Tracking and Analysis of Active Droplet Dynamics

from image processing to non-equilibrium statistical physics

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Introduction

- **Active matter systems** can **harness energy** from their surroundings and **propel themselves** away from equilibrium.

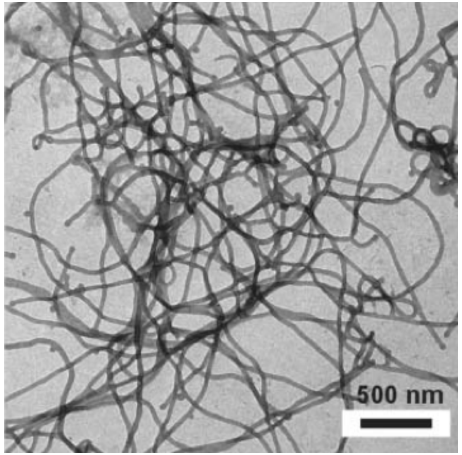
- **Even if composed by "simple" individual entities**, they show **complex collective behaviour** of dynamical **self-assembly.**

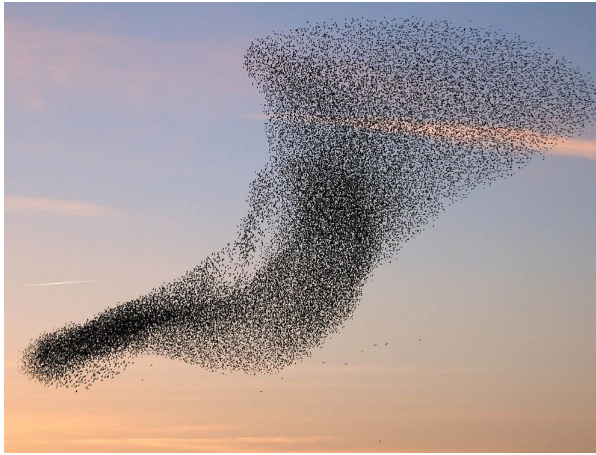
Introduction

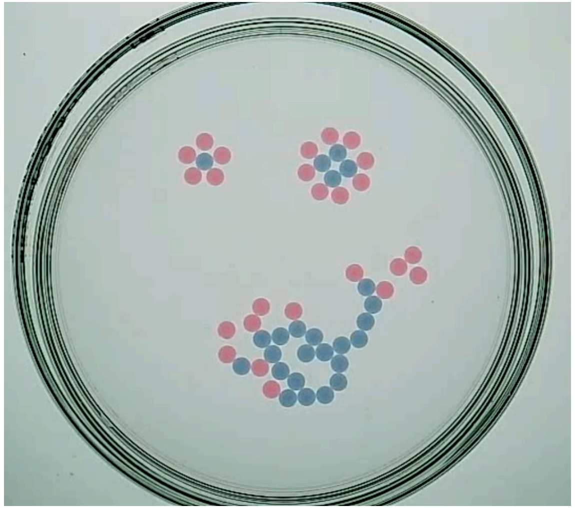
Realizations:

- **Biological**: Span all levels of living organisms.
- **Synthetic**: Systems capable of dynamical self-propelled behaviour akin to that found in living matter

Countless **applications**, e.g. bacterial micromotors [1], soft robotics, design of novel materials







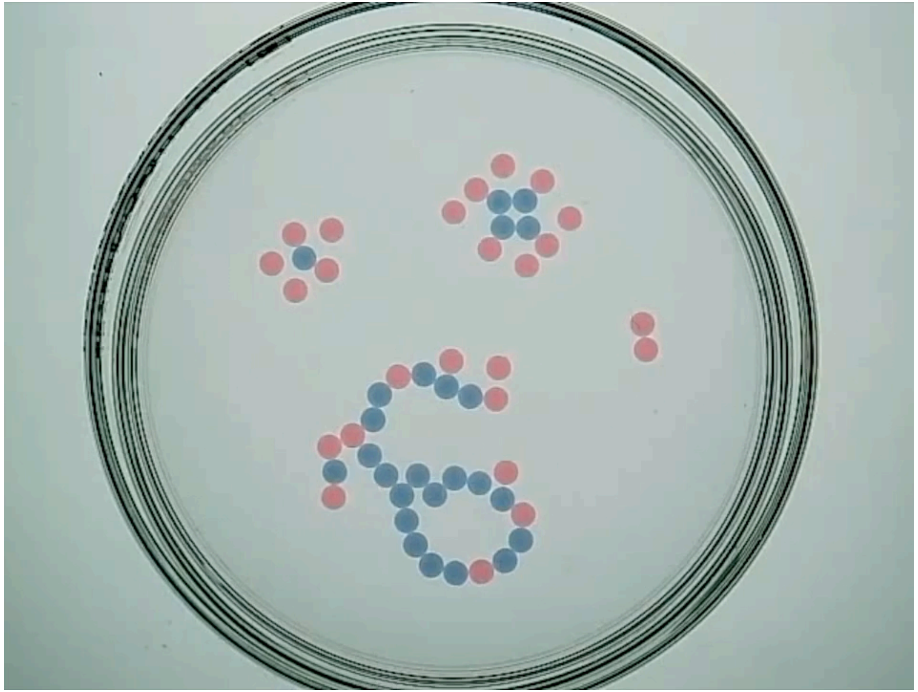
1. Vizsnyiczai, G., Frangipane, G., Maggi, C. *et al.* Light controlled 3D micromotors powered by bacteria. *Nat Commun* **8**, 15974 (2017). https://doi.org/10.1038/ncomms15974

Introduction

The **system under study** in this project is made of **synthetic active matter** droplets immersed in a solution:

- **Droplets**: Ethil Silicitate (ES) & Paraffin + Oil O Red dye for red droplets and Sudan B black dye for blue droplets [2], [3]
- **Solution**: Sodium dodecyl sulfate

Self propulsion arises due to the **evaporation of ES.**



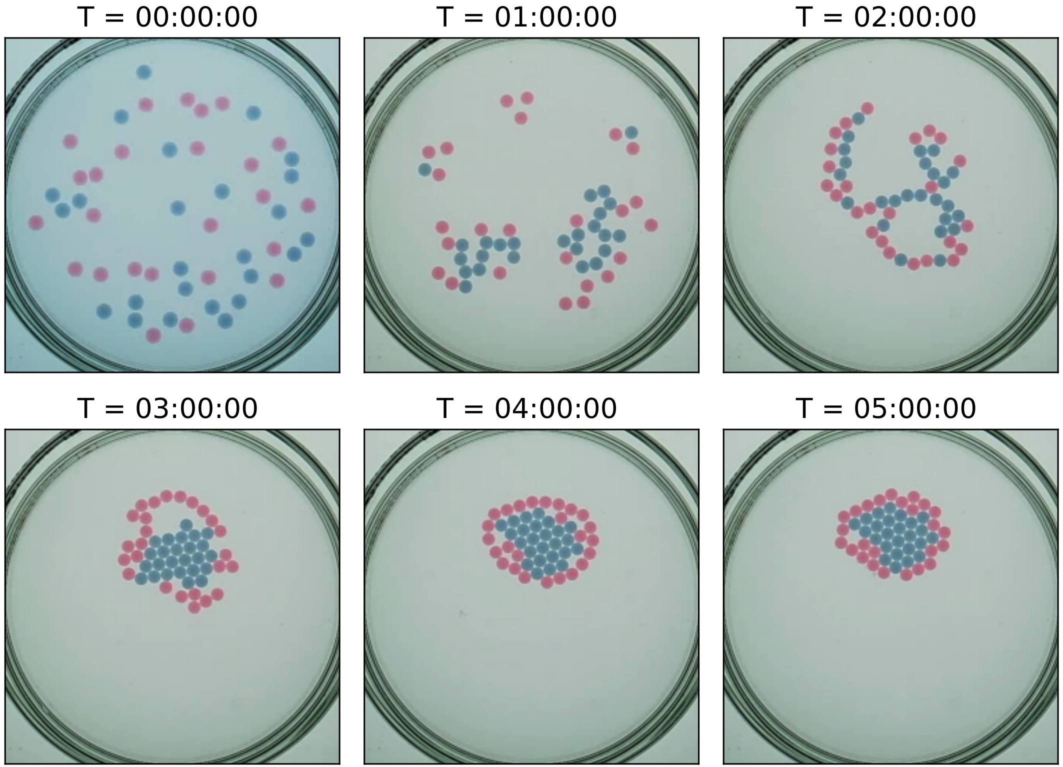
Video: dynamics of active droplets (25b25r) — 20 x

2. Muneyuki Matsuo, Hiromi Hashishita, Shinpei Tanaka, and Satoshi Nakata. Sequentially selective coalescence of binary self-propelled droplets upon collective motion. Langmuir, 39(5):2073–2079, 2023. PMID: 36692295.

3. R.J.G. Löffler. New Materials for Studies on Nanostructures and Spatio-temporal Patterns Self-organized by Surface Phenomena. 2021

Introduction

- **Stage 1**: Active "Brownian" motion with no structures
- **Stage 2**: Medium-sized semi-persistent structures
- **Stage 3**: Persistent arrangement in a quasi-regular structure



Objectives

The **long term goal** is to **predict large scale structures** and **dynamical assembly** of the droplets by **varying the system composition**

The **short term goal** is to **characterize the behaviour of the system** starting from the experimental video:

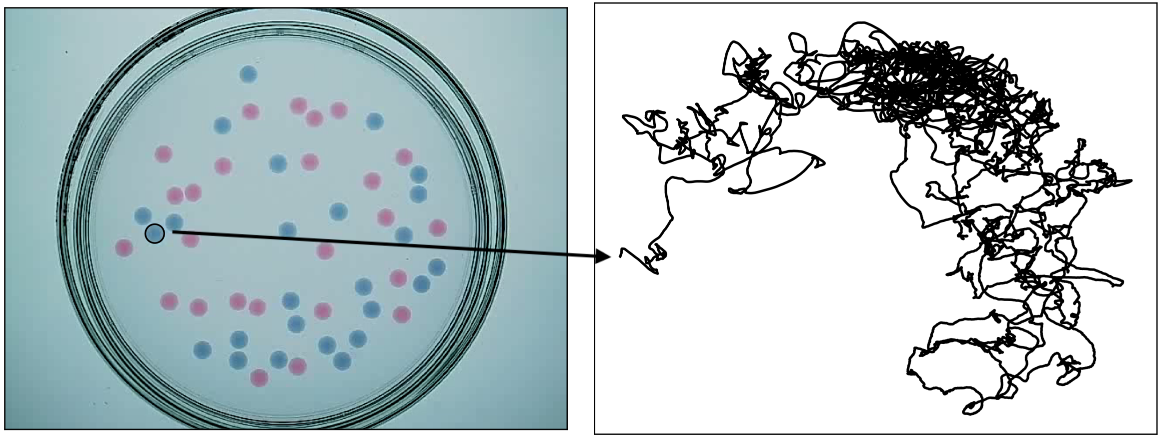
→

1. **Tracking procedure**
2. **Dynamical analysis**
3. **Structural analysis**

Tracking procedure

Tracking procedure

Accurate droplet positions and radii over time → **Quantitative characterization of the dynamics**



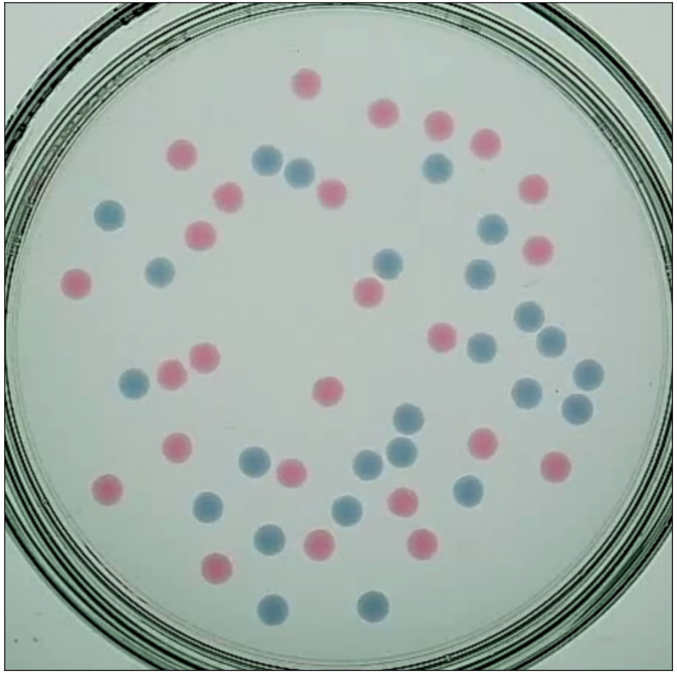
Steps of the pipeline:

1. Video preprocessing
2. Features detection
3. Linking

Tracking procedure - Video preprocessing

Preprocessing steps

- **Grey scaling** to simplify data format
- **Circular crop** to remove the petri dish from the frame
- **Sharpen kernel** to enhance the droplets' borders



Tracking procedure - Video preprocessing

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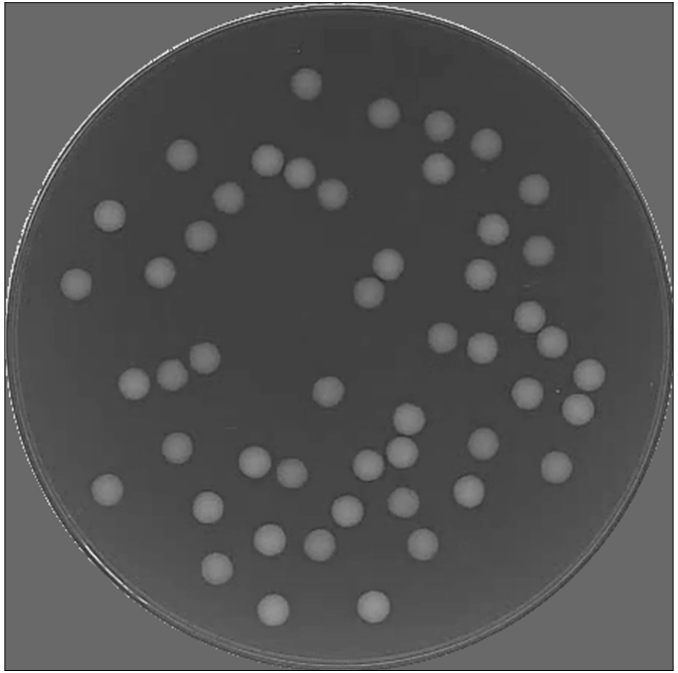
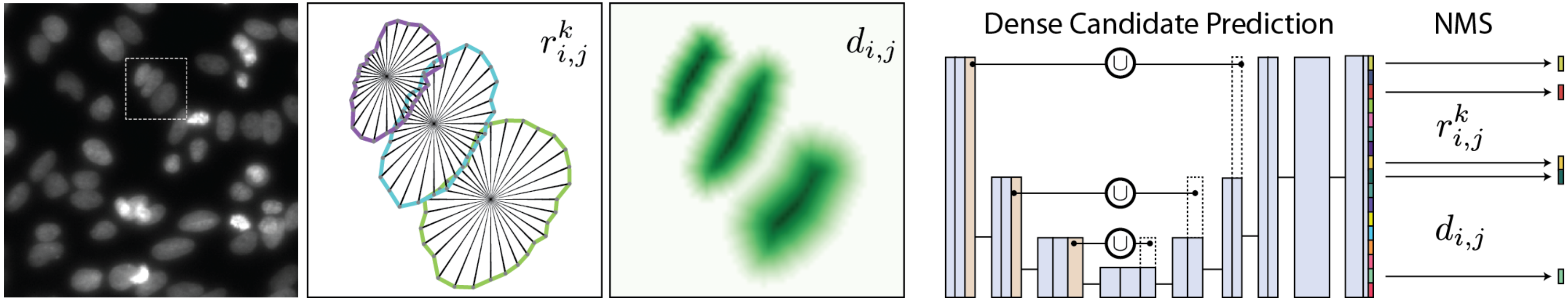


Tracking procedure - Features detection

Deep learning solution: → U-net architecture + Star convex prediction head

Stardist [4]



4. Martin Weigert, Uwe Schmidt, Robert Haase, Ko Sugawara, and Gene Myers. Star- convex polyhedra for 3d object detection and segmentation in microscopy. In The IEEE Winter Conference on Applications of Computer Vision (WACV), March 2020.

Tracking procedure - Features detection

Deep learning solution: → U-net architecture + Star convex prediction head

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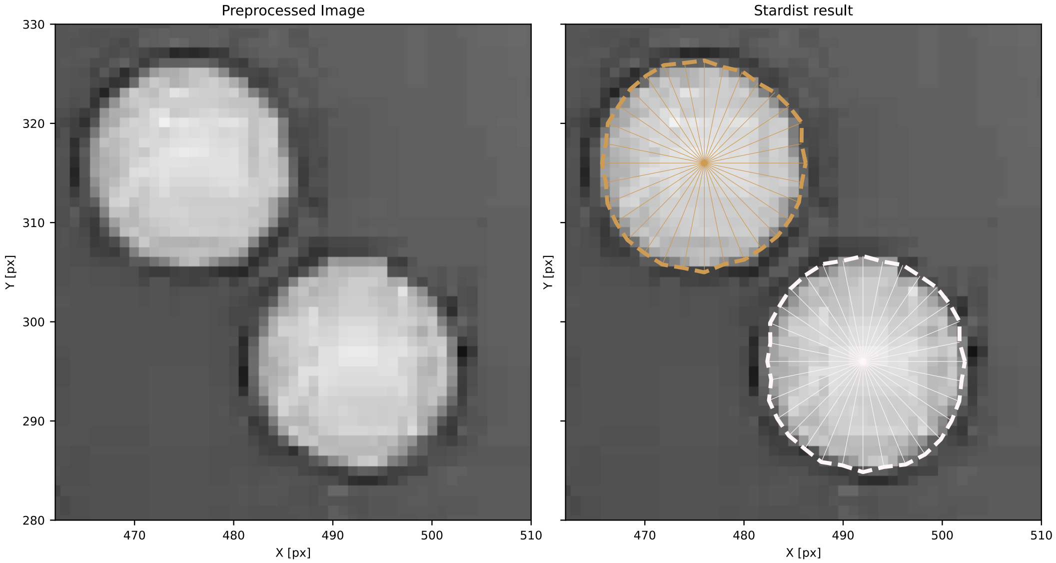
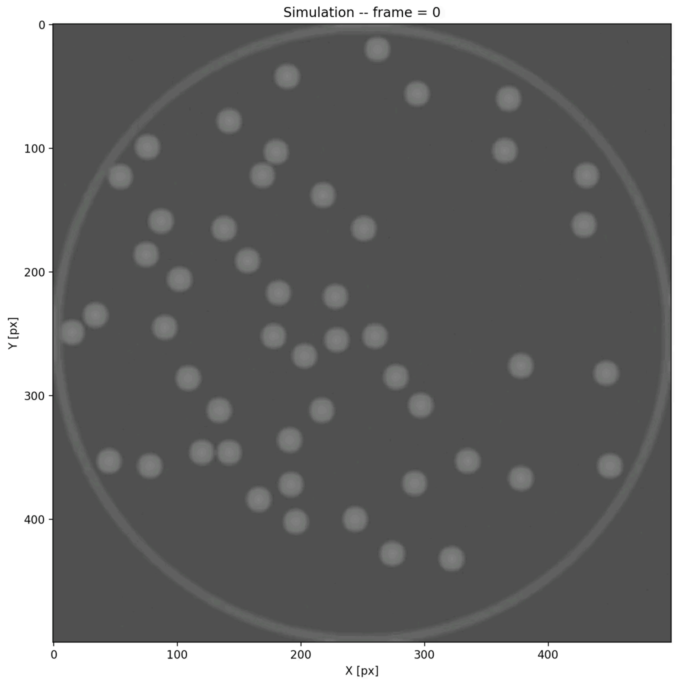


4. Martin Weigert, Uwe Schmidt, Robert Haase, Ko Sugawara, and Gene Myers. Star- convex polyhedra for 3d object detection and segmentation in microscopy. In The IEEE Winter Conference on Applications of Computer Vision (WACV), March 2020.

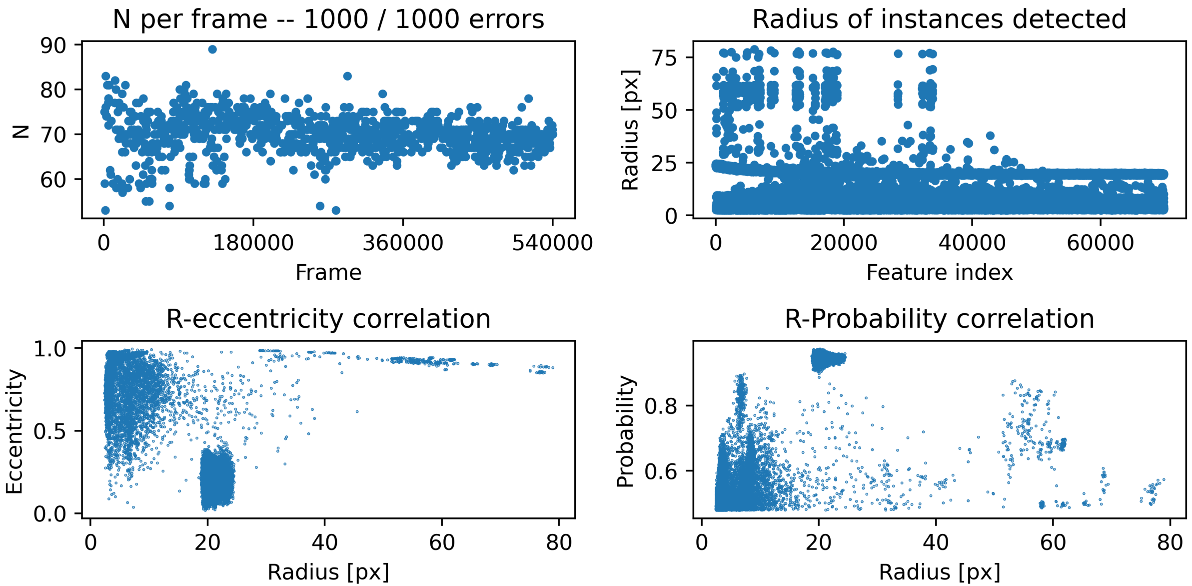
Tracking procedure - Features detection

To **train and/or optimize** the **Stardist network** we **simulated** an **interacting ABP** system and **generated synthetic images** resembling the post-processed data.



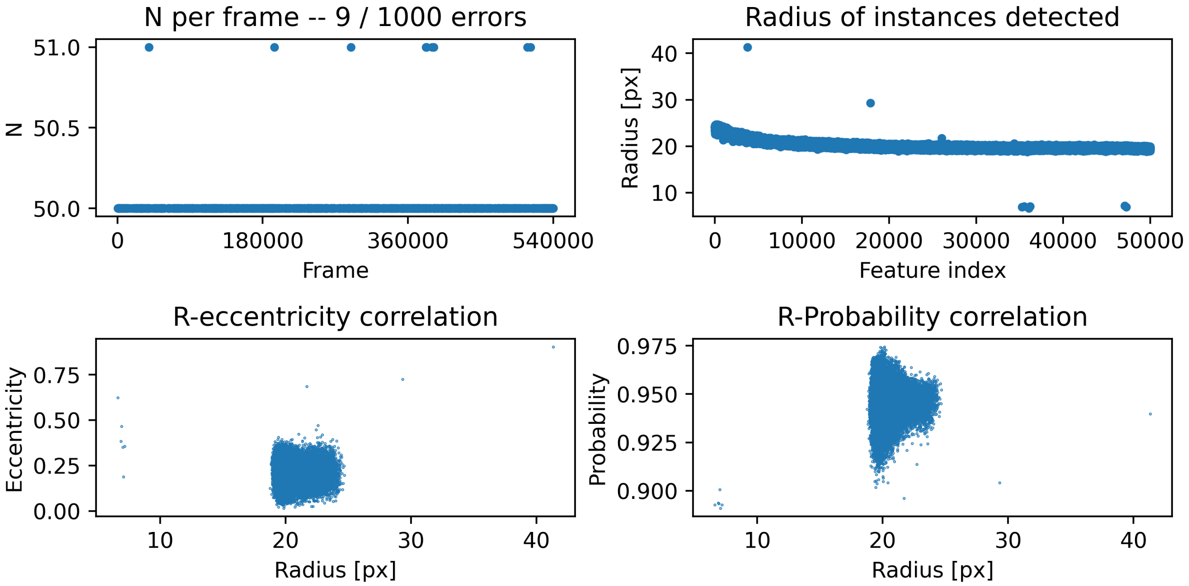
Tracking procedure - Features detection

Pretrained



Tracking procedure - Features detection

Pretrained + optimization



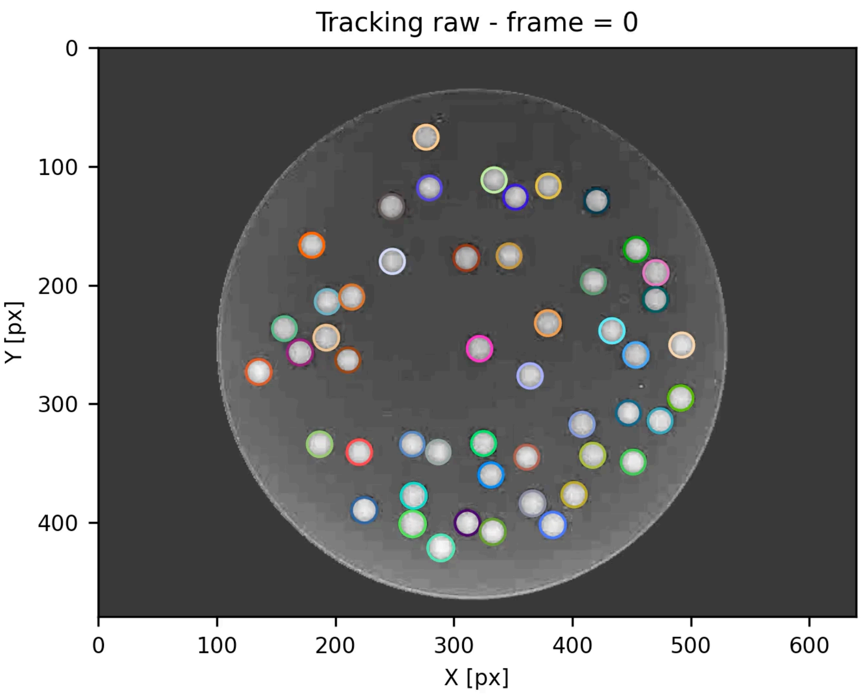
Tracking procedure - Linking

Instances' linking between frames, preserving droplets' identity

- **Probability** for the displacement of N non-interacting **Brownian particles**

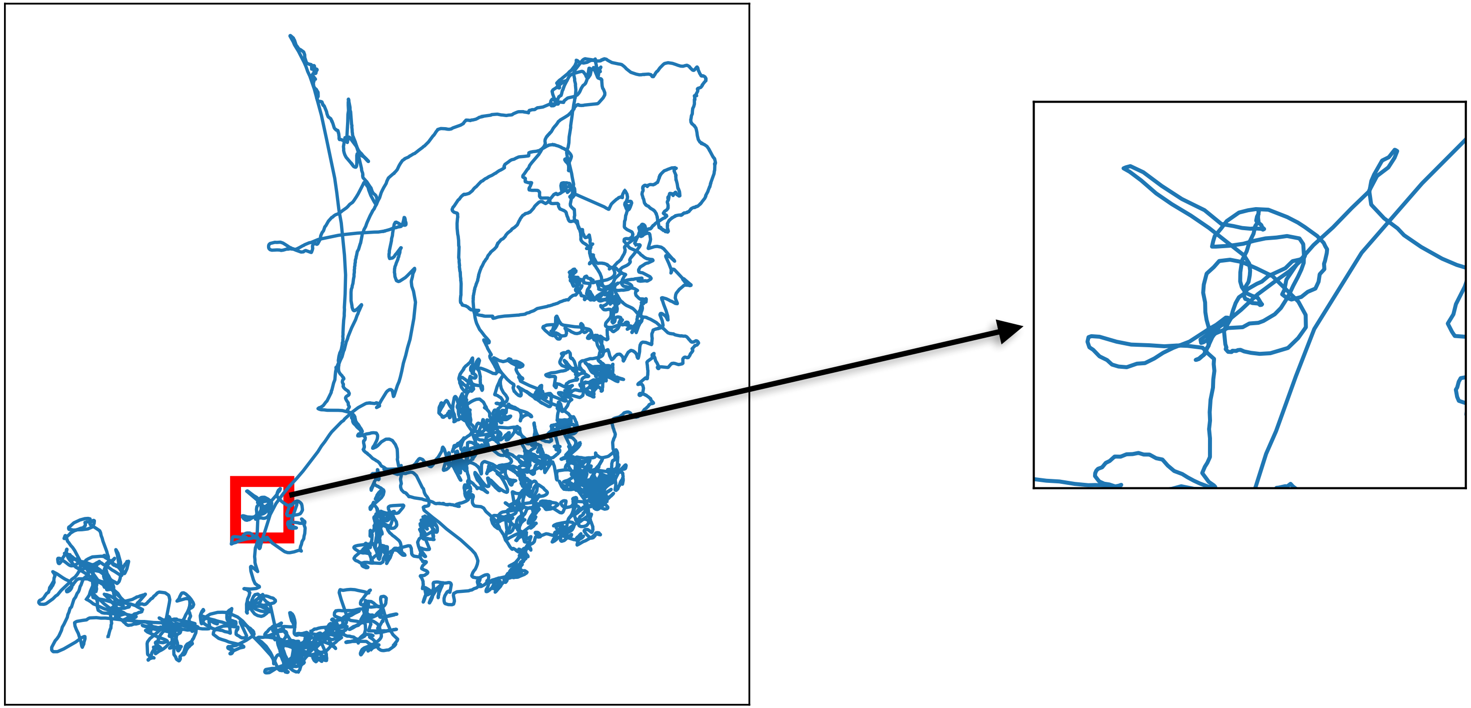
$$P\left(\{\delta_i\}\,|\,\tau\right) = \left(\frac{1}{4\pi D\tau}\right)^N exp\left(-\sum_{i=1}^{N}\frac{\delta_i^2}{4D\tau}\right)$$

most probable identity assignment across frames maximizes the probability



Tracking procedure - Outcomes

Result of the **tracking procedure**: highly **accurate trajectory of each droplet**.



Analysis

Analysis - Introduction

System characterization:

- **Activity**: Droplets’ depth in the solution
- **Dynamical properties**: MSD & Turning Angles distribution
- **Structural analysis**: Velocity Autocovariance & RDF

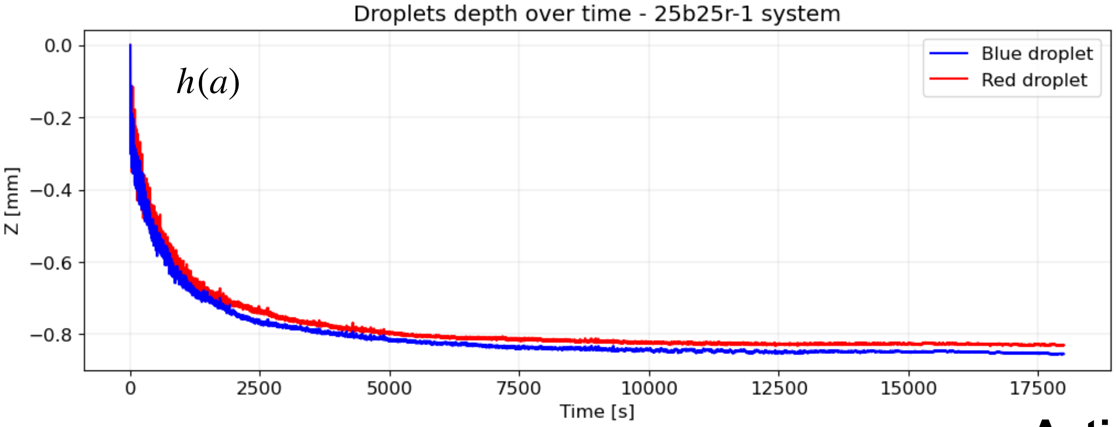
Analysis - Droplets' depth analysis

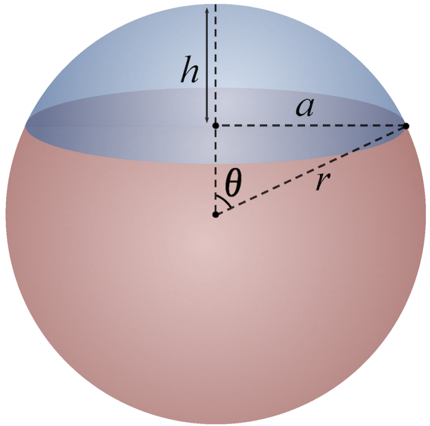
Assumptions:

- Perfectly **spherical droplets**
- **Droplets at frame 0** are **half submerged**

Radius as seen from above ⟶ a

$$\begin{cases} A_{cap} = 2\pi r h \\ A_{cap} = \pi(a^2 + h^2) \end{cases} \Longrightarrow h = h(a)$$





Activity decays as the droplet sinks

Analysis - Window-based analyses

Global time average analyses

(MSD, Turning Angles & VACF)

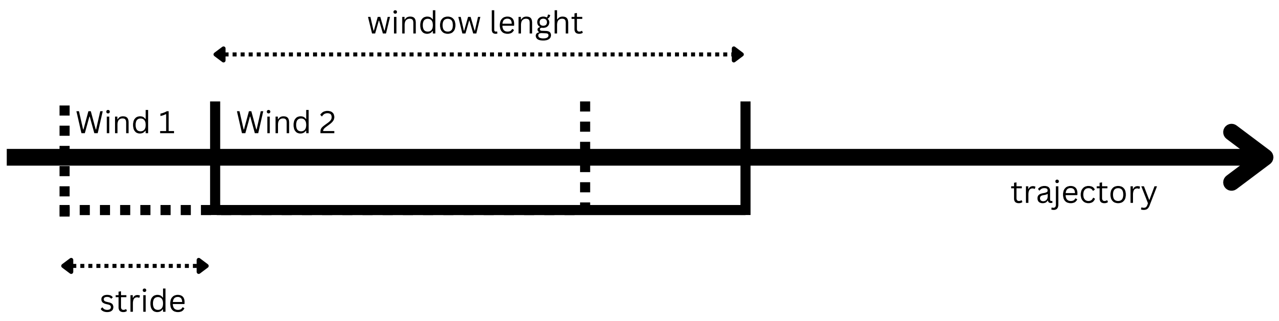
→

- **Not well-founded** since **time-translational invariance is not met** (activity decays over time)
- **Mixing different activity regimes**

For these reasons we perform a **window-based analysis**:

- **Trajectories are divided into windows** of 600 s
- **Window slides over the full trajectory** by a stride of 10 s

Analysis - Window-based analyses



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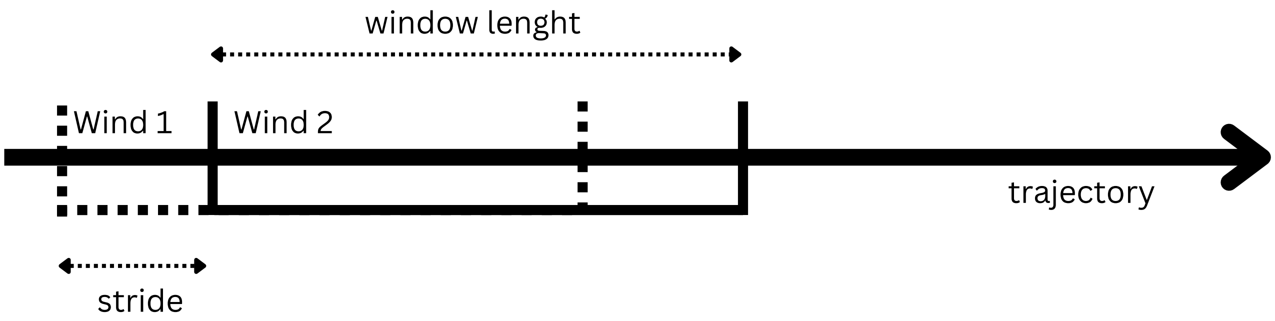
Analysis - Window-based analyses



Window-based analyses assume that the **macroscopic statistical properties** (activity) **do not change significantly** over the **window time extent**.

Analysis - Mean Squared Displacement (MSD)

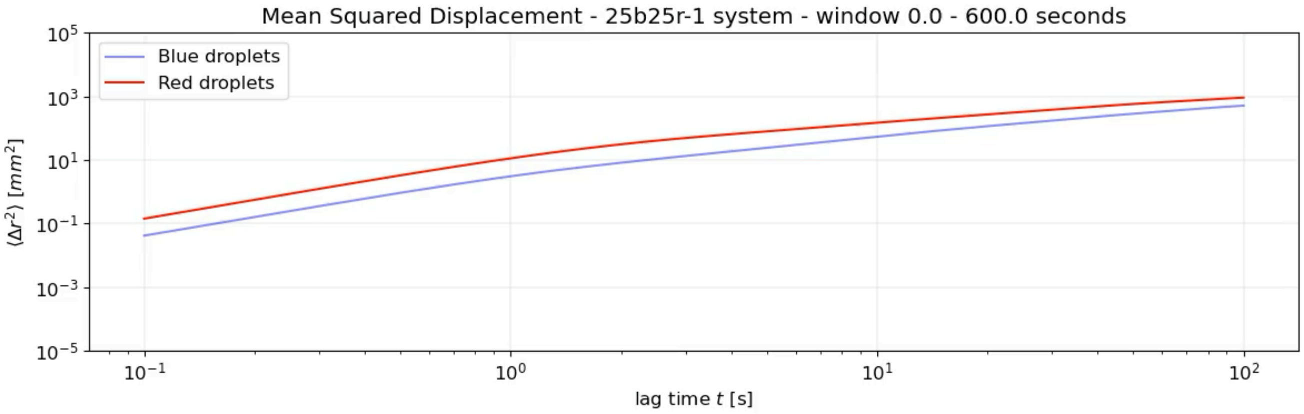
We compute the **time Average MSD** of droplets of same species over the window portion of the trajectory:

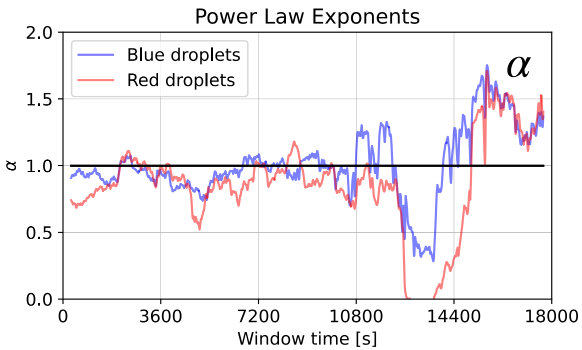
$$\langle \Delta \mathbf{r}^2(\tau) \rangle_\gamma = \frac{1}{N_\gamma} \sum_{k \in \gamma} \overline{\delta^2(\tau)}^k \text{ where } \overline{\delta^2(\tau)}^k = \langle (\mathbf{r}^k_{t+\tau} - \mathbf{r}^k_t)^2 \rangle_{t \in T} = \frac{1}{T - \tau} \sum_{t=0}^{T-\tau} (\mathbf{r}^k_{t+\tau} - \mathbf{r}^k_t)^2$$

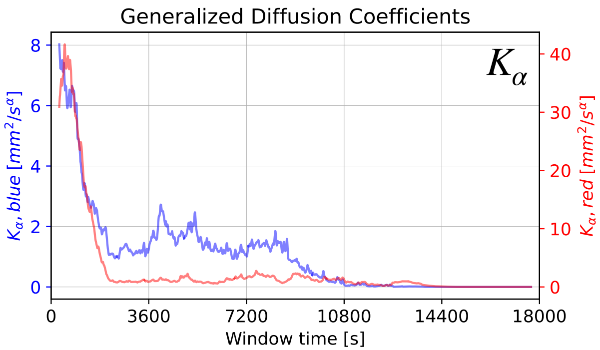
and perform **power law fit** in the [10 - 100] s region:

$$\langle \Delta \mathbf{r}^2(\tau) \rangle_\gamma = K_\alpha \tau^\alpha \qquad \begin{cases} \text{diffusive for } \tau \gg 10\,s \\ \text{ballistic for } \tau \ll 10\,s \end{cases}$$

Analysis - Mean Squared Displacement (MSD)







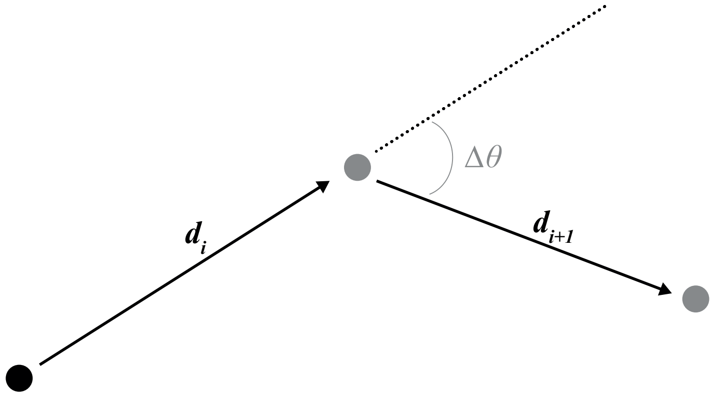
power law fit:

$$\langle \Delta \mathbf{r}^2(\tau) \rangle_\gamma = K_\alpha \tau^\alpha$$

Diffusive properties depend on the **activity** of the system.

Analysis - Turning Angles Distribution

We characterize the **droplet's rotational behaviour** as a **function of the activity.**

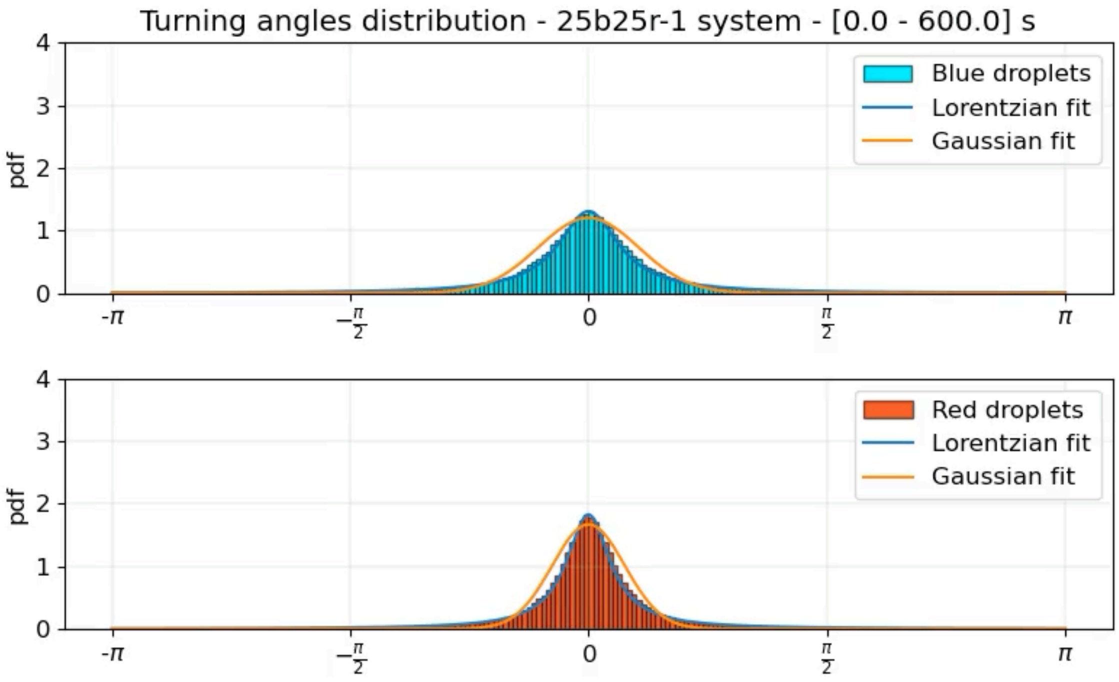


In the standard **ABP model turning angles** are **Gaussian distributed**:

$$P(\Delta\theta) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\Delta\theta - \mu)^2}{2\sigma^2}}$$

We perform the **window-based analysis** to **resolve** explicit **dependencies of the rotational diffusion of the droplets.**

Analysis - Turning Angles Distribution



Gaussian distribution not adequate

$$P(\Delta\theta) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\Delta\theta - \mu)^2}{2\sigma^2}}$$

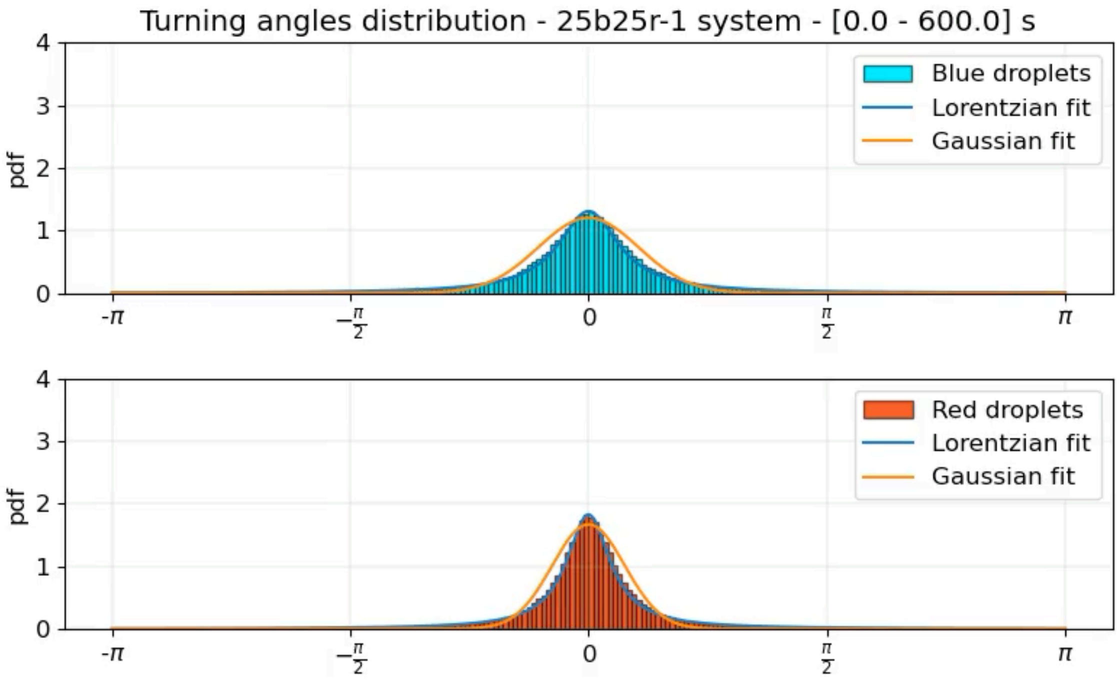
Lorentzian distribution adequate

$$P(\Delta\theta) = \frac{1}{\pi} \frac{\gamma}{(\Delta\theta - \mu)^2 + \gamma^2}$$

Lévy flight stochastic process for the rotational diffusion ? [5]

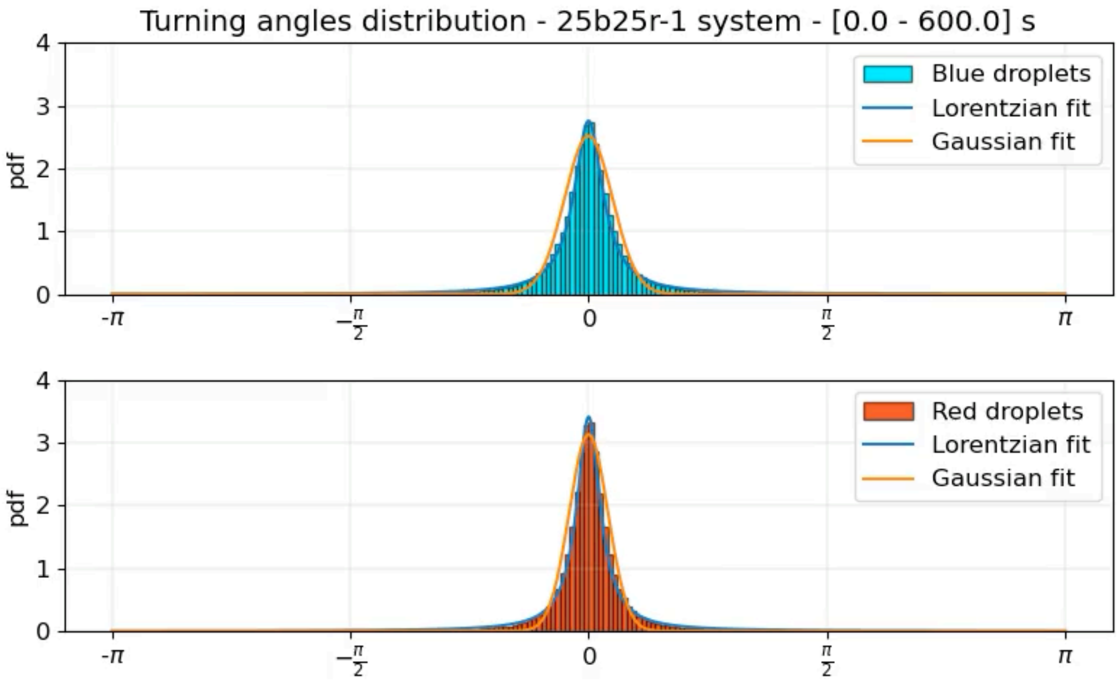
5. M.F. Shlesinger, G.M. Zaslavsky, and U. Frisch. Lévy Flights and Related Topics in Physics: Proceedings of the International Workshop Held at Nice, France, 27–30 June 1994. Lecture Notes in Physics. Springer Berlin Heidelberg, 1995

Analysis - Turning Angles Distribution



Discrepancies arise when droplets **move slow** and the **uncertainty of detection** becomes **relevant**

Analysis - Turning Angles Distribution - smooth



Discrepancies arise when droplets **move slow** and the **uncertainty of detection** becomes **relevant**

↓

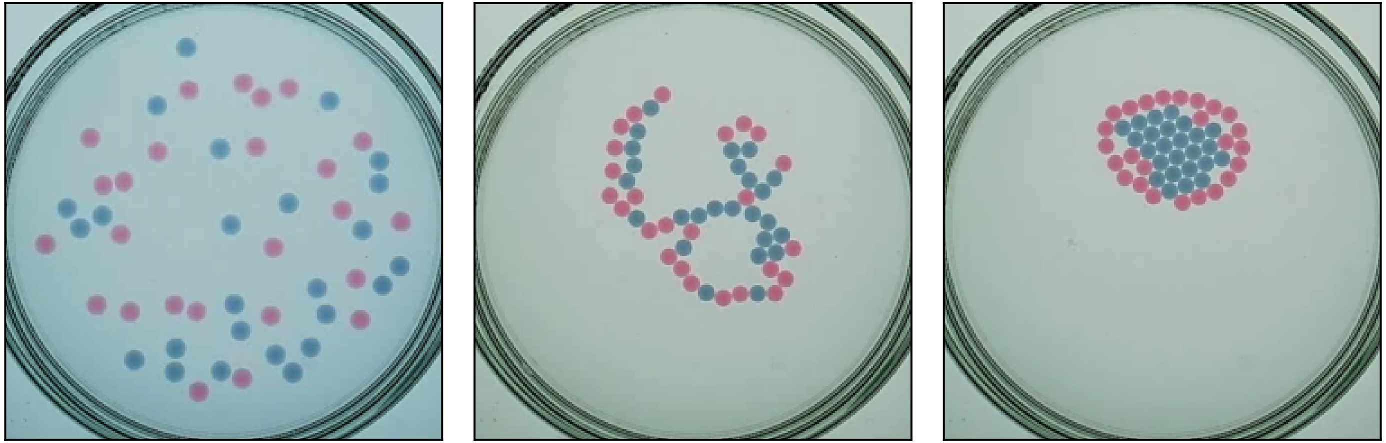
Savitzky-Golay filter smoothing of trajectories are applied

Lorentzian distribution is preserved

Analysis - Dynamical properties

Translational and **rotational diffusive properties** depend on the activity of the system

Stage 1 -- T = 00:00:00 Stage 2 -- T = 02:00:00 Stage 3 -- T = 04:00:00

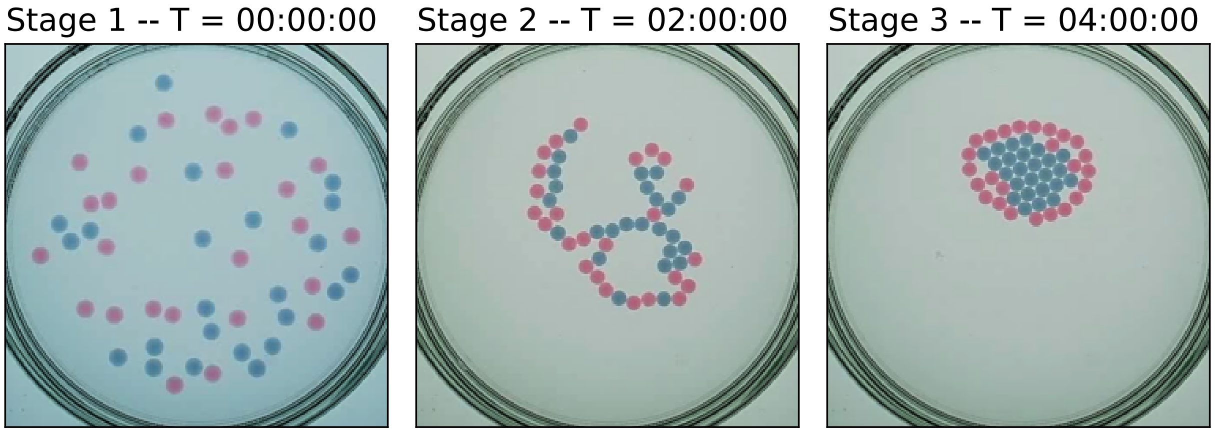


The next step is the characterization of the **relaxation dynamics** and **structure formation** through the means of VACF & RDF

Analysis - Velocity autocovariance function

VACF are employed to **investigate the structural arrest of a droplets' motion**

$$K^a(\tau) = \frac{1}{\sigma_\alpha^2}\frac{1}{N_\alpha}\sum_{i\in\alpha}\Big\langle (\mathbf{v}^i(t) - \langle \mathbf{v}^i(t)\rangle)\cdot(\mathbf{v}^i(t+\tau) - \langle \mathbf{v}^i(t+\tau)\rangle)\Big\rangle$$



Analysis - Velocity autocovariance function

High activity:

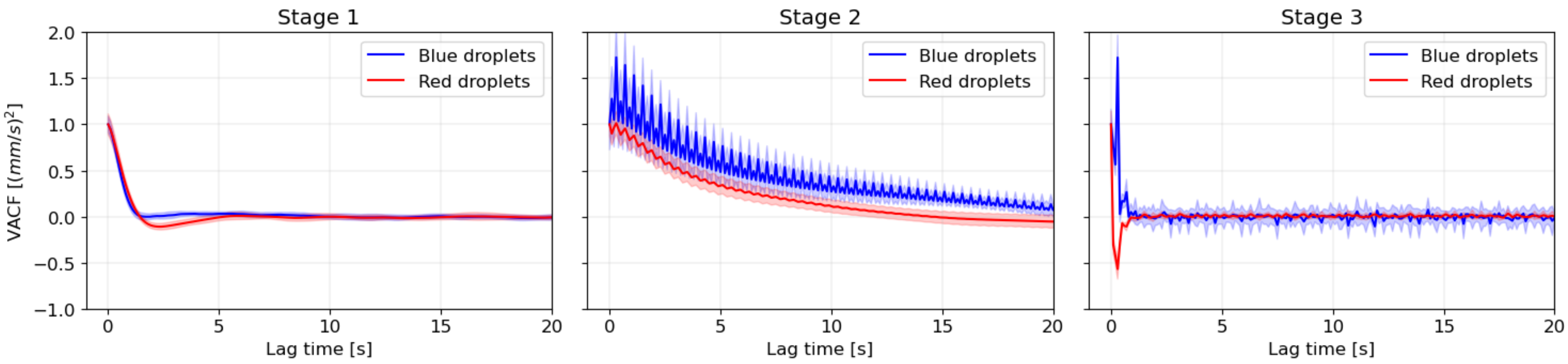
Fast decorrelation

Medium activity:

Persistent plateaus characteristic of arrested dynamics

Low Activity:

Regular arrangement, arrested state



Analysis - Velocity autocovariance function - smooth

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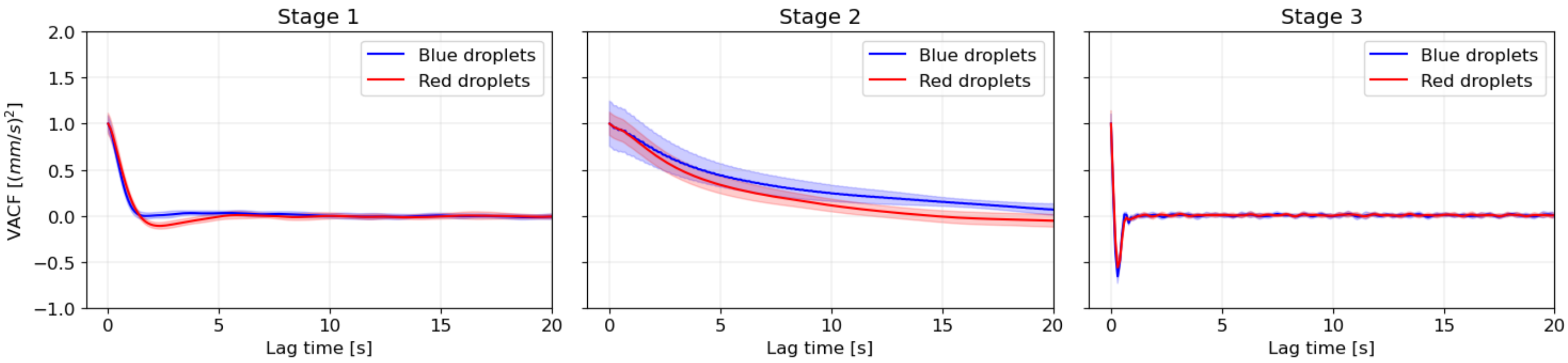
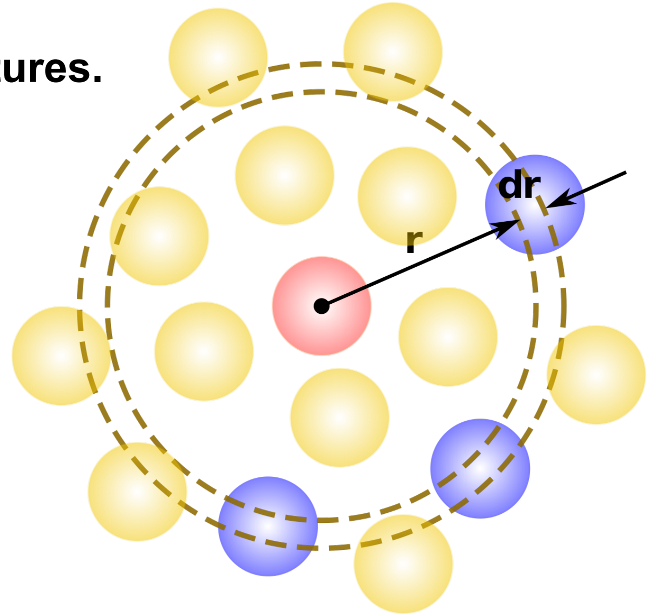


Analysis - Radial Distribution Function

Provides the **characterization of the spatial local structures.**

Approximation: Computed by dividing the average number of droplets at distance r by the the expected number of droplets assuming a homogeneous distribution.

$$g_{\alpha,\beta}(r) = \frac{\langle \rho_{\alpha,\beta}(r) \rangle}{N_\beta V} \quad \text{with} \quad V = \pi(\delta r^2 + 2r\delta r)$$

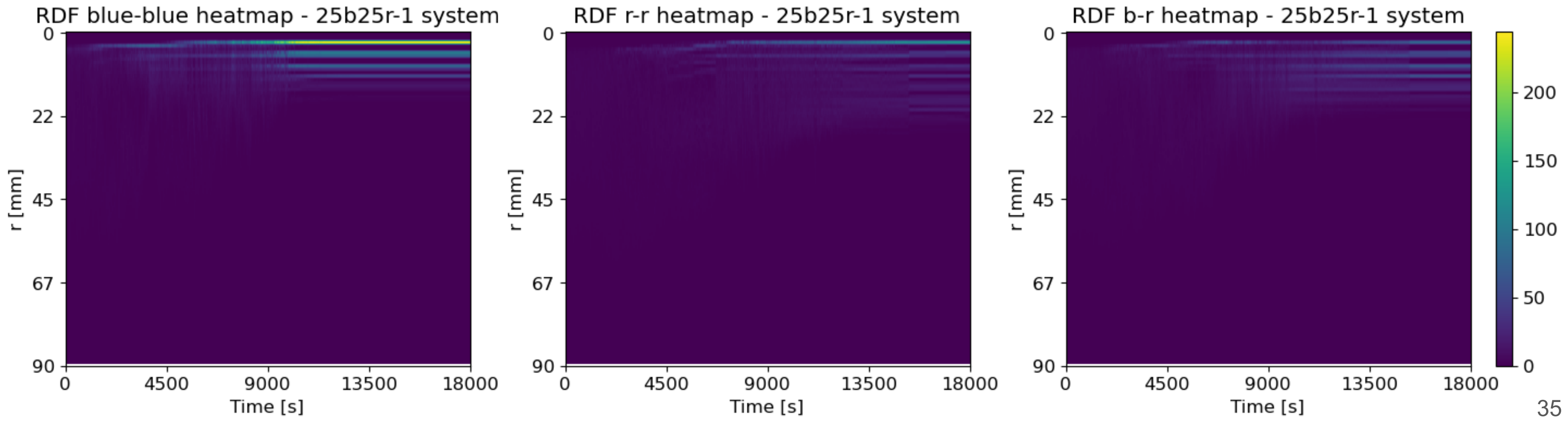


Analysis - Radial Distribution Function

Consistency with steric interaction: $g_{\alpha,\beta}(r < d_d) = 0$

The first **"solvation" shell appear** after 2000 s for blue droplets, after 5000 s for red droplets.

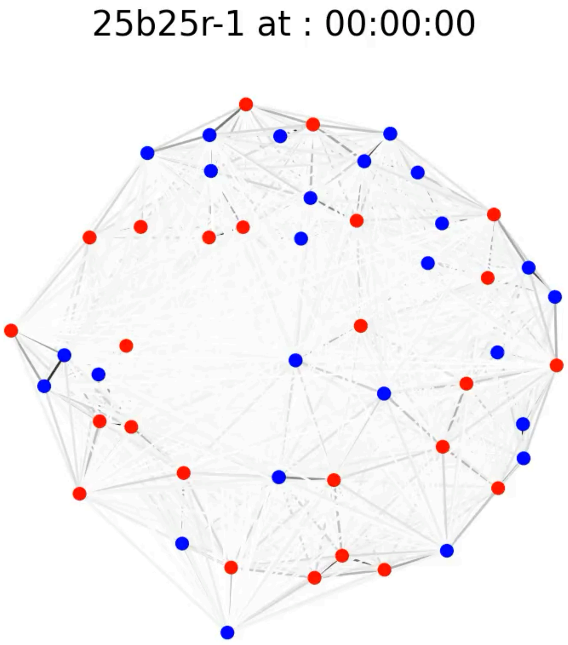
Structure observed also in the mixed species RDF



Future developments

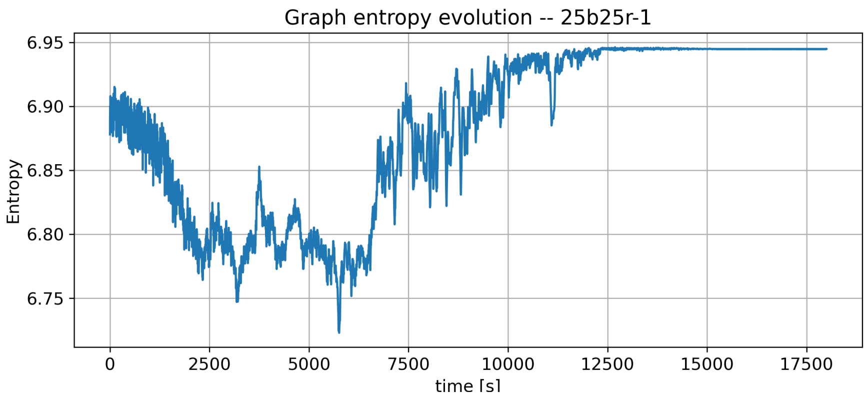
The future developments from this point are multiple:

- **Improve smoothing via Kalman Filter**
- **Network-based analysis**
- **Orientation alignment and Velocity vector field analysis**



Future developments

$$E(G,w) = -\sum_{uv \in E} p_{uv}\, log(p_{uv}) \qquad p_{uv} = \frac{w_{uv}}{\sum_{uv \in E} w_{uv}}$$



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Future developments - orientation alignment

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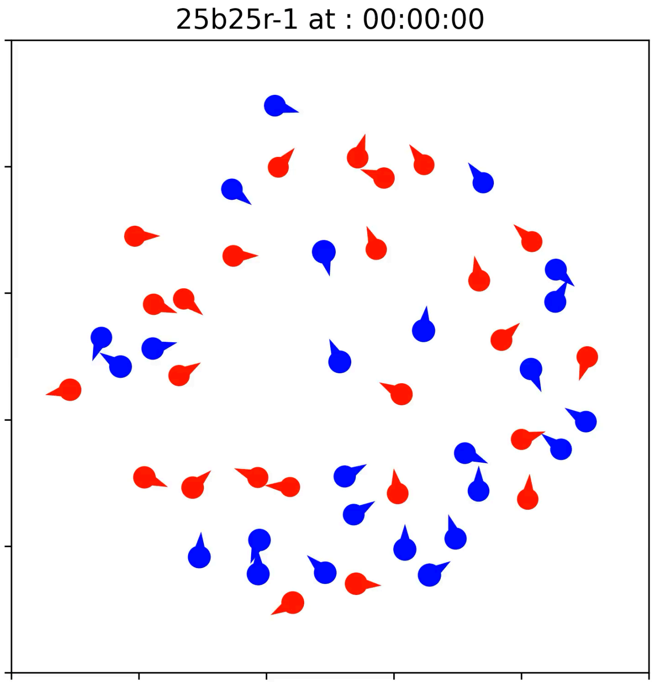

Future developments - velocity field

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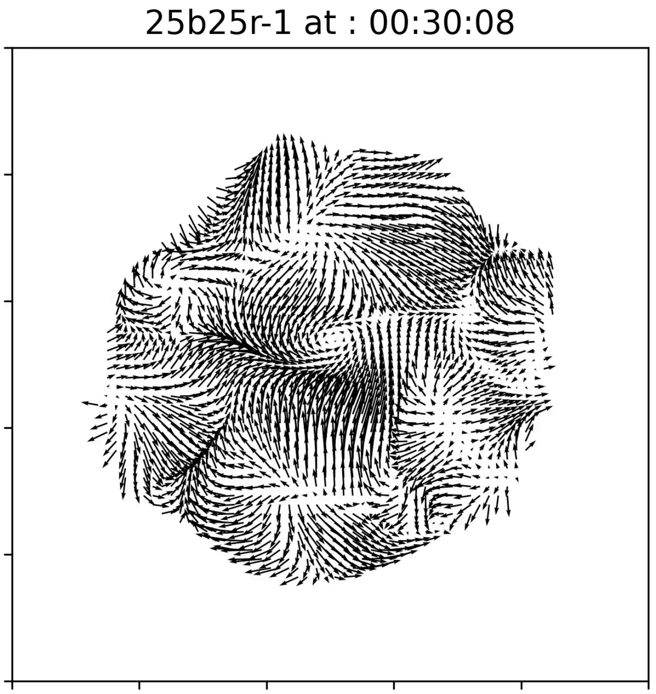

Thanks for your attention!

References

1. Vizsnyiczai, G., Frangipane, G., Maggi, C. *et al.* Light controlled 3D micromotors powered by bacteria. *Nat Commun* **8**, 15974 (2017).
2. Muneyuki Matsuo, Hiromi Hashishita, Shinpei Tanaka, and Satoshi Nakata. Sequentially selective coalescence of binary self-propelled droplets upon collective motion. Langmuir, 39(5):2073–2079, 2023. PMID: 36692295.
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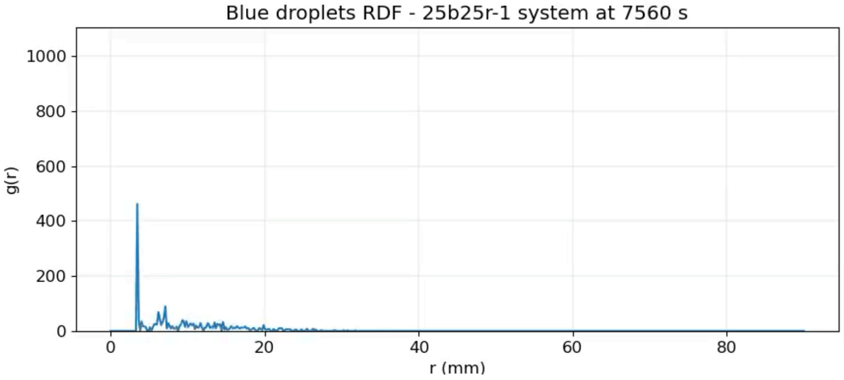
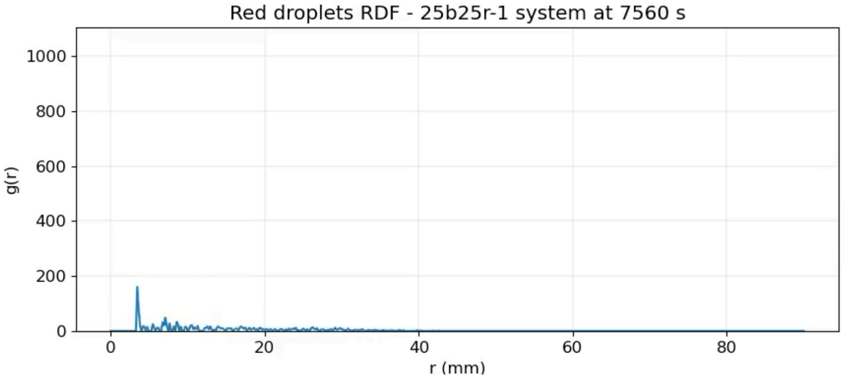
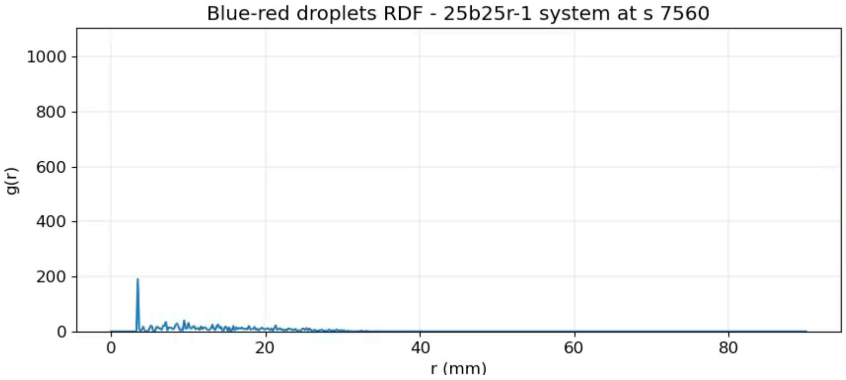
Extra Material - RDF

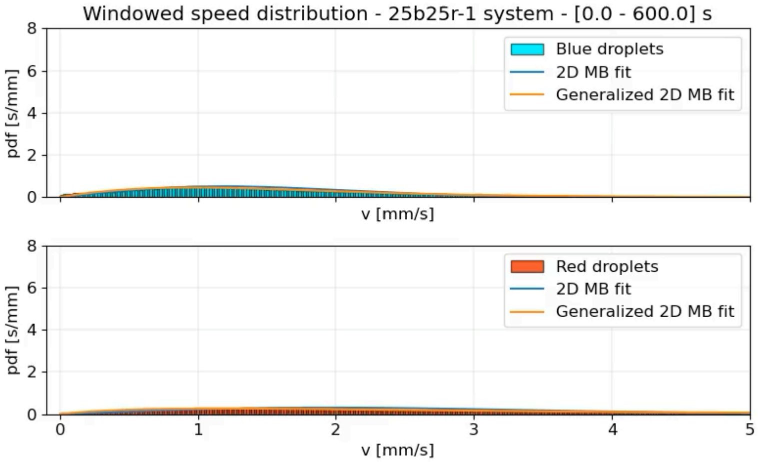




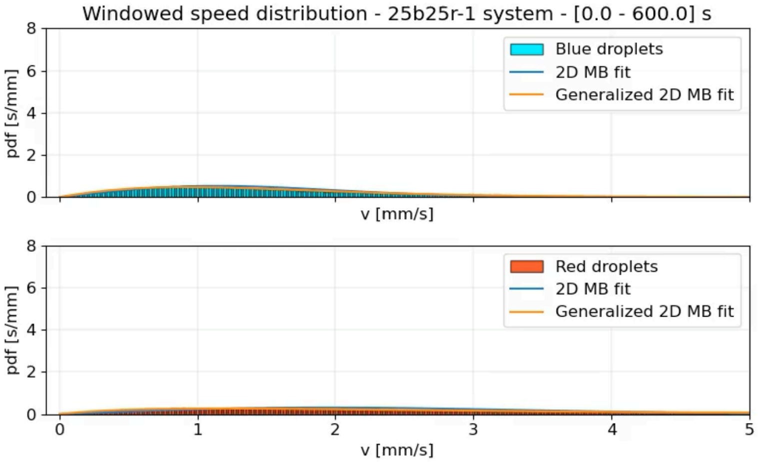


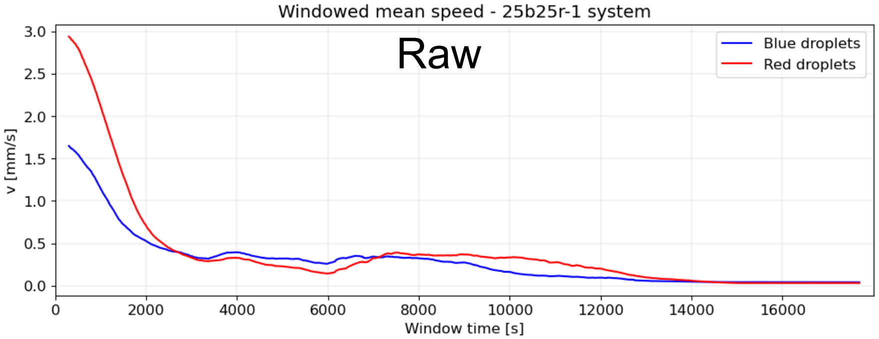
Extra Material - Speed distribution

Raw



Smooth





Extra Material - TDA on Graph

Persistent homology

Vietoris-Rips filtration