabla \mathbf{P} = -\underline{\underline{\Omega}} \cdot \mathbf{P} + \xi \underline{\underline{v}} \cdot \mathbf{P} - \frac{1}{\Gamma} \frac{\delta F}{\delta \mathbf{P}} + C\mathbf{u}$$

Simulations were performed by fixing ζ and varying *C.* Here, the results with periodic condition (PBC) on all the boundaries are shown. The initial conditions are **P**(**r**,0)=random and **u**(**r**,0)=0

Parameters:
system size=35x35

$w = 0$ shakers

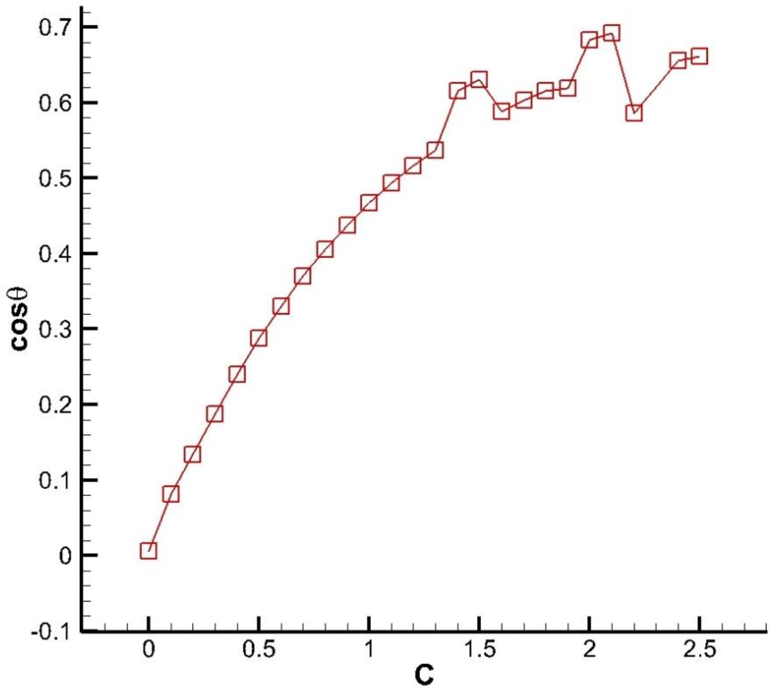
$\zeta = 0.01$ extensile

$a = b = 0.2$

$\kappa = 0.04$

$\Gamma = 1$ $\xi = 1.1$

$\tau = 2.5$

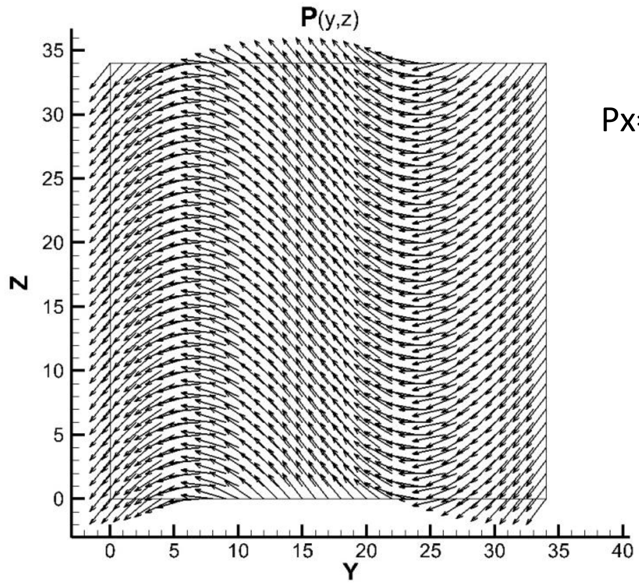


mean cosΘ as a function of *C,* where Θ is the angle between the vector **u** and **P**

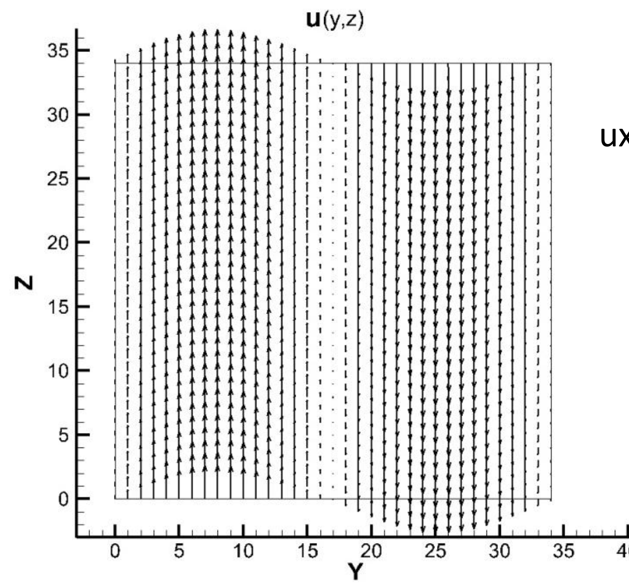
RESULTS WITH PBC

$C = 0.1$

$\zeta = 0.01$



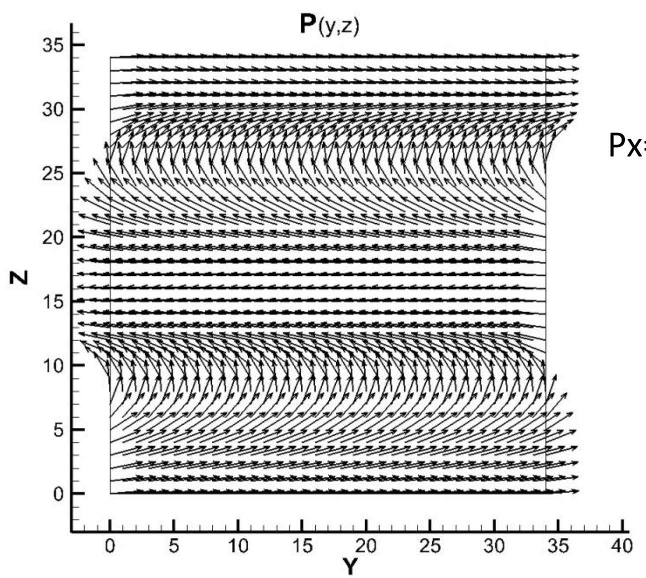
Px=0



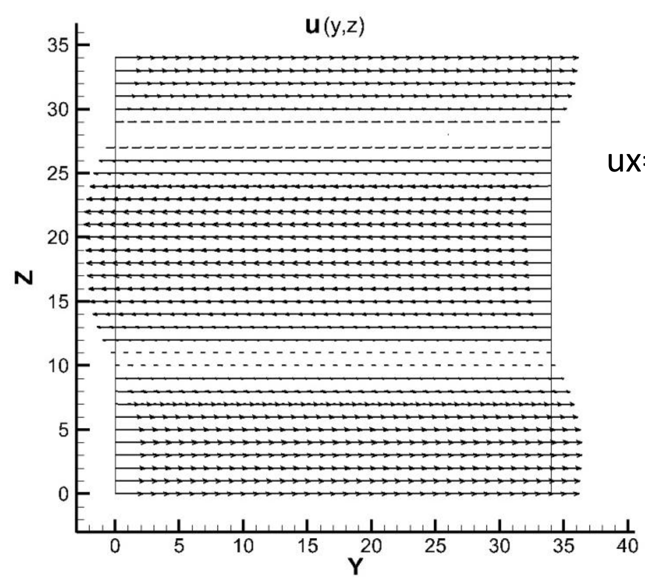
ux=0

$C = 2.1$

$\zeta = 0.01$



Px=0



ux=0

RESULTS WITH WALLS

non-slip walls at z=0 and z=L with strong anchoring conditions for the polarization field $\mathbf{P} = \hat{y}$

Parameters:
system size=35x35

$w = 0$ shakers

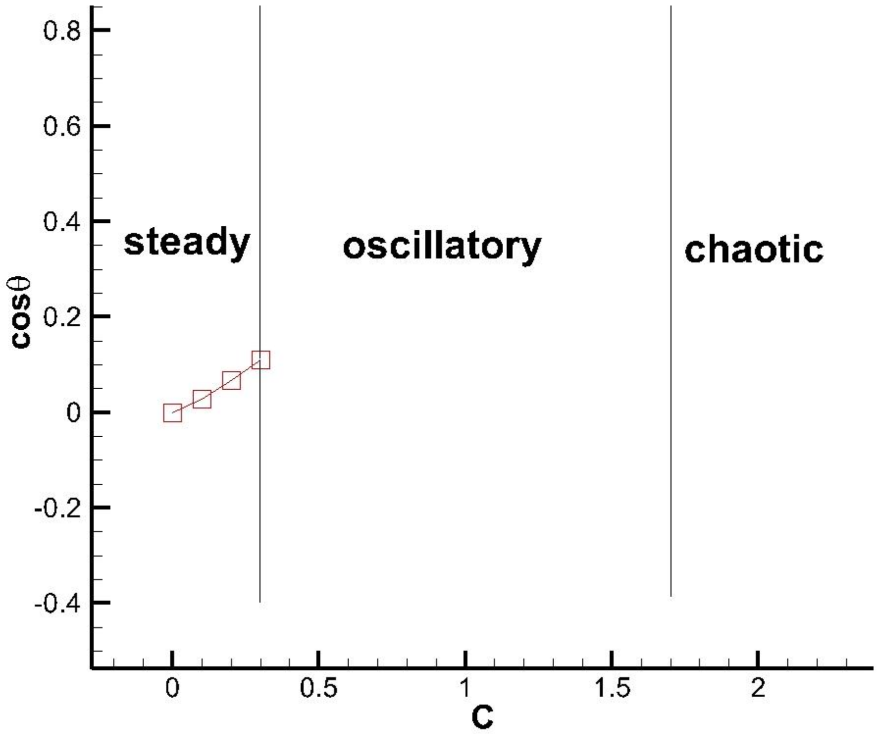
$\zeta = 0.01$ extensile

$a = b = 0.2$

$\kappa = 0.04$

$\Gamma = 1$ $\xi = 1.1$

$\tau = 2.5$



mean cosΘ as a function of *C,* where Θ is the angle between the vector **u** and **P**

SUMMARY

Polar active fluids studied by using a coarse-grained continuum model

Spontaneous flow transition in a quasi-2-dimensional geometry

three distinct steady states

large out-of-plane components

for higher activity the system becomes oscillatory or even chaotic

New phenomenological term to force the alignment between polarization and velocity vector

the system with PBC shows a continuous transition to aligned configurations

the system with WALLS shows an unstable behavior and it becomes oscillatory or even chaotic by increasing *C*