Stochastic process model of fatigue failure in glasses

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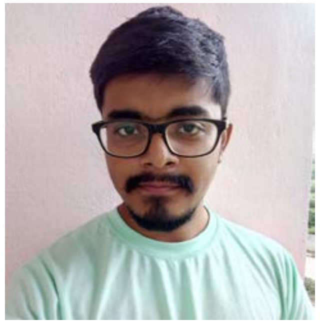
H. Bhaumik, G. Foffi and S. Sastry, Proc. Nat. Acad. Sci (USA) 118 (16) e2100227118 (2021) [arXiv:1911.12957]

S. Sastry, Phys. Rev. Lett. 126, 255501 (2021) [arXiv:2012.06726]

M. Mungan and S. Sastry, Phys. Rev. Lett 127, 248002 (2021) [arxiv:2106.13069]

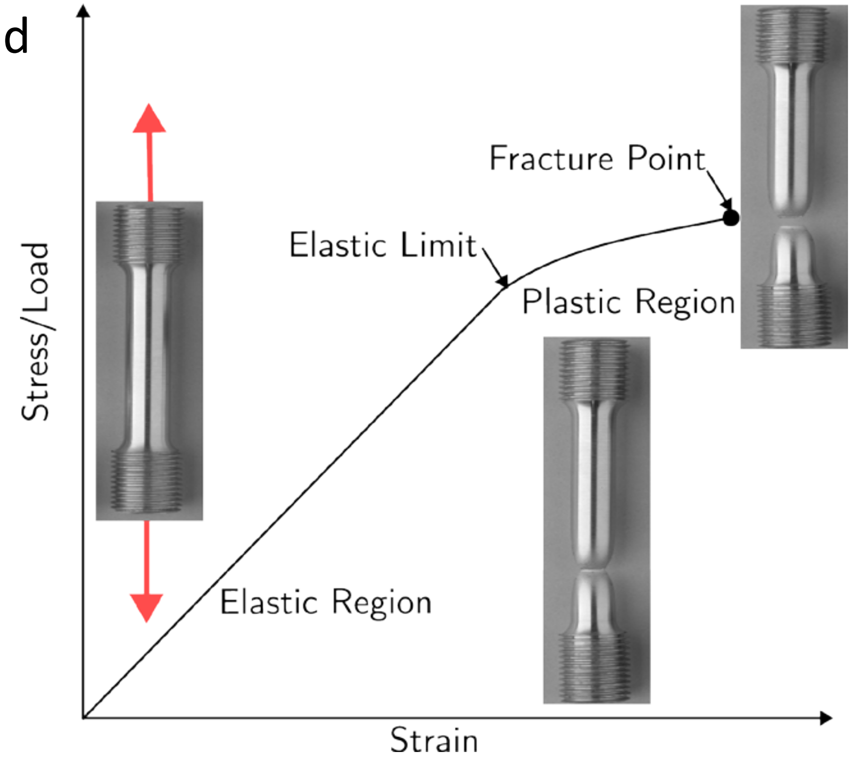
J. T. Parley, S. Sastry, P. Sollich, Phys. Rev. Lett. 128, 198001 (2022) [arxiv:2112.11578]

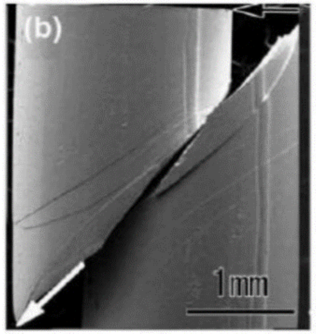
Y. Goswami, G. V. Shivashankar, S. Sastry) [arxiv:2312.01459] + ongoing work



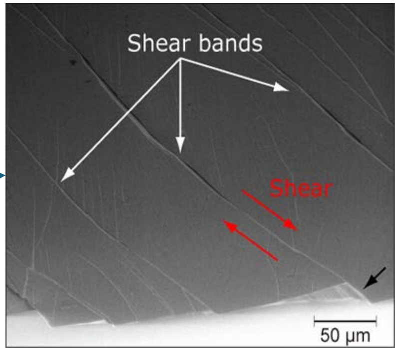

The mechanical behavior of solids

- Solids subjected to small external stresses/deformation respond elastically. Finite elastic moduli: **Reversible** behavior.
- Larger stresses lead to plasticity, yielding/failure. : **Irreversible** behavior.
- Understanding failure of obvious importance.





Failure mechanism



Uniform uniaxial load, Crystalline

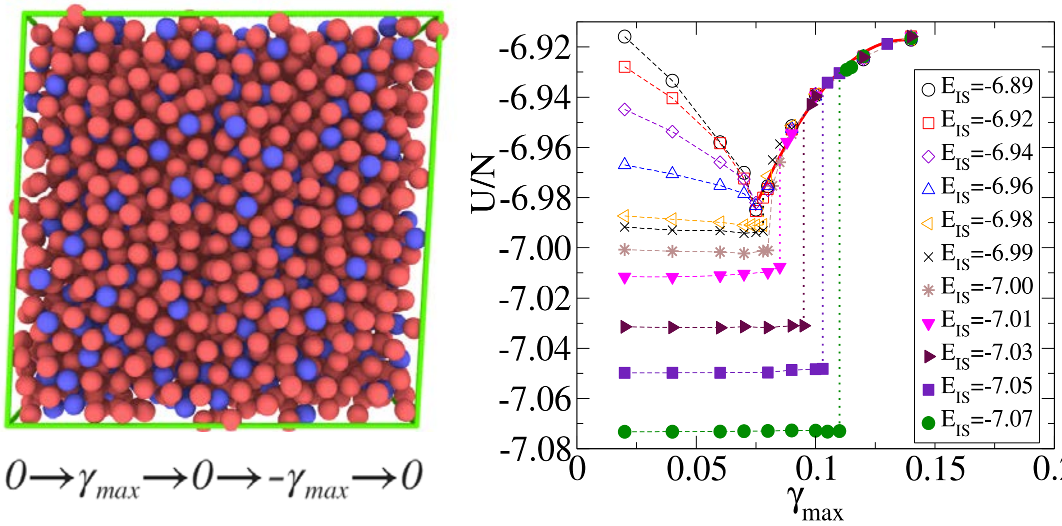
Uniform shear load, Amorphous

Aloha airline flight 243 fuselage failure (1988): Cyclic load, fatigue failure

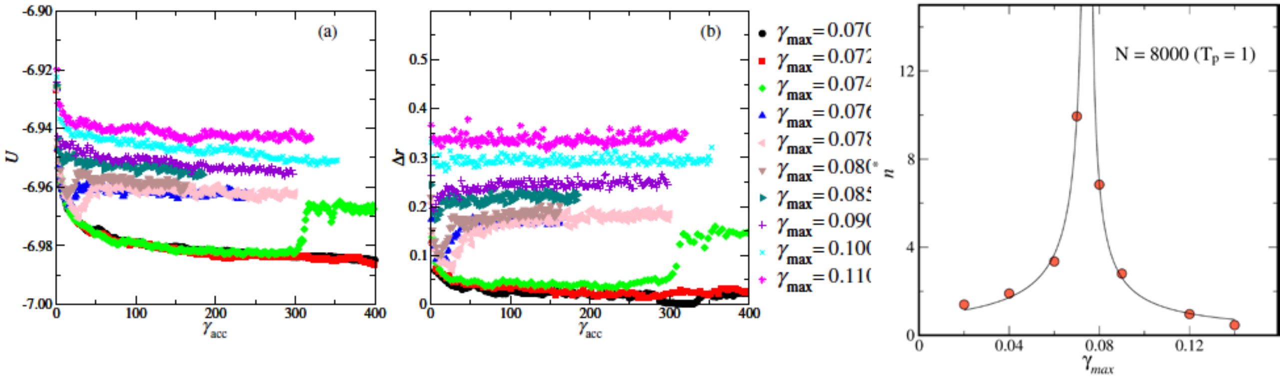
Simulations of cyclically sheared glasses

- Simulations of model glasses (Kob-Andersen BMLJ, BKS Silica, 2D BMLJ) applying athermal quasistatic or small shear-rate simulations.

- Cyclic shear – Shear back and forth in cycles with amplitude γ_{max} ($0 \rightarrow \gamma_{max} \rightarrow 0 \rightarrow -\gamma_{max} \rightarrow 0$)
- Leads to elastic and plastic response.
- Study properties of stroboscopic configurations.
- Yielding diagram displays dramatic dependence on degree of annealing.
- Non-monotonic change of energies and displacements with cycles.
- Divergence of time scales to reach steady states.

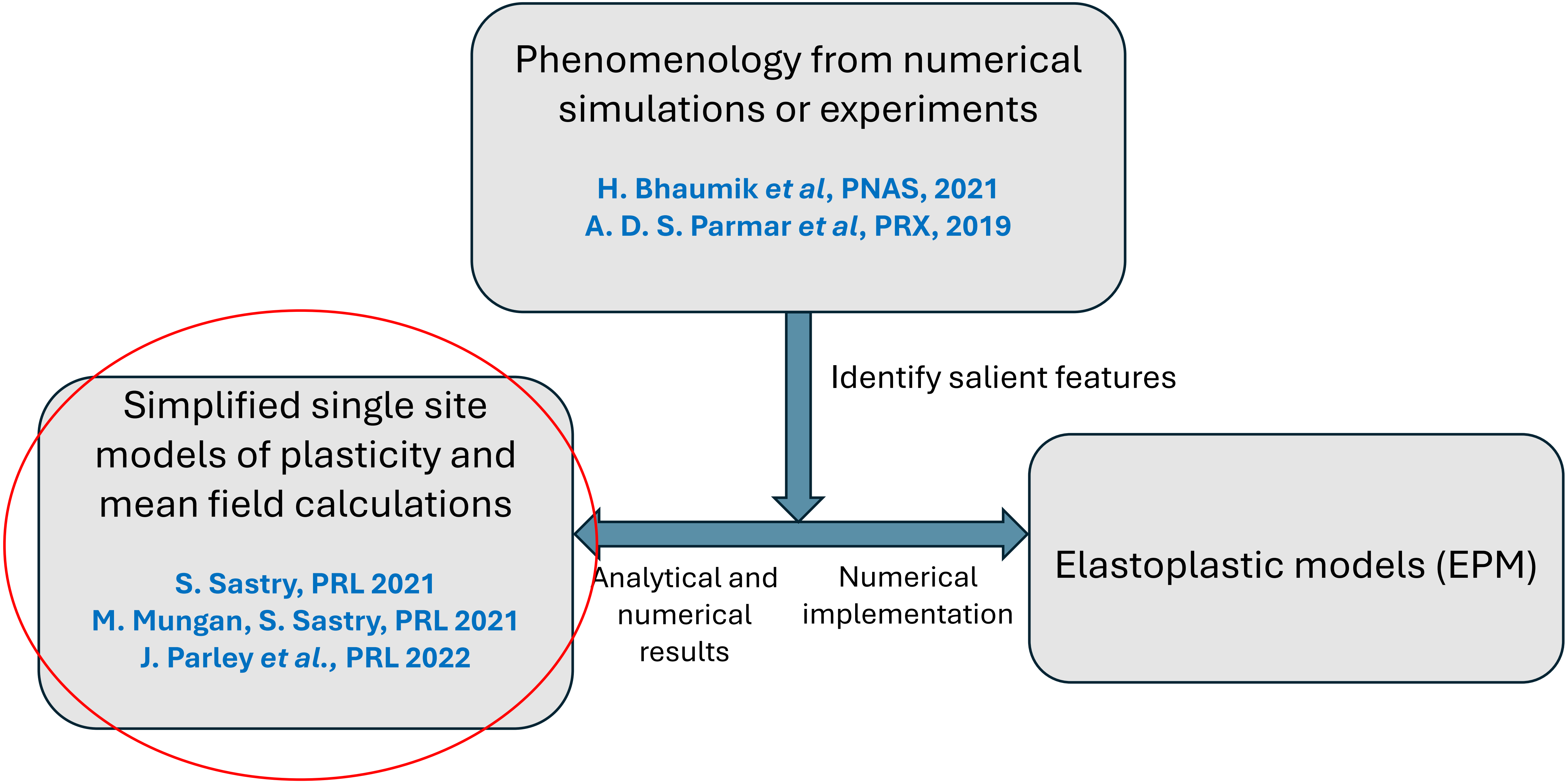


Bhaumik, Foffi, Sastry, PNAS 2021



Leishangthem, Parmar, Sastry, Nat. Comm. 2017
Parmar, Kumar, Sastry, PRX 2019

Amorphous solids under cyclic shear



A "meso-state" model of yielding

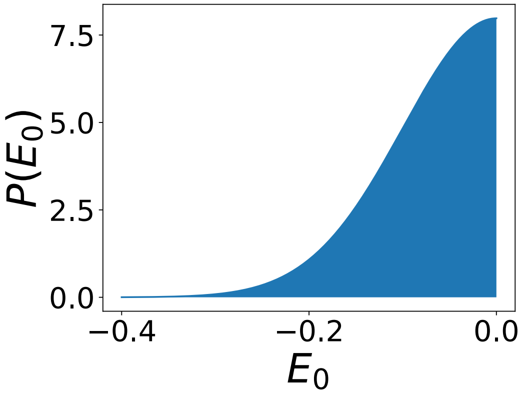
- The ("**one site**") model is specified in terms of a distribution of "**meso-states**", each characterized by an **(i)** minimum energy, **(ii)** a 'stress-free' plastic strain, **(iii)** a stability (strain) interval, and **(iv)** a maximum energy before instability/yield.
- When a minimum becomes unstable, a stochastic transition occurs to "allowed" minima, which must have lower energy **at the strain value** of the instability.
- Plastic strain γ_0 can be regularly spaced, or "uniformly" distributed.
- Allow transitions to ANY E_0 that qualifies or only within a range (constrained).

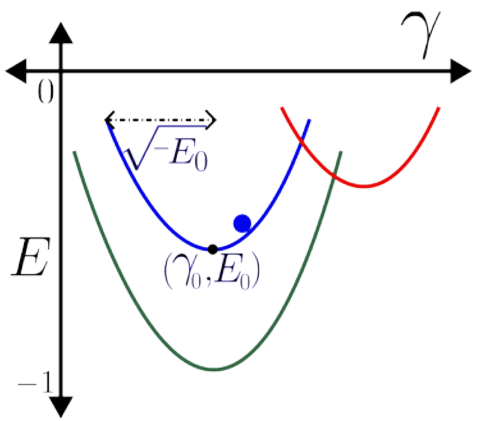
Qualitative features of simulations captured.

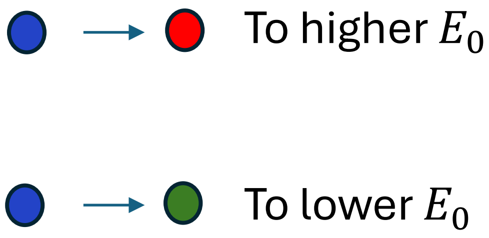
Energy vs strain: $E(\gamma, E_0, \gamma_0) = E_0 + \frac{\kappa}{2}(\gamma - \gamma_0)^2$

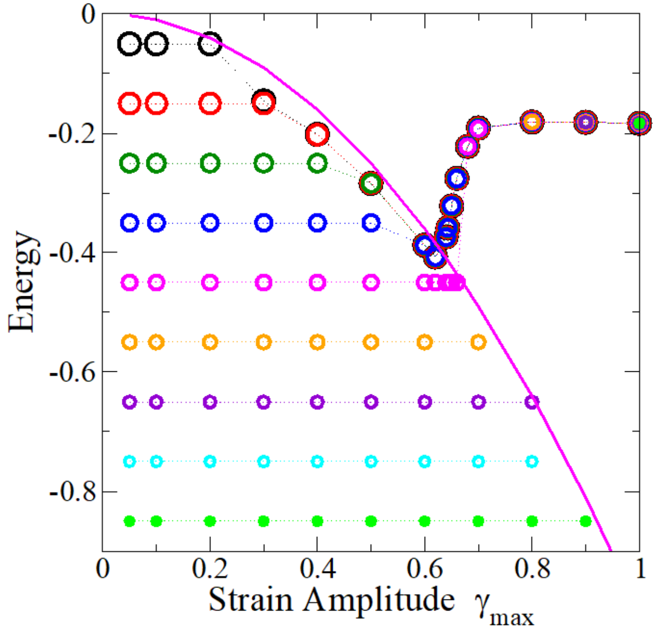
$$P_0(E_0) = \sqrt{\frac{2}{\pi\sigma^2}} \exp\left(-\frac{E_0^2}{2\sigma^2}\right)$$

Stability interval: $\gamma_\pm = \gamma_0 \pm \sqrt{-E_0}$









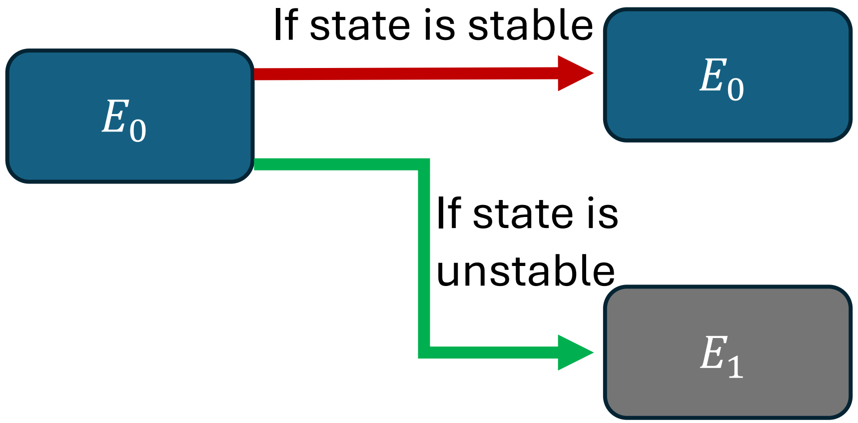
S. Sastry, PRL 2021

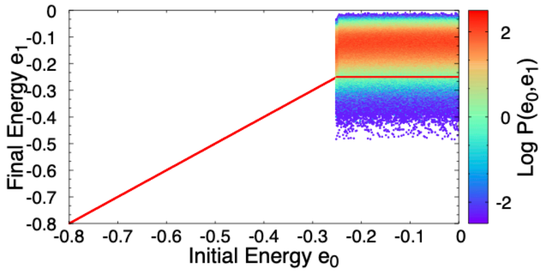
Cycle to Cycle dynamics

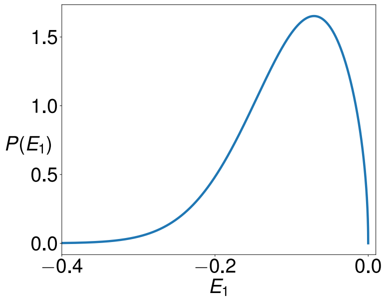
- ➢ energy at the end of a cycle vs at the beginning, at varying strain amplitude, reveals that either:
  - The energies do not change (stable), or
  - The distribution of new energies largely independent of initial energy.

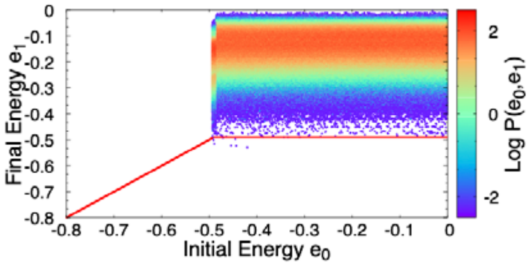
$E_0 < -\gamma_{max}^2$

Stable









Roughly 'invariant' w.r.t. initial energy E_0

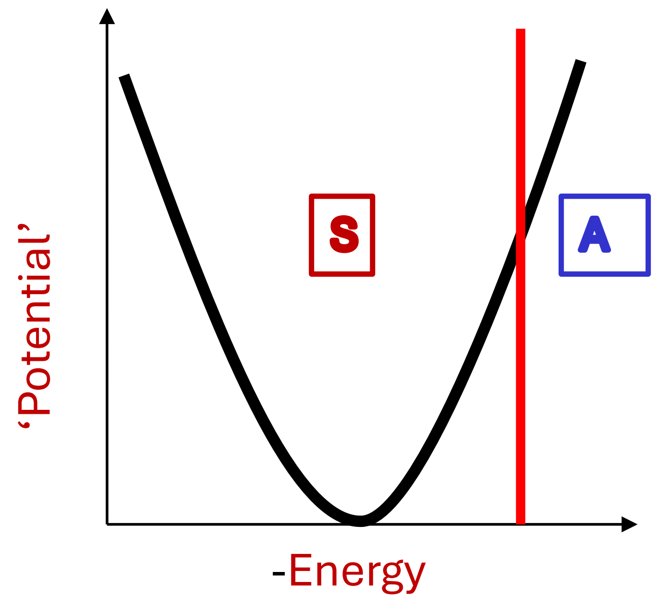
- ➢ "Invariant" distribution of final states for (unstable) states that undergo transitions.
- ➢ Leads to a simplifying picture of a random walk in a confining potential.
- ➢ **Yielding driven by entropy** – paucity of stable states vs abundance of high energy states.

Ehrenfest trap model

- **A simple map of dynamics** : Random walk along the **energy axis**, with a discrete set of energies, and transition probabilities.
- One can calculate the **trapping time** and the expected average energy as a function of time:

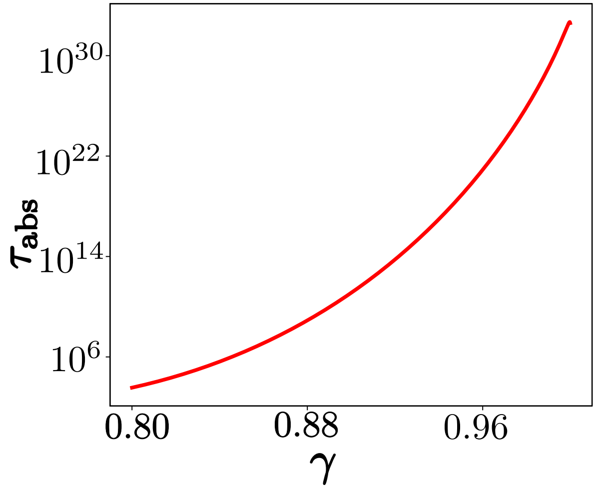
$$\tau_{abs}(\gamma) = 2\sqrt{\pi N}\sqrt{\epsilon_\gamma(1-\epsilon_\gamma)}\frac{e^{2NI(\epsilon_\gamma)}}{2\epsilon_\gamma - 1}$$

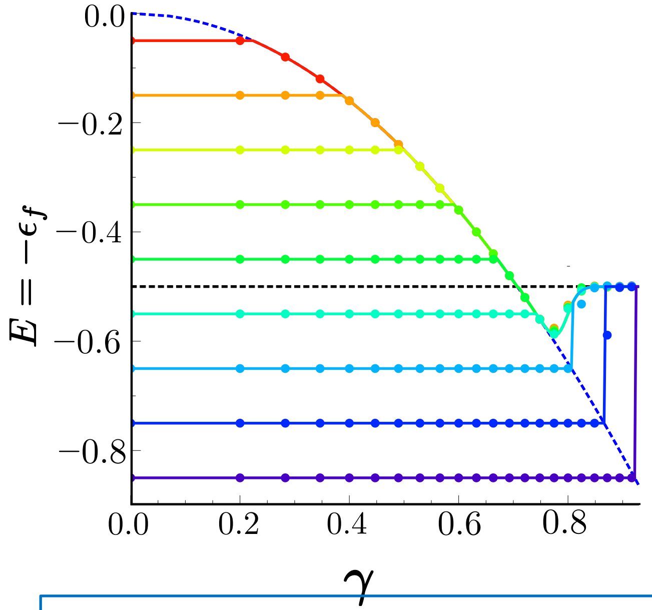
$$I(x) = \log 2 + x\log x + (1-x)\log(1-x)$$



- A yielding diagram like the previous model and a similar estimate of the yield amplitude that depends on number of cycles.

$$\gamma_y^2 = \frac{1}{2}\left(1 + \sqrt{\frac{1}{N}\ln\left(\pi^{-\frac{1}{2}}\frac{\tau}{N}\right)}\right)$$





- **Next**: Improve the model and incorporate activated escape for mechanically stable states.

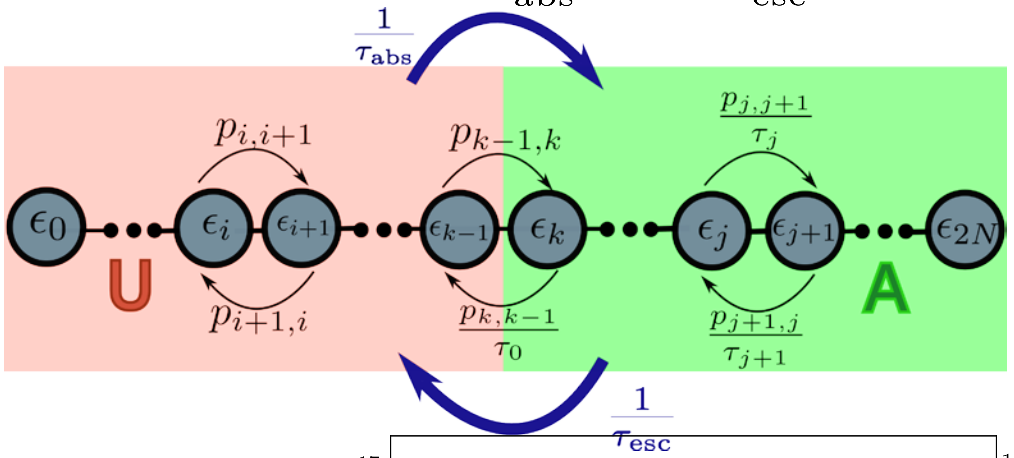
M. Mungan, S. Sastry, PRL 2021

Thermally activated escape

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} P_{\mathrm{U}}(t) \\ P_{\mathrm{A}}(t) \end{pmatrix} = \begin{pmatrix} -\frac{1}{\tau_{\mathrm{abs}}} & \frac{1}{\tau_{\mathrm{esc}}} \\ \frac{1}{\tau_{\mathrm{abs}}} & -\frac{1}{\tau_{\mathrm{esc}}} \end{pmatrix} \begin{pmatrix} P_{\mathrm{U}}(t) \\ P_{\mathrm{A}}(t) \end{pmatrix}$$

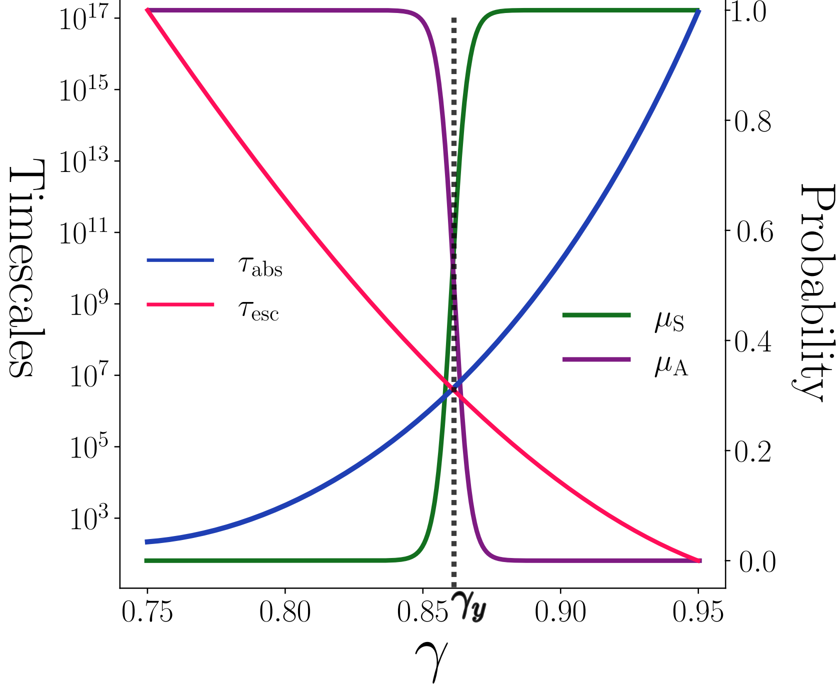
- System can escape the absorbing states due to thermal/ mechanical noise.
- Allowing for escape mechanism fixes yield point

$$\gamma_y^2 = \frac{1}{2}\left(1 + \sqrt{\frac{1}{N}\ln\left(\pi^{-\frac{1}{2}}\frac{\tau_{\mathrm{esc}}}{N}\right)}\right)$$



- Stable states get thermally activated after $\tau_j = \tau_0 e^{\beta \Delta E_j}$, $\Delta E_j = -\frac{\kappa}{2}(\epsilon_j - \gamma^2)$

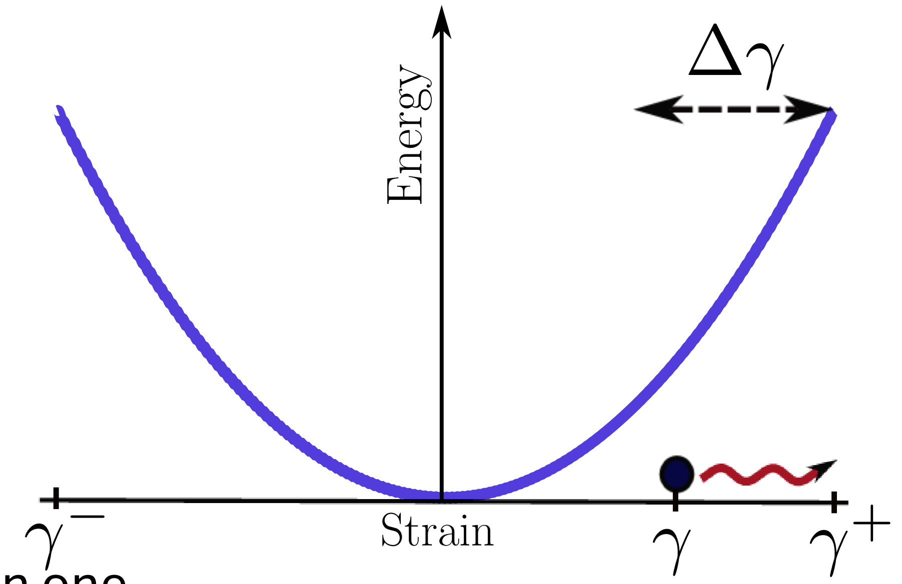
- $\tau_{\mathrm{esc}}(\gamma) = \frac{\tau_0}{\gamma^2}\sqrt{\pi N} e^{4N(\epsilon_{\max} - \gamma^2)^2}$, $\epsilon_{\max}$: Energy scale set by temperature.



- No sharp transition between elastic and yielded state due to temperature.

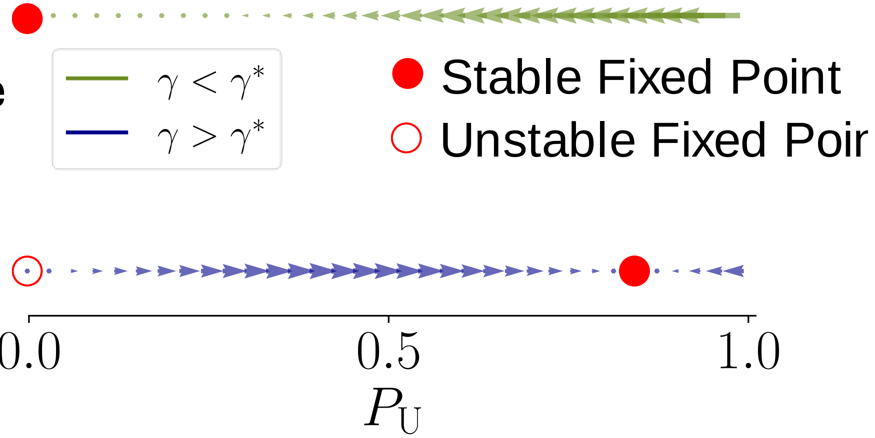
Activated escape-Mechanical noise

- Assume that activated escape can be described by imposing a waiting time τ_j at each site 'j' in the Ehrenfest model given by : $\tau_j = \tau_0 + \frac{\left(\sqrt{\epsilon_j}-\gamma\right)^2}{2D(t)}$, $D(t) = \alpha P_U(t)$
- Motivation : Considering escape happens by diffusion for strain interval $(\Delta\gamma)$: $\left(\sqrt{\epsilon_j} - \gamma\right)^2 \equiv (\Delta\gamma)^2$

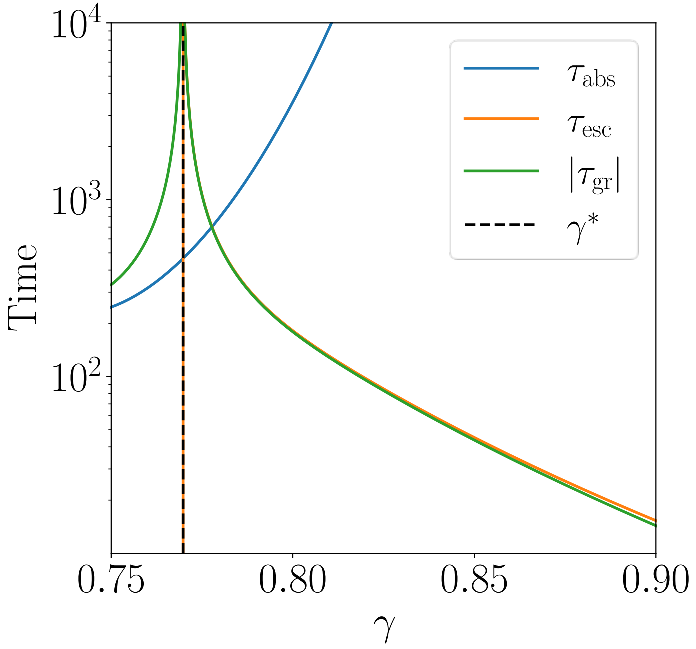


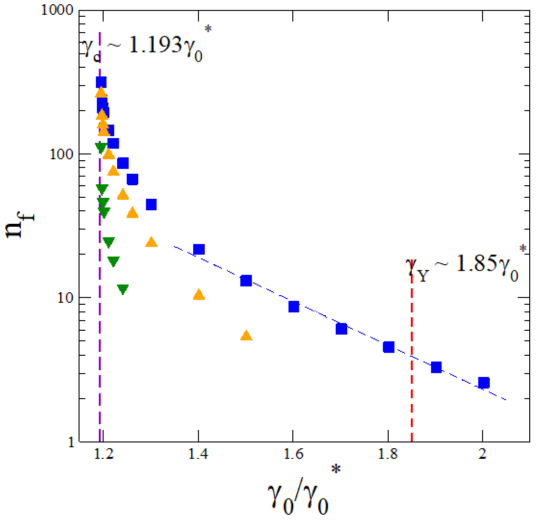
- U state: Set of states with low stability (will undergo transition within one cycle),
  is the primary source of noise. Higher $P_U \Longrightarrow$ More strength of noise $\Longrightarrow$ larger diffusion constant.
- α →Strength of coupling (In principle depends on the Eshelby kernel).
  Increase α → Stronger noise → Lesser strain amplitude to yield

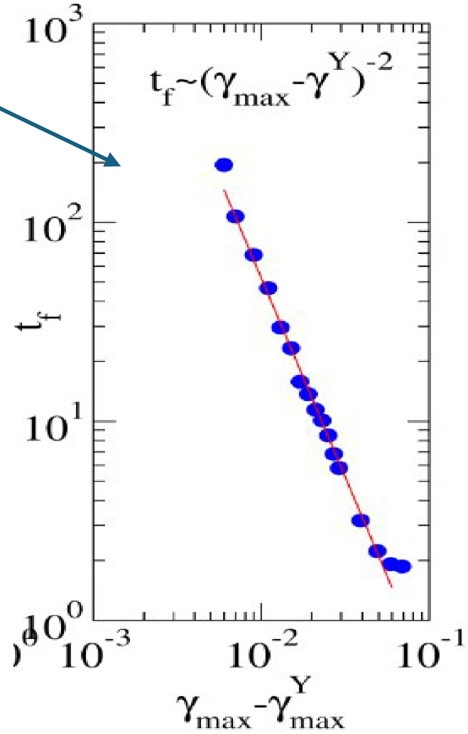
Analysis of time-scales

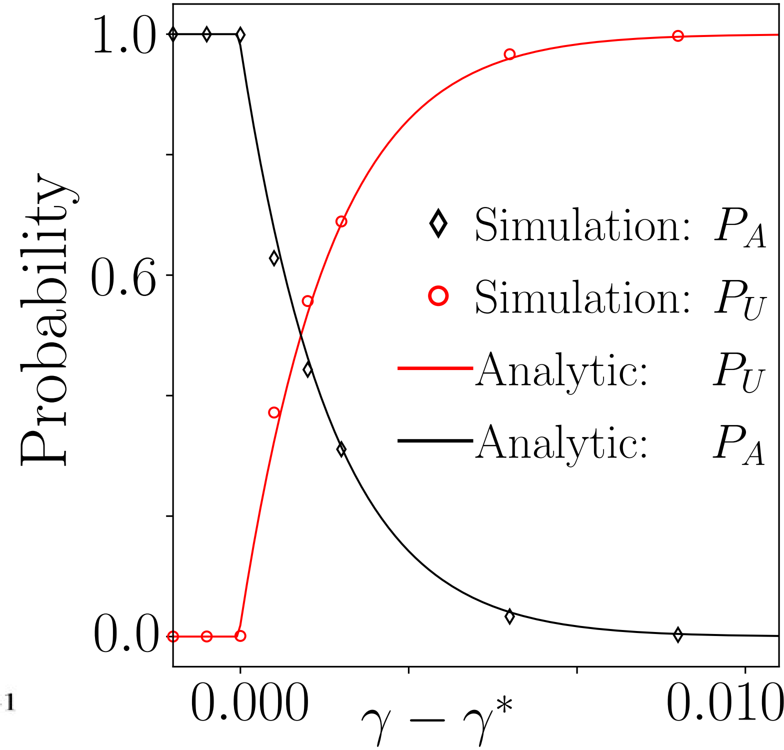


- Stochastic model as a dynamical system : System changes from one stable fixed point at zero activity for $\gamma < \gamma^*$ to a stable fixed point at finite activity (yielding) for $\gamma > \gamma^*$ with the zero activity fixed point becoming unstable.
- Divergence of timescales : key feature of yielding.
- Stochastic model : τ_{esc} diverges at γ^* ✓
- **The exponent of divergence for τ_{esc} is 1.**
- Exponent of divergence different in MD simulations







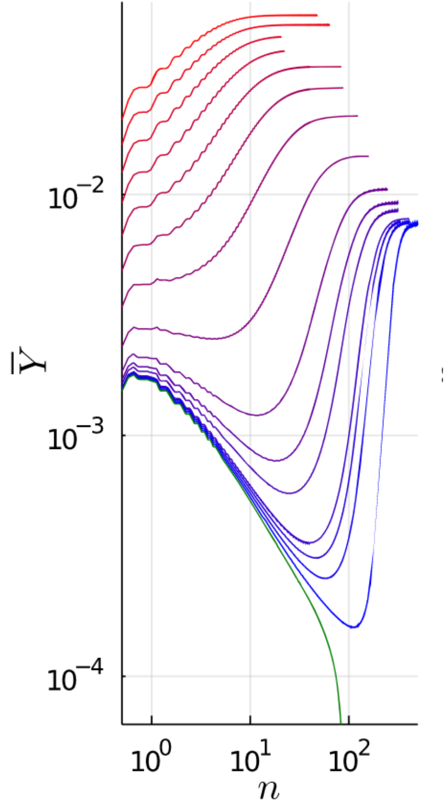


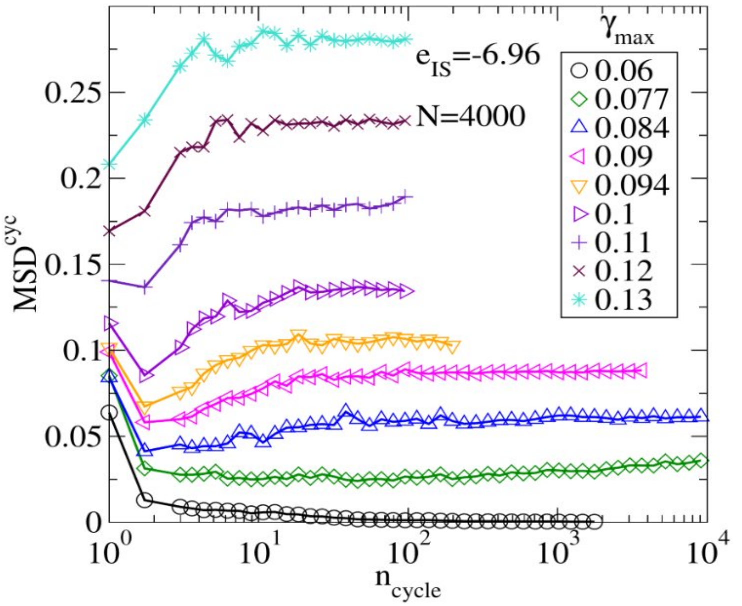
Steady state probabilities

Dynamics to failure

- Simulations and mean field calculations show non-monotonic evolution of activity with time: initial annealing followed by jump in energy, MSD
- Two-state coarse grained description: only one independent variable P_U.
- P_U will always approach fixed point monotonically.
- Two-state coarse graining not correct for capturing the dynamics.
- Define three ‘macrostates’: **U: Unstable** (states prone to yielding) , **T: Threshold** (states near the threshold of stability), **A: Absorbing** (highly stable states)
- Evaluate the effective rates governing the transition

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} P_{\mathrm{U}} \\ P_{\mathrm{T}} \\ P_{\mathrm{A}} \end{pmatrix} = \begin{pmatrix} -\frac{1}{\tau_{\mathrm{abs}}(\gamma)} & \frac{1}{\tilde{\tau}_{\mathrm{esc}}} & 0 \\ \frac{1}{\tau_{\mathrm{abs}}(\gamma)} & -\left(\frac{1}{\tilde{\tau}_{\mathrm{esc}}} + \frac{1}{\tau_{\mathrm{st}}}\right) & \frac{1}{\tau_{\mathrm{esc}}} \\ 0 & \frac{1}{\tau_{\mathrm{st}}} & -\frac{1}{\tau_{\mathrm{esc}}} \end{pmatrix} \begin{pmatrix} P_{\mathrm{U}} \\ P_{\mathrm{T}} \\ P_{\mathrm{A}} \end{pmatrix}$$





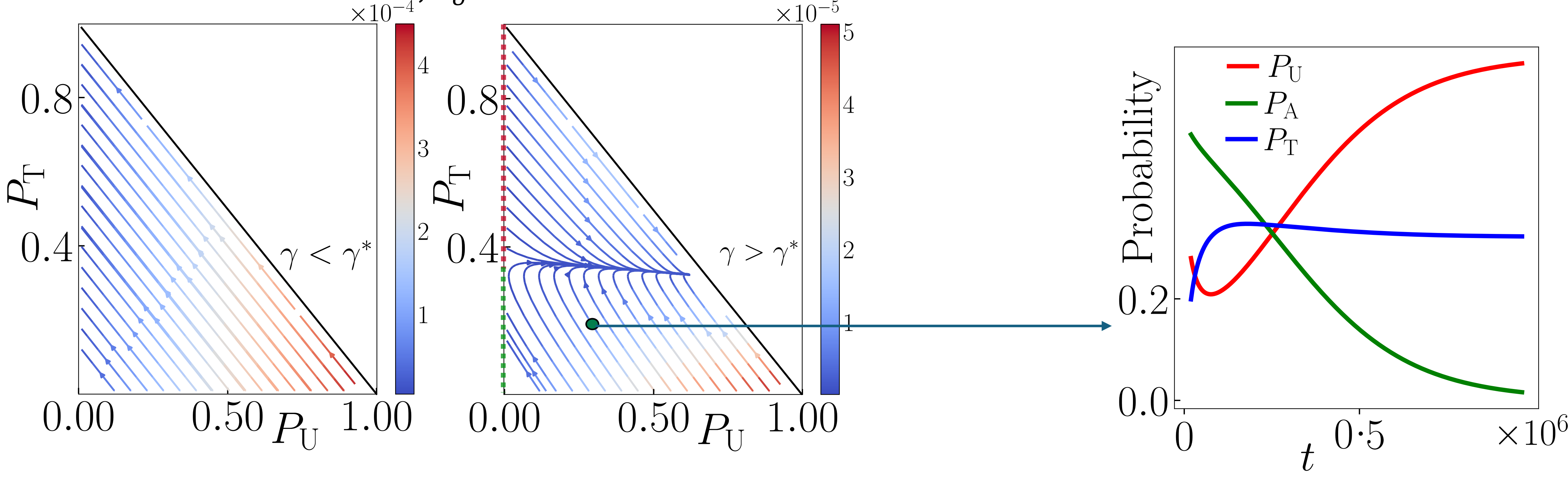
J. Parley, S. Sastry, P. Sollich, PRL 2022

Three state model

➢Well-annealed (low P_T, high P_A) glasses show non-monotonic evolution of activity.

➢Certain initial condition do not yield even for $\gamma > \gamma^*$ ⟹ Well-annealed samples have initial condition dependent γ_y.

➢Cause of non-monotonicity: If P_T is below a threshold value(green line), there is flow from U to T. Once the threshold exceeds, P_U increases.



Summary

- Yielding of glasses under cyclic shear exhibit (a) strong dependence on annealing, (b) divergence of time scales at the yield point, and (c) non-monotonic changes in energy and displacements on the way to yielding.
- A "landscape" based model captures qualitative behavior, but with no genuine transition.
- The dynamics can be mapped to a random walk in a potential with absorbing boundaries, leading to similar yielding behavior, but (again) no genuine transition.
- The incorporation of feedback through "mechanical noise" that depends on the population of unstable states leads to the presence of a genuine transition with diverging time scales.
- Coarse-graining the dynamics with sufficient (three) coarse-grained states also capture the observed non-monotonic behavior of properties.

Looking for postdocs to work in this and related areas!!