# Tackling collective motion in large-scale simulations with a highly scalable MPCD Code

**From single-swimmer motion to collective patterns under gravitational fields: A particle-based hydrodynamic study**

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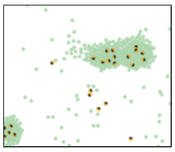
## In Short

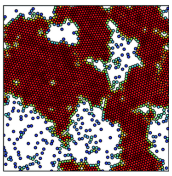
- Modeling different types of microswimmers using MPCD with domain decomposition to explore their collective behavior in quasi-2D and 3D
- Investigate the dependence of collective patterns on system size and perform extensive parameter studies
- Results: Observation and characterization of phase transitions in quasi-2D, sedimentation and convection dynamics under gravity in 3D, swarming motion of elongated microswimmers

Swimming on the micron scale, and understanding how microorganisms overcome the constraints of low Reynolds number hydrodynamics [1], has attracted a lot of attention among physicists. Both artificial swimmers [2] and biological organisms [3,4] are probed for the principal properties of their individual and collective motion [5], as well as locomotion under external fields such as gravity [6] or Poiseuille flow [7].

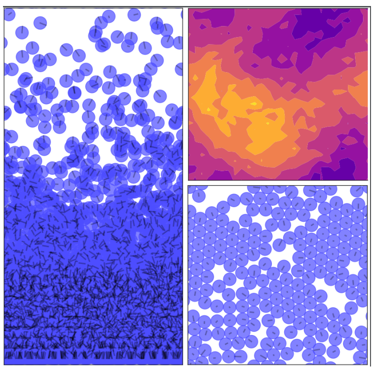
***Left: Observations of dynamic cluster formation*** *in active particle and squirmer simulations.* ***Right: Collective Sedimentation and Convection Dynamics*** *of squirmers (*Top right*: mean vertical squirmer current density shows convection cell.* Bottom right*: hexagonal packings at the bottom).*



*Stürmer et al, JCP 2019*



*Blaschke et al., Soft Mat. 2016*

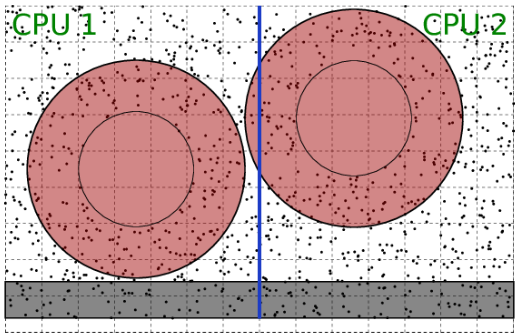


*Kuhr et al., Soft Mat. 2017*

The fluid environment and the flow fields initiated by microswimmers strongly determine both their isolated motion and their appealing collective patterns which they develop in non-equilibrium. The project investigates swimmers in their fluid environment in detail by using the particle-based mesoscale simulation technique of multi-particle collision dynamics (MPCD). In particular, we perform large-scale simulations to explore the collective dynamics of microswimmers in the thermodynamic limit. For this reason a large number of microswimmers of different complexity have to be simulated in their fluid environment at large system sizes. This requires extensive simulations with a parallel and highly scalable MPCD code for which sufficient access to parallel computing facilities is necessary.

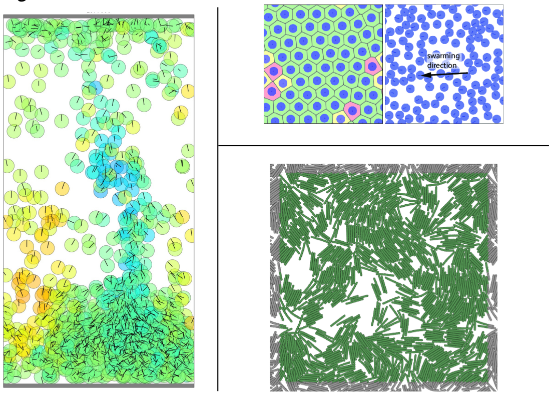
We implement spherical and non-spherical microswimmers within the MPCD method. In general, we pay attention to both the generic features of far-field hydrodynamics – characterized by the notion of pushers and pullers – and the near-field hydrodynamics close to the swimmers' surfaces. For that reason, we use the model swimmer called "squirmer" which can mimick both artificial swimmers such as Janus particles, and biological organisms such as *Chlamydomonas* and *Volvox*. At the current stage of the project we are interested in the collective dynamics and onset of dynamic patterns of (bottom-heavy) microswimmers under gravity. In addition, we perform large-scale simulations of the phase behaviour of active rods and filaments in quasi-2D. These studies aim to mimic the appealing patterns of convective plumes [3] and active turbulence [4] observed in biological matter.

***Parallel implementation of MPCD:*** *The dashed lines separate collision cells, the blue lines separate core sectors.*




In our work we employ a highly scalable parallel implementation of MPCD using system domain decomposition and MPI (*cf.* blue line in the plot). This enables us to simulate large systems with many squirmers (red circles). The MPCD method solves the Navier-Stokes equation on a coarse grained level, where the fluid is represented by point particles (*cf.* black points in the plot) interacting within grid cells (*cf.* dashed lines). This algorithm lends itself to parallelization: the simulation box is divided by a 2D Cartesian grid (core sectors), representing the borders between CPU cores. This scales exceptionally well as fluid particles interact only within their grid cells. MPI is used to communicate between CPU cores.

***Large scale simulations:*** Left: *Snapshot of a 3D system of bottom-heavy squirmers: plumes (light blue) sink towards a convection roll.* Top right: *In monolayers of squirmers confined by strong gravity various states occur, such as hydrodynamic Wigner fluidsand swarming states.* Bottom right: *Phase separation of elongated microswimmers*



In our previous work [8] we demonstrated that squirmers exhibit motility-induced phase-separation, whereby domains of low squirmer density coexist with stable clusters. With the help of the computing resources provided by the HLRN, we were able to extend the system size more than ten-fold, eliminating finite-size effects and to resolve the phase diagram quantitatively [9].

Furthermore, we have investigated the single-particle and collective dynamics of squirmers under the influence of gravity. We determined and analyzed the diverse motional states that a single squirmer shows depending on the details of its flow field [10]. On the other end of the size range we simulated several thousand squirmers [11], again relying heavily on HLRN resources. We observed layering of swimmers at the bottom wall and an exponential region above the layers, with an enhanced sedimentation length compared to passive systems.

We also studied the dynamics of a monolayer of swimmers created by a strong gravitational force [12]. Among other things, we identified swarming of pushers and hydrodynamic Wigner fluids for pullers and neutral squirmers (see picture above, top right).

Currently, we simulate systems of bottom-heavy squirmers that perform *gravitaxis*. We find that their exponential sedimentation profiles are inverted once the center-of-mass offset is sufficiently large. Interestingly, we can tune the gravitational force and torque such that continuous plumes and stable convection rolls occur (see left picture above).

We also perform simulations with active rods and active flexible filaments. They consist of several squirmers merged together to form elongated bodies (see picture above, bottom right). We find dynamic swarming states that are especially interesting for puller-type swimmers, where hydrodynamic interactions induce the formation of lanes with a buckling instability.

## WWW

http://www.itp.tu-berlin.de/stark/

## More Information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