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Particles in the ABC flow, and morphology of droplets in turbulent flows

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Part one: Particles in the turbulent ABC flow

Alessandro Chiarini, Ianto Cannon & Marco E. Rosti



Particles in turbulent flows

- Particle fluid interaction affects the **fluid motion** and the **paths of the particles**
- Modulation of the **large-scale flow** is relevant to sandstorms in engine cooling/cleaning

Sandstorm



Credit: Barcroft media, 2010

Pollen dispersal

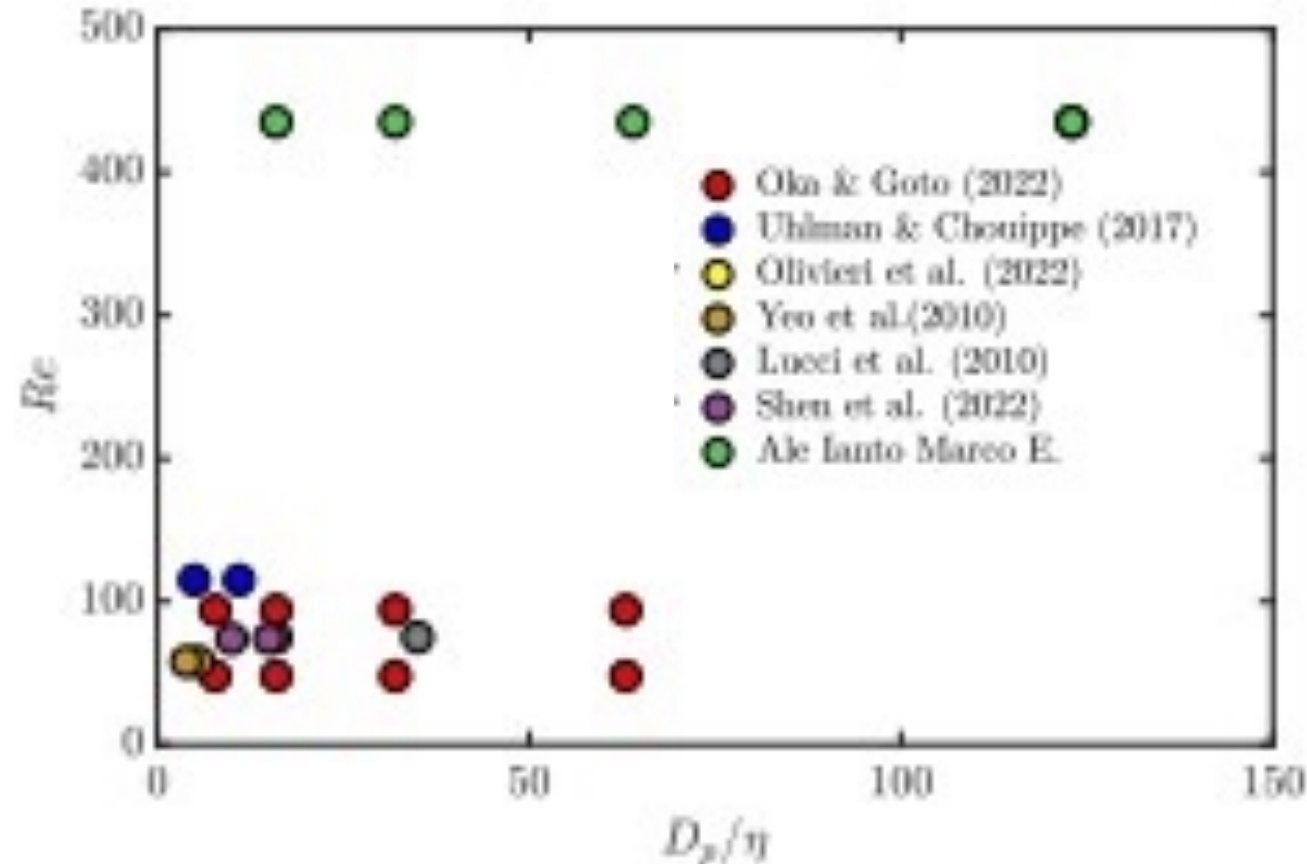


Credit: Robert J. Erwin



Recent work in particle-laden turbulence

- Recent reviews have stated a **gap in our understanding** between small particles and large massive particles
- We explore **intermediate size** particles ($\eta < D_p < L$)
- We investigate a **high turbulence intensity** ($Re_\lambda = 435$)



Brandt & Colletti *Ann. Rev. Fluid Mech.* (2021)

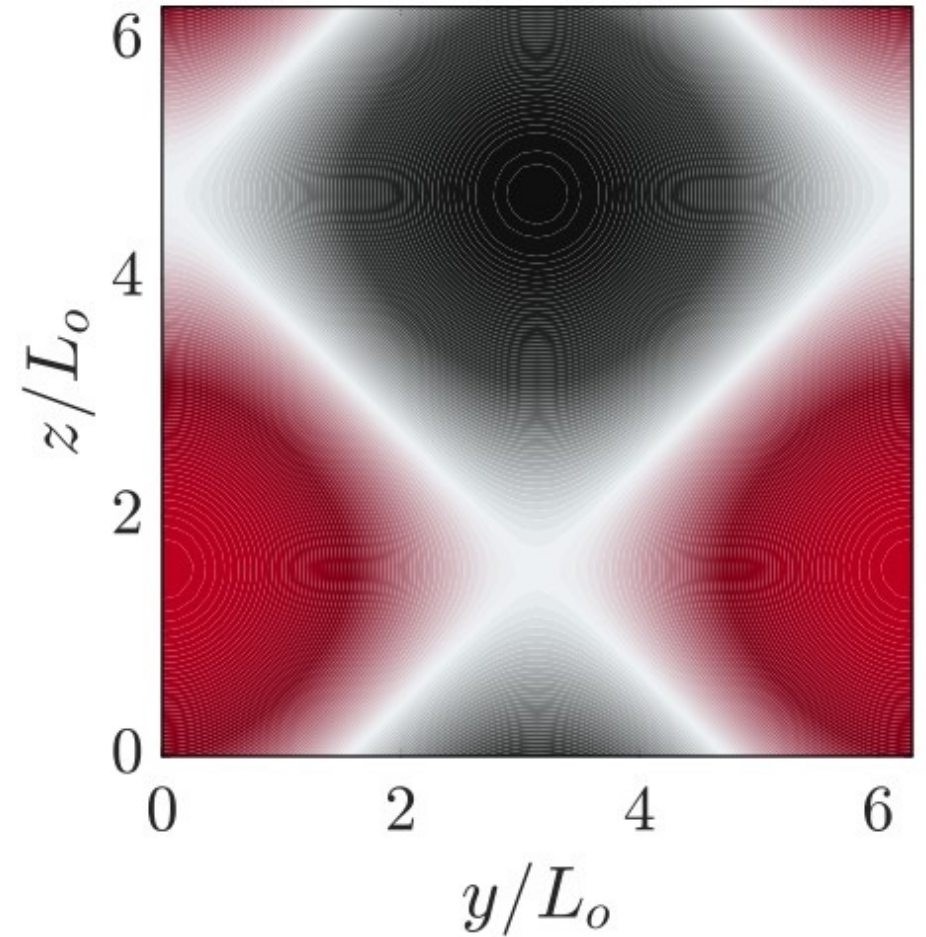
Oka & Goto, *J. Fluid Mech.* (2022)

Our goals

- How do solid particles modulate the *largest scales* of the flow?
- We choose Arnold-Beltrami-Childress (ABC) forcing with $A = B = C = 1$

$$\mathbf{f} = \left(\frac{2\pi}{L}\right)^2 F_o \begin{pmatrix} A \sin(2\pi z/L) + C \sin(2\pi y/L) \\ B \sin(2\pi x/L) + A \sin(2\pi z/L) \\ C \sin(2\pi y/L) + B \sin(2\pi x/L) \end{pmatrix}$$

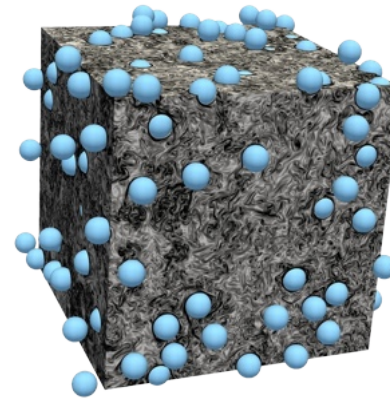
- Triperiodic cellular forcing
- Rotation symmetry in x, y, z
- 3D *mean shear*
- No need for walls
- How do particles *disperse* in the flow?



Musacchio & Boffetta, *Phys. Rev. E* (2014)

Podvigina, *Phys. D: Nonlin. Phenom.* (1994)

Numerical method



Two-way coupled IBM

- We solve the flow on a 1024^3 numerical with $Re_\lambda \approx 435$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho_f} \nabla p + \nu \Delta \mathbf{u} + \mathbf{f} + \mathbf{f}_F$$

$$\nabla \cdot \mathbf{u} = 0$$

- 10^4 spherical particles

$$m^p \frac{dU_i^c}{dt} = \oint_{\partial V^p} \sigma_{ij} n_j dA + F_i^{\text{ext}},$$

$$I^p \frac{d\Omega_i^c}{dt} = \oint_{\partial V^p} \epsilon_{ijk} r_j \sigma_{kl} n_l dA + T_i^{\text{ext}}$$

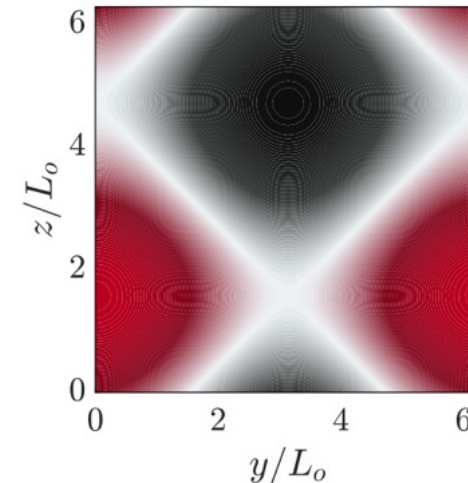
Hori et al, Comput. & Fluids, 2021

ABC forcing

- We vary the particle mass fraction

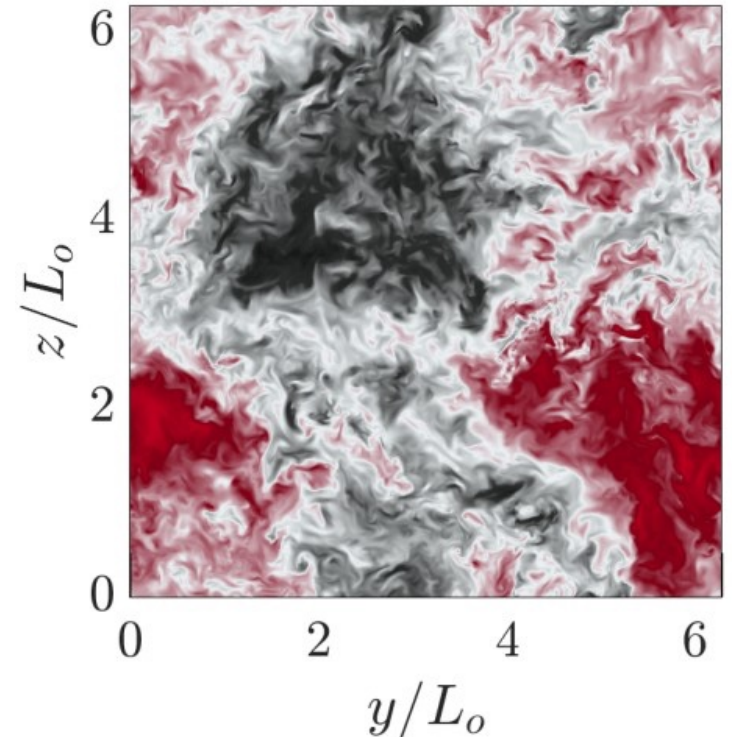
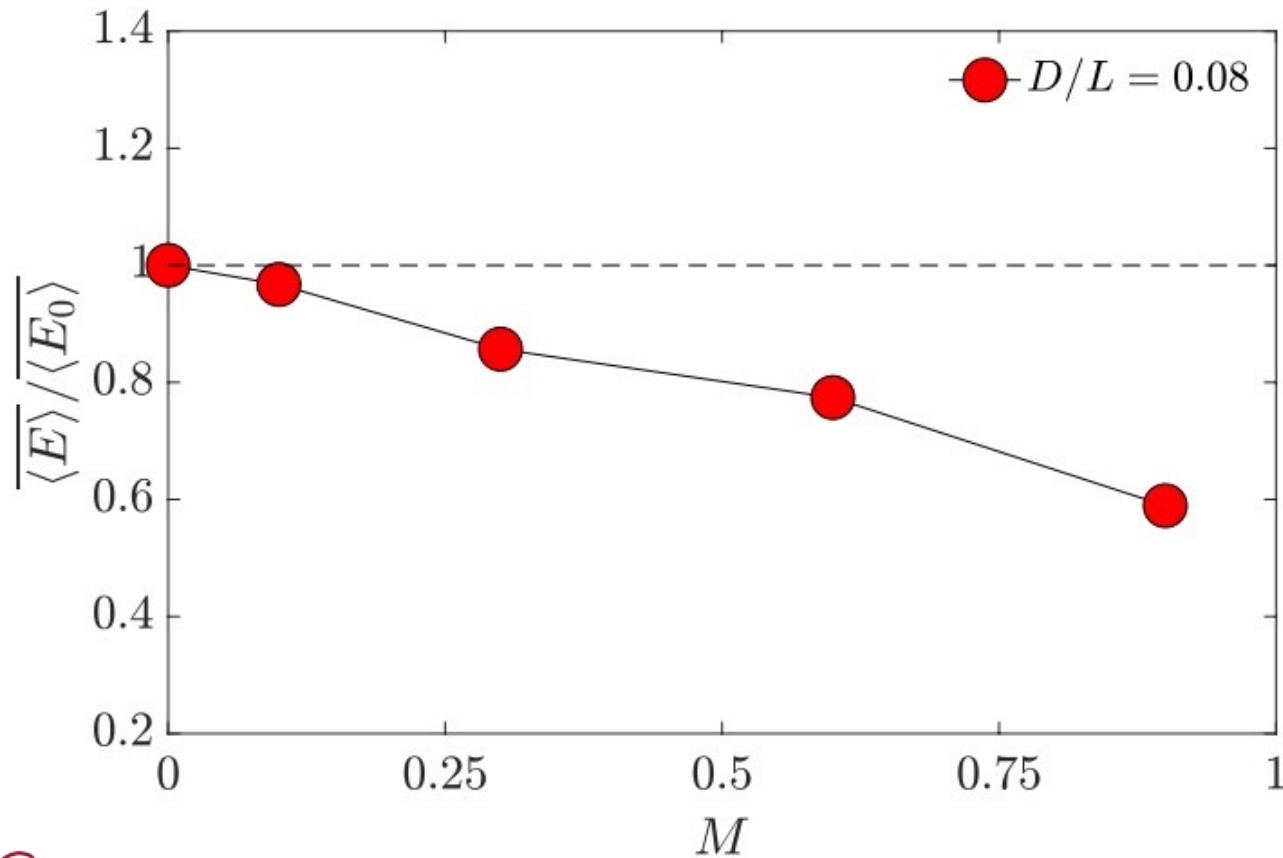
$$M \equiv \frac{m_p}{m_f + m_p}$$

- And the particle diameter D



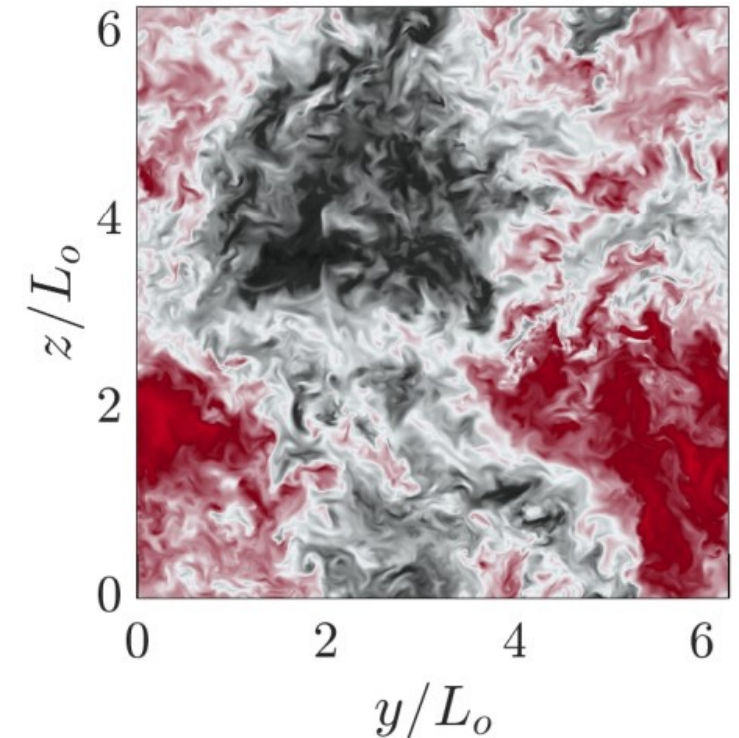
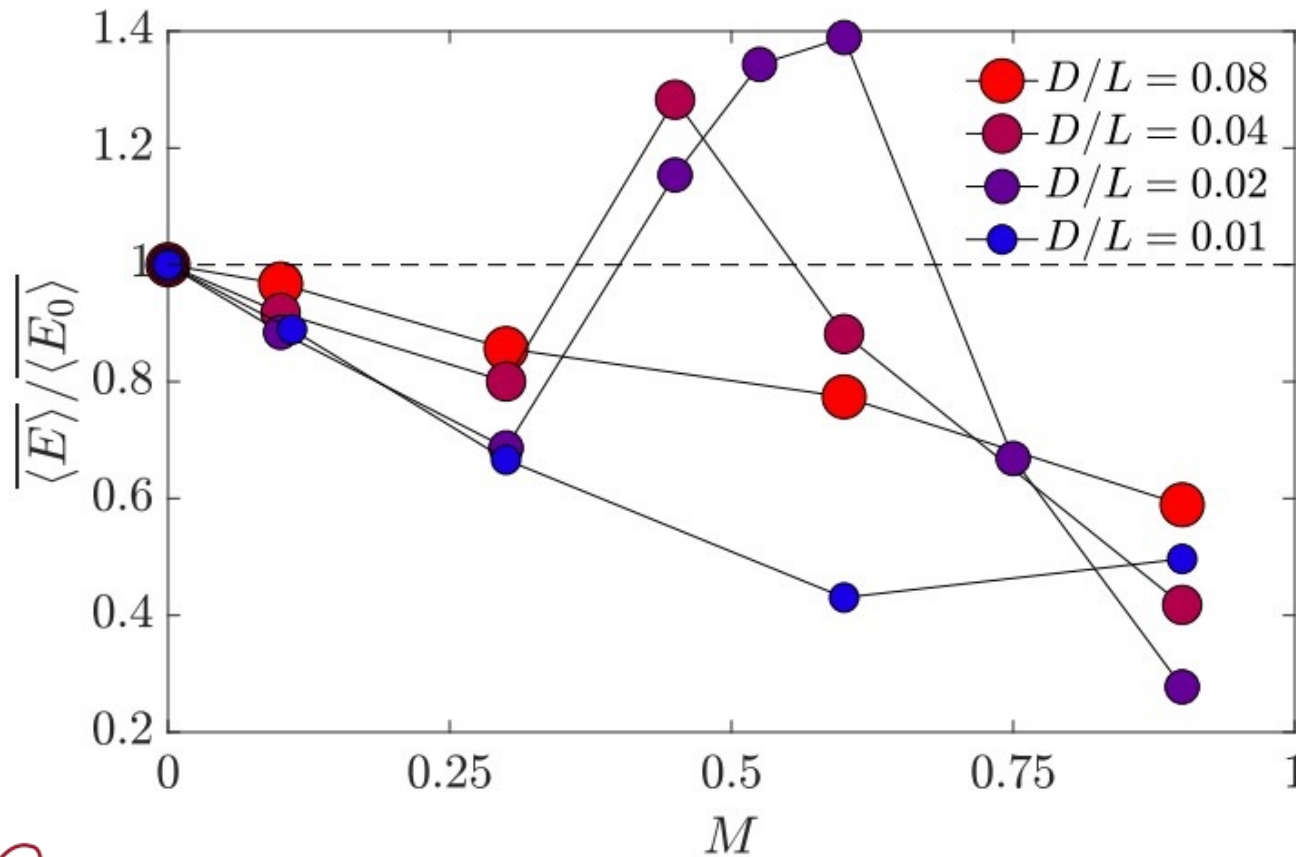
Kinetic energy modulation

- Generally as particle mass fraction increases, the energy of the flow is **suppressed**



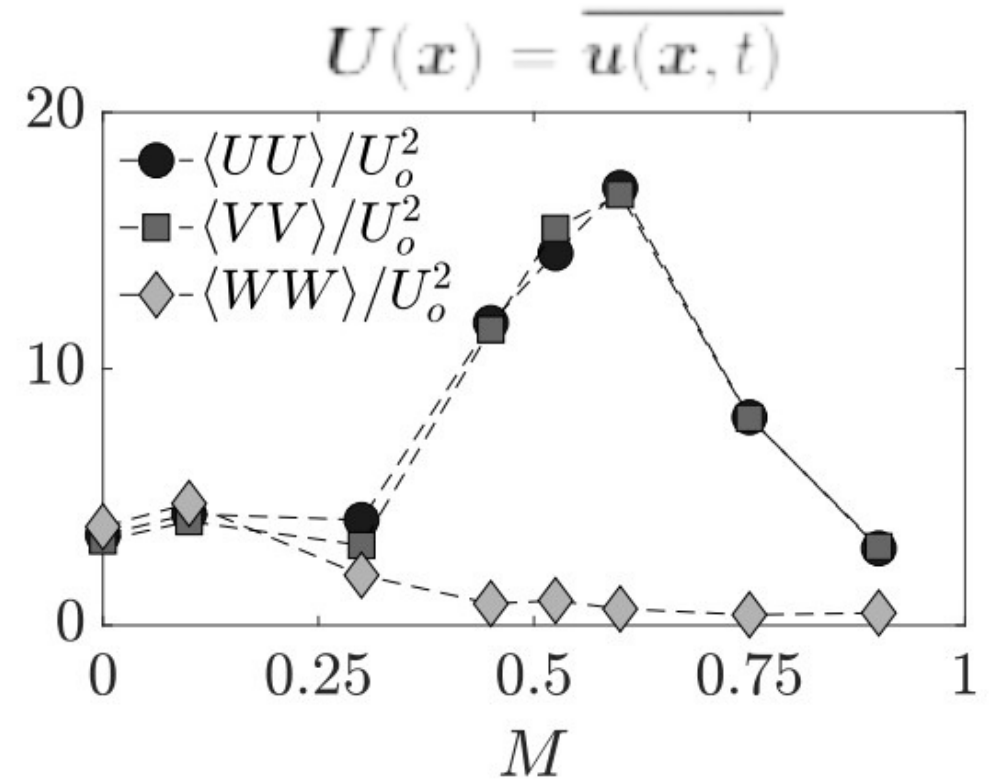
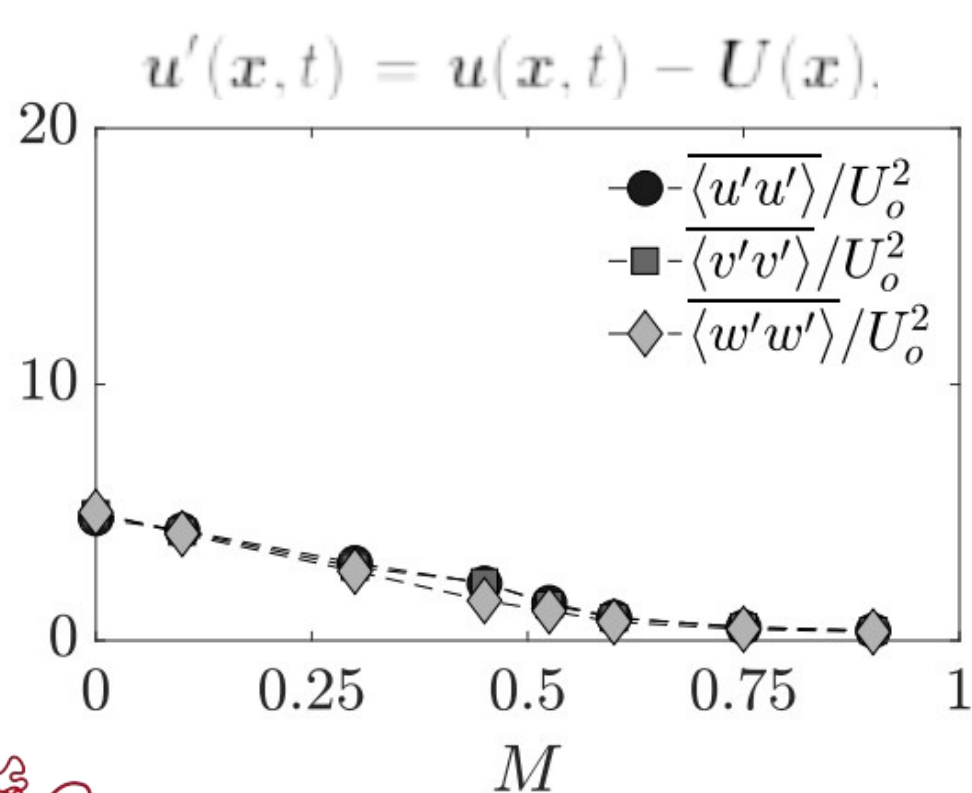
Kinetic energy modulation

- At some intermediate particle sizes, **energy is enhanced!**



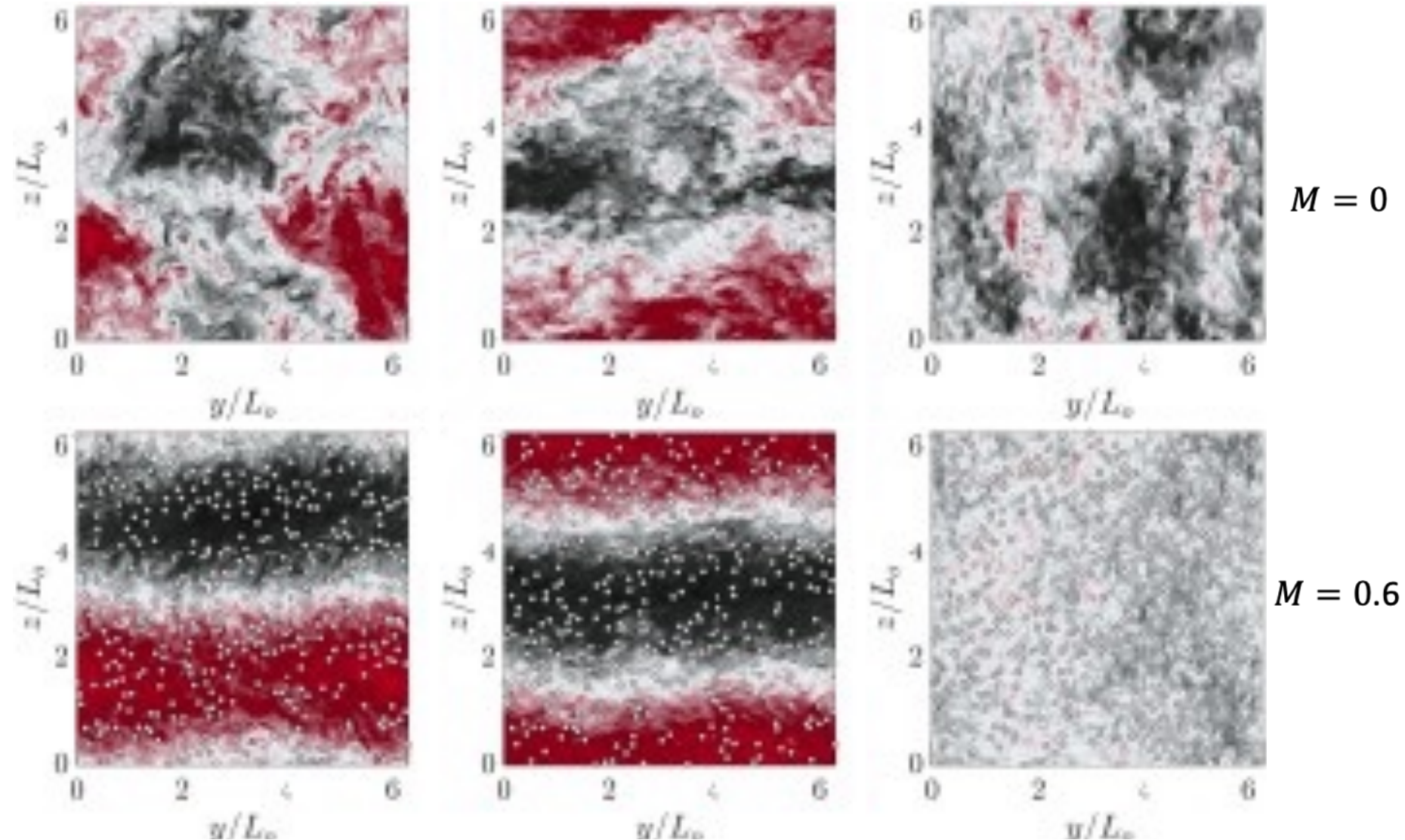
Turbulence modulation

- This is entirely due to an enhancement of the **mean (time averaged) flow**
- The mean flow is highly anisotropic

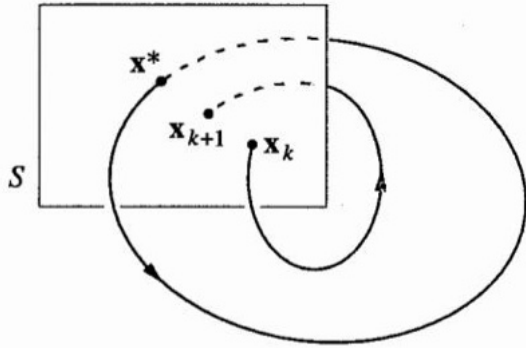


Anisotropy of the flow

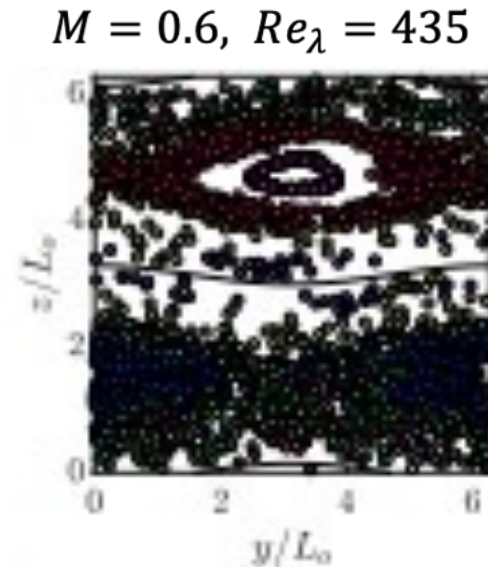
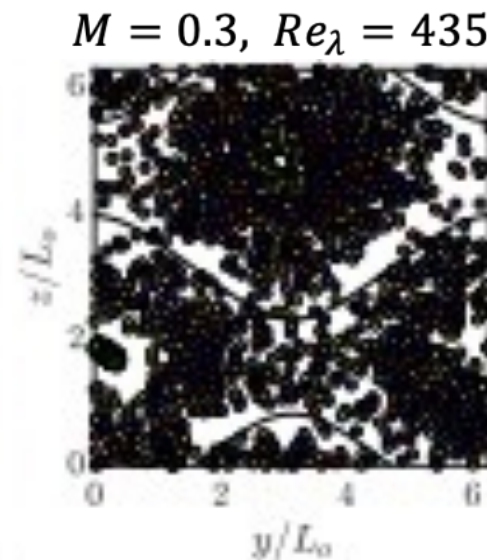
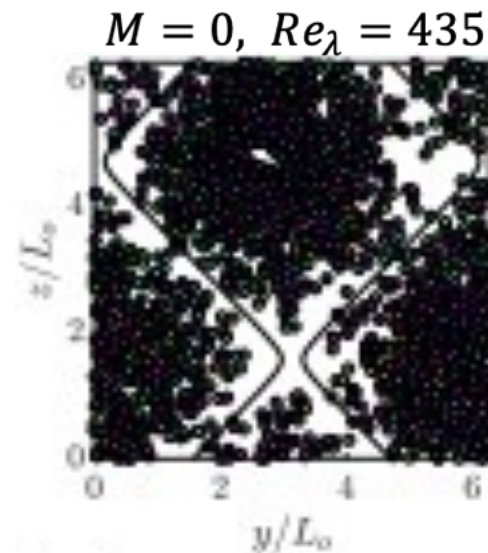
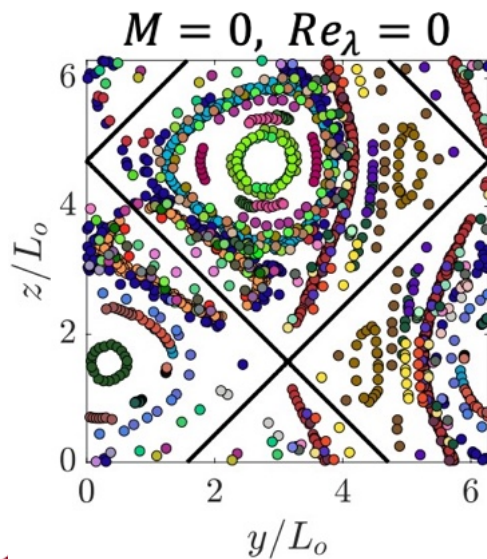
- The single phase flow resembles the forcing with turbulent fluctuations
- For large particle mass fractions, **one direction** (z) is suppressed
- the flow becomes almost two-dimensional



Poincaré maps

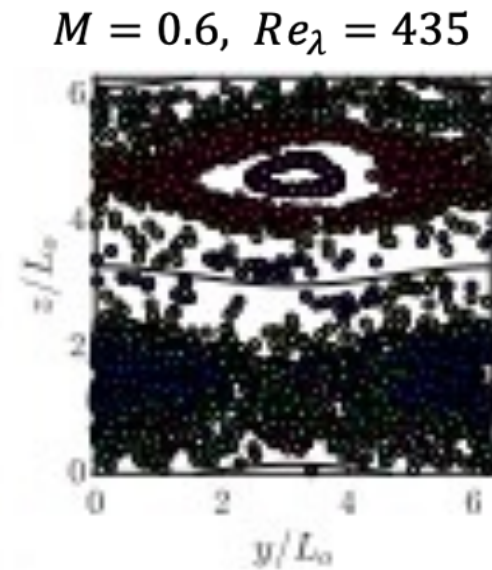
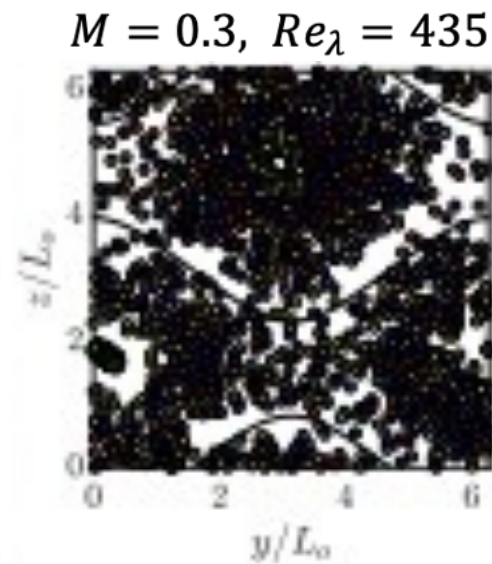
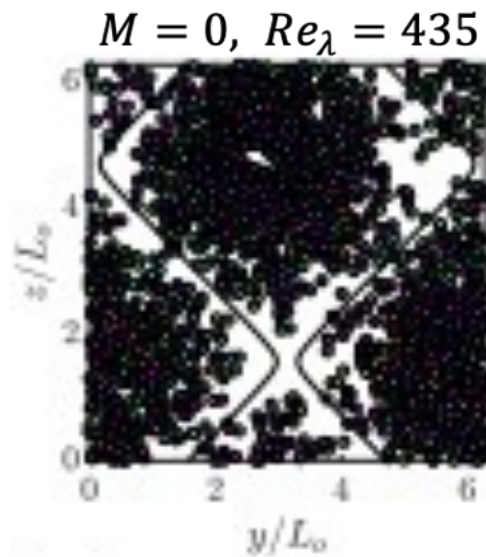
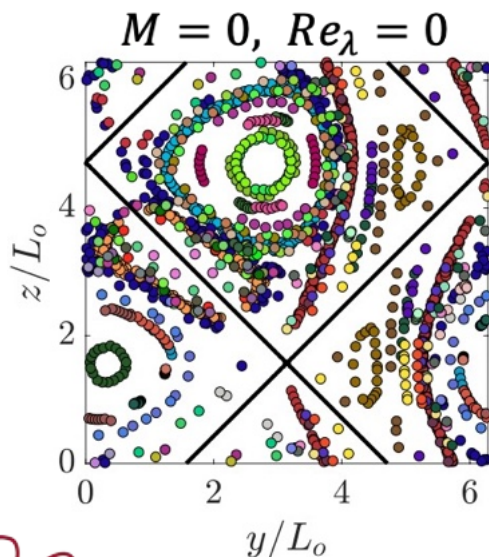
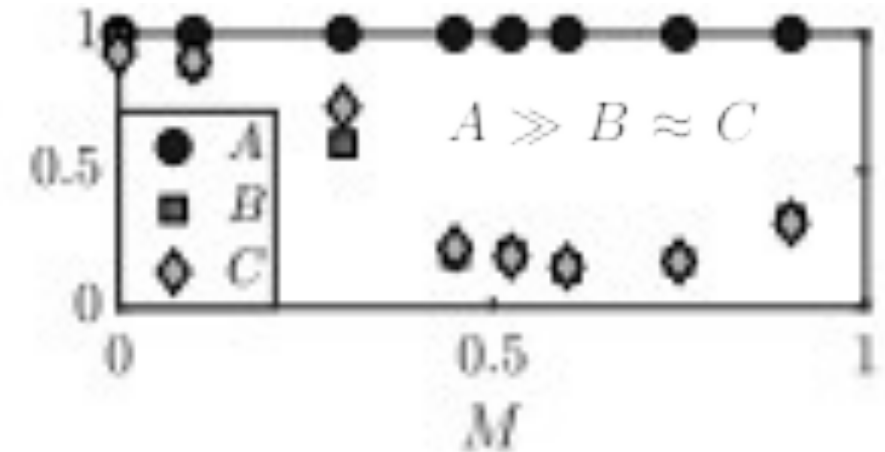


- We make Poincaré maps of the mean flow in the $x = L/2$ plane.
- This is done by following streamlines and marking successive intersections of the plane
- For $M=0.3$ and $M=0.6$, the spread of points in the z direction is reduced



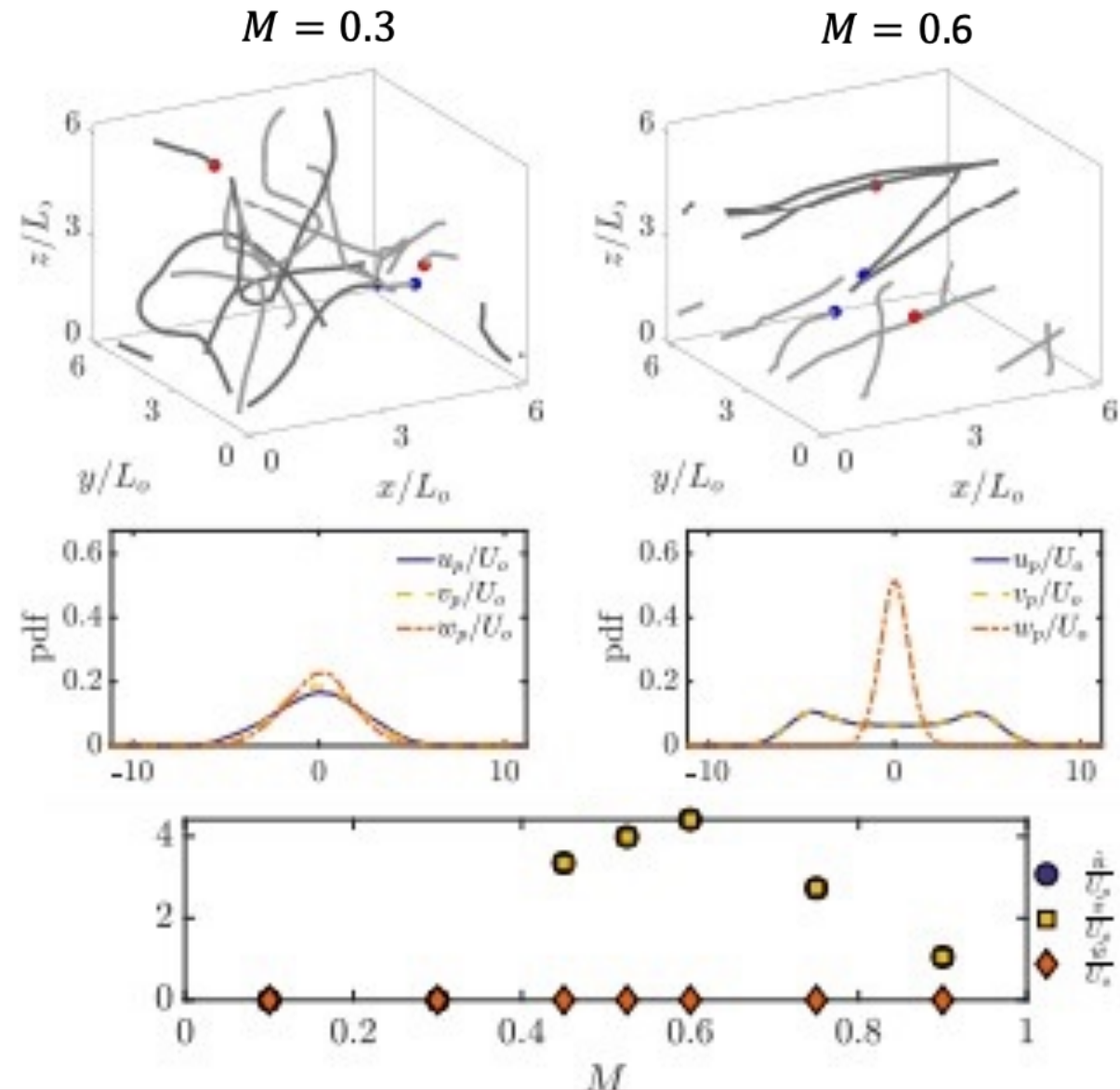
Shape of the mean flow

- We calculate the coefficients A,B and C
- For large mass fractions, a **new type of ABC flow** is seen with B and C reduced.
- We show the loci where the new ABC flow has $u = 0$.
- These coincide with low density regions in the Poincaré maps.



Particle trajectories

- Low mass particles **follow the chaotic flow**
- The three particle velocity components have the same probability distribution.
- Massive particles move in **straight lines**
- The z -velocity is strongly peaked at zero, whereas x and y -velocities become **bi-modal**
- Particles continuously **force the flow** towards the 2D state
- When $M > 0.3$, the modes depart from zero

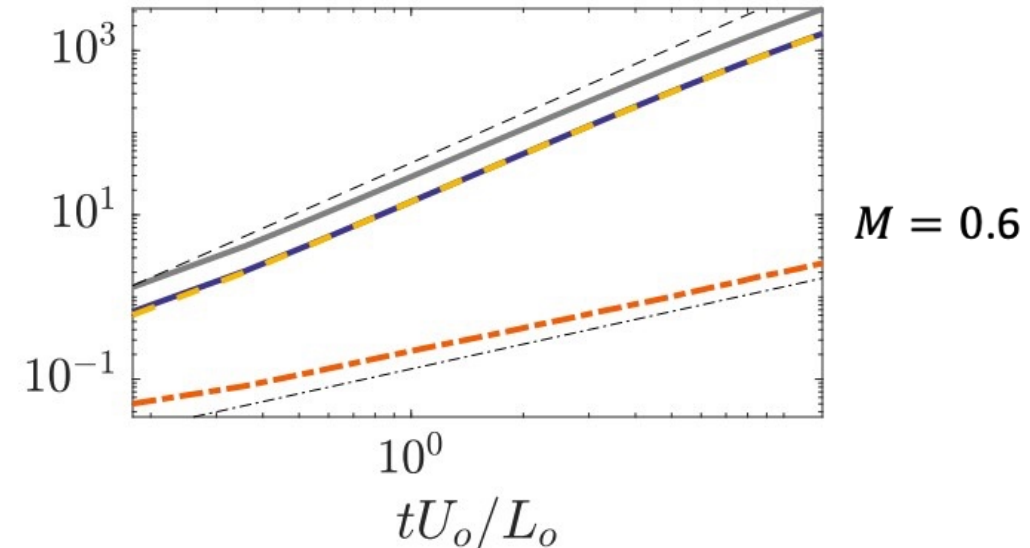
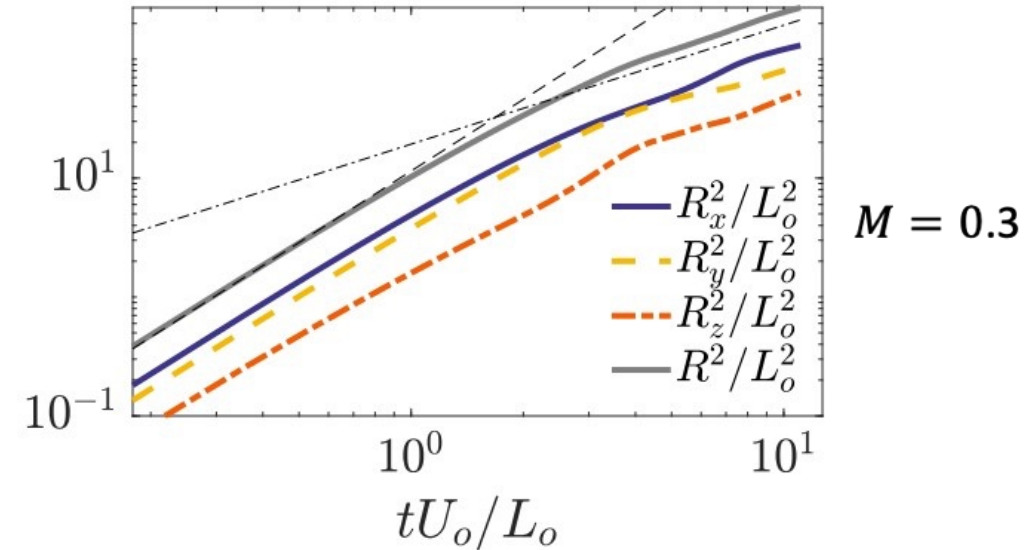


Particle displacement

- The **mean-squared displacement** of the particles is a measure of the distance travelled after a time t

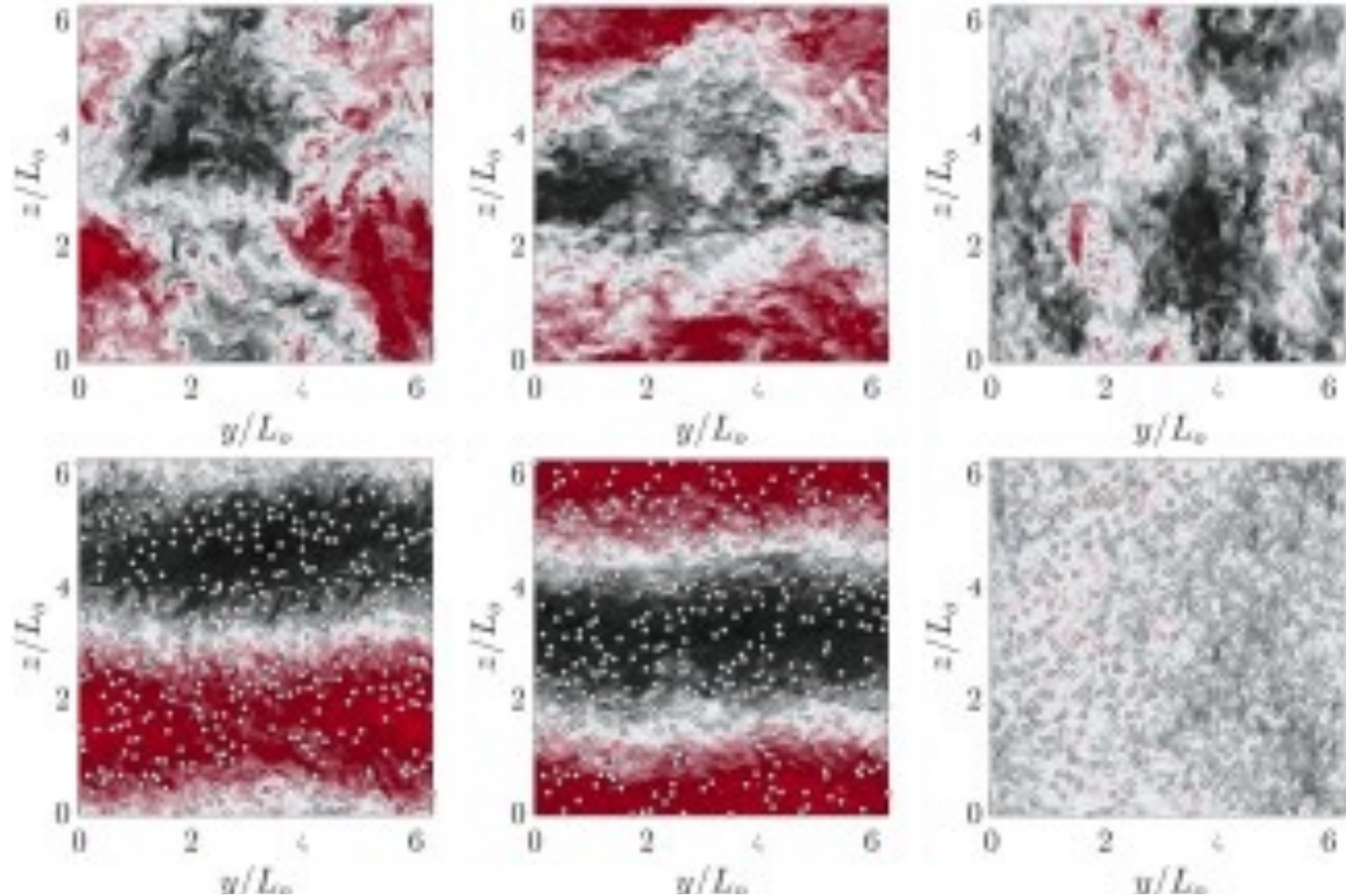
$$R(t)^2 = \langle |\mathbf{x}_p(t) - \mathbf{x}_p(0)|^2 \rangle_p \sim t^\alpha$$

- The low mass particles have
 - ballistic** motion $\alpha \approx 1$
 - followed by **diffusive** motion $\alpha \approx 2$
- The massive particles have
 - ballistic motion in **x and y** for all times
 - diffusive motion in **z** for all time
 - this is a type of **anomalous diffusion**



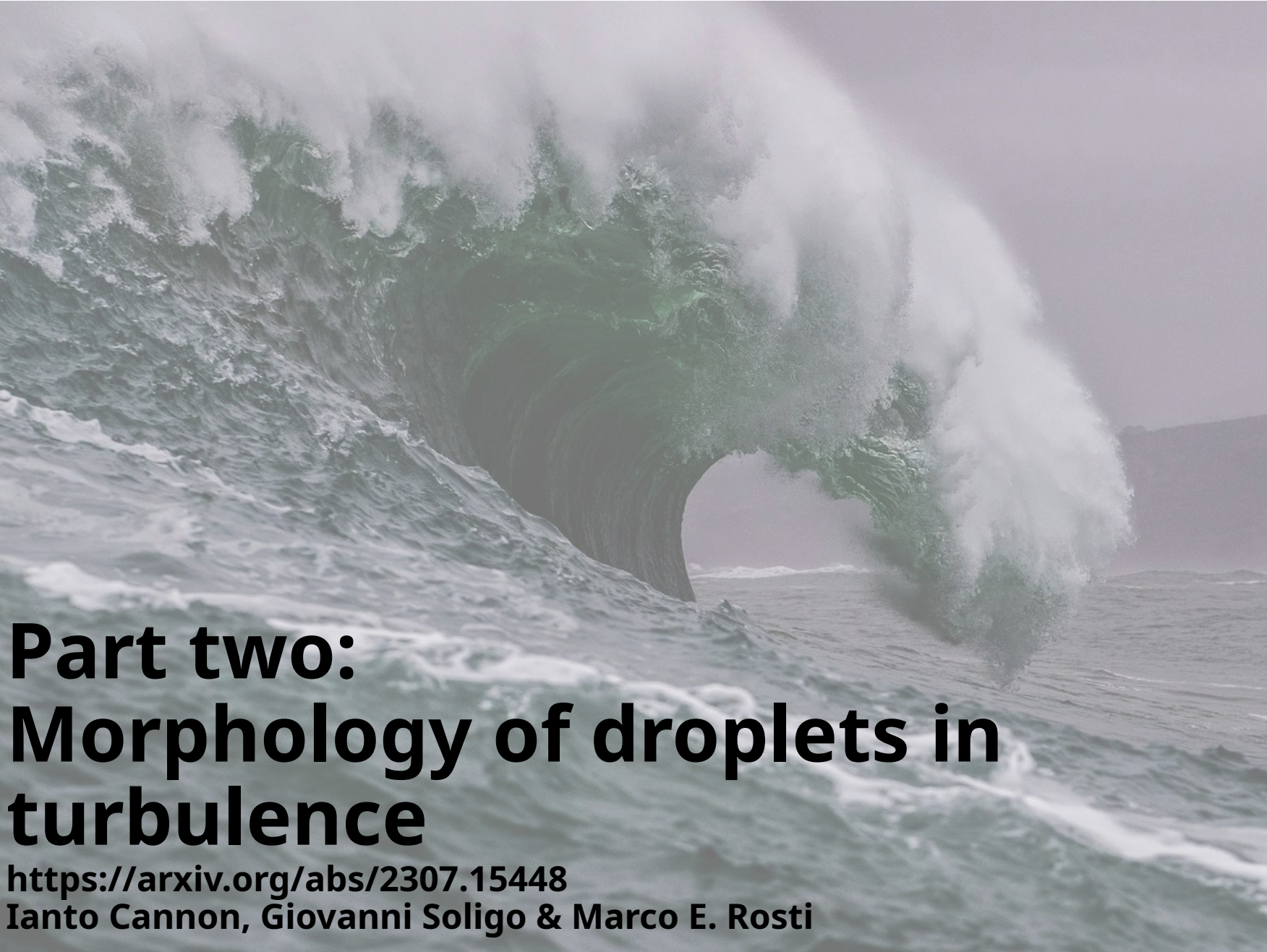
Part 1 conclusion

- The kinetic energy is enhanced at large particle mass fractions
- The flow becomes anisotropic
- This shows the potential to use particles to modify the large scale structures of the flow
- The particles exhibit anomalous diffusion
- Future work:
 - Can particles reduce recirculating regions?



$M = 0$

$M = 0.6$



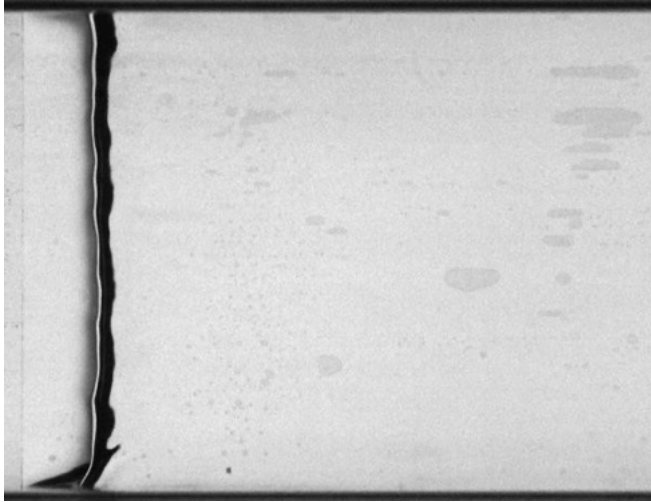
Part two: Morphology of droplets in turbulence

<https://arxiv.org/abs/2307.15448>

Ianto Cannon, Giovanni Soligo & Marco E. Rosti

Droplet breakup in nature

Droplet breakup during cough



Kant et al. *Phys. Rev. Fluids* 2023 Bag-mediated film atomization in a cough machine

CO₂ absorption by the ocean



Credit: Linda Gietka

What is the **morphology** of droplets in turbulence?

- Surfactants are **surface active agents**, compounds that decrease surface tension at an interface
- Eg., soap, lipids in the lungs, salts, and many impurities

How do **surfactants** affect morphology?



Numerical method

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right] + \nabla \cdot (\tau_c f_\sigma) + \mathbf{f}_s,$$

$$\nabla \cdot \mathbf{u} = 0,$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u} H) = 0,$$

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla \cdot (M_\psi \nabla \mu_\psi),$$

$$f_\sigma = \max[\sigma_{min}, \sigma_0(1 + \beta_s \log(1 - \psi))]$$

-fluid motion $Re_\lambda = 180$

-incompressibility

-volume-of-fluid field

-surfactant concentration

-surface tension

Engblom et al., *Comm. Comput. Phys.* (2013)

Yun et al., *Appl. Math. Comput.* (2014)

Soligo et al., *J. Comput. Phys.* (2019)

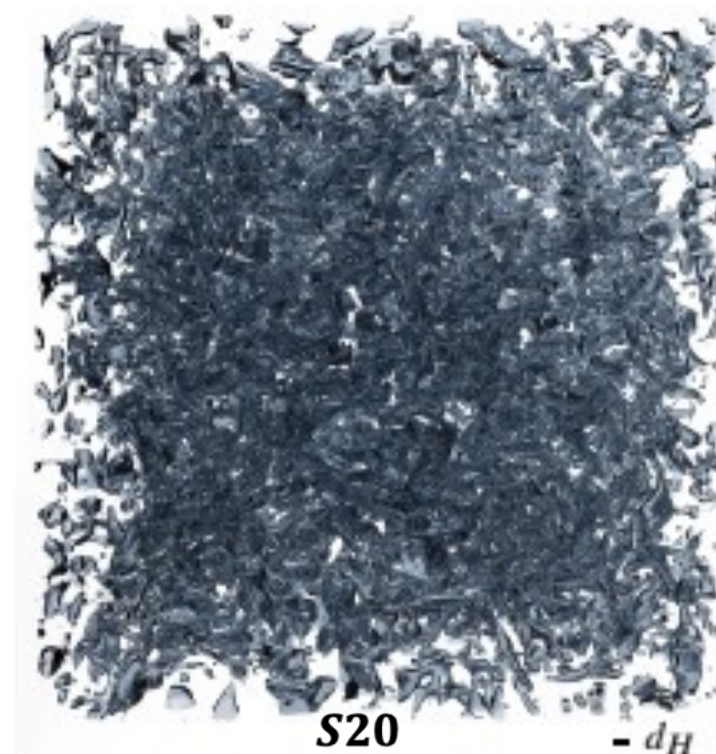
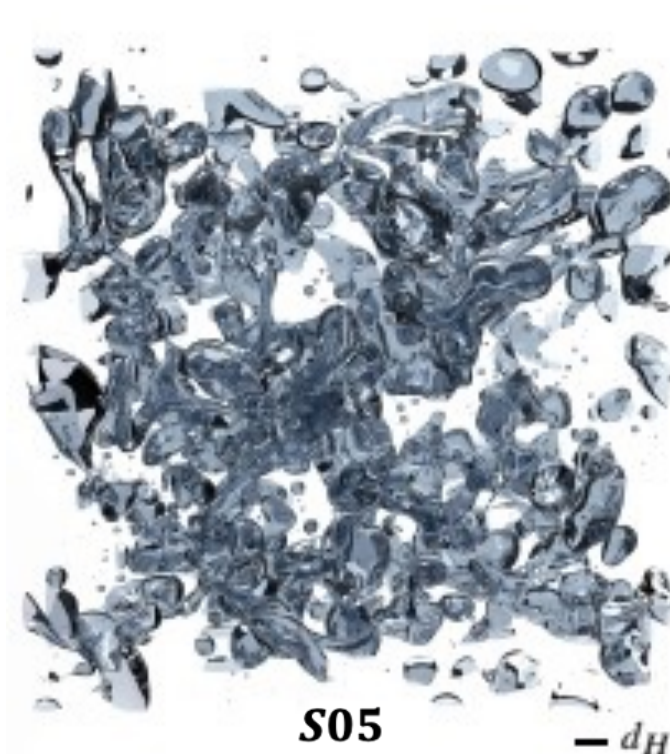


Simulation setup

- Statistically-steady turbulence in a triperiodic box with 500^3 grid points
- We define a **Kolmogorov-Hinze diameter** in the presence of surfactant

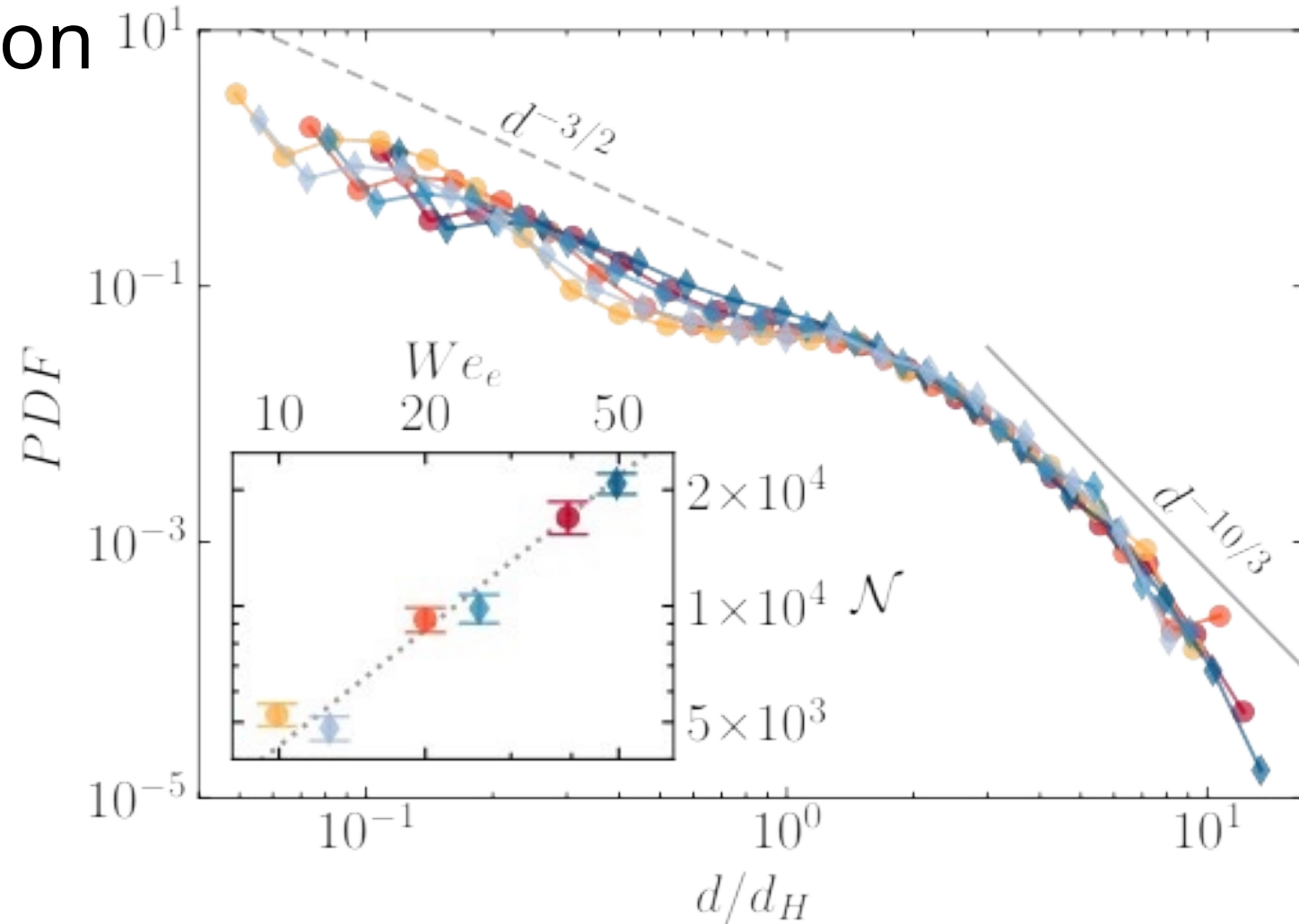
$$d_H \equiv 0.725 \langle \sigma \rangle^{3/5} \rho^{-3/5} \varepsilon^{-2/5}$$

case		$\langle \phi \rangle$	$\langle \psi \rangle$	We	$d_{H\sigma}/L$
SP	●	0	0	-	-
C10	●	0.1	0	10	0.0565
C20	●	0.1	0	20	0.0392
C40	●	0.1	0	40	0.0290
S05	◆	0.1	0.1	5	0.0370
S10	◆	0.1	0.1	10	0.0317
S20	◆	0.1	0.1	20	0.0241



Droplet size distribution

- We define an **equivalent diameter** for each droplet, $d \equiv (6V/\pi)^{1/3}$,
- The DSD shows two distinct scalings, which are known to result from coalescence and breakup



Garrett et al., *J. Phys. Oceanograph.* (2000)
Dean, Stokes, *Nature* (2002)

Droplet deformation

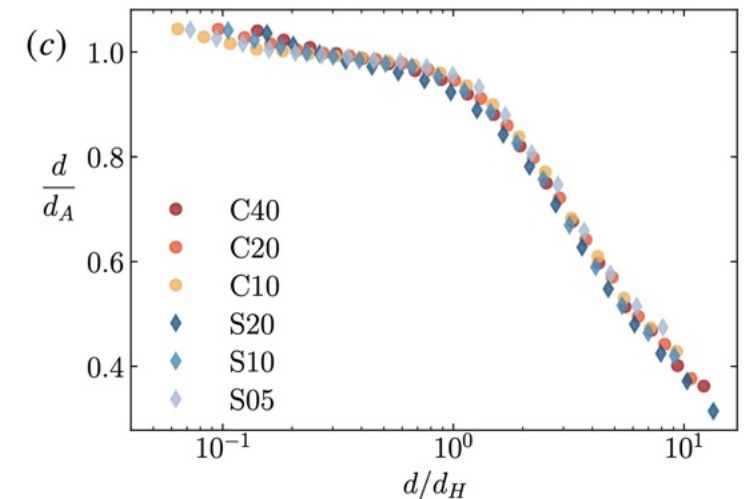
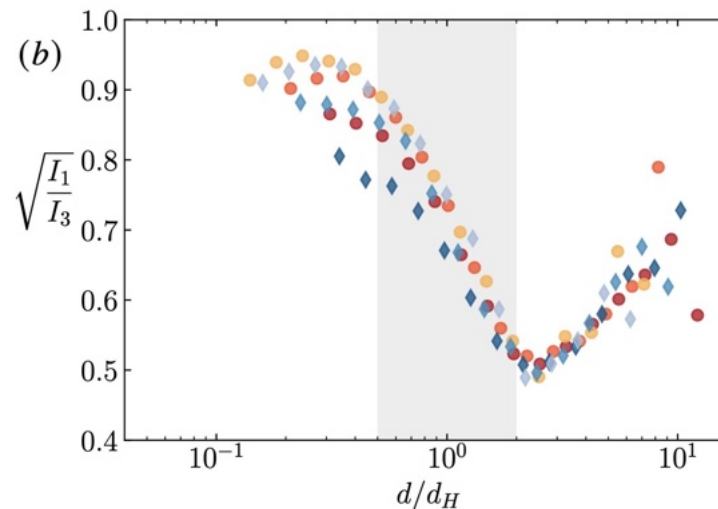
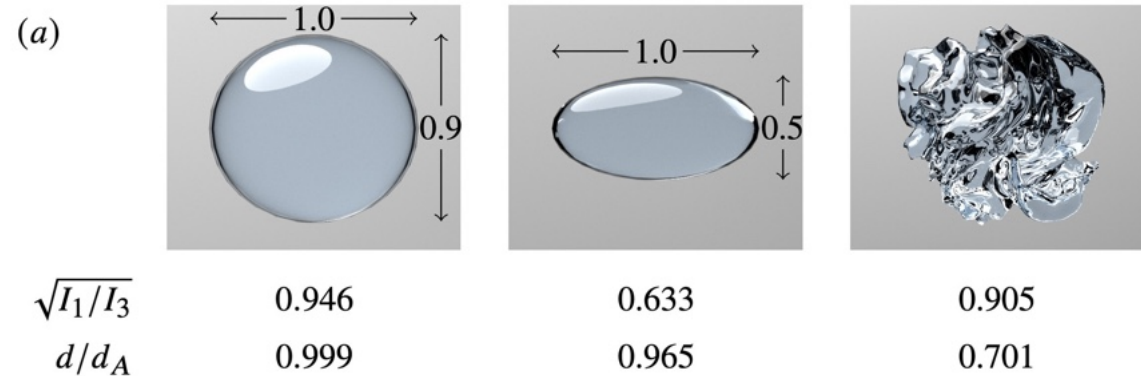
- We measure the aspect ratio

$$\sqrt{I_1/I_3}, \quad \mathbf{I} \equiv \int_V \rho(|\mathbf{r}|^2 \mathbf{I} - \mathbf{r} \otimes \mathbf{r}) dV,$$

- and the sphericity d/d_A , where

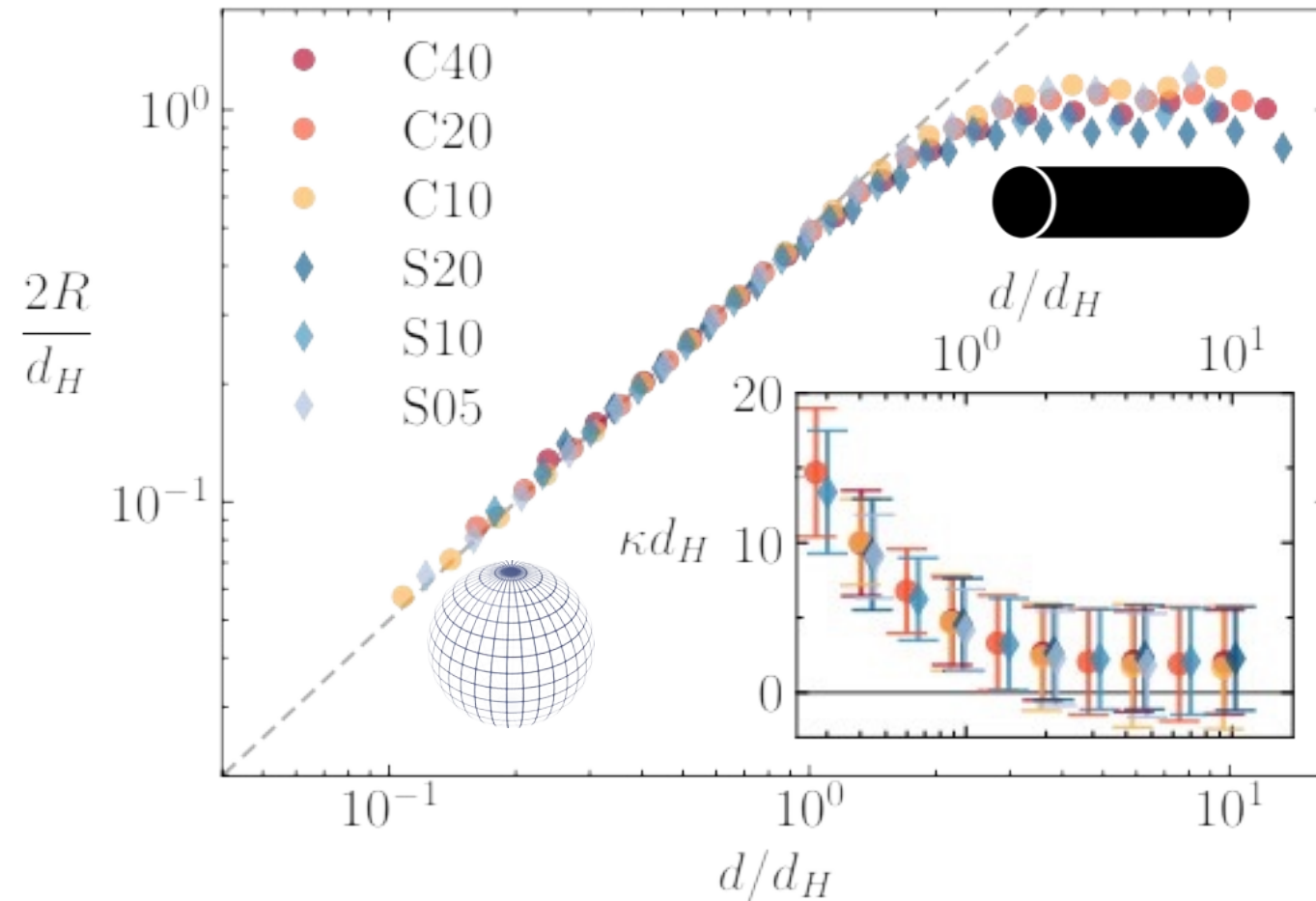
$$d \equiv (6V/\pi)^{1/3}, \quad d_A \equiv \sqrt{A/\pi}$$

- the aspect ratio decreases with droplet size, and rebounds in the breakup regime
- the sphericity decreases sharply in the breakup regime



Droplet radius of curvature

- We compute the curvature using the interface normal, $\kappa = \nabla \cdot \mathbf{n}$.
- The radius of curvature $R \equiv 1/\kappa$.
- Below the Hinze-scale $R \approx d/4$
- Above the Hinze-scale $R \approx d_H/2$

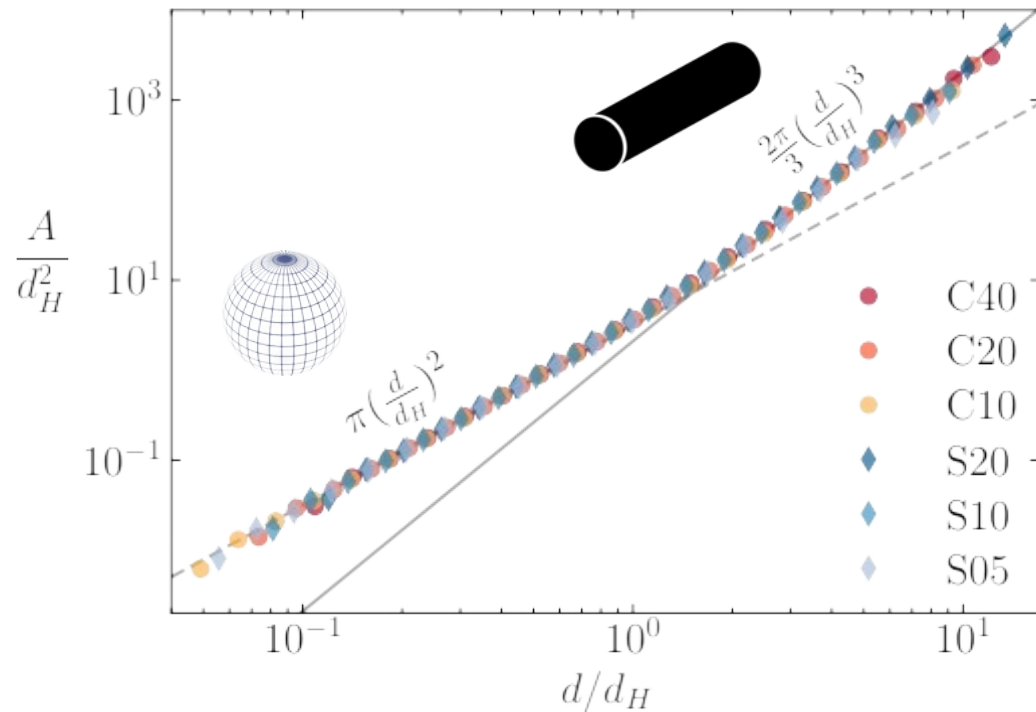


Droplet areas

Below the Hinze-scale the droplet areas scale as spheres

Above the Hinze-scale the droplet areas scale as filaments with diameter d_H

case	$\langle \phi \rangle$	$\langle \psi \rangle$	We
SP	0	0	-
C10	0.1	0	10
C20	0.1	0	20
C40	0.1	0	40
S05	0.1	0.1	5
S10	0.1	0.1	10
S20	0.1	0.1	20



Topology of the droplets

- We compute the Euler characteristic of the droplet interfaces $\chi = n - e + f$.

- This gives the number of handles h and voids v

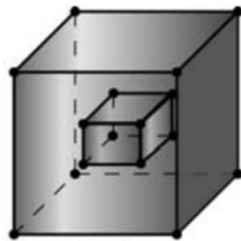
$$1 - \chi/2 = h - v,$$

$$h = 0, v = 0$$



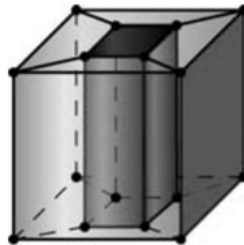
$$\begin{aligned} n &= 8 \\ e &= 12 \\ f &= 6 \\ \chi &= 2 \end{aligned}$$

$$h = 0, v = 1$$



$$\begin{aligned} n &= 16 \\ e &= 24 \\ f &= 12 \\ \chi &= 4 \end{aligned}$$

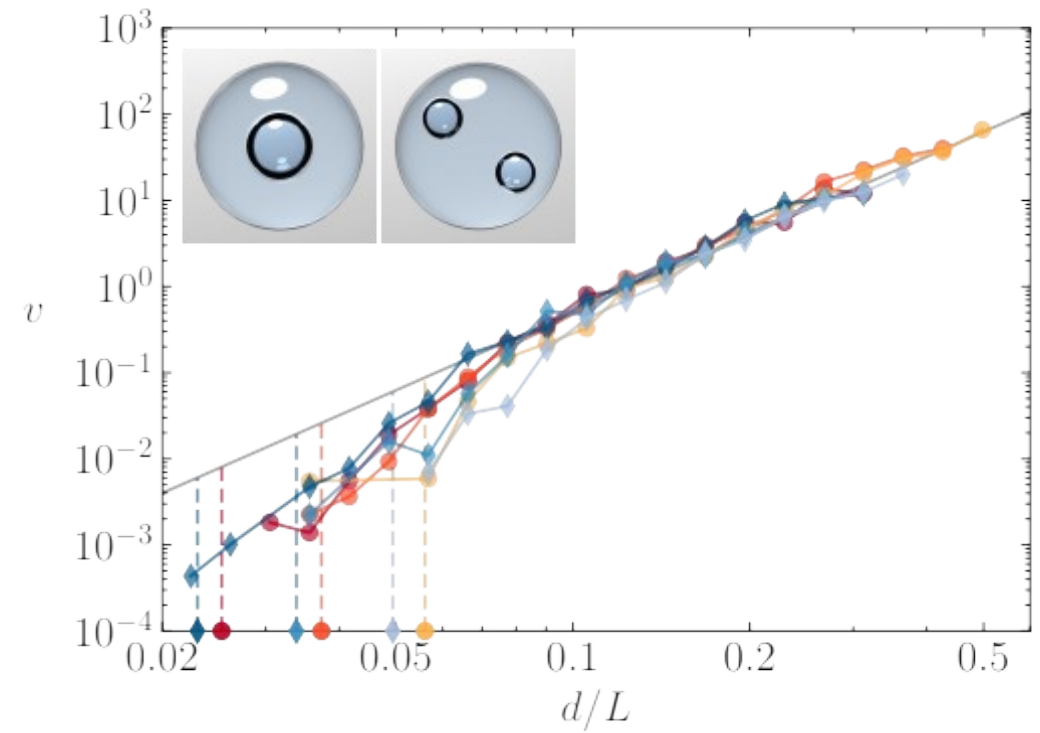
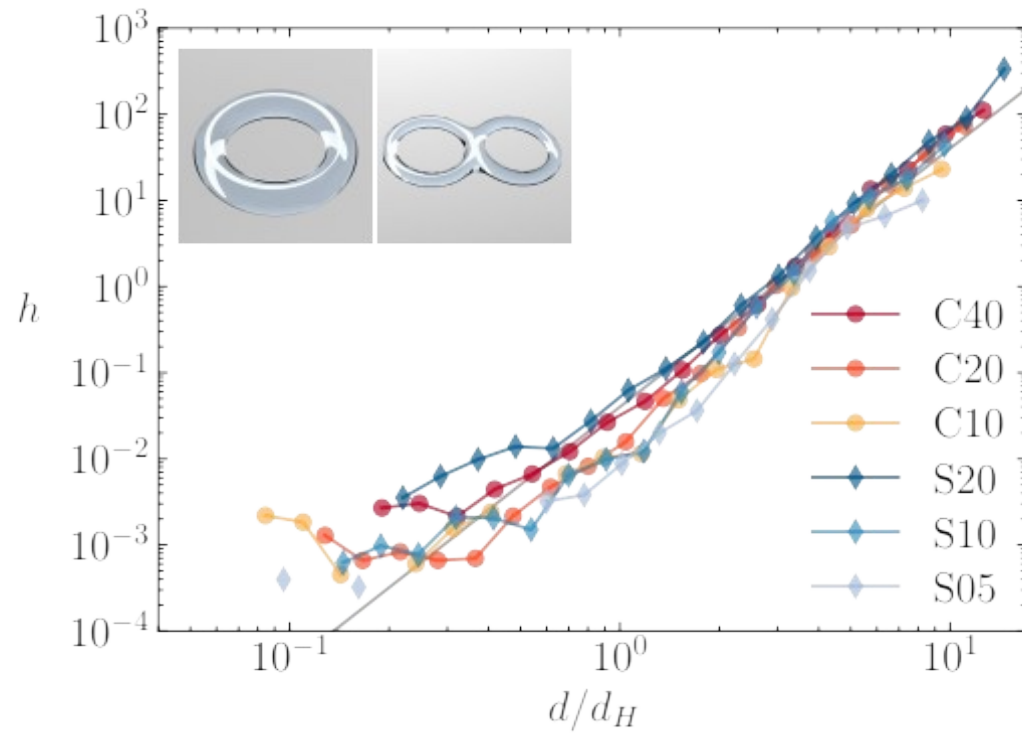
$$h = 1, v = 0$$



$$\begin{aligned} n &= 16 \\ e &= 32 \\ f &= 16 \\ \chi &= 0 \end{aligned}$$



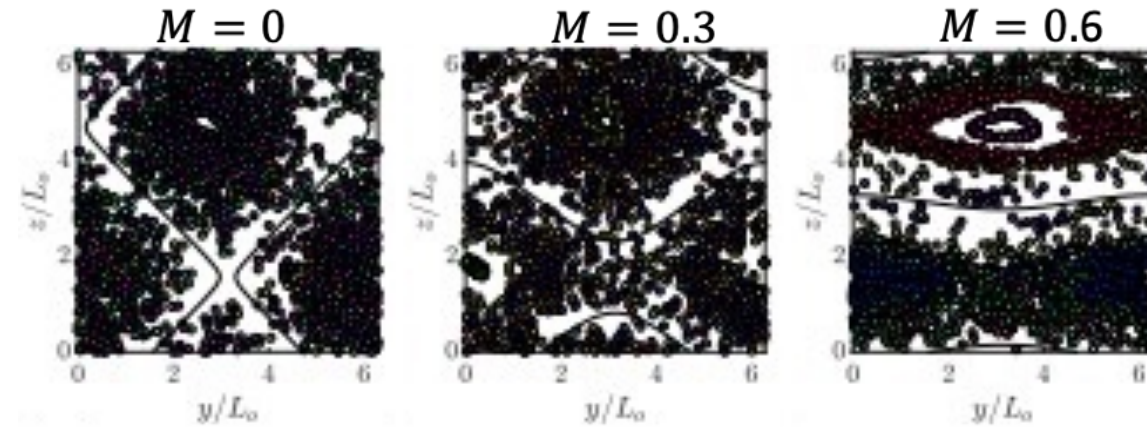
Handles and voids



Conclusions

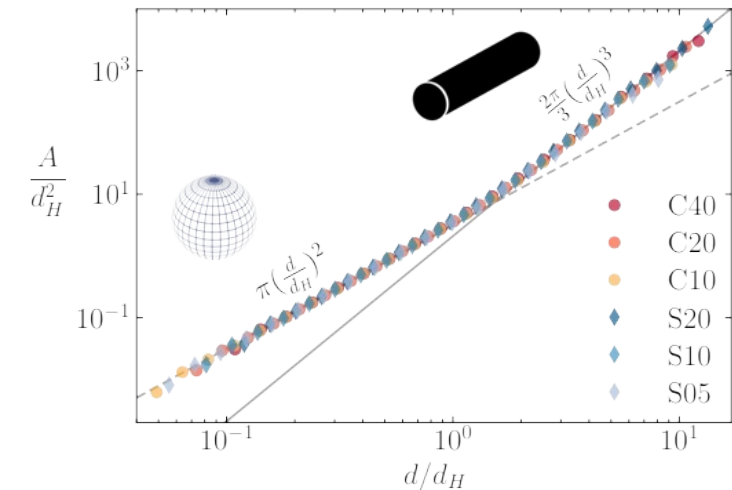
Part 1:

- The kinetic energy is enhanced at large particle mass fractions
- The flow becomes anisotropic
- The particles exhibit anomalous diffusion
- Chiarini, Cannon & Rosti, (2023). Anisotropic mean flow enhancement and anomalous transport of finite-size spherical particles in turbulent flows (*under review*)



Part 2:

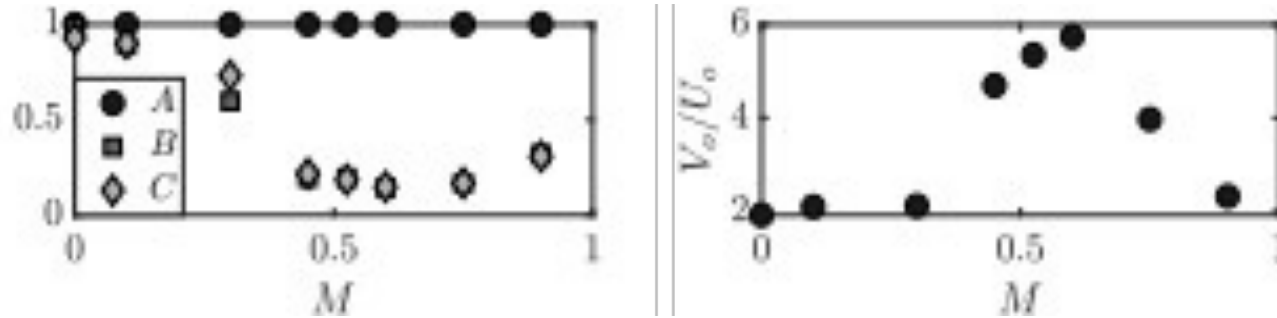
- The interface-averaged surface tension can be used to define the Hinze-scale in surfactant-laden flows
- Droplets smaller than the Hinze-scale are ellipsoidal
- Droplets larger than the Hinze-scale are filamentous
- Cannon, Soligo & Rosti, (2023). Morphology of clean and surfactant-laden droplets in homogeneous isotropic turbulence (*under review*) arxiv.org/abs/2307.15448



Thank you!

Poincaré maps

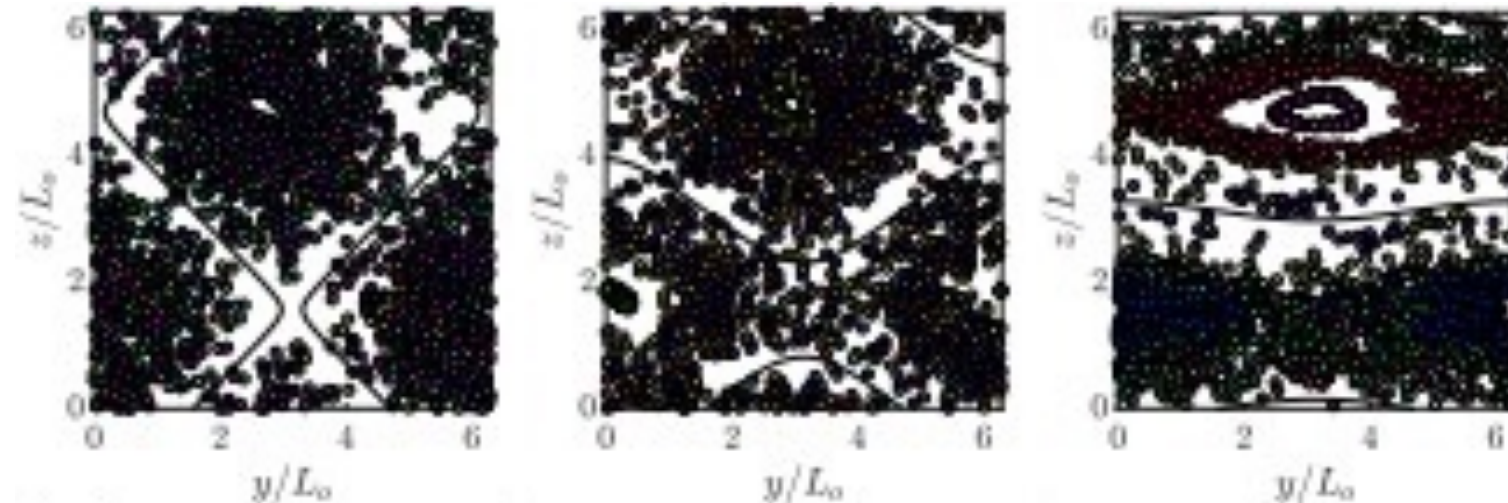
$$f = \left(\frac{2\pi}{L}\right)^2 F_o \begin{pmatrix} A \sin(2\pi z/L) + C \sin(2\pi y/L) \\ B \sin(2\pi x/L) + A \sin(2\pi z/L) \\ C \sin(2\pi y/L) + B \sin(2\pi x/L) \end{pmatrix}$$



$M = 0$

$M = 0.3$

$M = 0.6$



- Remarkably, the mean flow closely resembles the laminar ABC flow

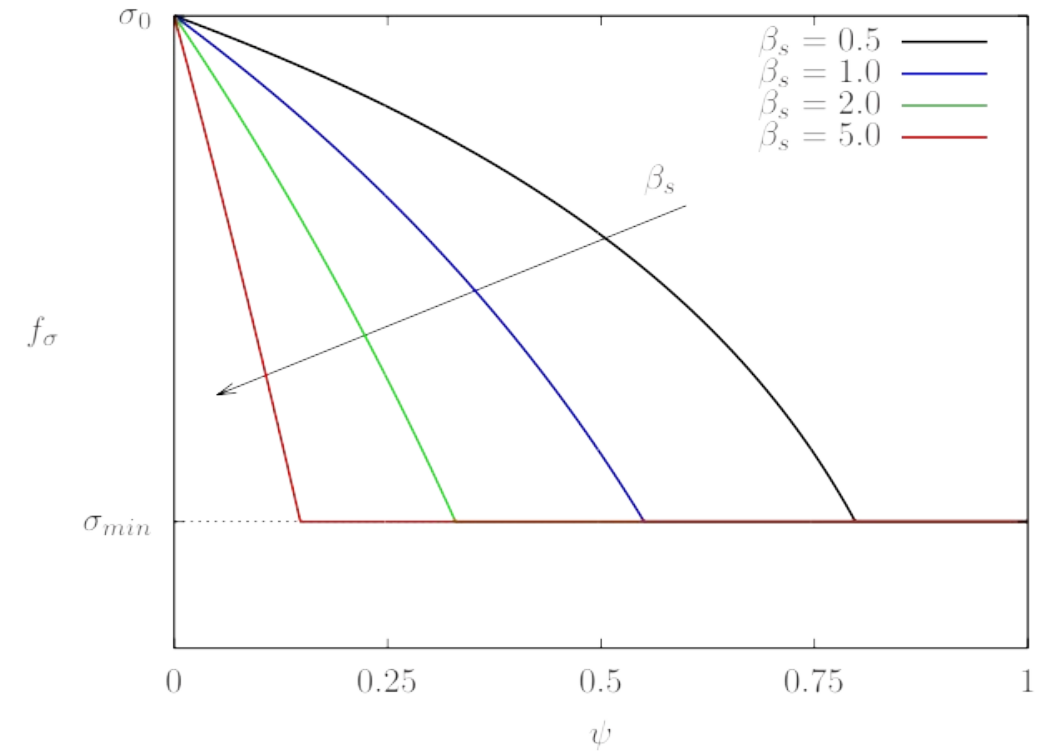
- We can calculate the corresponding coefficients A, B and C with,

$$V_o A = \frac{1}{L^3} \int_0^L \int_0^L \int_0^L (U \sin(z/L_o) + V \cos(z/L_o)) dz dy dx$$

- For large mass fractions, the flow becomes anisotropic, and a state with $A \gg B \approx C$ is reached
- We show in black, the loci where the laminar ABC flow has $u = 0$.

Musacchio, *Phys. Rev. E* (2014)

Langmuir equation of state



$$f_\sigma = \max[\sigma_{min}, \sigma_0(1 + \beta_s \log(1 - \psi))]$$

Muradoglu, & Tryggvason, *J. Comput. Phys.* (2008)

Kolmogorov-Hinze diameter

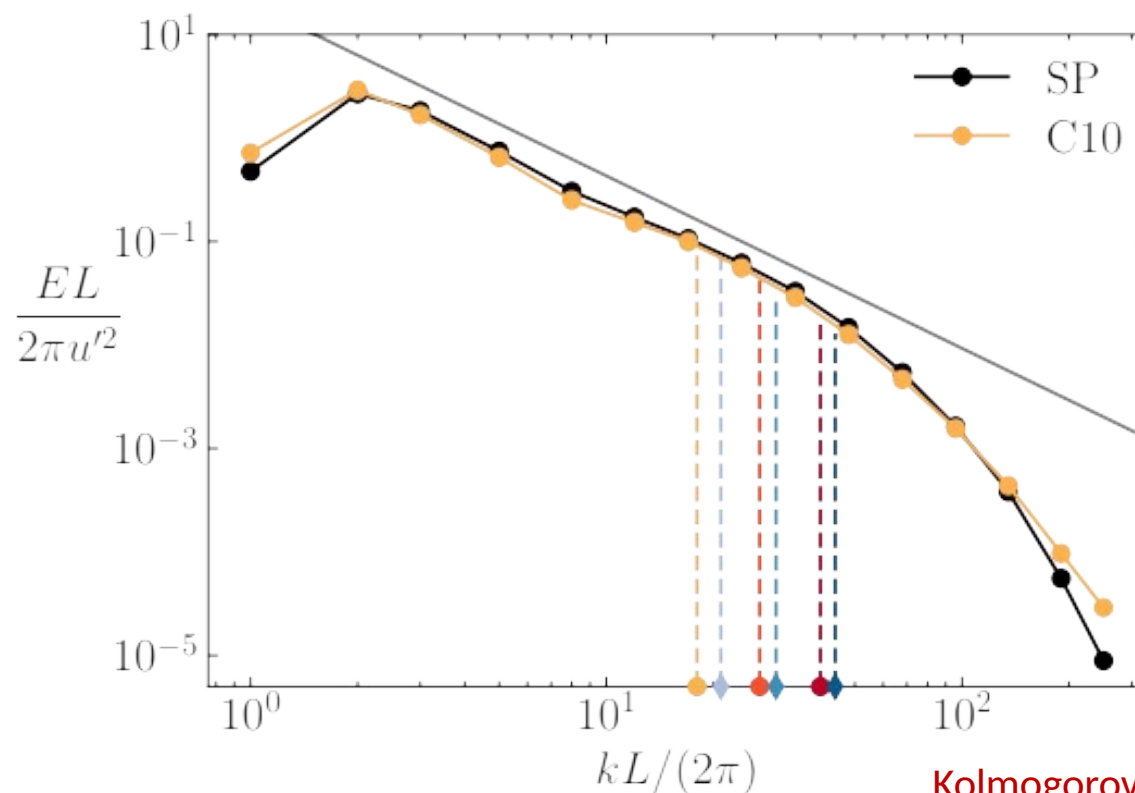
- The turbulent kinetic energy spectrum has an $E \sim k^{-5/3}$ scaling

- The **Kolmogorov-Hinze diameter** is an estimate of the largest droplet which is not broken by turbulent fluctuations

$$d_H \equiv 0.725 \langle \sigma \rangle_I^{3/5} \rho^{-3/5} \varepsilon^{-2/5}$$

- The effective Weber number takes surfactants into account $We_e \equiv \rho u'^2 L_b / \langle \sigma \rangle_I$
- The total number of droplets increases with Weber number
- We define an equivalent diameter for each droplet, $d \equiv (6V/\pi)^{1/3}$,
- Droplet breakup and coalescence produce two distinct scalings in the DSD

case	$\langle \phi \rangle$	$\langle \psi \rangle$	We
SP	0	0	-
C10	0.1	0	10
C20	0.1	0	20
C40	0.1	0	40
S05	0.1	0.1	5
S10	0.1	0.1	10
S20	0.1	0.1	20



Kolmogorov (1949)
Hinze, *AIChEJ* (1955)