Active particles inside moving droplet

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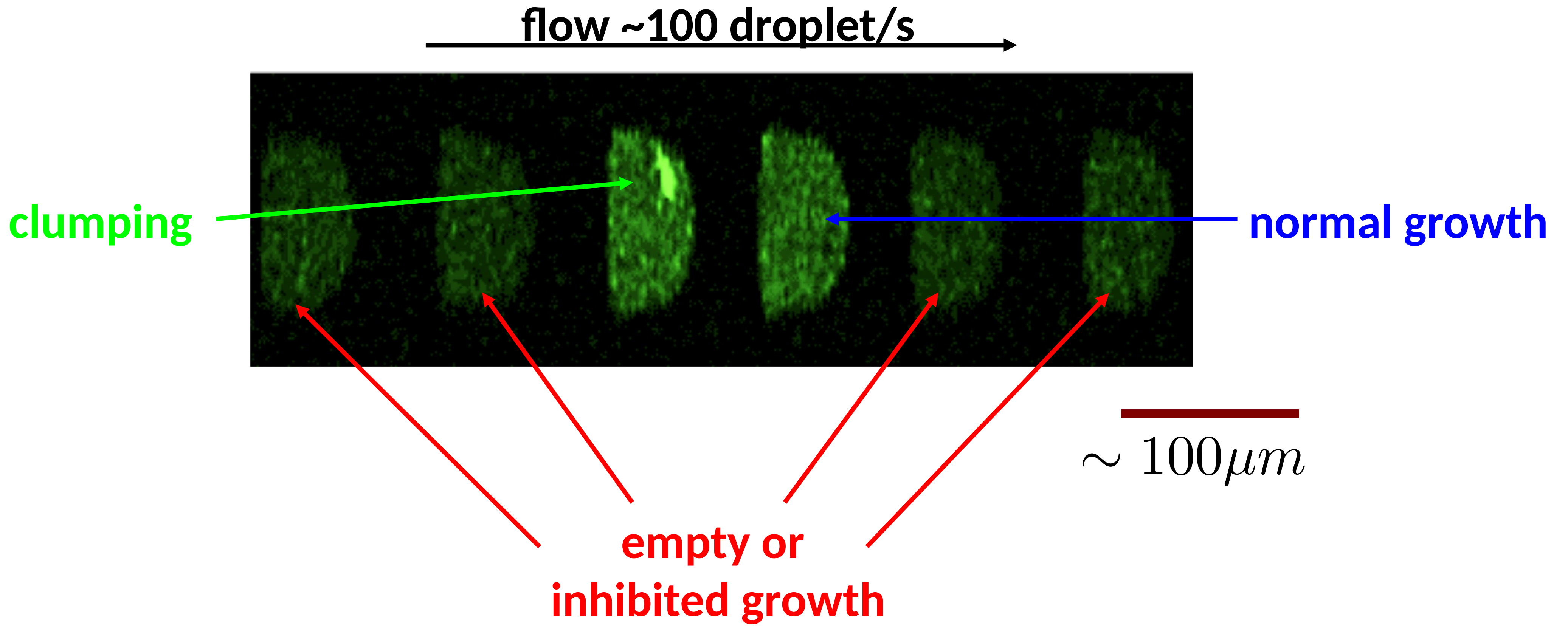
Motivation: experiments on antibiotic inhibition of bacteria growth inside droplets

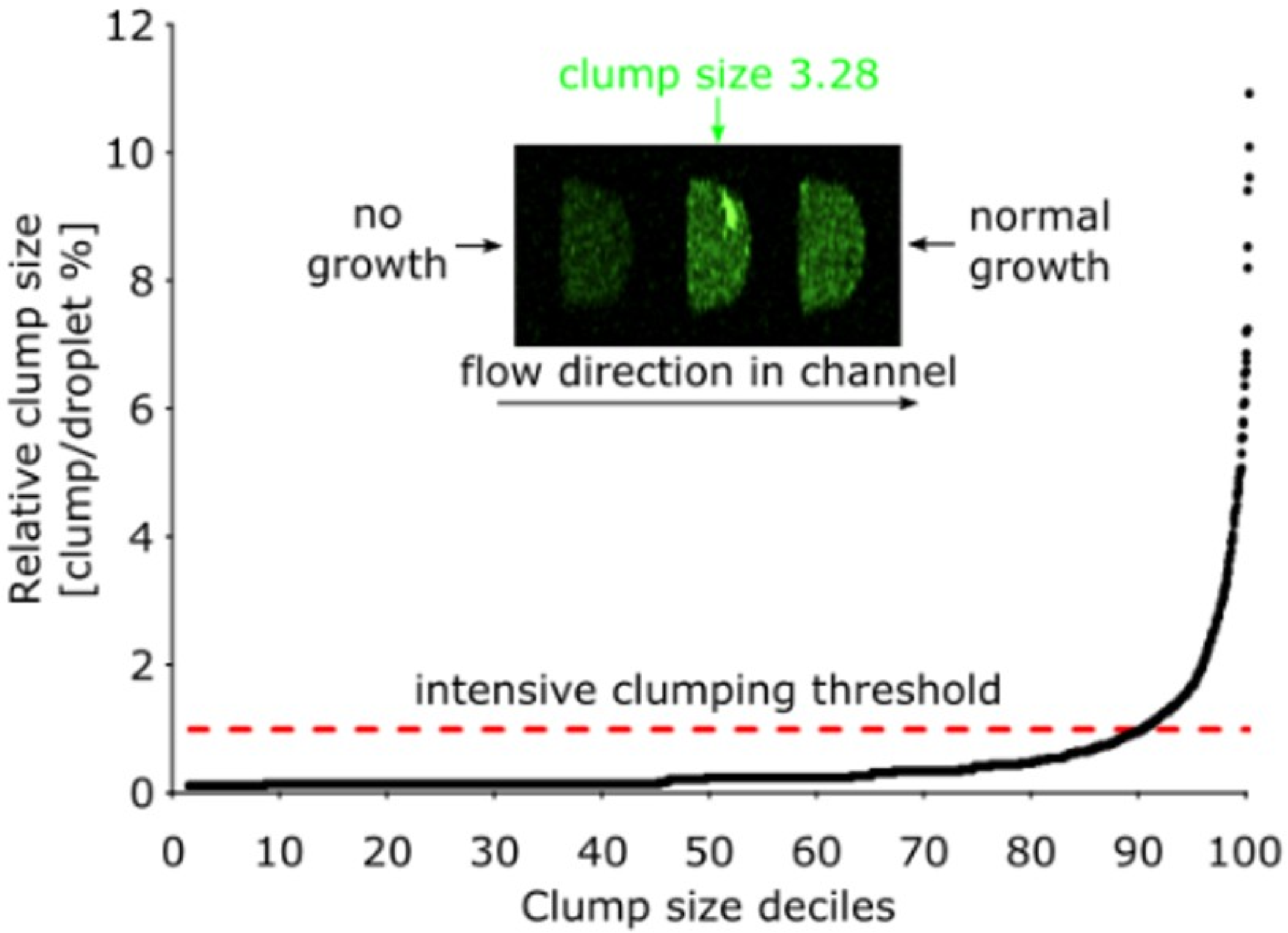
Scheler, Makuch, Debski, Horka, Ruszczak, Pacocha, Sozański, Smolander, Postek, Garstecki, submitted:

Detection of bacteria in droplets (~20 000) by confocal microscope:



Clumps are visible as regions of much higher fluorescent intensity

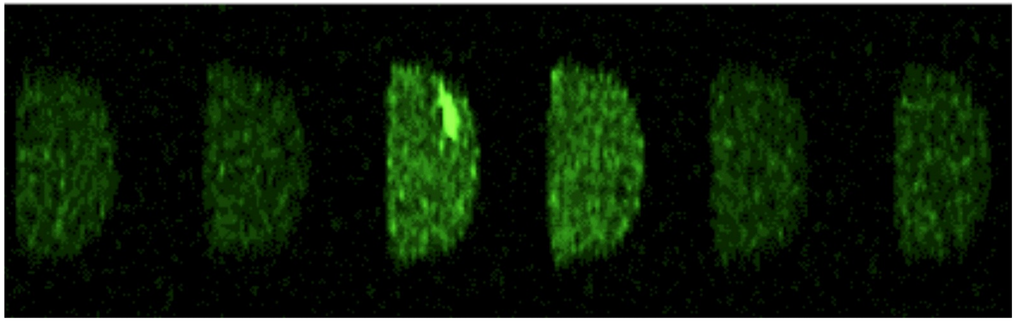
Statistic of clumps



How many droplets have clumps?
What is size distribution of clumps?

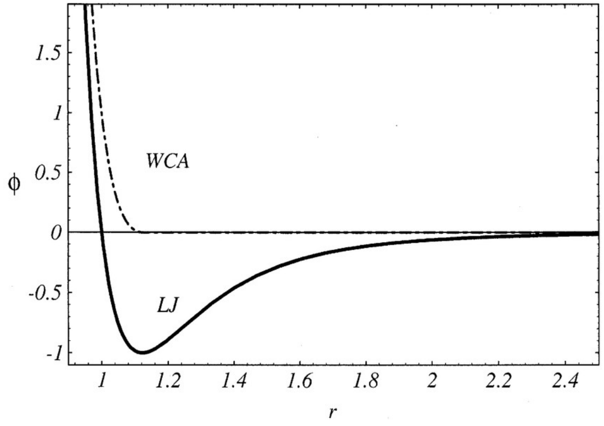
It is a motivation to study:
statistics of clumps of active particles in a droplet with recirculating flow

Model of active particles inside droplet



•Swimmers (d=1 μm, U_0=1μm/s) with Brownian rotation ($\tau_R=1/D_R$)

•confined in a droplet (d=100 μm) modeled by WCA potential ($r_{cut}=2^{1/6}d$),



•recirculating flow inside droplet: $A_{ext}\mathbf{v}_0(\mathbf{r})$,

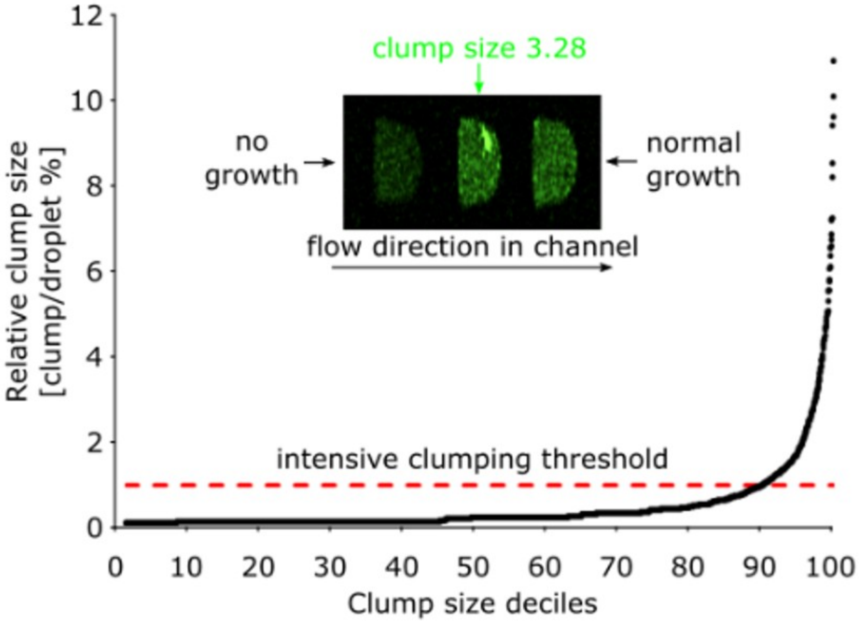
•no hydrodynamic interactions

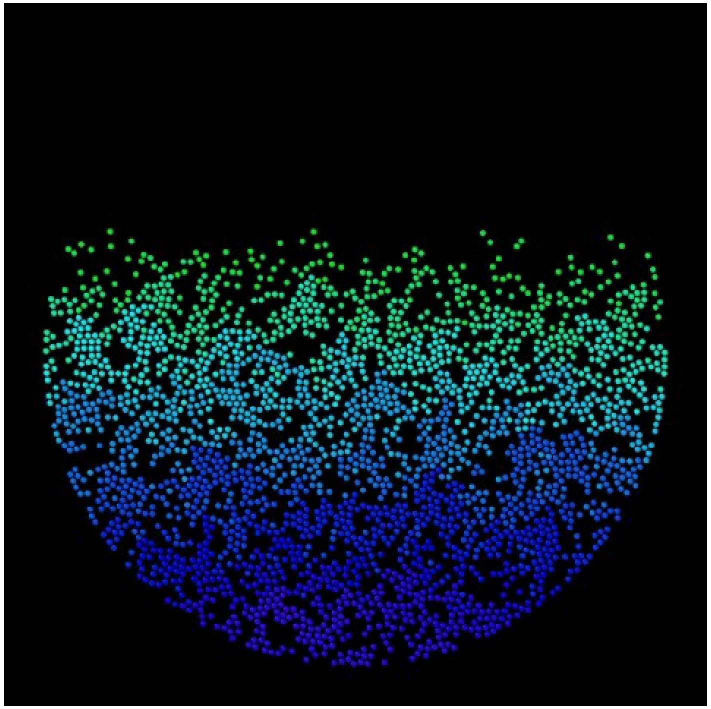
•excluded volume interactions between particles (WCA)

We study clumping for different:

volume fractions, φ, rotation times, τ_R and amplitudes of external flow, A_{ext}

Measurements of statistics of clumps





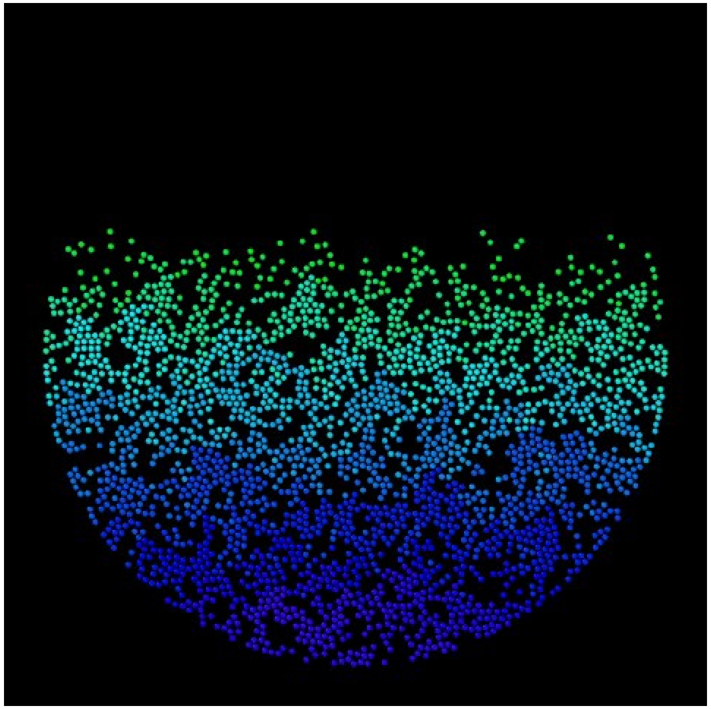
Experiment:
statistics from many droplets

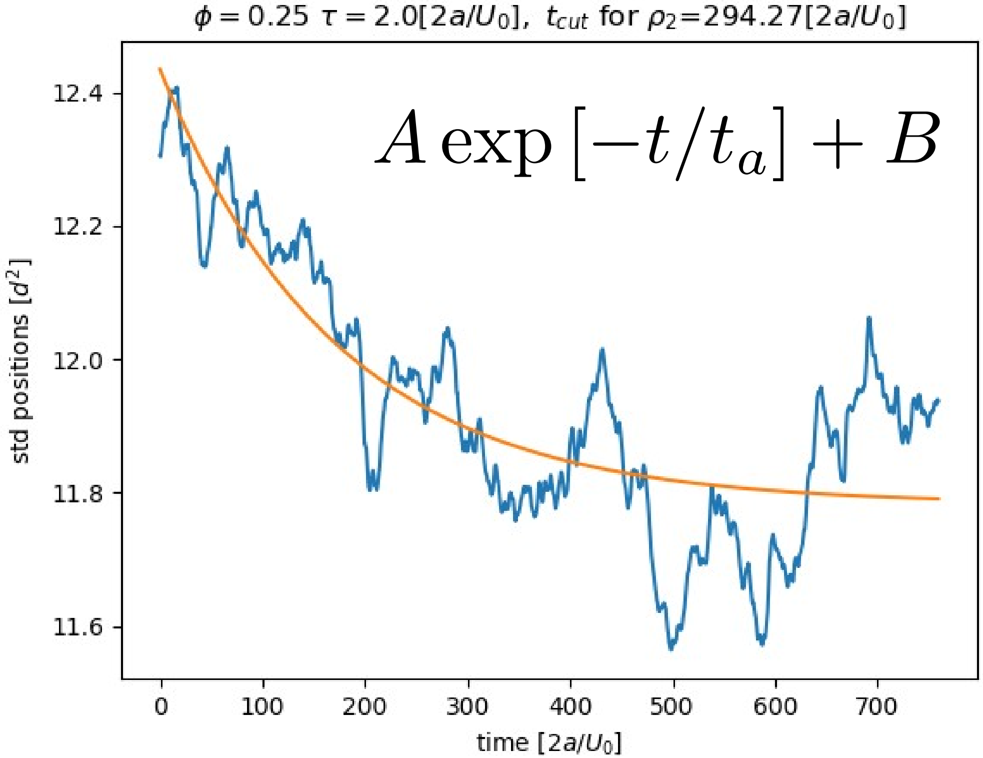
Simulations:
-achieve stationary state
-measure over independent configurations to get clump statistics

Stationary state

$$\rho_2(t) = \frac{1}{ND^2}\sum_{i=1}^{N}\mathbf{R}_i(t)^2\,,$$

$$\langle U\rangle(t) = \frac{1}{N}\sum_{i=1}^{N}|\mathbf{U}_i(t)|$$





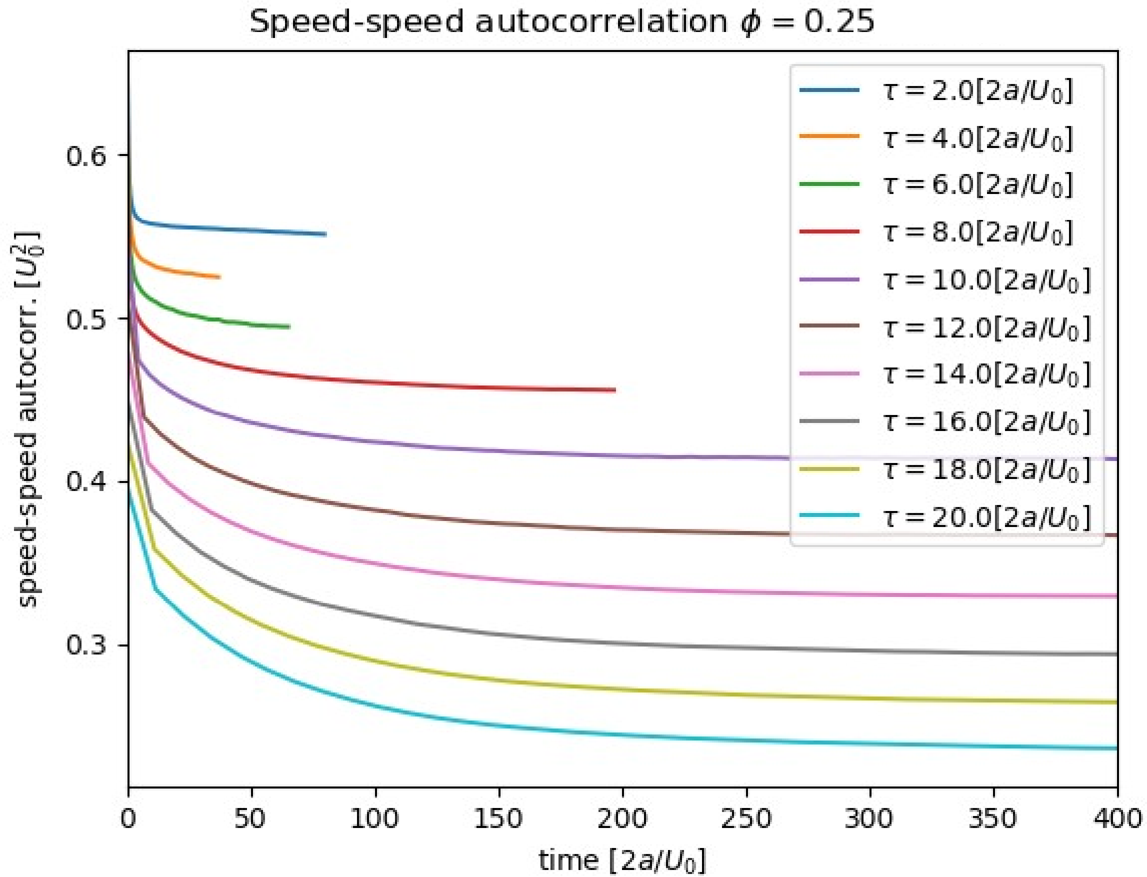
$$|A|\exp[-t/t_a]\,/\,|B| < \epsilon_{rr}$$

$$t_{cut} = -t_a\log[|B\epsilon_{rr}/A|]$$

Independent measurements

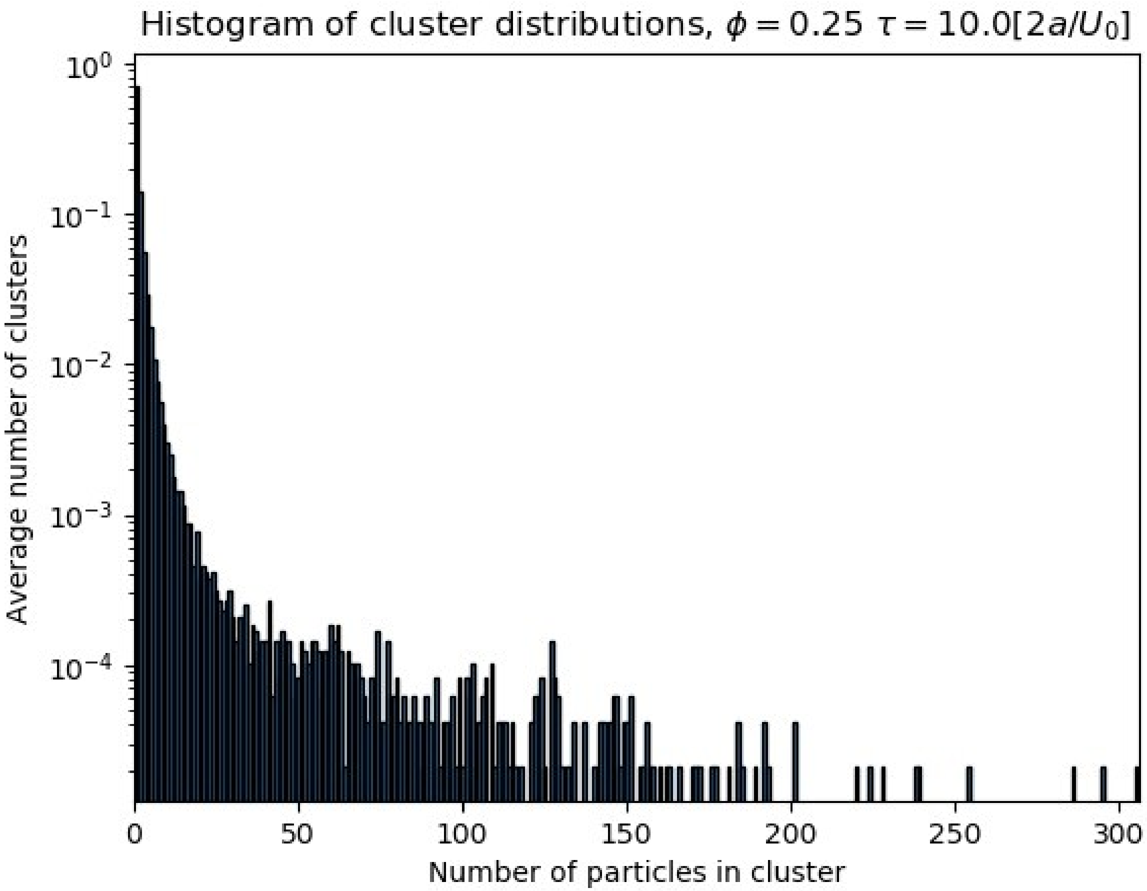
Autocorrelation time of measured quantity determines whether two measurements are independent
E.g. speed-speed autocorrelation:

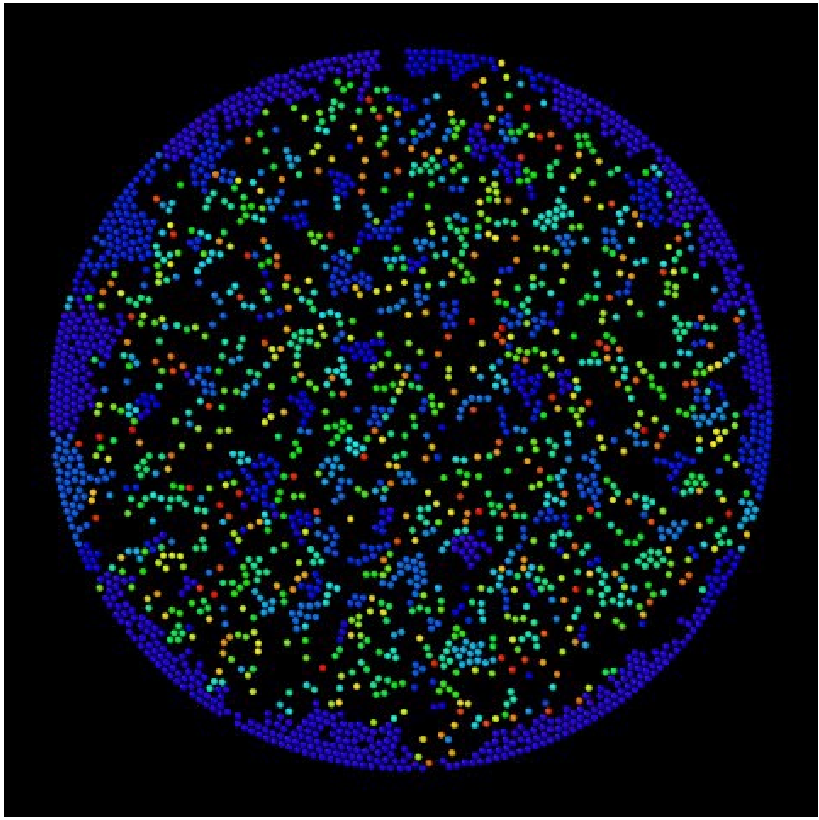
$$\left\langle U\left(t+\tau\right)U\left(t\right)\right\rangle_t = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{T}\int_0^T dt\ \left|\mathbf{U}_i\left(t+\tau\right)\right|\left|\mathbf{U}_i\left(t\right)\right|$$



Statistics of clumps

Clump: we define through distance r_{cut} in WCA potential





Summary

Done

✔automated procedure to measure clump statistics (volume fraction, rotation time, amplitude)
✔hoomd based code (thx: Austin and Stewart)
✔currently automated procedure for amplitude of torque

To do:

-change speed autocorrelation to autocorrelation of cluster size distribution (the quantity of interest)
OR (can it be reduced to density-density autocorrelation

$$F(\vec{k},t) = \frac{1}{N}\langle \rho_{\vec{k}}(t)\rho_{-\vec{k}}(0)\rangle$$

-apply external flow instead of uniform torque
(checked that it is easy modification of hoomd)

-from 2d to 3d - easy from the perspective of simulations in hoomd