Enhanced Order in Two-temperature Models of Scalar Activity

Chandan Dasgupta
Indian Institute of Science and
International Centre for Theoretical Sciences
Bangalore, India

Active Matter and Beyond
ICTS, Bangalore
November 6, 2023

Collaborators

S. Siva Nasarayya Chari (Indian Institute of Science, Currently at University of Allahabad, India)
Jayeeta Chattopadhyay (Indian Institute of Science, Currently at Niels Bohr Institute, Denmark)
Sriram Ramaswamy (Indian Institute of Science)
Prabal K. Maiti (Indian Institute of Science)

Soft Matter **15**, 7275 (2019)
Phys. Rev. E **104**, 054610 (2021)
Phys. Rev. E **107**, 024701 (2023)

What is scalar activity?

Activity is “vectorial” in nature in most model systems - it is represented by a self-propulsion force.

N. Ganai, S. Sengupta, G. I. Menon, Chromosome Positioning from Activity Based Segregation, Nucleic Acids Research, **42**, 4145 (2014):
Approximated differences in activity in different components by different “temperatures” for the components.

This is known as **scalar activity**

S. N. Weber, C. N. Weber and E. Frey, Phys. Rev Lett. **116**, 058301 (2016): Brownian dynamics simulation of a binary mixture of particles with different diffusivities in two dimensions.

J. Smrek and K. Kremer, Phys. Rev. Lett. **118**, 098002 (2017); Entropy **20**, 520 (2018): Molecular dynamics simulation of a mixture of hot and cold model polymer chains.

“Hot” and “Cold” components phase separate if the two temperatures are sufficiently different.

Theory of phase separation:

Y. Grosberg and J.-F. Joanny, Phys. Rev. E **92**, 032118 (2015); Polymer Sci. C **60**, 118 (2018).

E. Ilker and J.-F. Joanny, Phys. Rev. Res. **2**, 023200 (2020)

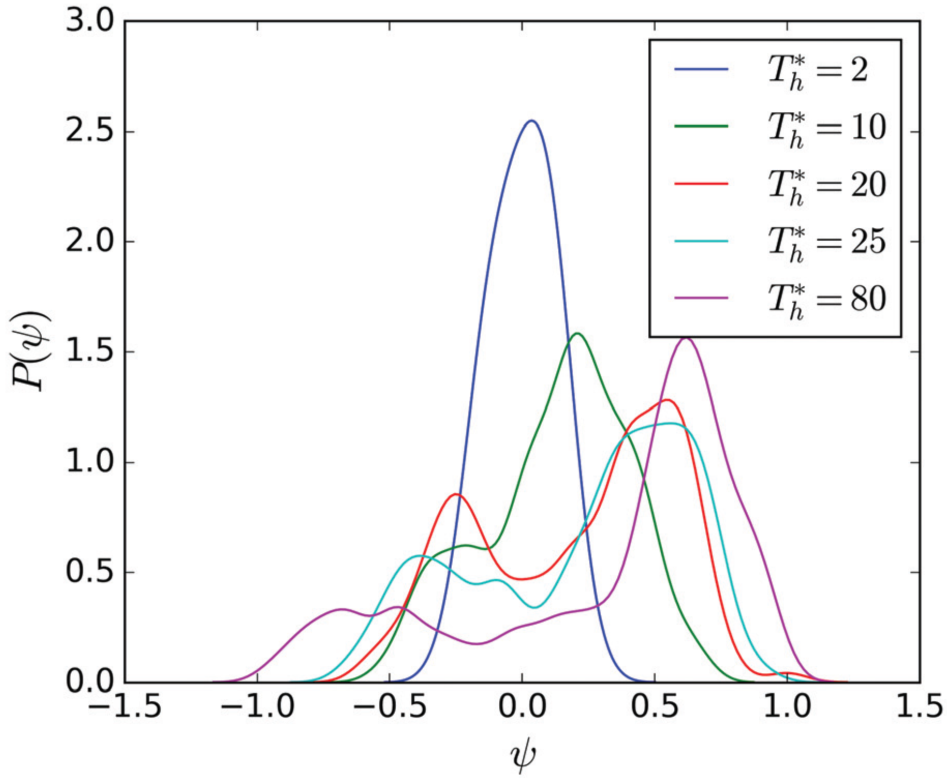
In two-temperature models of scalar activity, phase separation may lead to enhanced order in the cold component

I. Lennard-Jones particles in three dimensions
II. Soft repulsive spherocylinders in three dimensions

Half of the particles (labeled “hot”) are connected to a thermostat at a higher temperature T_h while the rest of the particles (labeled “cold”) remain connected to a thermostat at a lower temperature T_c equal to that of the initial equilibrium system.

Measure of scalar activity: $\chi = T_h/T_c - 1$

Lennard-Jones particles in three dimensions



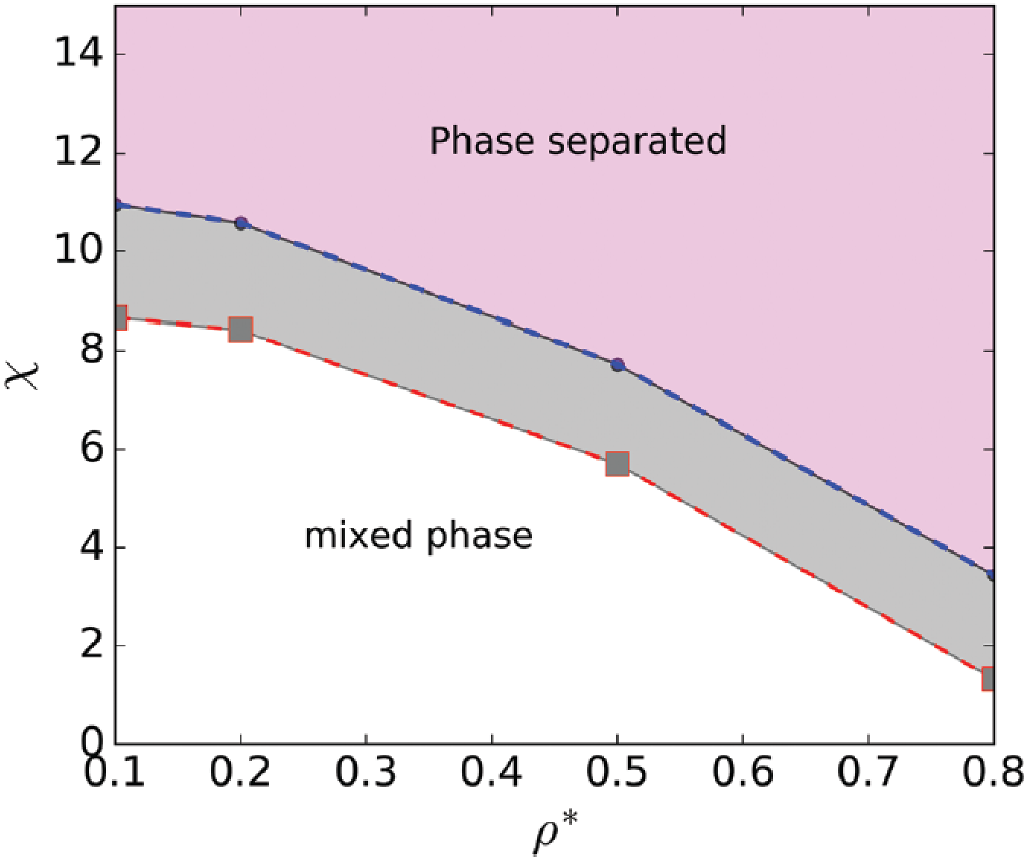
$$\psi = < (n_h - n_c)/(n_h + n_c) >$$

n_h (n_c): Number of hot (cold) particles in a sub-box

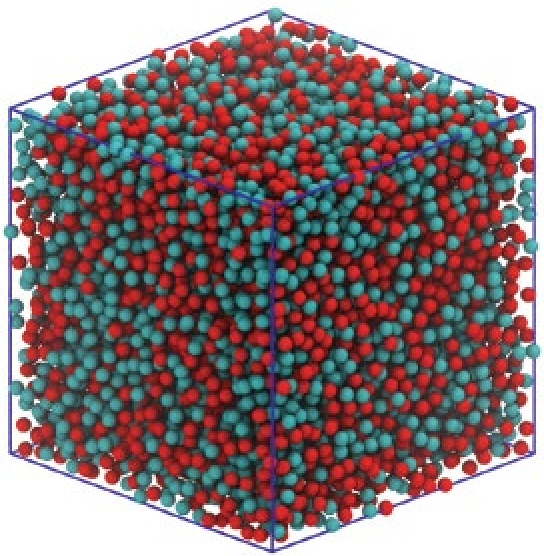
Distribution of ψ becomes bimodal after phase separation

Lennard-Jones particles in three dimensions

Phase Diagram

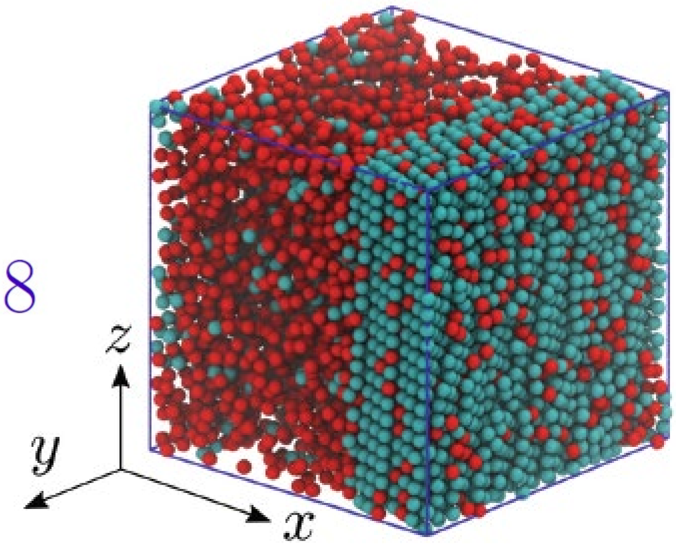


Lennard-Jones particles in three dimensions



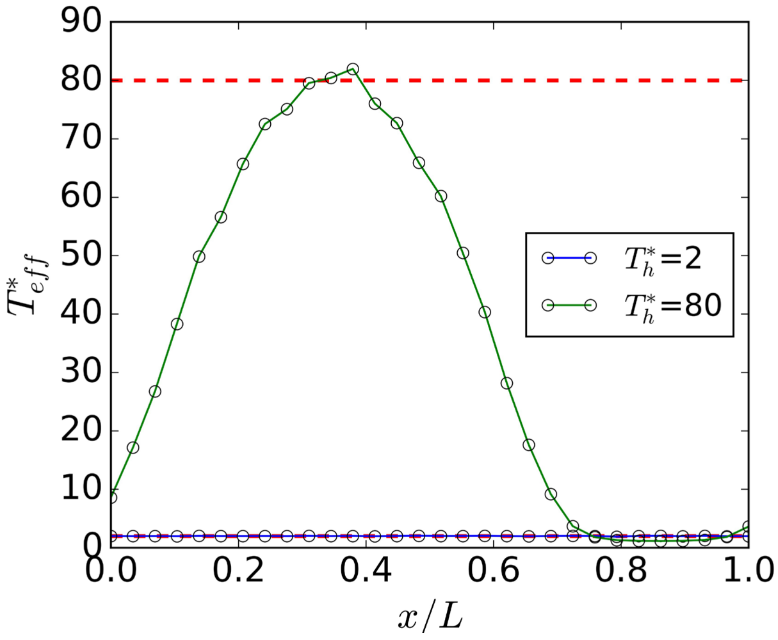
$T_c = T_h = 2.0$

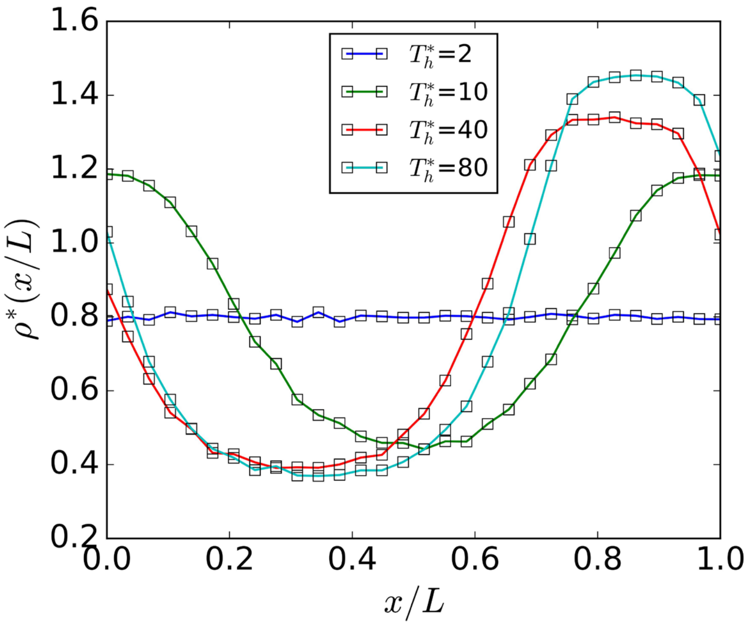
$\rho = 0.8$



$T_c = 2.0, \;\; T_h = 80.0$

Particles in the cold region exhibit crystalline order

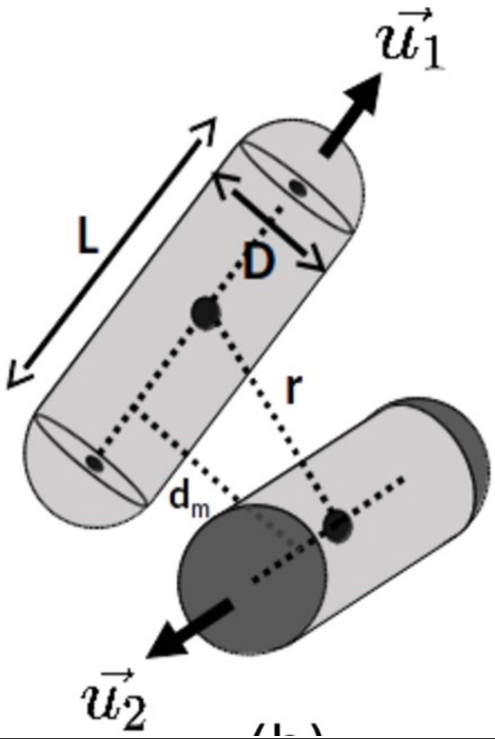


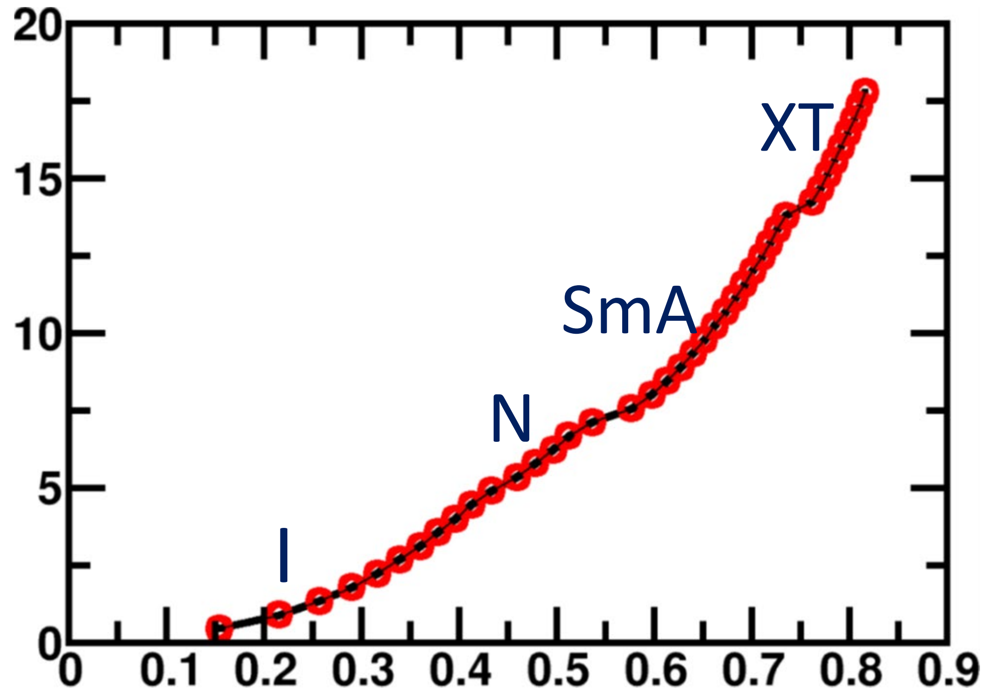


Equilibrium system at the density and effective temperature in the cold region **does not exhibit crystallization.**

Enhancement of order!

Soft repulsive spherocylinders in 3 dimensions





Length L and diameter D, truncated Lennard-Jones interaction (WCA potential)

Equation of state (pressure vs. packing fraction) for L/D = 5.0 at equilibrium at T=5.0

Phase behavior at equilibrium depends on A = L/D

A_{SRS}	A_{HSC}	$\chi = 0$	Phases at $\chi \neq 0$
5	5.28	I, N, Sm, K	I, N, Sm, K, multidomain K at $\eta = 0.36$
3	3.20	I, Sm, K	I, **N**, Sm, K at $\eta = 0.33$
2	2.11	I, K	I, **Sm**, K at $\eta = 0.45$

Shape parameter A = L/D, Packing fraction η

Activity parameter $\chi = T_h/T_c - 1$

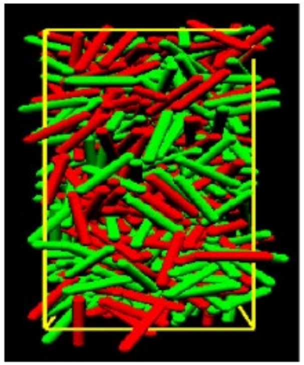
Liquid-crystalline order is determined from order parameters and orientational and translational correlation functions.

Nematic Order Parameter

$$Q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{3}{2} u_i^{\alpha} u_i^{\beta} - \frac{1}{2} \delta_{\alpha\beta} \right).$$

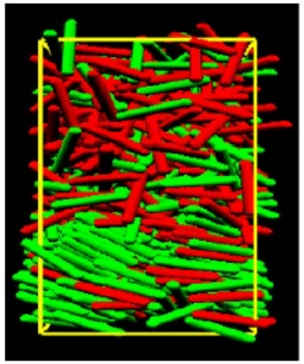
Scalar order parameter S: Largest eigenvalue of **Q**

Results for A = 5.0



$\chi = 0.00$

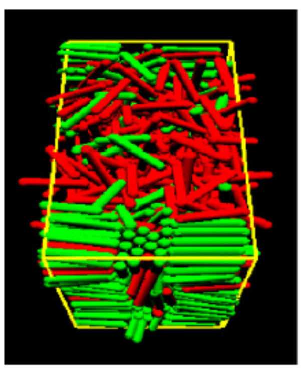
S= 0.02 -I



$\chi = 2.00$

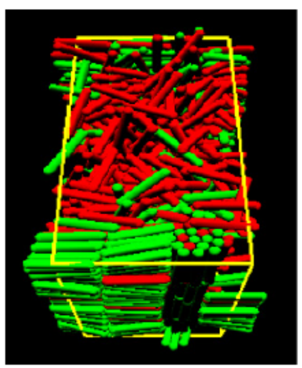
$S_{cold} = 0.50$ - N

$S_{hot} = 0.07$ - I



$\chi = 5.00$

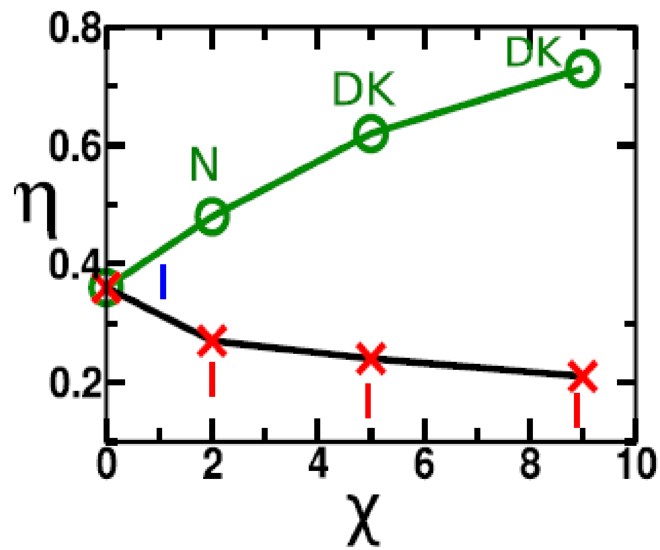
$S_{cold} = 0.62$-
Domain crystal
$S_{hot} = 0.06$- I



$\chi = 9.00$

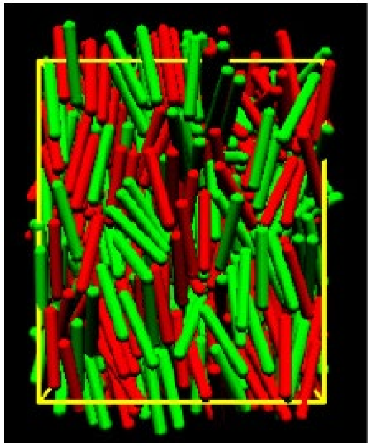
$S_{cold} = 0.64$ -
Domain crystal
$S_{hot} = 0.06$-I

Initial equilibrium state is in the isotropic phase



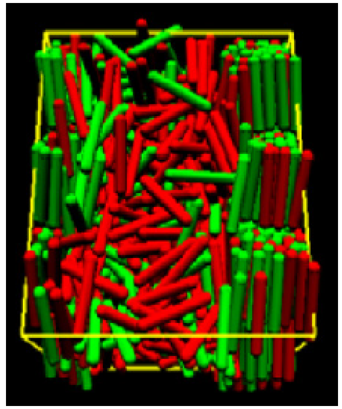
Heating half the particles leads to ordering of the other half of the particles

Results for A = 5.0



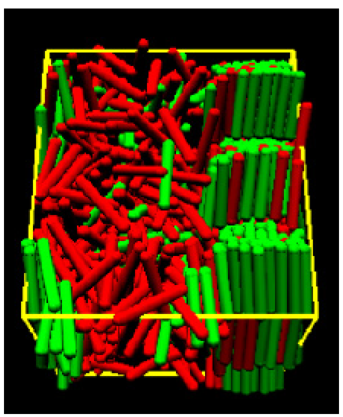
$\chi = 0.00$

$S = 0.75$-N



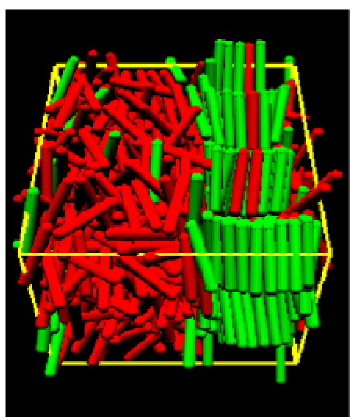
$\chi = 2.00$

$S_{cold} = 0.97$- SmA
$S_{hot} = 0.10$- I



$\chi = 5.00$

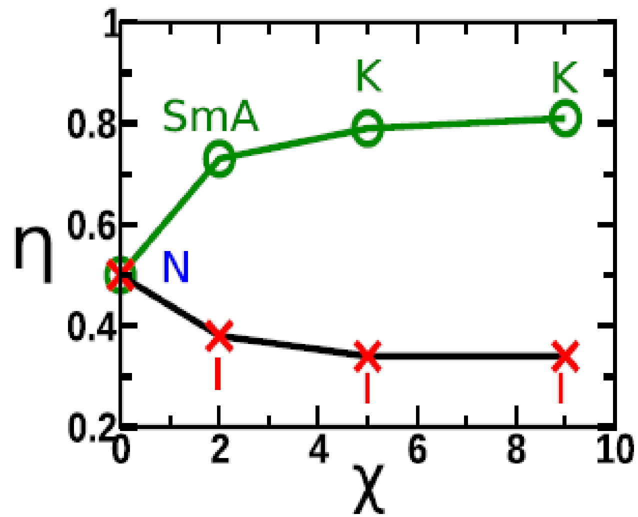
$S_{cold} = 0.99$- K
$S_{hot} = 0.10$- I



$\chi = 9.00$

$S_{cold} = 0.99$- K
$S_{hot} = 0.08$- I

Initial equilibrium state is in the nematic phase

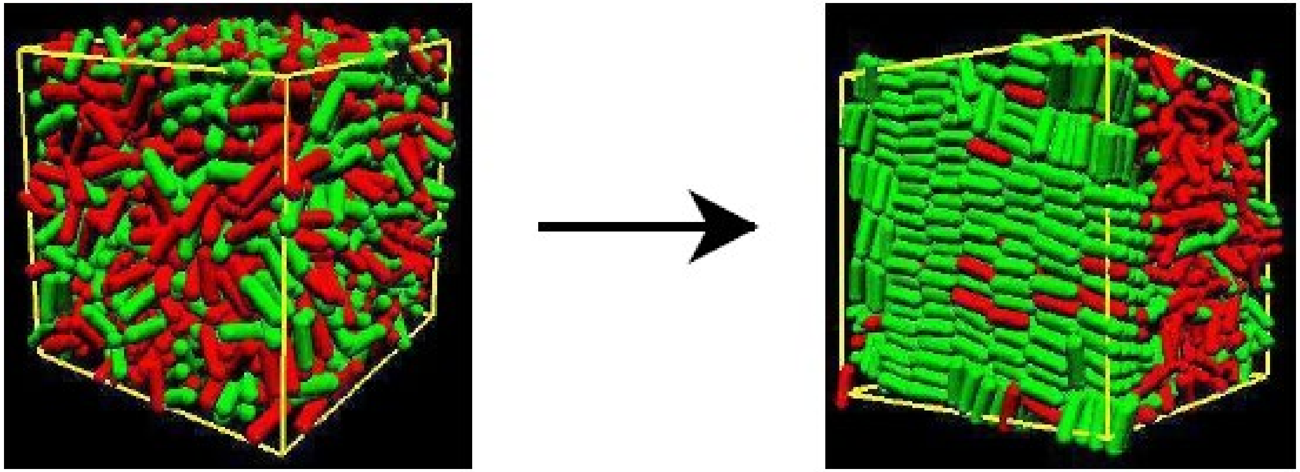


The degree of order in the cold region is higher than that in an equilibrium system under the same conditions.

Scalar activity may lead to the realization of phases that are not present at equilibrium

For L/D = 2, the nematic and smectic-A phases are absent at equilibrium.

$\eta = 0.45$



$\chi = 0$ [Isotropic]

$\chi = 9$

Smectic A phase is found in the cold region for $\chi = 9$

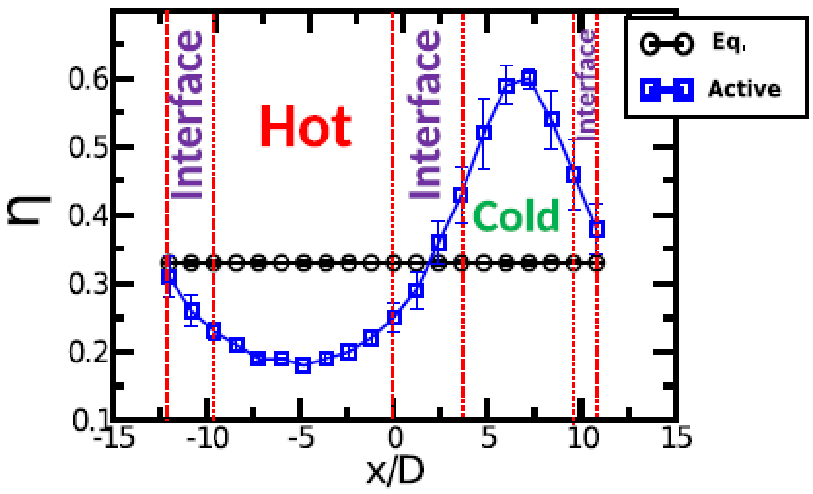
Conclusions from simulations:

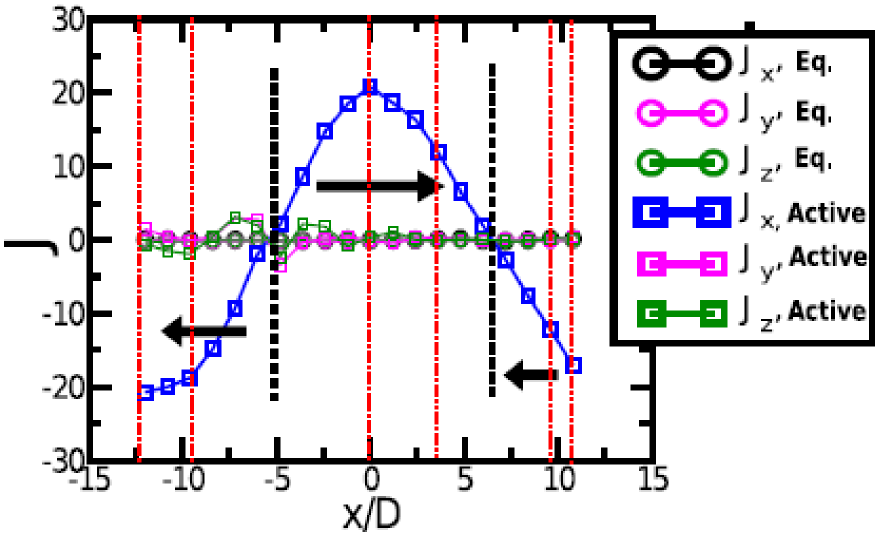
A. Scalar activity leads to enhanced order in the cold region.
B. Scalar activity induces phases that are inaccessible at equilibrium.

If the interface between hot and cold regions is sharp, then the particles in the bulk of the two regions should behave as if they are at equilibrium at the densities and temperatures in the bulk regions.

Density and temperature change smoothly in the direction normal to the interface.

$$L/D = 3.0, \quad \eta = 0.33, \quad \chi = 9.0$$





- ❑ Interfaces are not sharp.
- ❑ Heat flux normal to the interface is nonzero throughout the system.

Need to consider the phase behavior in the presence of a heat flux.

Thank You