Multi-Time Scaling Techniques for Accelerating Crystal Plasticity Fatigue Simulations of Additively Manufactured Inconel 718

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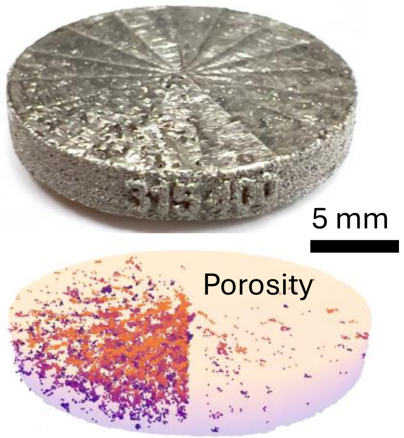
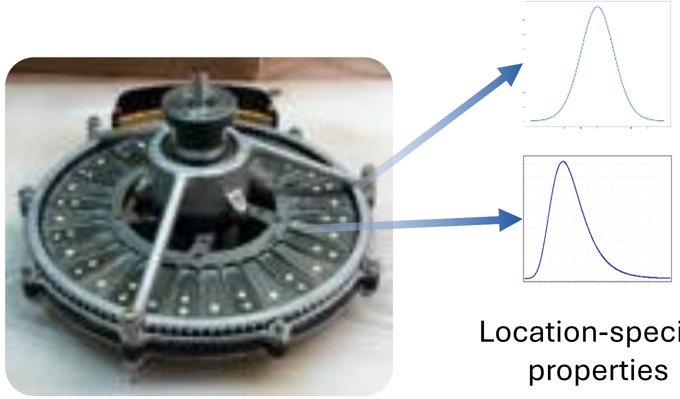
Computational Materials-Informed Qualification and Certification of Additively Manufactured (AM) Flight Hardware





Location-specific properties

Process → **Structure** → **Property / Performance**

Small deviations in process conditions → Potentially large variation in performance

Current approaches for qualification and certification of metallic materials are heavily dependent on test data

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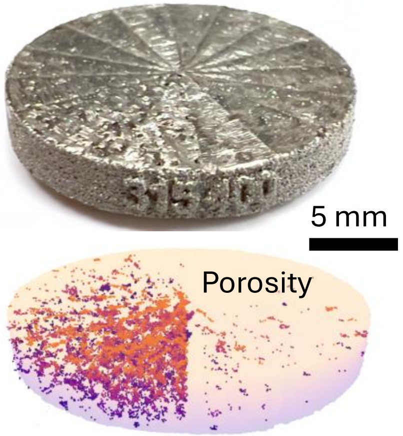

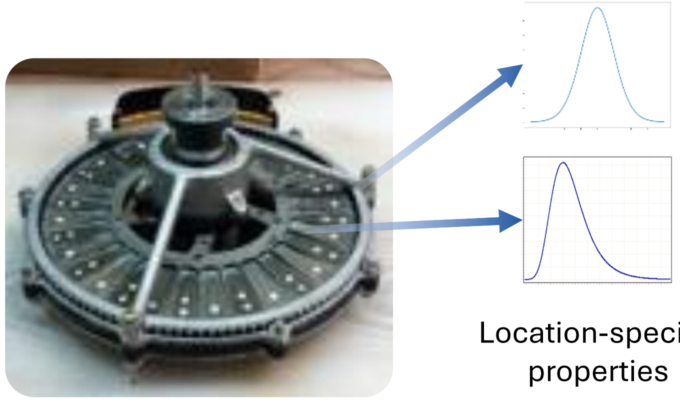

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Small deviations in process conditions → Potentially large variation in performance

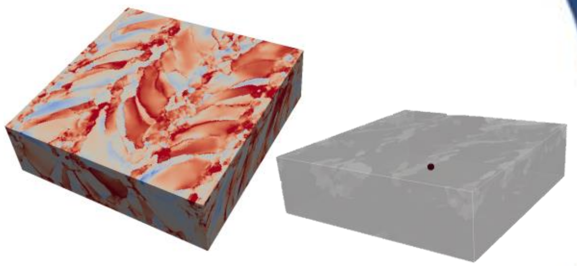
Goal: Change the Paradigm for Qualification and Certification

Develop a computational materials-informed ecosystem for quantifying sources of variability in fatigue performance of additively manufactured metallic materials through integrated multi-scale, multi-physics simulation, characterization and monitoring

Microstructure-informed Fatigue Simulation

Fatigue of AM materials with porosity

- Fatigue life is highly dependent on exact microstructure and defect configuration, which are dependent on process conditions
- Early stages of crack nucleation depend on *evolving* weakest links



Micromechanical simulation with porosity

Crack nucleation prediction requires microstructure simulation

- However, even low cycle fatigue demands thousands of loading cycles
- Physics-based simulations of a single loading cycle can take minutes to hours
- Experimental validation is limited by this computational efficiency

For a fixed simulation time, choose between trade-offs

↑ 100X **Number of Loading Cycles** 100X ? ↓ **Resolution / Domain Size** 100X ? ↓ **Solution Accuracy**

Can we simulate more loading cycles while reducing the corresponding trade-offs?

Combining Two Simulation Capabilities

(1) Elasto-viscoplastic fast Fourier transform (FFT) based micromechanical solver

Ricardo Lebensohn, Anand Kanjarla, Philip Eisenlohr. "An elasto-viscoplastic formulation based on fast Fourier transforms for the prediction of micromechanical fields in polycrystalline materials"

Core Features

- **FFT scaling:** FFT-based solution of micromechanical equilibrium and boundary conditions
- **"Voxel-based"**: Straightforward to model complex microstructures and defect configurations

(2) WATMUS: Wavelet transformation based multi-time scaling method

Deepu Joseph, Pritam Chakraborty, Somnath Ghosh. "Wavelet transformation based multi-time scaling method for crystal plasticity FE simulations under cyclic loading"

Core Features

- ~~**Multi-resolution Adaptive:** Reduced and adaptive wavelet basis for solving cyclic behavior~~
- **Cycle scale time integration:** Robust acceleration method to jump across loading cycles

Basic Crystal Plasticity

Anisotropic elasticity

$$\boldsymbol{\sigma} = \mathbb{C}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p)$$

Linear isotropic hardening

$$\dot{g} = h \sum_{\alpha} |\dot{\gamma}^{\alpha}|$$

Irreversible dislocation accumulation

Viscoplastic power law flow rule

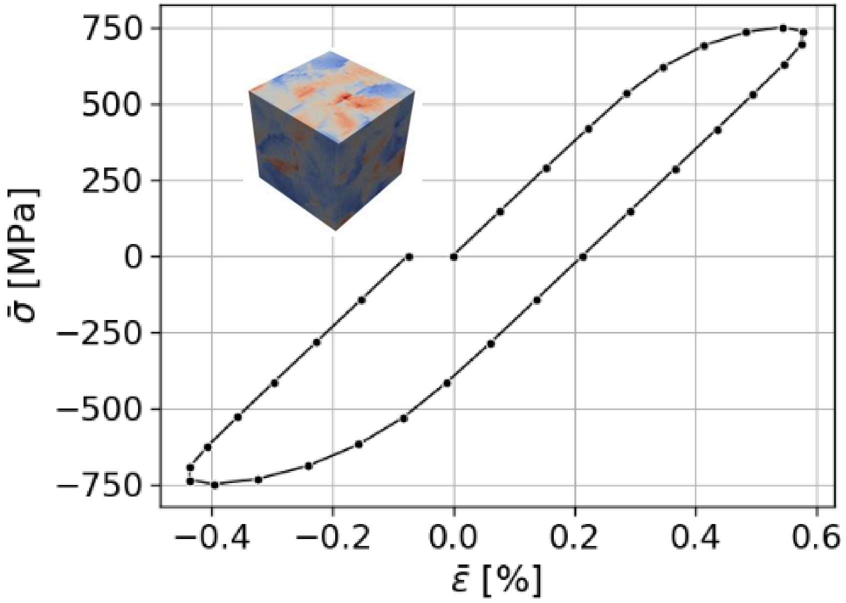
$$\dot{\gamma}^{\alpha} = a \left| \frac{\boldsymbol{\sigma} : \mathbf{s}^{\alpha}}{g} \right|^{1/m} \mathrm{sign}(\boldsymbol{\sigma} : \mathbf{s}^{\alpha})$$

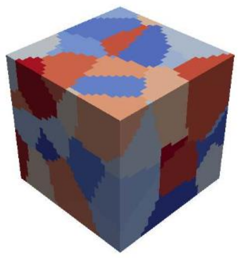
$$\dot{\boldsymbol{\varepsilon}}_p = \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{s}^{\alpha}$$

$\boldsymbol{\sigma}$:	stress	α :	slip system index
$\boldsymbol{\varepsilon}$:	total strain	a :	reference slip rate
$\boldsymbol{\varepsilon}_p$:	plastic strain	m :	strain rate sensitivity
g :	slip resistance	h :	hardening
$\mathbf{s}^{\alpha}$:	Schmid tensor		

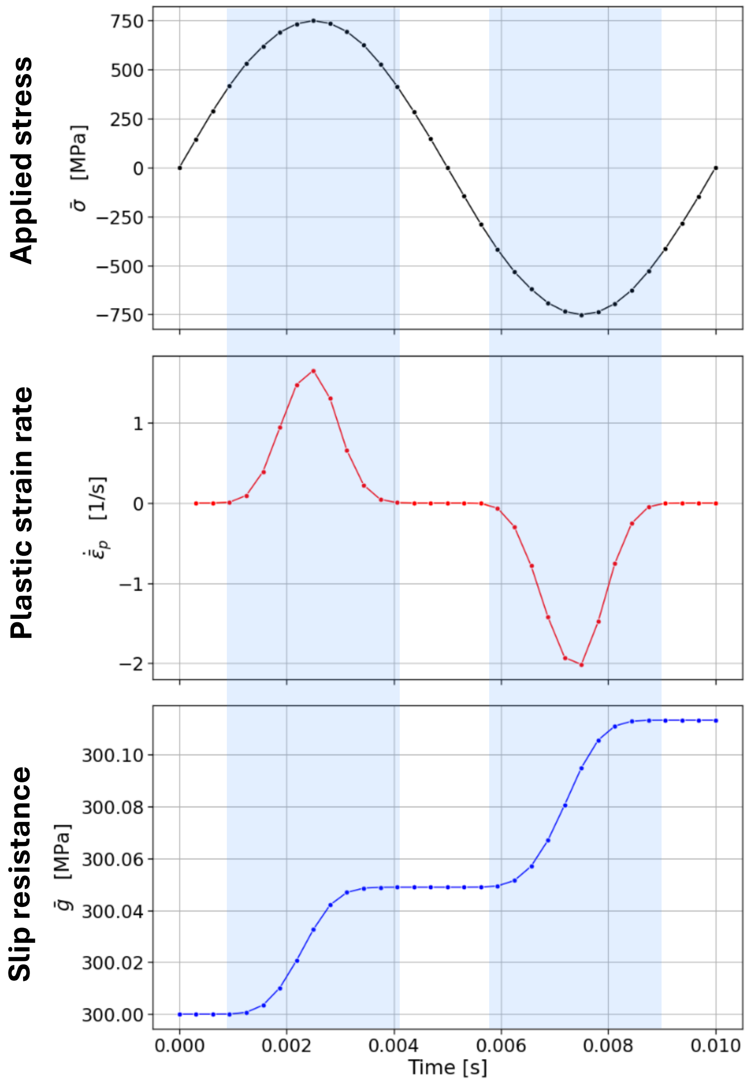
Model Response to Uniaxial Stress-controlled Loading

Stress-strain for single cycle





64 grain microstructure



Cyclic loading

$$\bar{\sigma} = \bar{\sigma}_0 \sin 2\pi f t$$

$$\bar{\sigma}_0 = 750\,\mathrm{MPa}$$
$$f = 100\,\mathrm{Hz}$$

Flow rule

$$\dot{\gamma}^\alpha = a \left| \frac{\boldsymbol{\sigma} : \mathbf{s}^\alpha}{g} \right|^{1/m} \mathrm{sign}(\boldsymbol{\sigma} : \mathbf{s}^\alpha)$$

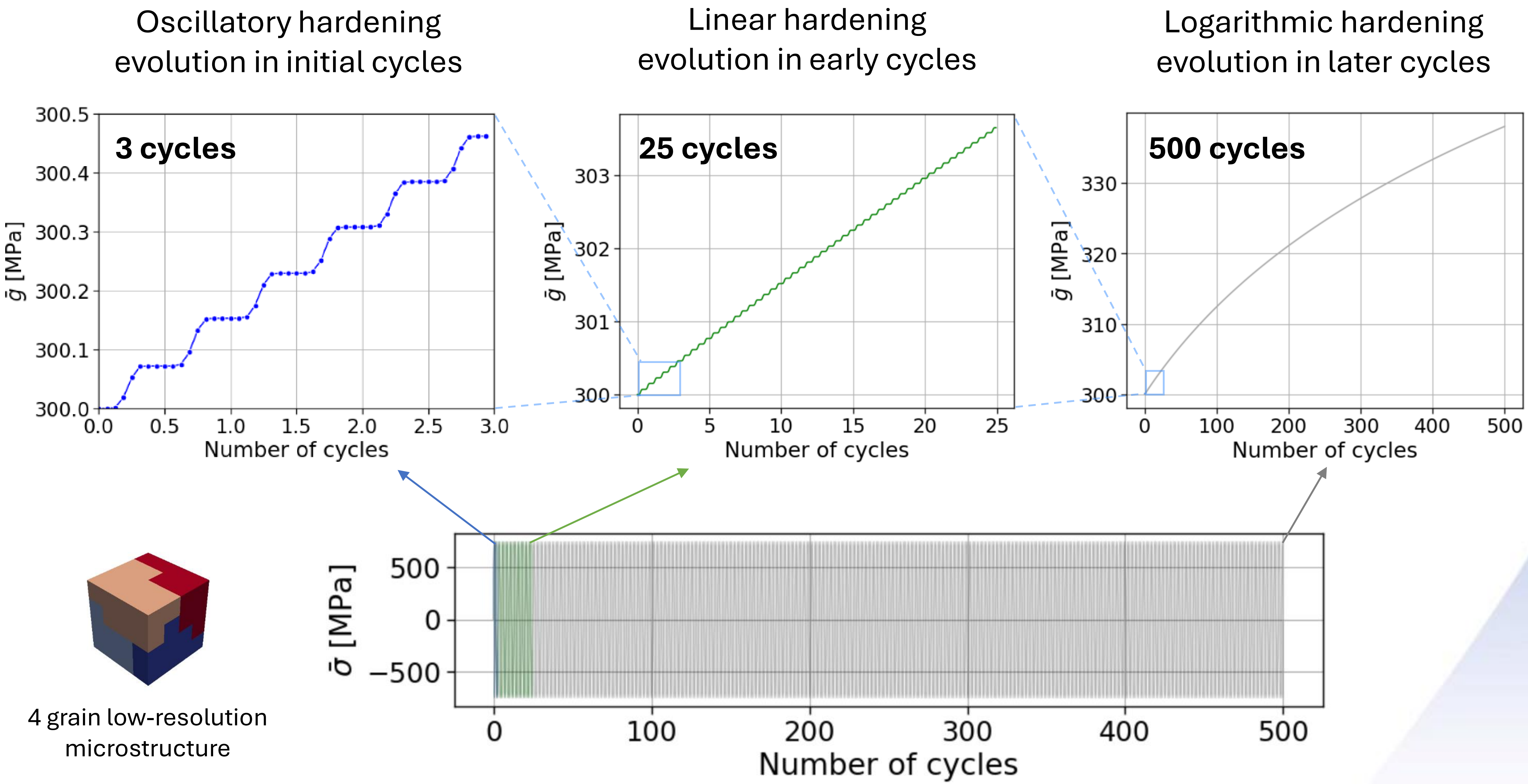
$$\dot{\varepsilon}_p = \sum_\alpha \dot{\gamma}^\alpha \mathbf{s}^\alpha$$

Hardening

$$\dot{g} = h \sum_\alpha |\dot{\gamma}^\alpha|$$

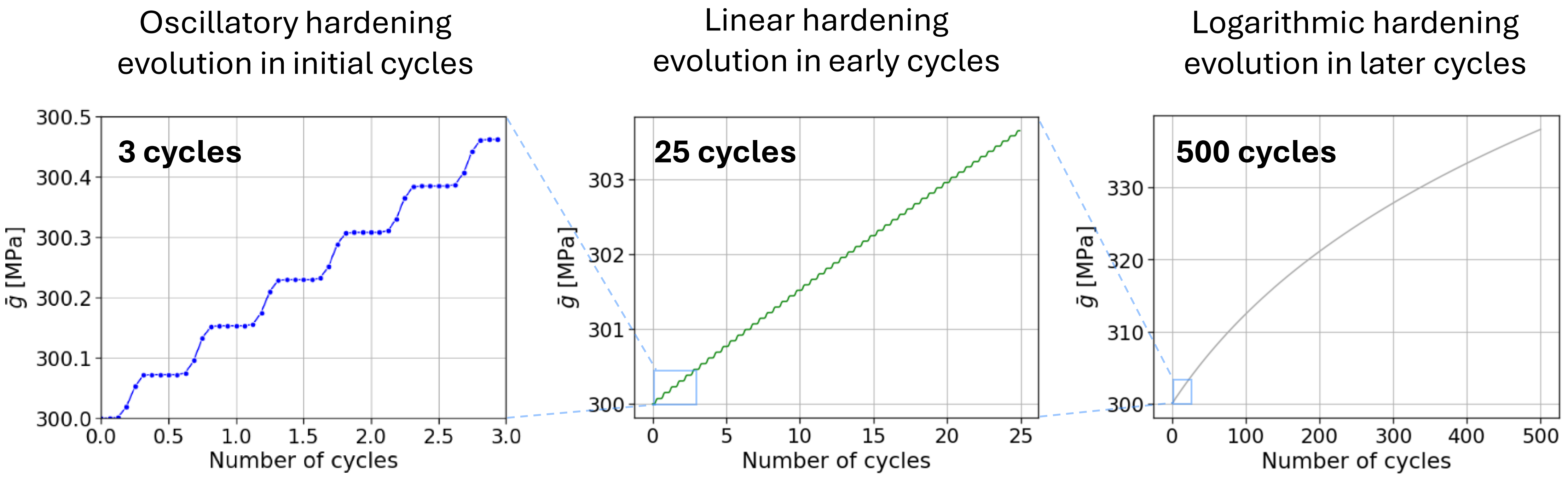
All quantities are volume averages (denoted by overbars) of components in the loading direction

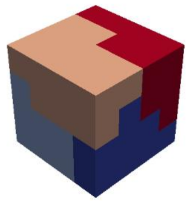
Material Behavior is Multi-scale in Fatigue



4 grain low-resolution microstructure

Material Behavior is Multi-scale in Fatigue





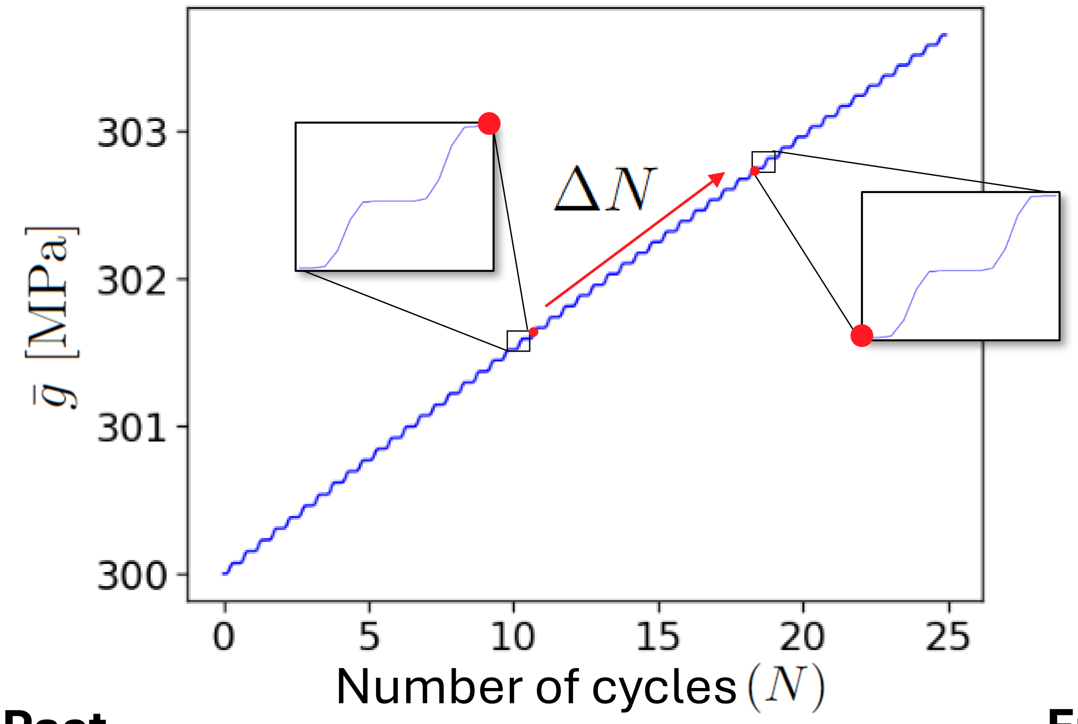
4 grain low-resolution microstructure

How can this continuity and predictability of the material state evolution be leveraged?

Cycle Scale Time Integration

Basic idea

Rather than solving for every time step of every cycle → integrate the material state across the *cycle time scale*



Past Cycle → **Future Cycle**

Cycle Scale Time Integration

Method to "jump" many cycles in time

Cycle Scale Time Integration

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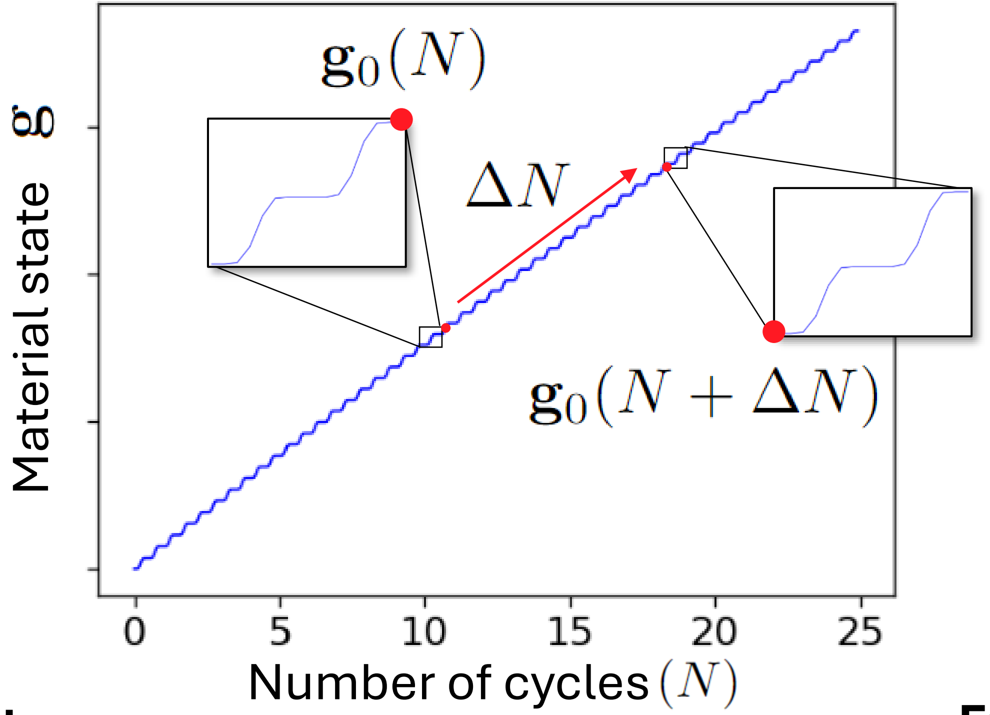


Past Cycle → **Future Cycle**

Cycle Scale Time Integration

Method to "jump" many cycles in time

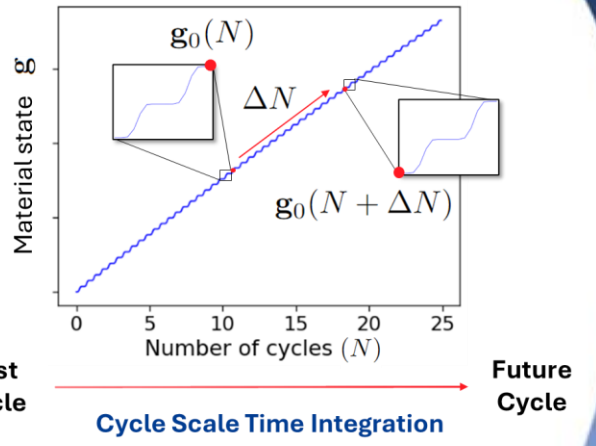
Focus on the ends of each cycle with a change of variables

Let $\mathrm{g}_0(N)$ *be a vector of all material state variables in the constitutive model at the start of a given cycle*

Cycle Scale Time Integration

Taylor approximation

$$\mathrm{g}_0(N+\Delta N) = \mathrm{g}_0(N) + \left(\left.\frac{\partial \mathrm{g}_0(N)}{\partial N}\right|_N\right)\Delta N + \frac{1}{2}\left(\left.\frac{\partial^2 \mathrm{g}_0(N)}{\partial N^2}\right|_N\right)\Delta N^2 + o(\Delta N^3)$$



Definitions of cycle scale derivatives

$$\left.\frac{\partial \mathrm{g}_0(N)}{\partial N}\right|_N = \frac{\mathrm{g}_0(N) - \mathrm{g}_0(N-\Delta N)}{\Delta N}$$

(Explicit time integration)

$$\left.\frac{\partial \mathrm{g}_0(N)}{\partial N}\right|_N = \frac{\mathrm{g}_0(N+\Delta N) - \mathrm{g}_0(N)}{\Delta N}$$

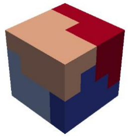
(Implicit time integration)

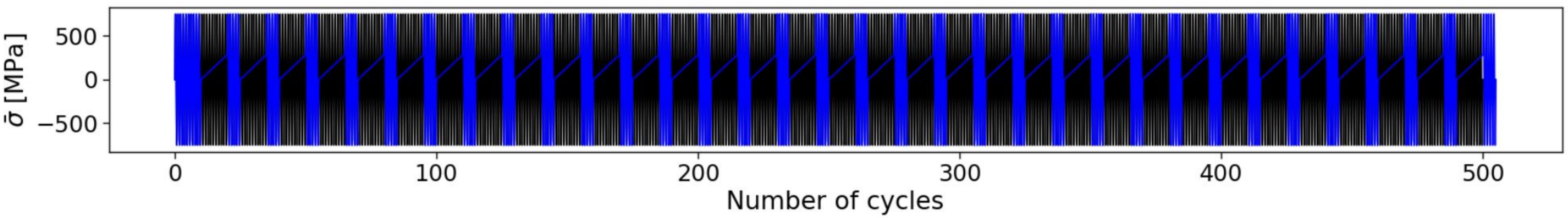
$$\boxed{\mathrm{g}_0(N+\Delta N) = \left(1 + \Delta N + \frac{1}{2}\Delta N^2\right)\mathrm{g}_0(N) - \left(\Delta N + \Delta N^2\right)\mathrm{g}_0(N-1) + \left(\frac{1}{2}\Delta N^2\right)\mathrm{g}_0(N-2)}$$

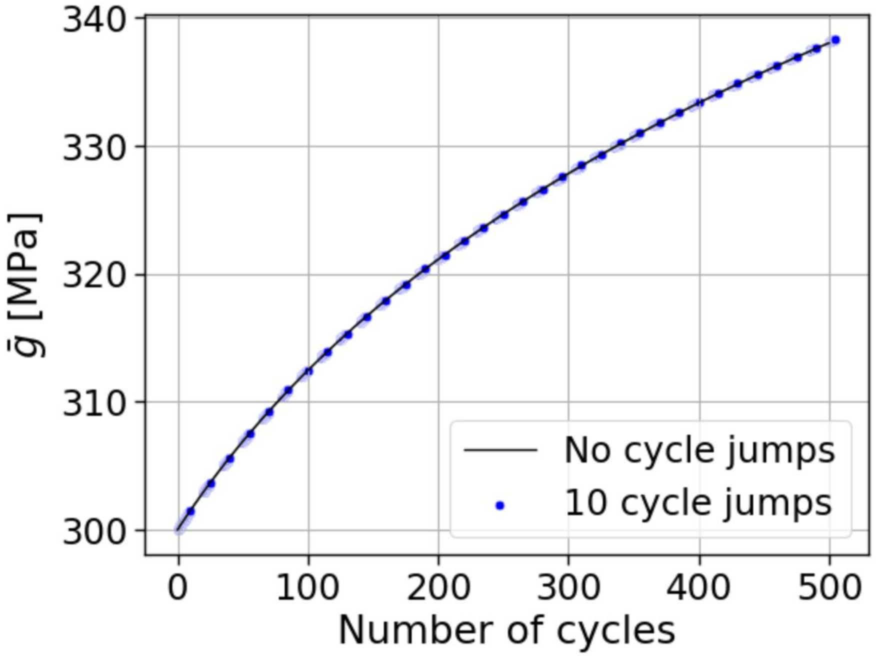
Material state after cycle jump is a function of previous cycle states

Cycle Jump Example Cases

750 MPa Stress-controlled loading for 500 cycles



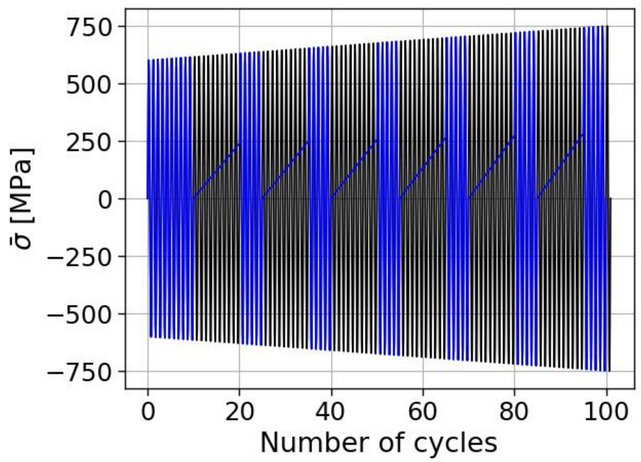


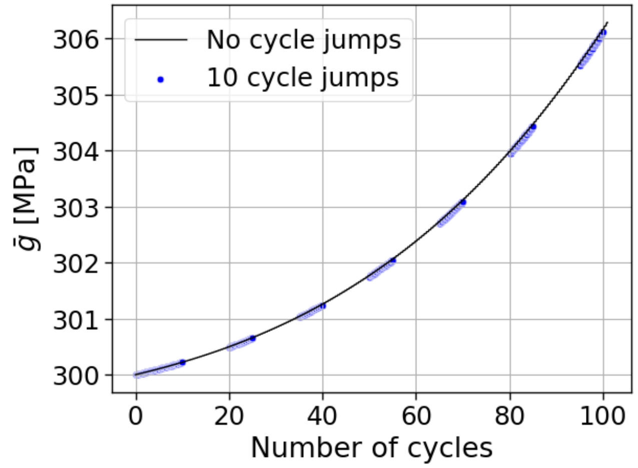


Hardening evolution is accurately maintained while jumping across the cycle scale

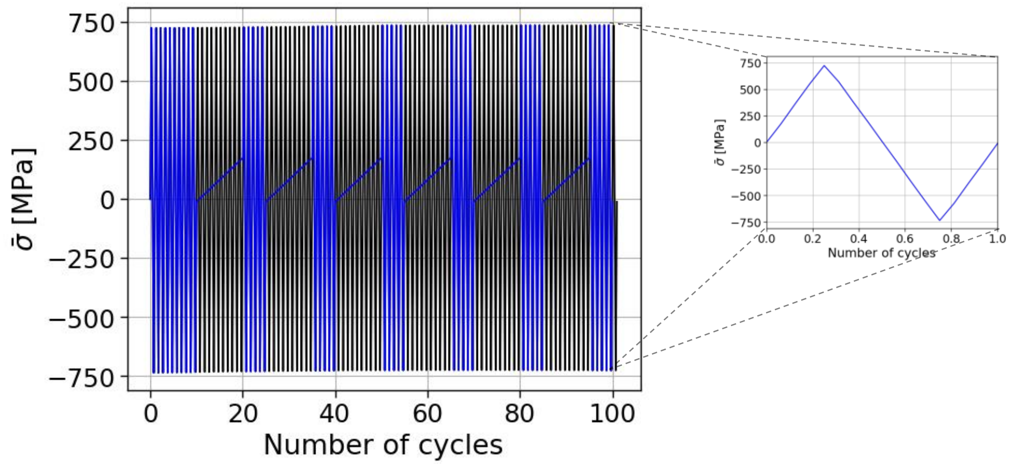
Cycle Jump Example Cases

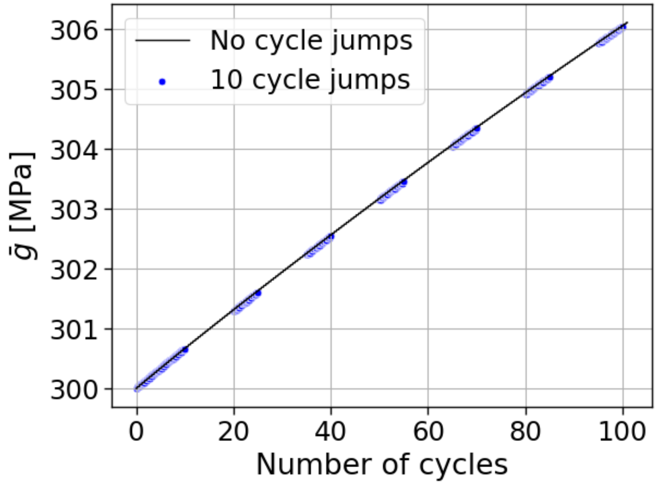
Ramped (aperiodic) loading for 100 cycles





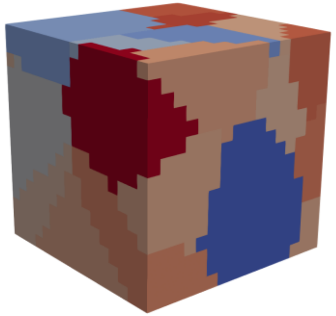
Triangular loading for 100 cycles



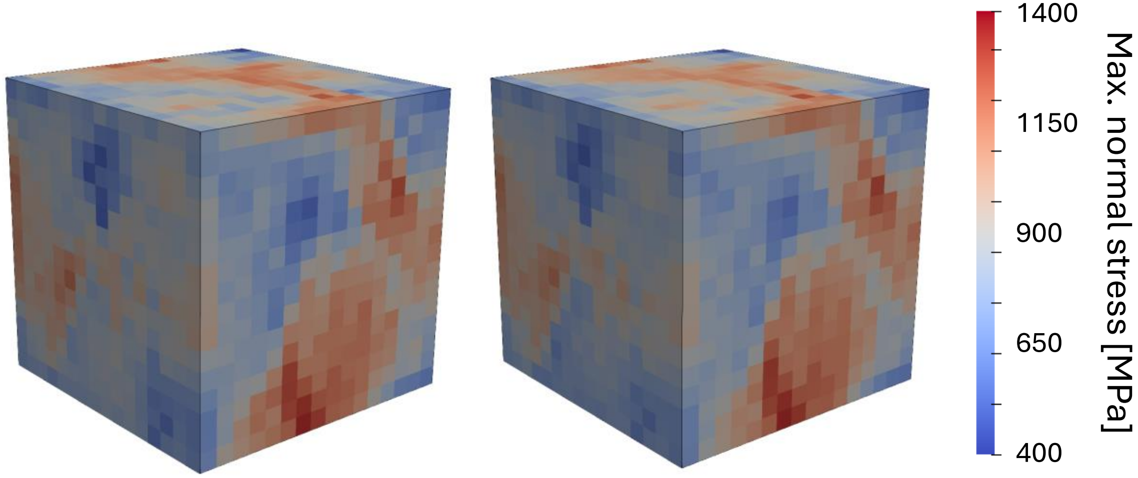


Stress Redistribution Throughout Cyclic Loading

24 grain microstructure with fully reversed stress-controlled 900 MPa loading

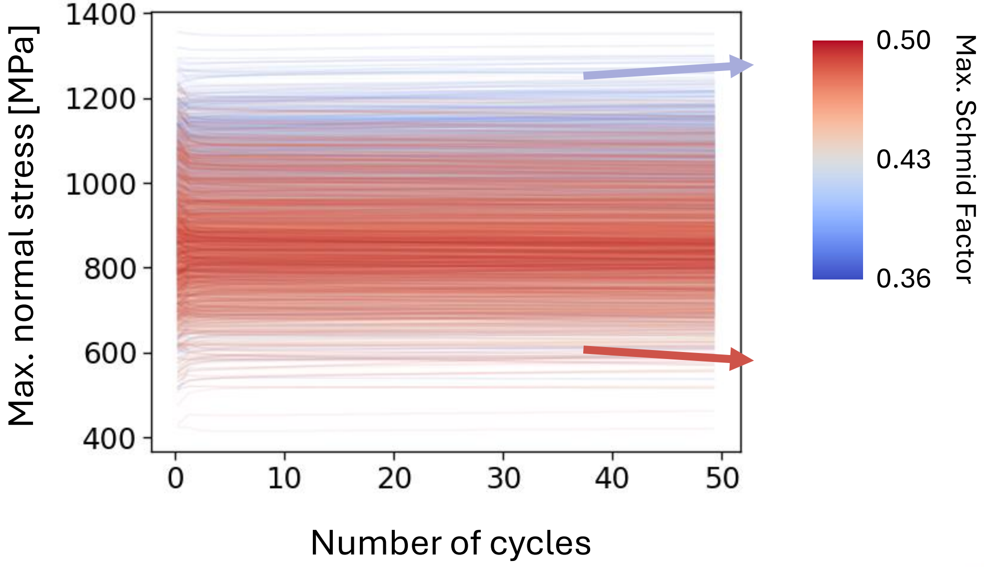


Uniform stress redistribution



Stress gradually localizes in concentrated areas over many cycles

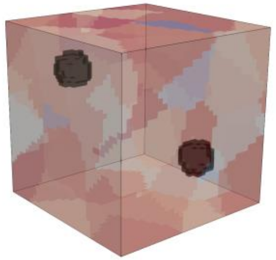
Early stress redistribution and gradual concentration



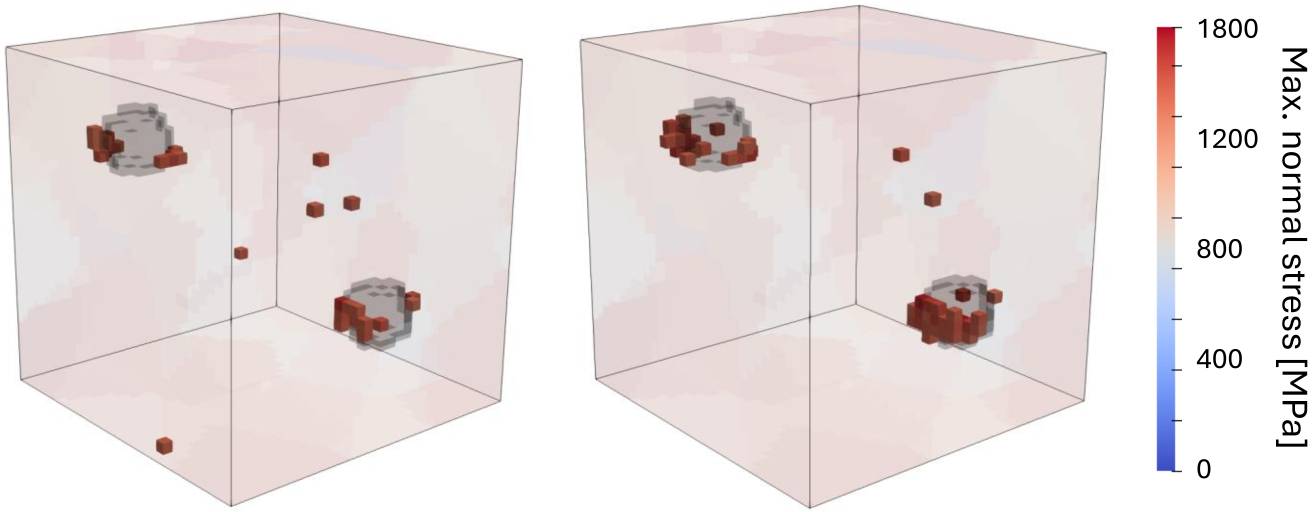
Each line is the history of a single material point at the peak load of each cycle

Stress Redistribution with Porosity

64 grain and 2 pore microstructure with fully reversed stress-controlled 900 MPa loading



Stress concentration locations shift and compete throughout cyclic loading

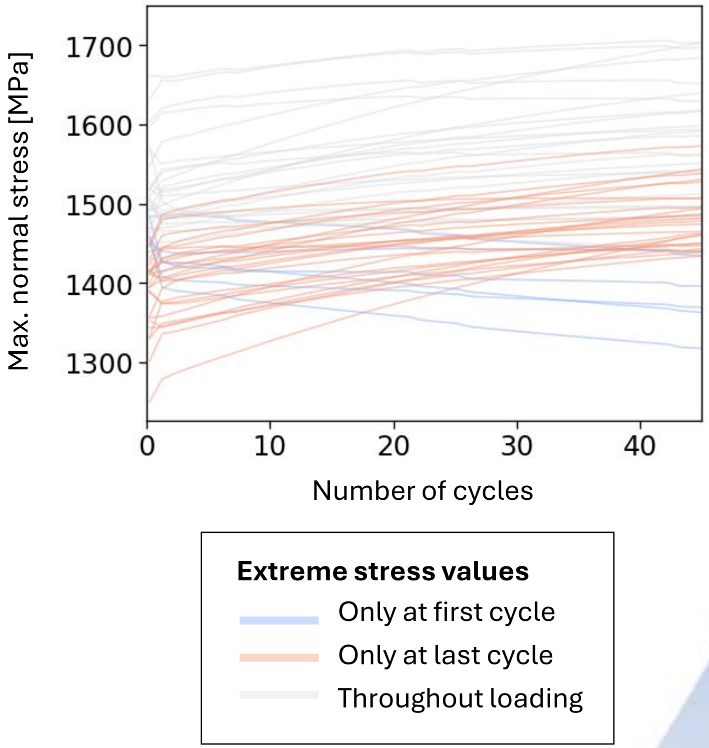


1st cycle

50th cycle

Threshold on material points where maximum normal stress is greater than 1450 MPa

Extreme stress value evolution at material points



Summary

- Combined elasto-viscoplastic FFT solver with cycle scale time integration to accelerate fatigue simulations
- Demonstration of explicit cycle scale time integration to accelerate crystal plasticity simulations
- Multi-time scale methods exhibit load-agnostic features
- Porosity induces changes in the rate and location of local stress redistribution

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Constitutive Parameters

Elastic Parameters

C_{1111} [GPa]	C_{1122} [GPa]	C_{2323} [GPa]
260	180	110

Plastic Parameters

g (initial) [MPa]	m	a [s^{-1}]	h [MPa]
300	0.1	1	10