Multiscale modelling of dislocation patterning

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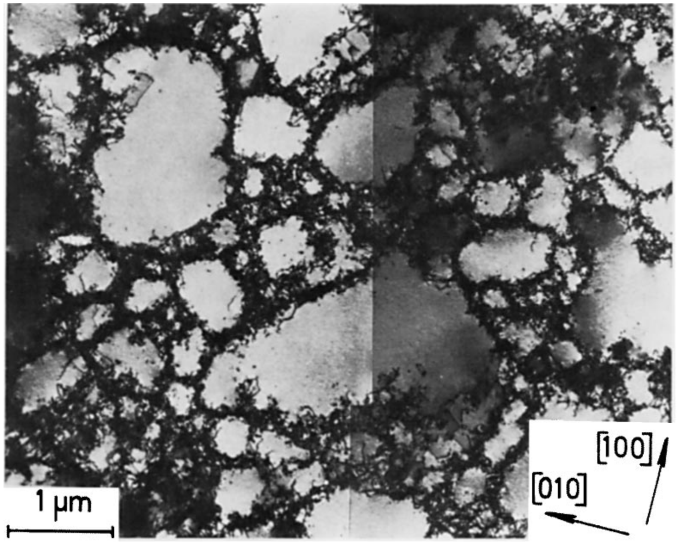
Motivation – dislocation patterns

- Multitude of observed dislocation patterns
  - Fractal, periodic, etc.
  - Crucial impact on plastic properties
  - May lead to strain localization and failure of the material



H Mughrabi, F Ackermann, K Herz, STP675, 1979

H Mughrabi, T Ungár, W Kienle, M Wilkens, Philos Mag, 1986

Dynamic modelling of PSBs

- Reaction-diffusion model:

$$\partial_t \rho_\mathrm{i} = D_\mathrm{i} \partial_x^2 \rho_\mathrm{i} + g(\rho_\mathrm{i}) - \bar{P}\rho_\mathrm{i} + c\rho_\mathrm{m}\rho_\mathrm{i}^2$$

$$\partial_t \rho_\mathrm{m} = D_\mathrm{m} \partial_x^2 \rho_\mathrm{m} + \bar{P}\rho_\mathrm{i} - c\rho_\mathrm{m}\rho_\mathrm{i}^2$$

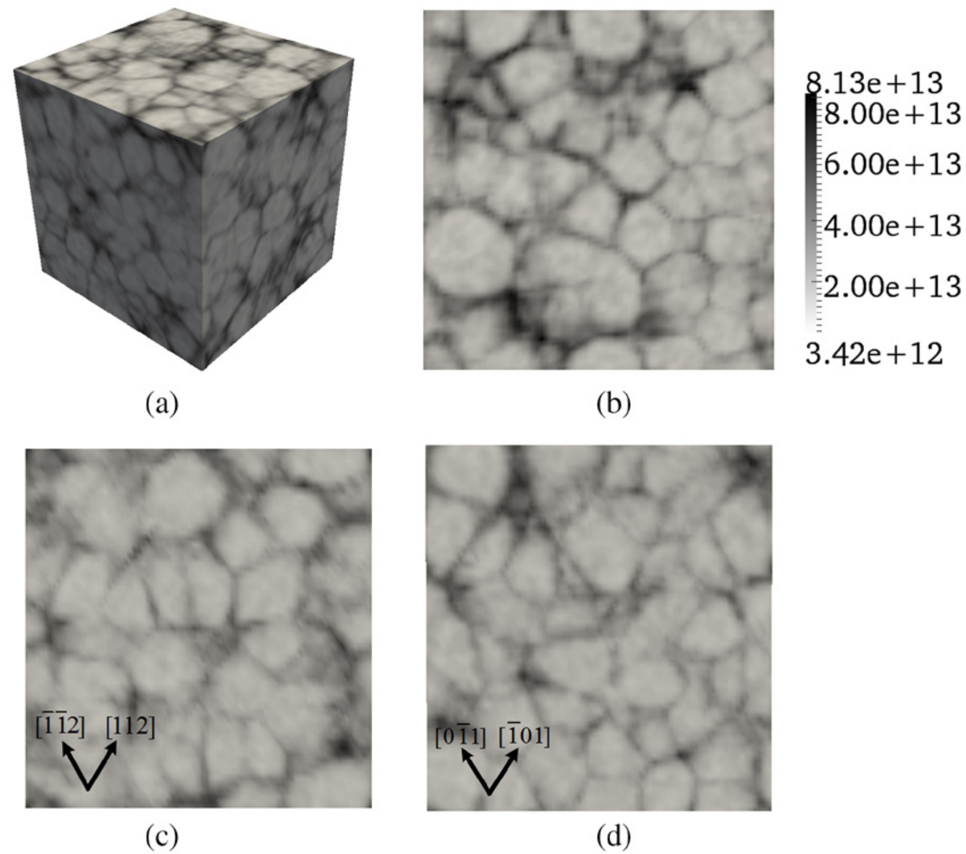
  - $\rho_\mathrm{m}, \rho_\mathrm{i}$: mobile and immobile dislocation densities
  - $g(\rho)$: dipole generation/loss function
  - $\bar{P}$: plastic strain rate
  - c : pinning rate

D Walgraef, EC Aifantis, J Appl Phys, 1985

EC Aifantis, Int J Plast, 1987

Continuum modelling of cell structures I.

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

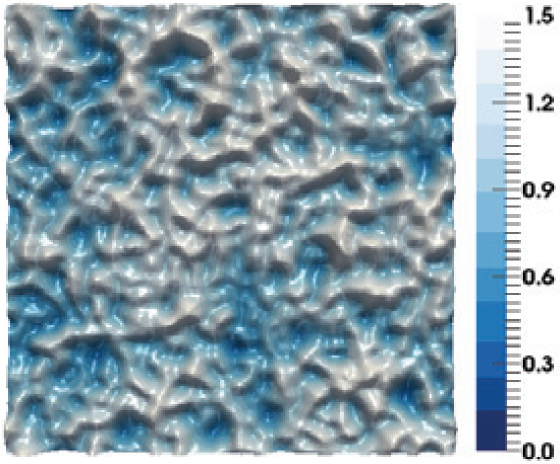


S. Xia and A El-Azab, Mod Simul Mater Sci Eng, 2015

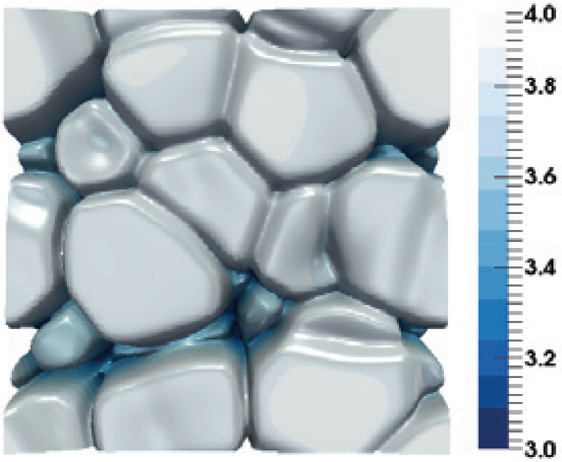
Continuum modelling of cell structures II.

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

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



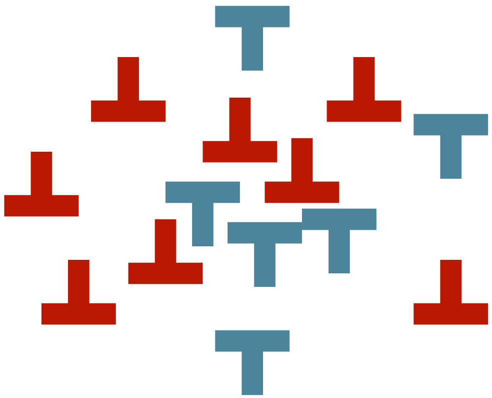
Initial



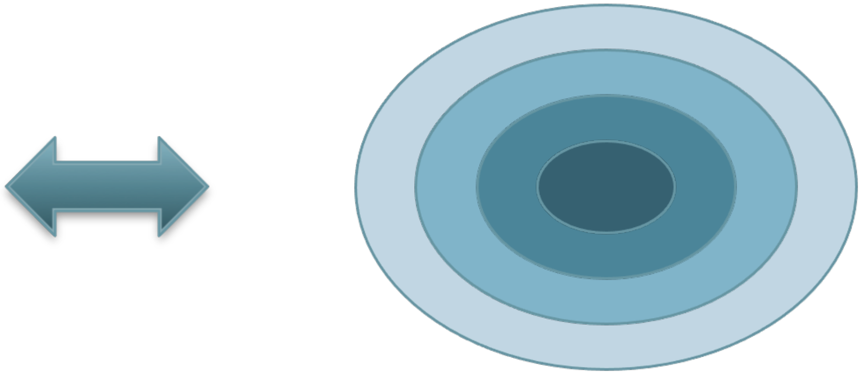
Stationary

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



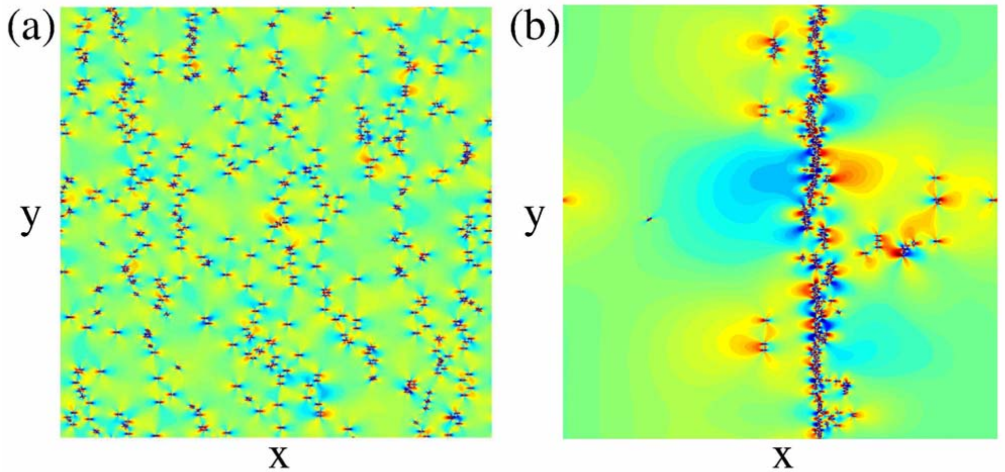
Discrete representation

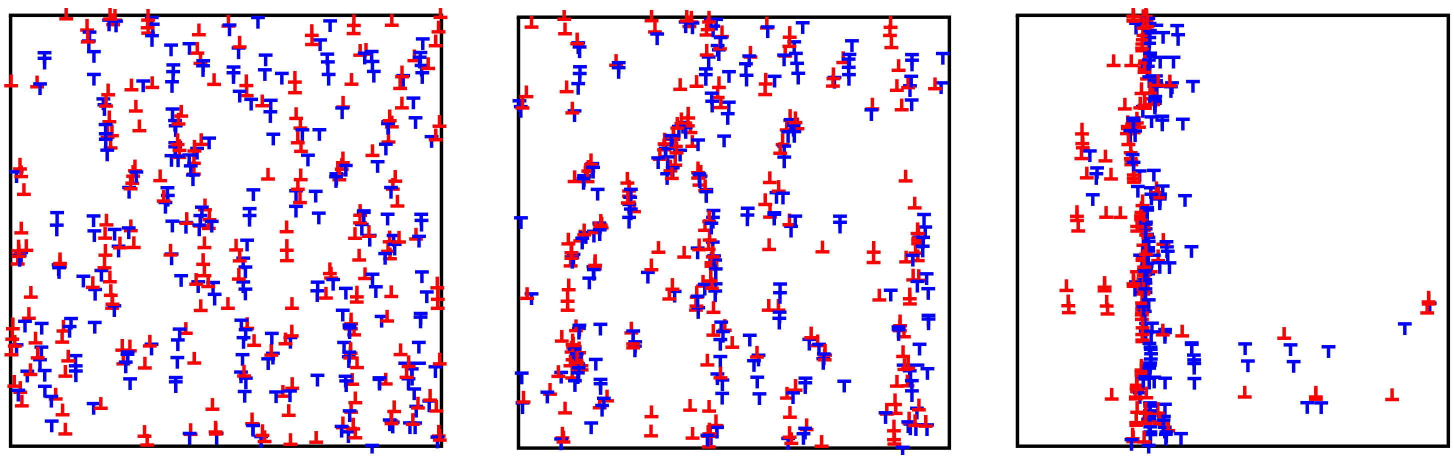


Continuum representation

Pattern evolution in 2D DDD

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





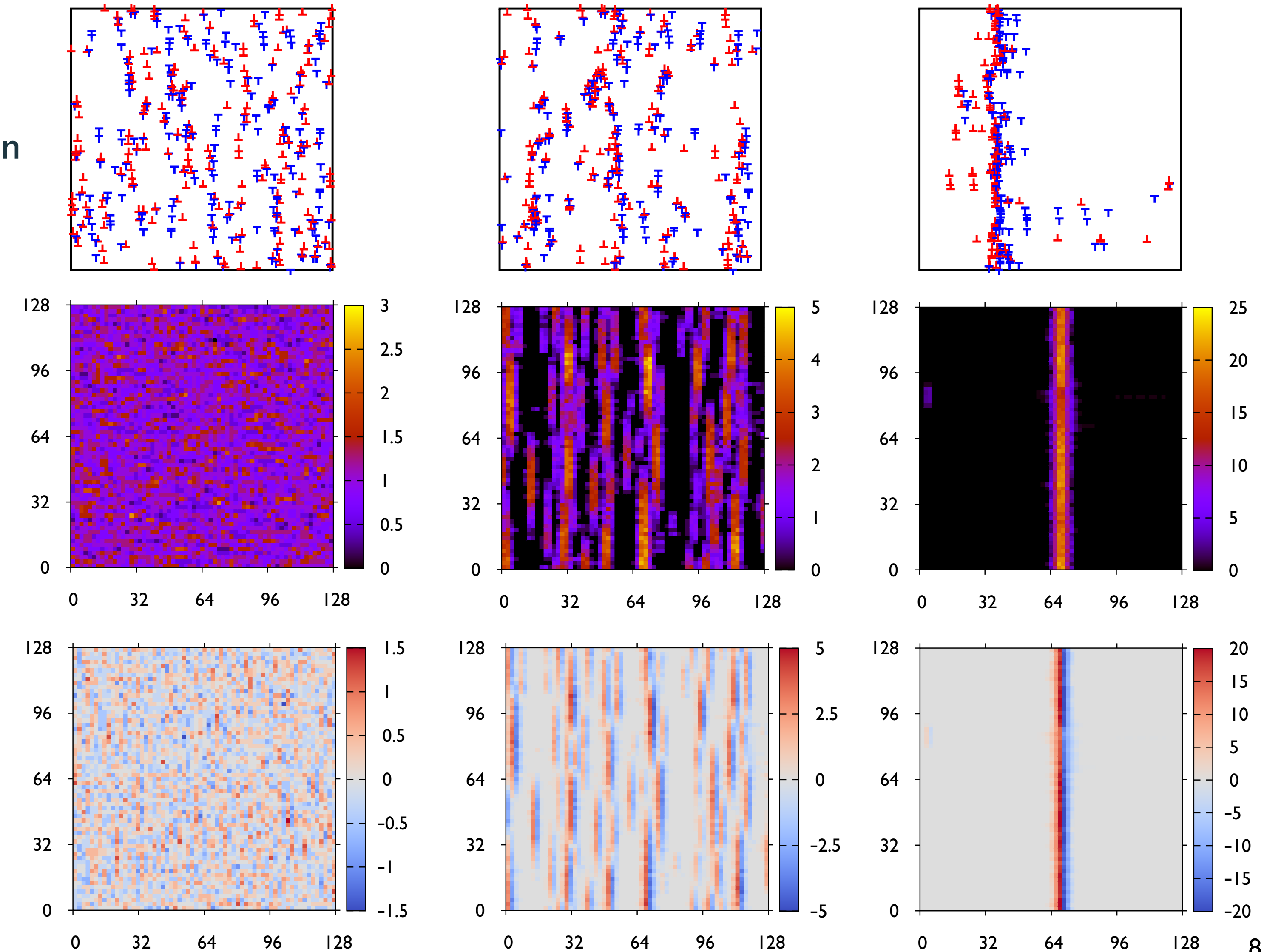
C Zhou, C Reichhardt, CJO Reichhardt, IJ Beyerlein, Sci Rep, 2015

Results: evolution of density patterns

DDD configuration

Continuum total density ρ

Continuum GND density κ



Continuum models

- Evolution equations of dislocations

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

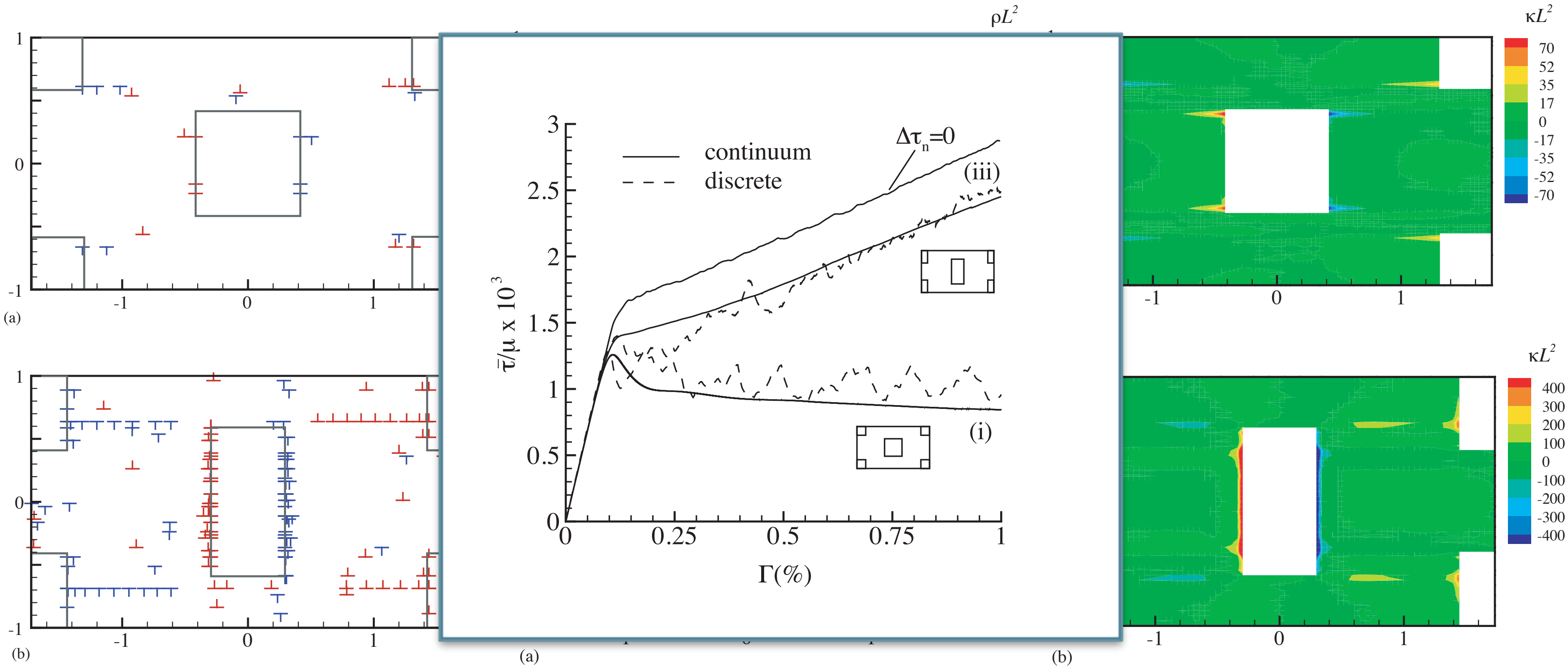
  - ρ_i: some scalar dislocation density field
  - $\boldsymbol{j}_i$: flux of the given density
  - f_{reaction}: multiplication, annihilation, cross-slip, etc.

- 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?
  - No multiplication, no annihilation
  - ???

Benchmark of continuum models

- Tensile test of a model composite material



DDD

$\rho = \rho_+ + \rho_-$

$\kappa = \rho_+ - \rho_-$

S Yefimov, I Groma, E van der Giessen, J Mech Phys Solids, 2004

Continuum model of Groma

Equation of motion of individual dislocations

↓ *Coarse graining*

Hierarchy of *N*-body densities

↓ *Assumption of short range correlations*

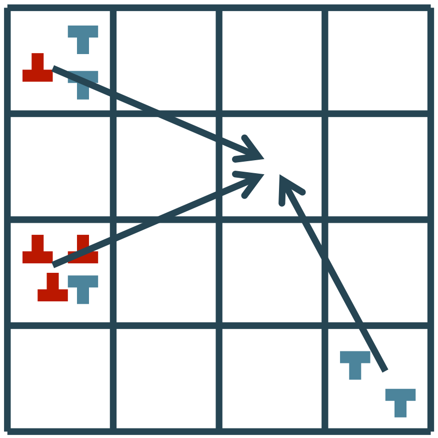
Closed set of evolution equations for ρ and κ

I Groma, Phys Rev B, 1997

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

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

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

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

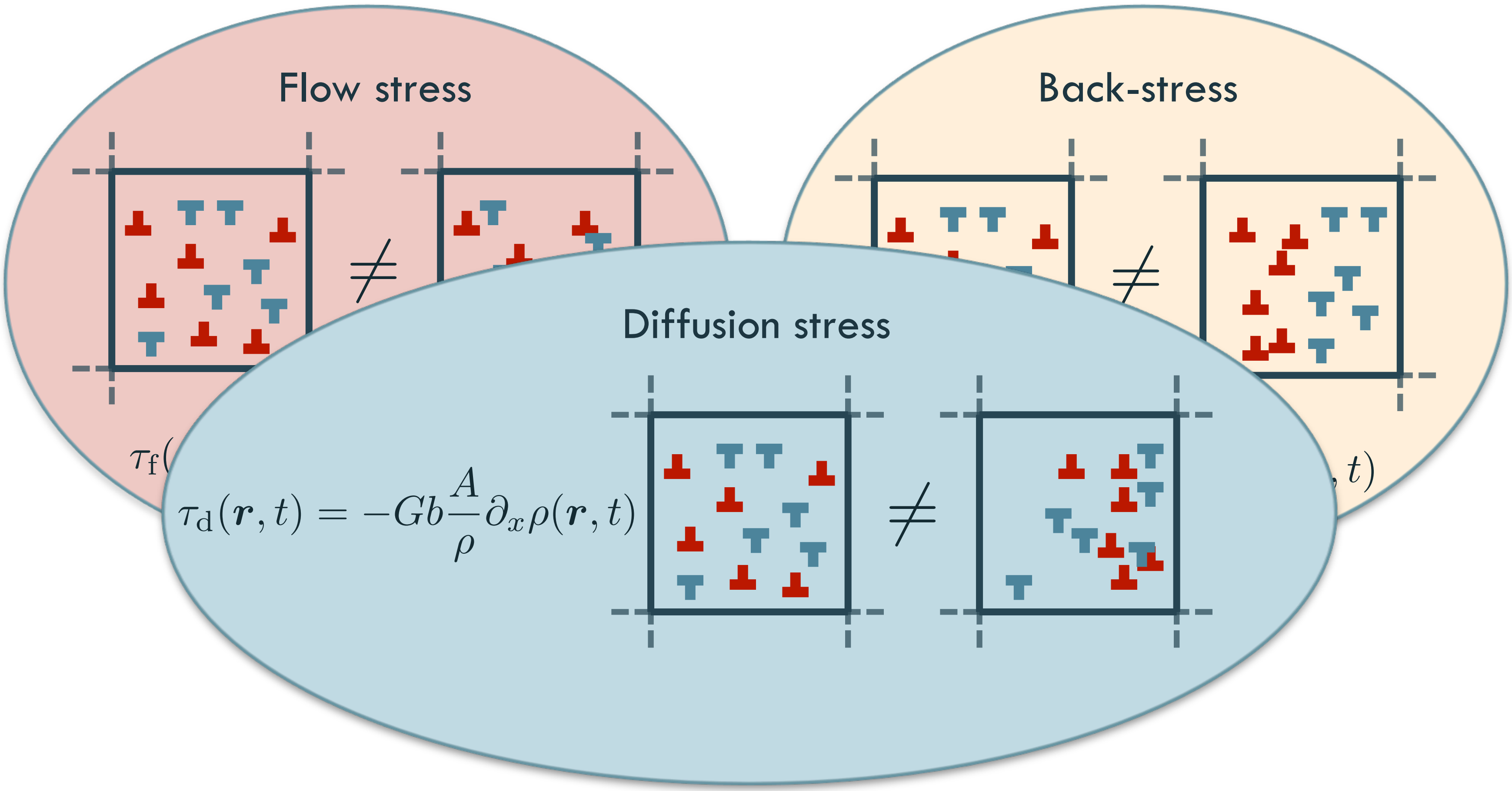
- Back-stress: $\tau_{\mathrm{b}}(\boldsymbol{r}, t) = -Gb \frac{D}{\rho} \partial_x \kappa(\boldsymbol{r}, t)$
- Diffusion stress: $\tau_{\mathrm{d}}(\boldsymbol{r}, t) = -Gb \frac{A}{\rho} \partial_x \rho(\boldsymbol{r}, t)$
- Flow stress: $\tau_{\mathrm{f}}(\boldsymbol{r}, t) = \alpha \mu b \sqrt{\rho(\boldsymbol{r},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

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

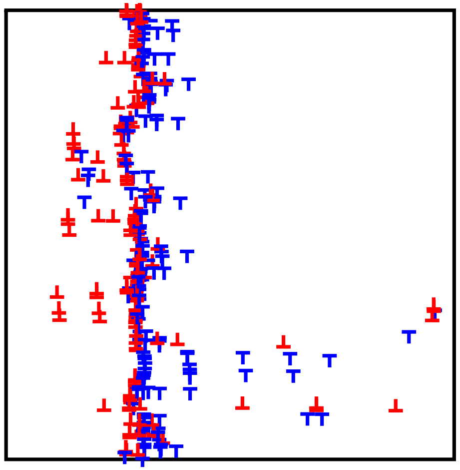
I Groma, M Zaiser, PD Ispánovity, Phys Rev B, 2016

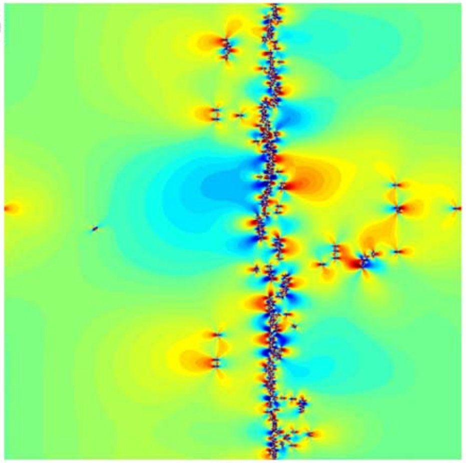
Correlation induced stress terms

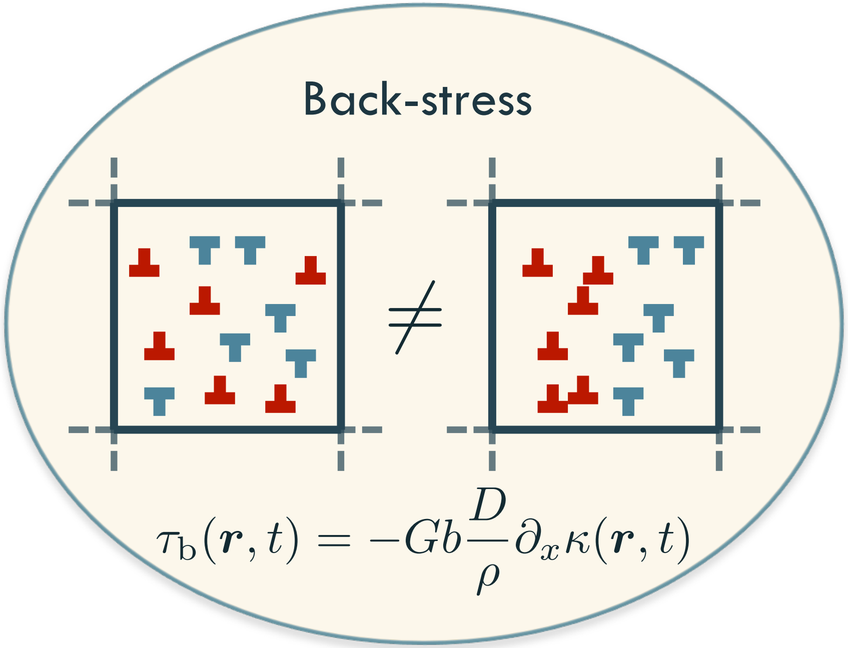
- The *representative volume element* (RVE) cannot resolve internal correlations



Strength of a dipolar wall







$$\tau_\mathrm{b}(\boldsymbol{r},t) = -Gb\frac{D}{\rho}\partial_x\kappa(\boldsymbol{r},t)$$

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

$$D < 0$$

Stochastic plasticity models

2D continuum equations

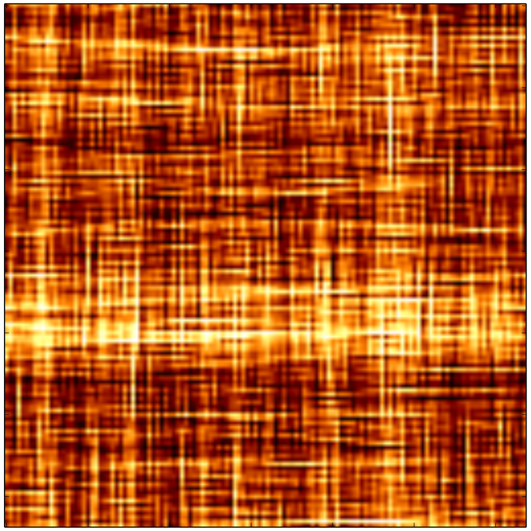
Assuming $\rho = \text{const.}$

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

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

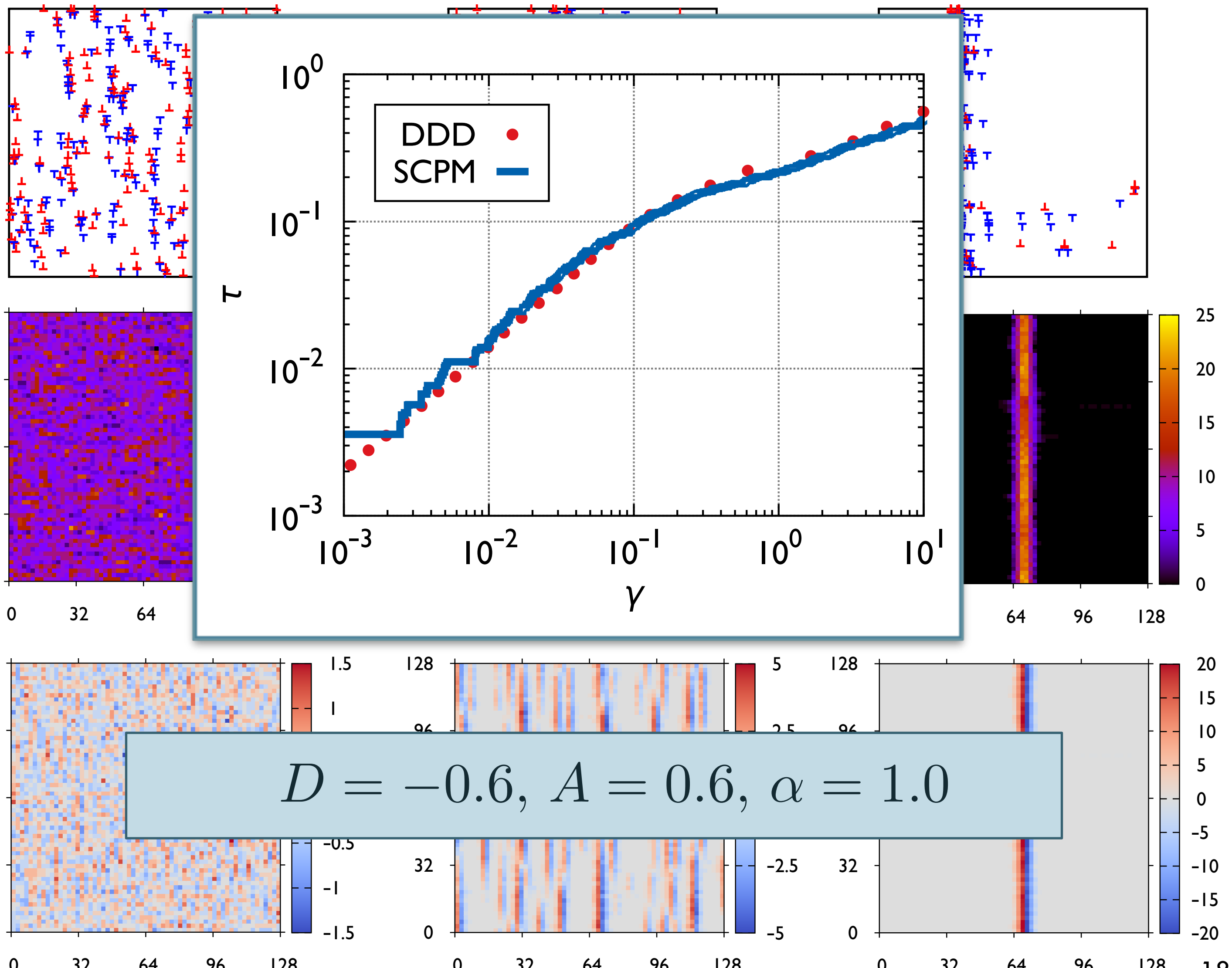
PD Ispánovity, D Tüzes, P Szabó, M Zaiser, I Groma, arXiv, 2016

Evolution of density patterns

DDD configuration

Continuum total density ρ

Continuum GND density κ



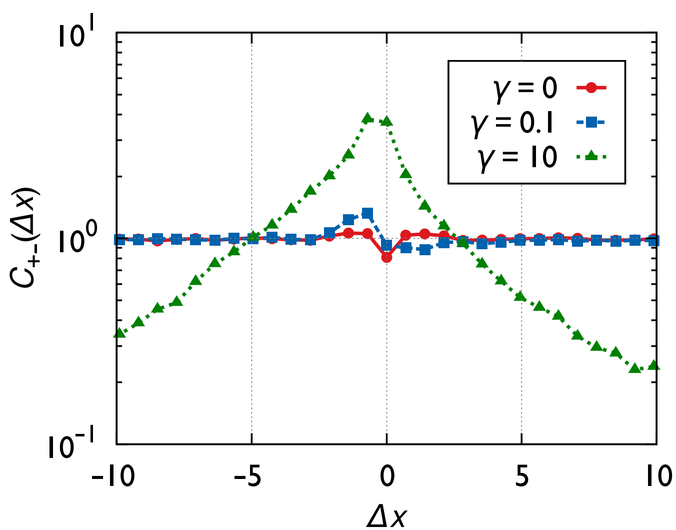
$$D = -0.6,\ A = 0.6,\ \alpha = 1.0$$

Characterization of pattern

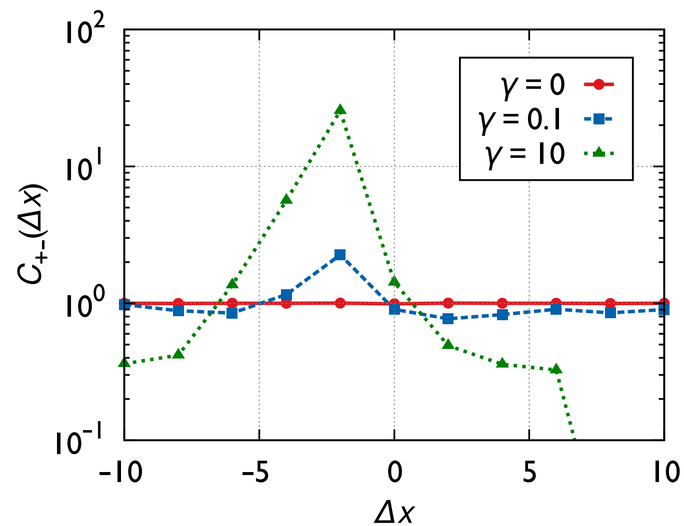
- Cross-correlation of + and – sign dislocations

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

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

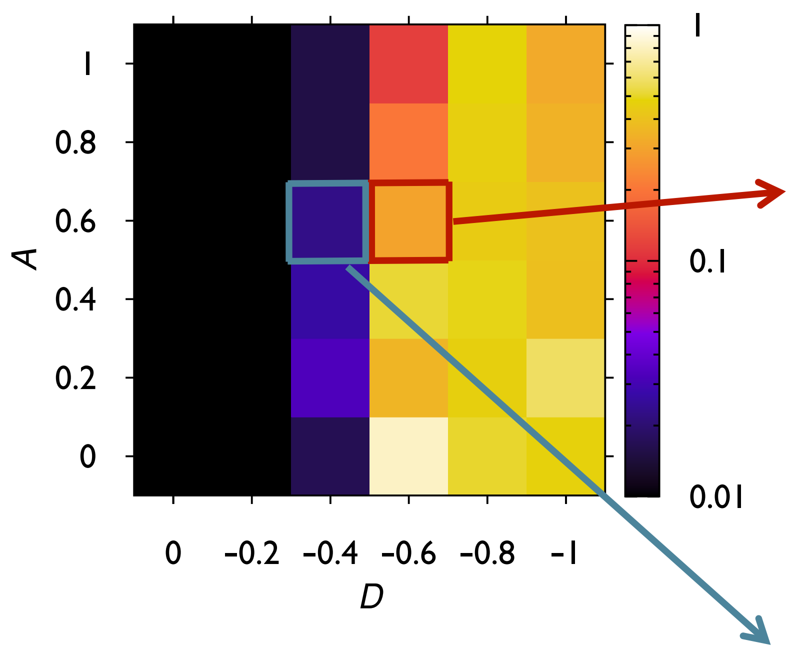


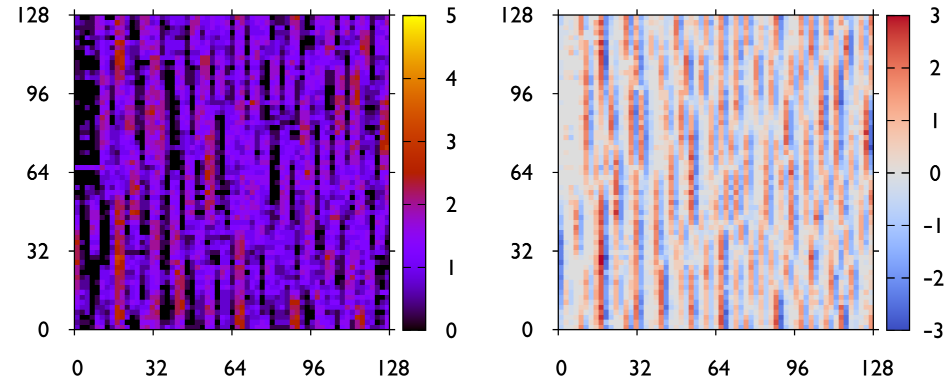
DDD



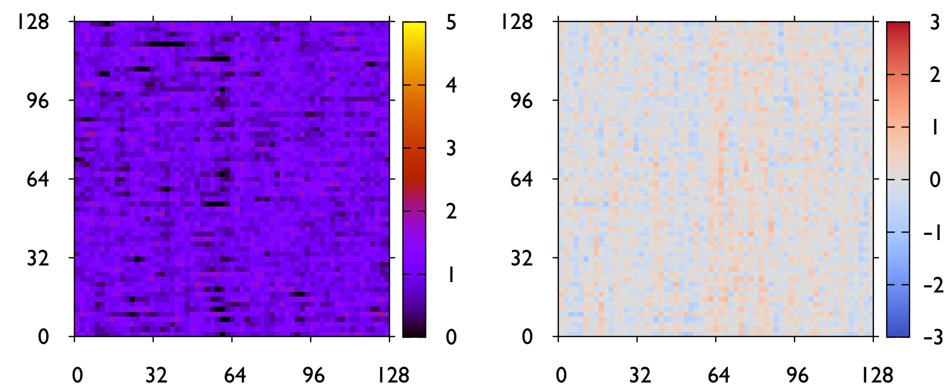
CDD

Effect of parmeter *D*





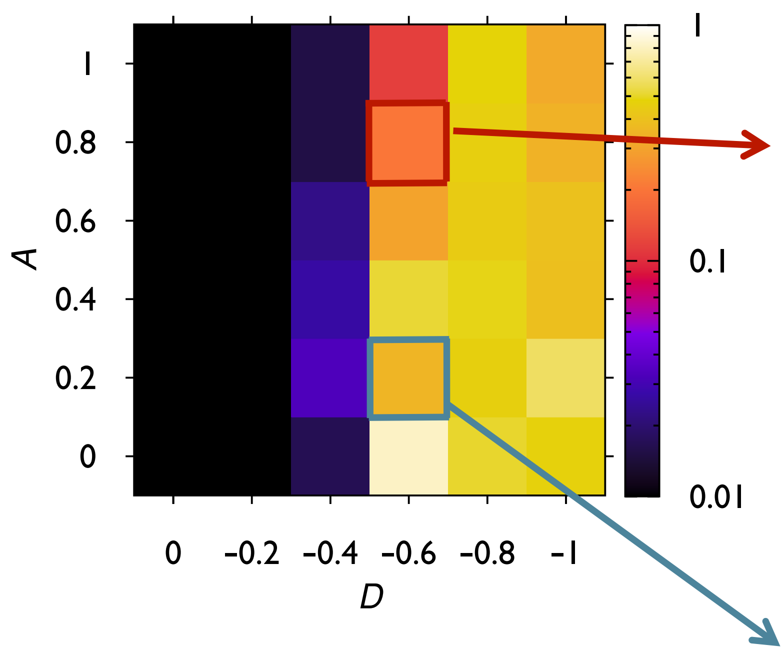
$D = -0.6$

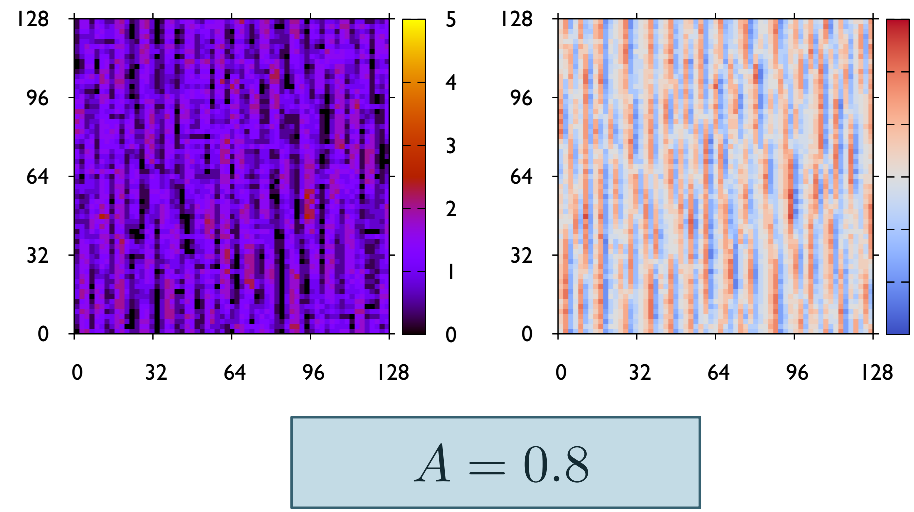


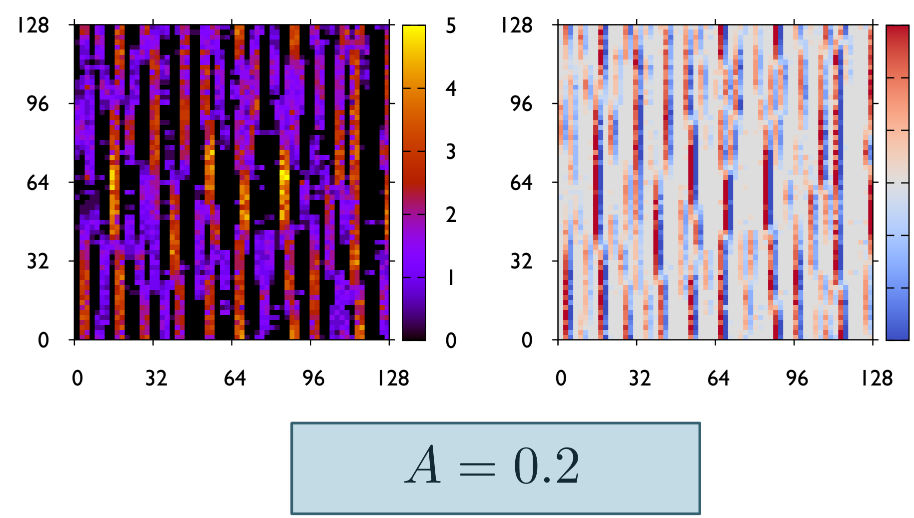
$D = -0.4$

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

Effect of parmeter *A*







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

Summary

- 2D continuum theory of dislocation dynamics
  - Derived analytically from the Eqs. of motion of discrete dislocations
  - It contains 3 dimensionless fitting parameters
  - There are no phenomenological assumptions, the gradient terms naturally emerge

- 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