FFT-Based Crystal Plasticity for Large Polycrystalline Systems

Physical Model • Mathematical Formulation • Numerical Implementation

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Outline

1. Physical Model

2. Mathematical Model

3. Numerical Implementation

What is Crystal Plasticity?

Metals are **polycrystalline** aggregates: many single crystals (grains) bonded together, each with a different lattice orientation.

- **Elastic deformation:**
  stretching of atomic bonds (reversible).
- **Plastic deformation:**
  motion of dislocations on crystallographic planes (irreversible).

Goal

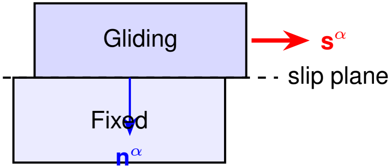
Predict the macroscopic stress–strain response of a polycrystal from the single-crystal constitutive law and the grain-level microstructure.

Slip Systems in FCC Metals

Dislocations glide on specific *slip planes* in specific *slip directions*.

Slip system α:

- Plane normal: $\mathbf{n}^\alpha \in \{111\}$
- Direction: $\mathbf{s}^\alpha \in \langle 110 \rangle$
- FCC $\Rightarrow$ **12 systems** (4 planes $\times$ 3 directions)



Schmid tensor (geometric projector):

$$\boldsymbol{P}^\alpha = \frac{1}{2}\left(\mathbf{s}^\alpha \otimes \mathbf{n}^\alpha + \mathbf{n}^\alpha \otimes \mathbf{s}^\alpha\right)$$

Resolved Shear Stress and Driving Force

The resolved shear stress on system α is:

$$\tau^\alpha = \boldsymbol{\sigma} : \boldsymbol{P}^\alpha = \sigma_{ij} \, P_{ij}^\alpha$$

Effective driving stress (Kocks–Argon–Ashby):

$$\tau_{\text{drive}}^\alpha = \tau^\alpha - \tau_{\text{back}}^\alpha, \qquad \tau_{\text{eff}}^\alpha = \left\langle |\tau_{\text{drive}}^\alpha| - S_{\text{ath}}^\alpha \right\rangle$$

- S_{ath}: athermal (long-range) resistance — grain boundaries, precipitates.
- $\langle \cdot \rangle$: Macaulay bracket — no slip if driving stress $<$ athermal resistance.

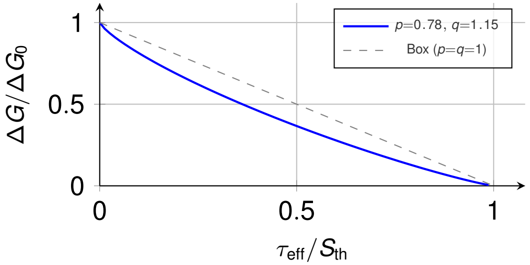
Thermally Activated Flow Rule

Dislocation motion is **thermally activated**. Slip rate on system α [1]:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_{\mathrm{ref}} \ \exp\left[-\frac{\Delta G_0}{k_B T}\left(1 - \left(\frac{\tau^{\alpha}_{\mathrm{eff}}}{S^{\alpha}_{\mathrm{th}}}\right)^{p}\right)^{q}\right] \mathrm{sgn}(\tau^{\alpha}_{\mathrm{drive}})$$

Parameters:

- $\dot{\gamma}_{\mathrm{ref}} = 10^7\ \mathrm{s}^{-1}$
- $\Delta G_0 = 9.5 \times 10^{-19}$ J
- $p = 0.78$, $q = 1.15$
- S_{th}: thermal resistance



Hardening: Voce Law

As plastic deformation proceeds, dislocation density increases and the crystal hardens. **Voce law** [2]:

$$\dot{s}^{\alpha} = \sum_{\beta} h_{\alpha\beta}\,|\dot{\gamma}^{\beta}|, \qquad h_{\alpha\beta} = q_{\alpha\beta}\; h_0\left(1 - \frac{s^{\beta}}{s_s}\right)$$

Parameter	**Symbol**	**Cu value**
Initial resistance	τ_0	50 MPa
Saturation resistance	s_s	200 MPa
Initial hardening rate	h_0	500 MPa
Latent hardening ratio	q_{lat}	1.4

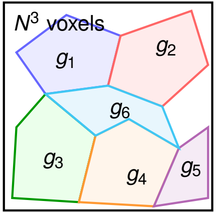
Self-hardening ($\alpha{=}\beta$): $q = 1$. Latent hardening ($\alpha{\neq}\beta$): $q = 1.4$.

Polycrystalline Microstructure

A real metal contains 10^3–10^6 grains. We represent a **Representative Volume Element (RVE)** on a regular grid.

Voronoi tessellation (periodic):

1. Seed N_g random points in $[0, 1)^3$.
2. Replicate to 3^3 periodic images.
3. Assign each voxel to nearest seed (KD-tree).
4. Random Bunge Euler angles $(\varphi_1, \Phi, \varphi_2)$ sampled with SO(3) Haar measure.



Each grain g has rotation $\mathbf{R}_g$ that rotates stiffness and slip systems into the sample frame.

Problem Statement: Equilibrium on an RVE

Given a periodic RVE with spatially varying stiffness $\boldsymbol{C}(\mathbf{x})$ and prescribed macroscopic stress $\bar{\boldsymbol{\sigma}}$ at the boundaries, find the local fields such that:

$$\begin{aligned}
\text{Equilibrium:} \quad & \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{0} && \text{(E1)} \\
\text{Constitutive:} \quad & \boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) && \text{(E2)} \\
\text{Compatibility:} \quad & \boldsymbol{\varepsilon} = \mathrm{sym}(\nabla \mathbf{u}), \;\; \mathbf{u} \text{ periodic} && \text{(E3)} \\
\text{Average stress:} \quad & \langle \boldsymbol{\sigma} \rangle = \bar{\boldsymbol{\sigma}} && \text{(E4)}
\end{aligned}$$

Key difficulty: $\boldsymbol{C}(\mathbf{x})$ varies sharply between grains — anisotropic cubic elastic constants rotated by different Euler angles.

Stress control: FFT solvers are natively strain-driven; we wrap them in a Newton iteration on $\bar{\boldsymbol{\varepsilon}}$ until $\langle \boldsymbol{\sigma} \rangle = \bar{\boldsymbol{\sigma}}$.

Lippmann–Schwinger Equation

Introduce a **homogeneous reference medium $\boldsymbol{C}^0$** and the **polarization**:

$$\boldsymbol{\tau}(\mathbf{x}) = \left[\boldsymbol{C}(\mathbf{x}) - \boldsymbol{C}^0\right] : \varepsilon(\mathbf{x})$$

Substituting into equilibrium and using the Green's function of $\boldsymbol{C}^0$ yields [3, 4]:

$$\boxed{\varepsilon(\mathbf{x}) = \bar{\varepsilon} - \left(\boldsymbol{\Gamma}^0 * \boldsymbol{\tau}\right)(\mathbf{x})}$$

- $\boldsymbol{\Gamma}^0$ is the periodic Green's operator of the reference medium.
- $*$ denotes spatial convolution.
- **Key:** in Fourier space, convolution $\rightarrow$ pointwise multiplication, so $\boldsymbol{\Gamma}^0$ is applied frequency by frequency.

Green's Operator via the Acoustic Tensor

For an **isotropic** reference medium (λ_0, μ_0), at wave direction $\mathbf{n} = \xi/|\xi|$:

Acoustic tensor:

$$A_{ik} = \mu_0\, \delta_{ik} + (\lambda_0{+}\mu_0)\, n_i n_k$$

Analytic inverse:

$$A^{-1}_{ik} = \frac{\delta_{ik}}{\mu_0} - \frac{\lambda_0{+}\mu_0}{\mu_0(\lambda_0{+}2\mu_0)}\, n_i n_k$$

Green's operator (Fourier space):

$$b_k = n_j\, \hat{\tau}_{kj}$$

$$\hat{u}_i = A^{-1}_{ik}\, b_k$$

$$\hat{\varepsilon}'_{ij} = \tfrac{1}{2}(n_i \hat{u}_j + n_j \hat{u}_i)$$

All operations in full (3×3) tensor form — no Voigt-notation factors needed, eliminating a common source of bugs.

Reference Medium and Stiffness Rotation

Reference medium from Voigt average:

$$\boldsymbol{C}^0 = \langle \boldsymbol{C}(\mathbf{x}) \rangle$$

$$K_V = \frac{C^0_{11}+C^0_{22}+C^0_{33}+2(C^0_{12}+C^0_{13}+C^0_{23})}{9}$$

$$\mu_V = \big(C^0_{11}+C^0_{22}+C^0_{33}-C^0_{12}-C^0_{13}-C^0_{23} \\ +\ 3(C^0_{44}+C^0_{55}+C^0_{66})\big)/15$$

$$\lambda_0 = K_V - \tfrac{2}{3}\mu_V$$

Stiffness rotation:

Each grain has the same (C_{11}, C_{12}, C_{44}) in its crystal frame but orientation $\mathbf{R}_g$:

$$C^{\text{sample}}_{ijkl} = R_{ip} R_{jq} R_{kr} R_{ls}\, C^{\text{crystal}}_{pqrs}$$

Anisotropy ratio $A = 2C_{44}/(C_{11}-C_{12})$:

Cu	Al	Ni	Fe
3.21	1.22	2.52	2.36

Basic Scheme (Moulinec–Suquet 1994)

Fixed-point iteration on the Lippmann–Schwinger equation [3, 4]:

1. Initialize $\boldsymbol{\varepsilon}^{(0)} = \bar{\boldsymbol{\varepsilon}}$
2. **Repeat** until $\|\Delta\boldsymbol{\varepsilon}\|/\|\boldsymbol{\varepsilon}\| < \text{tol}$:
   a. $\boldsymbol{\sigma}^{(n)} = \boldsymbol{C}(\mathbf{x}) : \boldsymbol{\varepsilon}^{(n)}$
   b. $\boldsymbol{\tau}^{(n)} = \boldsymbol{\sigma}^{(n)} - \boldsymbol{C}^0 : \boldsymbol{\varepsilon}^{(n)}$
   c. $\hat{\boldsymbol{\tau}}^{(n)} = \text{FFT}[\boldsymbol{\tau}^{(n)}]$
   d. $\hat{\boldsymbol{\varepsilon}}' = \boldsymbol{\Gamma}^0(\xi)\, \hat{\boldsymbol{\tau}}^{(n)}$ (pointwise, DC = 0)
   e. $\boldsymbol{\varepsilon}' = \text{IFFT}[\hat{\boldsymbol{\varepsilon}}']$
   f. $\boldsymbol{\varepsilon}^{(n+1)} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}'$

Cost per iteration: $\mathcal{O}(N^3 \log N)$ via FFT (vs. $\mathcal{O}(N^6)$ for direct FE assembly).

Conjugate Gradient Acceleration (Zeman 2010)

The basic scheme can be slow for high-contrast materials. CG [5] solves for the **strain fluctuation** $\tilde{\varepsilon}$:

$$\underbrace{\left(\boldsymbol{I} + \Gamma^0 \circ \Delta \boldsymbol{C}\right)}_{\boldsymbol{A}} \tilde{\varepsilon} = -\Gamma^0 \circ (\Delta \boldsymbol{C} : \bar{\varepsilon}) \equiv \mathbf{b}$$

where $\Delta \boldsymbol{C} = \boldsymbol{C}(\mathbf{x}) - \boldsymbol{C}^0$, $\varepsilon = \bar{\varepsilon} + \tilde{\varepsilon}$.

Standard CG on $\boldsymbol{A}\tilde{\varepsilon} = \mathbf{b}$:

- Each iter: 1 operator eval $=$ 2 FFTs
- Converges in $\sim$10 iterations
- Criterion: $\|\mathbf{r}\| / \|\mathbf{b}\| < \text{tol}$

Typical result (Cu, 16^3, 8 grains):

Solver	Iters (tol=10^{-5})
Basic	14
CG	11

Stress-Controlled Loading

FFT solvers are natively **strain-driven**: input $\bar{\varepsilon}$, output $\langle\boldsymbol{\sigma}\rangle$. To prescribe **boundary stresses** $\bar{\boldsymbol{\sigma}}$, we wrap the solver in a **Newton–Raphson** iteration on the macroscopic strain:

1. Initial guess: $\bar{\varepsilon}^{(0)} = (\boldsymbol{C}^0)^{-1} : \bar{\boldsymbol{\sigma}}$
2. Solve FFT with current $\bar{\varepsilon}^{(k)} \;\rightarrow\;$ obtain $\langle\boldsymbol{\sigma}\rangle^{(k)}$
3. Stress residual: $\Delta\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} - \langle\boldsymbol{\sigma}\rangle^{(k)}$
4. Update: $\bar{\varepsilon}^{(k+1)} = \bar{\varepsilon}^{(k)} + (\boldsymbol{C}^0)^{-1} : \Delta\boldsymbol{\sigma}$
5. Repeat steps 2–4 until $\|\Delta\boldsymbol{\sigma}\|/\|\bar{\boldsymbol{\sigma}}\| < \mathrm{tol}_\sigma$

Convergence: Typically 3–5 Newton iterations (each containing one full CG solve).

Example (Cu, 8^3, uniaxial $\sigma_{11} = 500$ MPa):
4 Newton iters, total 32 FFT iters $\;\rightarrow\; \langle\sigma_{11}\rangle = 500.0$ MPa, $\langle\varepsilon_{11}\rangle = 0.33\%$.

OTIS Automatic Differentiation Engine

For **elasto-viscoplasticity (EVPFFT)**, we need $\partial\dot{\gamma}/\partial\tau$ for Newton convergence.

OTIS uses **forward-mode AD**: each variable carries value + gradient vector:

$$\Big(\underbrace{f}_{\text{value}},\ \underbrace{\frac{\partial f}{\partial \tau},\ \frac{\partial f}{\partial s_{\text{th}}},\ \ldots}_{\text{gradients}}\Big)$$

Derivatives propagate exactly via the chain rule at every arithmetic operation — no finite differences, no truncation error.

Tracked sensitivities (per system):

- $\partial\Delta\gamma/\partial\tau$
- $\partial\Delta\gamma/\partial\tau_{\text{back}}$
- $\partial\Delta\gamma/\partial S_{\text{th,SSD}}$
- $\partial\Delta\gamma/\partial S_{\text{ath,SSD}}$

Enables **quadratic (Newton) convergence** in the non-linear constitutive update.

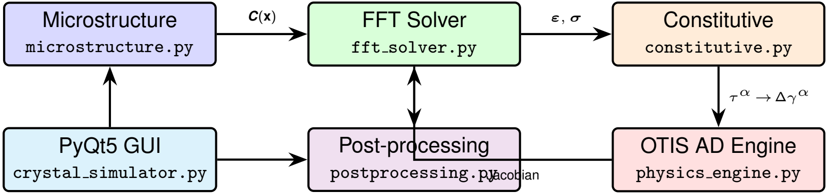
EVPFFT: Incremental Loading

The elasto-viscoplastic solver [6, 7] extends the elastic FFT to incremental plasticity:

1. Divide total loading into N_{inc} increments.
2. At each increment, iterate:
   - **Constitutive update** at every voxel:
     - $\tau^\alpha = \boldsymbol{\sigma} : \boldsymbol{P}^\alpha \ \rightarrow$ OTIS flow rule $\rightarrow \ \Delta\gamma^\alpha$
     - $\Delta\boldsymbol{\varepsilon}^p = \sum_\alpha \Delta\gamma^\alpha \, \boldsymbol{P}^\alpha$
     - Update hardening: $s^\alpha \leftarrow s^\alpha + \sum_\beta h_{\alpha\beta} |\Delta\gamma^\beta|$
   - **FFT equilibrium** solve with updated stress field.
3. Converge when $\|\Delta\boldsymbol{\varepsilon}\| / \|\boldsymbol{\varepsilon}\| < \text{tol}$.

Output: full-field stress, strain, accumulated slip, and texture evolution.

Software Architecture



- Pure **NumPy/SciPy** — no Fortran dependencies.
- FFT via `numpy.fft` (drop-in `pyFFTW` replacement for speed).
- Full (3×3) tensor arithmetic avoids Voigt-notation pitfalls.

Boundary Conditions and 3D Visualization

The GUI provides **stress-controlled** input with clear loading visualization:

Boundary stress input:

- Full symmetric stress tensor $\bar{\boldsymbol{\sigma}}$ in MPa
- Presets: uniaxial, biaxial, hydrostatic, pure shear
- Each preset describes *which faces* receive traction

3D preview:

- Wireframe RVE cube
- Traction arrows on each face
- Red $=$ tension, blue $=$ compression

Result visualization:

- **3D**: Von Mises stress on grain boundaries with loading arrows overlaid
- **2D slices**: σ_{VM}, σ_{11}, ε_{11}, hydrostatic pressure, grain map
- Reports achieved $\langle \boldsymbol{\sigma} \rangle$ and resulting $\langle \boldsymbol{\varepsilon} \rangle$

Key Implementation Details

1. Tensor-based Green's operator:

- Fields stored as $(N, N, N, 3, 3)$
- $\mathbf{A}^{-1}(\mathbf{n})$ pre-computed $\rightarrow (N, N, N, 3, 3)$
- 9 component-wise FFTs per field

2. Periodic Voronoi via KD-tree:

- Seeds replicated to $3^3{=}27$ images
- Query cost: $\mathcal{O}(N^3 \log N_g)$

3. Convergence criteria:

- Basic scheme: relative strain change $\|\boldsymbol{\varepsilon}^{(n+1)} - \boldsymbol{\varepsilon}^{(n)}\| / \|\boldsymbol{\varepsilon}^{(n)}\|$
- CG: residual norm $\|\mathbf{r}\| / \|\mathbf{b}\|$
- Stress control: $\|\Delta\bar{\boldsymbol{\sigma}}\| / \|\bar{\boldsymbol{\sigma}}\|$

4. Spectral equilibrium (diagnostic):

$\|\xi_j \hat{\sigma}_{ij}\| / \|\hat{\sigma}\|$ has $\sim$7% floor at sharp grain boundaries — this is a discretization artifact, not a convergence failure.

Validation and Results

1. Homogeneous medium ($\boldsymbol{C}=$ const): error $=0$ in one iteration. ✓

2. Polycrystalline copper (C_{11}=168.4, C_{12}=121.4, C_{44}=75.4 GPa):

Test	Grid	E_{eff} (GPa)	CG iters	Control
8 grains	16^3	≈ 202	11	strain
4 grains	8^3	—	8/Newton	stress

Bounds: $E_R = 133$ GPa (Reuss) $< E_H \approx 171$ (Hill) $< E_{\text{FFT}} \approx 200 < E_V = 210$ GPa (Voigt). ✓

3. Stress-controlled test ($\sigma_{11} = 500$ MPa, Cu 8^3):
4 Newton iters, $\langle \sigma_{11} \rangle = 500.0$ MPa, $\langle \varepsilon_{11} \rangle = 0.33\%$. ✓

Stress heterogeneity: VM stress range $\approx$ 500–1500 MPa (factor $\sim 3\times$) under 1% uniaxial strain.

Scalability and Future Work

Current capabilities:

- Elastic and EVPFFT simulations
- Strain- and stress-controlled loading
- Arbitrary grains on N^3 grids
- Interactive PyQt5 GUI with 3D views
- 3D boundary stress visualization

Planned extensions:

- 64^3–128^3 grids (`pyFFTW` + r2c transforms)
- Finite-strain: $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$
- Texture evolution tracking
- Non-local EVPFFT [8]
- Phase-field: damage & recrystallization

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