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Title: Direct multiscale embedding of viscoplastic self-consistent (VPSC)
polycrystal plasticity enabled by adaptive sampling

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Direct multiscale embedding of viscoplastic self-consistent (VPSC) polycrystal plasticity enabled by adaptive sampling

Nathan Barton (LLNL) and Ricardo Lebensohn (LANL)

Adaptive sampling: improved mechanics without undue computational expense - Taylor (fcc) and now VPSC (hcp):

Previous Barton's et al. work: Arsenlis et al., CMAME, 2006; Barton et al., IJP, 2008; Knap et al., IJNME, 2008; Bernier et al., JEMT, 2008; Barton et al., IJNME 2011.

AS-VPSC new work: N.R. Barton, J.V. Bernier, R.A. Lebensohn and D.E. Boyce: “The use of discrete harmonics in direct multi-scale embedding of polycrystal plasticity”, Computer Methods in Applied Mechanics and Engineering, in press.

Adaptive Sampling builds response on the fly

- Coarse scale model queries database for fine-scale material response
- If possible, approximate response from past evaluations
- Otherwise perform fine scale evaluation
- Fine-scale evaluations grow database

Speedup and error control are well behaved

- **250X speedup**: drawing, Taylor, with 512 grains at the fine-scale
- Full evaluation simulation: roughly 2.3 processor-years

$$\text{AS speedup} \approx \frac{NW}{nW + Nw}$$

- **N** : fine-scale queries
- **n** : fine-scale evaluations under AS
- **W** : fine-scale work
- **w** : AS work in lieu of fine-scale evaluation

Low symmetry and low-SFE cubic single crystals often twin, substantially affecting polycrystal response

HCP Metals: Zr (Nuclear), Ti (Aero), Mg (Auto), Be (defense):

Slip:

Twinning:

Rapid texture changes, anisotropic hardening:

alpha-U, orthorhombic:

Slip:

Twinning:

Strong anisotropy, tension-compression asymmetry:

FCC, BCC, low SFE, high strain-rate:

Slip:

Twinning:

ViscoPlastic Self-Consistent (VPSC) formulation

Lebensohn and Tome, Acta Mater (1993)

- VPSC model:

- VPSC vs Taylor:

Unlike under Taylor model, each grain deforms differently according to its directional properties.

- VPSC code:

Distribution version: widely used in Universities, Laboratories and Industry.

- VPSC-based Abaqus UMAT:

Available (Segurado, Lebensohn, Tome, IJP, 2012), based on “full evaluation”.

- Material systems studied with VPSC:

Metals: Al-alloys, Cu-alloys, Zr-alloys, Ti-alloys, Mg-alloys, Be, Ni-alloys, steels, U-alloys, etc. **Geomaterials:** ice, calcite, quartzite, halite, olivine, etc. **Polymers:** Polyethylene

VPSC-Abaqus prediction of bending of rolled Ti bars

Eglin's Ti plate, orthotropic texture (*):

4-point bending jig:

4 different configurations:

Animated simulation:

Different final 3-D shapes:

(*) Nixon et al. IJP, 2010; (**) Knezevic et al, MSE A, 2013

Uniaxial tests: anisotropic, tension $\neq$ compress (twinning!) (*):

VPSC-Abaqus (green symbols) vs experimental cross-sections (photographs) ():**

Previous AS implementation (Taylor) employed a simple fine-scale state description

- Scalar hardness variable(s) $\mathcal{H} = \{h_1, h_2\}$
 - no texture variation or evolution beyond rigid rotation
 - ≈ 10 dimensional sampling space
 - adequate for initial anisotropy, strain localization, pressure and temperature sensitivity

AS-VPSC makes use of a more expansive fine-scale state description

$$\mathcal{H} = \{h_1, h_2, h_3, \dots, A_{ij}, c_k\}$$

grain shape

texture

Texture (ODF) evolution follows from standard conservation equation, and allows for twinning

Conservation equation:	$\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = \Theta$
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Weak form:
$$\int_{\mathcal{R}} \left(\frac{\partial \rho}{\partial t} \phi + \phi \text{div}(\rho \mathbf{v}) \right) d\mu = \int_{\mathcal{R}} \left(\frac{\partial \rho}{\partial t} \phi - \rho \mathbf{v} \cdot \nabla \phi \right) d\mu \quad \forall \phi$$

Time discretization:
$$\frac{\partial \rho}{\partial t} \sim (\rho_{n+1} - \rho_n) / \Delta t$$

Forward-Euler integration:

$$\int_{\mathcal{R}} \rho_{n+1} \phi d\mu = \int_{\mathcal{R}} (\rho_n \phi + (\Delta t)(\rho_n \mathbf{v} \cdot \nabla \phi + \Theta_n \phi)) d\mu$$

Spatial discretization, no twinning:
$$\bar{\rho}_{n+1} = \bar{\rho}_n + L^{-1} G(\bar{\rho}_n \bar{V}) \Delta t$$

Twinning operators constructed similarly:
$$\bar{f} \cdot (L_t \bar{g}) = \int_{\mathcal{R}} f(\mathbf{r}) g(\mathbf{r} \mathbf{r}_t) d\mu$$

Or using orthonormal basis functions:	$\rho = \sum_i c_i H_i \quad c_i = \int_{\mathcal{R}} \rho H_i d\mu$
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$$\frac{dc_i}{dt} = \int_{\mathcal{R}} \frac{\partial \rho}{\partial t} H_i d\mu = \int_{\mathcal{R}} (\Theta - \text{div}(\rho \mathbf{v})) H_i d\mu = \int_{\mathcal{R}} \rho \mathbf{v} \cdot \nabla H_i d\mu + \int_{\mathcal{R}} \Theta H_i d\mu$$

Pre-computation is unfeasible: Even reducing to a small (coarse) harmonic basis, computation time is daunting

- VPSC calculation takes ≈ 1 second
- Evaluation results depend on current texture, so need to span space of harmonic basis and deformation conditions ... say 8^{60} evaluations, or 10^{46} processor-years

$$\mathcal{Y} = f_{\mathcal{Y}}(\bar{\tau}', \mathcal{H}, p, \theta) \quad \mathcal{H} = \{h_1, h_2, h_3, \dots, A_{ij}, c_k, v_{\text{tw}}\}$$

- But a given simulation samples a comparatively low-dimensional manifold in this high-dimensional space!

Discrete harmonics offer an appealing basis

Spherical harmonics are eigenfunctions of the negative Laplacian on the n-sphere:

$$-\Delta u = \lambda u$$

Weak form:

$$\int \nabla u \nabla \phi = \lambda \int u \phi, \quad \forall \phi$$

Discrete harmonics satisfy the generalized eigenvalue problem:

$$H\bar{u} = \lambda L\bar{u}$$

	hex. symm.						
PF deg.	0	2	4	6	7	8	9
quat. deg.	0	4	8	12	14	16	18
dimen.	1	5	9	26	15	34	19

Increasing degree

Twinning operators amount to non-local source/sink relationships

- Twinning operators involve the construction of modified 2-form “mass” (L-2 inner product) matrices:

$$\bar{f} \cdot (L_t \bar{g}) = \int_{\mathcal{R}} f(\mathbf{r}) g(\mathbf{r} \mathbf{r}_t) d\mu$$

- Example: image of Gaussian at the origin under six twinning operators

Uniaxial deformation to 25% strain illustrates convergence

Direct evolution with full DOF:

0.468057
1627.46

0.466554
1635.77

0.234315
1624.98

0.233312
1624.75

0.160327
1641.73

0.149172
1644.25

L_2 norm of difference with direct evolution

strength measure (MPa)

Discrete aggregate results agree with direct continuous evolution methods

Discrete
aggregate

Direct
evolution

Even under monotonic loading, sampling provides benefit

Evaluation fraction < 0.1

Example application – four-point bend of textured titanium

- Initial texture from pole figures
- Project onto harmonics to get initial coefficients

Nixon, Lebensohn, Cazacu, & Liu,
Acta Mat., 2010

Harmonic-based scheme captures salient features of the response

- Compared to (points) PTR scheme with many more degrees of freedom & distinct hardening in each grain
- Do not expect complete agreement – models employ different assumptions

Four-point bend results demonstrate utility in component-scale simulations

Shape of cross-sections for two different bend orientations – agree with published results (Knezevic *et al.*, *Mat. Sci. Eng. A*, 2013)

Summary

- Adaptive sampling working with more detailed state descriptions:
 - ODF expansion with 10s of terms
 - Maintains benefit from sampling
- Convergence versus expansion order is well behaved
- Gross texture evolution from twinning is captured
- VPSC derivatives: in parallel on remote processes
- AS-VPSC improves AS-Taylor accounting for texture evolution, twinning effects.
- ALE3D-AS-VPSC (this work) vs COEVP-AS-VPFFT (ExMatEx scale-bridging app):
 - homogenization-based model (VPSC) implies no fine-scale spatial resolution, allowing us to account for microstructure evolution by solving a PDE (flux equation with source and sinks) for ODF.
 - with VPFFT we still need to find appropriate and numerically tractable microstructure representation for AS.
- Do we want to pursue a COEVP-AS-VPSC scale-bridging app?

$$\frac{dc_i}{dt} = \int_{\mathcal{R}} \rho \mathbf{v} \cdot \nabla H_i d\mu + \int_{\mathcal{R}} \Theta H_i d\mu$$

$$\rho = \sum_i c_i H_i$$