Clustering and Flow of Self-Propelled Particles in Channels

S. Othman, T. Auth, J. Midya, G. Gompper
Theoretical Physics of Living Matter, Forschungszentrum Jülich, Germany

Motivation

- Examples for flow of granular matter in channels are abundant on the microscale (e.g., microfluidics of fluids containing colloids) and macroscale (e.g., pedestrians in tunnels)
- Flow can be driven externally (e.g., by a gravitational or electric field or a pressure difference) or internally by self-propelled agents.
- Targeted drug delivery in the human blood vessels may be achieved with the help of self-propelled particles as delivery vehicles.
- Formation of dense phases (e.g., particle clusters) can act as obstacle and clog channels, in particular for complex channel geometries.
- We aim to determine phase diagrams of self-propelled particles to predict parameter ranges for dilute and dense phases
- We aim to determine the influence of channel walls and an external alignment field on the distribution of the particles in the channels.

Active matter

Flock of starlings (NanoWerk.com)

- Bird flocks and fish schools show amazing collective motion.
- Active matter consists of self-propelled agents which consume energy to generate propulsion forces [1].
- A generic model system for active matter is active Brownian particles (ABPs) where the individual agents are subject to thermal motion in addition to their self-propulsion.
- In two dimensions, ABPs refers to circular discs that are subject to translational and rotational thermal motion; rotational thermal motion changes the direction of self-propulsion.

Model & Methods

- We simulate ABPs that interact via a Lennard-Jones potential

$$V_{LJ} = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- We use Brownian Dynamics (BD) simulations for ABPs

$$d\mathbf{r} = \gamma^{-1}\mathbf{F}dt + \sqrt{2k_BT\gamma^{-1}}dW_t + v_0\hat{e}_i + p\,\hat{e}_i \cdot B^*$$

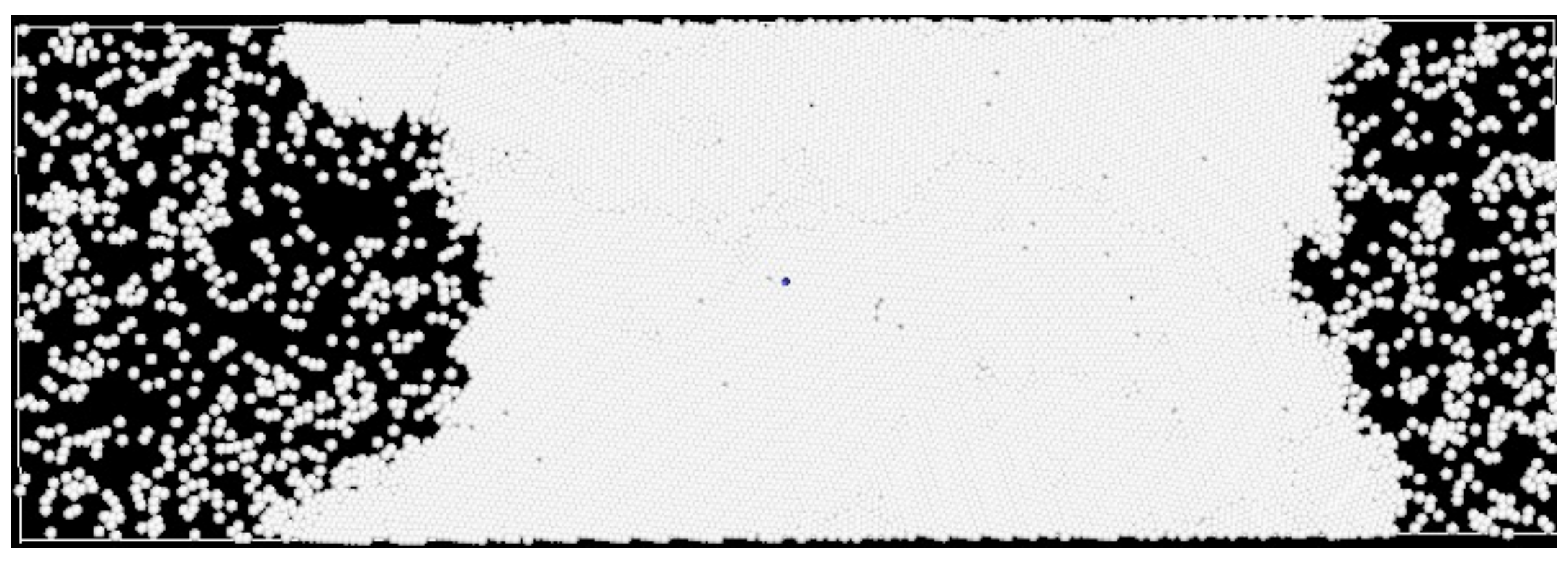
with
$v_0 = \frac{\mathrm{Pe}}{d_{BH}}$, $\hat{e}_i = \begin{pmatrix} cos\varphi \\ sin\varphi \end{pmatrix}$, $D_r = \frac{3}{d_{BH}^2}$

σ: distance (size of the particle)
ϵ: depth of the potential well
r: particle position
γ: drag force coefficient
F : total external force
W_t : noise with zero mean and unit variance
v_0: self-propulsion velocity
$\hat{e}_i$: unit vector for direction of self-propulsion force
Pe : Péclet number
d_{BH} : Baker-Henderson diameter
$p\,\hat{e}_i$: particle dipole moment
B*: alignment field

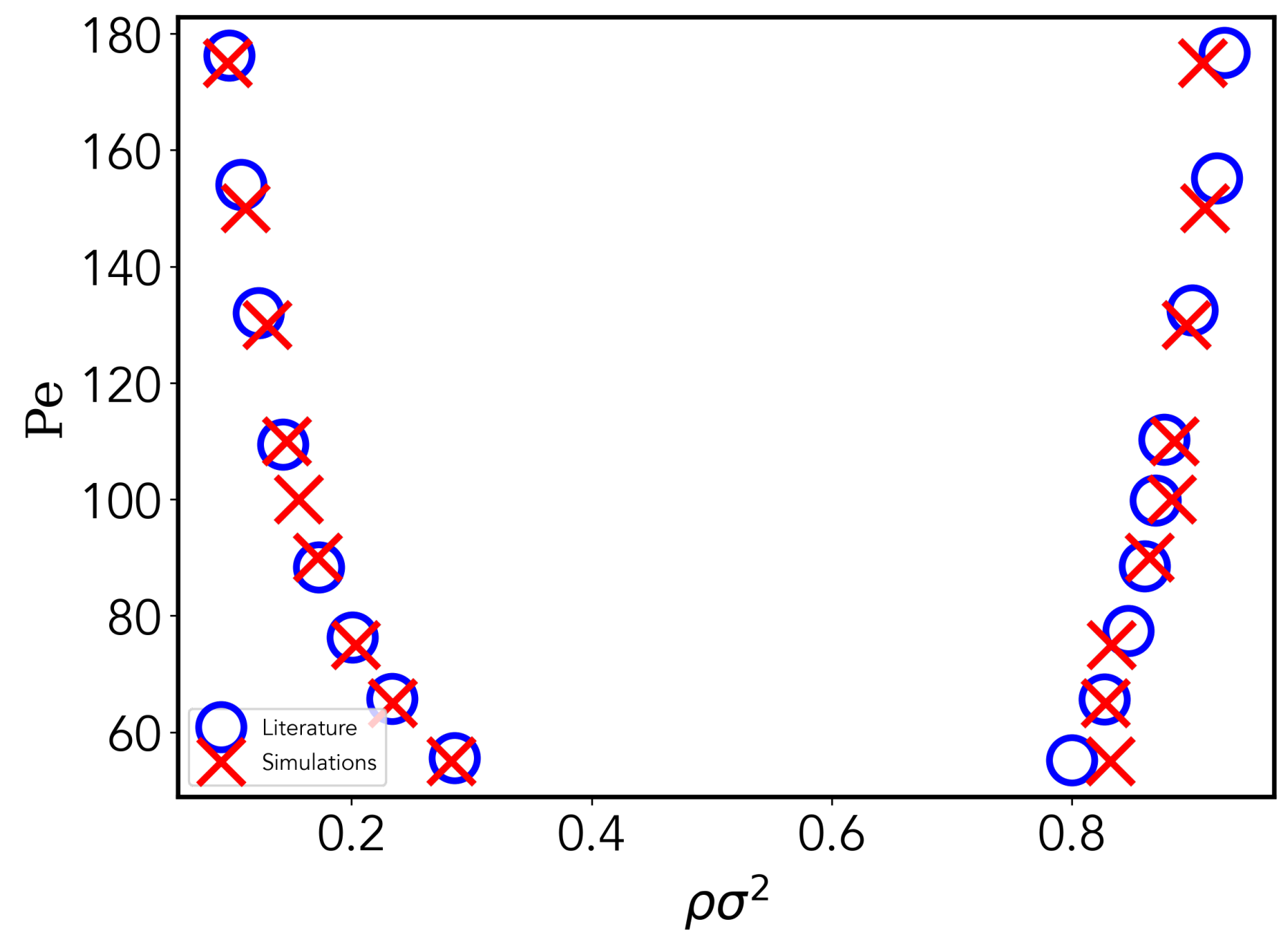
- Alignment field for particle orientation $\hat{e}_i$ aligns direction of self-propulsion force
- Simulations are done with a Verlet algorithm using LAMMPS [2]
- Periodic boundary conditions except mentioned otherwise
- We analyze the data using Python to extract local particle densities and generate phase diagrams.

Results

Phase diagram of ABPs in bulk



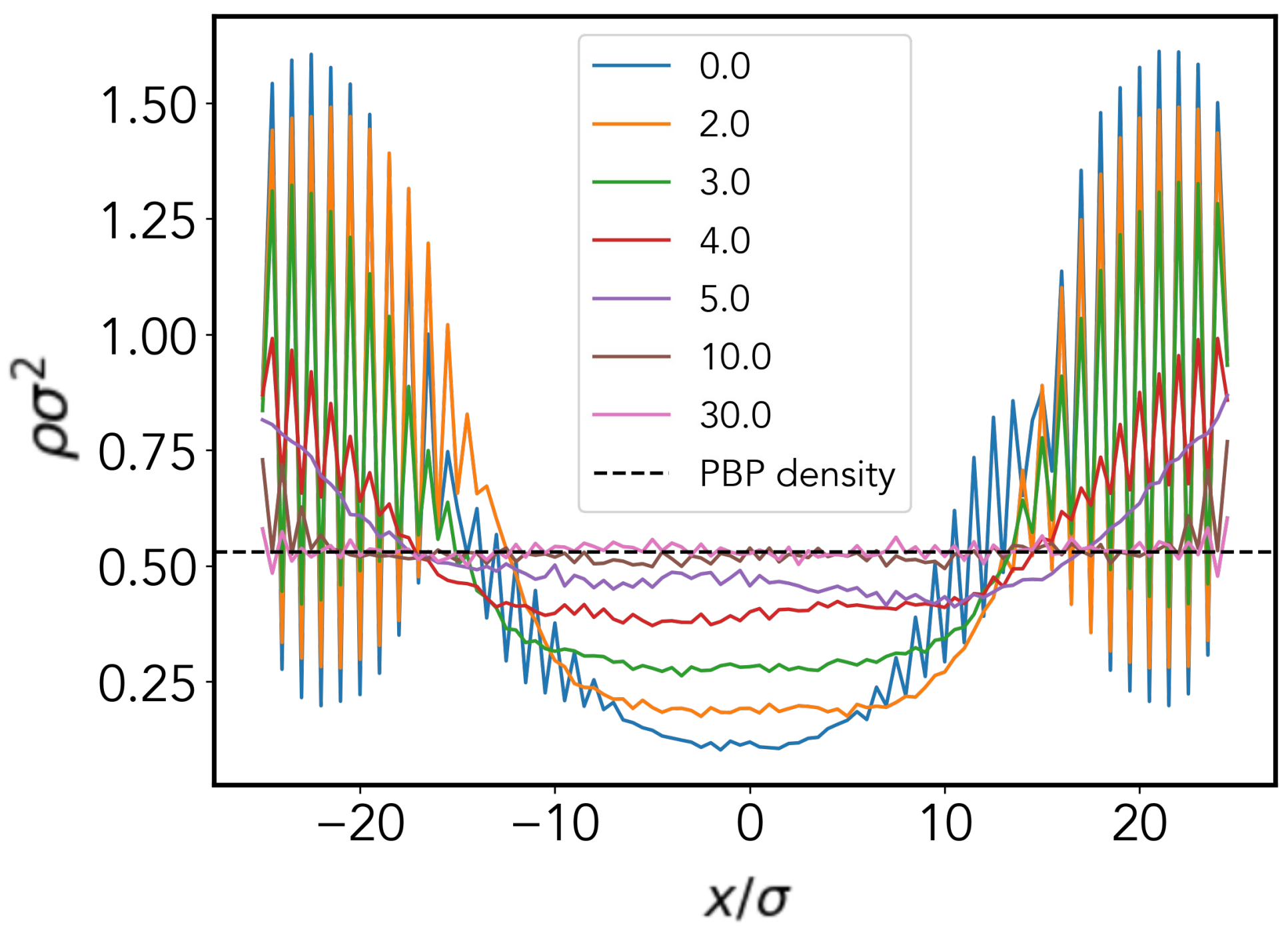
- We do steady-state runs for 10M steps and production runs for 800M steps with around 12,000 particles in 2D at various Pe.
- Self-propulsion leads to self-trapping of the ABPs and phase separation into a dense, liquid and a dilute, gas phase.
- We use simulation boxes with aspect ratio 1:3, where the liquid phase forms perpendicular to the long direction of the box.



- With decreasing Pe, the gas phase extents to higher and the liquid phase to lower particle densities ρ.
- A critical point where the two-phase region vanishes has been reported at rho = 0.62 and Pe= 40 [3].

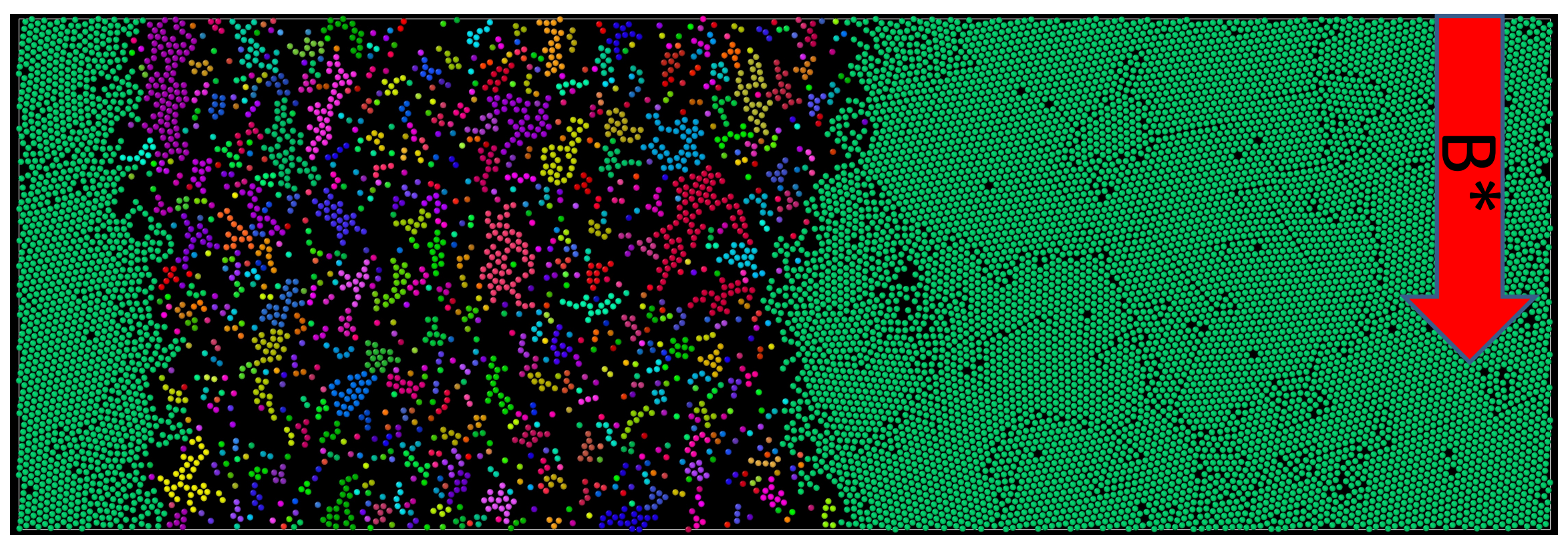
ABPs in straight channels

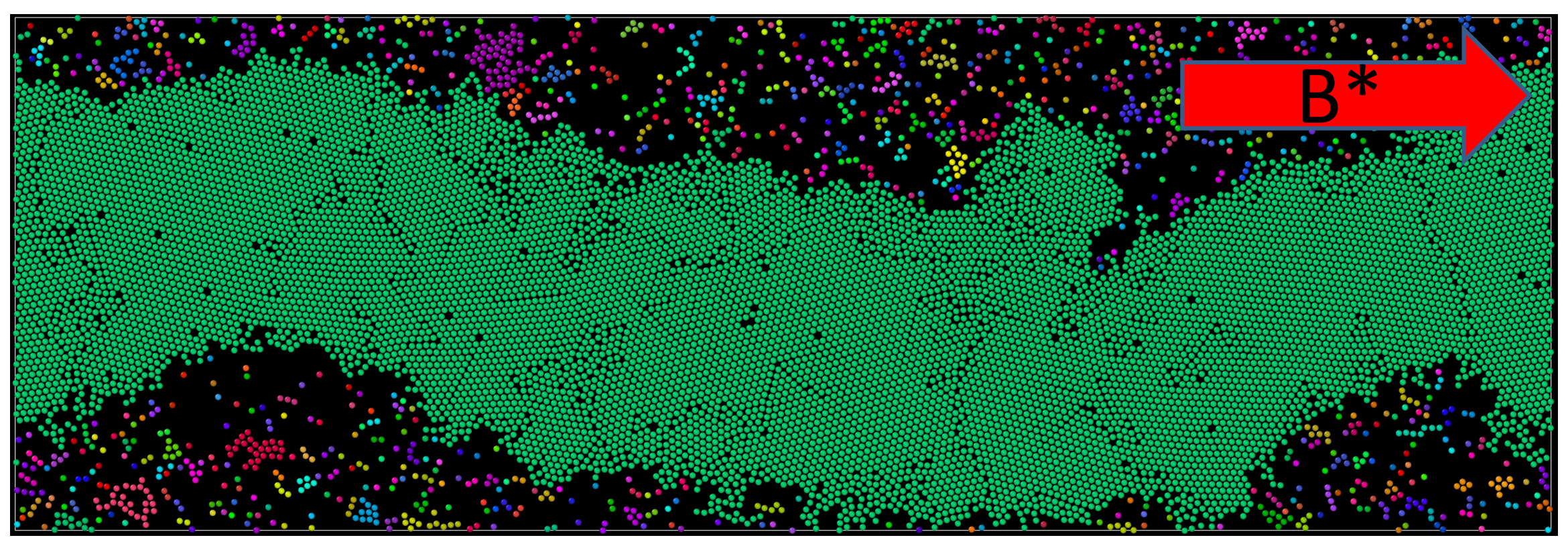
- For channels with reflective walls, the particles crystallize close to the wall, which leads to an oscillating density.



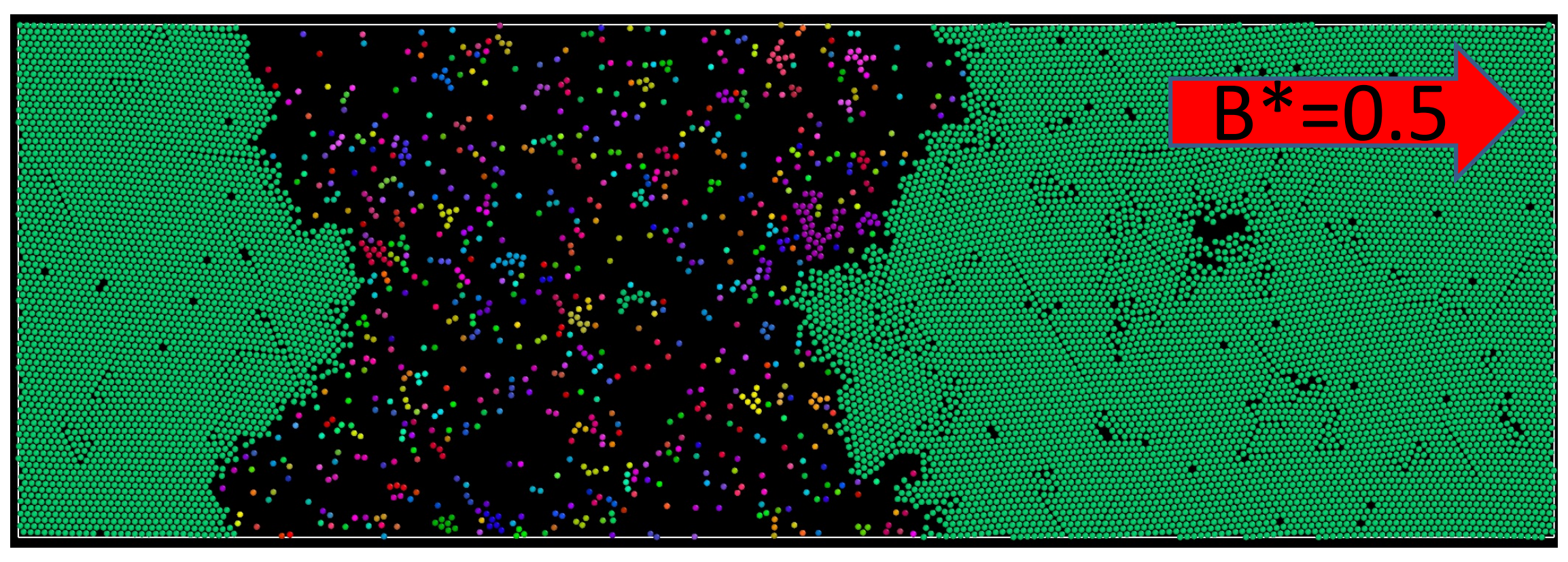
ABPs with alignment field in bulk

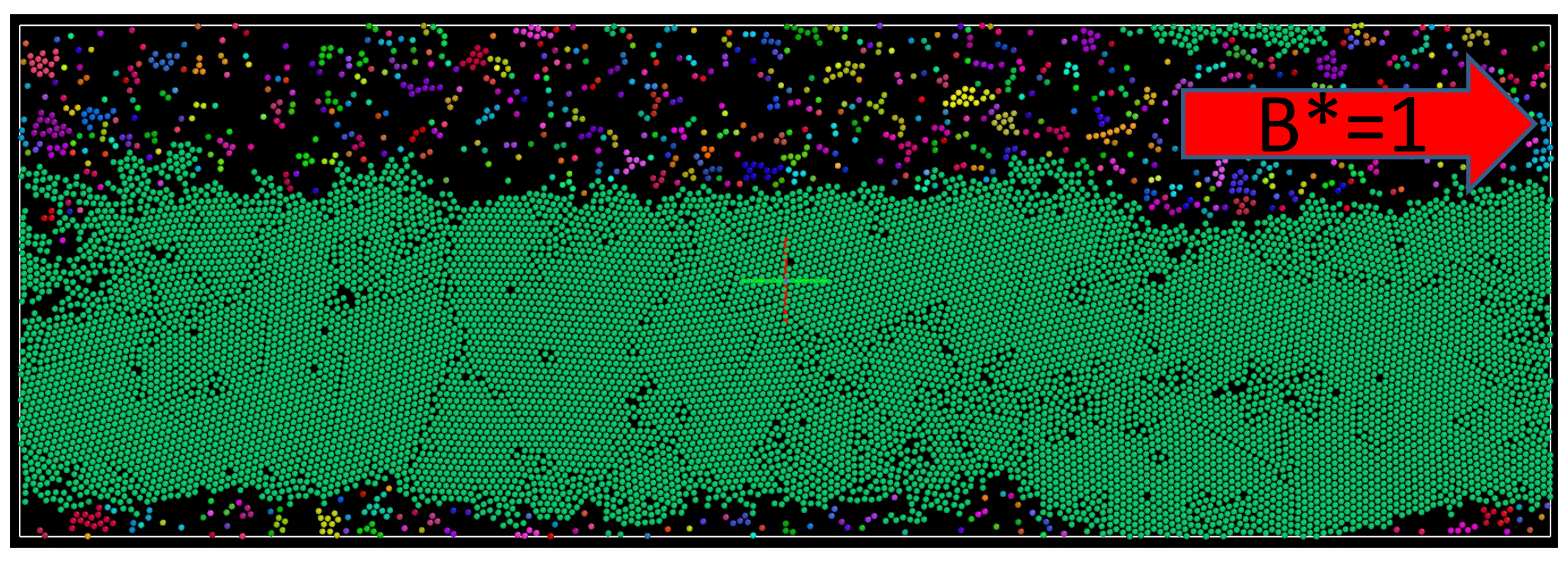
- For a strong alignment field, the phase boundaries are parallel to the direction of the field.



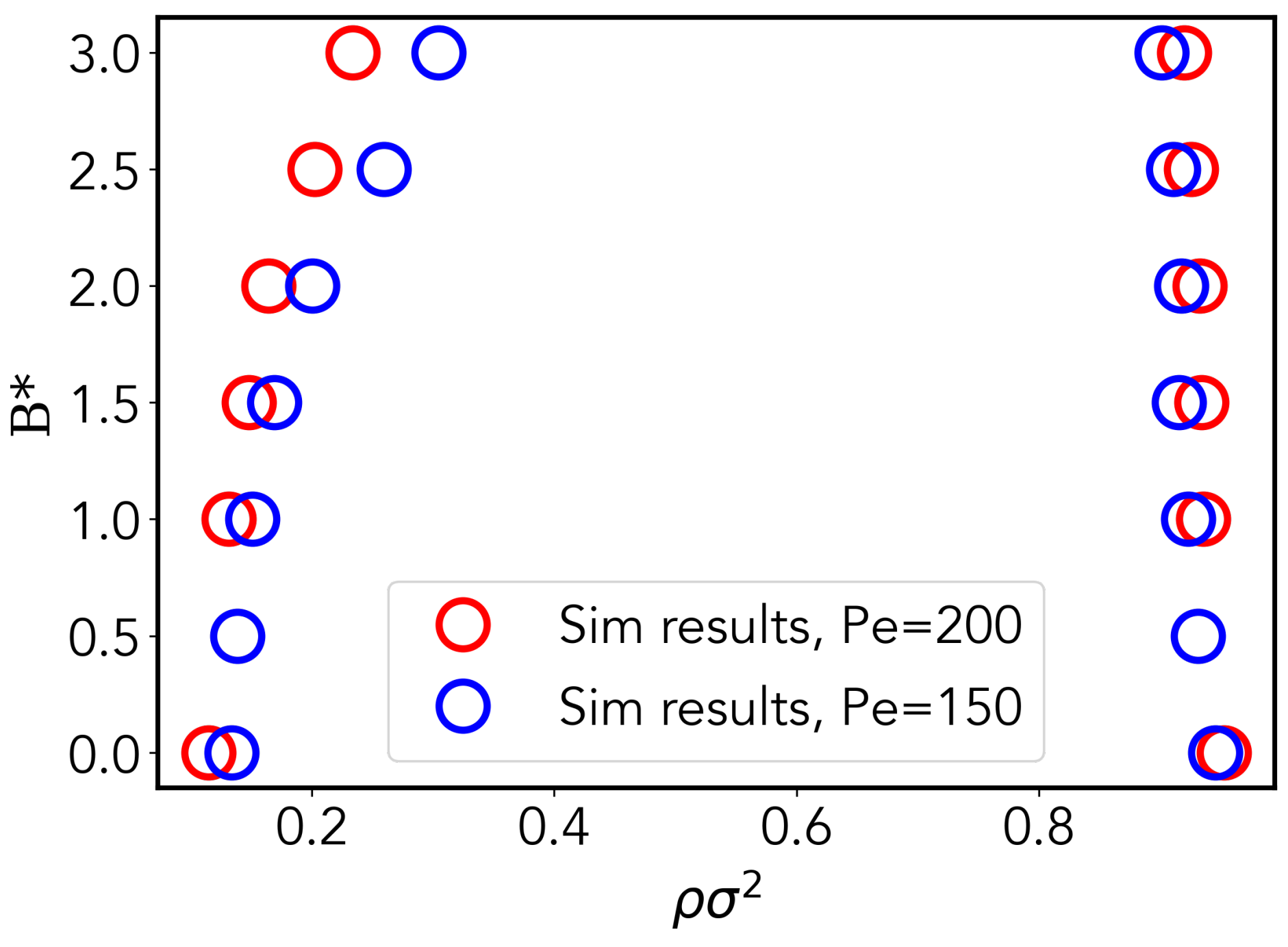


- For a weak alignment field, the cluster will still orient perpendicular to the direction of the simulation box.
- For high alignment field strengths, the effective self-propulsion strength parallel is lower than perpendicular to the alignment field.





- With increasing strength of the alignment field **B***and for fixed **Pe**, the gas phase extents to higher and the liquid phase to lower particle densities ρ.
- We expect to find a critical point beyond a critical field strength **B***.



Conclusions

- ABPs form a liquid phase at high Péclet numbers and densities
- In channels ABPs aggregate at the walls and show crystalline, fluid, and gas structure.
- A sufficiently strong alignment field for the particle self-propulsion force aligns phase boundaries in field direction
- For strong alignment field, the effective propulsion force is stronger perpendicular than parallel to the field direction.

Outlook

- Calculate critical points and exponents for fixed Pe and various strengths of the alignment field; calculate Binder cumulants
- Identify gas, liquid, and one-phase parameter regimes in $\mathbf{B}^*-$ Pe phase diagram.
- Characterize flow of ABPs in straight channels of various widths (with reflective walls) for several combinations of B and Pe
- Characterize local particle order in straight channels with various widths for several combinations of $\mathbf{B}^*$and Pe
- Simulate flow in straight channels with obstacles and/or varying channel width
- Study complex channel geometries and networks.

References

[1] Elgeti, Jens, Roland G. Winkler, and Gerhard Gompper. *Rep. Prog. Phys.* **78** (2015) 056601
[2] A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in 't Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, S. J. Plimpton, Comp Phys Comm, 271 (2022) 10817.
[3] Jonathan Tammo Siebert, Florian Dittrich, Friederike Schmid, Kurt Binder, Thomas Speck, and Peter Virnau Phys. Rev. E **98**, (2022) 030601(R)