Crystallization in Granular Shear Flows

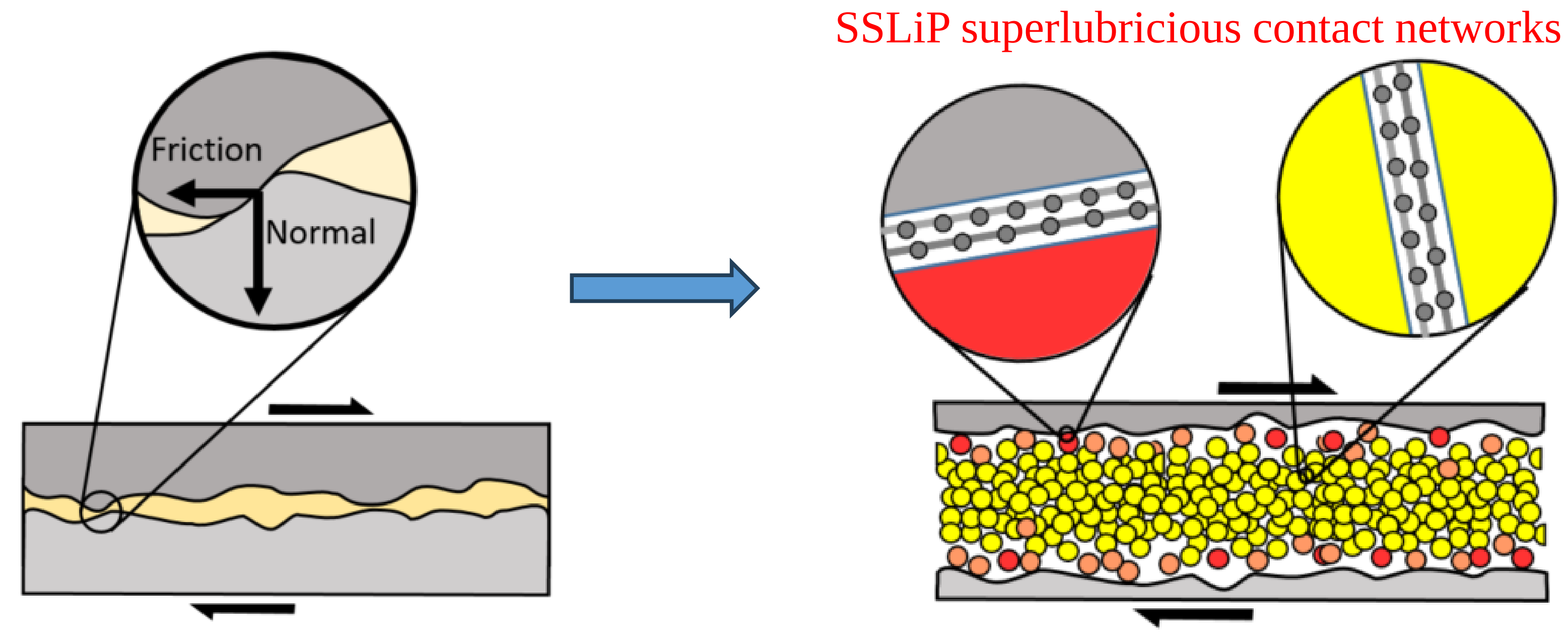
Esma Kurban, Dalila Vescovi, Diego Berzi

Department of Civil and Environmental Engineering, Politecnico di Milano, Italy

INTRODUCTION

An estimated 25% of world energy consumption and 75% of mechanical failure is due to friction, the force resisting relative motion between contacting objects. The Scaling-up Superlubricity into Persistence (SSLiP) project aims to reduce friction between contacting objects by an interdisciplinary approach combining surface science, granular and soft condensed matter, statistical physics, and tribology. The fundamental mechanism of superlubricity, which is generally defined to be friction coefficient $\mu < 0.01$, is an atomic lattice misfit between clean, flat, rigid crystalline surfaces [1].

SSLiP superlubricious contact networks



Standard boundary lubrication friction

Dynamic topology of tribocolloids

In the scope of the SSLiP, ploughing asperity contacts of standard boundary lubrication friction at rough surfaces are replaced by the dynamic topology of colloids coated with atomic flat 2D materials. We aim to optimize the properties of colloidal/granular particles to achieve and sustain superlubricity under extreme conditions (high loads, shear rates). These properties include restitution coefficient, inter-particle friction coefficient, and size distribution.

METHODS

Molecular dynamics simulations

Shear flows of superlubric granular/colloidal particles are simulated in LAMMPS.

$N = 3150$ flowing spheres (yellow)

density $\rho_p = 1$,

stiffness $k_n = 2 \cdot 10^5\, \rho_p d\, V^2$,

restitution coefficient $e_n = 0.4$,

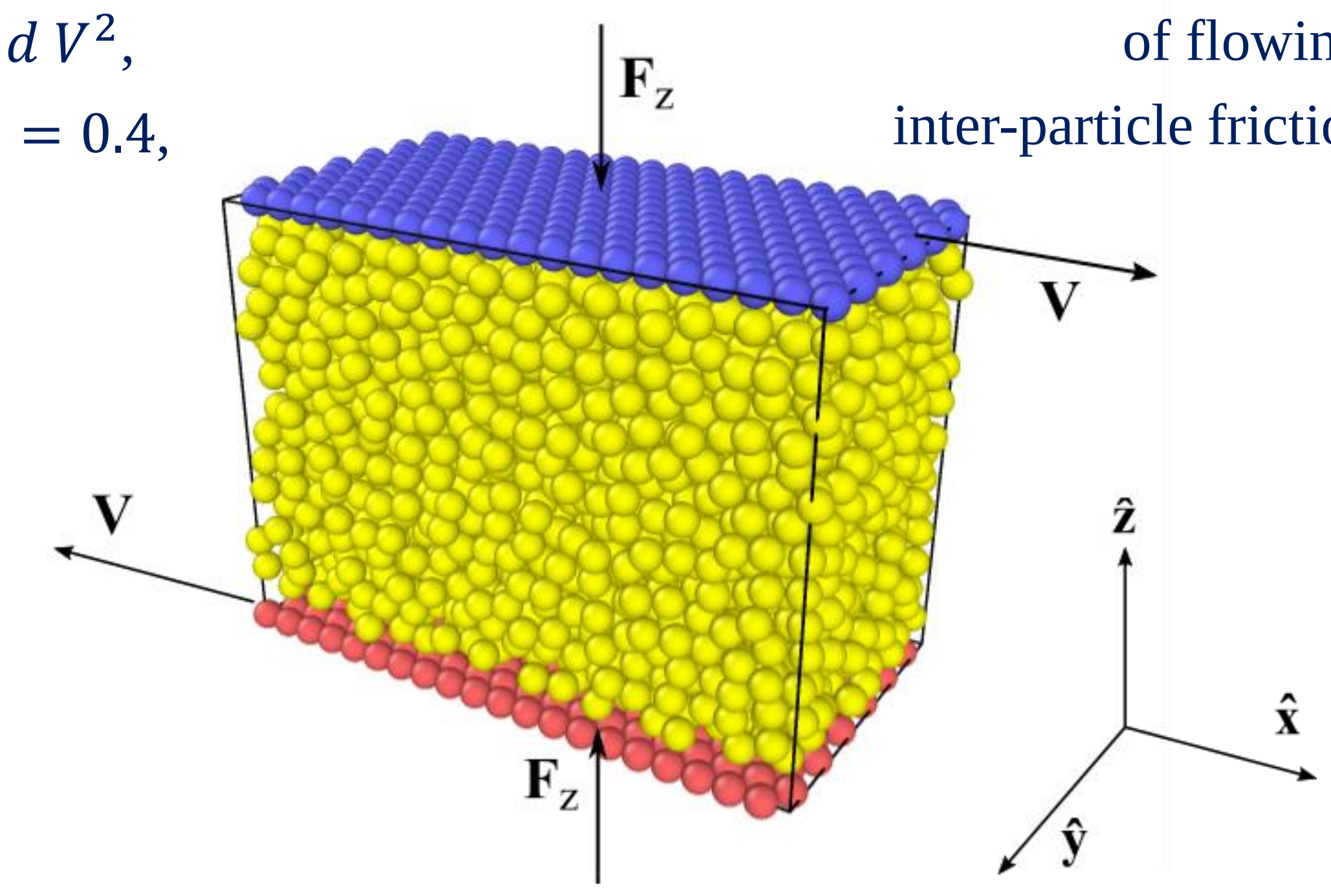
diameter d=1,

inter-particle friction μ_p

N_w=480 wall spheres (blue and red)

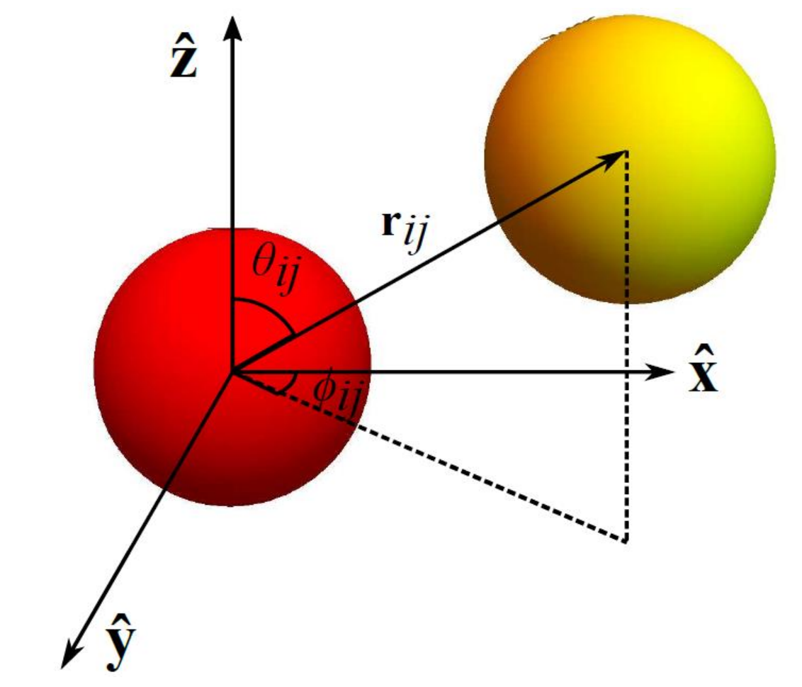
same ρ_p, k_n, e_n,d of flowing spheres,

inter-particle friction $\mu_w = 0$



- Absence of gravity, nondimensional units.
- Periodic boundary conditions in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions.
- The walls are constructed in hexagonal close-packed arrangement, exposed to a constant vertical load F_z and a shear velocity V=1.
- Hookean force between contacting spheres.
- Data are taken in the steady state and averaged over $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and in time.
- Measurement of the macroscopic friction $\mu = \frac{F_x}{F_z}$, F_x is the horizontal force at walls.
- Average volume fraction $\nu = \frac{N * vs}{v_t}$, v_s is volume of a sphere and v_t is the total volume occupied by the flowing particles.
- Effect of inter-particle friction coefficient μ_p and vertical load F_z.

Ordering Analysis by bond orientational order parameters



$\mathbf{r}_{ij}$: the bond vector between particle i (red) with j (yellow).

$\bar{\tilde{q}}_6$ helps to distinguish between liquid and crystals. $\bar{\tilde{q}}_4$ is sensitive to the crystal type.

Associate a set of spherical harmonics with every bond joining a particle i and its neighbours $N_b(i)$:

$$q_{lm}(i) = \frac{1}{|N_b(i)|} \sum_{j \in N_b(i)} Y_{lm}(\theta_{ij}, \phi_{ij})$$

$$q_l(i) = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |q_{lm}(i)|^2}$$

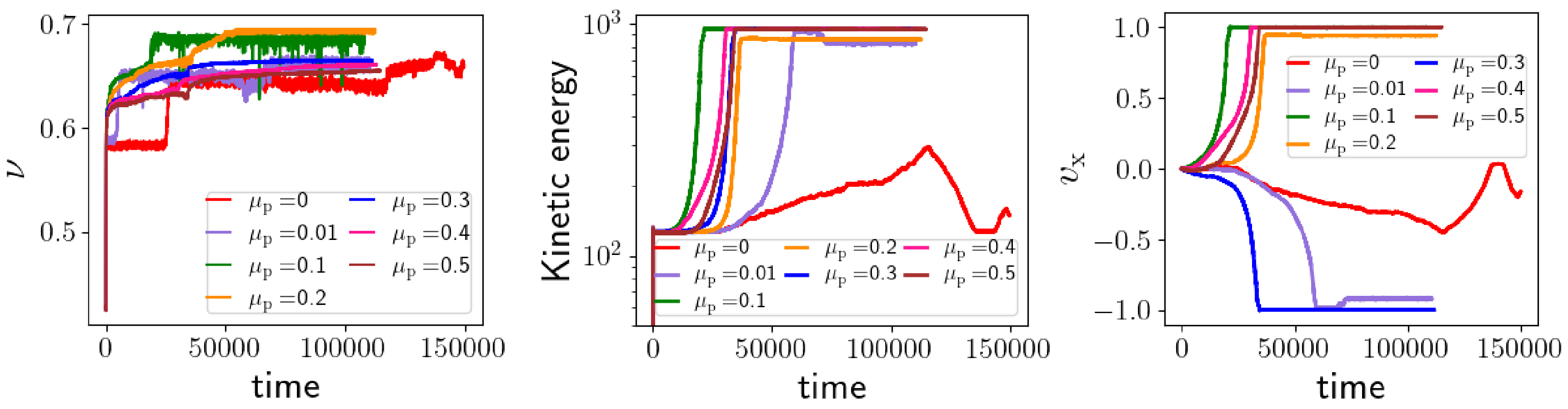
New local bond orientational order parameters $\tilde{q}_l(i) = \boldsymbol{q}_l(i) \cdot \boldsymbol{q}_l(j)$ are averaged over the nearest neighbours of particle i [2]:

$$\bar{\tilde{q}}_l(i) = \frac{1}{1 + |N_b(i)|} \left[\tilde{q}_l(i) + \sum_{j \in N_b(i)} \tilde{q}_l(j) \right]$$

RESULTS

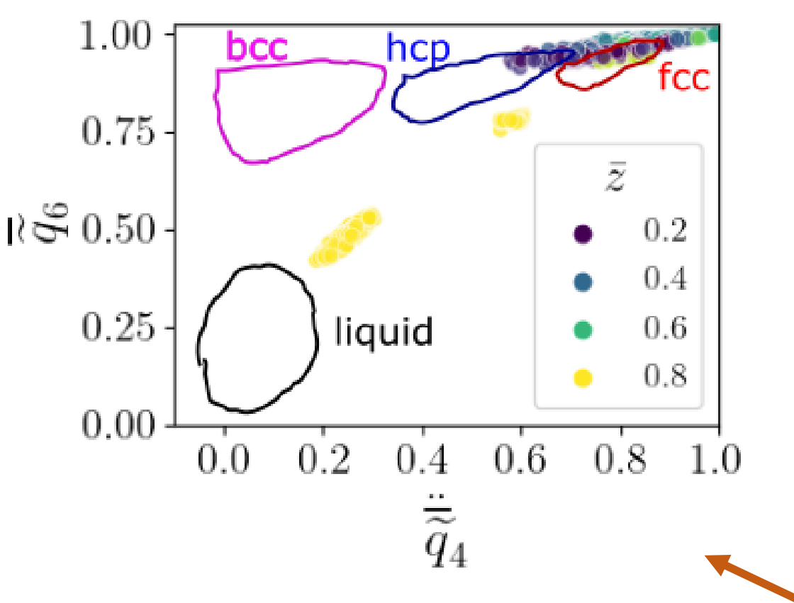
Crystallization

F_z=2.4 $\rho_p d^2\, V^2$, Time evolution

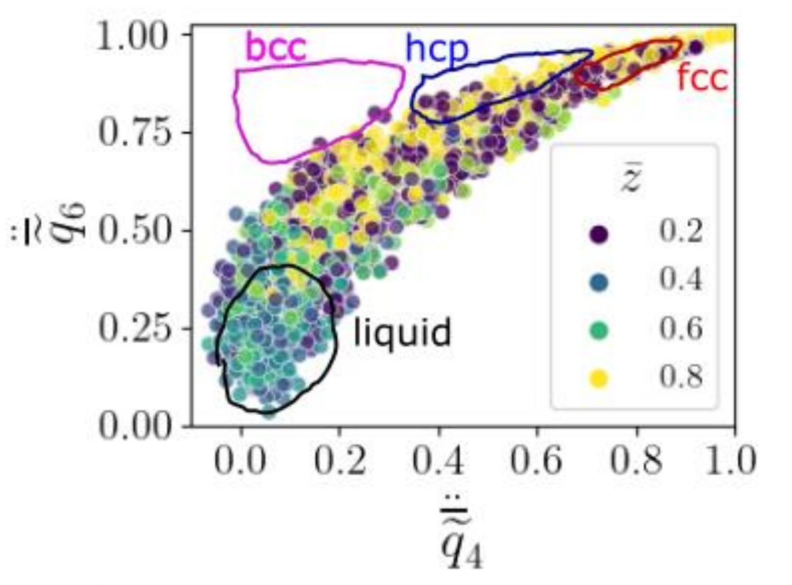


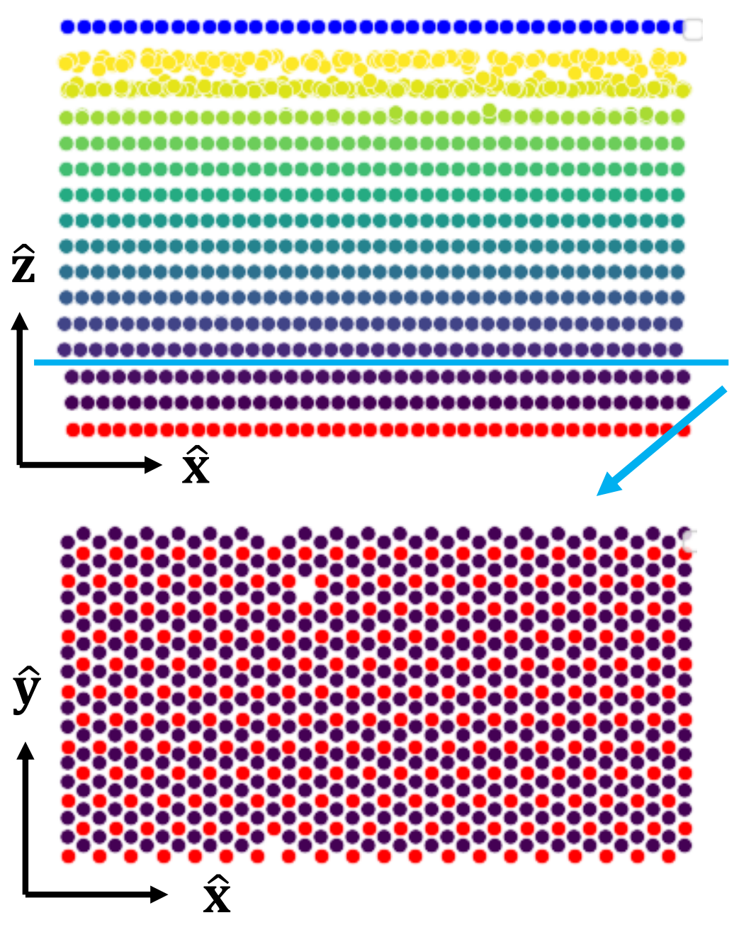
v_x: the velocity of center of mass of the flowing particles in the $\hat{\mathbf{x}}$ -direction.

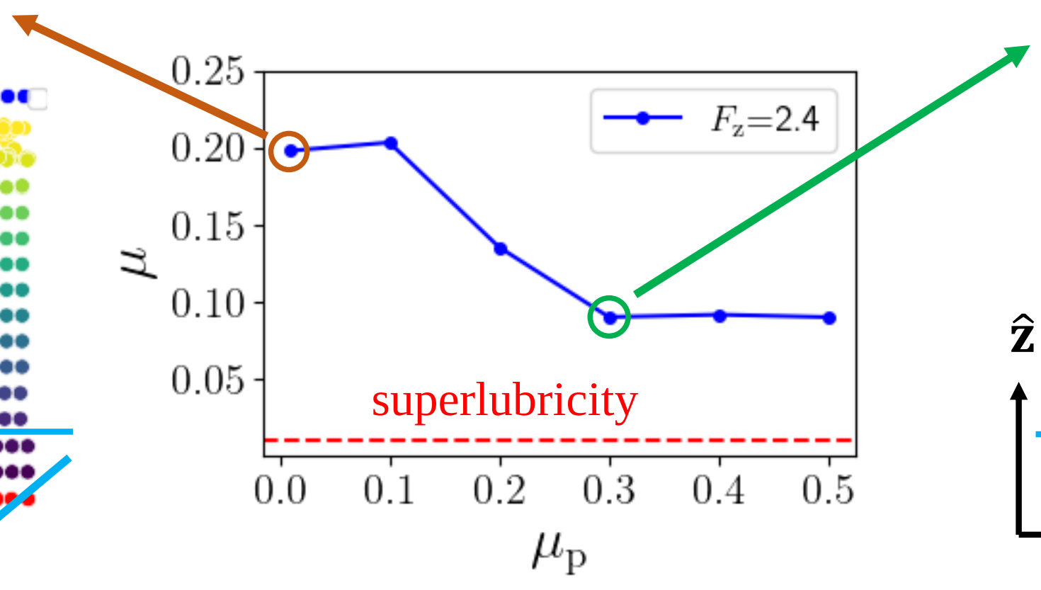
F_z=2.4 $\rho_p d^2\, V^2$, Ordering Analysis

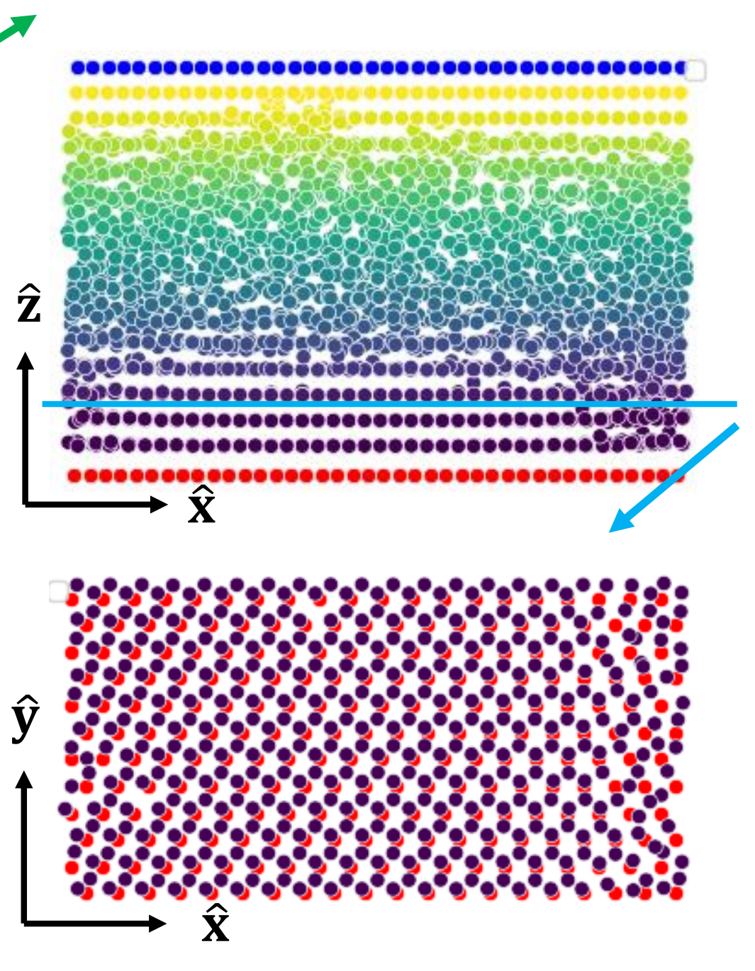


bcc: body-centered cubic, hcp: hexagonal close-packed, fcc: face-centered cubic, liquid phases of Leonard-Jones particles at melting point [2] are shown as reference.







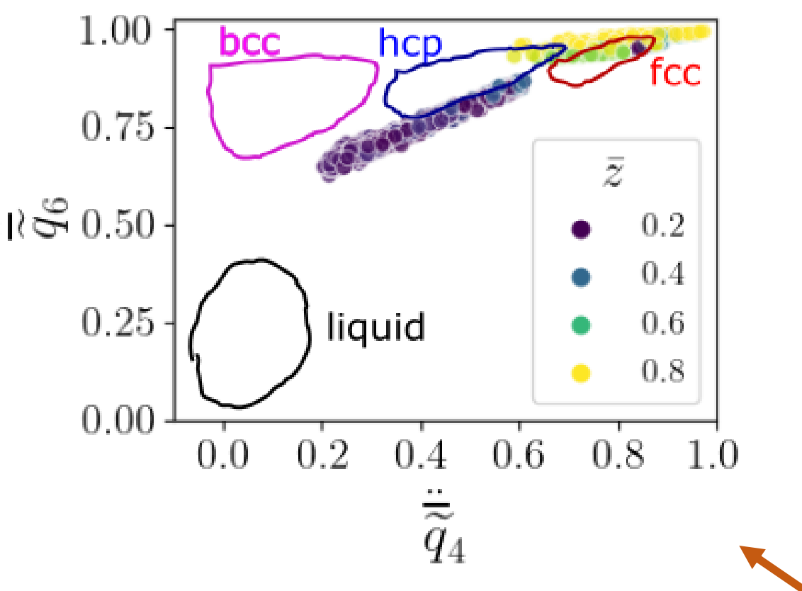


As the flowing particles become more frictional, the macroscopic friction(μ) reduces up to 50% due to incommensurate structures near the walls.

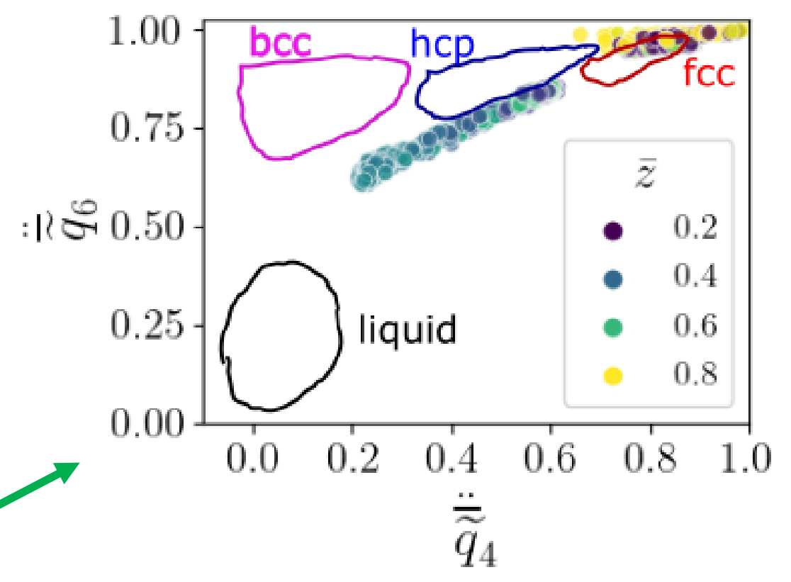
Commensurate structures, fcc layering

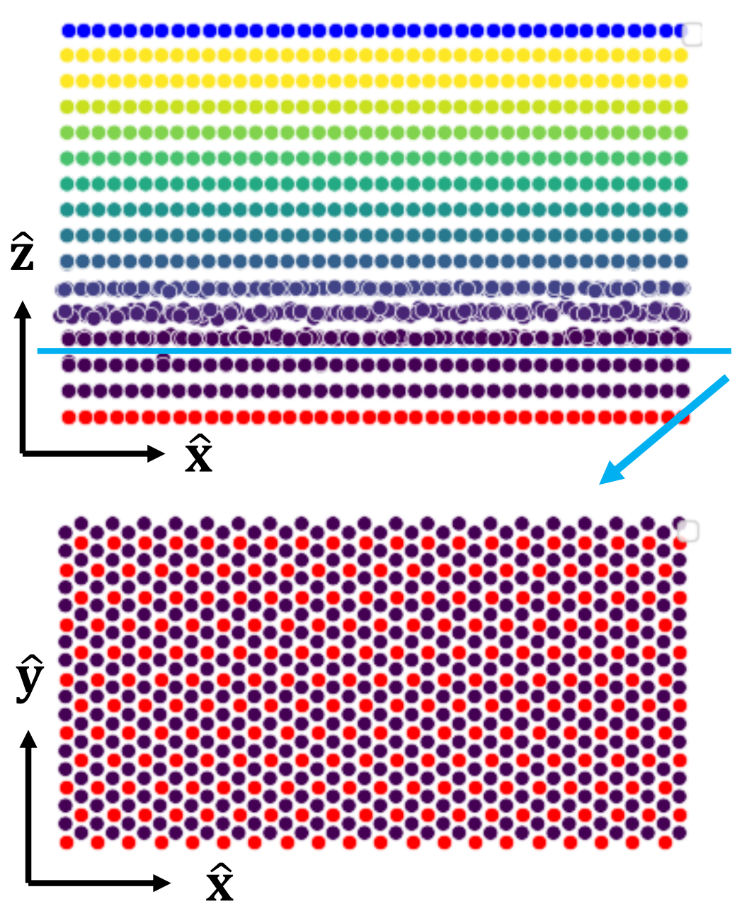
Incommensurate structures

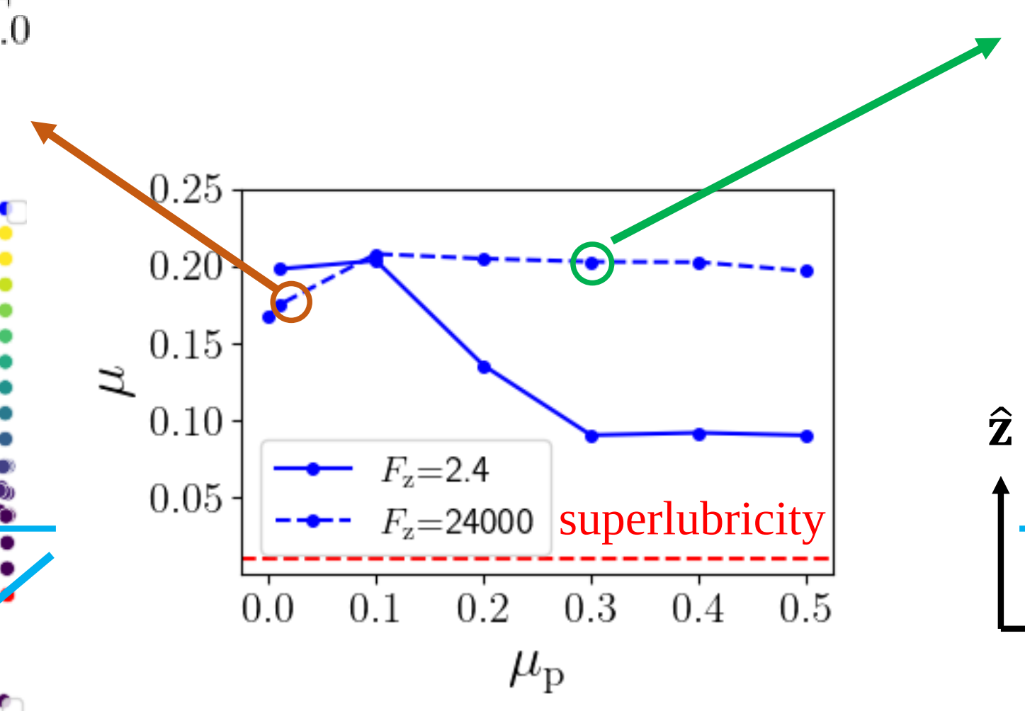
F_z=24000 $\rho_p d^2\, V^2$, Ordering Analysis

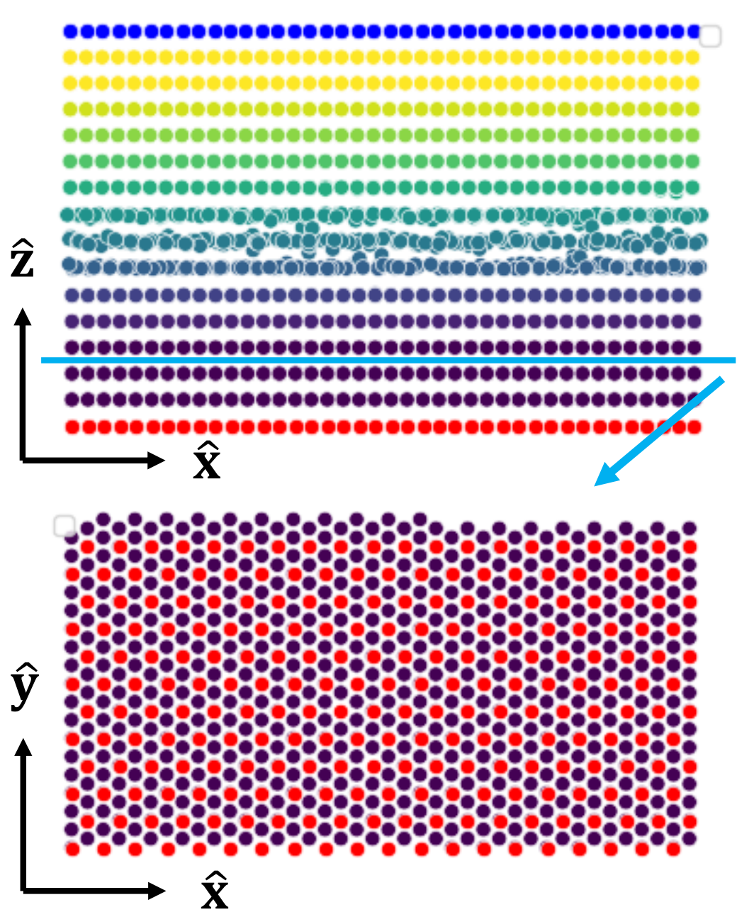


As the vertical load increases, the effect of inter-particle friction is eliminated by yielding similar structures near the boundaries.









Commensurate structures, fcc layering near the walls

REFERENCES

1. K. Shinjo and M. Hirano, “Dynamics of friction: superlubric state”, Surf. Sci., vol. 283, Mar. 1993.
2. H. Eslami, P. Sedaghat, and F. Muller-Plathe, “Local bond order parameters for accurate determination of crystal structures in two and three dimensions”, Physical Chemistry Chemical Physics, vol. 20, Oct. 2018.

ACKNOWLEDGEMENTS

- HORIZON-EIC-2021-PATHFINDEROPEN-01, Project number: 101046693, SSLiP: Scaling-up Superlubricity into Persistence https://www.sslip.eu/.

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Commision. Neither the European Union nor the granting authority can be held responsible for them.

Funded by the European Union

CONTACT

Mail address: esma.kurban@polimi.it