Yield Transition and Controlled Fluidization of Soft-Glassy Materials

SM&FT 2017

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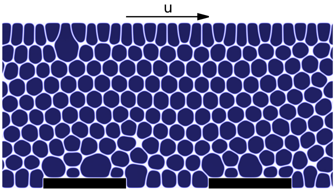
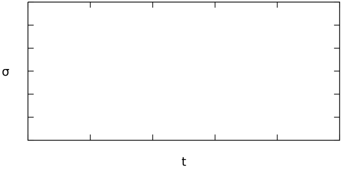
[3] High performance data network:
Convergenza di metodologie e integrazione di infrastrutture
per il calcolo HPC e HTC - FONDI CIPE

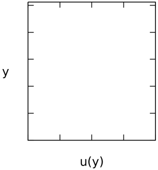
December the 13th, 2017

What are Soft-Glassy Materials*?

Class of materials (gels, pastes,...)
Sharing a **complex** phenomenology (elasticity, yielding, ageing,...)
A good example: **Emulsions**







Ensembles of Droplets that do not coalesce - surfactants...

Display both solid and liquid features: yield stress $\sigma_Y \left[\frac{\text{force}}{\text{area}}\right]$

- **Solid-like behaviour - elastic response:** $\sigma < \sigma_Y$,
- **Liquid-like behaviour - flow is non-Newtonian:** $\sigma > \sigma_Y$.

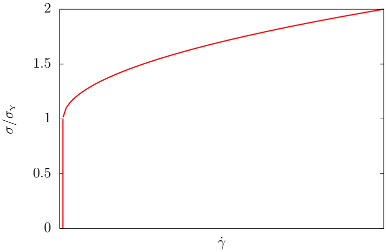
*R. G. Larson "The Structure and Rheology of Complex Fluids", Oxford University Press, (1999)

How do they flow? (Rheology)

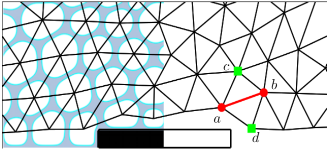
- Relation between σ and $\dot{\gamma} \propto \frac{\partial u}{\partial y}$ (shear rate)
- **Stress-dependent viscosity** $\eta(\sigma) = \frac{\sigma}{\dot{\gamma}}$
- Simple fluids: constant viscosity

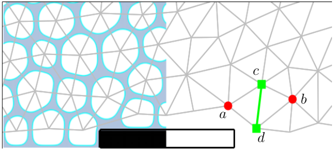
Herschel-Bulkley relation

$$\sigma = \sigma_{\mathsf{Y}} + A\dot{\gamma}^n, \ \sigma > \sigma_{\mathsf{Y}}$$



The flow is due to **irreversible plastic rearrangements** of the droplets
How to detect them?
Changes in **Delaunay Triangulation** of droplets **centers of mass**





Rearrangements happen at a **rate** $\Gamma(x)$ which is **space-dependent**

Rich physics involved

- There are **non-local** effects in confined (micro-channels) flows
  Finite-size effects: for fixed stress σ, the viscosity η depends on the channel size
  KEP model*: Fluidity $f(x) = \dfrac{\dot{\gamma}}{\sigma} \propto \Gamma(x)$

$$\xi^2 \nabla^2 f(x) = f(x) - f_{\mathsf{b}}(\sigma),$$

  ξ: **cooperativity length**

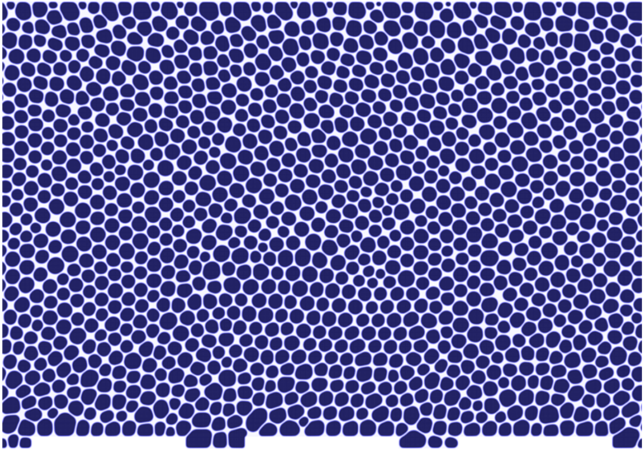
- Non-trivial **Boundary Effects**: Wall Fluidity $f(x_{\mathsf{w}}) = f_{\mathsf{w}}$
  1) Is it possible to **tune** the wall fluidity in a **controlled** way?
  2) Can **surface roughness** tune fluidity?

- **Yield-stress transition**
  1) Rheology at the transition in stress-driven flows?
  2) Correlations at the yield-stress point?

*L. Bocquet *et al.*, *Phys. Rev. Lett.* **103**, 036001 (2009)

HPC for Emulsions

- Efficient simulations for emulsions with **multi-GPU** implementations of **Lattice Boltzmann** method*
- *General* **Prompt Tracking** of topological changes†



*M. Bernaschi, L. Rossi, R. Benzi, M. Sbragaglia & S. Succi, *Phys. Rev. E*, **80**, 066707 (2009)
†M. Bernaschi, ML & M. Sbragaglia, *Comp. Phys. Comm.*, **213**, 19 - 28 (2017)

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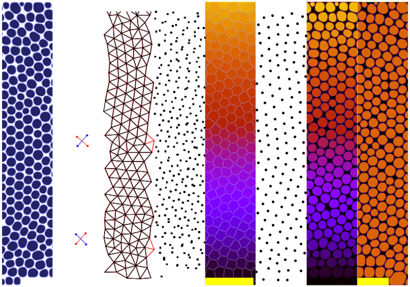

What can we do?

- Analyze centers of mass **displacements**
- Track topological changes
- Analyze Voronoi tesselation (elastic stress)

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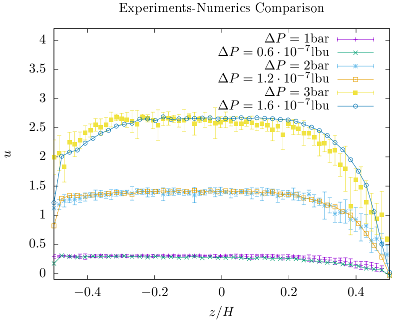
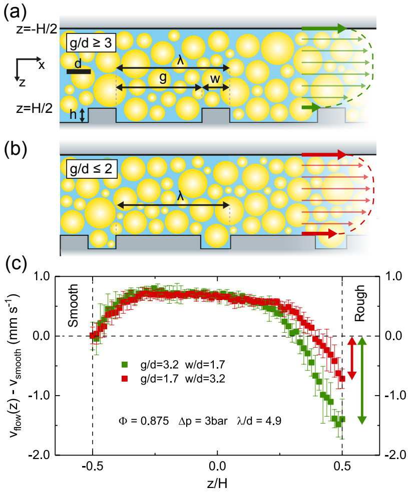
Controlled Fluidization*: Experimental Setup

- Pressure driven flow in microchannels with patterned wall
- Slip on the rough wall depends on roughness parameters
- Good **fluidization measure**

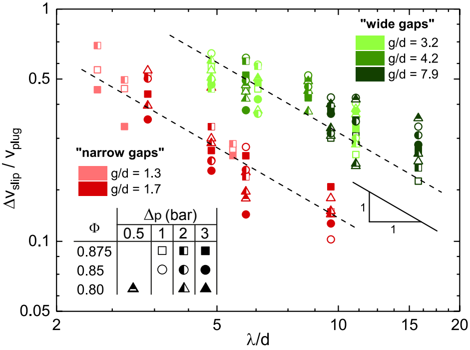
$$\Delta v_{\text{slip}} = v_{\text{smooth}} - v_{\text{rough}}$$





*L. Derzsi, D. Filippi, G. Mistura, M. Pierno, ML, M. Sbragaglia, M. Bernaschi & P. Garstecki, *Phys. Rev. E*, **95**, 052602 (2017)

Controlled Fluidization*: Experimental Results



Systematic Study - Parameters

∇P	Pressure Gradient
Φ	Packing Fraction
λ	Periodicity of the grooves
w	Width between the grooves
g	Gap between the grooves

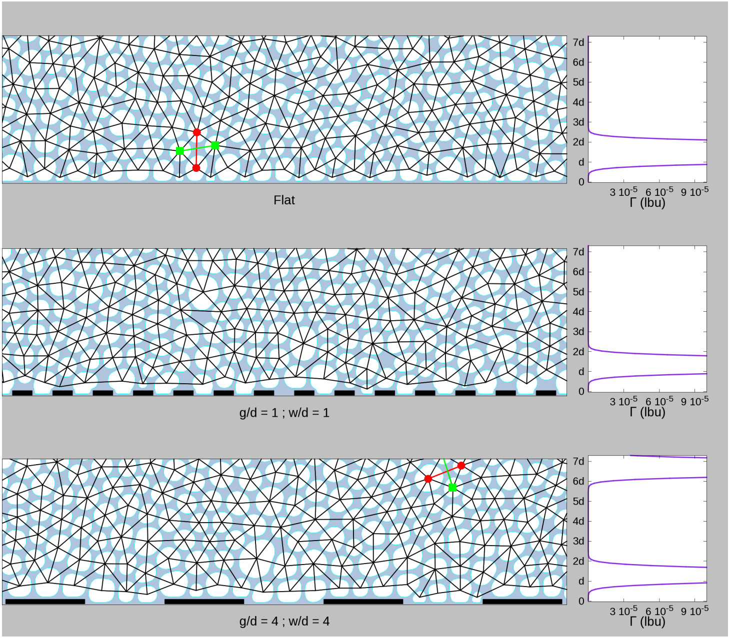
Very Different Load Conditions

$$\frac{\Delta v_{\text{slip}}}{v_{\text{plug}}}$$

Experimental data scale on **two master curves**
Wide Gaps - Narrow Gaps

*L. Derzsi, D. Filippi, ML, G. Mistura, M. Bernaschi, P. Garstecki, M. Sbragaglia & M. Pierno (under review *Soft Matt.*)

Controlled Fluidization: Numerical Results



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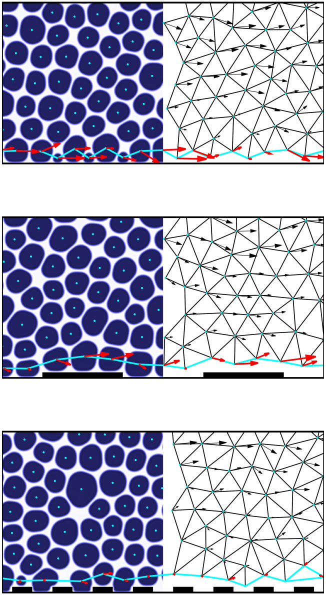
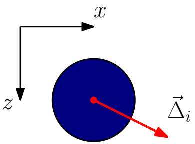
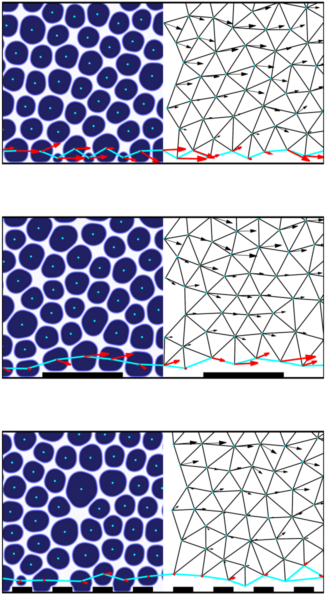


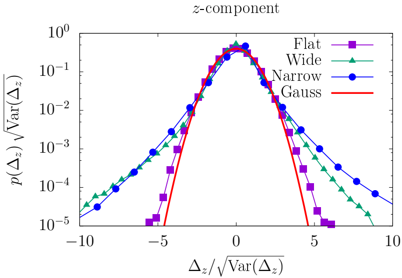
More information from Boundary Dynamics
Droplets **Displacements**...

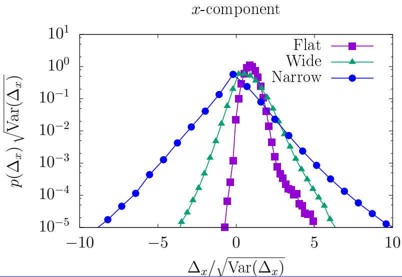


...at the **topological Boundary**
(no need to specify height cutoff...)

Controlled Fluidization: Numerical Results





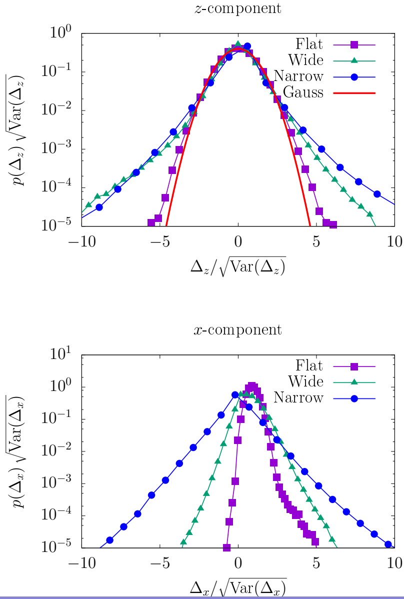


Controlled Fluidization: Numerical Results

Trapped vs. **Get-in-Get-out**

Very different boundary displacements statistics

First ab initio study of fluctuations

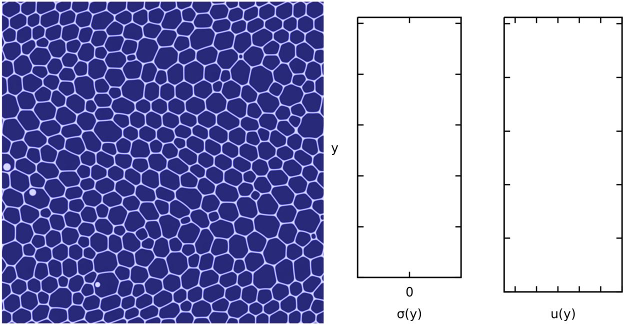


Yield-stress transition*: Numerical Setup

Fully periodic **densely packed** emulsion near the **yield-stress**

- Periodic forcing **in space** - **stress-controlled** flow - $\sigma_{\mathrm{p}} \simeq \sigma_{\mathrm{Y}}$

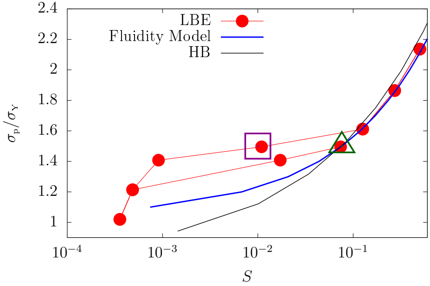
$$\sigma_{xy}(x, y) = \sigma_{\mathrm{p}} \cos\left(\frac{2\pi}{L} y\right),$$

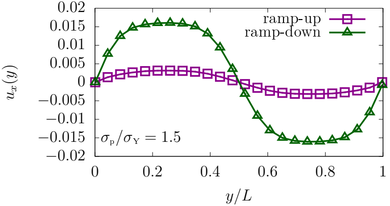


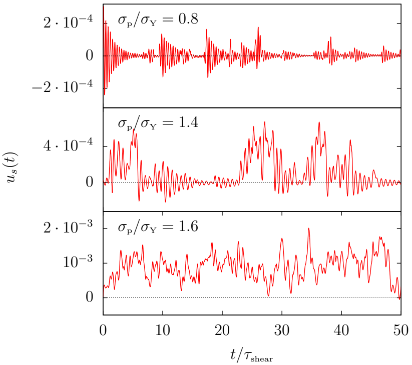
Yielding is not a stationary phenomenon!
How to characterize such behaviour?

*R. Benzi, ML & M. Sbragaglia arXiv:1710.00686 [cond-mat.soft] (under review at *PRX*)

Yield-stress transition*: Metastability and Hysteresis







Projection onto viscous profile

$$u_s(t) = \frac{1}{L}\sum_{y=0}^{L-1} u_x(y)\sin\left(\frac{2\pi}{L}y\right),$$

$$\tau_{\text{shear}} = \dot{\gamma}^{-1}$$

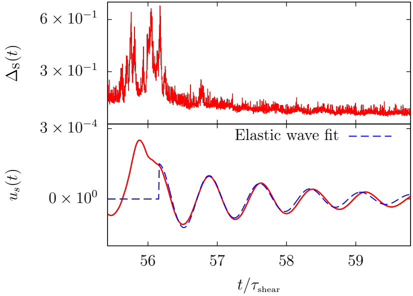
Elastic waves hamper u_s signal, let's look at **displacements**...

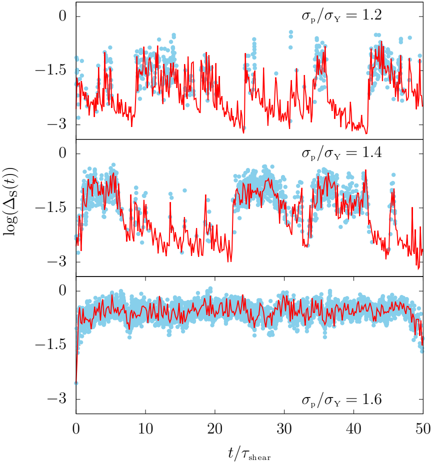
* R. Benzi, ML & M. Sbragaglia arXiv:1710.00686 [cond-mat.soft] (under review at *PRX*)

Yield-stress transition*: Displacements Analysis

Flow properties linked to droplets displacements: $\vec{\Delta}_i = \vec{x}_i(t) - \vec{x}_i(t - \delta t)$,

- We are interested in extreme events $\Delta_{\mathsf{S}}(t) \equiv \sup_i |\vec{\Delta}_i(t)|$,



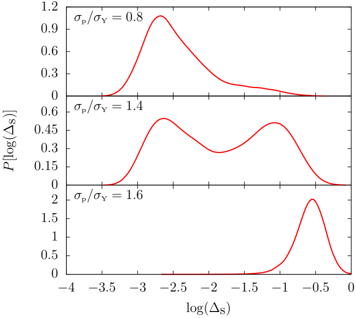


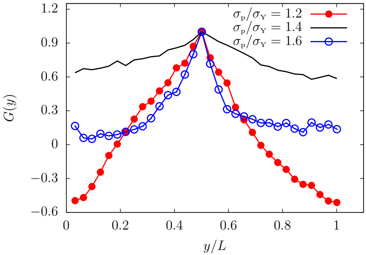
- Take the log to tame intermittency...

Clear link to plastic events! (blue dots)

*R. Benzi, ML & M. Sbragaglia arXiv:1710.00686 [cond-mat.soft] (under review at *PRX*)

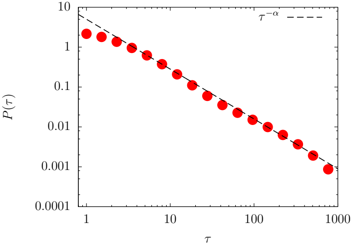
Yield-stress transition: Bimodality and Correlations





Results robust for realistic flows

- Repeated transitions in time from solid to fluid phase and back
- Bimodal probability distribution for $\log(\Delta_S)$
- Qualitatively different from stick-slip (!)



- **Largest correlations** (dynamic heterogeneities) at bimodality
- Trapping time with power-law distribution (as in sheared p-spin glasses)

Conclusions & Perspectives

Controlled Fluidization[a]

[a] L. Derzsi, D. Filippi, G. Mistura, M. Pierno, ML, M. Sbragaglia, M. Bernaschi & P. Garstecki, *Phys. Rev. E*, **95**, 052602 (2017) + (under review *Soft Matt.*)

1) First systematic experimental study of wall roughness
2) Scaling law for fluidization as λ^{-1}
3) According to g: **Trapped** vs. **Get-in-get-out**
4) First *ab initio* characterization of droplets dynamics fluctuations
5) Study the interplay between boundary and elasticity

Yield-stress transistion[b]

[b] R. Benzi, ML & M. Sbragaglia arXiv:1710.00686 [cond-mat.soft] (under review at *PRX*)

1) In a stress-driven flow **yielding** is **not stationary**
2) System **intermittently tunnels** from a solid to a fluid phase and back
3) Largest Dynamic Heterogeneity & power-law trapping time distribution at bimodality
4) Close relation to mean-field spin glasses phenomenology

HPC research[†] and resources crucial for these results

[†] M. Bernaschi, ML & M. Sbragaglia, *Comp. Phys. Comm.*, **213**, 19 - 28 (2017)

Conclusions & Perspectives