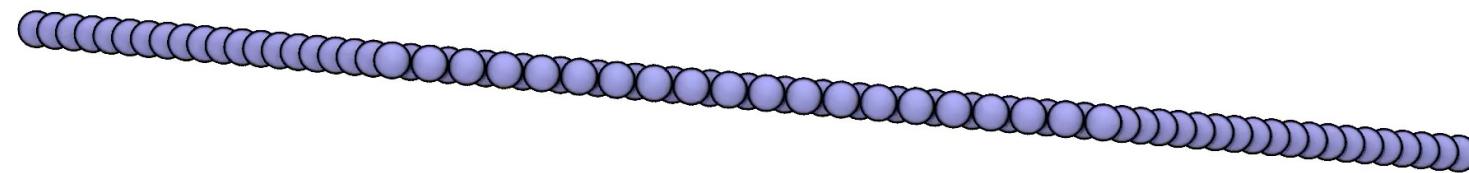


Buckling, Crumpling, and Tumbling of Semiflexible Sheets in Simple Shear Flow



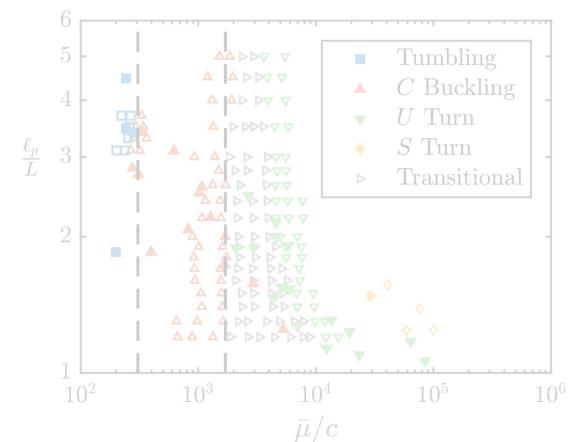
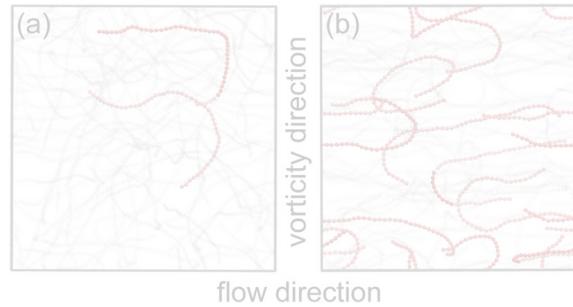
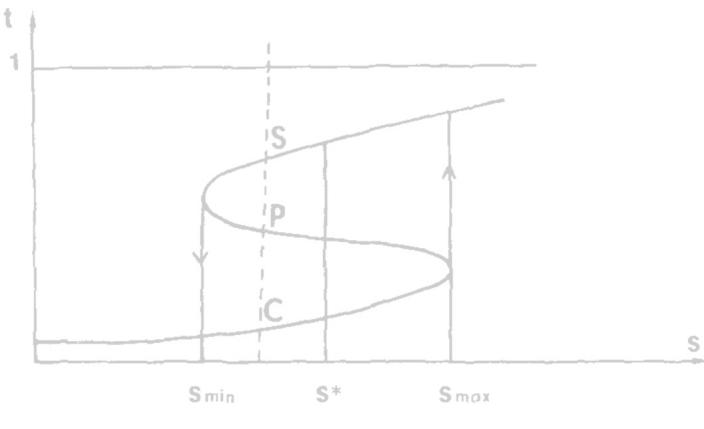
Kevin Silmore
Michael Strano
James Swan
July 19, 2021



Fluid-structure interactions are prevalent in soft matter



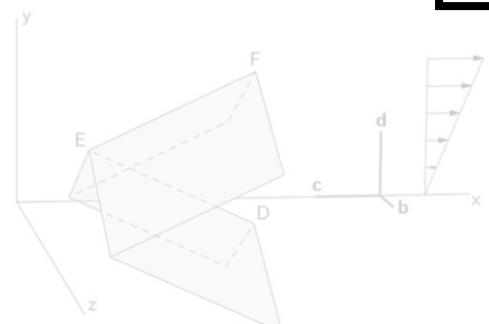
M. Harasim et al., Phys. Rev. Lett. **110**, 108302 (2013).



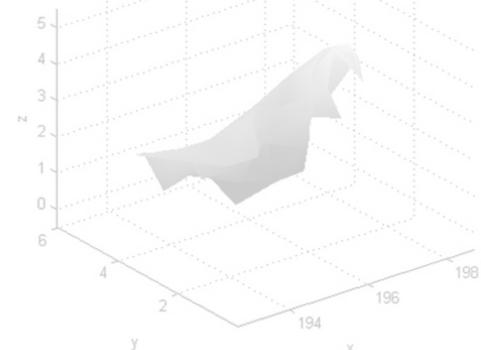
iu et al., PNAS **115**, 9438 (2018).

What do 2D sheets do when subjected to shear flow at low Reynolds number?

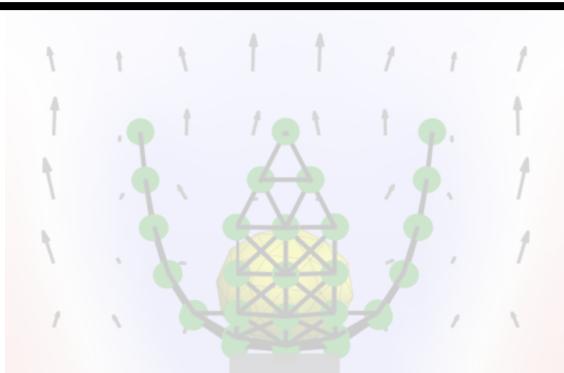
$$\text{Re} = \frac{\rho U L}{\eta} \ll 1$$



S. Dutta and M. D. Graham, Soft Matter **13**, 2620 (2017).



Y. Xu and M. J. Green, J. Chem. Phys. **141**, 024905 (2014).

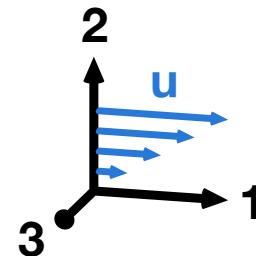
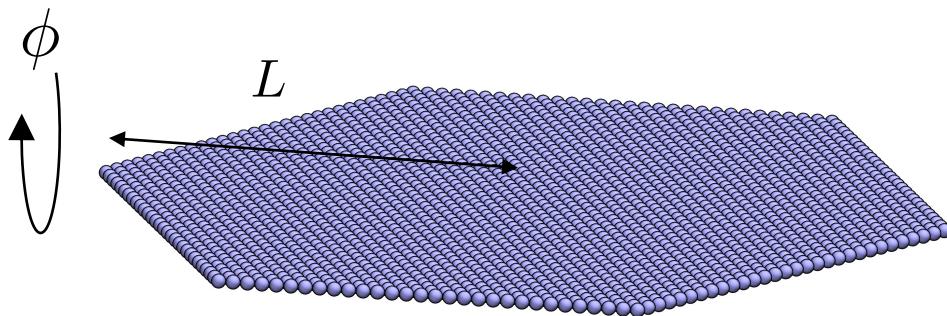


A. Laskar et al., Sci. Adv. **4**, eaav1745 (2018).



F. Tardani et al., Langmuir **34**, 2996 (2018).

A triangulated model is constructed for thin, isotropic 2D sheets



RPY mobility matrix Shear flow

$$d\mathbf{x}_i = \left(- \sum_j \mathcal{M}_{ij} \frac{\partial U}{\partial \mathbf{x}_j} + \mathbf{Lx}_i \right) dt$$

In-plane stretching:

$$U_{\text{bond}}(r) = \frac{k}{2}(r - r_0)^2$$

Out-of-plane bending:

$$U_{\text{bend}}(\Delta_i, \Delta_j) = \kappa(1 - \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j)$$

Hard-sphere repulsion:

$$U_{\text{HS}}(r) = \begin{cases} \frac{16\pi\eta a^2 [2a \ln(\frac{2a}{r}) + (r - 2a)]}{\Delta t} & 0 \leq r \leq 2a \\ 0 & r > 2a \end{cases}$$

Bending soft relative to stretching

$$FvK = \frac{kL^2}{\kappa} > 10^4$$

$$S = \frac{\kappa}{\pi\eta\dot{\gamma}L^3}$$

D. M. Heyes and J. R. Melrose, J. Non-Newtonian Fluid Mech. **46**, 1 (1993).

G. Gompper and D. M. Kroll, Journal de Physique I **6**, 1305 (1996).

M. J. Bowick, A. Košmrlj, D. R. Nelson, and R. Sknepnek, Phys. Rev. B **95**, 104109 (2017).

J. Rotne and S. Prager, J. Chem. Phys. **50**, 4831 (1969).

H. Yamakawa, J. Chem. Phys. **53**, 436 (1970).

Calculating the mobility matrix is challenging due to long-ranged interactions

Electrostatics

$$\epsilon \Delta \phi = -\rho_c$$

Solution for a sphere:

$$\phi(r) = \frac{Q}{4\pi\epsilon r}$$

Stokes flow

$$\begin{aligned}\eta \Delta \mathbf{u} - \nabla p &= -\mathbf{f} \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

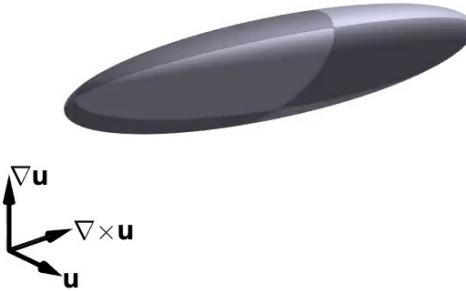
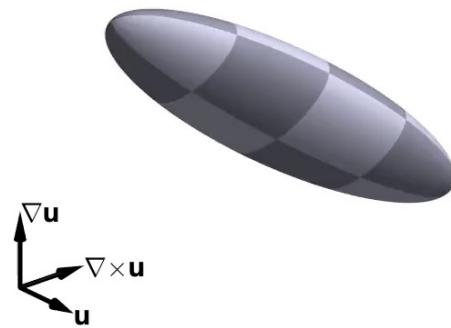
$$\mathbf{u}(\mathbf{x}) = \left(\frac{3a}{4r} \left[\mathbf{I} + \frac{\mathbf{xx}}{r^2} \right] + \frac{3a^3}{4r^3} \left[\frac{1}{3} \mathbf{I} - \frac{\mathbf{xx}}{r^2} \right] \right) \cdot \mathbf{U}$$

Pairwise interaction calculations can be accelerated on GPUs



Jeffery's equations govern the motion of ellipsoids in Stokes shear flow

$$\dot{\omega} = f(\omega, \nabla u, a_1, a_2, a_3)$$



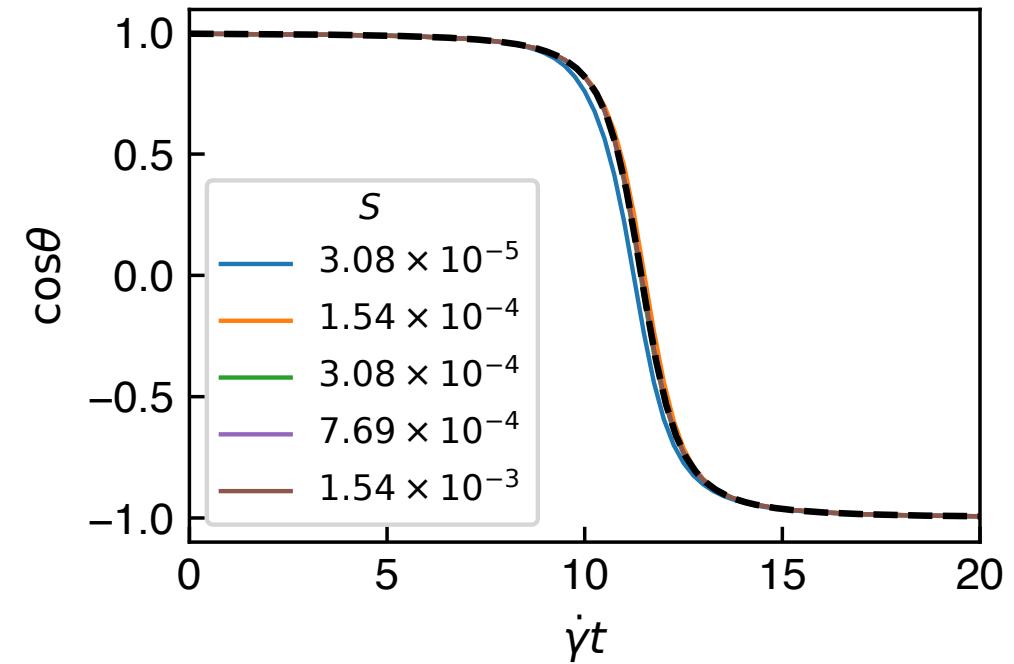
Sheet trajectories for $\phi=0^\circ$ follow Jeffery orbits

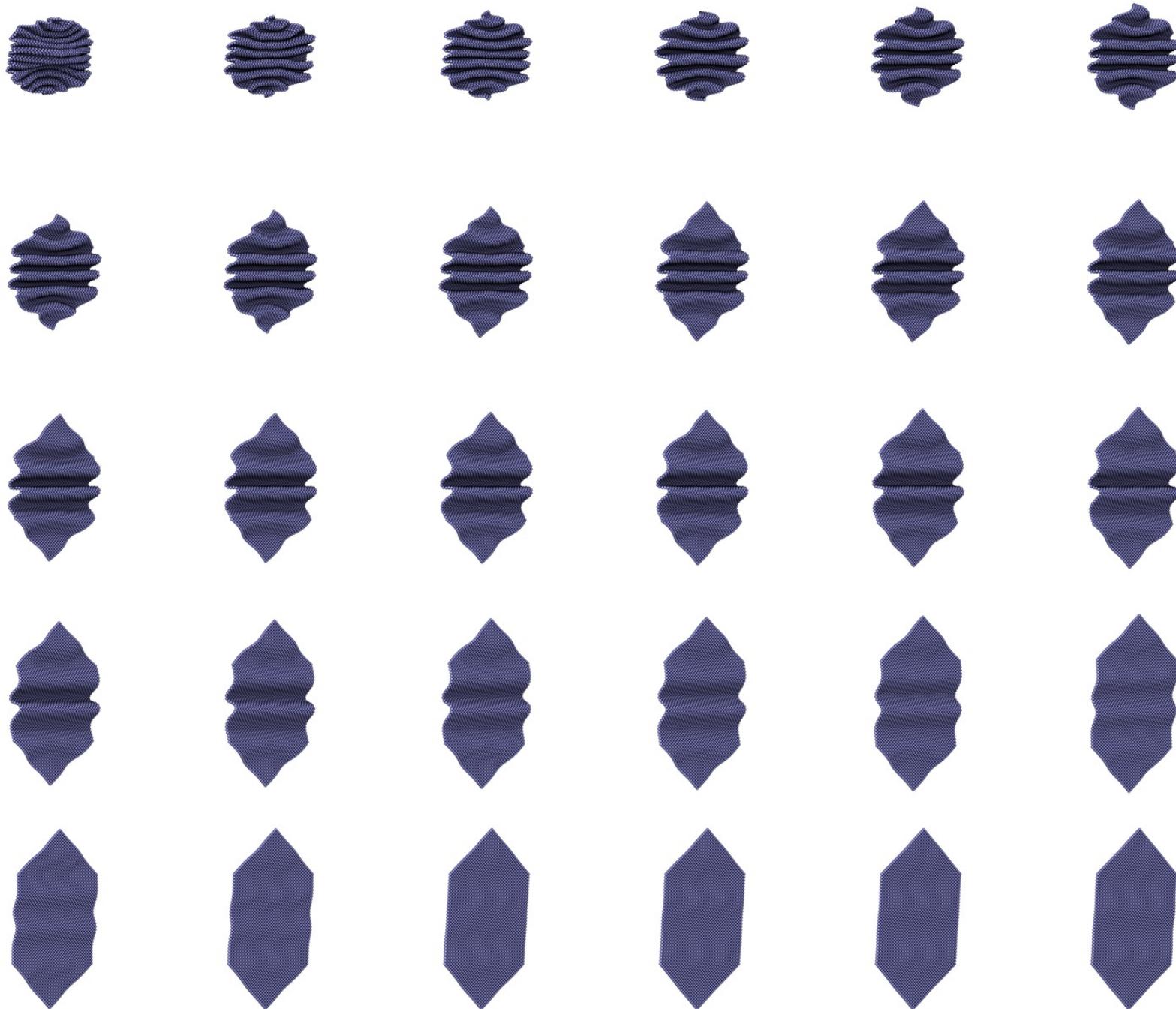
Jeffery orbit for infinitesimally thin spheroids:

$$\dot{\mathbf{p}} = \boldsymbol{\Omega}\mathbf{p} - [(\mathbf{I} - \mathbf{p}\mathbf{p}^T)(\mathbf{E}\mathbf{p})]$$

$$\begin{aligned}\boldsymbol{\Omega} &= (\mathbf{L} - \mathbf{L}^T)/2 \\ \mathbf{E} &= (\mathbf{L} + \mathbf{L}^T)/2\end{aligned}$$

$$\mathbf{L} = \nabla \mathbf{u} = \dot{\gamma} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$





Sheets exhibit
different buckling
modes for $\phi = 0^\circ$

$$\dot{\gamma}t = 11.5$$

S increasing from left to right

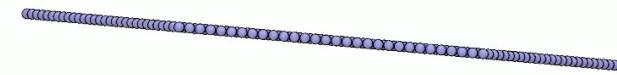
$$S = \frac{\kappa}{\pi\eta\dot{\gamma}L^3}$$

Sheets exhibit different buckling modes

$t = 0.0$

$t = 0.0$

$t = 0.0$



$$S = 3.08 \times 10^{-5}, \phi = 0^\circ$$

$$S = 6.15 \times 10^{-4}, \phi = 0^\circ$$

$$S = 3.08 \times 10^{-3}, \phi = 0^\circ$$

$$S = \frac{\kappa}{\pi \eta \dot{\gamma} L^3}$$

Buckling can be predicted with a 1D quasi-static elasticity model

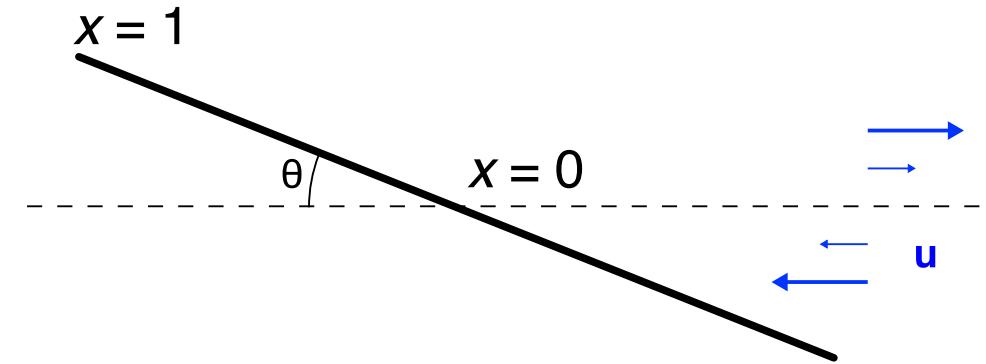
Assuming θ governed independently by Jeffery orbit

$$S \frac{d^2}{dx^2} \left(f(x) \frac{d^2 w}{dx^2} \right) = q_{\perp}(x) + q_{\parallel}(x) \frac{dw}{dx} + r_{\parallel}(x) \frac{d^2 w}{dx^2}$$

changing width out-of-plane stress in-plane stress

$w(0) = w''(0) = w''(1) = w'''(1) = 0$

symmetry at $x = 0$ free end at $x = 1$



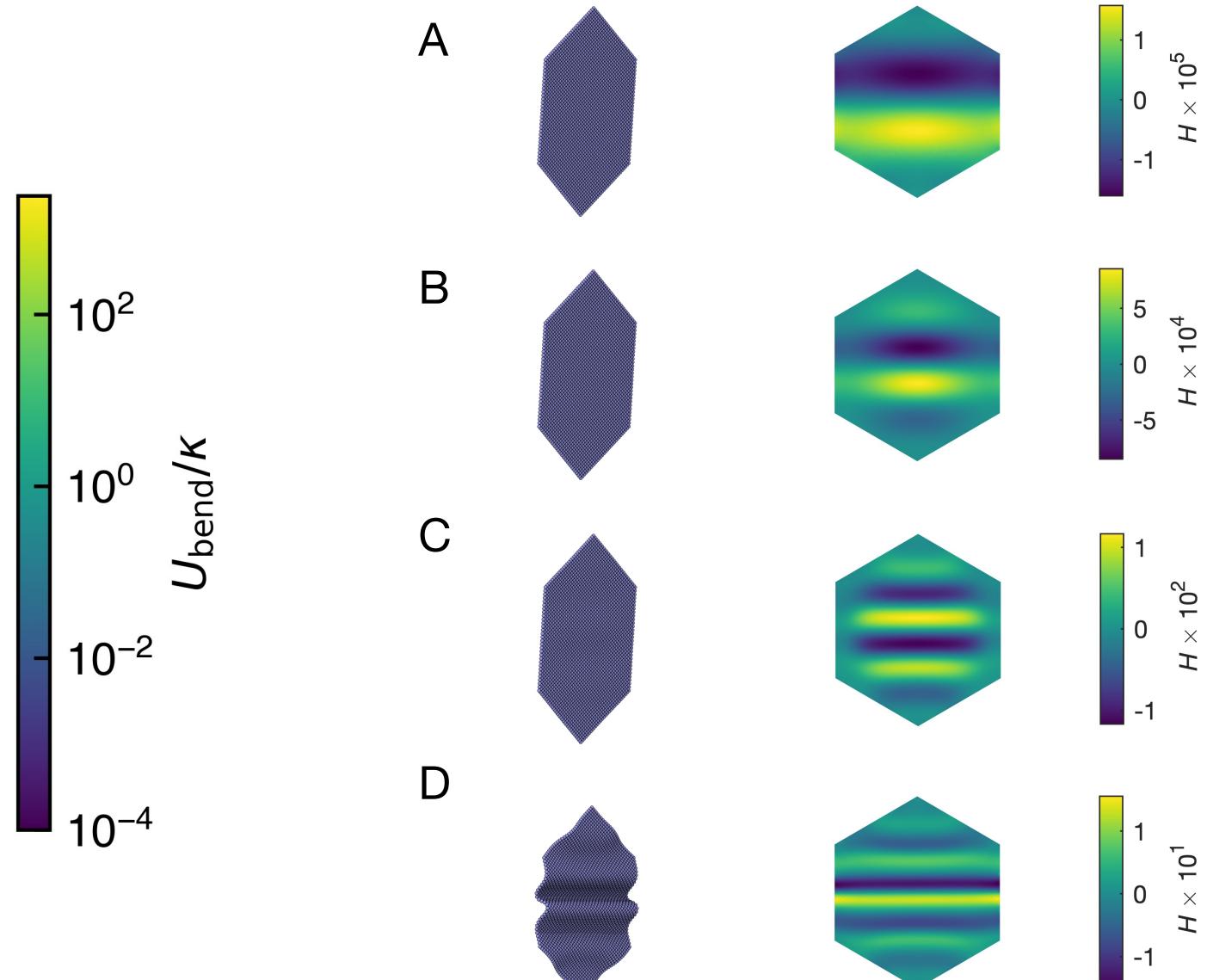
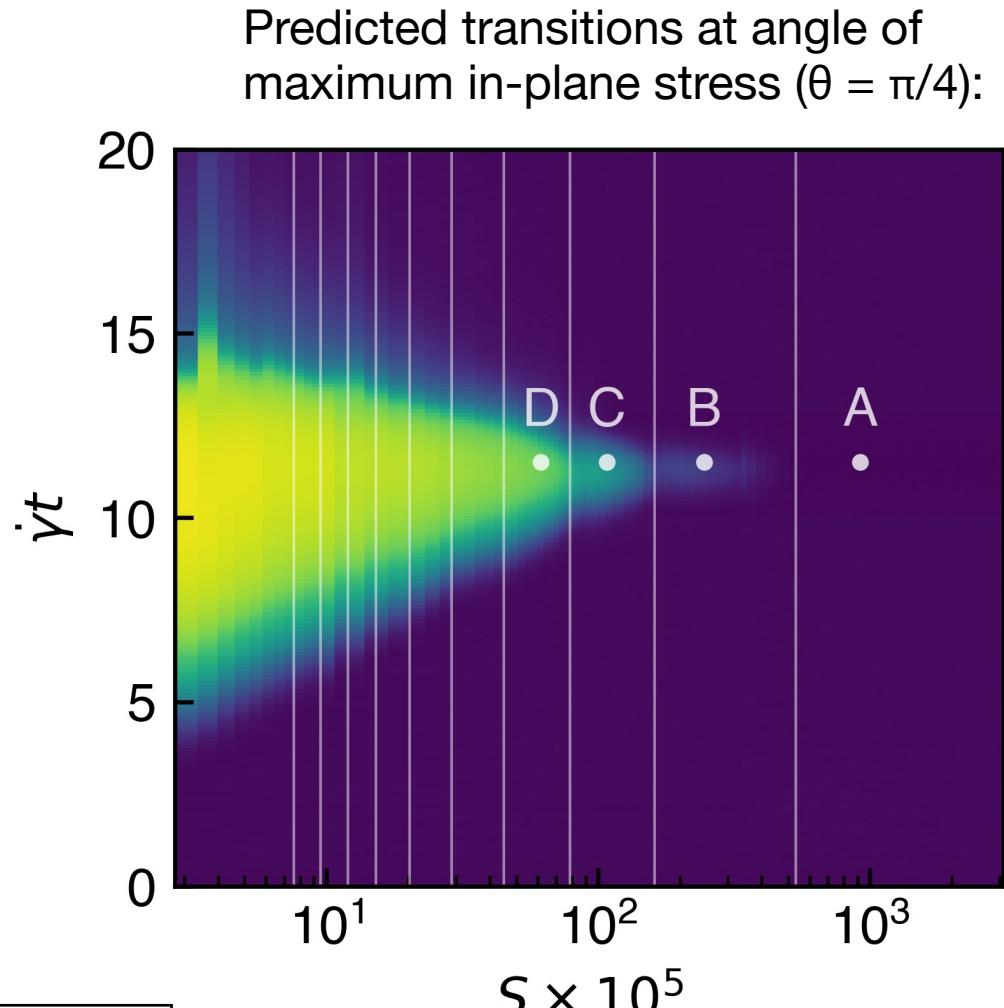
Buckling transitions from generalized eigenvalue problem of homogeneous part:

$$\mathbf{A}\mathbf{w}^h = S^{-1}\mathbf{B}\mathbf{w}^h$$

basis expansion in polynomials

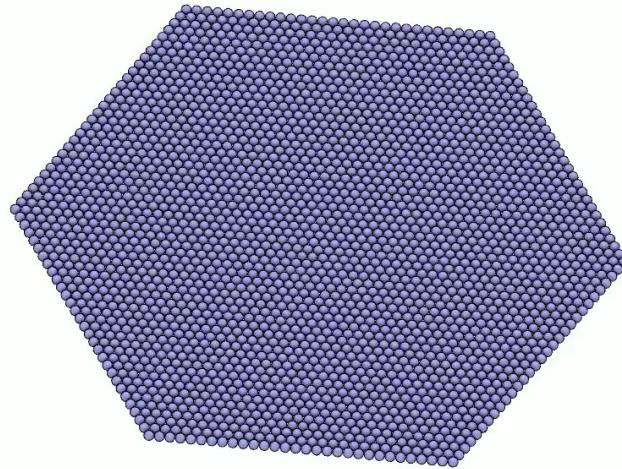
$$S = \frac{\kappa}{\pi\eta\dot{\gamma}L^3}$$

Buckling can be predicted with a 1D quasi-static elasticity model



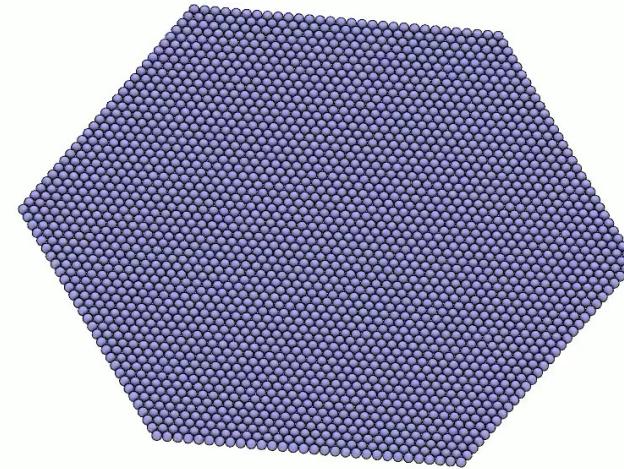
Some sheets tumble at different initial orientations

t = 0.0



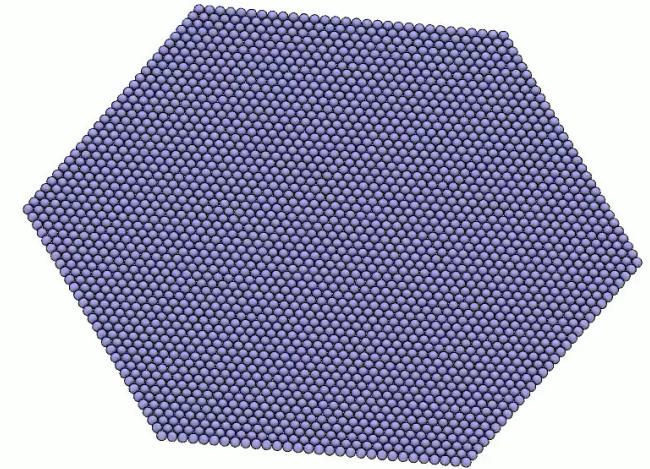
$S = 3.08 \times 10^{-5}, \phi = 54^\circ$

t = 0.0



$S = 6.15 \times 10^{-4}, \phi = 54^\circ$

t = 0.0



$S = 3.08 \times 10^{-3}, \phi = 54^\circ$

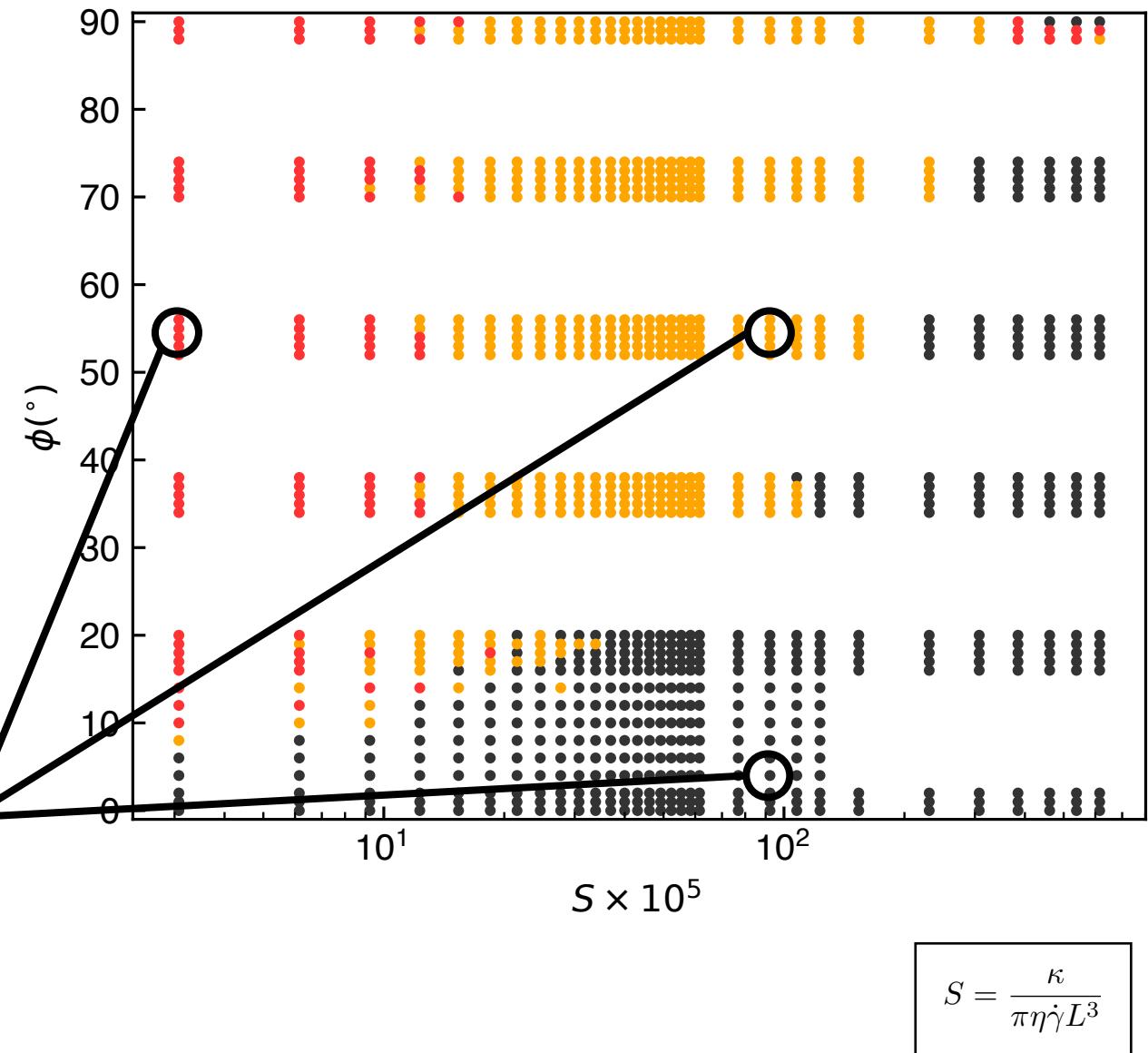
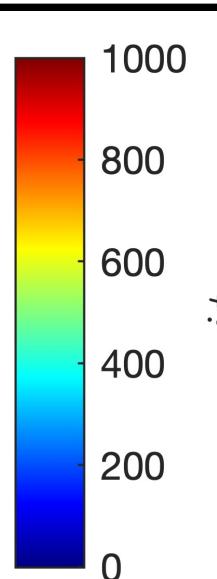
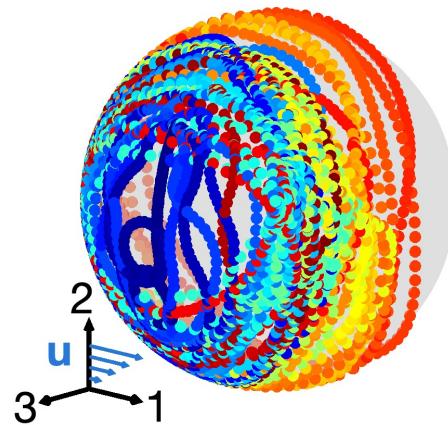
$$S = \frac{\kappa}{\pi \eta \dot{\gamma} L^3}$$

Sheets can be classified into different dynamical states

Mean orientation via Fréchet mean:

$$\bar{\mathbf{n}} = \arg \min_{\mathbf{x} \in S^2} \sum_{i \in \{\Delta\}} A_i \text{dist}(\mathbf{x}, \hat{\mathbf{n}}_i)^2$$

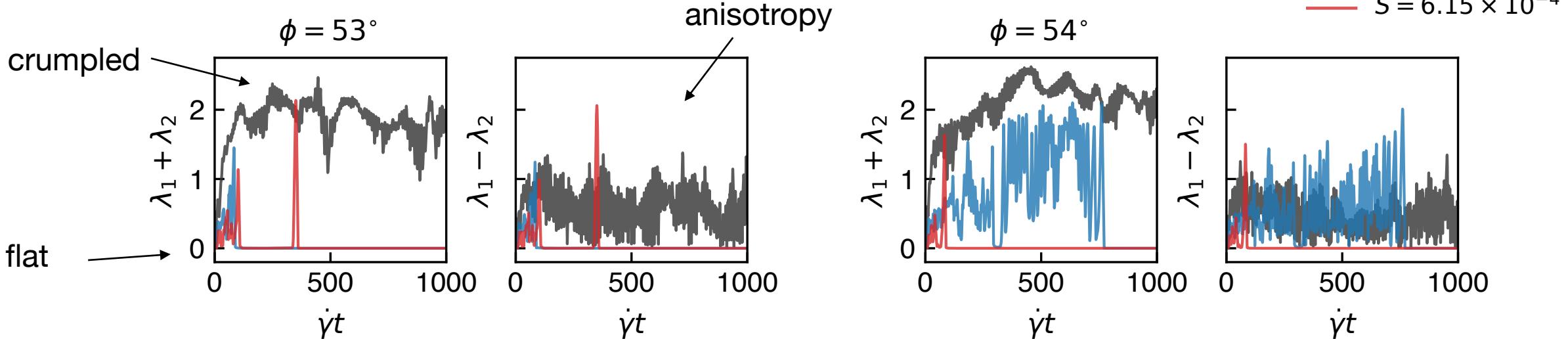
Quasi-Jeffery
Initially tumbling
Continuously tumbling



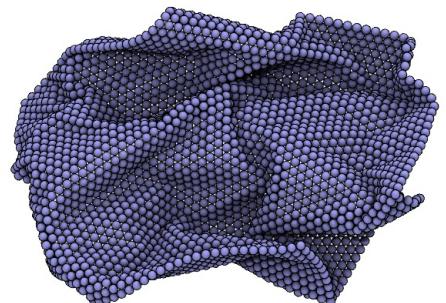
$$S = \frac{\kappa}{\pi \eta \dot{\gamma} L^3}$$

Chaos and crumpling can be characterized with covariance

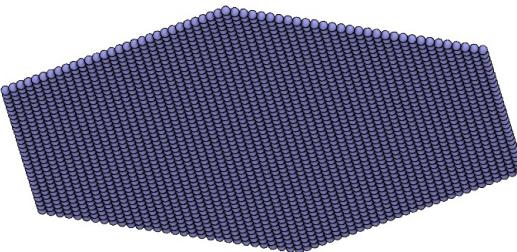
Eigenvalues of orientational covariance matrix:



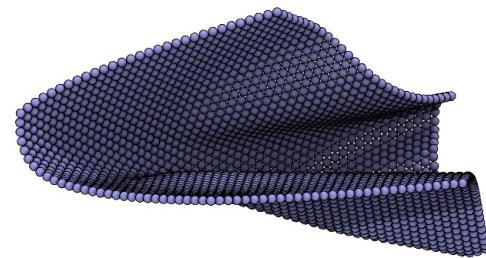
$$\lambda_1, \lambda_2 > 0$$



$$\lambda_1 = \lambda_2 = 0$$

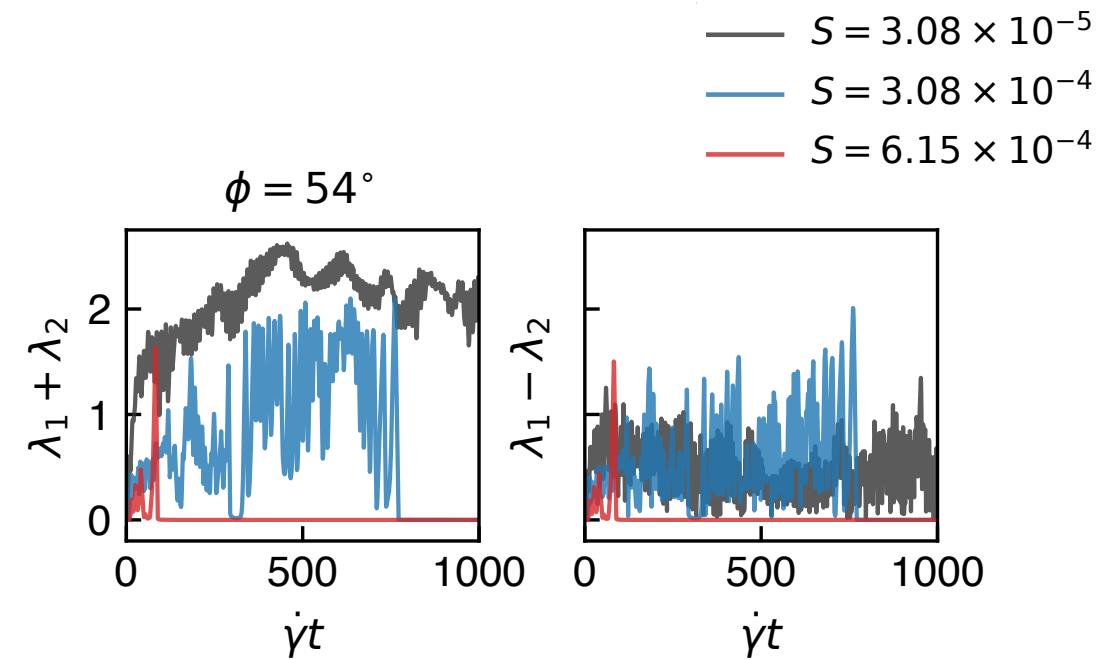
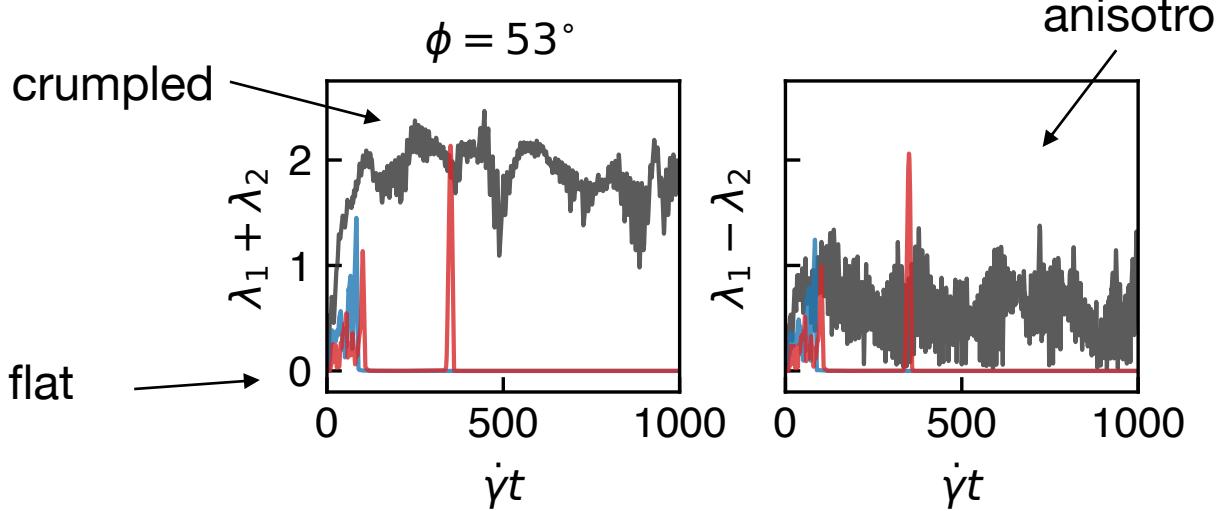


$$\lambda_1 > 0, \lambda_2 \approx 0$$



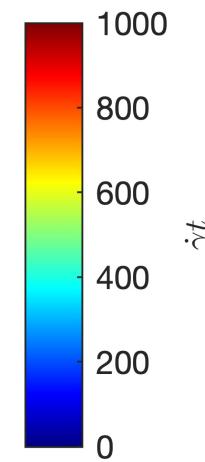
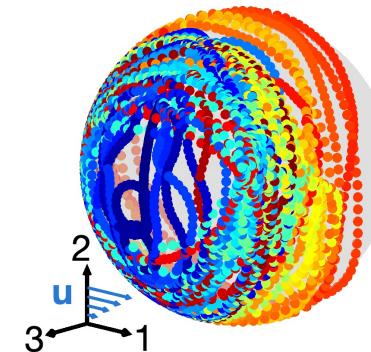
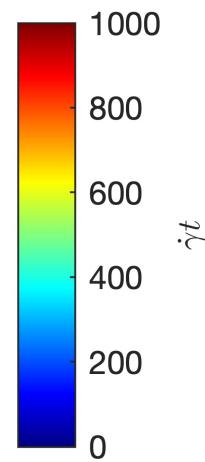
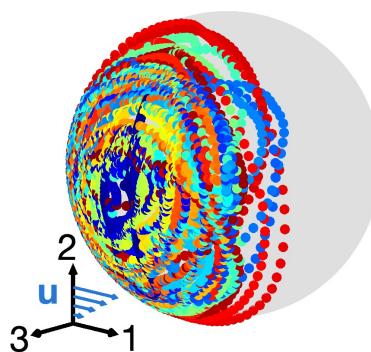
Chaos and crumpling can be characterized with covariance

Eigenvalues of orientational covariance matrix:

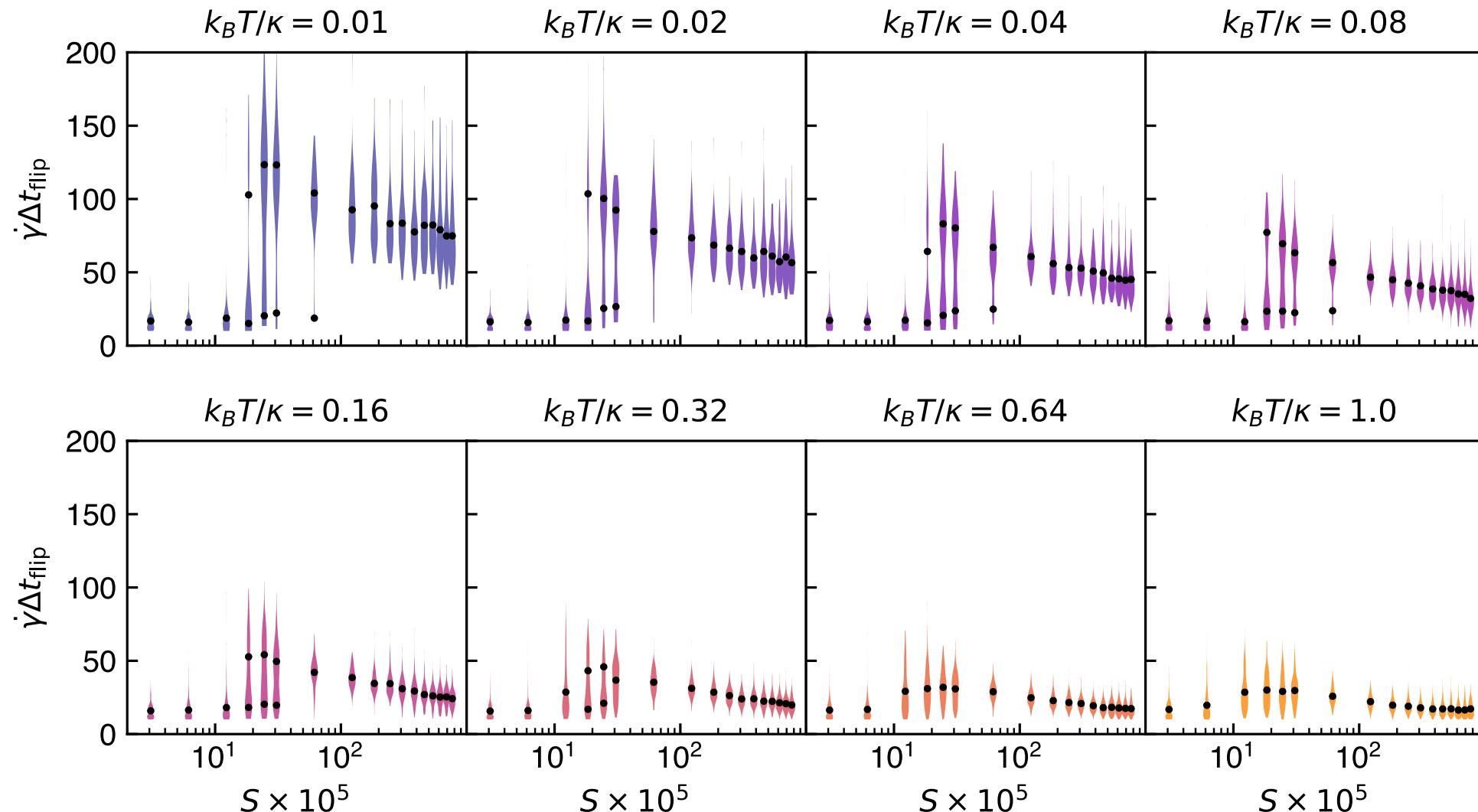


— $S = 3.08 \times 10^{-5}$

Tumbling
is chaotic

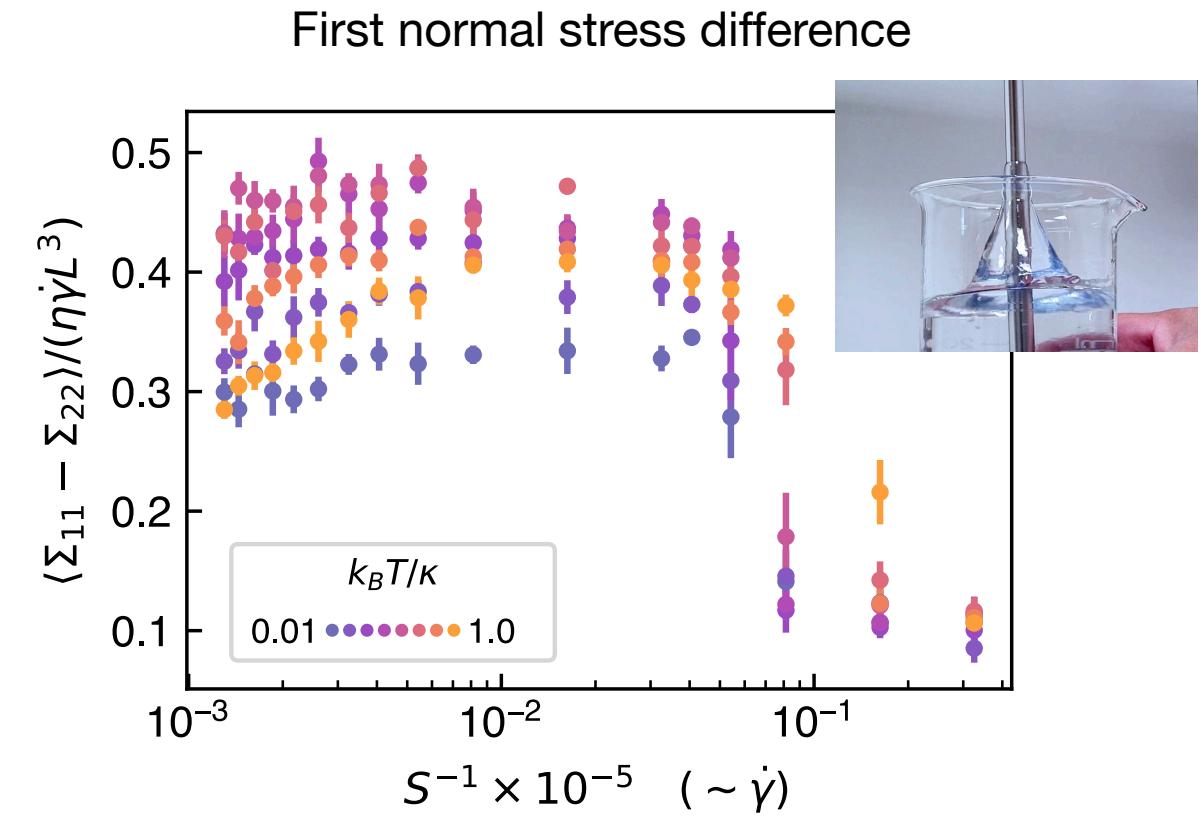
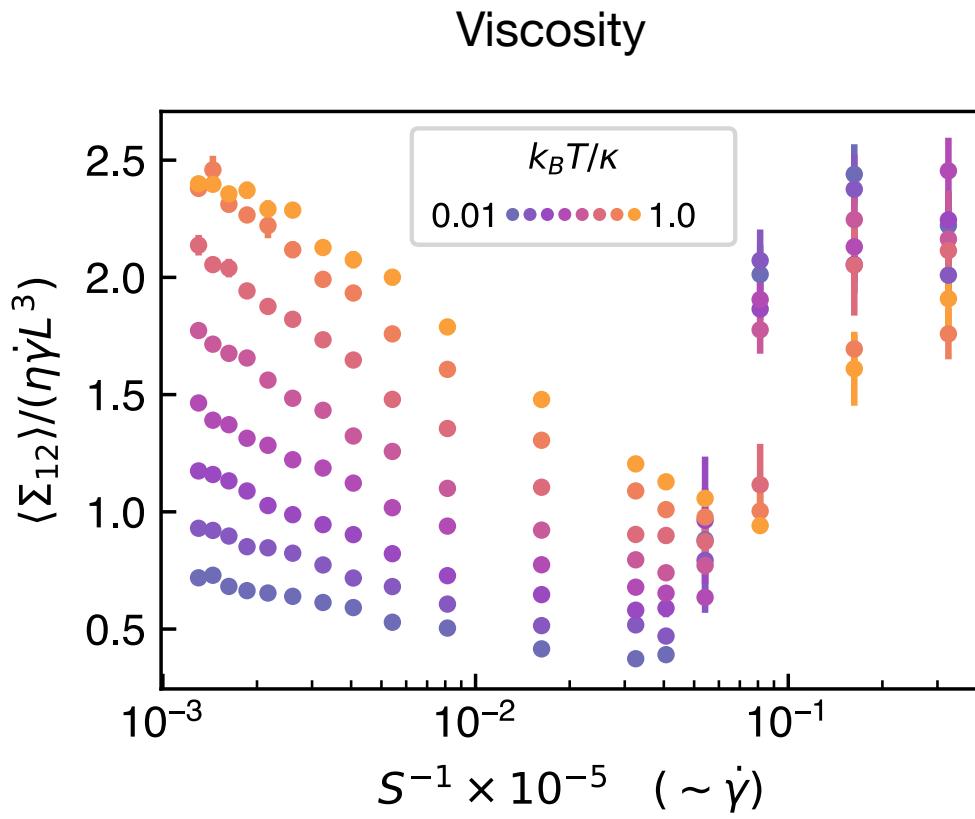


Thermal fluctuations cause stochastic flipping



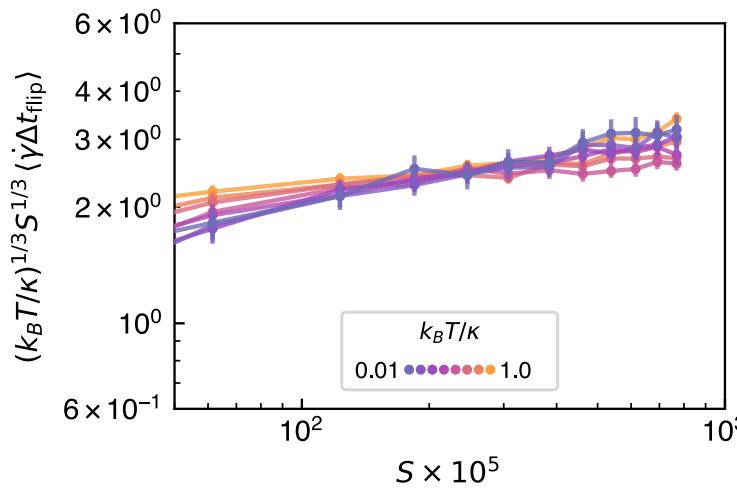
$$S = \frac{\kappa}{\pi \eta \dot{\gamma} L^3}$$

Rheological properties can be calculated from sheet conformations

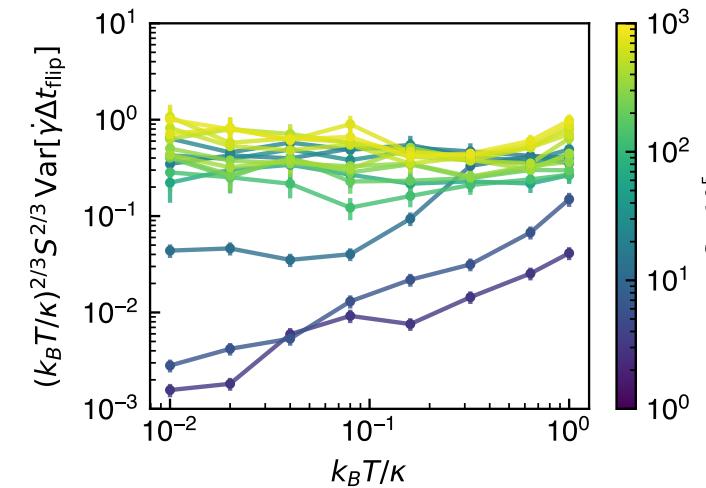


Universal scaling laws can be predicted by balancing rotational diffusion with convection

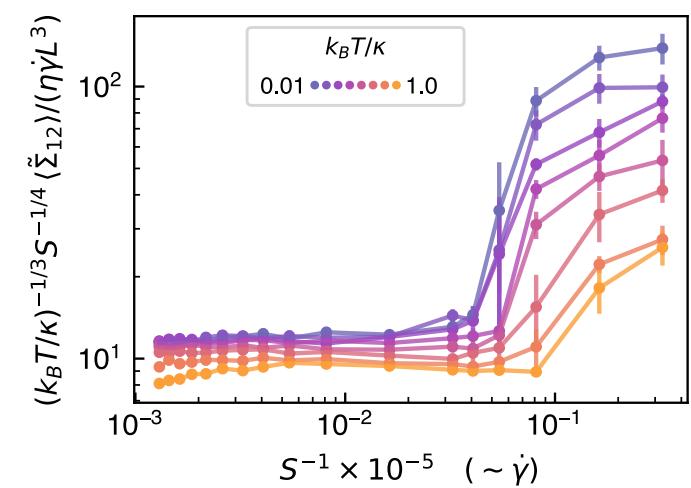
Mean flipping time



Flipping time variance



Viscosity



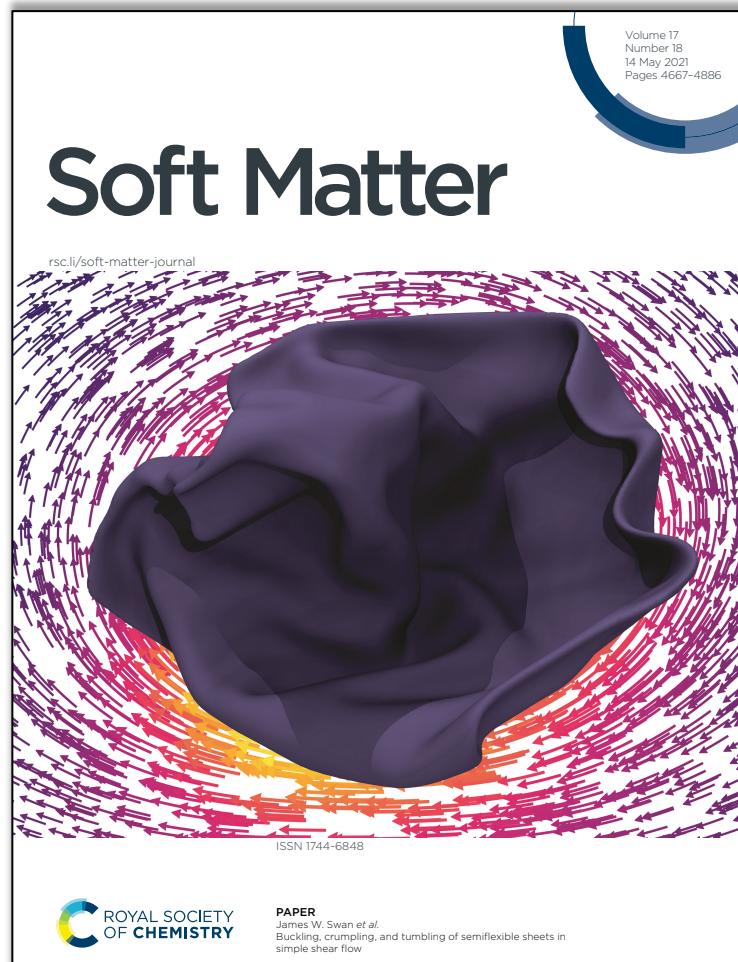
$$S = \frac{\kappa}{\pi \eta \dot{\gamma} L^3}$$

Acknowledgments

- Swan group
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- Pat Doyle
- Gareth McKinley
- Nikta Fakhri



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Conclusions

Transient buckling occurs for $\phi=0^\circ$ with modes predicted by 1D quasi-static elasticity model

Smaller values of S can result in chaotic, continuously tumbling trajectories, but not for all initial orientations

Sheets that do not tumble are described well by Jeffery orbits

Thermal fluctuations cause stochastic flipping of sheets and lead to interesting bulk rheological behavior

$$S = \frac{\kappa}{\pi \eta \dot{\gamma} L^3}$$