A mesoscale approach for dislocation density motion using a Runge-Kutta discontinuous Galerkin method

Katrin Schulz | Lydia Wagner | Christian Wieners
Length scales in plasticity

- **Microscopic (nm)**: defects in atomic lattice
- **Mesoscopic (μm)**: dislocations as line objects, ensembles of dislocations
- **Macroscopic (mm)**: polycrystalline aggregate, material as continuum
Outline

Basic framework in single crystal plasticity
We recall quasi-static single crystal plasticity and a mesoscale evolution model for dislocation densities.

Transport systems for dislocation densities
We recall analytic and numerical properties of linear conservation laws applied to dislocation densities.
We introduce a stable splitting scheme for dislocation densities and curvature.
The method is evaluated by a series of numerical experiments.

Coupling dislocation evolution with elasticity
We consider the fully coupled model combining static elasticity and the evolution of dislocation densities.

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Small Strain Single Crystal Plasticity

Let $B \subset \mathbb{R}^3$ be a bounded Lipschitz domain with Dirichlet and Neumann boundary $\partial_D B \cup \partial_N B = \partial B$. The infinitesimal strain $\varepsilon$ is given by

$$\varepsilon = \varepsilon(u) = \text{sym}(D u)$$

and the distortion tensor is decomposed additively into elastic and plastic parts

$$D u = \beta^e + \beta^p.$$
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$$\varepsilon = \varepsilon(u) = \text{sym}(Du)$$

and the distortion tensor is decomposed additively into elastic and plastic parts

$$Du = \beta^\text{el} + \beta^\text{pl}.$$

Plastic slip is assumed to take place on $N$ slip systems with local ONB $\{d_s, l_s, m_s\}$, where $d_s = \frac{1}{b_s} b_s$ is slip direction, $b_s$ is the Burgers vector of length $b_s = |b_s|$, $m_s$ the slip unit normal, and $l_s = m_s \times d_s$.

The plastic shear strain in the slip system $s$ is denoted by $\gamma_s$. We assume

$$\beta^\text{pl} = \sum_s \gamma_s d_s \otimes m_s.$$

The plastic strain depends on the plastic shear strains $\gamma = (\gamma_1, \ldots, \gamma_N)^\top$ by

$$\varepsilon^\text{pl} = \varepsilon^\text{pl}(\gamma) = \text{sym}(\beta^\text{pl}) = \sum_s \gamma_s \text{sym}(d_s \otimes m_s).$$

This defines the elastic strain

$$\varepsilon^\text{el} = \varepsilon^\text{el}(u, \gamma) = \varepsilon(u) - \varepsilon^\text{pl}(\gamma).$$
Small Strain Single Crystal Plasticity

The macroscopic equilibrium equation is given by

\[- \text{div} \sigma = f_B \quad \text{in} \quad B,\]

with the body force $f_B$ and the constitutive relation for the Cauchy stress tensor

$$\sigma = C[\varepsilon^\text{el}] = C[\varepsilon - \varepsilon^\text{pl}]$$

depending on the elasticity tensor $C$. The macroscopic boundary conditions are

$$u = u_D \quad \text{on} \quad \partial_D B, \quad \sigma n = t_N \quad \text{on} \quad \partial_N B,$$

where $u_D$ is a prescribed boundary displacement and $t_N$ is an applied traction.
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Let $U = \{ u \in H^1(B, \mathbb{R}^3) : u = 0 \text{ on } \partial_D B \}$, and assume that $u_D$ extends to $B$.

Then, for given $\varepsilon^{\text{pl}} = \varepsilon^{\text{pl}}(\gamma)$, we have in weak form: find $u \in u_D + U$ such that

$$\int_B C[\varepsilon(u^n) - \varepsilon^{\text{pl}}] \cdot \varepsilon(\delta u) \, dx = \int_B f_B \cdot \delta u \, dx + \int_{\partial_N B} t_N \cdot \delta u \, da, \quad \delta u \in U.$$

Depending on $\gamma$, this equation holds for every time $t \in [0, T]$.

The system is closed by determining the evolution of the plastic shear strains $\gamma_s$. 
Dislocation-based Plasticity

We assume that the plastic shear strain is determined by Orowan’s relation

$$\partial_t \gamma_s = b_s \rho_s \nu_s$$

depending on the dislocation density $\rho_s$ and the dislocation velocity $\nu_s$.

The dislocation density tensor (the so-called Kröner-Nye tensor)

$$\alpha = \nabla \times \beta^\text{pl} = \sum_s \rho_s,\rightharpoonup \mathbf{l}_s \otimes \mathbf{d}_s + \rho_s,\rightharpoonup \mathbf{d}_s \otimes \mathbf{d}_s$$

is determined by the edge and screw dislocation densities

$$\rho_s,\rightharpoonup = -\mathbf{d}_s \cdot \nabla \gamma_s, \quad \rho_s,\rightharpoonup = \mathbf{l}_s \cdot \nabla \gamma_s.$$
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$$\alpha = \nabla \times \beta^\text{pl} = \sum_s \rho_{s,\parallel} l_s \otimes d_s + \rho_{s,\perp} d_s \otimes d_s$$

is determined by the edge and screw dislocation densities

$$\rho_{s,\parallel} = -d_s \cdot \nabla \gamma_s, \quad \rho_{s,\perp} = l_s \cdot \nabla \gamma_s.$$ 

Defining the dislocation density vectors

$$\kappa_s = -m_s \times \nabla \gamma_s = \frac{1}{b_s} \left( \rho_{s,\parallel} l_s + \rho_{s,\perp} d_s \right), \quad \kappa_s^\perp = -m_s \times \kappa_s$$

yields $\alpha = \sum_s \kappa_s \otimes b_s$. By Orowan’s relation, the evolution of $\kappa_s = m_s \times \kappa_s^\perp$ is

$$\partial_t \kappa_s = \nabla \times \left( \rho_s \nu_s m_s \right).$$
Averaged Continuum Dislocation Dynamics

Following Hochrainer et al., we consider the system

\[
\begin{align*}
\partial_t \rho_s &= -\nabla \cdot \left( v_s \kappa_s^\perp \right) + v_s q_s , \\
\partial_t \kappa_s &= \nabla \times \left( \rho_s v_s m_s \right) , \\
\partial_t q_s &= -\nabla \cdot f_s(\rho_s, \kappa_s, q_s) ,
\end{align*}
\]

where \( q_s \) is the dislocation curvature density, and the curvature density flux is

\[
f_s(\rho_s, \kappa_s, q_s) = \frac{q_s}{\rho_s} \kappa_s^\perp v_s + \frac{1}{2|\kappa_s|^2} \left( (\rho_s + |\kappa_s|) \kappa_s \otimes \kappa_s - (\rho_s - |\kappa_s|) \kappa_s^\perp \otimes \kappa_s^\perp \right) \nabla v_s .
\]

The system is closed by a constitutive law \( v_s = v_s(\tau_s, \rho) \) for the dislocation velocity, where \( \tau_s = \sigma d_s \cdot m_s \) is the resolved stress and \( \rho = (\rho_1, \ldots, \rho_N)^T \).
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**Definition**

\((\rho_s, \kappa_s, q_s) \in L_1((0, T) \times B; \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R})\) is weak solution of the above system, if

\[
0 = \int_{(0, T) \times B} \left( \rho_s \partial_t \delta \rho_s + \kappa_s \cdot \partial_t \delta \kappa_s + q_s \partial_t \delta q_s \\
- v_s \kappa_s^\perp \cdot \nabla \delta \rho_s - v_s q_s \delta \rho_s - \rho_s v_s m_s \cdot \nabla \times \delta \kappa_s - f_s(\rho_s, \kappa_s, q_s) \cdot \nabla \delta q_s \right) \, dt \, dx
\]

for all smooth test functions \((\delta \rho_s, \delta \kappa_s, \delta q_s)\) with compact support in \((0, T) \times B\).
The Dislocation Velocity

The CDD system is closed by a constitutive law for the dislocation velocity

\[ v_s(\tau^{\text{eff}}_s, \rho_1, \ldots, \rho_S) = \frac{b_s}{B} \text{sgn}(\tau^{\text{eff}}_s) \max \left\{ 0, |\tau^{\text{eff}}_s| - \tau^y_s(\rho_1, \ldots, \rho_S) \right\} \]

depending on the effective stress \(\tau^{\text{eff}}_s\) in the slip system \(s\), a drag coefficient \(B > 0\), and a yield stress \(\tau^y_s\).

The effective stress is given as \(\tau^{\text{eff}}_s = \tau_s - \tau^b_s\) and is computed from the resolved shear stress \(\tau_s = \sigma \cdot \mathbf{M}_s\) including the dislocation eigenstresses and a back stress

\[ \tau^b_s = \frac{D\mu b_s}{\rho_s} \nabla \cdot \kappa^\perp_s \]

accounting for short-range dislocation interaction depending on a material parameter \(D\) that acts as a back stress parameter.

The back stress can be evaluated from the plastic shear strain by

\[ \tau^b_s = \frac{D\mu}{\rho_s} \nabla \cdot \left( \mathbf{m}_s \times (\mathbf{m}_s \times \nabla \gamma_s) \right) = \frac{D\mu}{\rho_s} \nabla_s \cdot \nabla_s \gamma_s \]

with the projected gradient \(\nabla_s = \mathbf{d}_s (\mathbf{d}_s \cdot \nabla) + \mathbf{l}_s (\mathbf{l}_s \cdot \nabla)\).

Including material dependent interaction coefficients \(a_{sn}\), the yield stress is given by

\[ \tau^y_s(\rho_1, \ldots, \rho_S) = \mu b_s \sqrt{\sum_n a_{sn}\rho_n} \]
Analytic Properties of Linear Conservation Laws

We consider the case $\nu \equiv \text{const.}$ and $q \equiv 0$. Define $w = (\rho, \kappa)$ and the flux function $F$ with $\nabla \cdot F(w) = \begin{pmatrix} \nabla \cdot (\nu \kappa) \\ -\nabla \times (\rho \nu \mathbf{m}) \end{pmatrix}$.

For the equation $\partial_t w + \nabla \cdot F(w) = b$ holds:

- The matrix $\mathbf{n} \cdot F$ is symmetric for all $\mathbf{n}$ with eigenvalues $0$ and $\pm \nu |\mathbf{m} \times \mathbf{n}|$. Thus, the system is hyperbolic and solutions propagate with speed $\nu$. 
Analytic Properties of Linear Conservation Laws

We consider the case \( v \equiv \text{const.} \) and \( q \equiv 0 \).

Define \( w = (\rho, \kappa) \) and the flux function \( F \) with \( \nabla \cdot F(w) = \left( \frac{\nabla \cdot (v \kappa^\perp)}{-\nabla \times (\rho v \mathbf{m})} \right) \).

For the equation \( \partial_t w + \nabla \cdot F(w) = b \) holds:

- The matrix \( n \cdot F \) is symmetric for all \( n \) with eigenvalues 0 and \( \pm v |m \times n| \). Thus, the system is hyperbolic and solutions propagate with speed \( v \).

- Conservative for \( b \equiv 0 \): \( \int w(t) \, dx \equiv \text{const.} \) \( \int |w(t)|^2 \, dx \equiv \text{const.} \).
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For the equation $\partial_t w + \nabla \cdot F(w) = b$ holds:

- The matrix $n \cdot F$ is symmetric for all $n$ with eigenvalues $0$ and $\pm v|m \times n|$. Thus, the system is hyperbolic and solutions propagate with speed $v$.

- Conservative for $b \equiv 0$: $\int w(t) \, dx \equiv \text{const.}$ \quad $\int |w(t)|^2 \, dx \equiv \text{const.}$

- The operator $Sw = \nabla \cdot F(w)$ generates a semigroup depending on the domain of the operator $\mathcal{D}(S) \subset L_2(\mathbb{R}^3, \mathbb{R} \times \mathbb{R}^3)$.
  
  This extends to the case that $v$ is sufficiently smooth.
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- If the initial value \( w(0) \) and the right-hand side \( b \) are sufficiently smooth, a unique solution of the linear PDE exists. This solution is obtained by adding viscosity, i.e., \( \partial_t w^\varepsilon + \nabla \cdot F(w^\varepsilon) = b + \varepsilon \Delta w^\varepsilon \), and passing to the limit \( \varepsilon \to 0 \).
Analytic Properties of Linear Conservation Laws

We consider the case \( \nu \equiv \text{const.} \) and \( q \equiv 0 \).

Define \( w = (\rho, \kappa) \) and the flux function \( F \) with \( \nabla \cdot F(w) = \left( \nabla \cdot (\nu \kappa^\perp) \right) - \nabla \times (\rho \nu \mathbf{m}) \).

For the equation \( \partial_t w + \nabla \cdot F(w) = b \) holds:

- The matrix \( \mathbf{n} \cdot F \) is symmetric for all \( \mathbf{n} \) with eigenvalues 0 and \( \pm \nu |\mathbf{m} \times \mathbf{n}| \).
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- Conservative for \( b \equiv 0 \): \( \int w(t) \, d\mathbf{x} \equiv \text{const.} \quad \int |w(t)|^2 \, d\mathbf{x} \equiv \text{const.} \)

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- If \( w(0) \in BV(\mathbb{R}^3, \mathbb{R} \times \mathbb{R}^3) \) and \( b \in L^1(\mathbb{R}^3, \mathbb{R} \times \mathbb{R}^3) \), a weak solution in \( BV((0, T) \times \mathbb{R}^3, \mathbb{R} \times \mathbb{R}^3) \) exists.
Riemann Solutions of the Dislocation System

We consider $v_s \equiv \text{const.}$ and straight dislocation densities with $q_s \equiv 0$ of the form

$$\rho_s(t, x) = A_s(\lambda t - x \cdot n)$$

corresponding to a Riemann solution traveling in the direction $n$ with speed $\lambda$ and amplitude $A_s(\cdot)$.
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Then, $\partial_t \rho_s = \lambda A'_s$, and $\nabla \rho_s = -A'_s n$ yields

$$\partial_t \kappa_s = \nabla \times (\rho_s \nu_s m_s) = -\nu_s m_s \times \nabla \rho_s = -\nu_s A'_s m_s \times n.$$ 

Thus, with

$$\kappa_s(t, x) = \frac{1}{\lambda} A_s(\lambda t - x \cdot n) m_s \times n, \quad \lambda = \nu_s |m_s \times n|$$

we obtain a solution of the dislocation system.
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If $A_s(\cdot)$ is discontinuous, this is a weak solution of the dislocation system.
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we obtain a solution of the dislocation system.

If $A_s(\cdot)$ is discontinuous, this is a weak solution of the dislocation system.

A linear combination of discontinuous Riemann solutions with $\rho_s(0) \in \mathbb{Z}$ a.e. in $\mathbb{R}^3$ results in $\rho_s(t) \in \mathbb{Z}$ a.e. in $\mathbb{R}^3$, and the boundary of $\rho_s^{-1}(n)$ for $n \in \mathbb{Z}$ in every slip plane $\Gamma_{s,d} = \{x \in \mathbb{R}^3 : x \cdot m_s = d\}$ has finite length in every compact region.
We set $n = l_s + 2d_s$ and $A_s(z) = \begin{cases} 1 & z > 0, \\ -1 & z < 0. \end{cases}$
A Riemann Solution for the Dislocation System

We set \( n = l_s + 2d_s \) and \( A_s(z) = \begin{cases} 
1 & z > 0 , \\
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\end{cases} \)

Note that phase field models for dislocations with energy contribution \( \frac{1}{\varepsilon} \text{dist}(\rho_s, \mathbb{Z})^2 \)
for \( \varepsilon \rightarrow 0 \) also result into solutions in \( BV(\mathbb{R}^3, \mathbb{Z}) \), cf. Conti-Garroni-Müller 2011.
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General Observation
Monotone schemes are diffusive and of low order, high order schemes oscillate.
A BV Solution for the Dislocation System

We start with $\rho_s(0) \in BV(\mathbb{R}^3, \mathbb{Z})$. 

finite volume ($P_0$)                      discontinuous Galerkin ($P_2$)
Numerical Approximation of Linear Conservation Laws

Let $\mathcal{B} = \bigcup K$ be a decomposition into tetrahedral elements $K$ with faces $f \subset \partial K$. In every slip system $s$, we consider discontinuous approximations in

$$V_h = \left\{ w_h \in L_2(\mathcal{B}, \mathbb{R} \times \mathbb{R}^3) : w_h \in P_k(K, \mathbb{R} \times \mathbb{R}^3) \right\}.$$

- The central flux $n_f \cdot F^c(w_h) = \frac{1}{2} \left( n_f \cdot F(w_K) + n_f \cdot F(w_K^f) \right)$ converges with

$$\| w - w_h \| = O(h^k).$$
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- The upwind flux $n_f \cdot F^{\text{up}}(w_h)$ obtained by solving the Riemann problem yields

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- Stable implicit Runge-Kutta schemes require no time step limitation.
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- The central flux \( n_f \cdot F^c(w_h) = \frac{1}{2} \left( n_f \cdot F(w_K) + n_f \cdot F(w_{K_f}) \right) \) converges with

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\| w - w_h \| = O(h^k).
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- The upwind flux \( n_f \cdot F^{up}(w_h) \) obtained by solving the Riemann problem yields

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\| w - w_h \| = O(h^{k+1/2}).
\]

- Explicit time stepping schemes require \( \Delta t \leq h/v \) (CFL condition).

- Stable implicit Runge-Kutta schemes require no time step limitation.

- Reversible Runge-Kutta schemes with central flux are energy conserving.

- Runge-Kutta schemes with upwind flux are monotone (for \( k = 0 \)).
A DG Scheme for the Dislocation System

Strategy (in every slip system $s$)

- upwind flux for monotone schemes
- explicit splitting in $(\rho, \kappa)$ and $q$
- implicit midpoint rule in both systems
  (a stable implicit reversible Runge-Kutta scheme)
A DG Scheme for the Dislocation System

Strategy (in every slip system $s$)
- upwind flux for monotone schemes
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Time integration for dislocation densities

Weak solutions $\mathbf{w} = (\rho, \kappa)$ satisfying

$$(\partial_t \mathbf{w}, \delta \mathbf{w})_K - (\mathbf{F}(\mathbf{w}), \nabla \delta \mathbf{w})_K + \sum_{f \subset \partial K} (\mathbf{n}_f \cdot \mathbf{F}(\mathbf{w}), \delta \mathbf{w})_f = (\nu q, \delta \mathbf{w})_K$$

are approximated at $t_n$ by $\mathbf{w}_h^n \in V_h$ for given $\nu_{h-1}^n$ and $q_{h-1}^n$ by

$$\frac{1}{t_n - t_{n-1}} (\mathbf{w}_h^n - \mathbf{w}_{h-1}^n, \delta \mathbf{w}_h)_K - (\mathbf{F}(\mathbf{w}_h^{n-1/2}), \nabla \delta \mathbf{w}_h)_K$$

$$+ \sum_{f \subset \partial K} (\mathbf{n}_f \cdot \mathbf{F}^{\text{up}}(\mathbf{w}_h^{n-1/2}), \delta \mathbf{w}_h)_f = (\nu_{h-1}^n q_{h-1}^n, \delta \mathbf{w}_h)_K$$

for all $\delta \mathbf{w}_h \in V_h$, where $\mathbf{w}_h^{n-1/2} = \frac{1}{2} (\mathbf{w}_h^n + \mathbf{w}_h^{n-1})$. 
A DG Scheme for the Dislocation System

Time integration for the curvature density

Weak solutions $q$ with

$$(\partial_t q, \delta q)_K - (f(\rho, \kappa, q), \nabla \delta q)_K + \sum_{f \subset \partial K} (n_f \cdot f(\rho, \kappa, q), \delta q)_f$$

$$= (g(\rho, \kappa), \nabla \delta q)_K - \sum_{f \subset \partial K} (n_f \cdot g(\rho, \kappa), \delta q)_f,$$

$$f(\rho, \kappa, q) = \frac{v}{\rho} \kappa^\perp, \quad g(\rho, \kappa) = \frac{1}{2|\kappa|^2} \left( (\rho + |\kappa|) \kappa \otimes \kappa - (\rho - |\kappa|) \kappa^\perp \otimes \kappa^\perp \right) \nabla v$$

are approximated at $t_n$ by $q^n_h \in V^q_h$ for given $v^{n-1}_h$ and $(\rho^n_h, \kappa^n_h)$ by

$$\frac{1}{t_n - t_{n-1}} (q^n_h - q^{n-1}_h, \delta q^n_h)_K - (f_{n,h}(q^{n-1/2}_h), \nabla \delta q^n_h)_K + \sum_{f \subset \partial K} (n_f \cdot f_{n,h}^{up}(q^{n-1/2}_h), \delta q^n_h)_f$$

$$= (g_{n,h}, \nabla \delta q^n_h)_K - \sum_{f \subset \partial K} (n_f \cdot g_{n,h}, \delta q^n_h)_f,$$

$$f_{n,h}(q_h) = f(K_h * \rho^n_h, K_h * \kappa^n_h, q_h), \quad g_{n,h} = g(K_h * \rho^n_h, K_h * \kappa^n_h),$$

for all $\delta q^n_h \in V^q_h$ using continuous approximations of $\rho^n_h, \kappa^n_h,$ and $K_h * v^{n-1}_h,$ obtained by convolution with a kernel function $K_h(\cdot, \cdot)$ with small support of size $h.$
A Radial Solution for Constant Velocity

Let $\mathbf{r}$ be the projection of $\mathbf{x} \in \Omega$ on to $\Gamma = \text{span}\{\mathbf{d}, \mathbf{l}\}$ and $z = \mathbf{x} \cdot \mathbf{m}$. Then,

$$
\rho(t, \mathbf{x}) = \frac{1}{2\pi s_r s_z} \exp \left( -\frac{1}{2s_r^2} (|\mathbf{r}| - R(t))^2 - \frac{1}{2s_z^2} z^2 \right)
$$

$$
\kappa(t, \mathbf{x}) = \rho(t, \mathbf{x}) \mathbf{m} \times \frac{\mathbf{r}}{|\mathbf{r}|}
$$

$$
q(t, \mathbf{x}) = \frac{1}{|\mathbf{r}|} \rho(t, \mathbf{x})
$$

solves the CDD system for constant velocity $v$ and radius $R(t) = R_0 + vt$. 
A Radial Solution for Constant Velocity

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$$

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q(t, \mathbf{x}) = \frac{1}{|\mathbf{r}|} \rho(t, \mathbf{x})
$$

solves the CDD system for constant velocity $v$ and radius $R(t) = R_0 + vt$. 

![Images of $\rho$, $\kappa \cdot \mathbf{d}$, $\kappa \cdot \mathbf{l}$, and $q$.]
A Radial 3d-Solution with Open Boundary

We set $\nu \equiv 1$, and we start with $(\rho_s, \kappa_s, q_s)(0, x) = A_s(0, r_s, z_s) \left(1, \frac{1}{r_s} m_s \times r_s, \frac{1}{r_s}\right)$. 

\begin{align*}
\rho(0) & \\
\rho(T) & 
\end{align*}
Convergenc (3d) for Different Polynomial Degrees

\[ \| \rho - \rho_h \|_2 \quad \| q - q_h \|_2 \]

\[ O(n^{-0.5}) \quad O(n^{-2.5}) \]

degrees of freedom \( n \) for \((\rho, \kappa)\) in \(d\)-direction

degrees of freedom \( n \) for \(q\) in \(d\)-direction
Algorithm for the Fully Coupled Model

[A0] Set initial values for $\gamma^0_s, w_s = (\rho^0_s, \kappa^0_s)$ and $q^0_s$ for $s = 1, \ldots, N$. Set $n = 0$ and $t_0 = 0$.

[A1] Set $\varepsilon^{pl,n} = \varepsilon^{pl}(\gamma^n)$ and compute $u^n$ with $u^n(x) = u_D(t_n, x)$ and
\[
\int_B C[\varepsilon(u^n) - \varepsilon^{pl,n}] \cdot \varepsilon(\delta u) \, dx = \int_B f_B(t_n) \cdot \delta u \, dx + \int_{\Gamma_N} t_N(t_n) \cdot \delta u \, da.
\]
Set $\sigma^n = C[\varepsilon(u^n) - \varepsilon^{pl,n}], \tau^n_s = \sigma^n d_s \cdot m_s$, and $v^n_s = v_s(\tau^n_s, \rho^n_s)$. 
Algorithm for the Fully Coupled Model

[A0] Set initial values for $\gamma_0^s, w_s = (\rho_0^s, \kappa_0^s)$ and $q_0^s$ for $s = 1, \ldots, N$. Set $n = 0$ and $t_0 = 0$.

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Set $\sigma^n = C[\varepsilon(u^n) - \varepsilon^{pl,n}]$, $\tau^n_s = \sigma^n d_s \cdot m_s$, and $v^n_s = v_s(\tau^n_s, \rho^n_s)$.

[A2] Choose $M \in \mathbb{N}$. For $m = 1, \ldots, M$ and $s = 1, \ldots, N$ compute $w_{s}^{n+m/M}$ with
\[
\frac{M}{\Delta t_n} (w_{s}^{n+m/M} - w_{s}^{n+(m-1)/M}, \delta w)_K - (F_s(w_{s}^{n-(m-1/2)/M}), \nabla \delta w)_K
+ \sum_{f \subset \partial K} (n_f \cdot F_{s,up}(w_{s}^{n-(m-1/2)/M}), \delta w)_f = (v_{s}^{n+(m-1)/M}q_{s}^{n+(m-1)/M}, \delta w)_K
\]
and then $q_{s}^{n+m/M}$ with
\[
\frac{M}{\Delta t_n} (q_{s}^{n+m/M} - q_{s}^{n+(m-1)/M}, \delta q)_K - (f_{s,n+m/M}(q_{s}^{n+(m-1/2)/M}), \nabla \delta q)_K
+ \sum_{f \subset \partial K} (n_f \cdot f_{s,up,n+m/M}(q_{s}^{n+(m-1/2)/M}), \delta q)_f = (g_{s,n+m/M}, \nabla \delta q)_K - \sum_{f \subset \partial K} (n_f \cdot g_{s,n+m/M}, \delta q)_f
\]
set $v_{s}^{n+m/M} = v_s(\tau^n, \rho^{n+m/M})$, and $\gamma_{s}^{n+m/M} = \gamma_{s}^{n+(m-1)/M} + \frac{M}{\Delta t_n} b_s \rho_{s}^{n+m/M} v_{s}^{n+m/M}$.  

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Algorithm for the Fully Coupled Model

[A0] Set initial values for $\gamma_s^0, w_s = (\rho_s^0, \kappa_s^0)$ and $q_s^0$ for $s = 1, \ldots, N$. Set $n = 0$ and $t_0 = 0$.

[A1] Set $\varepsilon^{pl,n} = \varepsilon^{pl}(\gamma^n)$ and compute $u^n$ with $u^n(x) = u_D(t_n, x)$ and

$$\int_B [C(\varepsilon(u^n) - \varepsilon^{pl,n}) \cdot \varepsilon(\delta u) \, dx] = \int_B f_B(t_n) \cdot \delta u \, dx + \int_{\Gamma_N(t_n)} t_N(t_n) \cdot \delta u \, d\mathbf{a}.$$ 

Set $\sigma^n = C(\varepsilon(u^n) - \varepsilon^{pl,n})$, $\tau^n_s = \sigma^n d_s \cdot m_s$, and $v^n_s = v_s(\tau^n_s, \rho^n_s)$.

[A2] Choose $M \in \mathbb{N}$. For $m = 1, \ldots, M$ and $s = 1, \ldots, N$ compute $w_s^{n+m/M}$ with

$$\frac{M}{\Delta t_n} (w_s^{n+m/M} - w_s^{n+(m-1)/M}, \delta w)_K - (F_s(w_s^{n-(m-1)/M}), \nabla \delta w)_K$$

$$+ \sum_{f \subset \partial K} (n_f \cdot F_{up}^s(w_s^{n-(m-1)/M}), \delta w)_f = (v_s^{n+(m-1)/M} q_s^{n+(m-1)/M}, \delta w)_K$$

and then $q_s^{n+m/M}$ with

$$\frac{M}{\Delta t_n} (q_s^{n+m/M} - q_s^{n+(m-1)/M}, \delta q)_K - (f_{s,n+m/M}(q_s^{n+(m-1)/M}), \nabla \delta q)_K$$

$$+ \sum_{f \subset \partial K} (n_f \cdot f_{up}^s(q_s^{n+(m-1)/M}), \delta q)_f = (g_{s,n+m/M}, \nabla \delta q)_K - \sum_{f \subset \partial K} (n_f \cdot g_{s,n+m/M}, \delta q)_f$$

set $v_s^{n+m/M} = v_s(\tau^n, \rho^{n+m/M})$, and $\gamma_s^{n+m/M} = \gamma_s^{n+(m-1)/M} + \frac{M}{\Delta t_n} b_s \rho_s^{n+m/M} v_s^{n+m/M}$.

[A3] If $t_n < t_{\text{max}}$, select $\Delta t_n > 0$, set $t_n = t_{n-1} + \Delta t_n$, $n := n + 1$, and go to [A1].
A Tricrystall Experiment

We consider three cubic single-crystalline grains for the comparison of DDD simulations and a gradient plasticity model presented in Bayerschen et al. 2015.

Each grain is assumed to be face-centered cubic with \( N = 12 \) slip systems where the \( \langle 100 \rangle \)-axis corresponds to the \( x_1 \)-axis. For \( B_1 \) and \( B_2 \), the \( \langle 010 \rangle \)- and \( \langle 001 \rangle \)-axis are oriented in \( x_2 \)- and \( x_3 \)-direction. The central grain \( B_2 \) is rotated by an angle \( \alpha \) around the \( x_1 \)-axis.

In each slip system \( s = 1, \ldots, 12 \), a constant initial dislocation and curvature density is chosen. We assume that there are no GNDs in the beginning. In \( x_1 \)-direction, a uni-axial loading is applied on the left boundary and homogeneous Neumann boundary on the other boundaries. We choose the back stress parameter \( D = 0.255 \). The length of the Burgers vector is \( b_s = 2.56 \cdot 10^{-4} \) \( \mu m \), and we use the interaction parameters given by Kubin et al. 2008.
Tricristall – Results

Stress-strain curve for $\alpha = 5^\circ, 35^\circ$ using 8640 cells, local degree $k = 2$ in $V_h$ and $\Delta t = 0.5 \text{ ns}$ compared with DDD results (gray) from Bayerschen et al. 2015.
Tricristall – Results

Distribution of the screw part of the dislocation density.

\[ \kappa_{\pm} \cdot d_{\pm} \]

For different angles \( \alpha = 5^\circ \) and \( \alpha = 35^\circ \):

- \( \kappa_{+} \) and \( \kappa_{-} \) for various strains:
  - \( \varepsilon_{11}^{\text{pl}} = 0.001 \)
  - \( \varepsilon_{11}^{\text{pl}} = 0.002 \)
  - \( \varepsilon_{11}^{\text{pl}} = 0.003 \)
Tricristall – Results

Distribution of the plastic strain along $x_1$ (averaged in $(x_2, x_3)$)

$\alpha = 5^\circ$

$\alpha = 35^\circ$

$\varepsilon_{11}^{pl} = 0.1\%$
$\varepsilon_{11}^{pl} = 0.2\%$
$\varepsilon_{11}^{pl} = 0.3\%$
Tricristall – Results

Distribution of the plastic strain along $x_1$ (averaged in $(x_2, x_3)$)

$\alpha = 5^\circ$

$\alpha = 35^\circ$

$\varepsilon_{11}^{pl} = 0.1\%$  
$\varepsilon_{11}^{pl} = 0.2\%$  
$\varepsilon_{11}^{pl} = 0.3\%$

Reference data (grey): Bayerschen et al. 2015
Summary and Outlook

Combining a finite element method for elasto-plasticity with an implicit Runge-Kutta discontinuous Galerkin scheme for the dislocation microstructure allows for the efficient approximation of a 3d dislocation based continuum model.

The next steps are:
- Numerical analysis of the approximation scheme.
- Convergence to / comparison with gradient plasticity.
- Interface modeling and polycrystal simulations with more grains.