Linear stability analysis of discrete dislocation systems

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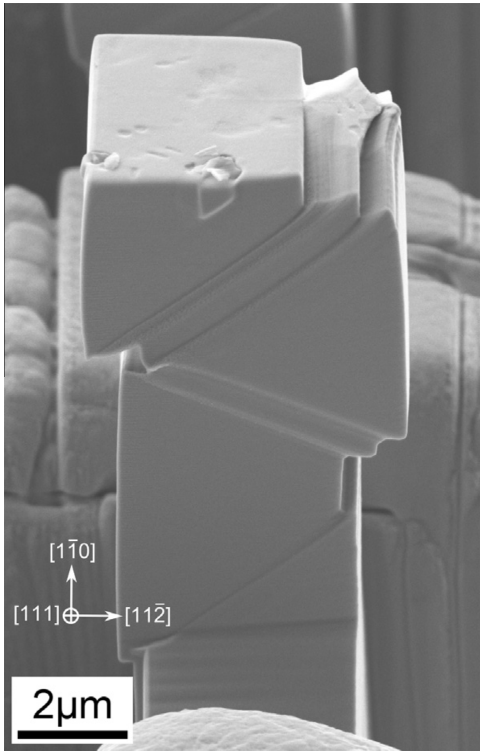
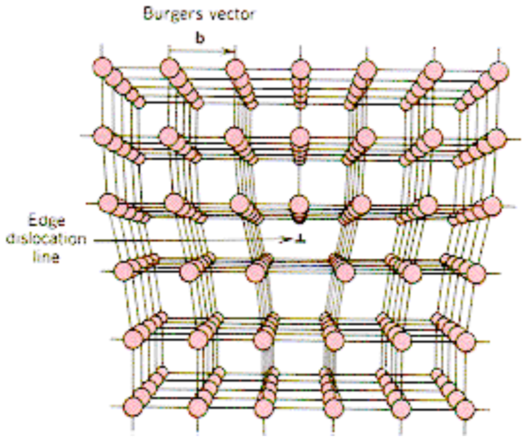
Motivation

- Large stochastic fluctuations arise during the deformation of small (few um) crystalline samples
  - Makes predictable deformation impossible
- Power-law distributions characterize intermittency
- The question of universality is still open
  - What physical processes affect the critical behaviour and how?

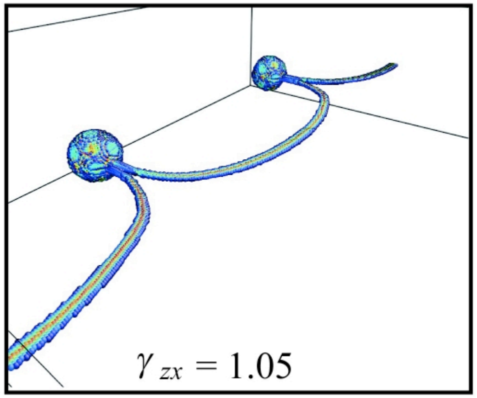


Relevant lenght scales

Atomic scale

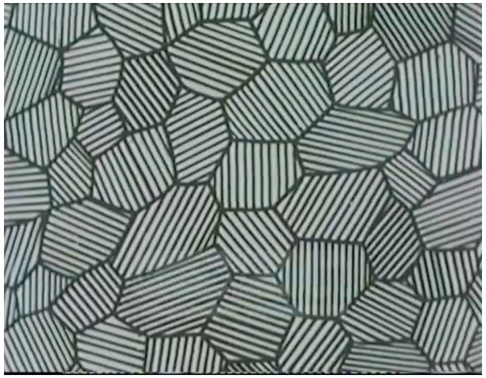


Quenched disorder

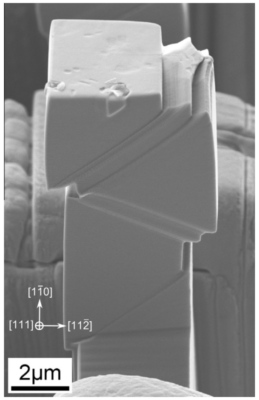


Dislocation pattern

Grain size



Specimen size



Outline

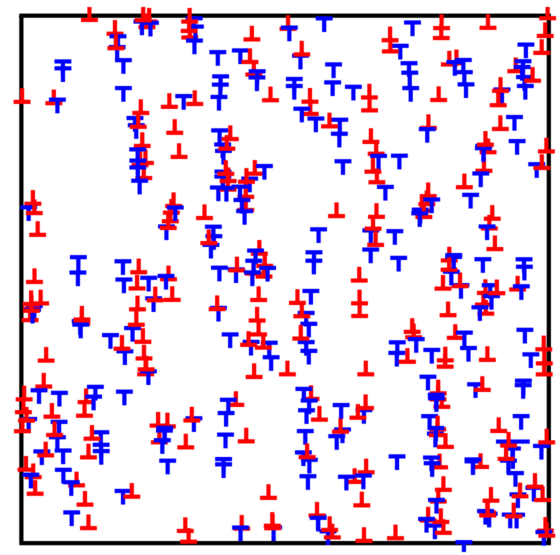
- 2D discrete dislocation dynamics model
- Extended criticality and effect of quenched pinning
- Local yield thresholds
  - Anomalous scaling
- Linear stability analysis
  - Dynamical correlations in the system
  - Prediction of events
  - Quenched pinning

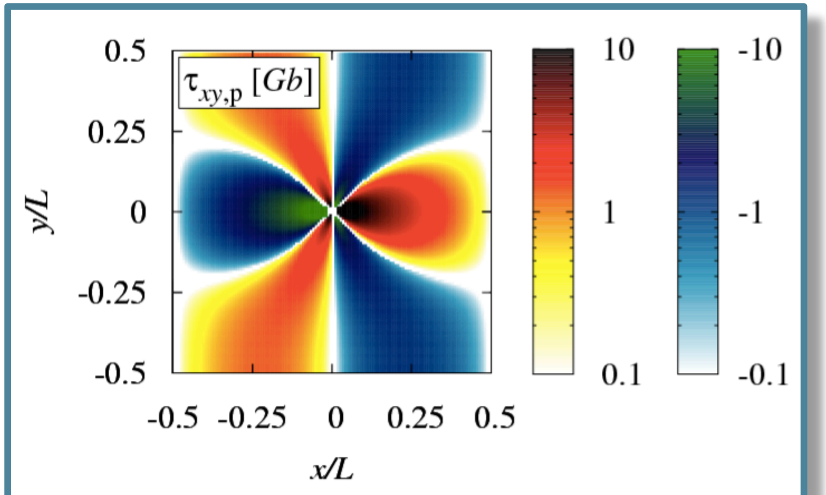
2D dislocation model

2D DDD

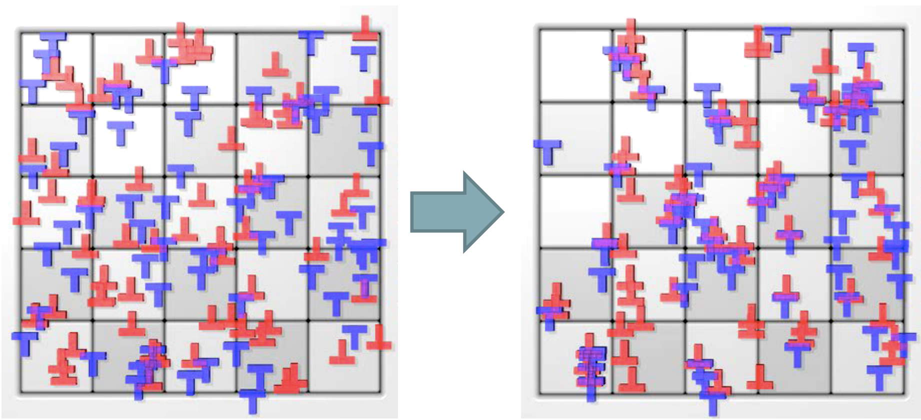
- Parallel edge dislocations in single slip
- Periodic boundary conditions
- Number of dislocations: *N*
- Sign of dislocations: $s_i = \pm 1$
- Stress-field of an individual dislocation: τ_{xy}
- Overdamped motion:

$$\dot{x}_i = s_i \left[\sum_{j=1, j\neq i}^{N} s_j \tau_{xy}(\boldsymbol{r}_i - \boldsymbol{r}_j) + \tau_{\text{ext}} \right]$$

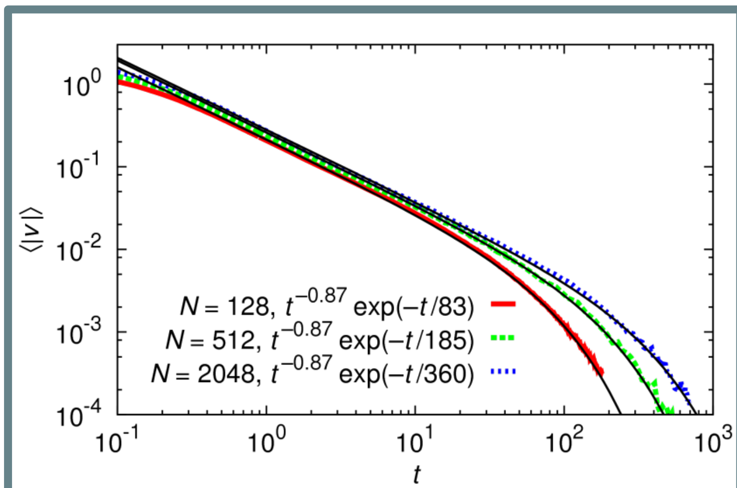


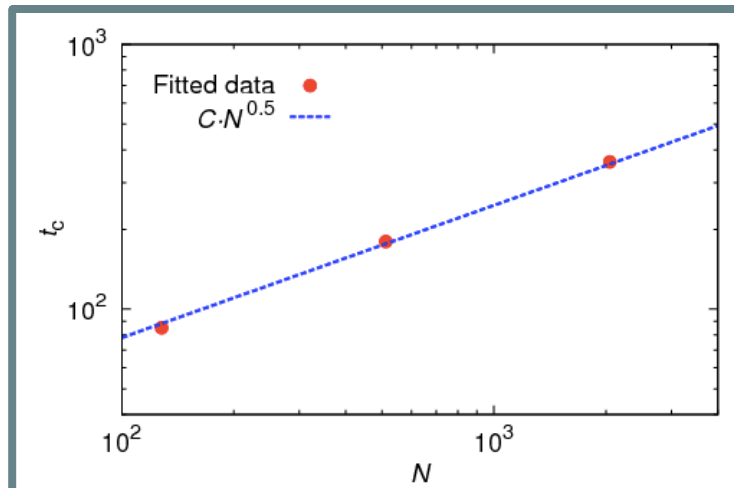


Relaxation from a random initial state



- Average absolute velocity: $\langle |v(t)| \rangle \propto t^{-\alpha}, \quad \alpha \approx 0.87$
- The cut-off t_c diverges with system size

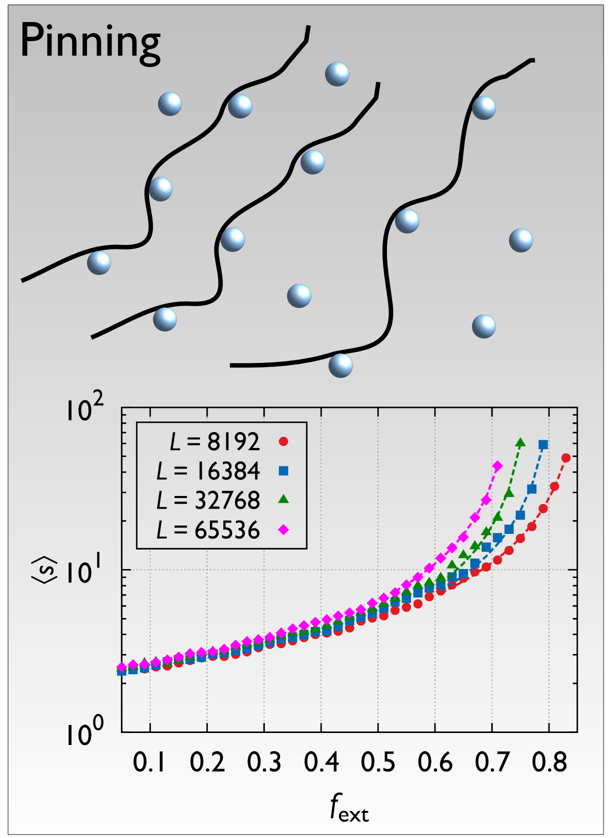


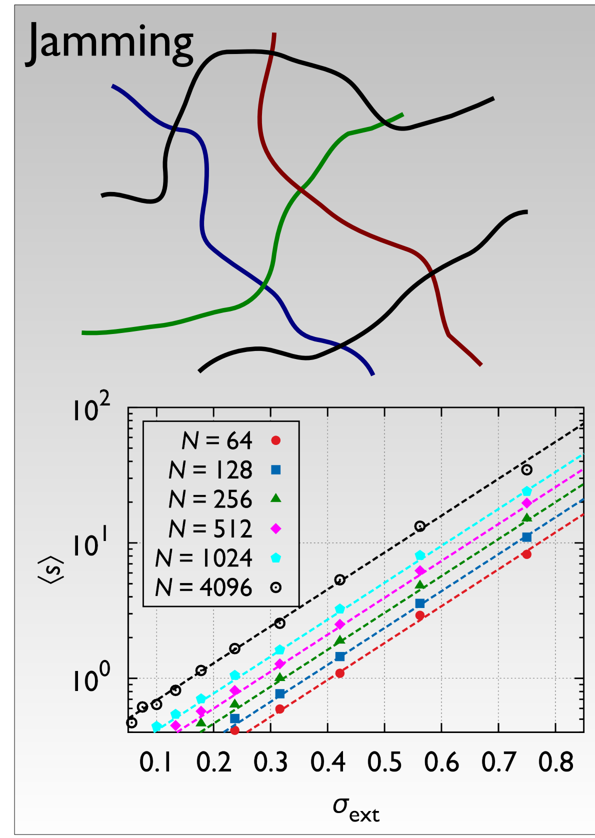


F. F. Csikor *et al.*, JSTAT, 2009; P. D. Ispánovity *et al.*, PRL, 2011

Extended criticality

- The system is always critical
  - $\langle s \rangle \propto L^{0.8}$
  - $\langle \Delta\gamma \rangle \propto L^{-1.2}$
  - Avalanches always span the whole system
  - Also true in 3D





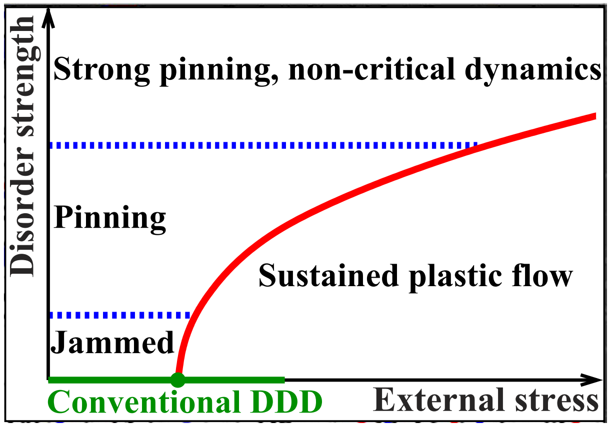
PD Ispánovity, L Laurson, M Zaiser, I Groma, S Zapperi, M Alava, PRL, 2014

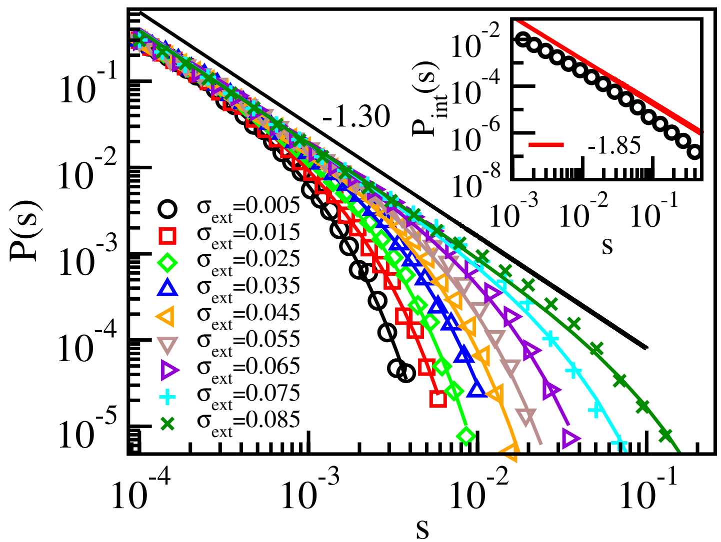
A Lehtinen, G Costantini, M Alava, S Zapperi, L Laurson, PRB, 2016

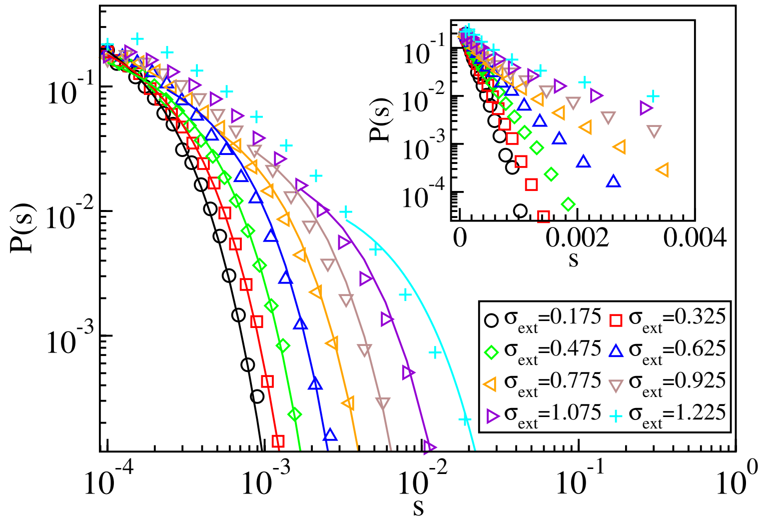
M Ovaska, A Lehtinen, M Alava, L Laurson, S Zapperi, PRL, 2017

Effect of quenched pinning

- A new length-scale leads to:
  - 1.0 → 1.3 → Gaussian
  - jamming → pinning → non-critical dynamics



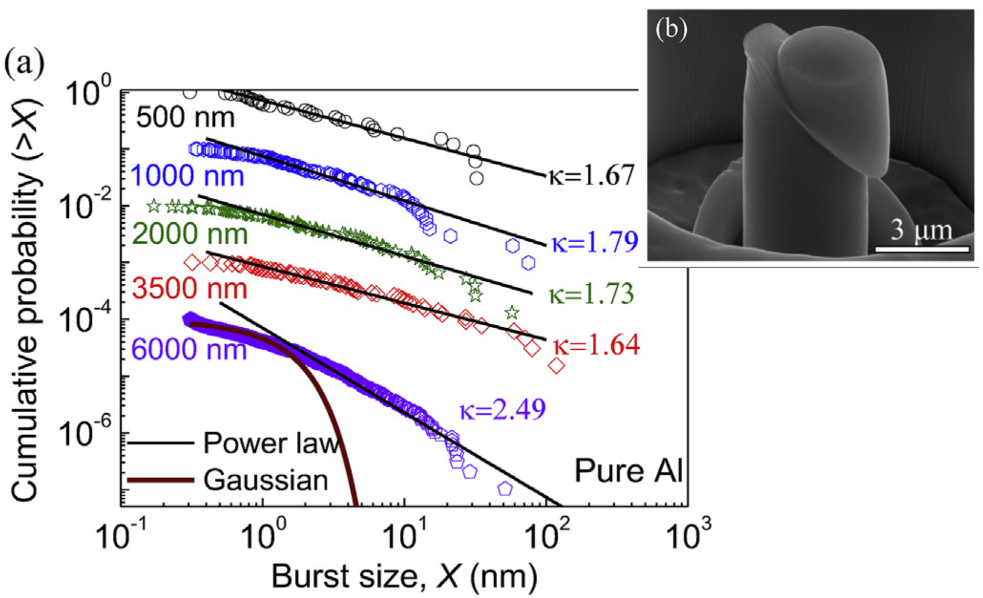


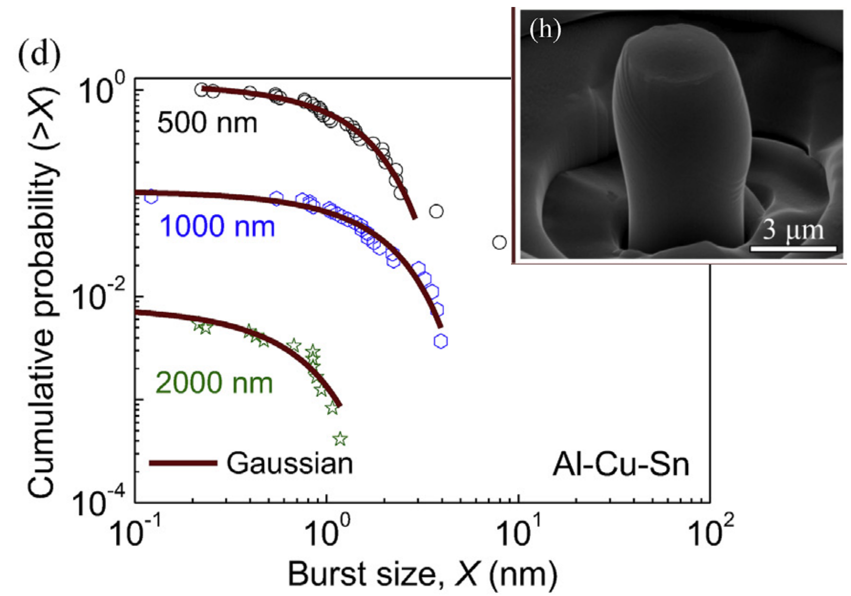


[Ovaska, Laurson, Alava, Sci. Rep. (2015)]

Micropillar deformation

- Alloying introduces a length-scale
  - Critical → smooth dynamics

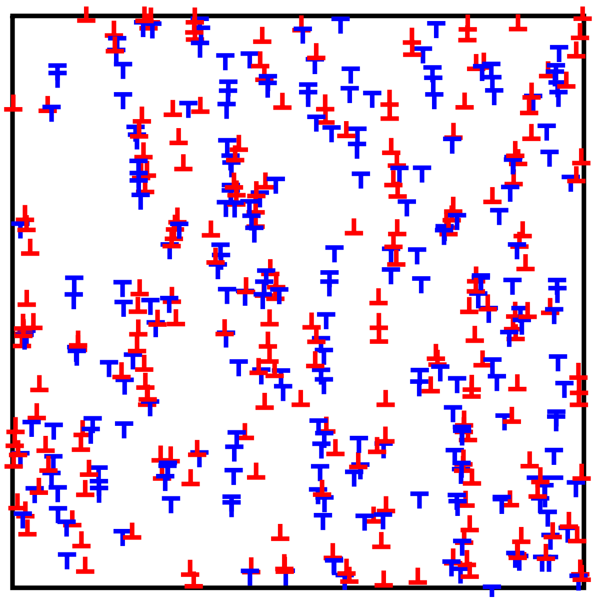




[Zhang *et al*, Acta Mater. (2017)]

Stochastic modelling

- What should be the threshold distribution of the stochastic model?
- What is the size of the Representative Volume Element?



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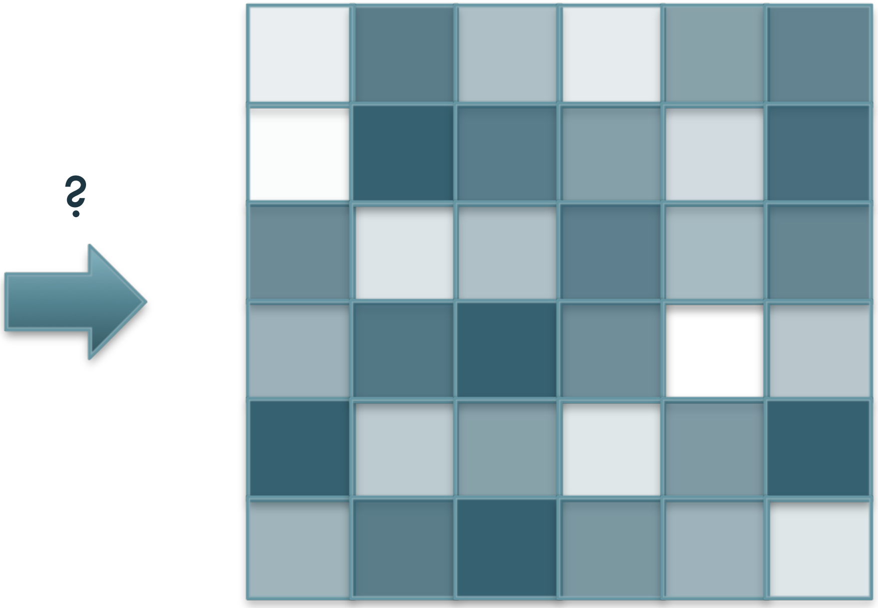
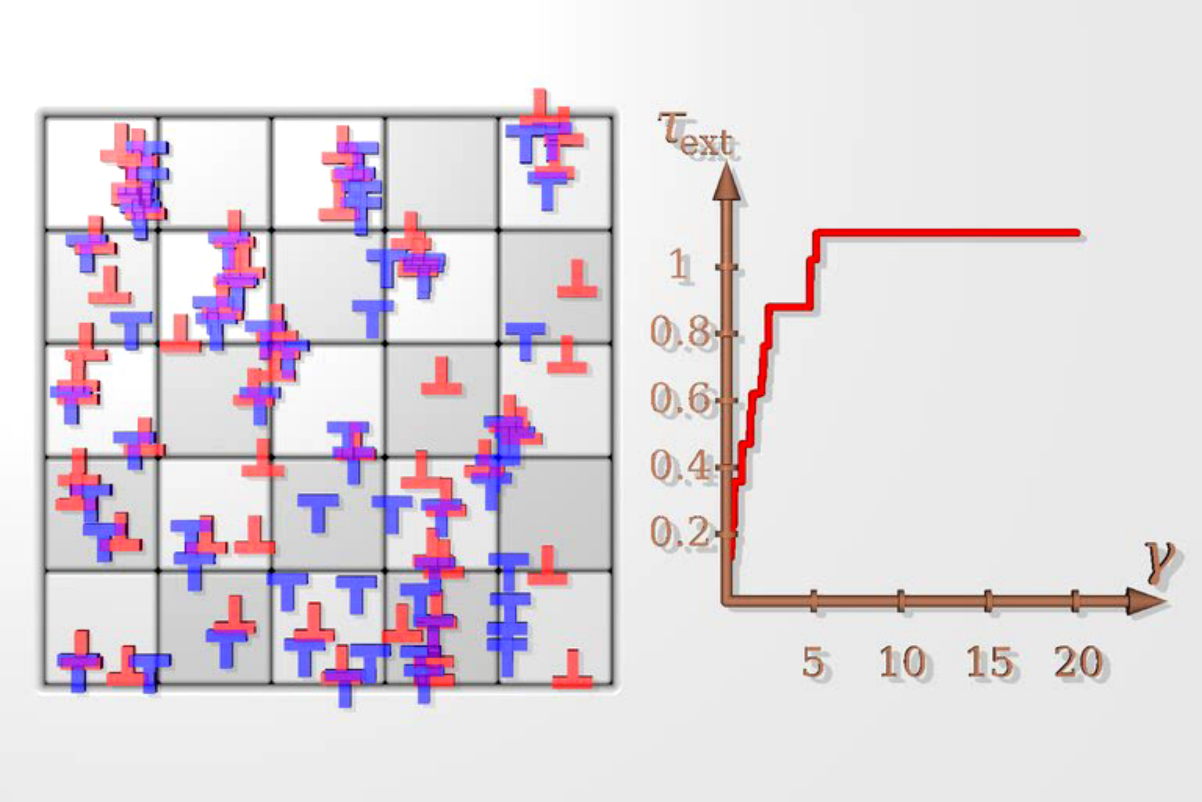
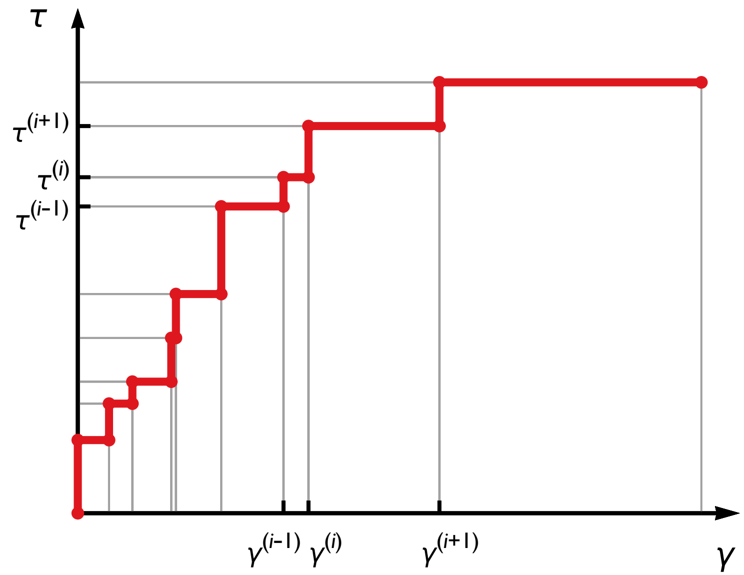


[Ispánovity, Tüzes, Szabó, Zaiser, Groma, PRB, (2017)] Single slip plastic quasi-static shear in 2D



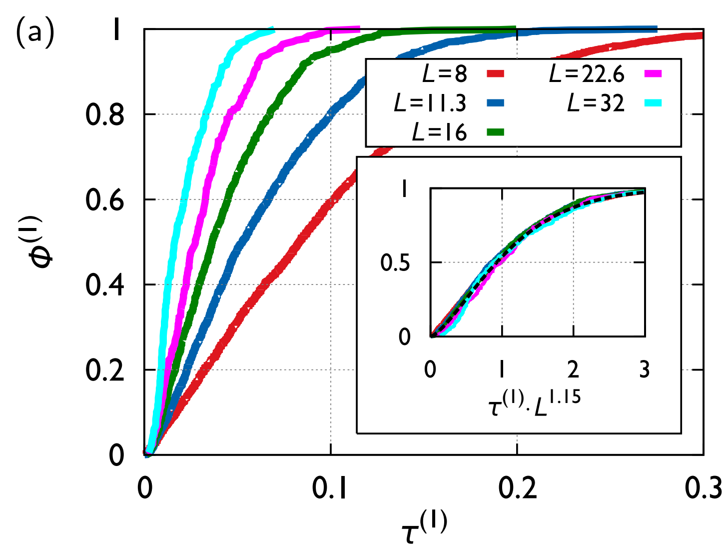
Local yield threshold distribution



- Number of links: $M \propto L^{1.6}$
- Average stress increment: $\Delta\tau \propto L^{-1.2}$
- Average strain jump: $\Delta\gamma \propto L^{-1.2}$
- Local yield thresholds are correlated

[Ispánovity, Tüzes, Szabó, Zaiser, Groma, PRB, (2017)]

Cumulative distribution of $\tau^{(1)}$



$$\Phi^{(1)}(\tau^{(1)}) = 1 - \exp\left(-\frac{1}{M}\left(\frac{\tau^{(1)}}{\tau_0}\right)^{\beta}\right)$$

Shape parameter: $\beta = 1.4$

Linear stability analysis

- EOM: $\dot{x}_i(t) = s_i \left[\tau_{\text{ext}} + \sum_{j \neq i} s_j \tau_{\text{xy}}(\boldsymbol{r}_i(t) - \boldsymbol{r}_j(t)) \right] =: f_i(t); \quad \dot{y}_i(t) = 0$
- El. energy: $E_{\text{el}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \frac{1}{2} \sum_{i,j=1, i \neq j}^{N} s_i s_j E_{\text{int}}(\boldsymbol{r}_i - \boldsymbol{r}_j)$

$$E_{\text{int}}(\boldsymbol{r}) = -\ln\left(\frac{r}{R}\right) - \frac{y^2}{r^2}$$

- Initially $\tau_{\text{ext}} = 0, x_i, \dot{x}_i = 0$ ⇒ $\tau_{\text{ext}} \neq 0, x_i + \Delta x_i, \dot{x}_i = 0$

$$-\sum_{j=1}^{N} \Lambda_{ij} \Delta x_j + \tau_{\text{ext}} s_i = 0$$, where $$\Lambda_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} E_{\text{el}}$$

dynamical matrix

[Derlet, Maass, PRE (2016)]

Linear stability analysis

- Dyn. matrix: $$\Lambda_{ij}(\boldsymbol{r}_1,\dots,\boldsymbol{r}_N)=\begin{cases}-s_i\sum_{j\neq i}s_j\partial_x\tau_{\text{xy}}(\boldsymbol{r}_i-\boldsymbol{r}_j), & \text{if } i=j,\\ s_is_j\partial_x\tau_{\text{xy}}(\boldsymbol{r}_i-\boldsymbol{r}_j), & \text{else.}\end{cases}$$
- Eigenmodes: $$\sum_{i=1}^{N}\Lambda_{ij}u_j^{(n)}=e^{(n)}u_i^{(n)}$$

$$\Delta x_i=\tau_{\text{ext}}\sum_n\frac{\sum_j s_ju_j^{(n)}}{e^{(n)}}u_i^{(n)}$$

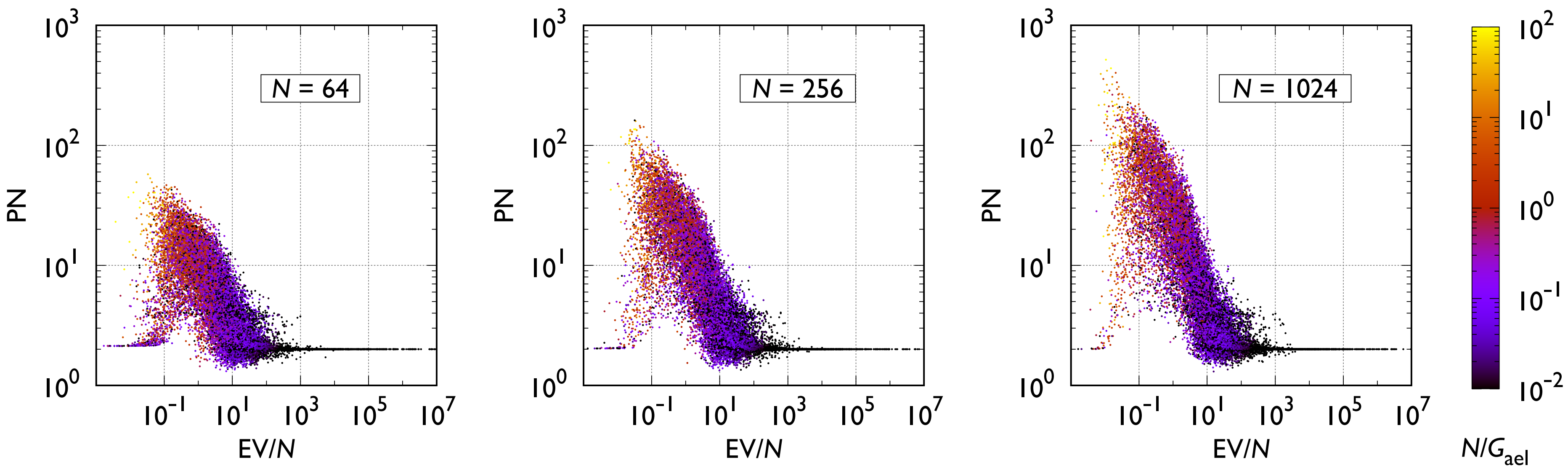
$$\Delta\gamma=\tau_{\text{ext}}\sum_n\frac{\left(\sum_j s_ju_j^{(n)}\right)^2}{e^{(n)}}=\tau_{\text{ext}}\sum_n\frac{1}{G_{\text{ael},n}}$$

- When one eigenvalue gets negative the satability analysis breaks down → event
- The displacements are proportional to the given eigenvector

[Derlet, Maass, PRE (2016)]

Spectrum

- Wide distribution of eigenvalues
- Participation number: $PN = \left[\sum_i \left(u_i^{(n)} \right)^4 \right]^{-1}$
- Large number of soft modes with large number of participant dislocations

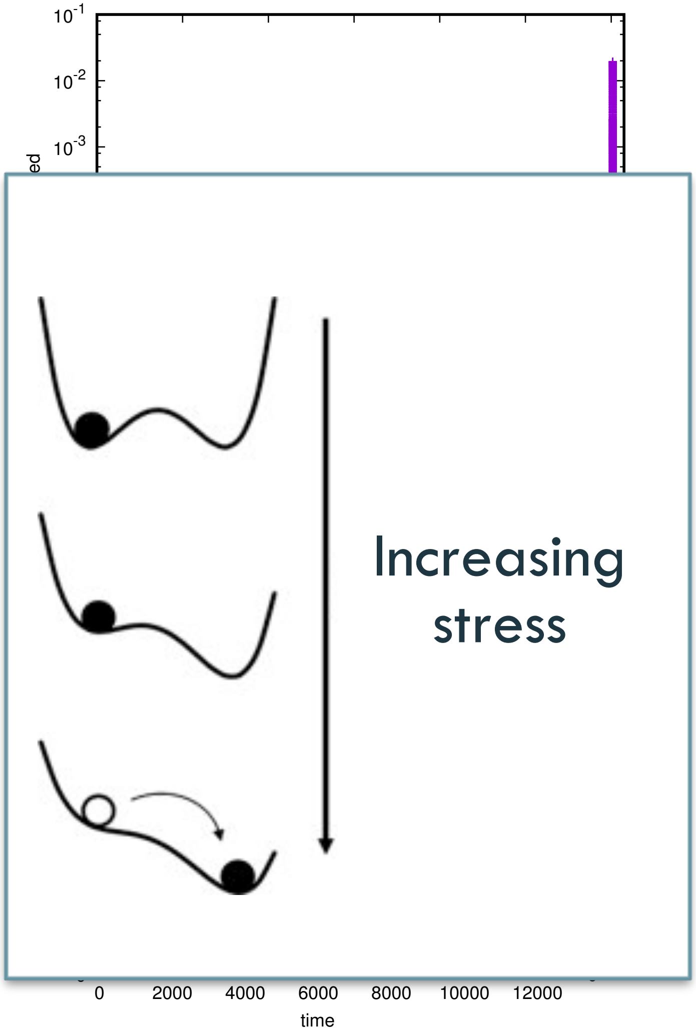


Individual events

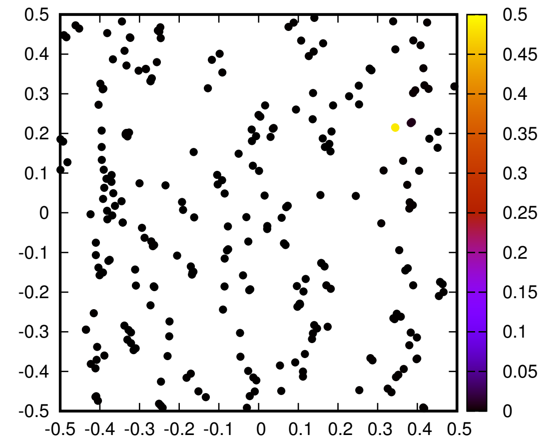
- $N = 256$
- Linear loading:

  $$\tau_{\text{ext}} \propto t$$

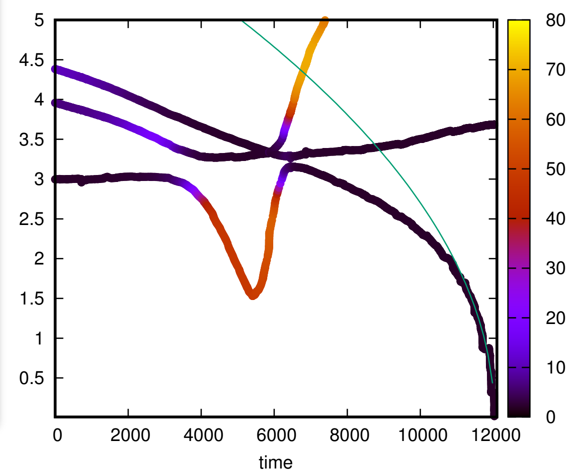
- Color code: PN
- Small event
  - Invloves a single dislocation dipole
- Close to instability: fold catastrophe



(c)



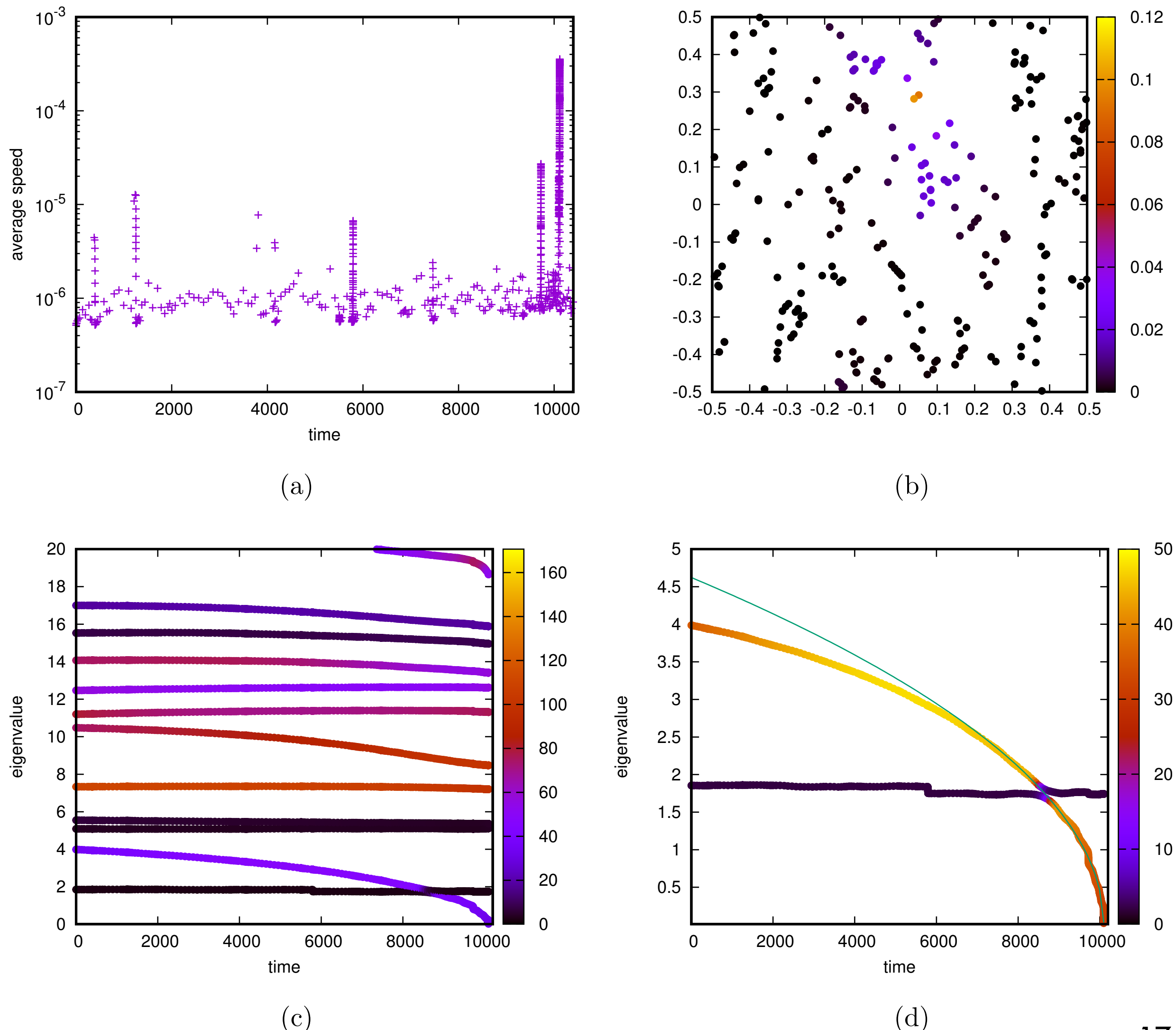
(b)



(d)

Individual events

- Large event
  - Invloves ~40 dislocations
- Close to instability: fold catastrophe



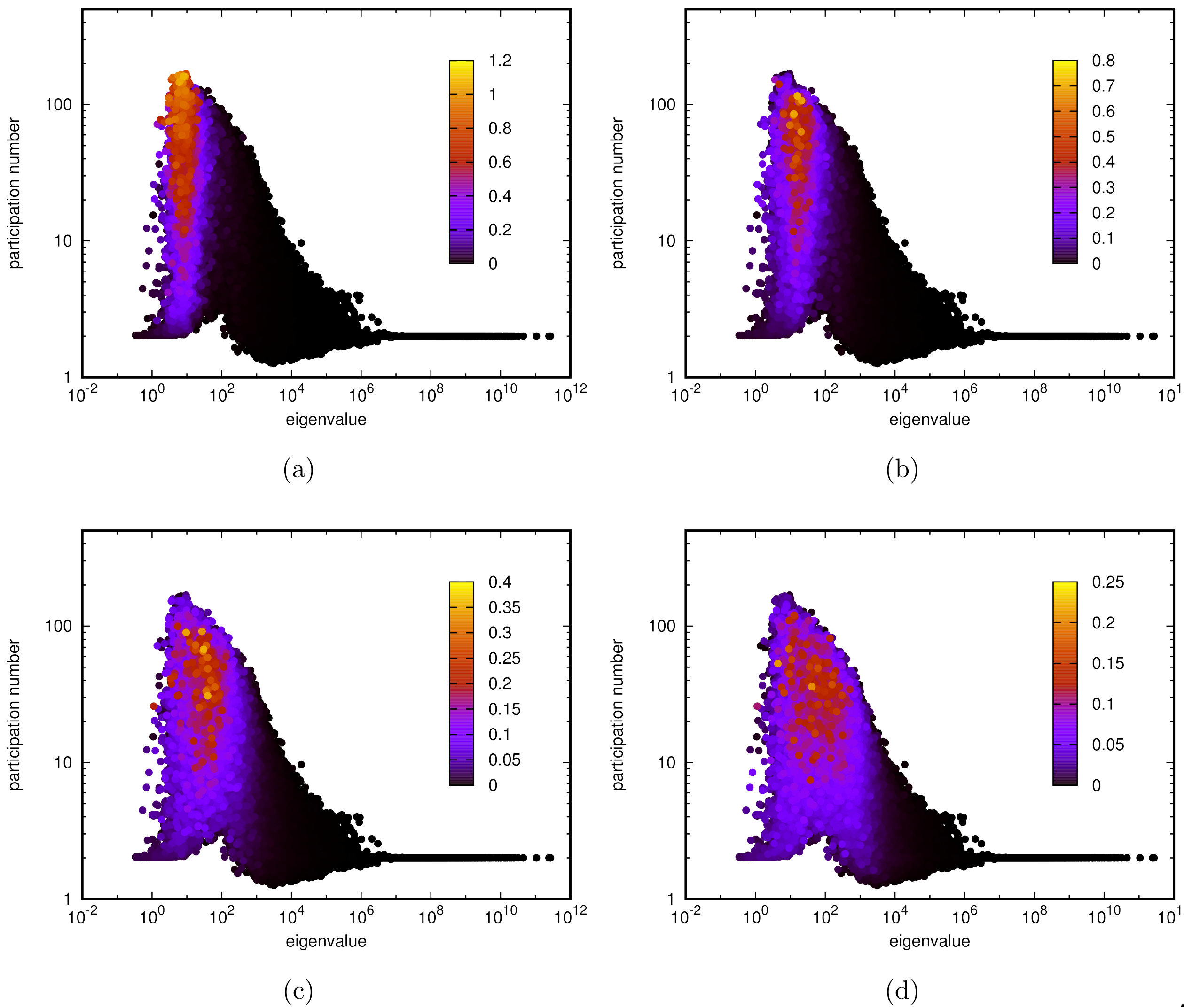
(a) (b) (c) (d)

Spatial structure

Color code:

Fourier weight corresponding to wavelenghts

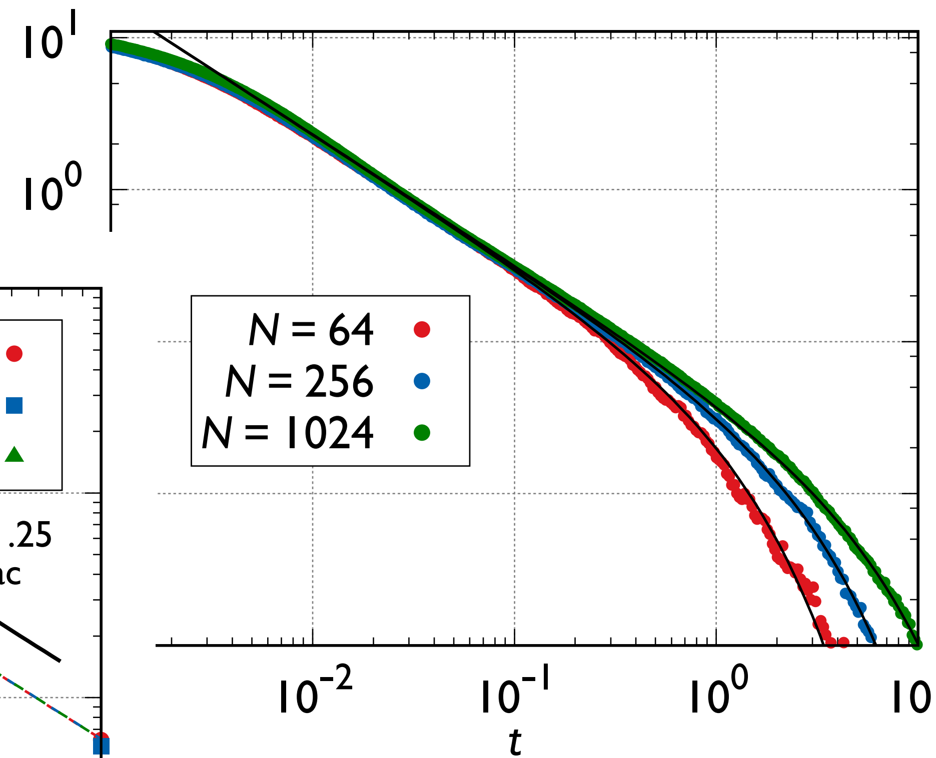
$k_x = 2\pi n / L$

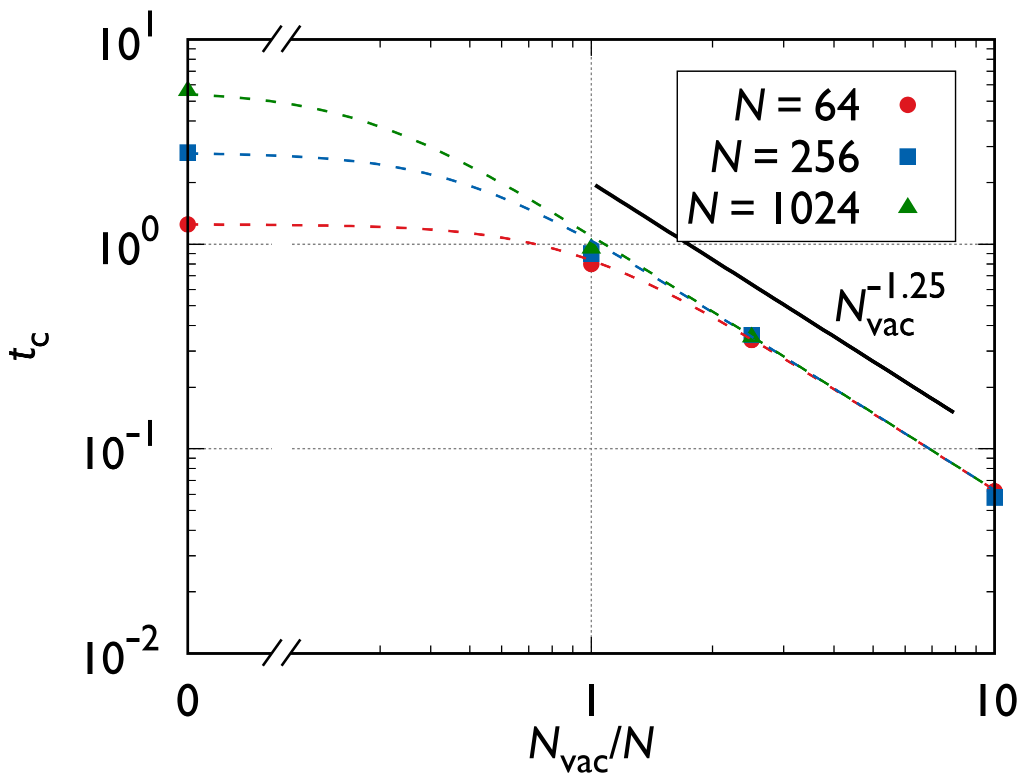


Addition of quenched disorder

- Quenched pinning points with short-range potential:

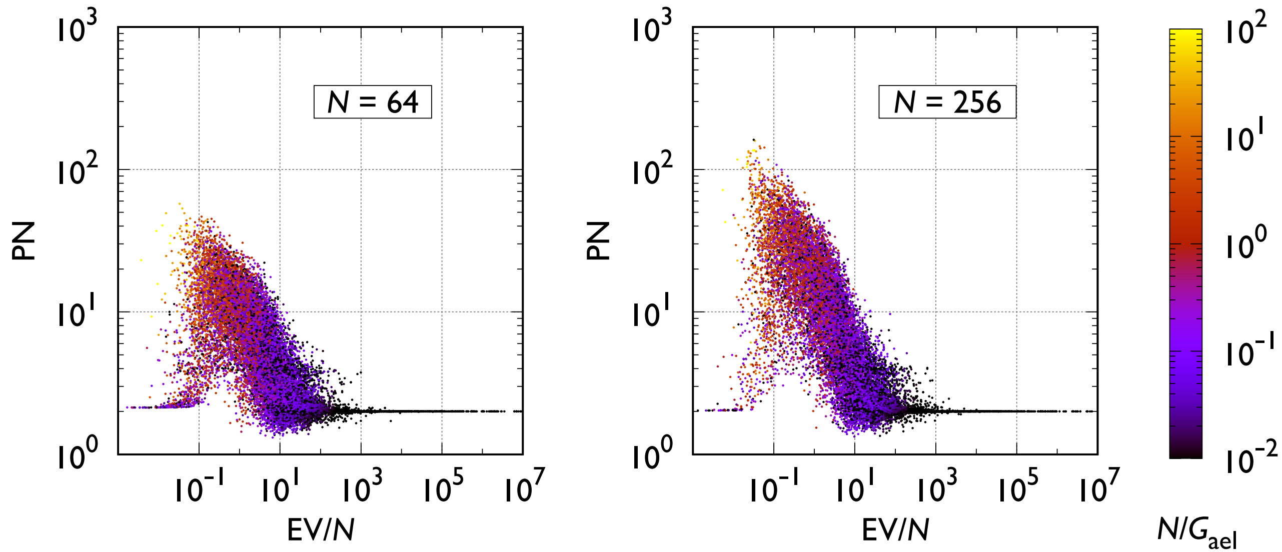
$$U(\boldsymbol{r}) = A\frac{\sin\varphi}{\ldots}\left(1 - e^{-k^2 r^2}\right)$$



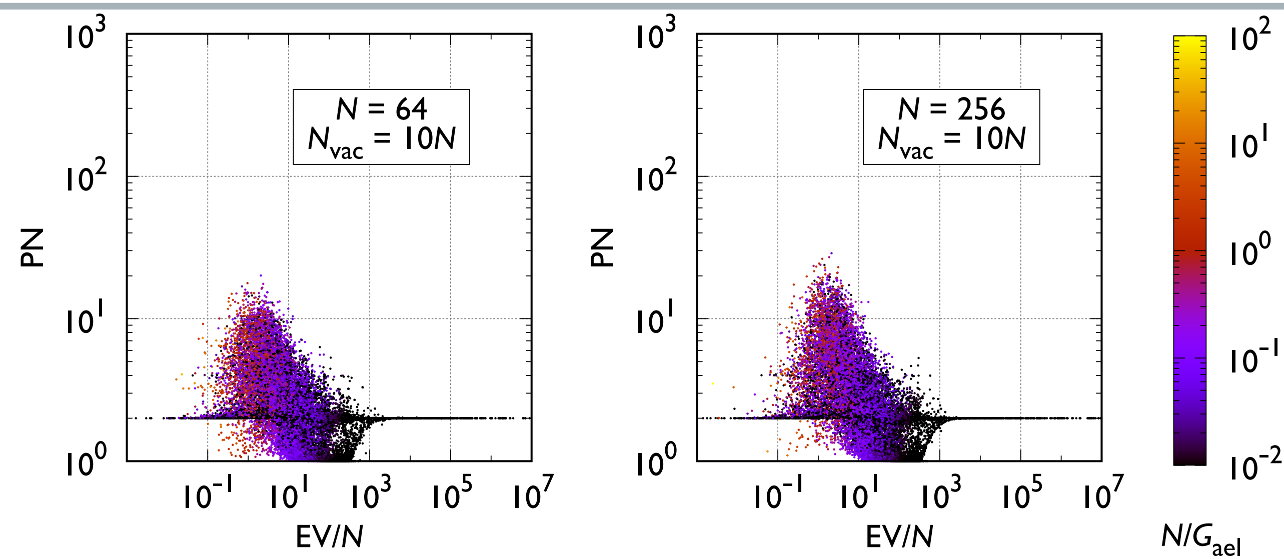


Spectra

Without pinning



With pinning



Summary

- Dynamical matrix describes local heterogeneities of the energy landscape
- Transition from extended to depinning-like criticality
- Opens new possibilities to understand system dynamics:
  - Exploring relevant internal length scales through dynamical correlations
    - Long- and short-range, RVE in stochastic modelling
  - Predictions of avalanches
  - Local yield threshold distribution
  - Additional effects: Peiers-stress (friction) or multiple slip systems
  - Can be generalized to 3D systems