Modelling shear jamming and fragility of concentrated suspensions

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Our goal

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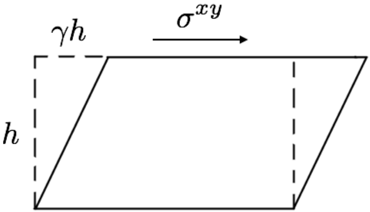
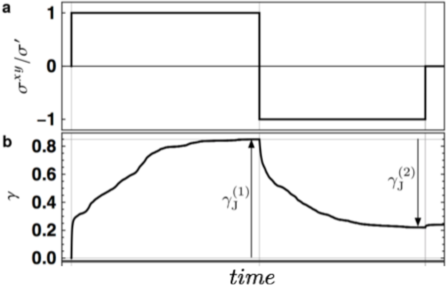
Start from experimental observations of the phenomena of **shear jamming**, **yielding**, and **viscoelasticity**

Develop a tensorial constitutive model able to capture those effects while remaining **as simple as possible**

Introduce a suitable **functional framework** for the analysis of the corresponding partial differential equations

Phenomenology of shear jamming





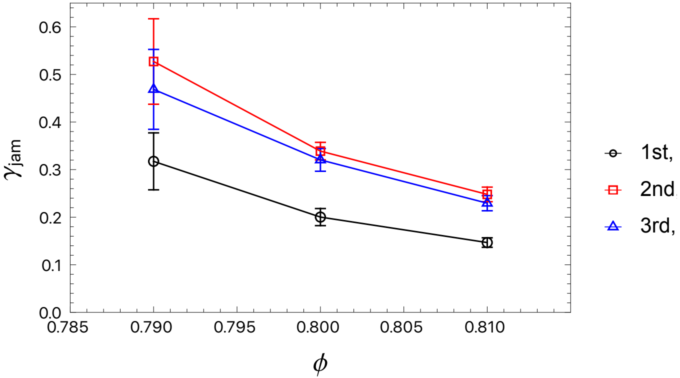
A **solidification** of the suspension that occurs under a simple shear deformation after a certain strain.

The constant traction applied to the suspension is **balanced** by the solid-like response of the jammed medium.

If we reverse the traction the suspension flows again and stops after some time: the jammed state is **fragile**.

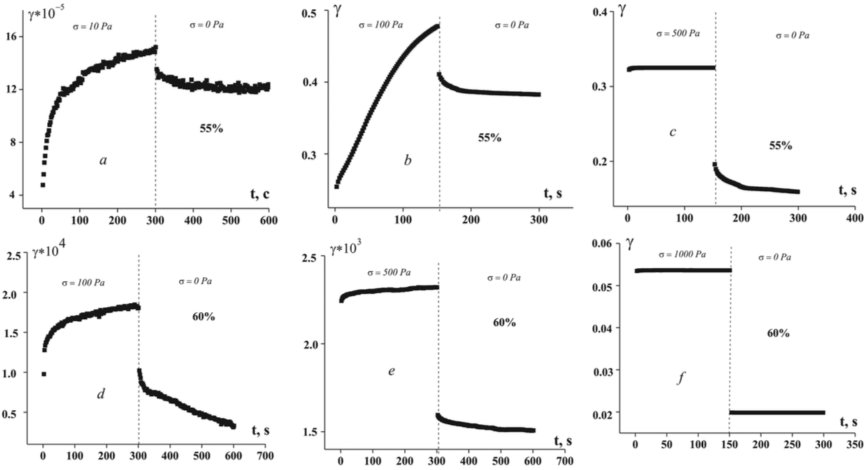
Figure from Seto et al., Granular Matter 21, 2019

Fragility and boundedness of the fluid state



To reach a second jammed state after inversion of the applied traction takes usually longer, but if we iterate the inversion we reach a third jammed state in about the same strain as the second one.

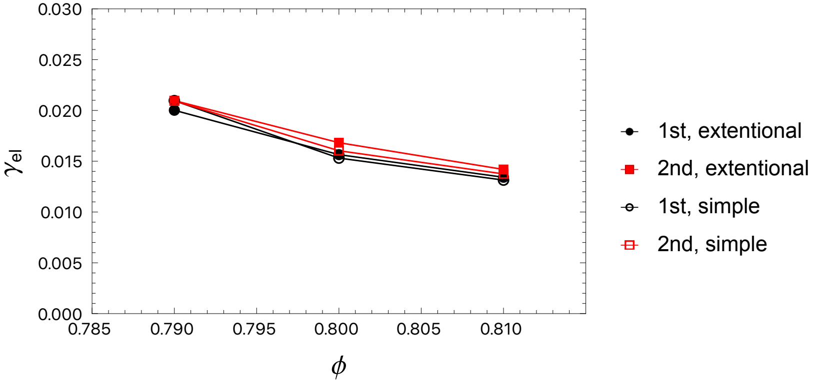
Elastic recoil



We may observe a partial elastic recoil if the traction is simply removed.

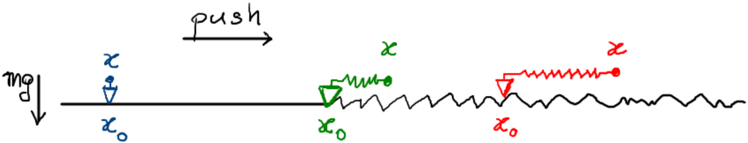
Figure from Malkin et al., J. Rheol. 64, 2020

Elastic recoil



In simulations, the elastic recoil may depend on penalization strategies, but it is also influenced by the developed microstructure.

A zero-dimensional analogue



$$m\dot{v}(t) = f_{\rm el}(x, x_0, v, v_0) + f_{\rm visc}(x, x_0, v, v_0)$$

$$\dot{x} = v(t)$$

$$x_0(t) : \begin{cases} \text{equals } x(t) \text{ in the smooth region} \\ \text{stuck on the boundary of the rough region if } |x - x_0| \le \ell^* \\ \text{follows } x(t) \text{ to reach } x(t) - \ell^* \text{ in the rough region} \end{cases}$$

Evolution equations

A crucial role in describing jamming is played by the history of the deformation that builds the suspension microstructure.

- Evolution equation for the *divergence-free* velocity field $\boldsymbol{u}$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \operatorname{div} \mathbf{T},$$

  driven by the Cauchy stress tensor $\mathbf{T}$.

- Evolution equation for the deformation gradient tensor $\mathbf{F}$ in *spatial coordinates* given by

$$\frac{\partial \mathbf{F}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\mathbf{F} = (\nabla \boldsymbol{u})\mathbf{F}.$$

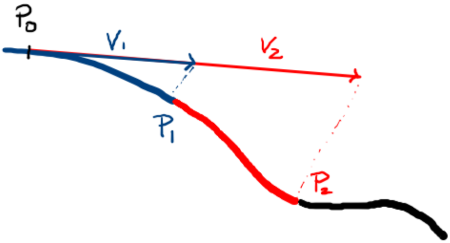
The tensor $\mathbf{F} = \nabla \chi$ is the gradient of the mapping that sends positions of material points at time zero into their position at time t.

Generalized forces on nonlinear state spaces

State space is a manifold $\Longrightarrow$ must distinguish points and tangent vectors

Generalized velocities and forces belong to tangent spaces

Exponential and logarithm connect tangent vectors to geodesic paths



Logarithmic measure of strain I

We can construct a tensorial measure of the local strain by setting

$$\mathbf{F} = \mathbf{V}\mathbf{R}, \qquad \mathbf{B} = \mathbf{F}\mathbf{F}^{\mathsf{T}} = \mathbf{V}^2 \quad \text{and} \quad \mathbf{L} = \frac{1}{2}\log \mathbf{B} = \log \mathbf{V}$$

where log denotes the matrix logarithm. This is well defined because the left Cauchy–Green tensor **B** is symmetric and positive definite.

L is the Eulerian counterpart of the Hencky strain, with the characteristic of neglecting rigid rotations.

Evolution equation for **B** in *spatial coordinates* given by

$$\frac{\partial \mathbf{B}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\mathbf{B} = (\nabla \boldsymbol{u})\mathbf{B} + \mathbf{B}(\nabla \boldsymbol{u})^{\mathsf{T}}.$$

Logarithmic measure of strain II

For an incompressible material, **F** and **B** live on manifolds determined by the nonlinear constraints $\det \mathbf{F} = 1$ and $\det \mathbf{B} = 1$.

We use the matrix logarithm to obtain local coordinates in a linear space for points on the manifold of **B**: the space of traceless tensor fields, since

$$\det(e^{\mathbf{A}}) = e^{\mathrm{tr}\,\mathbf{A}}.$$

Defining

$$\mathcal{C}[\mathbf{M}] := \int_0^T \int_\Omega (\det \mathbf{M} - 1),$$

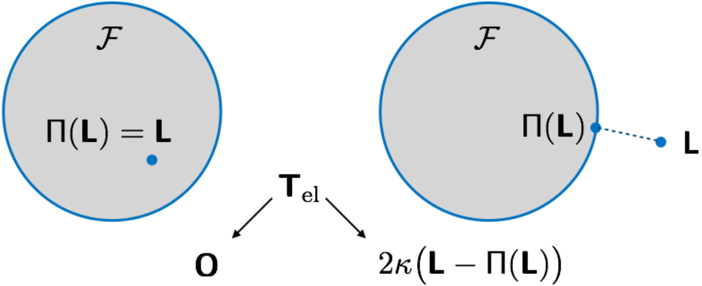
we obtain that **B** evolves on the manifold of isochoric strains since

$$\langle \delta\mathcal{C}[\mathbf{B}], \nabla \boldsymbol{u}\mathbf{B} + \mathbf{B}\nabla \boldsymbol{u}^{\mathsf{T}} \rangle = \int_0^T \int_\Omega \mathrm{tr}\left(\mathbf{B}^{-1}(\nabla \boldsymbol{u}\mathbf{B} + \mathbf{B}\nabla \boldsymbol{u}^{\mathsf{T}})\right) = \int_0^T \int_\Omega 2\,\mathrm{tr}(\nabla \boldsymbol{u}).$$

Unilateral soft constraint

$\mathcal{F}$: region *in the space of strains* within which the material is fluid

Elastic response proportional to how far is $\mathbf{L}$ from the fluid region



$\Pi_{r,\mathbf{L}_0}$: Projection onto $\mathcal{F}$

We take $\mathcal{F}$ as a ball of radius $r > 0$, a material parameter describing how much we can deform before jamming occurs, and centered at $\mathbf{L}_0 = \mathbf{0}$.

Constitutive prescriptions

We assume the following form for the Cauchy stress:

$$\mathbf{T} = -p\mathbf{I} + 2\eta\mathbf{D} + \mathbf{T}_{\mathrm{el}} = -p\mathbf{I} + 2\eta\mathbf{D} + 2\kappa\big(\mathbf{L} - \Pi_{r,\mathbf{L}_0}(\mathbf{L})\big),$$

where the material parameter $\kappa > 0$ represents an elastic stiffness and $\eta > 0$ is an effective viscosity.

On top of the usual viscous effects, an elastic response is activated whenever the logarithmic measure of strain $\mathbf{L}$ leaves the region $\mathcal{F}$.

It is important to observe that $\mathbf{T}_{\mathrm{el}}$ is generally **not aligned** with $\mathbf{D}$.

The value of κ can be estimated from the elastic recoil, while the value of r from the strain between to jammed states obtained by shearing in opposite directions.

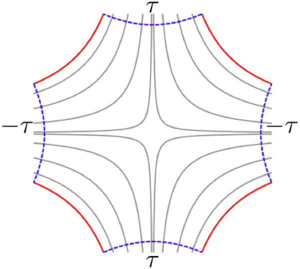
Extensional flow

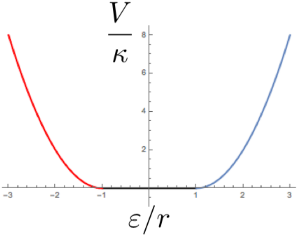
$$\mathbf{F} = \begin{pmatrix} e^{\varepsilon(t)} & 0 \\ 0 & e^{-\varepsilon(t)} \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} \varepsilon(t) & 0 \\ 0 & -\varepsilon(t) \end{pmatrix}$$

$$\boldsymbol{u} = (\dot{\varepsilon}(t)x, -\dot{\varepsilon}(t)y),$$

$$\mathbf{D} = \begin{pmatrix} \dot{\varepsilon}(t) & 0 \\ 0 & -\dot{\varepsilon}(t) \end{pmatrix}$$

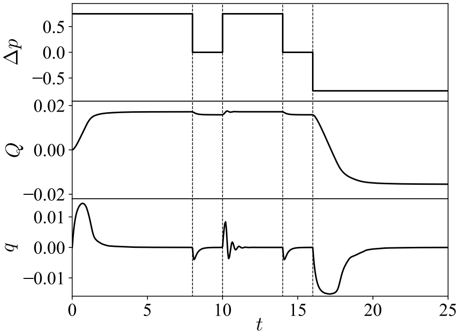




The linearized equations governing the motion are

$$\frac{\rho\ell^2}{2}\ddot{\varepsilon}(t) + 2\eta\dot{\varepsilon}(t) - \tau = \begin{cases} -2\kappa[\varepsilon(t) + r] & \text{if } \varepsilon < -r \\ +0 & \text{if } -r \le \varepsilon \le r \\ -2\kappa[\varepsilon(t) - r] & \text{if } \varepsilon > r \end{cases}$$

Clogging and unclogging in pressure driven flows



By driving the pressure difference we observe shear jamming in a contraction.

Intensity of the elastic response proportional to $\lambda = \|\mathbf{L} - \Pi(\mathbf{L})\|$.

Giusteri & Seto, *Phys. Rev. Lett.* 127, 138001 (2021)

A viscoelastic solid model

By setting $r = 0$ the elastically neutral region reduces to a point. We get

$$\mathbf{T} = -p\mathbf{I} + 2\eta\mathbf{D} + \kappa \log \mathbf{B}.$$

Evolution equations with $\det \mathbf{B} = 1$ and $\operatorname{div} \boldsymbol{u} = 0$:

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \eta \Delta \boldsymbol{u} + \kappa \operatorname{div} \log \mathbf{B},$$

$$\frac{\partial \mathbf{B}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\mathbf{B} = (\nabla \boldsymbol{u})\mathbf{B} + \mathbf{B}(\nabla \boldsymbol{u})^{\mathsf{T}}.$$

We introduce $\mathcal{M} := \{\mathbf{M} \in \mathrm{Mat}_d(\mathbb{R}) : \mathbf{M}^{\mathsf{T}} = \mathbf{M}, \operatorname{tr} \mathbf{M} = 0\}$ and

$$\mathcal{B}_T := \left\{ \begin{array}{c} \mathbf{B} : [0, T] \times \Omega \to \mathrm{Mat}_d(\mathbb{R}) : \mathbf{B} = \mathbf{B}^{\mathsf{T}},\ \det \mathbf{B} = 1, \\ \text{and } \log \mathbf{B} \in L^2([0, T] \times \Omega; \mathcal{M}) \cap L^\infty([0, T]; L^2(\Omega; \mathcal{M})) \end{array} \right\}$$

Solutions for the tensorial transport equation I

Definition. Let H and V denote the spaces of divergence-free L^2 and H^1 functions. Given $\boldsymbol{u} \in L^\infty([0,T];H) \cap L^2([0,T];V)$ and $\mathbf{B}_0 \in \mathcal{B}$, we say that $\mathbf{B} \in \mathcal{B}_T$ is a *charted weak solution* of the corresponding transport equation with initial datum $\mathbf{B}_0$ if there exist two sequences $\{\boldsymbol{u}_k\}$ and $\{\log \mathbf{B}_{0,k}\}$ of smooth fields that satisfy

- $\boldsymbol{u}_k \overset{*}{\rightharpoonup} \boldsymbol{u}$ in $L^\infty([0,T];H) \cap L^2([0,T];V)$,
- $\log \mathbf{B}_{0,k} \rightharpoonup \log \mathbf{B}_0$ in $L^2(\Omega;\mathcal{M})$,

and such that the corresponding sequence of smooth solutions $\{\mathbf{B}_k\}$ with advecting field $\boldsymbol{u}_k$ and initial condition $\mathbf{B}_{0,k}$ satisfies

$$\log \mathbf{B}_k \overset{*}{\rightharpoonup} \log \mathbf{B} \quad \text{in } L^\infty([0,T];L^2(\Omega;\mathcal{M})).$$

We say that $\mathbf{B}$ is the limit of $\{\mathbf{B}_k\}$ with respect to the *charted weak topology* on $\mathcal{B}_T$.

Solutions for the tensorial transport equation II

Theorem. For any $\mathbf{B}_0 \in \mathcal{B}$ and $\boldsymbol{u} \in L^\infty([0,T];H) \cap L^2([0,T];V)$ there exists a charted weak solution $\mathbf{B} \in \mathcal{B}_T$ of the related transport equation, which satisfies

$$\|\log \mathbf{B}\|_{L^\infty([0,T];L^2)} \leq 16T\|\nabla \boldsymbol{u}\|_{L^2([0,T];L^2)} + 2\|\log \mathbf{B}_0\|_{L^2}.$$

Moreover, if the sequence $\{\boldsymbol{u}_k\}$ that defines the solution is such that

$$\nabla \boldsymbol{u}_k \to \nabla \boldsymbol{u}, \quad \text{in } L^1_{\mathrm{loc}}((0,T)\times\Omega),$$

then the charted weak solution is unique and it satisfies,
for a.e. $(t,x) \in (0,T)\times\Omega$, the formula

$$\mathbf{B}(t,x) = e^{\int_0^t \nabla \boldsymbol{u}(s,\boldsymbol{\Phi}(s,t,x))ds}\mathbf{B}_0(\boldsymbol{\Phi}(0,t,x))e^{\int_0^t \nabla \boldsymbol{u}^\mathsf{T}(s,\boldsymbol{\Phi}(s,t,x))ds},$$

with $\boldsymbol{\Phi}(s,t,x)$ a regular Lagrangian flow associated with $\boldsymbol{u}$.

Key *a priori* estimates

We multiply the evolution equation with smooth $\boldsymbol{u}_k$ by $\mathbf{B}_k^{-1} \log \mathbf{B}_k$ and integrate to get

$$\frac{d}{dt} \| \log \mathbf{B}_k \|_{L^2}^2 + \int_\Omega (\boldsymbol{u}_k \cdot \nabla)(\log \mathbf{B}_k : \log \mathbf{B}_k)$$
$$= 2 \int_\Omega \nabla \boldsymbol{u}_k : \log \mathbf{B}_k \leq \frac{1}{\varepsilon} \| \nabla \boldsymbol{u}_k \|_{L^2}^2 + \varepsilon \| \log \mathbf{B}_k \|_{L^2}^2,$$

from which

$$\| \log \mathbf{B}_k(t, \cdot) \|_{L^2}^2 \leq \frac{1}{\varepsilon} \| \nabla \boldsymbol{u}_k \|_{L^2([0,T];L^2)}^2 + \varepsilon \| \log \mathbf{B}_k \|_{L^2([0,T];L^2)}^2 + \| \log \mathbf{B}_{0,k} \|_{L^2}^2,$$

$$(1 - \varepsilon T) \| \log \mathbf{B}_k \|_{L^2([0,T];L^2)}^2 \leq \frac{T}{\varepsilon} \| \nabla \boldsymbol{u}_k \|_{L^2([0,T];L^2)}^2 + T \| \log \mathbf{B}_{0,k} \|_{L^2}^2.$$

Solutions for the viscoelastic solid problem

By Galerkin approximation and fixed-point arguments we can prove the global-in-time existence of solutions for the coupled evolution of the velocity field $\boldsymbol{u}$ and the tensor $\mathbf{B}$, with $\boldsymbol{u} \in L^\infty([0,T];H) \cap L^2([0,T];V)$ of Leray type and $\mathbf{B} \in \mathcal{B}_T$ a charted weak solution of the transport equation.

The pair $(\boldsymbol{u}, \mathbf{B})$ satisfies, for almost every $t \in [0,T]$, the energy inequality

$$\rho\|\boldsymbol{u}(t,\cdot)\|_{L^2}^2 + \frac{\kappa}{2}\|\log \mathbf{B}(t,\cdot)\|_{L^2}^2 + 2\eta\int_0^t \|\nabla \boldsymbol{u}(s,\cdot)\|_{L^2}^2\, ds \\ \leq \rho\|\boldsymbol{u}_0\|_{L^2}^2 + \frac{\kappa}{2}\|\log \mathbf{B}_0\|_{L^2}^2.$$

The balance between the estimates on $\boldsymbol{u}$ and on $\log \mathbf{B}$ is crucial

We cannot deal directly with $\mathbf{B}$ in a linear space setting

Take-home messages

We defined a local tensorial model with the following features:

- It represents materials able to switch, reversibly, between a fluid-like and a solid-like behavior, capturing shear jamming and fragility
- It is not developed by fitting data in a restricted set of geometries, and can thus be applied to generic flows.

Addressing tensorial transport equations is required:

- Tensor fields involved in describing the elastic (and plastic) response of the material typically belong to nonlinear manifolds
- Logarithmic strains allow to cast in a linear setting the analytical results and obtain global-in-time existence of solutions

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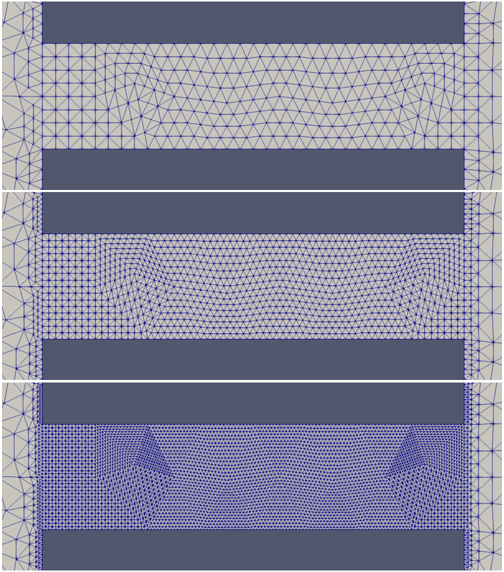
Thanks for your attention . . .

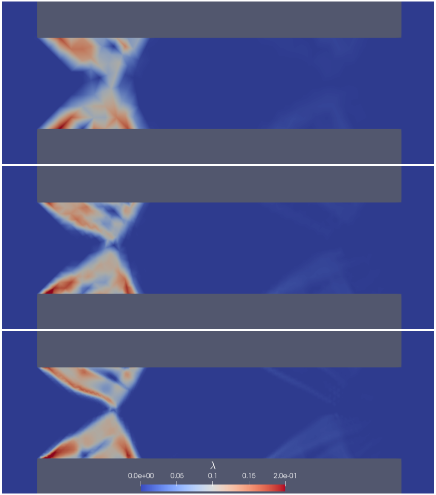
. . . and questions are welcome!

Shape of jammed domains: mesh refinement

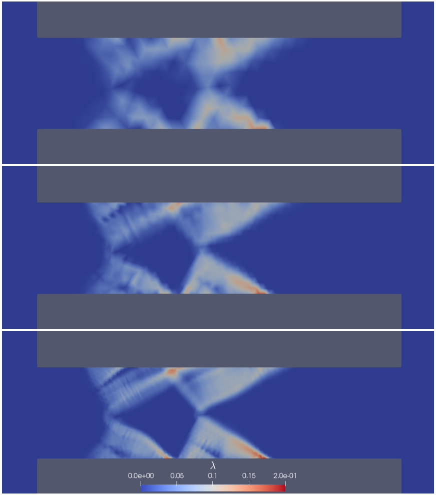


Shape of jammed domains

Jamming at $t = 8$ s

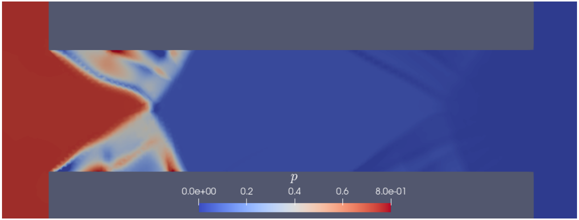


Jamming at $t = 25$ s



Shape of jammed domains: uniform-pressure basins

Pressure at $t = 8$ s



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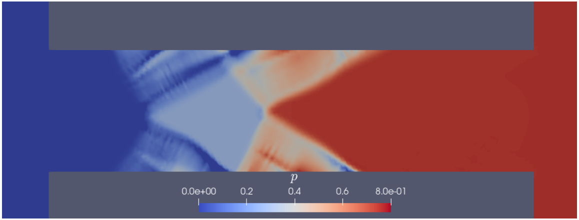
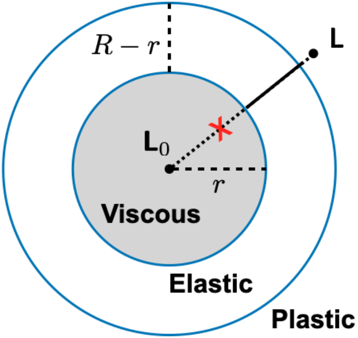


Yielding at high stress

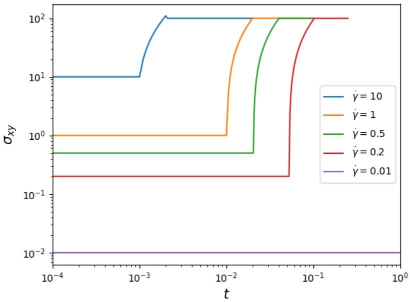
At high stresses, the granular component of the jammed suspension can undergo plastic reorganization, producing a plastic flow.

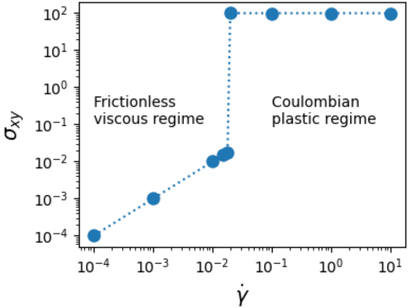
In the context of shear jamming, plasticity can be represented by an evolution of the center $\mathbf{L}_0$ of the elastically neutral region.



Rate-dependent behavior: Discontinuous Shear Thickening

In the fluid regime $\mathbf{B}_0$ and $\mathbf{B}$ are aligned and the eigenvalues β_0 of $\mathbf{B}_0$ follow those of $\mathbf{B}$ via: $\frac{\partial}{\partial t}\ln\beta_0 + (\boldsymbol{u}\cdot\nabla)\ln\beta_0 = \frac{2}{\tau_r}\left(\ln\beta - \ln\beta_0\right)$





Rate-controlled simulation of simple shear flow. Parameters: $\kappa = 10^4$, $r = R - r = 10^{-2}$, ρ, η, τ_r and channel width are set equal to unity.