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Fragmentation processes in turbulent flows

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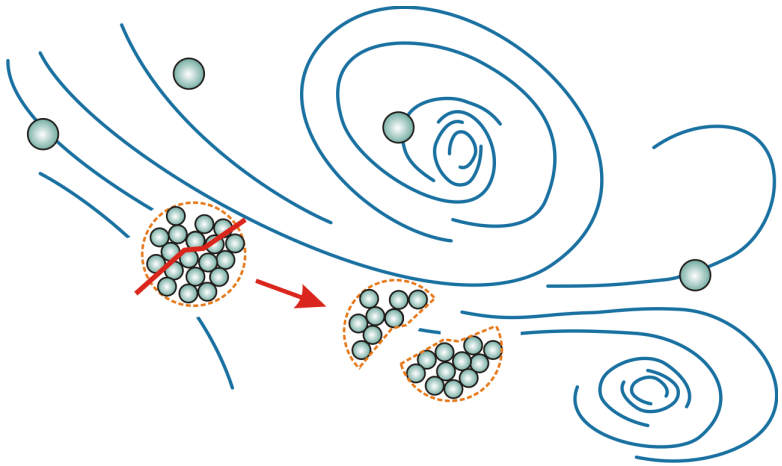
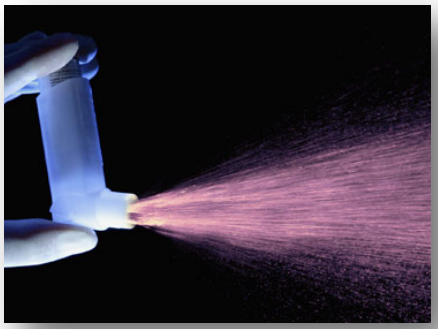


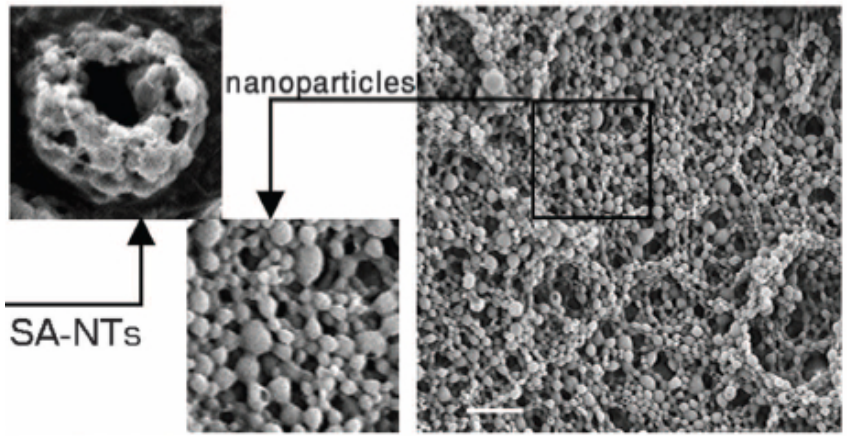
How many breakup events per unit time ?

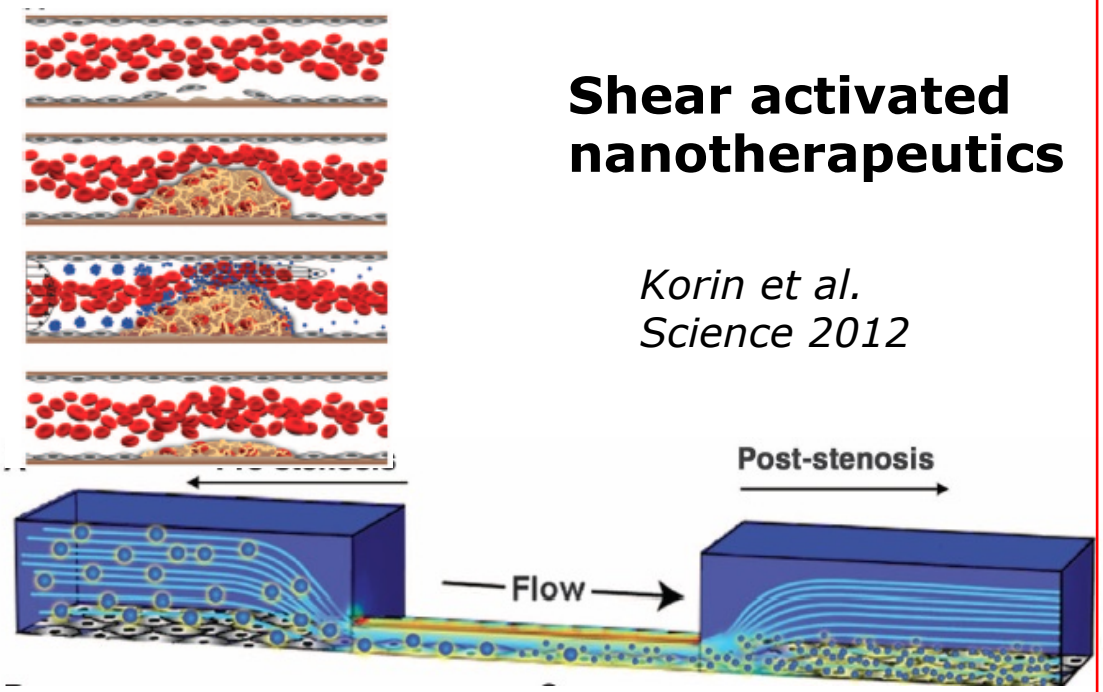
From plankton dynamics to nano drugs

- Industrial processing of polymer colloids
- Suspended particulate matter in environmental systems:
  e.g., marine snow or aerosols
- Dispersion of powder aggregates
  e.g. inhalation drugs



- Nano-particles for thrombus lysis in blood vessels



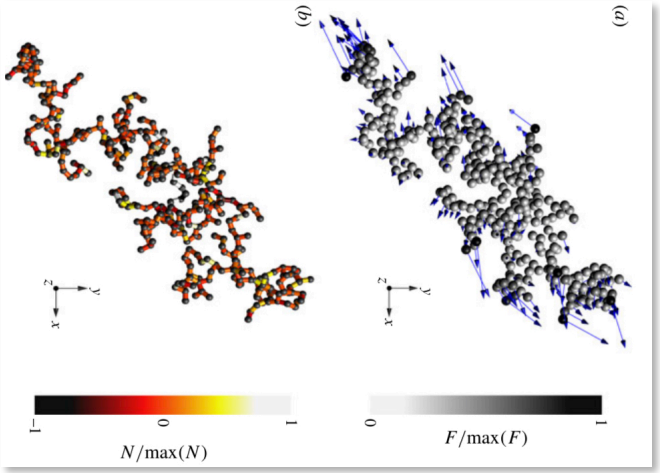


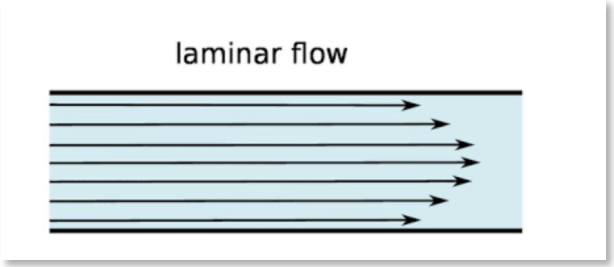
Shear activated nanotherapeutics

Korin et al.
Science 2012

Modeling approach: *no easy way out*

- **SOLVE INTERNAL DEGREES of FREEDOM, & NEGLECT TURBULENT MOTIONS**
  - Aggregate structure held together by surface forces at intermonomer bonds
  - Stokesian Dynamics relating forces, torques and stresslets on each monomer with the flow field through a mobility matrix
  - Aggregates moving in **simple laminar flows**

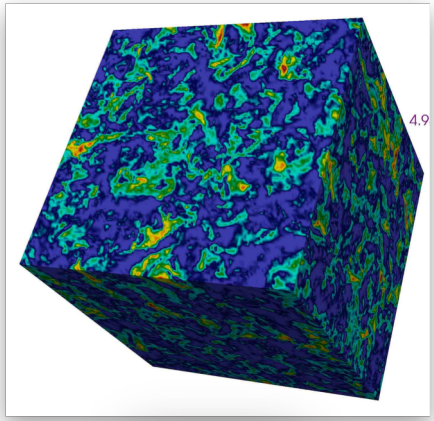


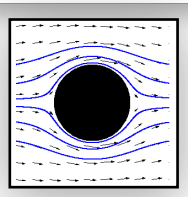


- **SOLVE TURBULENT MOTIONS, & NEGLECT INTERNAL D.o.F.**
  - Flow configurations need to resolve turbulent motions on wide range of scales

$\mathbf{Re}_\lambda \sim (L/\eta)^{2/3}$ #DoF ~ $\mathbf{Re}_\lambda^{9/2}$

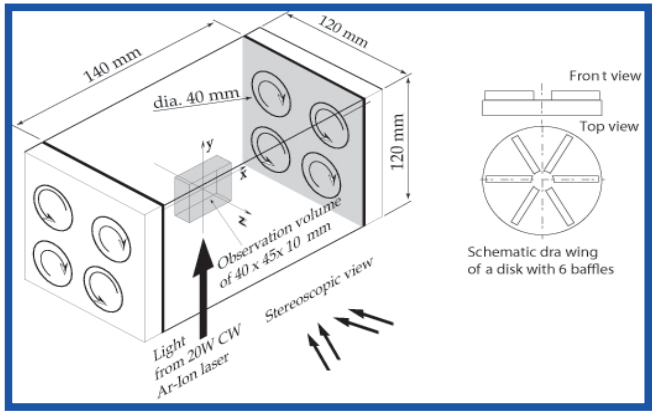
e.g. if $\mathbf{Re}_\lambda \sim \mathbf{400}$ you need #DoF => $N^3 = 2048^3$ grid points

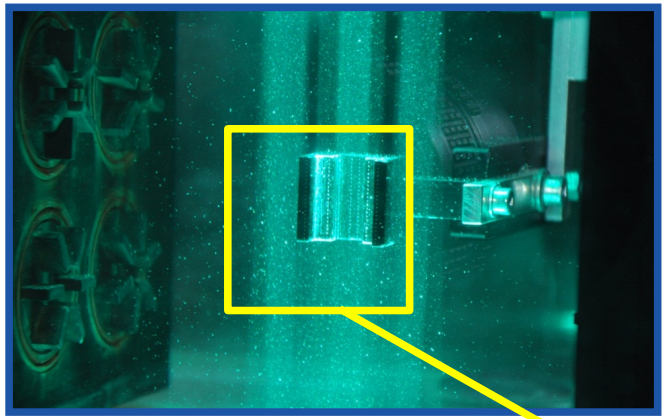


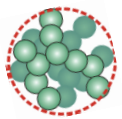


- Small aggregates as point-like "spherical" particles in a creeping flow
- Breakup due to mechanical stress only

Breakup of Finite-Size Colloidal Aggregates







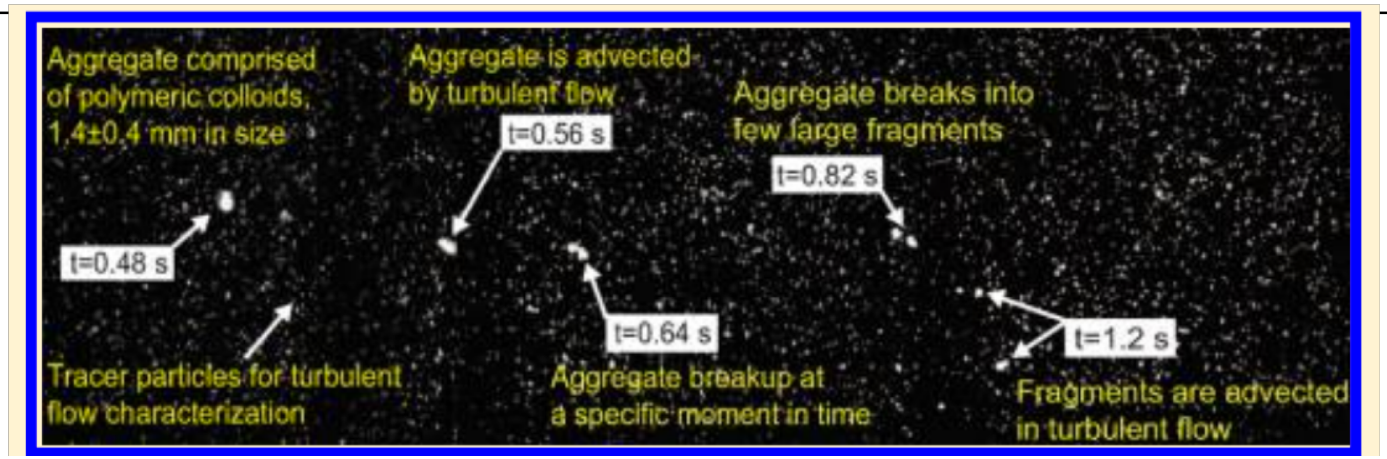
Aggregates:
d_f = 2.2
Size = 1.4 mm

Tracers for PTV:
Neutrally buoyant
Size = 0.1 mm

Flow forcing: eight counter rotating disks
Operating at 100 rpm
Tank : 420 mm x 420 mm x 440 mm

Observation domain,
30mm × 30mm × 40 mm
Camera 7Khz, 1024x1024 px

U_{rms}	L	η	ε	Re_λ	τ_η	Shear rate	images/τ_η
0.04 ms^{-1}	25mm	0.15 mm	1.9e-3 m^2s^{-3}	**117**	0.023 s	44 s^{-1}	6s^{-1}

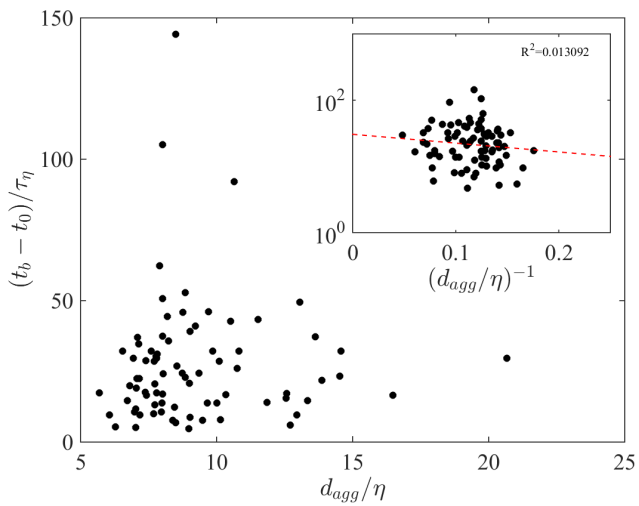


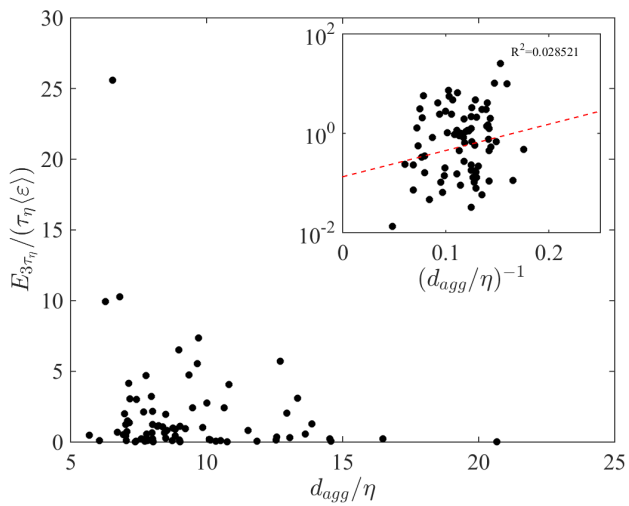
Saha et al. *Langmuir 2016, 32, 55–65*

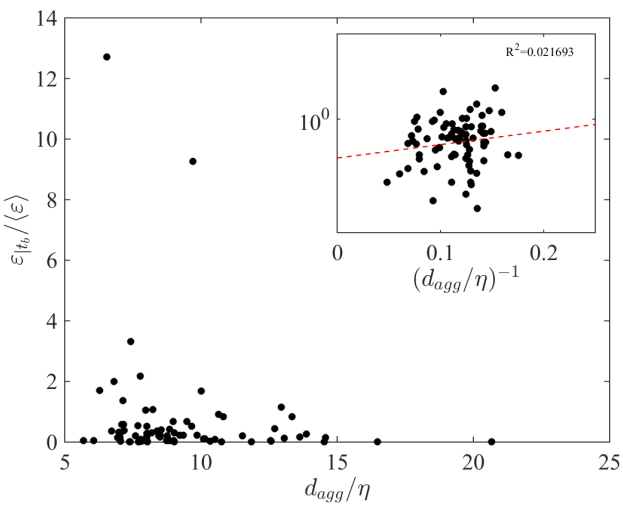
Breakup criteria

- Monitoring breakup events by PTV
- Aggregate strength decreases with increasing aggregate size

$$R_g \sim \sigma_{cr}^{-a}; \quad R_g \sim \xi^{1/d_f}$$







Criteria 1: "Slow breakup"
Breakup is controlled by slow internal dynamics inside the aggregate, i.e., rearrangement of primary particles. Turbulent fluctuations do not influence breakup.

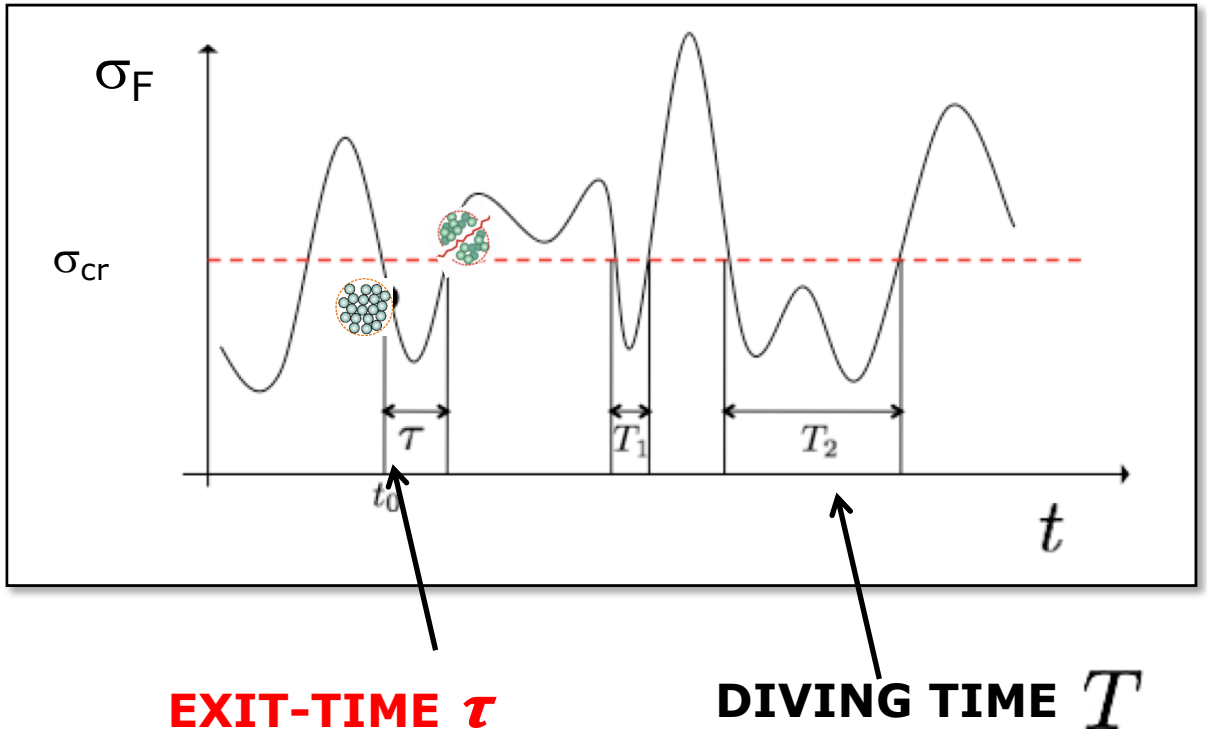
Criteria 2: "Intermediate breakup:" Breakup requires accumulation of stress.

$$E_\Delta = \int_{t_b-\Delta t_b}^{t_b} \varepsilon(t)dt$$

Criteria 3: "Fast or instantaneous breakup"
Local stress (local in time and space) controls breakup. Breakup upon crossing a critical threshold

Numerical experiments

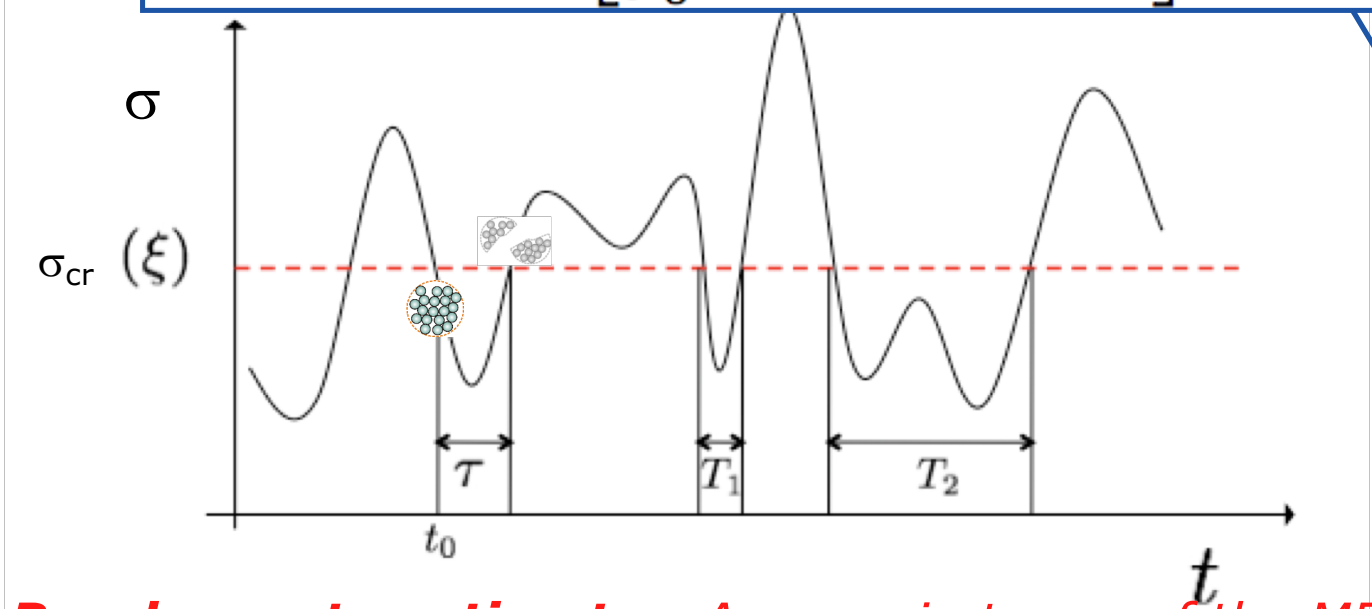
- In a turbulent flow, consider aggregates of mass ξ and strength $\sigma_{cr}(\xi)$
- Brittle limit: Aggregate break up when the mechanical-hydrodynamic stress exceeds a critical value $\sigma_{cr}(\xi)$
- At time t_0, release aggregate at random where $\sigma_F < \sigma_{cr}$
- Instantaneous break-up when local stress σ_F exceeds critical value $\sigma_F > \sigma_{cr}(\xi)$



The time from the release to the break-up is the first ***EXIT-TIME τ***
The ***DIVING TIME T*** is the mean time below critical threshold

Breakup rate natural def.: *Lagrangian* ***measure*** *from MEAN EXIT-TIME* τ

$$f_{LAG}(\sigma_{cr}) \equiv \left[\int_0^\infty d\tau\, \tau\, P_{\sigma_{cr}}(\tau)\right]^{-1} \equiv \frac{1}{\langle \tau(\sigma_{cr}) \rangle}$$



$$\langle \tau(\epsilon_{cr}) \rangle = \frac{\langle T^2(\epsilon_{cr}) \rangle}{\langle T(\epsilon_{cr}) \rangle}$$

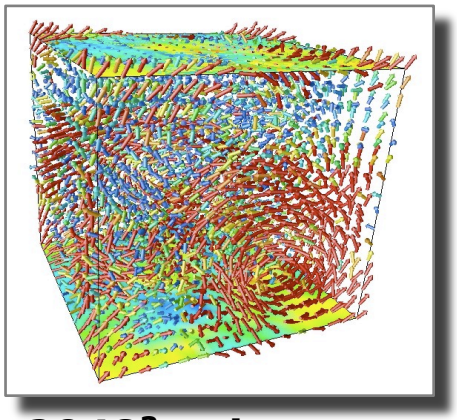
Breakup rate estimate: *A proxy in terms of the MEAN DIVING TIME* T

$$f_{EUL}(\sigma_{cr}) \equiv \frac{1}{\langle T(\sigma_{cr}) \rangle} = \frac{\int_0^\infty d\dot{\sigma}\, \dot{\sigma}\, p_2(\sigma_{cr}, \dot{\sigma})}{\int_0^{\sigma_{cr}} d\sigma\, p(\sigma)} = \frac{\text{number of up cross}}{\text{fraction of time below}}$$

V.I. Loginov (1985) + S.O. Rice Theorem for upcrossings events number estimate (1945)

Direct Numerical Simulations of 3D HIT

Fluid



2048^3 points
$Re_\lambda \sim 400$

- Incompressible, **H**omogeneous and **I**sotropic **T**urblent flow **u**
- Non-linear interaction of "eddies" of scales $\eta \leq r \leq L$
- Flow is controlled by turbulent dissipation $\epsilon = \nu(\partial u_i/\partial x_j)^2$ and Reynolds number $\mathbf{Re}_\lambda$
- Flow is seeded with 10^9 non-interacting point-particles

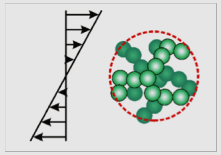
Particles motion

- Tracer Aggregates

$R << \eta$

$\rho_a \sim \rho_f$

$$\frac{d\mathbf{X}}{dt} = \mathbf{u}(\mathbf{X}, t)$$



$$\sigma = \sqrt{\frac{2}{15}}\mu\left(\frac{\varepsilon}{\nu}\right)^{1/2}$$

- Inertial aggregates

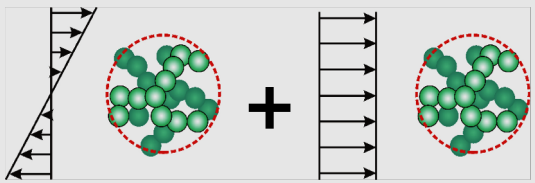
$R << \eta$

$\rho_a >> \rho_f$

$$\frac{d\mathbf{V}}{dt} = \frac{\mathbf{u}(\mathbf{X}, t) - \mathbf{V}}{\tau_a}$$

Stokes time

$$\tau_a = \left(\frac{\rho_f + 2\rho_a}{\rho_f}\right)\frac{R_g^2}{3\nu}$$



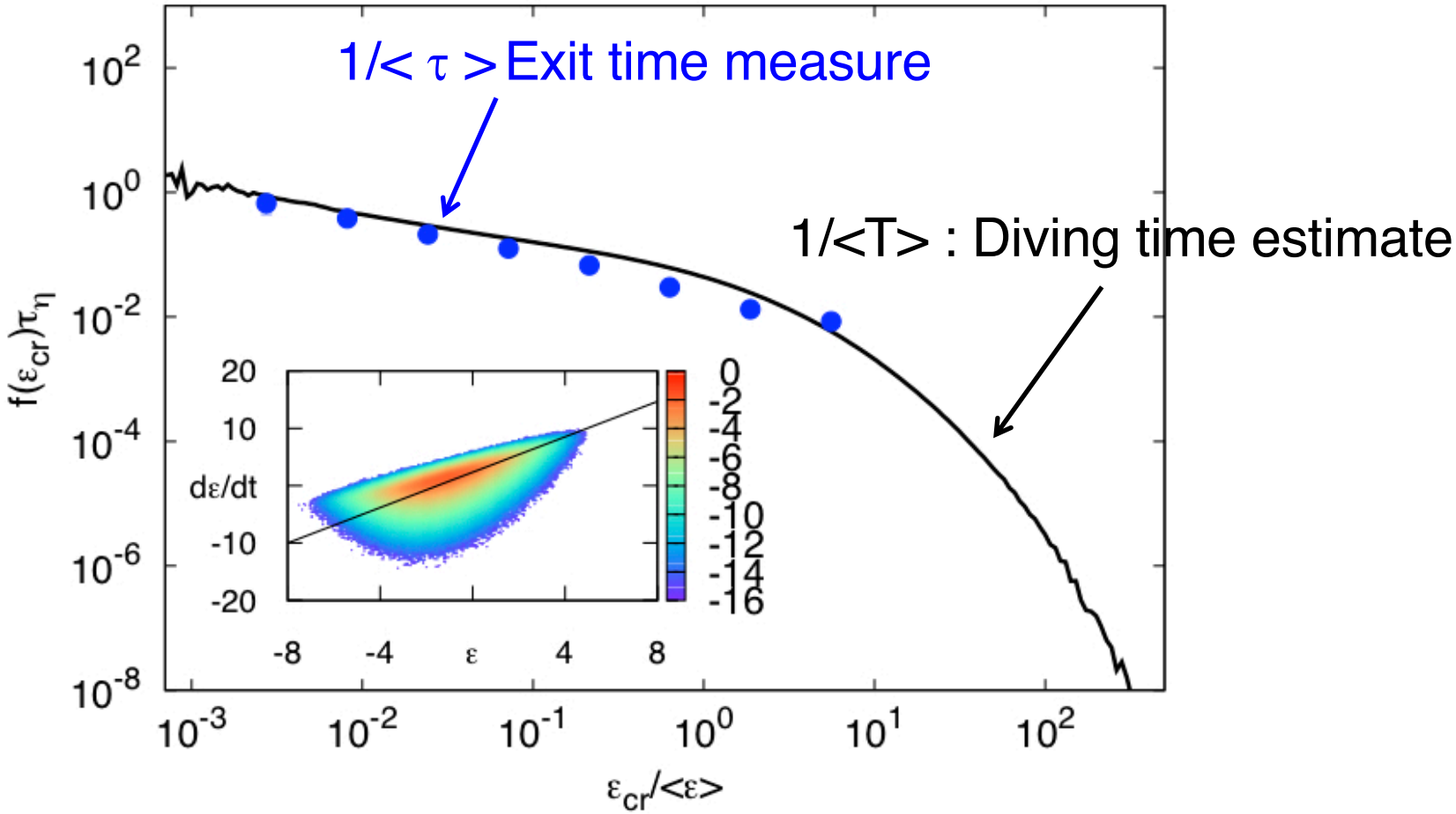
$$\sigma = \sqrt{\frac{2}{15}}\mu\left(\frac{\varepsilon}{\nu}\right)^{1/2} + \frac{2}{3}\mu\frac{|\boldsymbol{v} - \boldsymbol{u}|}{R}$$

Breakup rate:
Lagrangian measure vs Eulerian estimate

Results for TRACERS aggregates subject to shear stress only

$$\epsilon_{cr} = \frac{15\nu}{2\mu^2}\sigma_{cr}^2$$

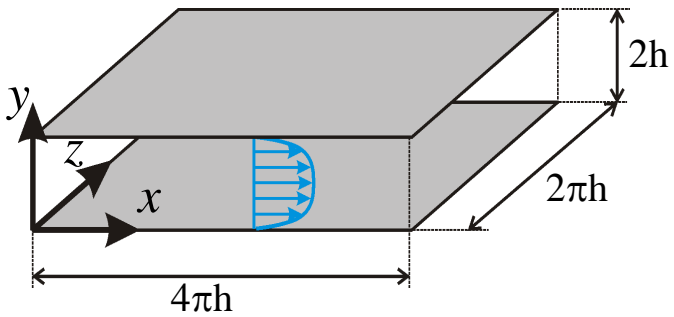
$$\epsilon = \nu(\partial u_i/\partial x_j)^2$$



NOTE: exit-time measure at large stress requires too long trajectories

What if we change flow configurations ?

Channel flow



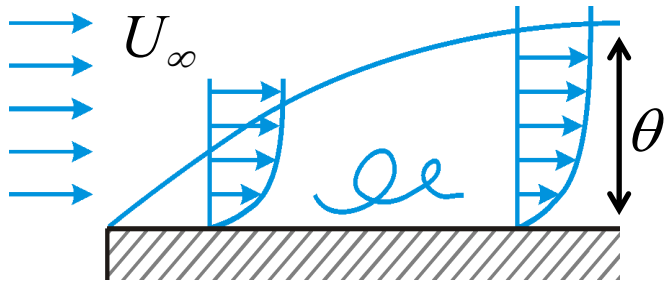
- $R_\tau = u_\tau h / \nu = 150$

(u_τ = shear velocity)

- Small aggregates released:

1. Center-plane
2. Near-wall region

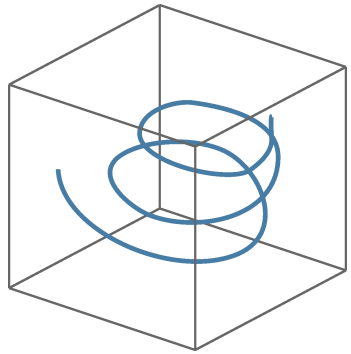
Developing boundary layer flow



- $R_\theta = U_\infty \theta / \nu = 200\text{-}2500$
  (θ=momentum-loss thickness)
- Small aggregates released:

1. Inside the boundary layer
2. Outside the boundary layer

H.I.T.



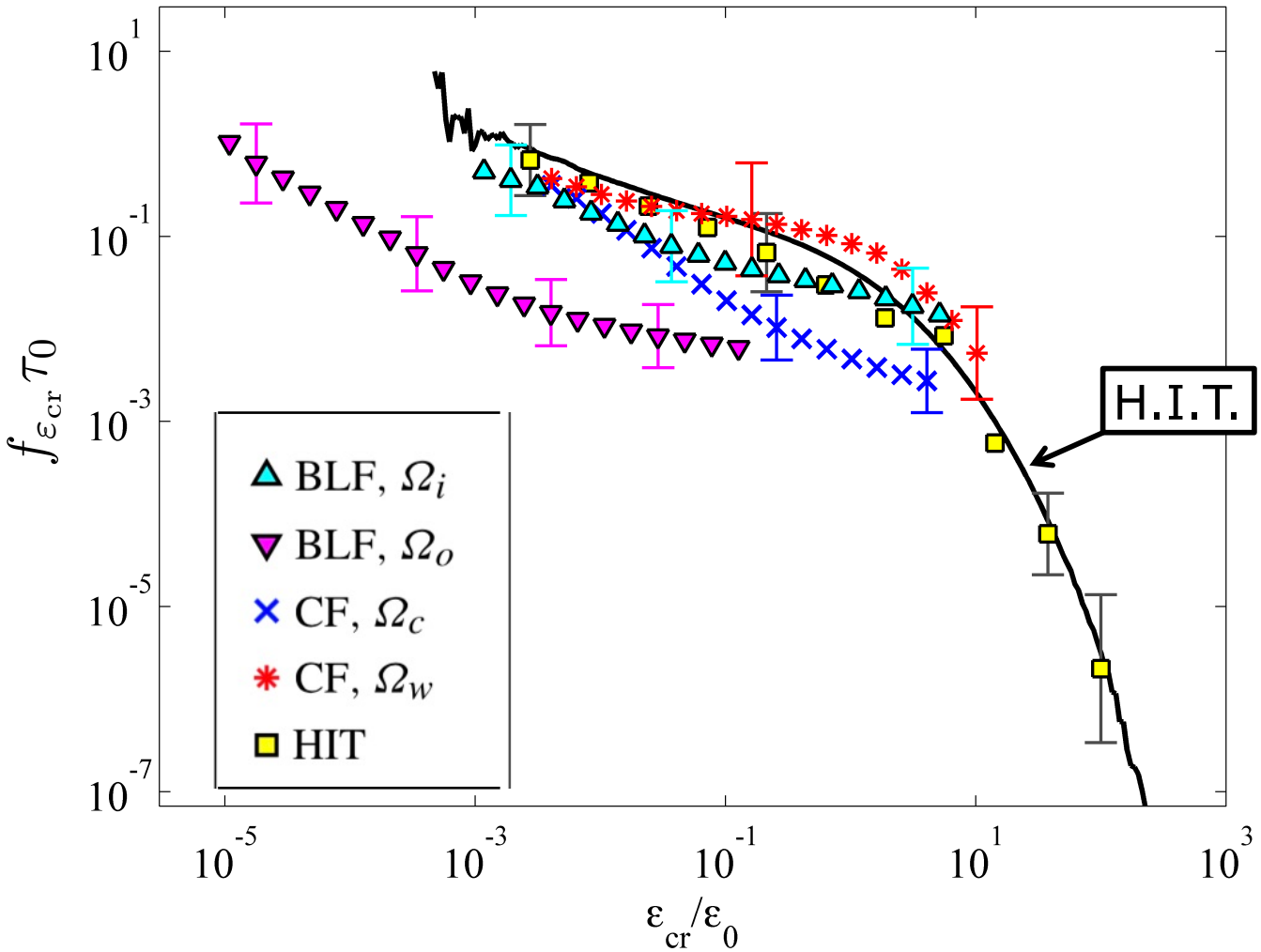
- $Re_\lambda \sim 400$
- Small aggregates are released homogenously

Results for tracer aggregates in diff flows

- **Channel flow**
  ε_0=volume average
  $\tau_0=(\nu/\varepsilon_0)^{1/2}$

- **Boundary layer**
  ε_0=volume average
  in the seeding region
  $\tau_0=(\nu/\varepsilon_0)^{1/2}$

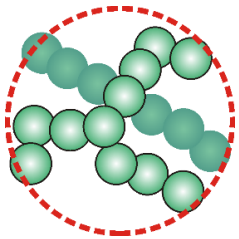
- **H.I.T.**
  ε_0=mean dissipation
  $\tau_0=(\nu/\varepsilon_0)^{1/2}$



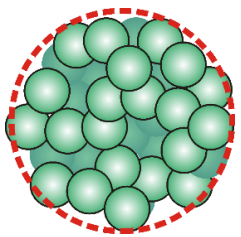
Aggregates with inertia

$$\sigma_{tot} = \mu\sqrt{\frac{2\epsilon}{15\nu}} + \frac{3\mu}{2}\frac{|\mathbf{u}-\mathbf{V}|}{R}$$

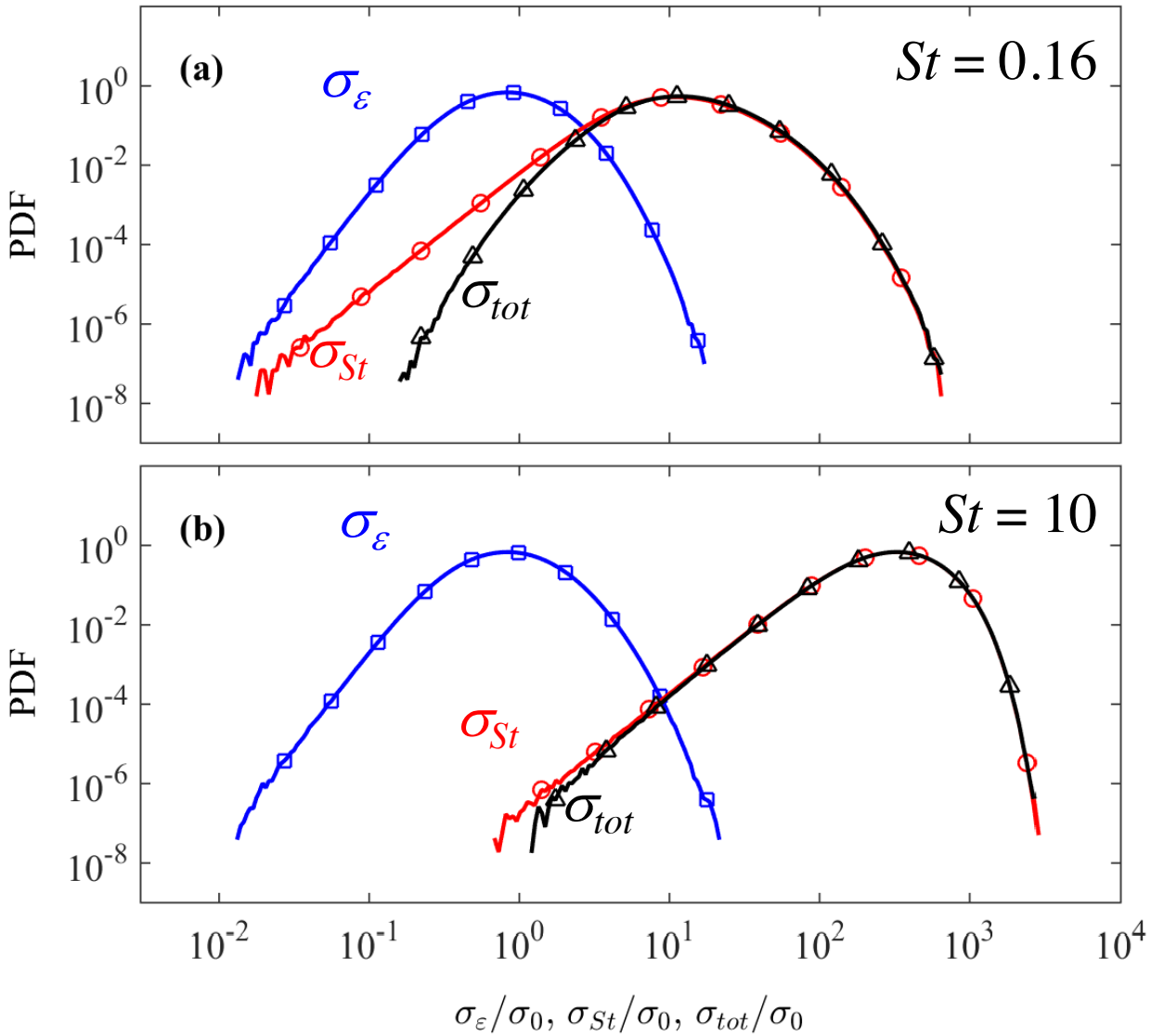
- Aggregates of size $R/\eta = 0.1$ and varying density



Open aggregate
Low density
$\rho_a > \rho_f$

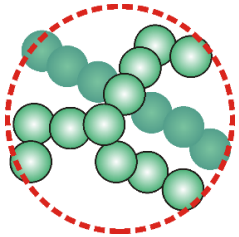


Compact aggregate, high density
$\rho_a >> \rho_f$

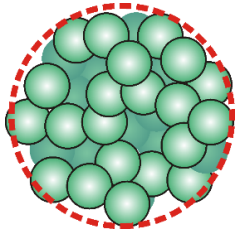


Breakup rate for inertial aggregates in H.I.T.

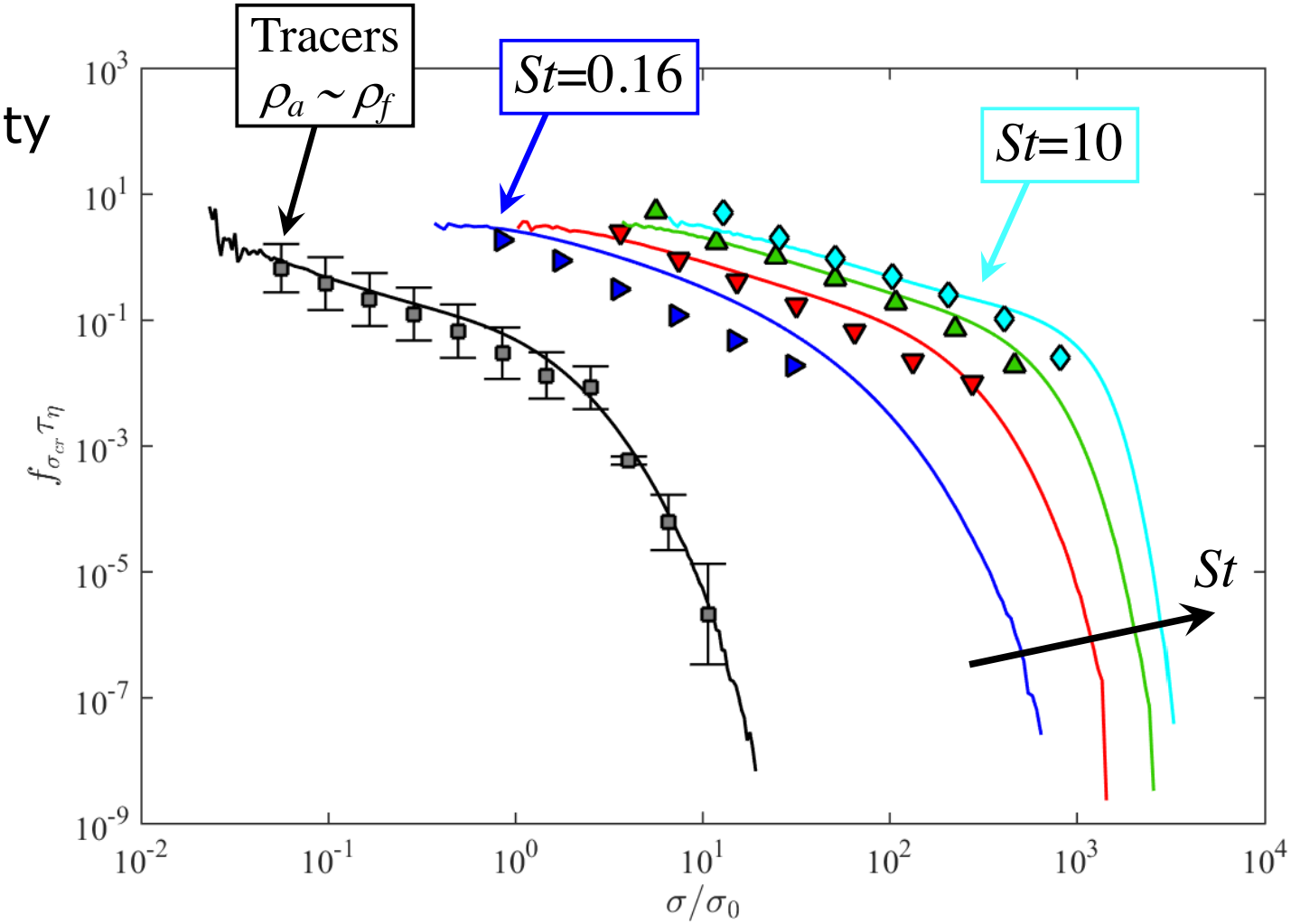
- Aggregates of size $R/\eta = 0.1$ and varying density



Open aggregate Low density



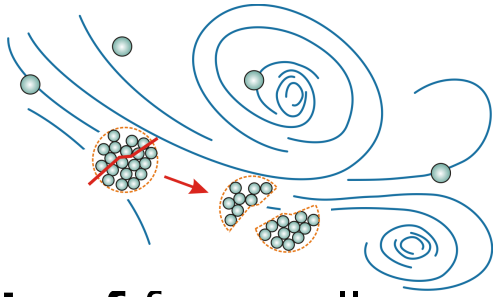
Compact aggregate, high density



Universal power law at small stress: *controlled by Gaussian fluctuations*

Non universal tail at large stress

Summary



MAIN OUTCOME:
An operational definition of breakup rates f for small *aggregates* diluted in a turbulent flow.

Exit time measure <τ> is a natural one, but requires high Lagrangian sampling & long trajectories.
Diving time estimate <T> is useful when Lagrangian tracking is difficult.

The power-law behaviour of the breakup rate f at small σ_{cr} is ~ universal with respect to *flow configurations and aggregates inertia*.
It is crucial to study breakup/coalescence dynamics via population balance equations.

The exponential tail of the break-up rate for large values of σ_{cr} is where rare turbulent fluctuations and inertia play a role

REFS:

- Babler, Biferale, Lanotte, *Phys. Rev. E* (2012)
- De Bona, Lanotte, Vanni, *Journal Fluid Mech* (2014)
- Babler et al., *Journal Fluid Mech* (2015)
- Babler, Biferale, Lanotte, *in preparation (2018)*