Universität Bremen

DLES 15
ERCOFTAC Workshop
Direct & Large Eddy Simulation

CENTER OF
APPLIED SPACE TECHNOLOGY
AND MICROGRAVITY
ZARM

Discerning the causality of drop breakup using massive ensembles of simulations



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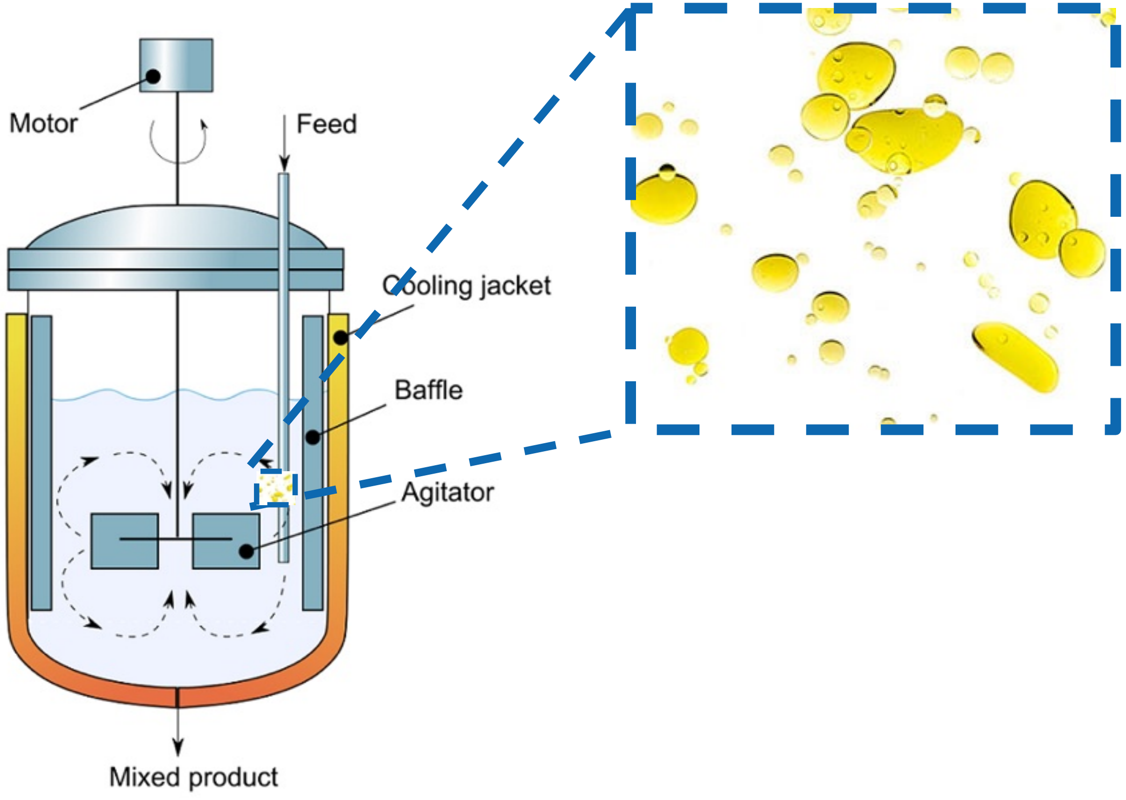
Drop breakup

Occurs in the production of emulsions,
e.g., food, pharmaceuticals, paint

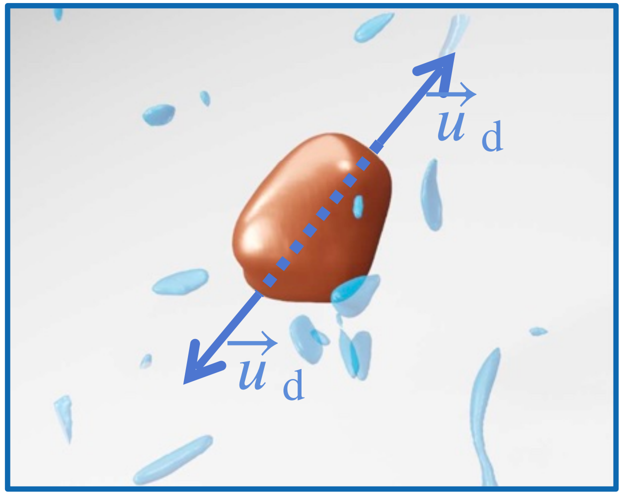
Håkansson, *Annu. Rev. Food Sci. Technol.* 2019
Mathijssen *et al.*, *Rev. Mod. Phys.* 2023

Emulsification



- Turbulent forces cause drop breakup

The Weber number



$$We = \frac{\text{kinetic energy}}{\text{surface energy}} = \frac{\frac{1}{2}\rho\, d^3\, u_d^2}{\sigma\, d^2}$$

Assumptions:

- Deformation by ‘eddies’ of size ~ d,
- resistance by surface tension σ

The Kolmogorov-Hinze diameter

Kolmogorov, *Dok. Akad. Nauk.* 1949, Hinze, *AIChE J.* 1955

Kolmogorov and Hinze proposed that drops will break as long as: $We > We_c$
Rearranging gives a critical diameter

$$\boxed{d_{KH} = We_c^{-3/5}\,\sigma^{3/5}\rho^{-3/5}\epsilon^{-2/5}, \qquad We_c \approx 2}$$

- ✅ Simple yes or no prediction of breakup
- ✅ Confirmed by many studies in different flows

Shinnar *J. Fluid Mech.* 1961, Vankova *et a. J. Colloid Interface Sci.* 2007, Perlekar *et al. Phys. Fluids* 2012; Cannon *et al. J. Fluid Mech. 2023,* Ni, Annu. *Rev. Fluid Mech.* 2024

- ❌ Different values of the constant We_c
- ❌ Static: No information on the dynamics, e.g. breakup time

Our questions

1. **What is the lifetime of a drop?**

2. **Can we make a simple mechanistic model of drop breakup?**

Method: direct numerical simulations

Vela-Martín & Avila, *J. Fluid Mech.* (2021)

- homogeneous isotropic turbulence
- sustained by forcing on modes k<2
- pseudo-spectral method
- optimised CUDA code
- 256^3 grid fits on a single GPU
- initial condition: spherical drop
- 2080 breakup simulations
- across 7 Weber numbers

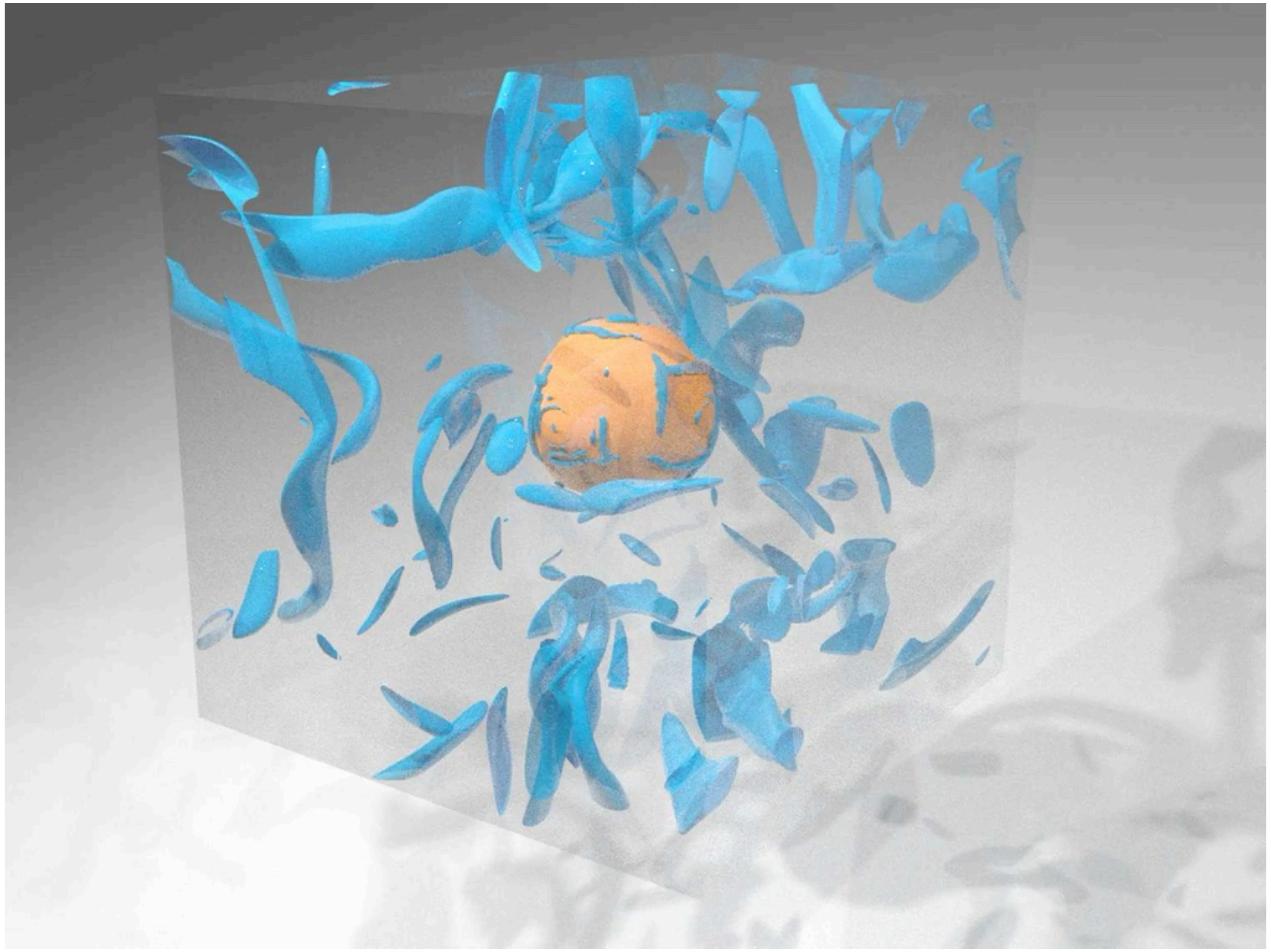
	We	N
◀	1.2	180
▲	1.3	200
▼	1.4	200
▶	1.6	200
●	1.8	200
■	2.9	500
◆	3.6	600

$t = 0.6\ [t_d]$

$Re_\lambda = 58\ ,\ \ We = 1.82$

* Jaqmin *J. Comput. Phys.* (1999), Magaletti *et al. J. Fluid Mech.* (2013)

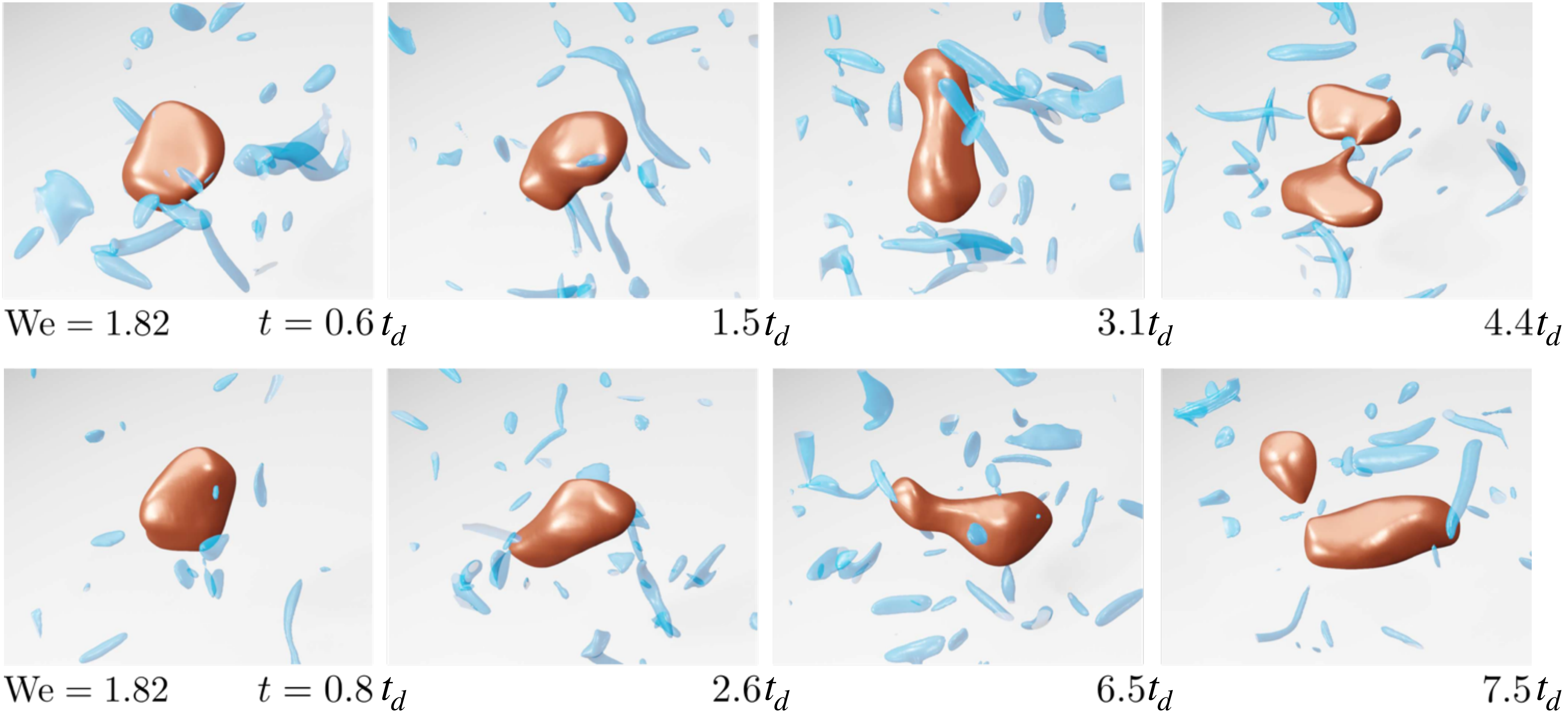
DNS of drop breakup in HIT



https://youtu.be/AEsZjPGtYoA?si=glVKadQIIz-KLPIn

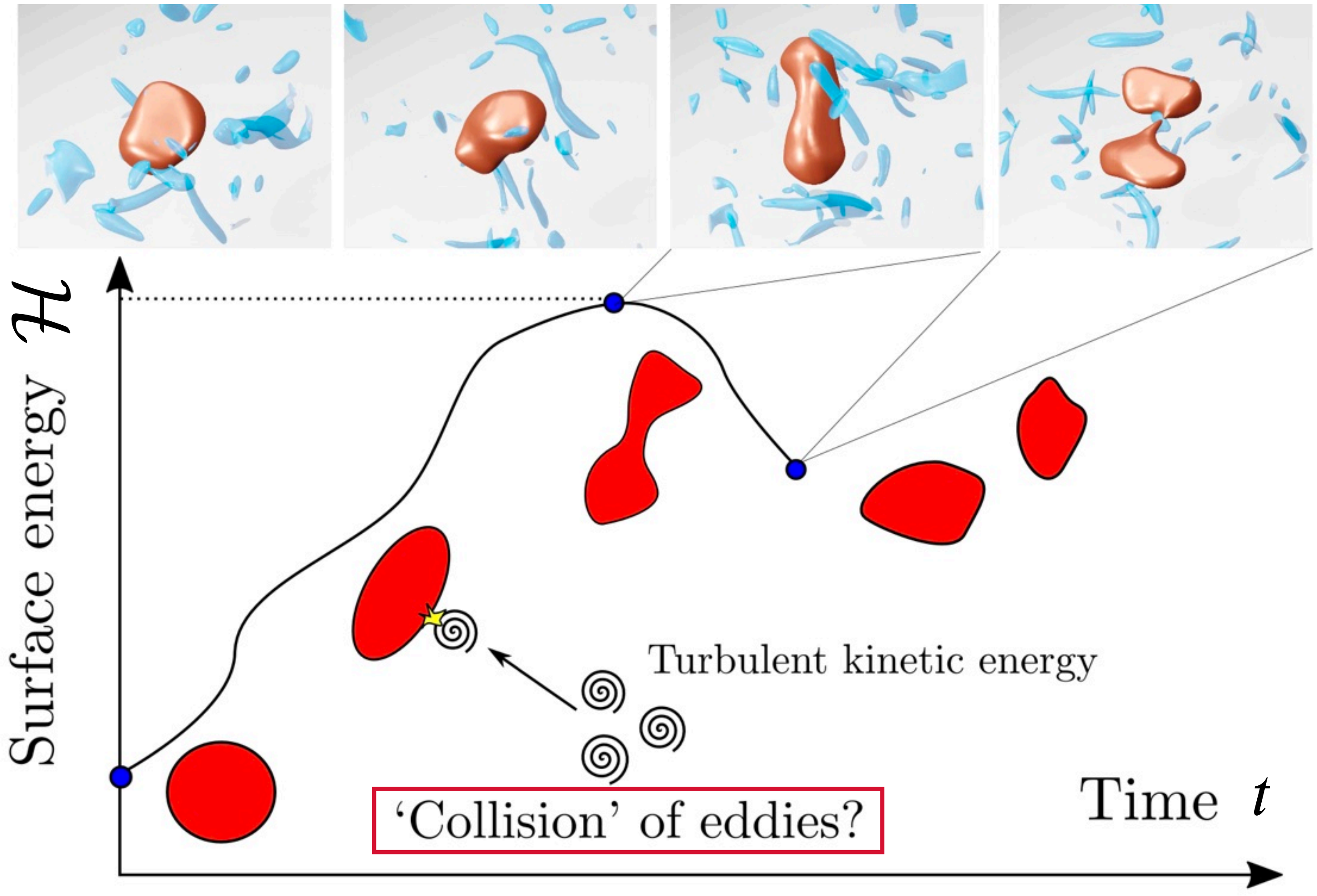
Drop breakup is a stochastic process

$t_d = d/u_d$

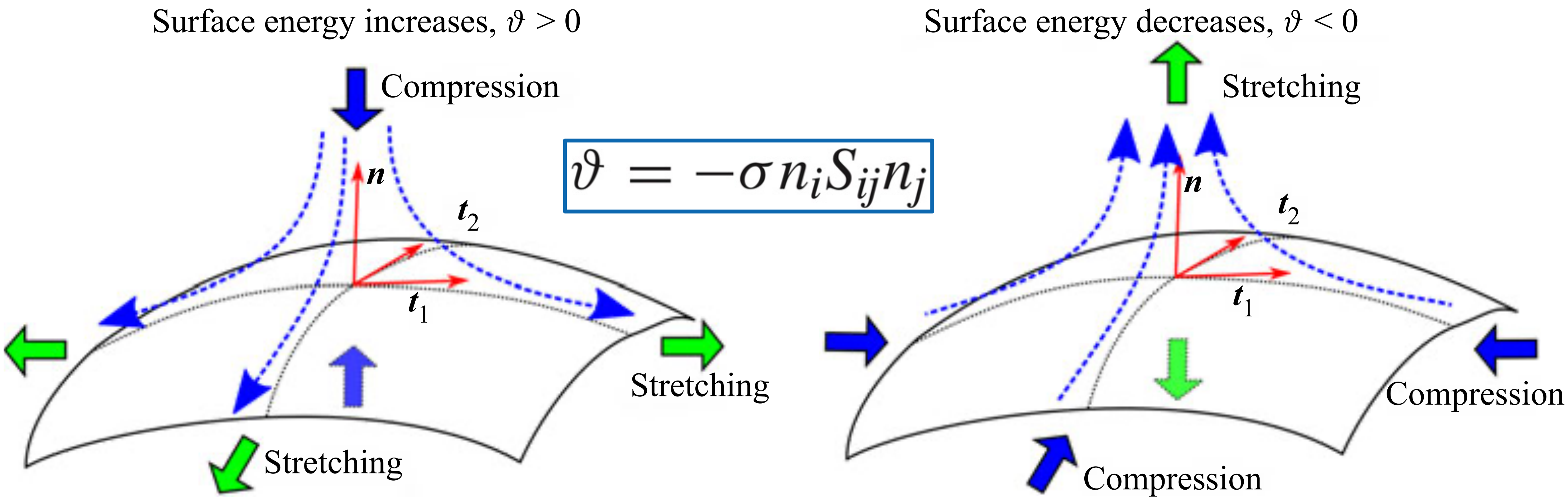


Vela-Martín & Avila, *Sci. Adv.* 2022

Drop deformation by ‘collision’ of eddies



Drop deformation by straining motions



$$\boxed{\vartheta = -\sigma n_i S_{ij} n_j}$$

Exact equations:
$$\mathrm{d}_t E = \mathcal{P} - \epsilon - \langle \vartheta \rangle_S$$
$$\mathrm{d}_t \mathcal{H} = \langle \vartheta \rangle_S$$

Vela-Martín & Avila, *J. Fluid Mech.* 2021

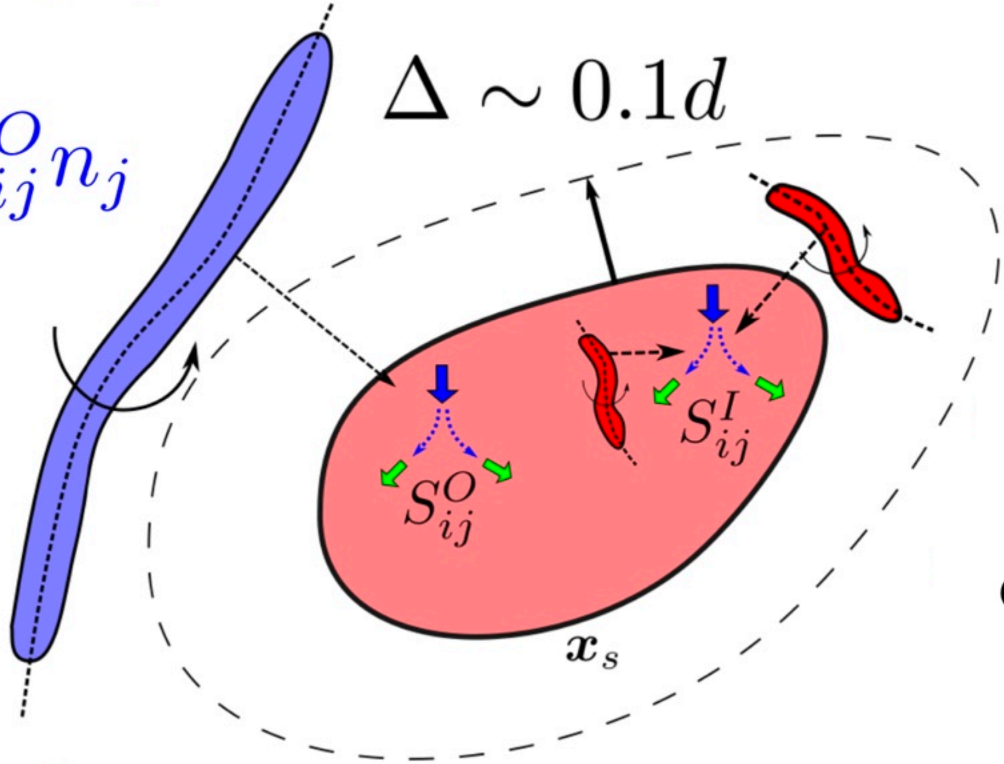
Stretching by outer/inner eddies

Decomposition of the rate-of-strain tensor (Biot-Savart law):

$$S_{ij} = S^I_{ij} + S^O_{ij}$$

$$\vartheta^O = -\sigma n_i S^O_{ij} n_j$$

$$\vartheta^I = -\sigma n_i S^I_{ij} n_j$$



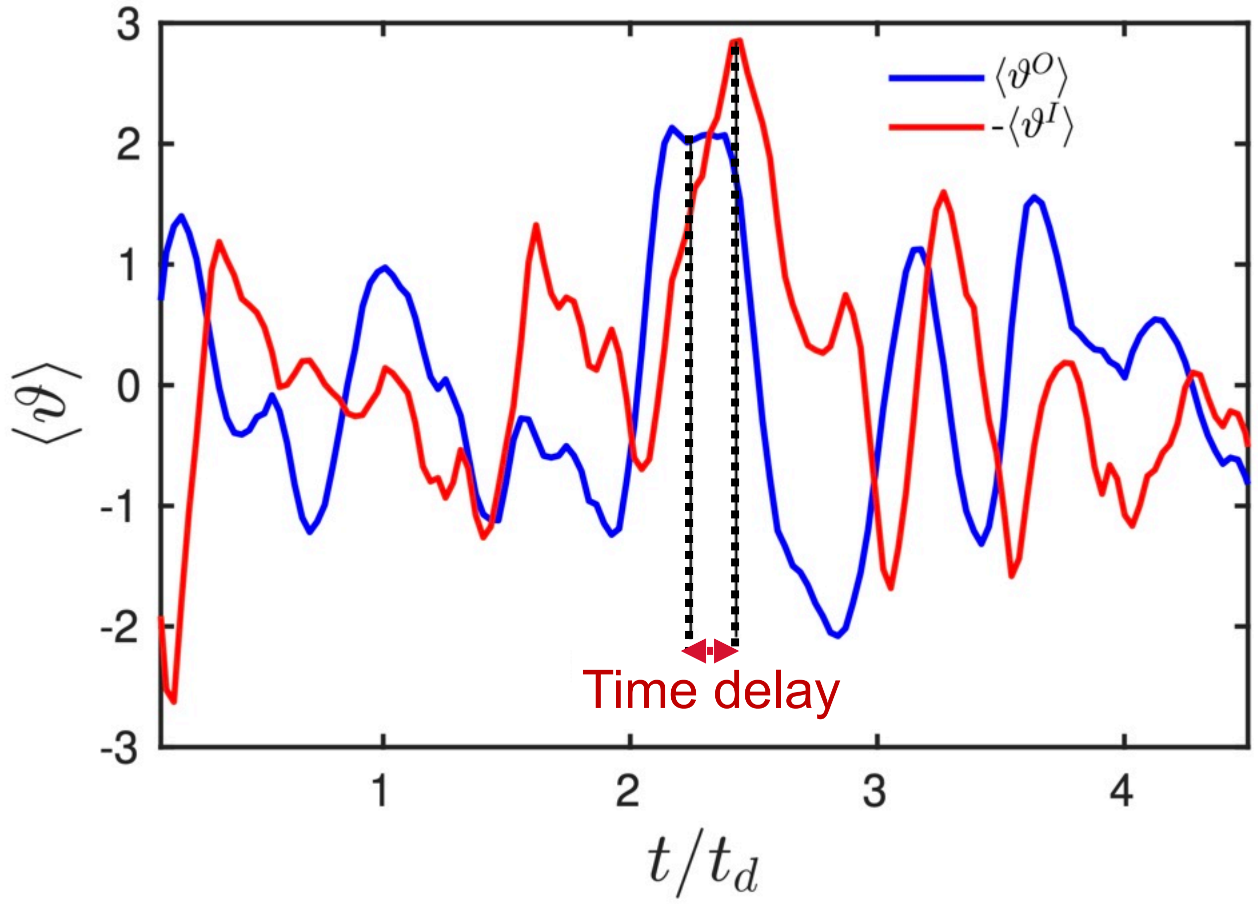
Modeling approach:

$$\mathrm{d}_t \mathcal{H} = \vartheta_O + \vartheta_I$$

Vela-Martín & Avila, *J. Fluid Mech.* 2021; borrowed from Ohkitani & Kishiba 1995 + Hamlington, Schumacher & Dahm 2008

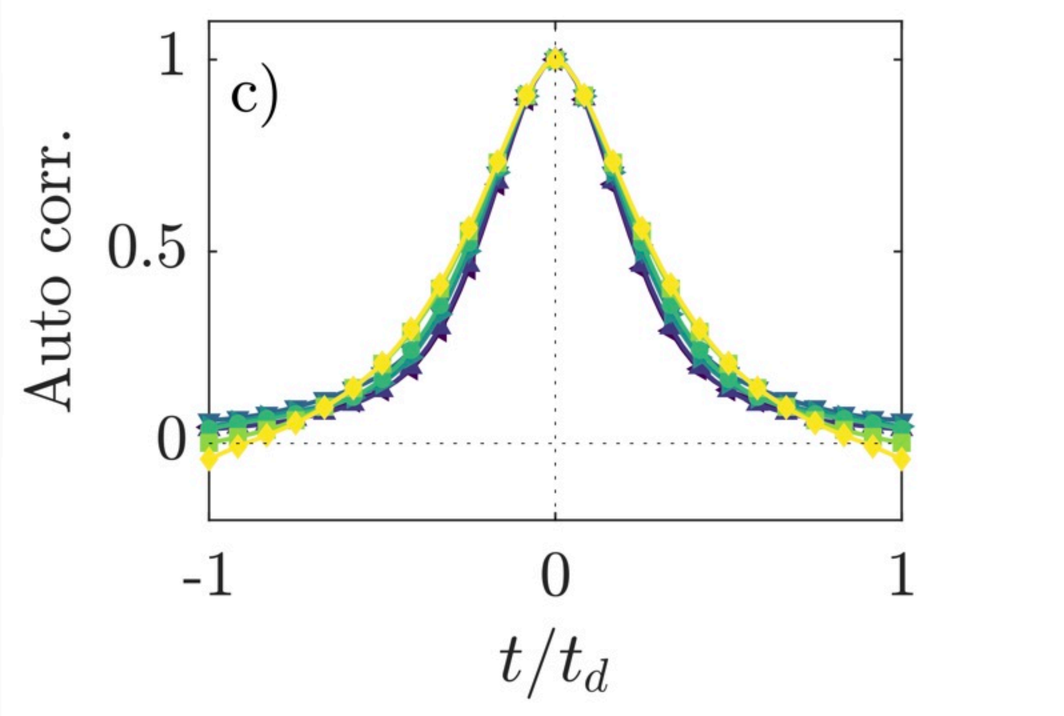
Outer eddies drive deformation

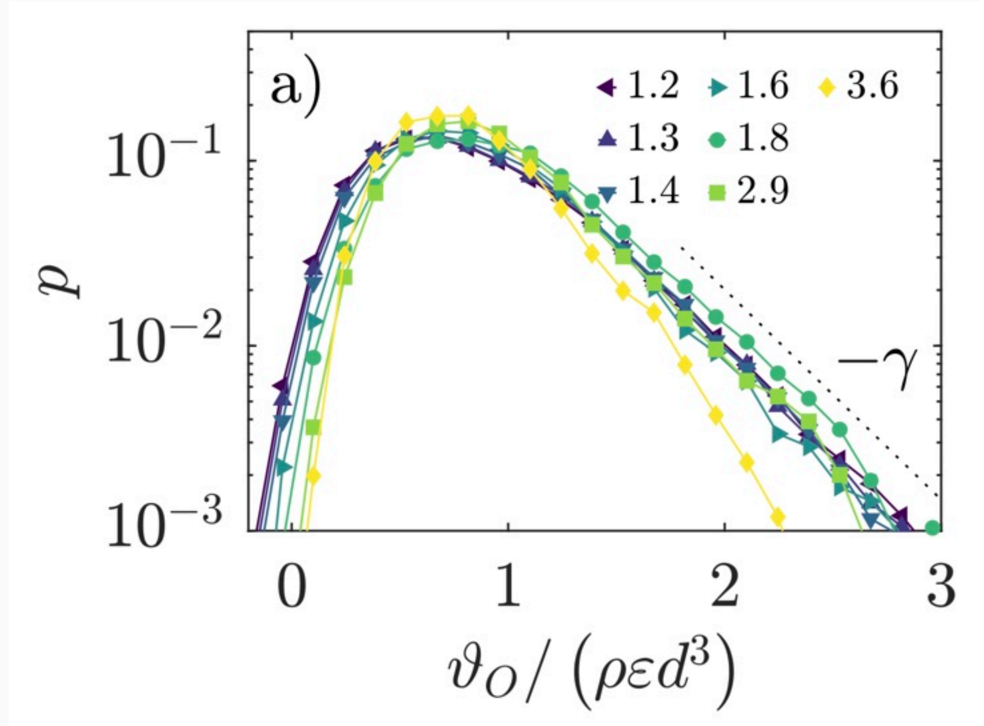
$We = 1.8$



Model of outer stretching

$\langle(\nu_O(t_0+t)-\langle\nu_O\rangle)(\nu_O(t_0)-\langle\nu_O\rangle)\rangle_{t_0}/\sigma^2_{\nu_O}$

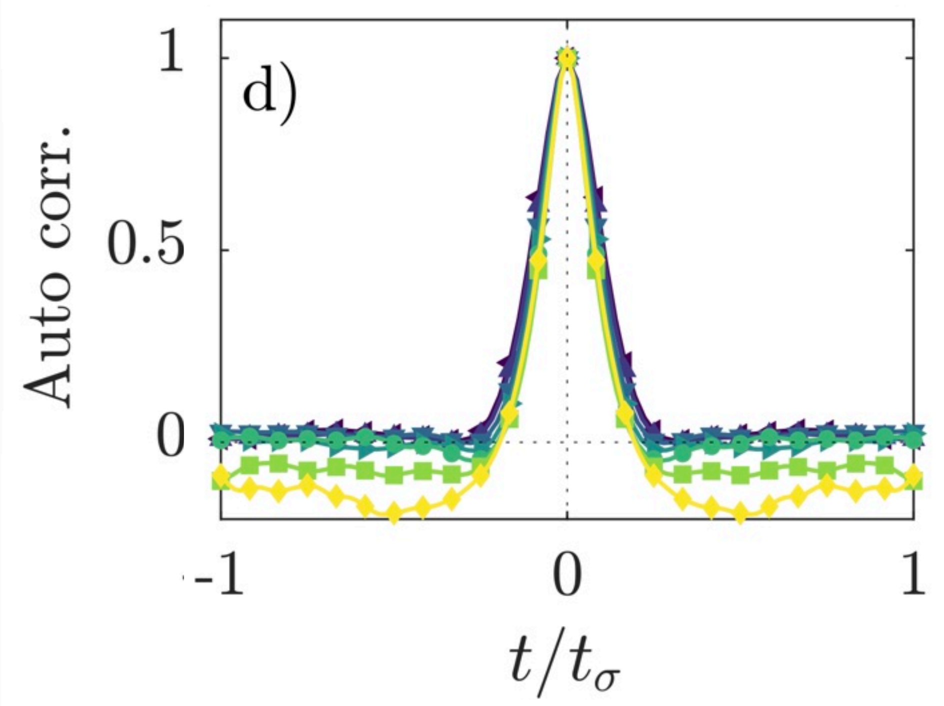


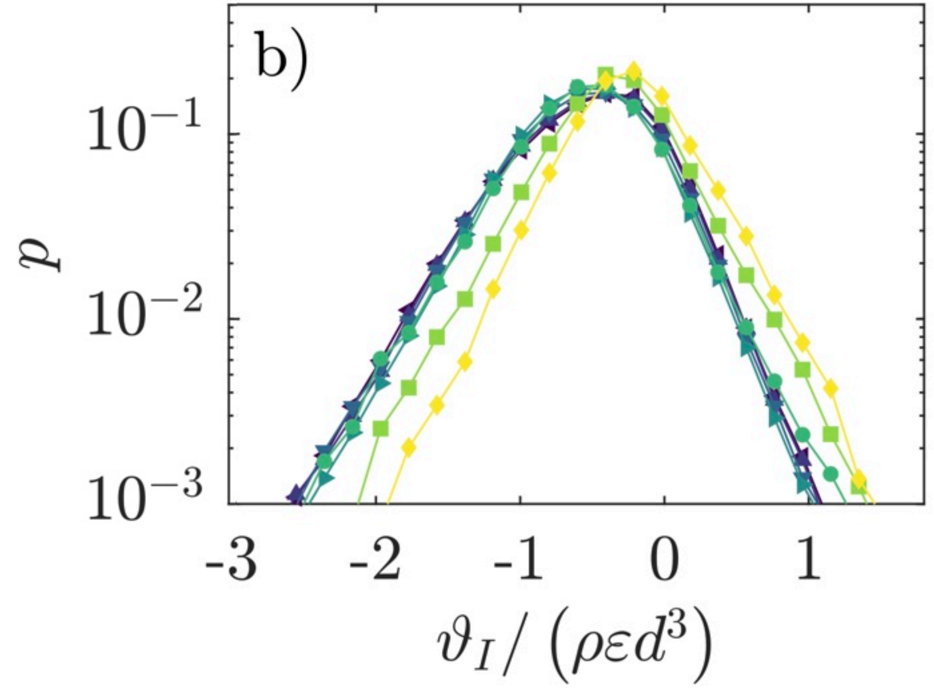


- varies with 0.1 eddy turnover times $t_d = d/u_d$
- value is positive and exponentially distributed. $\boxed{P\left(\hat{\vartheta}_O \geq \hat{\vartheta}_O^e\right) \propto e^{-\gamma\hat{\vartheta}_O^e}}, \gamma = 2.6$

Model of inner stretching

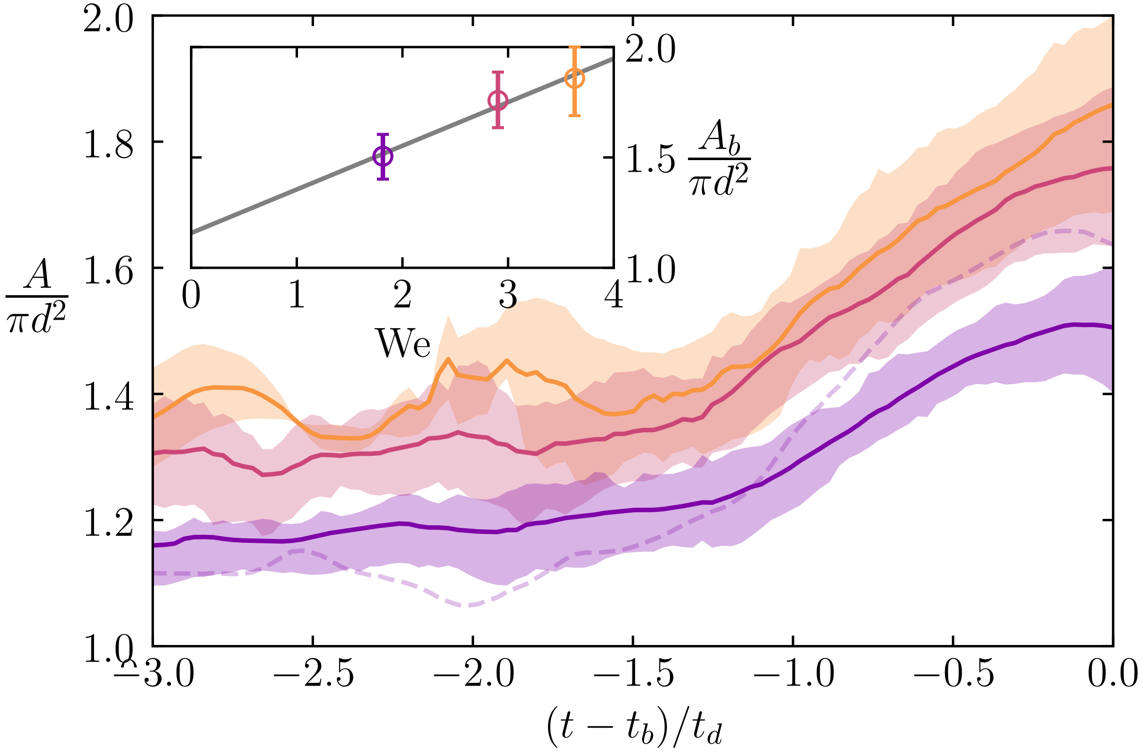
$$\langle(\nu_I(t_0+t)-\langle\nu_I\rangle)(\nu_I(t_0)-\langle\nu_I\rangle)\rangle_{t_0}/\sigma^2_{\nu_I}$$





- varies with 1/3.5 capillary times $t_\sigma = \sqrt{\rho d^3/\sigma}$
- value is negative and depends on the drop area $\boxed{\vartheta_I \approx -\frac{c_d}{t_\sigma}(\mathcal{H}-\mathcal{H}_0)}$, $c_d = 3.5$

Area at breakup



Area increase at breakup is constant $\frac{A_b - \langle A \rangle}{\pi d^2} = 0.27$

Breakup rate

- drop energy is a competition $\mathrm{d}_t\mathcal{H} = \vartheta_O + \vartheta_I$
- probability of exceeding the breakup energy $\boxed{P_b \propto e^{-\chi\,\mathrm{We}^{-3/2}}}$

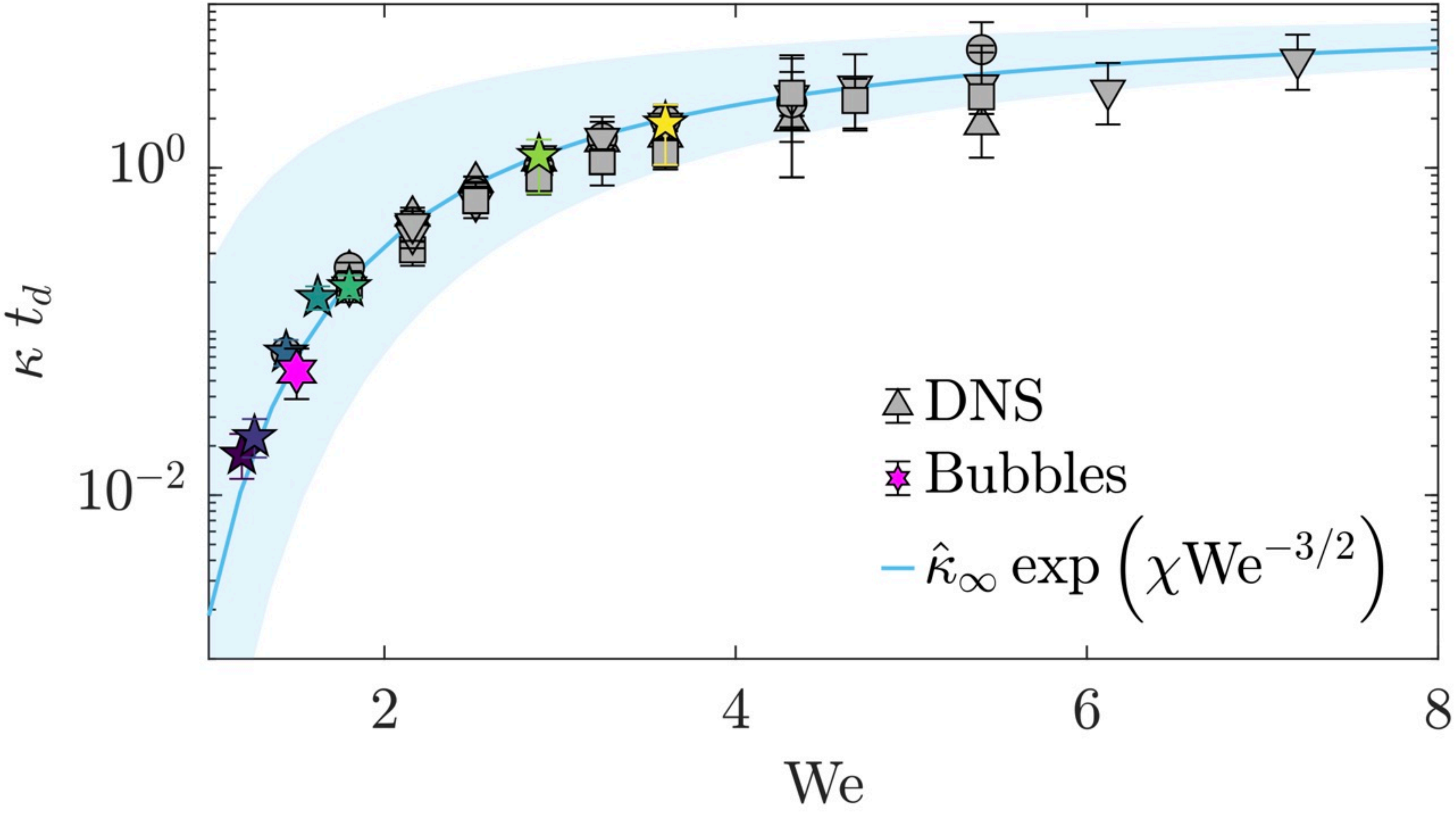
$$\chi = \gamma\,\pi\,\xi_c\,c_d/(1-\delta)$$

$$\delta = e^{-c_d\,\hat{t}_{\vartheta_O}\,\mathrm{We}^{-1/2}}$$

- outer stretching events occur ~10 times per eddy turnover $\boxed{\hat{\kappa} = \hat{\kappa}_\infty\,e^{-\chi\,\mathrm{We}^{-3/2}}}$

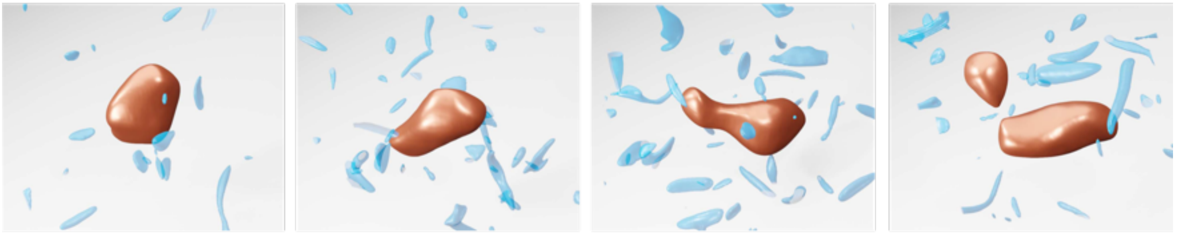
$$\hat{\kappa}_\infty = 10/t_d$$

Breakup rate



S. Perrard, A. Rivière, W. Mostert, and L. Deike, Bubble deformation by a turbulent flow, J. Fluid Mech. 2021
A. Vela-Martín and M. Avila, Memoryless drop breakup in turbulence, Sci. Adv. 8, 2022

Conclusions



- The drop is stretched by outer eddies and relaxes via inner eddies
- Outer stretching events occur every $0.1 t_d$
- Outer stretching intensity is exponentially distributed with $\gamma = 2.6$
- Inner stretching has a rate of $3.5 t_\sigma$
- The area increase at breakup is $0.27 \pi d^2$
- The breakup rate is $\kappa_\infty t_d^{-1} \exp\left(-\chi \mathrm{We}^{-3/2}\right)$
- Scaling constants can be determined a priori from measurements of the flow
- Model is generalisable to other flows; e.g., non-Newtonian
- Morón, Cannon, Vela-Martín, & Avila, “Causal mechanisms of drop breakup in turbulent flows,” https://arxiv.org/abs/2605.07504
- Thank you!