Multiscale modelling of dislocation patterning

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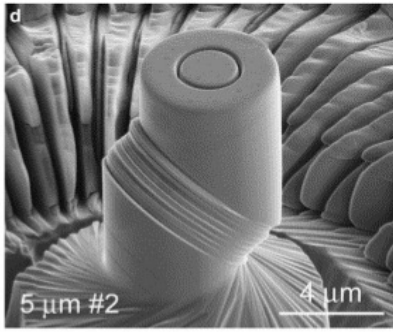
Motivation

- Crystal plasticity is undoubtedly a critical phenomenon
  - Power-law distributions, scaling laws
  - Details unclear
- Complex system far from equilibrium

- Dislocations tend to form patterns
  - Various patterns under different conditions
  - Details unclear
- Complex system far from equilibrium



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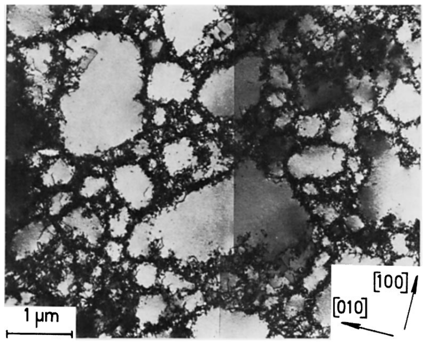


Outline

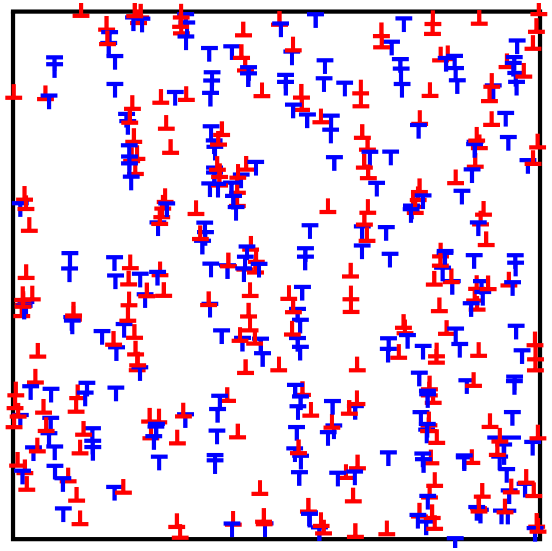
- Properties of 2D dislocation systems
  - Avalanche distributions – extended criticality
  - Formation of dipolar walls
- Continuum modelling
  - Stochastic modelling
  - Deterministic continuum models
- 2D stochastic continuum framework
  - Evolution equations – backstress, flow stress
  - Dipolar wall formation
  - Comparison with DDD
- Summary

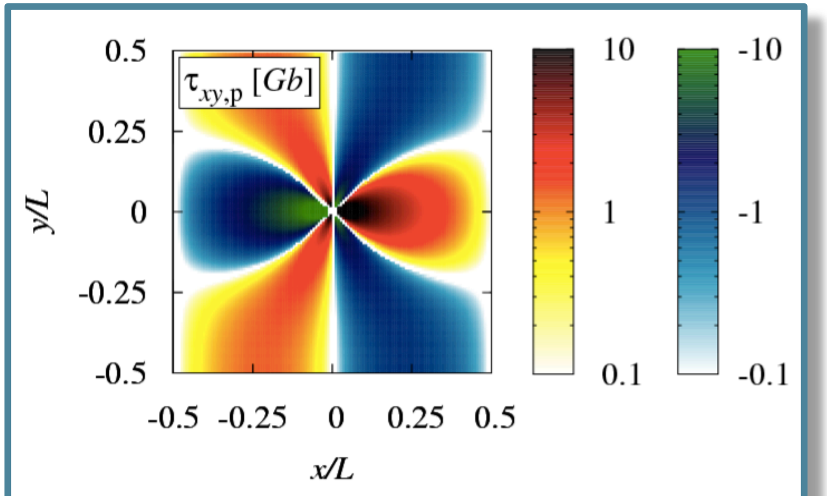
2D dislocation model

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: σ_{xy}
- Overdamped motion:

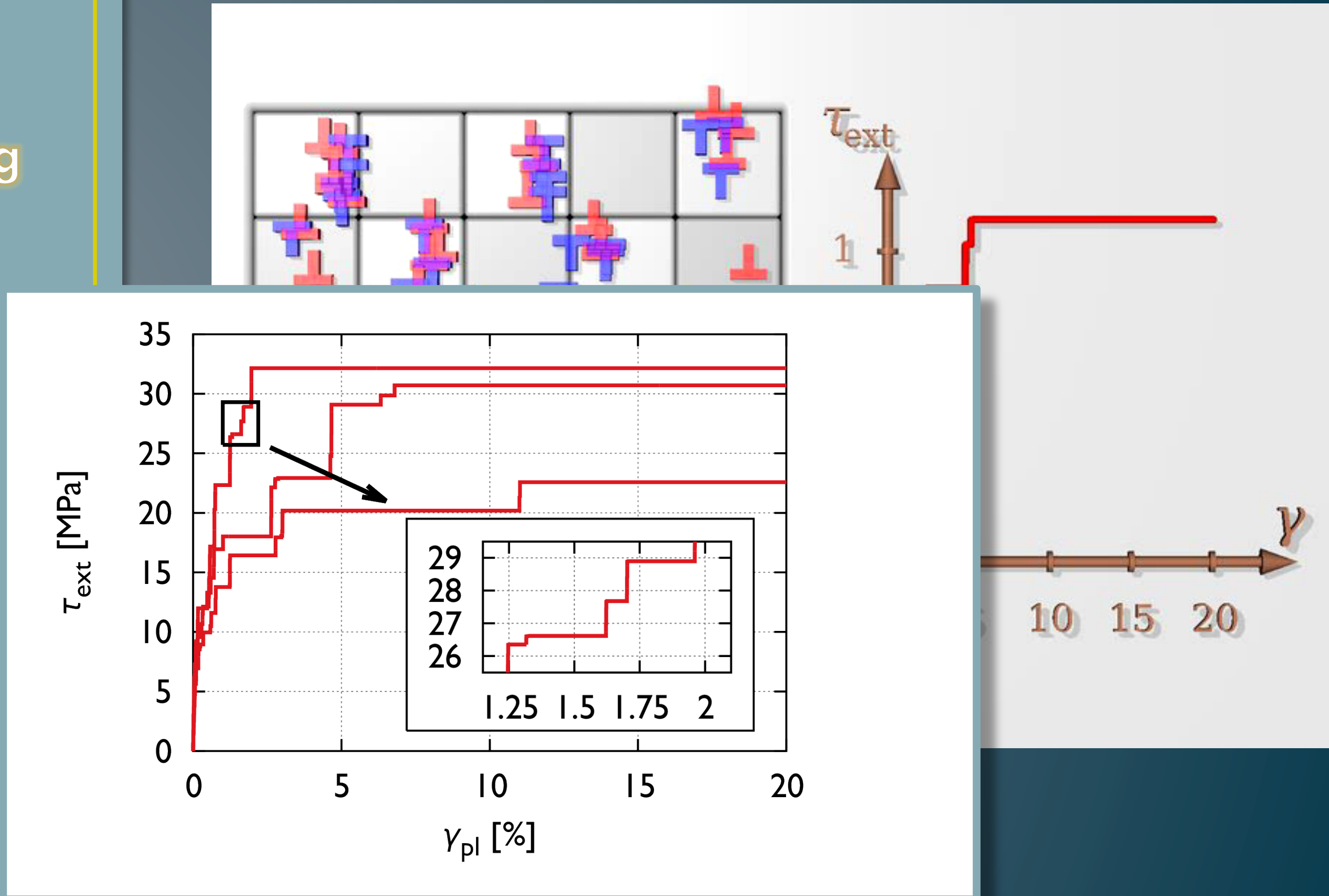
$$\dot{x}_i = s_i \left[\sigma_{\text{ext}} + \sum_{i=1}^{N} s_j \sigma_{xy}(\boldsymbol{r}_i - \boldsymbol{r}_j) \right]$$





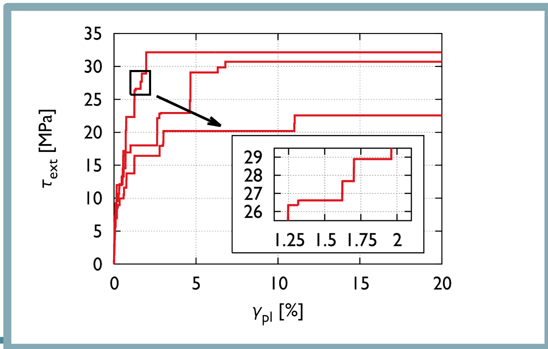
Plastic shearing in 2D

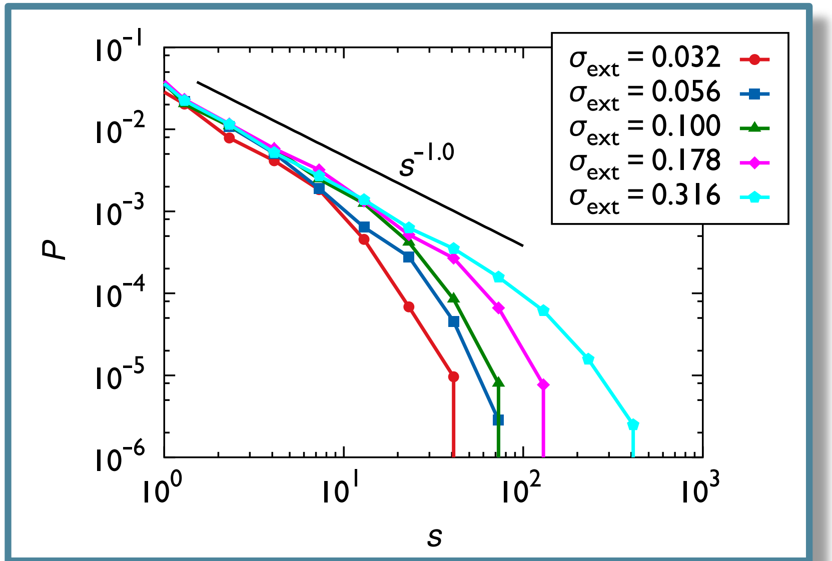
- Initial relaxati[cut off]
  step
- Quasi-static
  stress increase



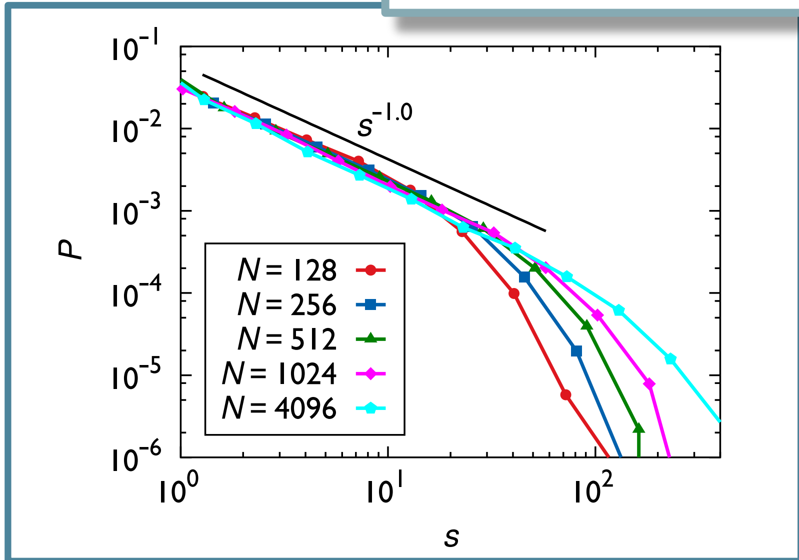
Strain burst distributions

- Avalanche size *s* is the total area swept
- System size: $L = \sqrt{N}$





Dependence on the applied stress (N = 4096)

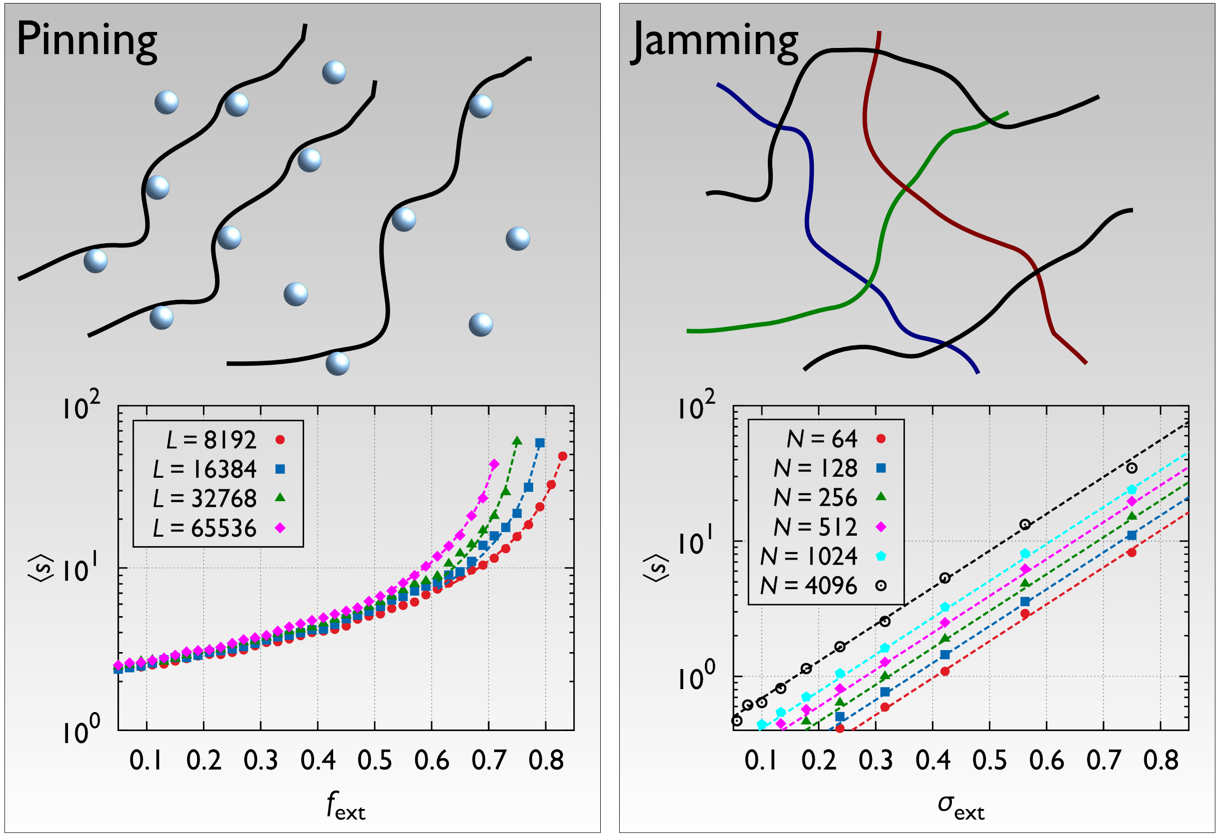


Dependence on the system size (σ_{ext} = 0.316)

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

Extended criticality

- The system is always critical
  - Other indications (relaxation, system size scaling, pseudo gap)
  - 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

Conclusions of 2D results

Disadvantages

- Toy model
- No multiple slip
- No short-range interactions
- No curvature

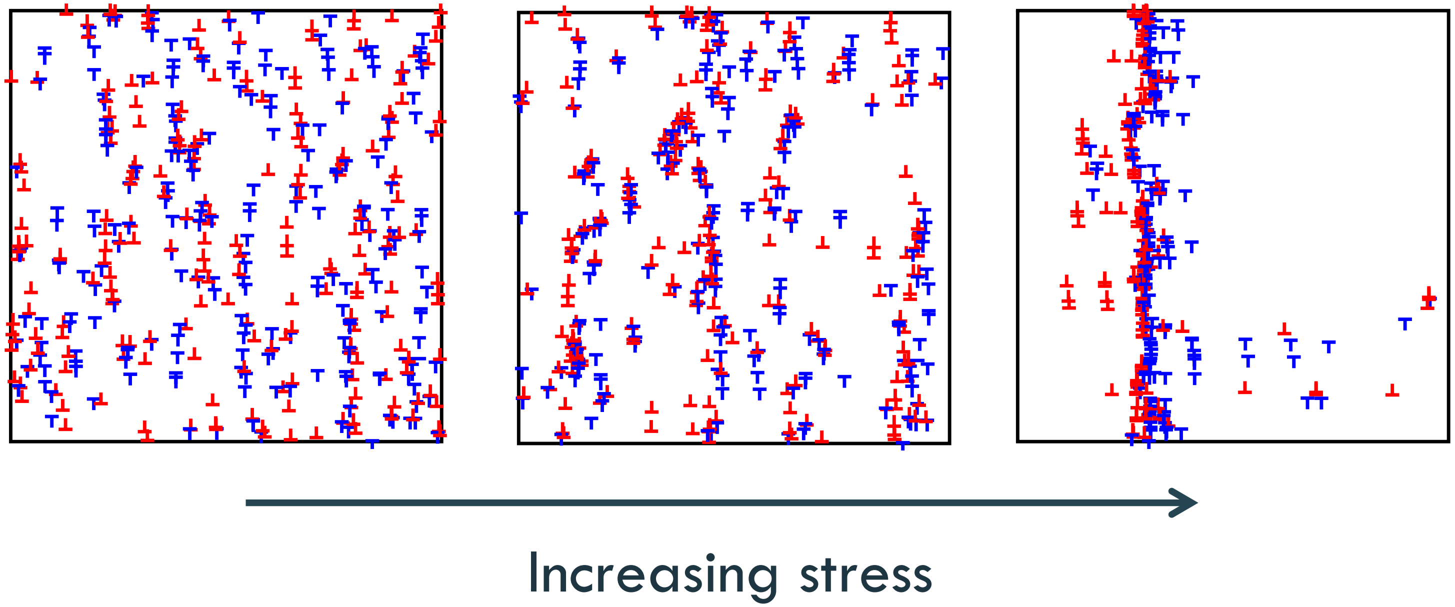
Advantages

- Toy model
  - Numerically feasible
  - Theoretically feasible
- Dislocations
  - Long-range interactions
  - Constrained motion

- The 2D system is a limiting case theoretical models should be capable of describing
- It is ideal for developing concepts and methods for describing and understanding collective phenomena

Pattern evolution in 2D DDD

- With increasing stress dipolar walls form
- These are the 'strongest' objects in 2D single slip

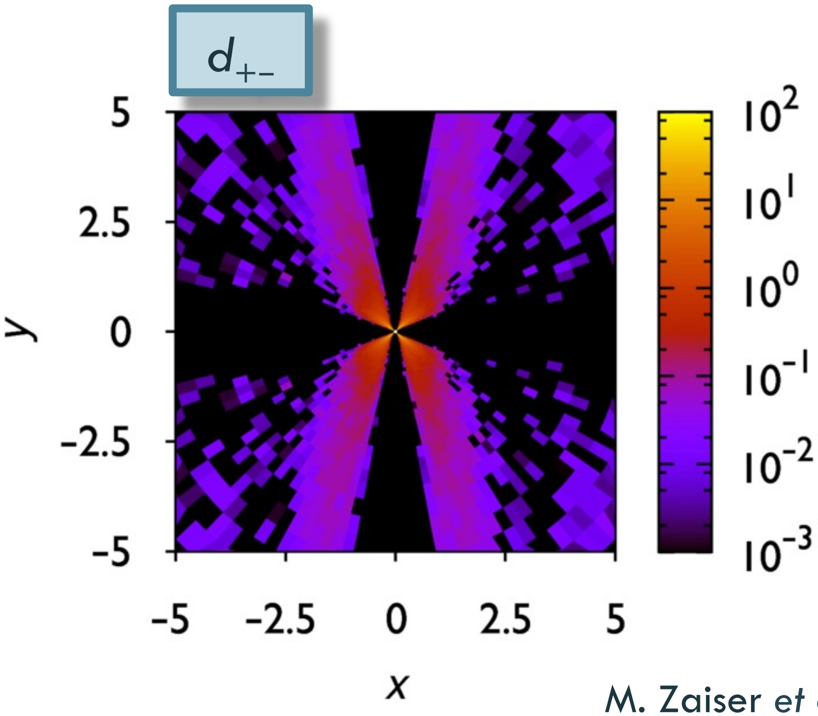


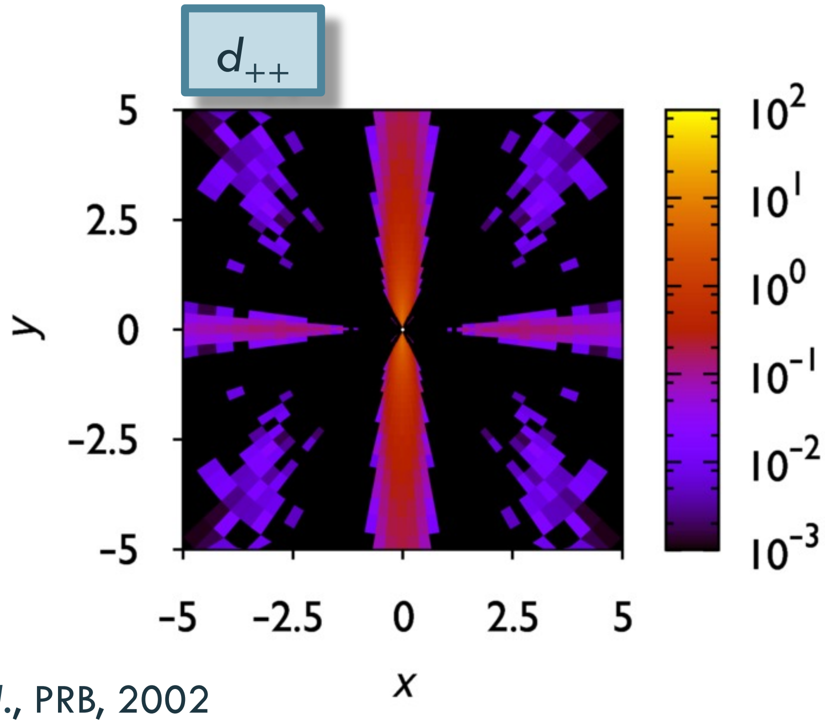
C Zhou, C Reichhardt, CJO Reichhardt, IJ Beyerlein, Sci Rep, 2015

P Szabó, PD Ispánovity, I Groma, PRB, 2015

Spatial correlation functions

- Correlation functions: dislocation density around a randomly chosen positive sign dislocation
  - d_{+-} : relative density of the negative sign dislocations
  - d_{++}: relative density of the positive sign dislocations





M. Zaiser *et al.*, PRB, 2002

Continuum modelling of dislocations

Stochastic elastoplastic models

- Aim: modelling strain bursts
  - Local yield threshold distributions

Continuum dislocation dynamics

- Aim: modelling local strain evolution and patterns
  - Local dislocation density fields
    - Deterministic

Stochastic plasticity models

2D continuum equations

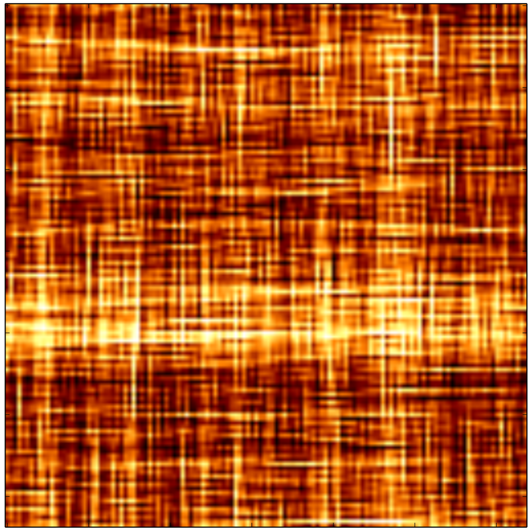
Assuming $\rho = \text{const.}$

Evolution equation for plastic strain

$$\dot{\gamma} = \rho b M_0 (\tau_{\text{mf}} - \tau_{\text{f}})$$

Considering τ_{f} *as a stochastic variable*

Stochastic CA model for plasticity



Strain pattern upon shear

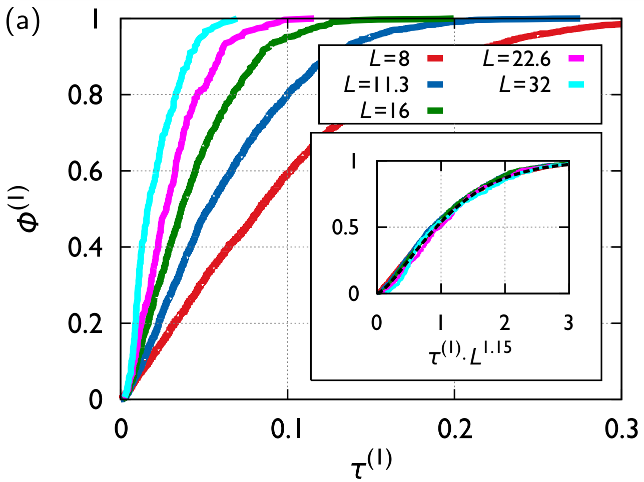
M Zaiser, P Moretti, J Stat Mech, 2005
S Sandfeld et al, J Stat Mech, 2015

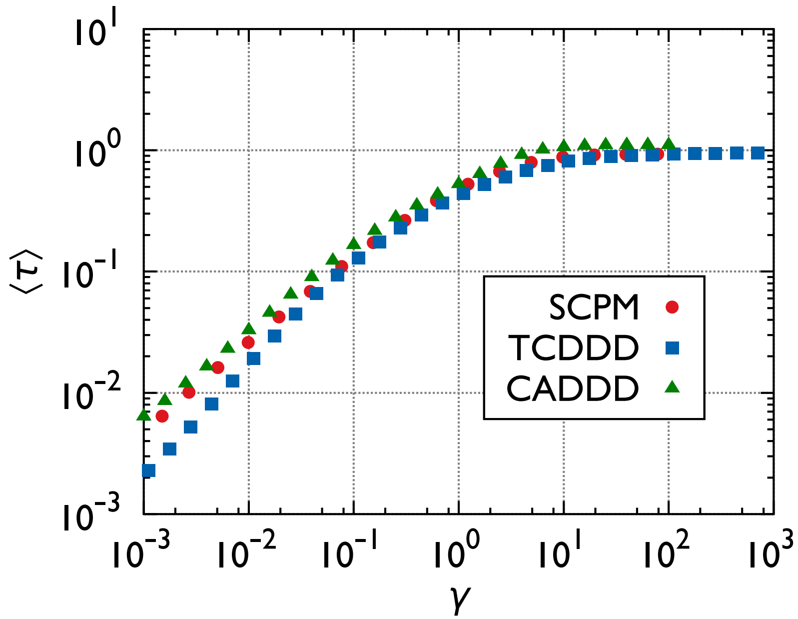
Setting the yield threshold distribution

The distribution of the stress at the first strain burst

- Shape parameter: $\beta = 1.4$

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



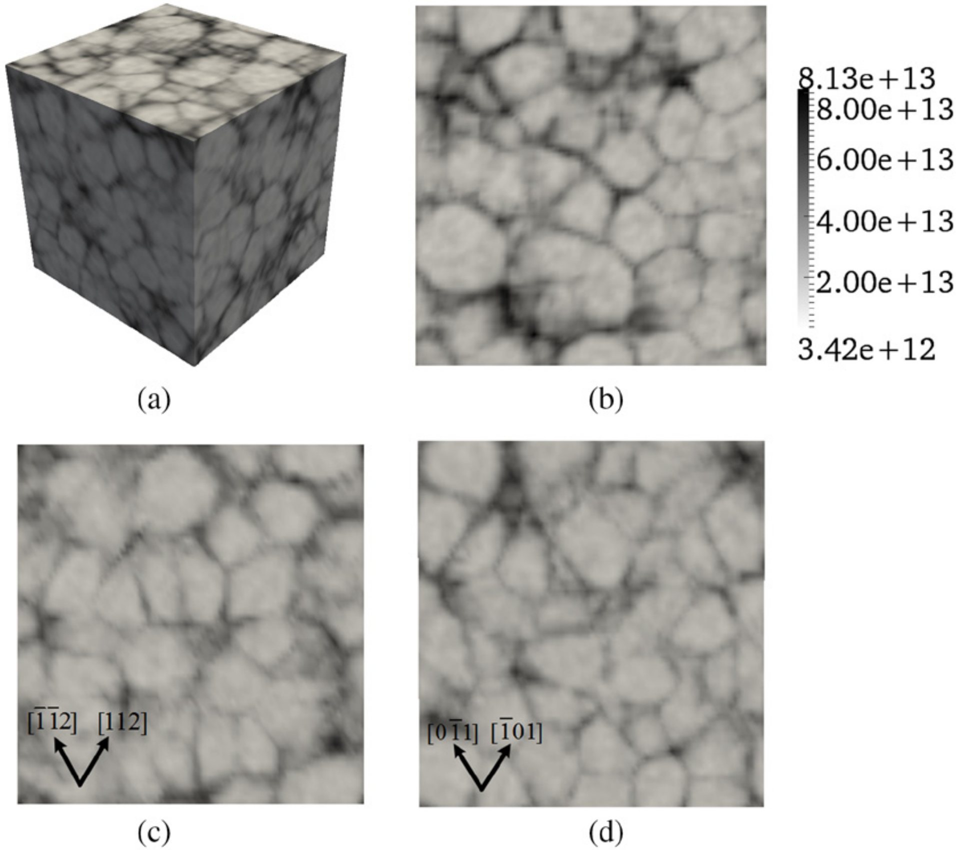


$$\Phi^{(1)}(\tau^{(1)}) = 1 - \exp\left(-\frac{1}{M}\left(\frac{\tau^{(1)}}{\tau_0}\right)^{\beta}\right)$$

PD Ispánovity, D Tüzes, P Szabó, M Zaiser, I Groma, PRB, 2017

Continuum modelling of cell structures I.

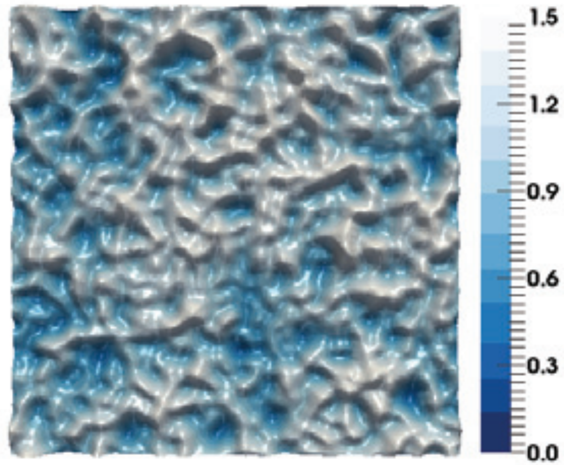
- Mean-field 3D continuum dislocation dynamics model
- Enabling cross-slip leads to the formation of a cell structure



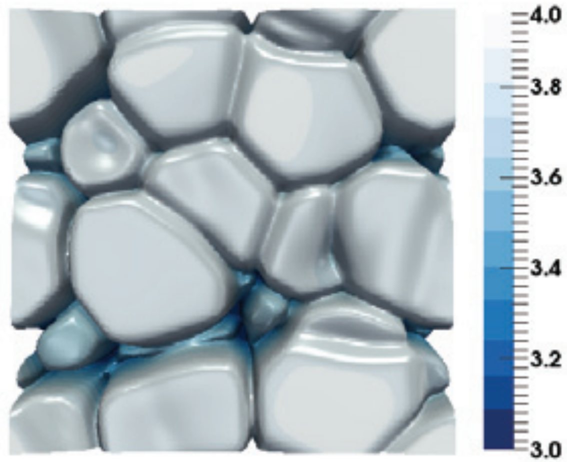
S. Xia and A El-Azab, Mod Simul Mater Sci Eng, 2015

Continuum modelling of cell structures II.

- CDD model of Hochrainer and co-workers
- Neglecting elastic stress interactions and keepeng a Taylor-like friction stress leads to a cellular pattern



Initial

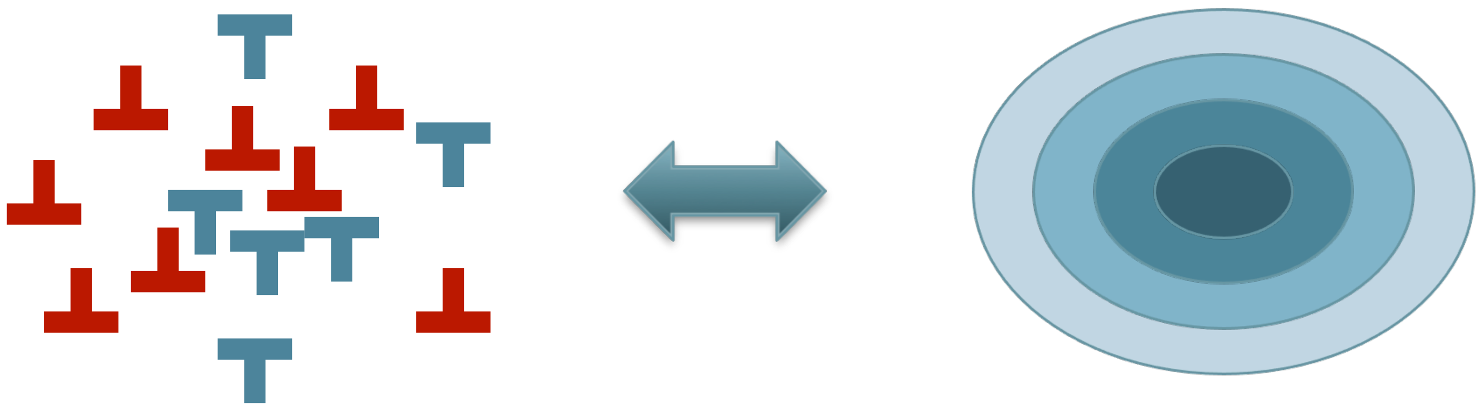


Stationary

S Sandfeld, M Zaiser, Mod Simul Mater Sci Eng, 2015

Objectives

- Multiscale modelling of dislocation patterning
  - Quantitative comparison of *discrete* and *continuum* models
  - Validation of the continuum model, e.g. back-stress
  - Systematic determination of the fitting parameters of the continuum model
  - Simplest case: 2D single slip



Discrete representation | Continuum representation

Continuum models

- Evolution equations of dislocation densities

$$\partial_t \rho_i + \nabla \boldsymbol{j}_i = f_{\mathrm{reaction}}(\rho_i, \tau_{\mathrm{ext}}, \dots)$$

  - ρ_i: some scalar dislocation density field
  - $\boldsymbol{j}_i$: flux of the given density
  - f_{reaction}: multiplication, annihilation, cross-slip, etc.

- Question:
  - What scalar densities to use?
  - What is the reaction term?
  - How to compute the fluxes?

- In 2D single slip:
  - SSD (ρ) and GND (κ) densities?
    - $\rho = \rho_+ + \rho_-$
    - $\kappa = \rho_+ - \rho_-$
  - No multiplication, no annihilation

Continuum model of Groma

Equation of motion of individual dislocations

↓ *Coarse graining*

Hierarchy of *N*-body densities

↓ *Assumption of short range correlations*

Closed set of evolution equations for ρ and κ

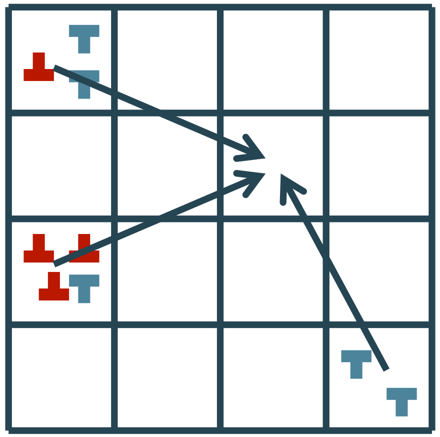
I Groma, Phys Rev B, 1997

I Groma, M Zaiser, FF Csikor, Acta Mater, 2003

I Groma, M Zaiser, PD Ispánovity, PRB, 2016

Evolution equations w/o correlations

$$\partial_t \rho(\boldsymbol{r},t) = -M_0 b \partial_x [\kappa \tau_{\mathrm{mf}}]$$
$$\partial_t \kappa(\boldsymbol{r},t) = -M_0 b \partial_x [\rho \tau_{\mathrm{mf}}]$$



- M_0 : dislocation mobility
- b : Burgers vector
- τ_{mf} : mean-field stress
  - External load & long-range stresses generated by the GNDs

$$\tau_{\mathrm{mf}}(\boldsymbol{r},t) = \tau_{\mathrm{ext}} + \int \kappa(\boldsymbol{r}-\boldsymbol{r}')\tau_{\mathrm{ind}}(\boldsymbol{r}')\mathrm{d}^2 r'$$

  - Measurable quantity: the average local stress around a dislocation
  - Plastic strain: $\partial_t \kappa(\boldsymbol{r},t) = -(1/b)\partial_x \dot{\gamma}(\boldsymbol{r},t)$

I Groma, P Balogh, Acta Mater, 1999

Evolution equations with correlations

$$\partial_t \rho(\boldsymbol{r},t) = -M_0 b \partial_x [\kappa \tau_{\mathrm{mf}} - \kappa \tau_{\mathrm{b}} + \rho \tau_{\mathrm{d}}]$$

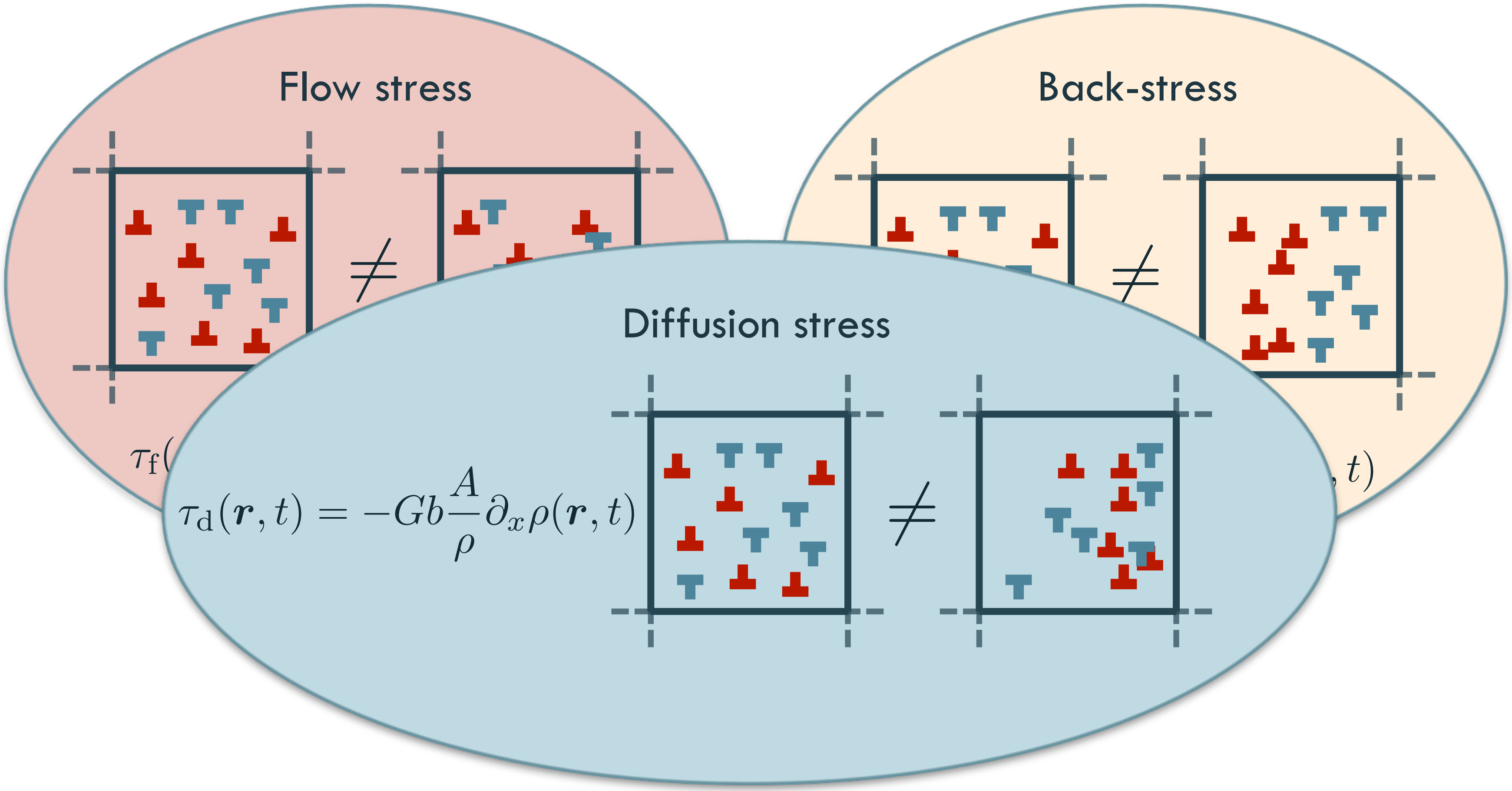
$$\partial_t \kappa(\boldsymbol{r},t) = -M_0 b \partial_x \left[\rho \tau_{\mathrm{mf}} - \rho \tau_{\mathrm{b}} - \rho \left(1 - \frac{\kappa^2}{\rho^2}\right) \tau_{\mathrm{f}} + \kappa \tau_{\mathrm{d}}\right]$$

- Back-stress: $\tau_{\mathrm{b}}(\boldsymbol{r},t) = -Gb\frac{D}{\rho}\partial_x \kappa(\boldsymbol{r},t)$
- Diffusion stress: $\tau_{\mathrm{d}}(\boldsymbol{r},t) = -Gb\frac{A}{\rho}\partial_x \rho(\boldsymbol{r},t)$
- Flow stress: $\tau_{\mathrm{f}}(\boldsymbol{r},t) = \alpha \mu b \sqrt{\rho(\boldsymbol{r},t)}$
- Dimensionless fitting parameters: $D,\ A,\ \alpha$

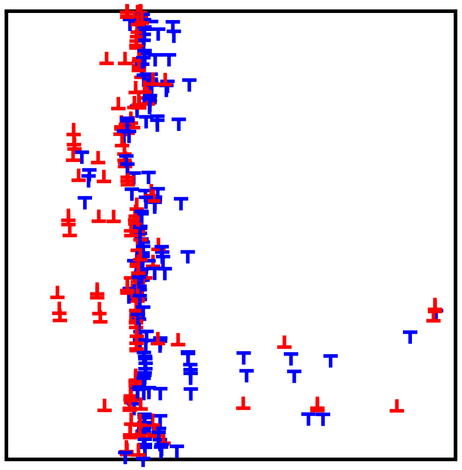
I Groma, M Zaiser, PD Ispánovity, Phys Rev B, 2016

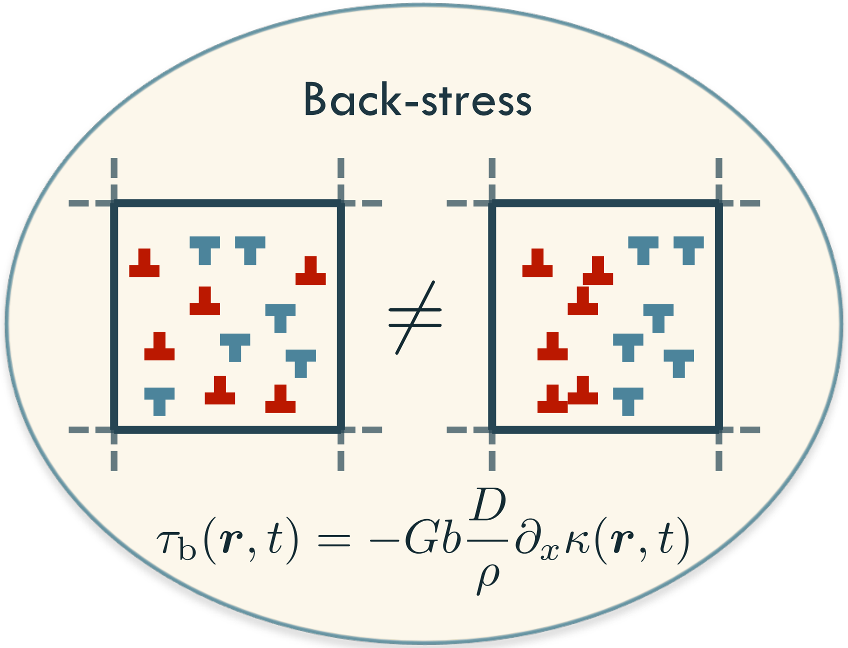
Correlation induced stress terms

- The *representative volume element* (RVE) cannot resolve internal correlations



Strength of a dipolar wall





- In the middle of a dipolar wall: $\partial_x \rho = 0$ and $\partial_x \kappa < 0$
- The back-stress must be negative

$$D < 0$$

Implementation

$$\partial_t \rho(\boldsymbol{r}, t) = -M_0 b \partial_x [\kappa \tau_{\mathrm{mf}} + \kappa \tau_{\mathrm{b}} + \rho \tau_{\mathrm{d}}]$$

$$\partial_t \kappa(\boldsymbol{r}, t) = -M_0 b \partial_x \left[\rho \tau_{\mathrm{mf}} + \rho \tau_{\mathrm{b}} - \rho \left(1 - \frac{\kappa^2}{\rho^2}\right) \tau_{\mathrm{f}} + \kappa \tau_{\mathrm{d}}\right]$$

- CA implementation with extremal dynamics
- Dimensionless fitting parameters: D, A, α
- Flow stress is a stochastic variable
- No phenomenological assumptions

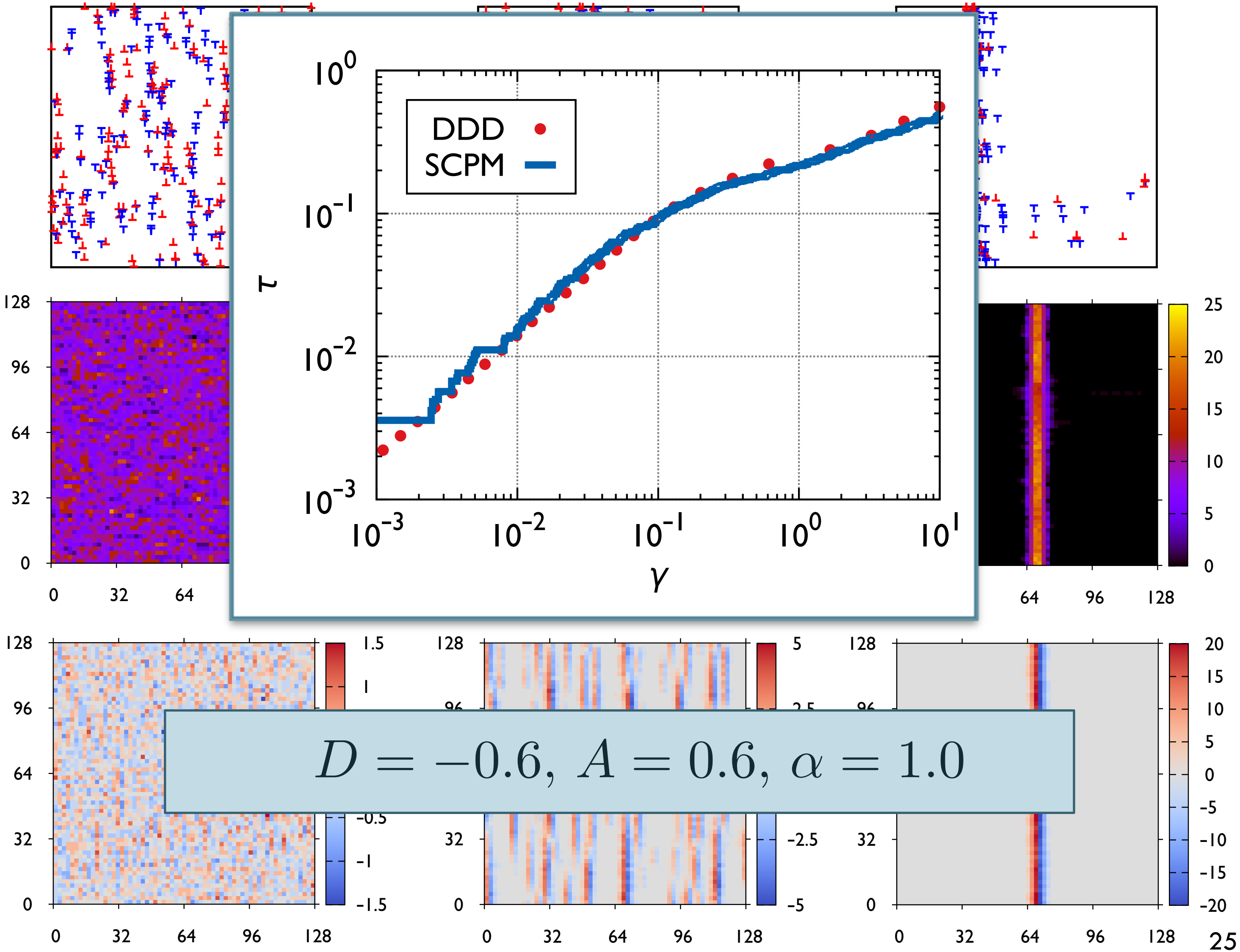
PD Ispánovity, D Tüzes, P Szabó, M Zaiser, I Groma, arXiv, 2016

Evolution of density patterns

DDD configuration

Continuum total density ρ

Continuum GND density κ



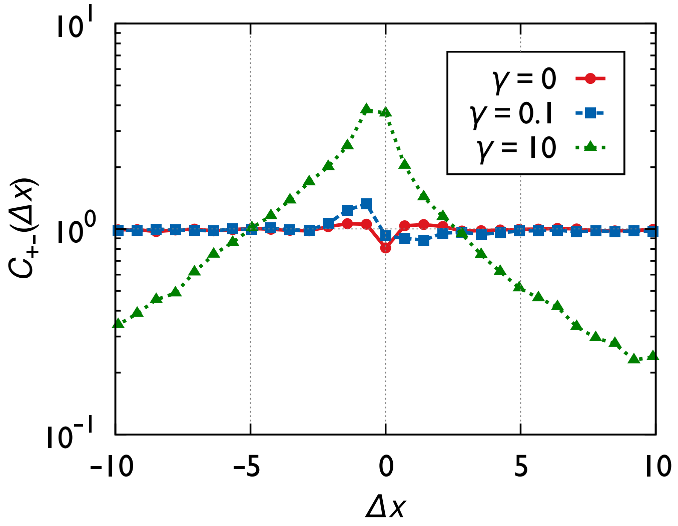
$$D = -0.6,\ A = 0.6,\ \alpha = 1.0$$

Characterization of pattern

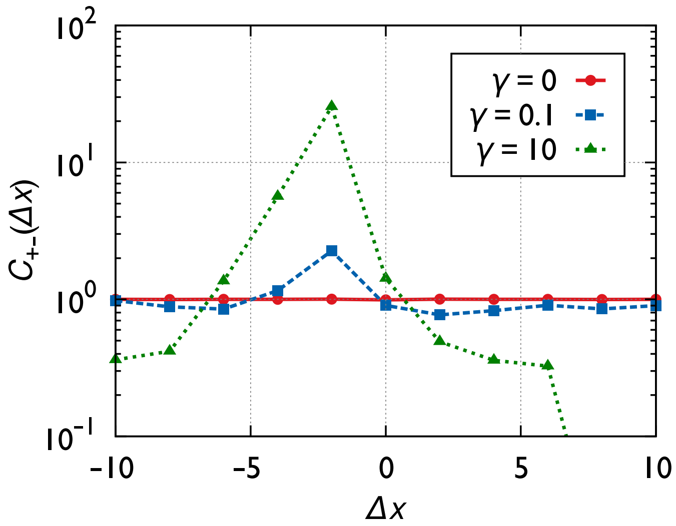
- Cross-correlation of + and – sign dislocations

$$C_{+-}(\Delta x, \Delta y) = \int \rho_+(x', y')\rho_-(x' + \Delta x, y' + \Delta y)\mathrm{d}x'\mathrm{d}y'$$

- $C_{+-}(\Delta x) := \langle C_{+-}(\Delta x, \Delta y)\rangle_{\Delta y}$:

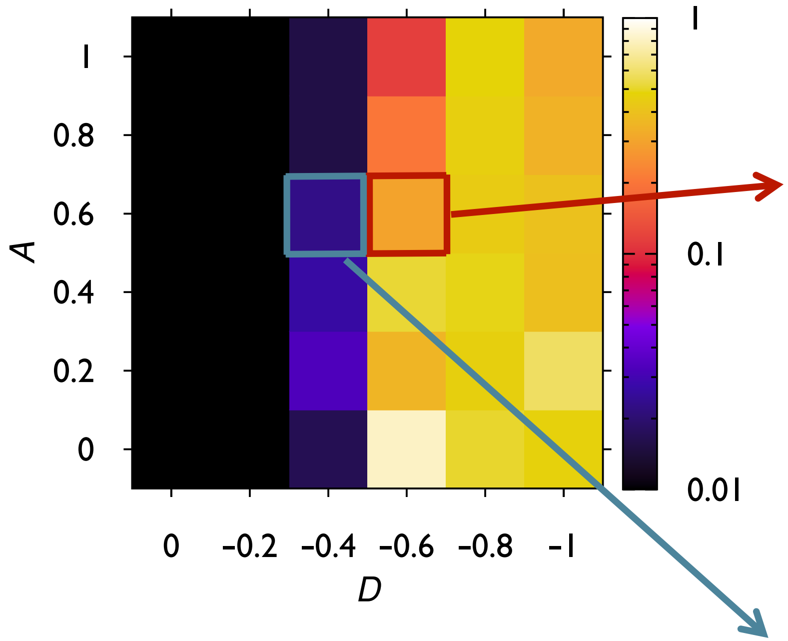


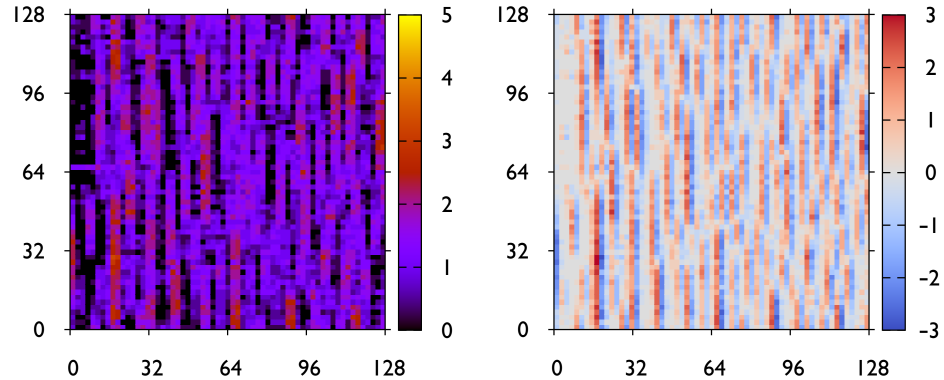
DDD



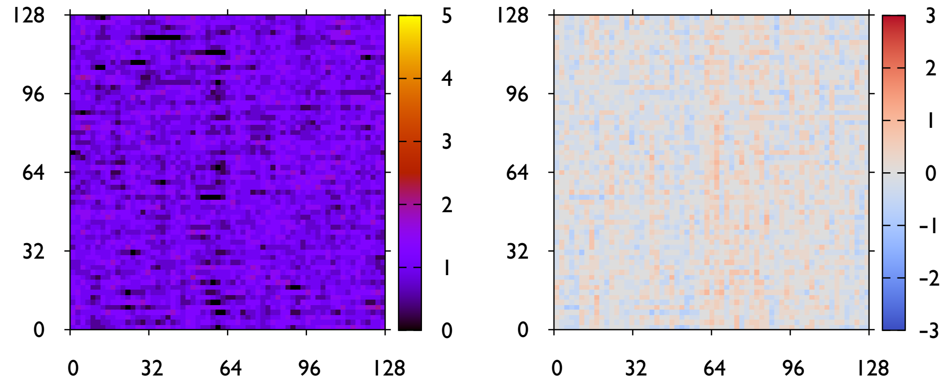
CDD

Effect of parmeter *D*





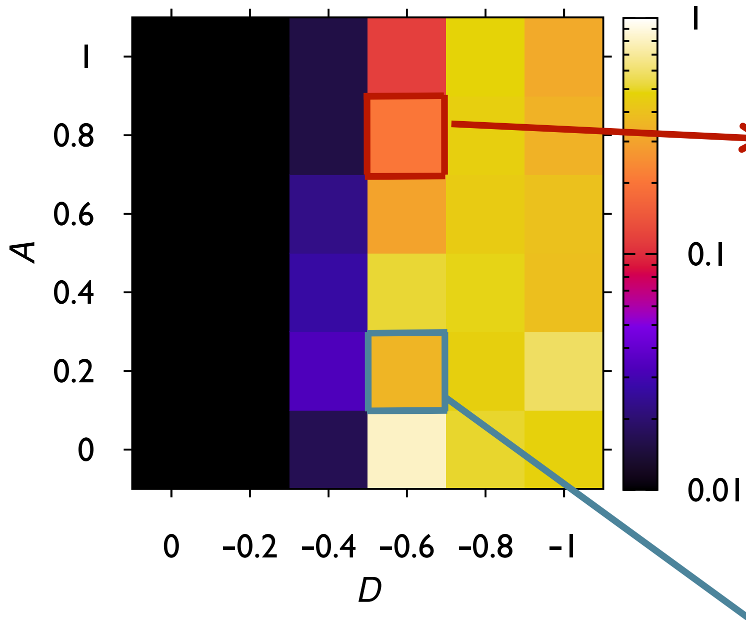
$D = -0.6$

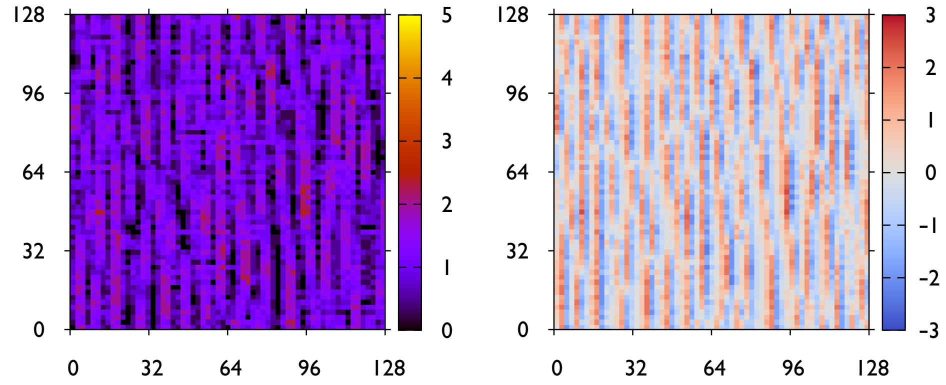


$D = -0.4$

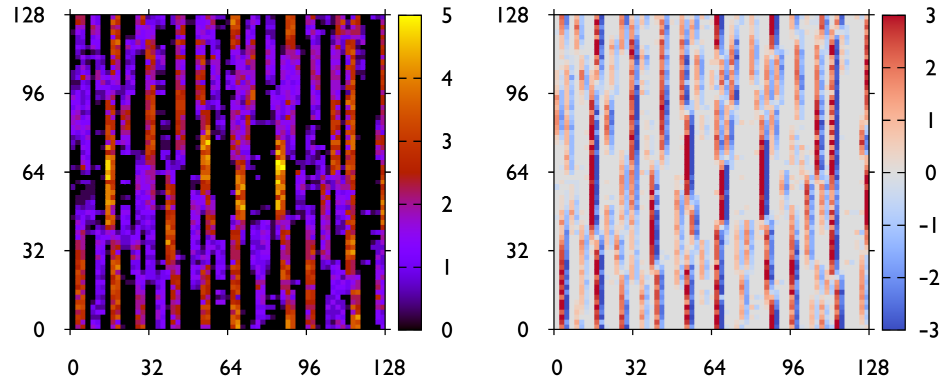
- Order parameter: level of asymmetry in $C_{+-}(\Delta x)$

Effect of parmeter *A*





$A = 0.8$



$A = 0.2$

- Order parameter: level of asymmetry in $C_{+-}(\Delta x)$

Summary

- 2D DDD is a simple toy model with very complex dynamics
  - Extended criticality
  - Anomalous system size dependence
- 2D continuum theory of dislocation dynamics
  - Derived analytically from the Eqs. of motion of discrete dislocations
  - There are no phenomenological assumptions, the gradient terms naturally emerge
  - Gradient terms are related to features of the microstructure: back-stress – dipolar walls
- The 2D continuum theory properly captures the patterning and the strain response of 2D DDD simulations
- Inclusion of back-stress is necessary for pattern formation