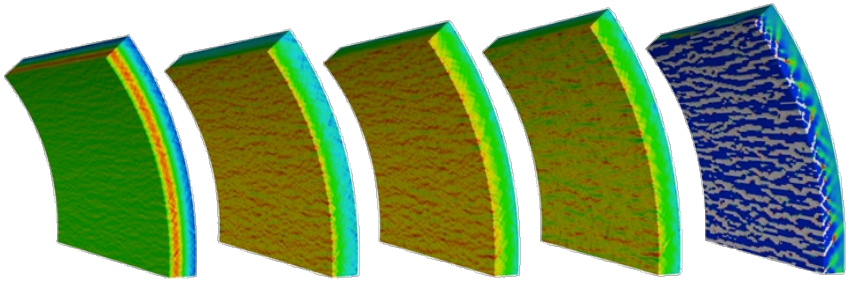
Direct multiscale embedding of viscoplastic self-consistent (VPSC) polycrystal plasticity enabled by adaptive sampling

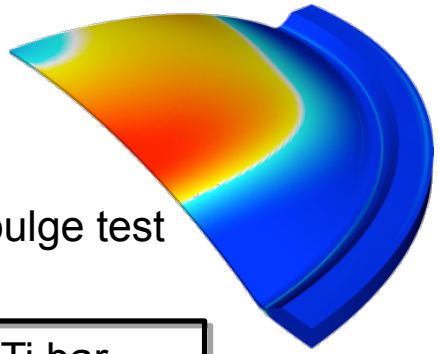
Nathan Barton (LLNL) and Ricardo Lebensohn (LANL)

LA-UR-14-28102

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



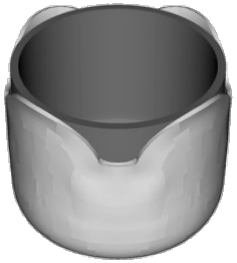
over-pressured tube



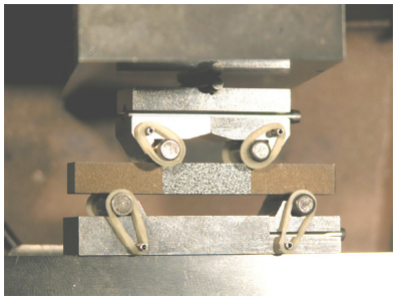
bulge test

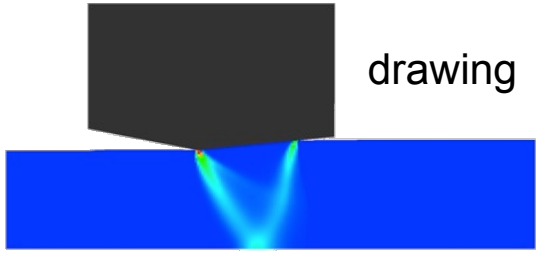
barreling

cup drawing



bending of Ti bar





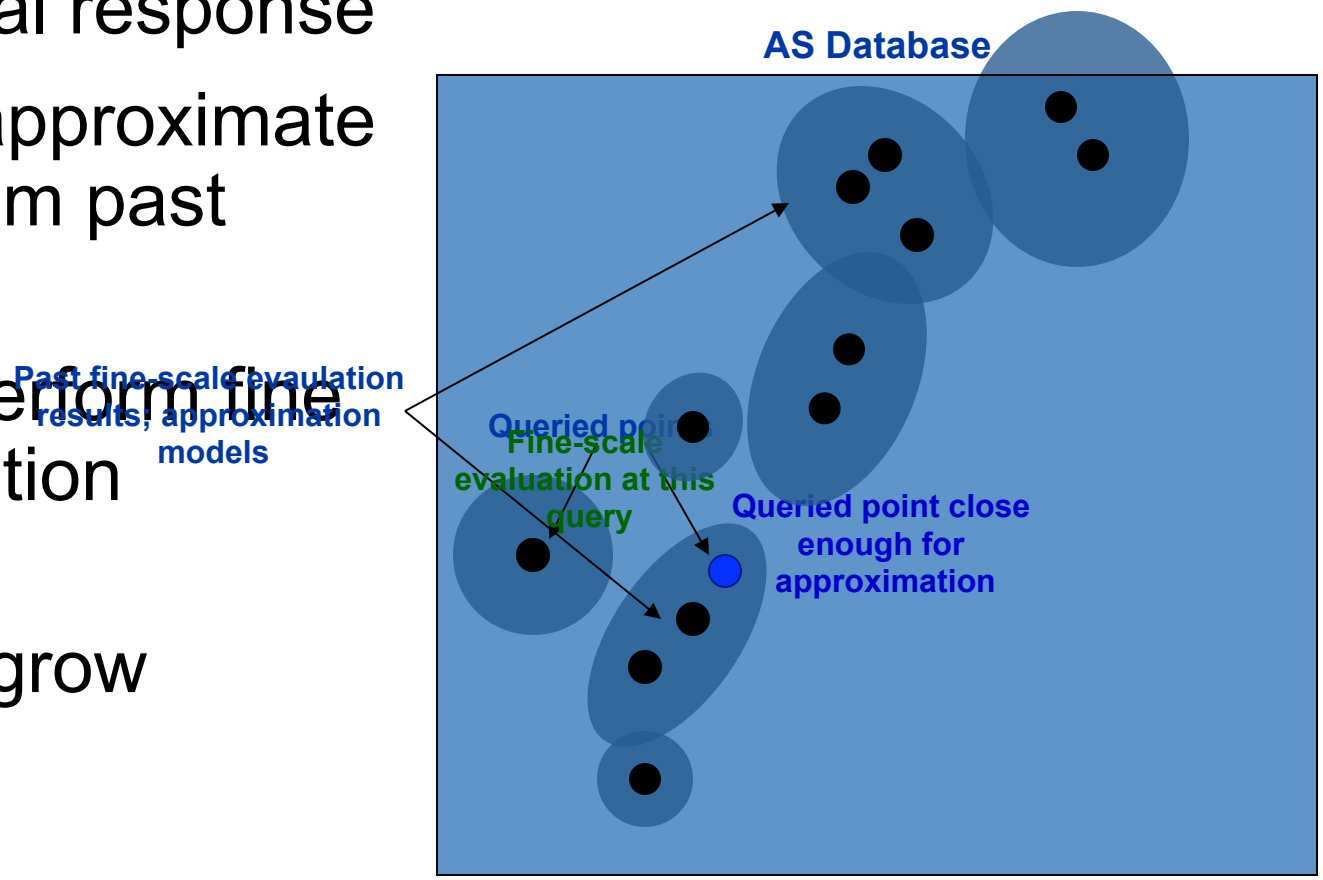
drawing

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 283, 224-242 (2015).

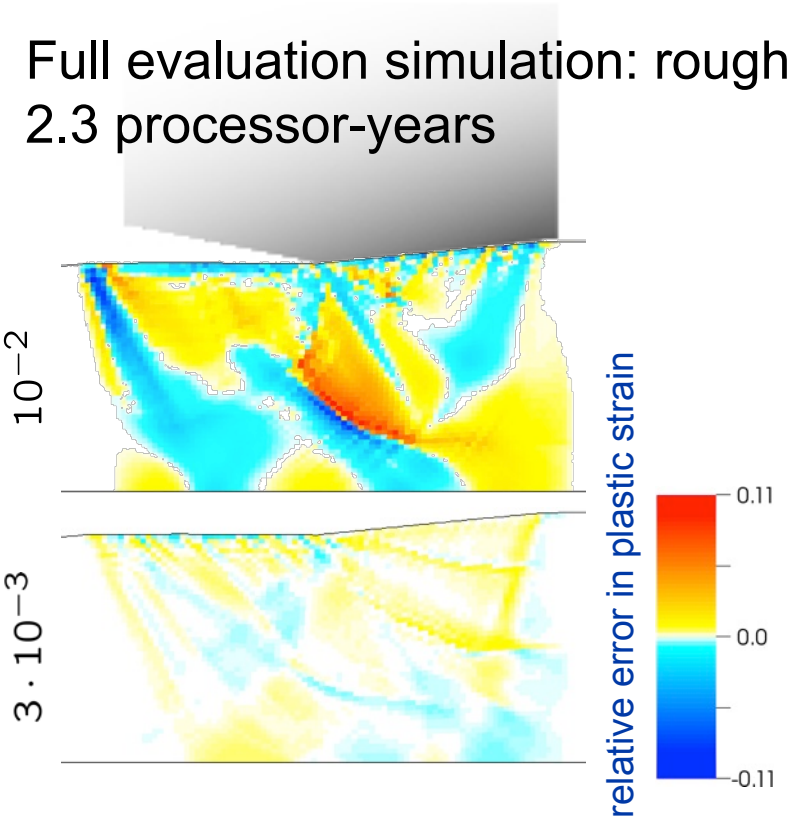
Adaptive Sampling builds response on the fly

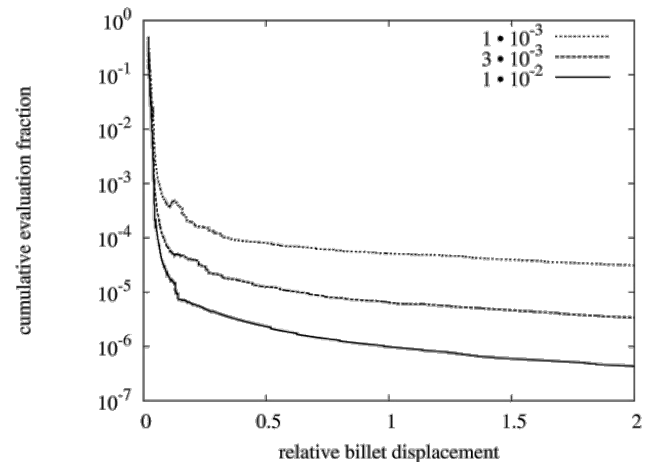
- Coarse scale model queries database for fine-scale material response
- If possible, approximate response from past evaluations
- Otherwise perform fine scale evaluation
- Fine-scale evaluations grow database

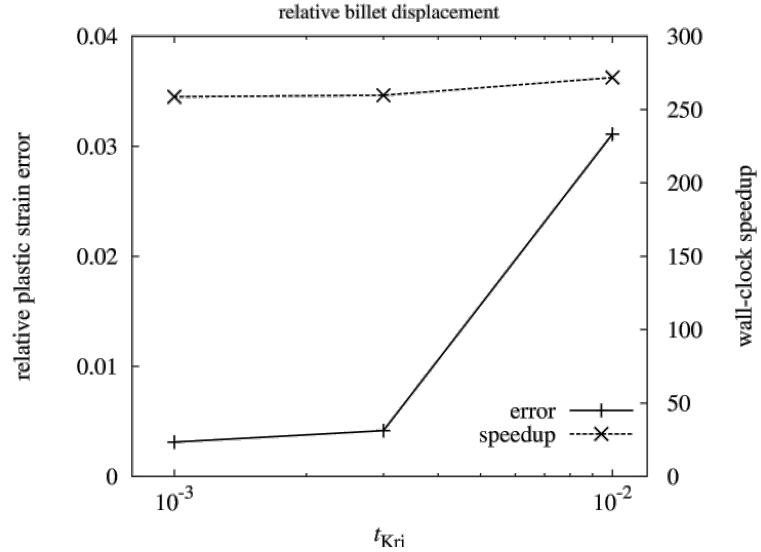


Speedup and error control are well behaved

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







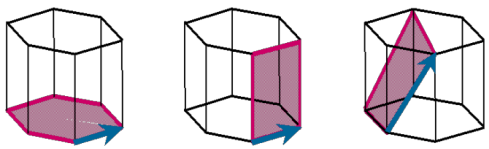
$$\text{AS speedup} \approx \frac{NW}{nW + Nw}$$

- ***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:

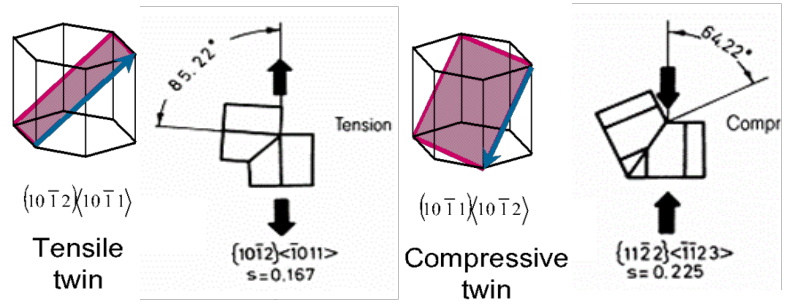


$\langle 0001\rangle\langle 11\bar{2}0\rangle$ Basal slip

$\langle 10\bar{1}0\rangle\langle 11\bar{2}0\rangle$ Prismatic slip

$\langle 11\bar{2}2\rangle\langle 11\bar{2}3\rangle$ Pyramidal slip

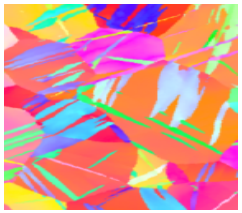
Twinning:



$\langle 10\bar{1}2\rangle\langle 10\bar{1}1\rangle$ Tensile twin

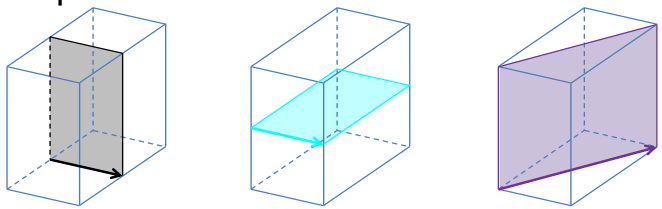
$\langle 10\bar{1}1\rangle\langle 10\bar{1}2\rangle$ Compressive twin

Rapid texture changes, anisotropic hardening:



alpha-U, orthorhombic:

Slip:

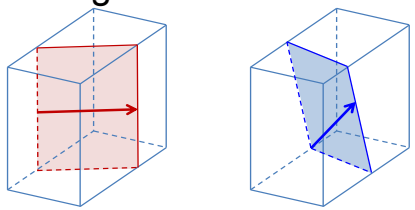


(010)[100] 1 System

(001)[100] 1 System

{110}⟨110⟩ 2 Systems

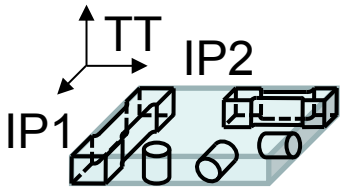
Twinning:

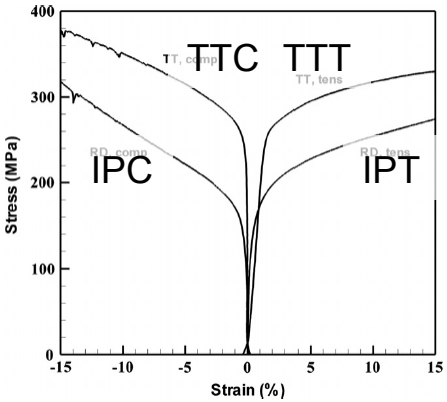


{130}⟨310⟩ 2 Variants

'{172}'⟨312⟩ 4 Variants

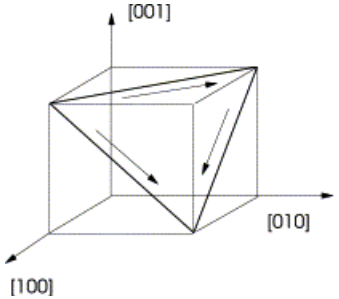
Strong anisotropy, tension-compression asymmetry:





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

Slip:



Twinning:

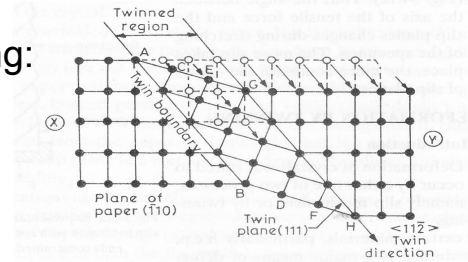
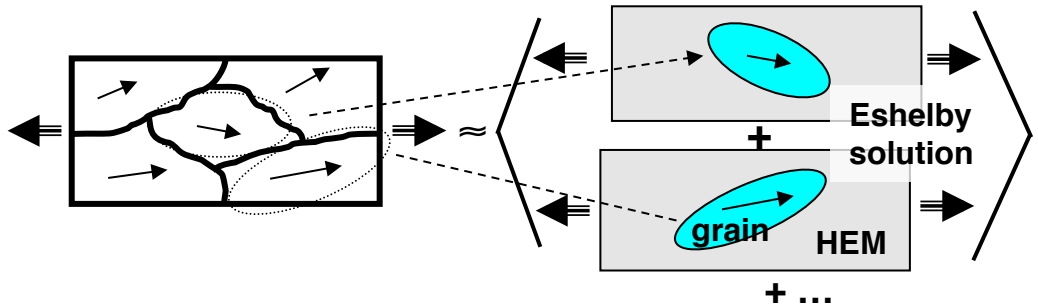


Fig. 54.13. Twinning in an f.c.c. lattice.

ViscoPlastic Self-Consistent (VPSC) formulation

Lebensohn and Tome, Acta Mater (1993)

- **VPSC model:**



- **VPSC vs Taylor:**

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

- **VPSC code:**

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

- **VPSC-based Abaqus UMAT:**

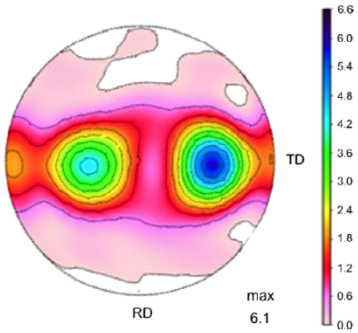
Available (Segurado, Lebensohn, Tome, IJP, 2012), based on "full evaluation".

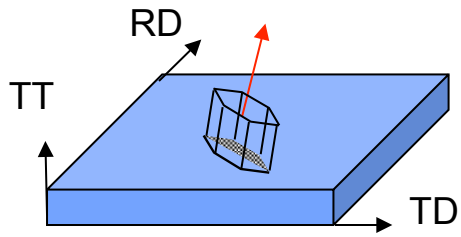
- **Material systems studied with VPSC:**

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**

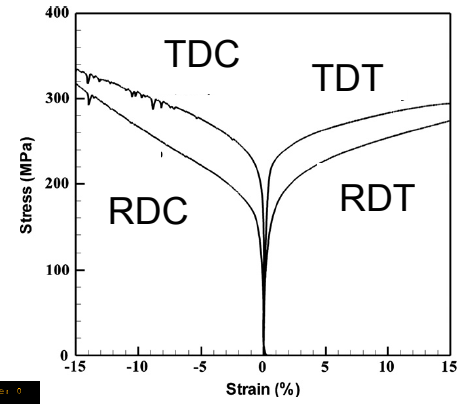
VPSC-Abaqus prediction of bending of rolled Ti bars

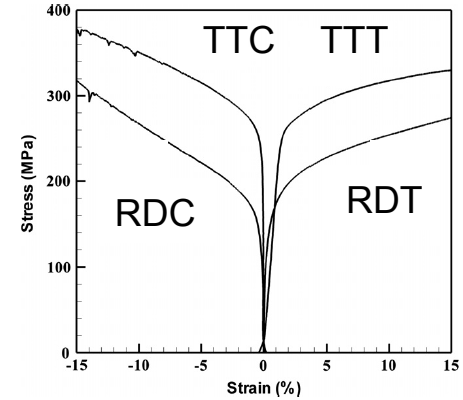
Eglin's Ti plate, orthotropic texture (*):



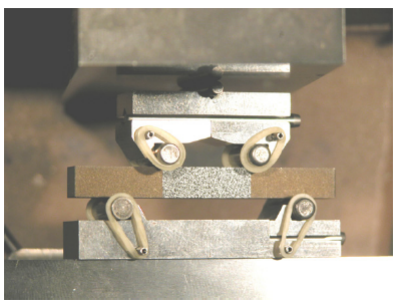


Uniaxial tests: anisotropic, tension ≠ compres (twinning!) (*):

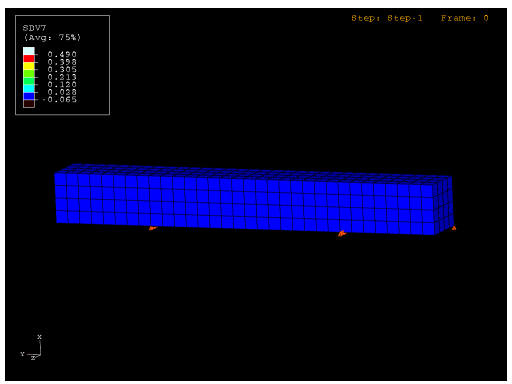




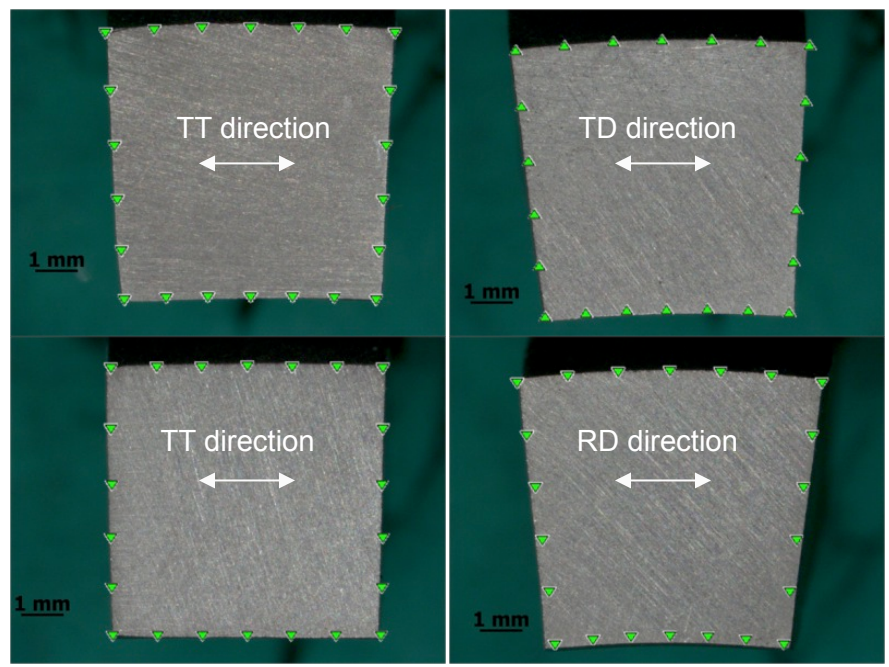
4-point bending jig:



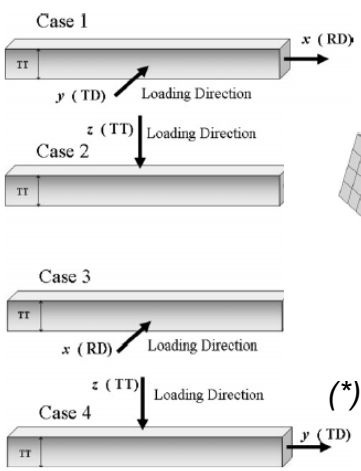
Animated simulation:



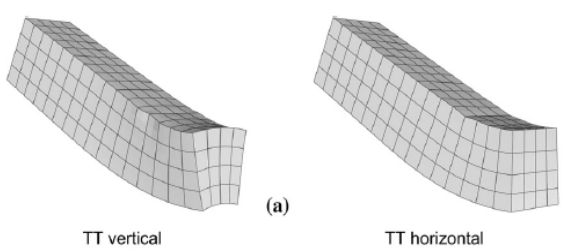
VPSC-Abaqus (green symbols) vs experimental cross-sections (photographs) (**):



4 different configurations:

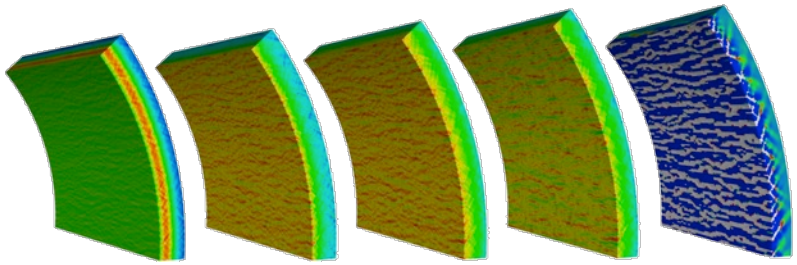


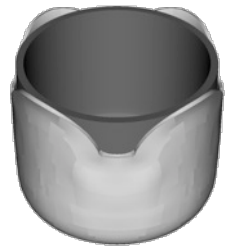
Different final 3-D shapes:

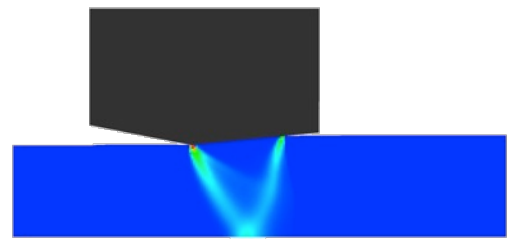


(*) Nixon et al. IJP, 2010; (**) Knezevic et al, MSE A, 2013

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

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

grain shape **texture**

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

Conservation equation: $\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \mathbf{v}) = \Theta$

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

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

Forward-Euler integration:

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

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: $\bar{f} \cdot (L_{\mathrm{t}} \bar{g}) = \int_{\mathcal{R}} f(\mathbf{r}) g(\mathbf{r}\mathbf{r}_{\mathrm{t}}) \mathrm{d}\mu$

Or using orthonormal basis functions: $\rho = \sum_i c_i H_i \qquad c_i = \int_{\mathcal{R}} \rho H_i \mathrm{d}\mu$

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = \int_{\mathcal{R}} \frac{\partial \rho}{\partial t} H_i \mathrm{d}\mu = \int_{\mathcal{R}} (\Theta - \mathrm{div}(\rho \mathbf{v})) H_i \mathrm{d}\mu = \int_{\mathcal{R}} \rho \mathbf{v} \cdot \nabla H_i \mathrm{d}\mu + \int_{\mathcal{R}} \Theta H_i \mathrm{d}\mu$$

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

$$\mathcal{Y} = f_{\mathcal{Y}}(\bar{\boldsymbol{\tau}}', \mathcal{H}, p, \theta) \qquad \mathcal{H} = \{h_1, h_2, h_3, ..., A_{ij}, c_k, v_{\mathrm{tw}}\}$$

- 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:

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

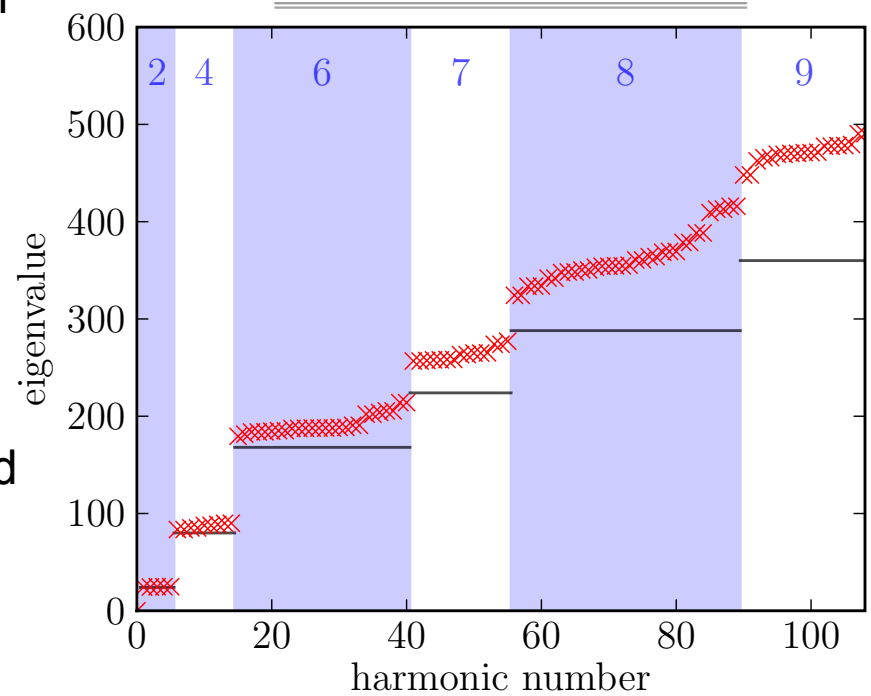
Weak form:

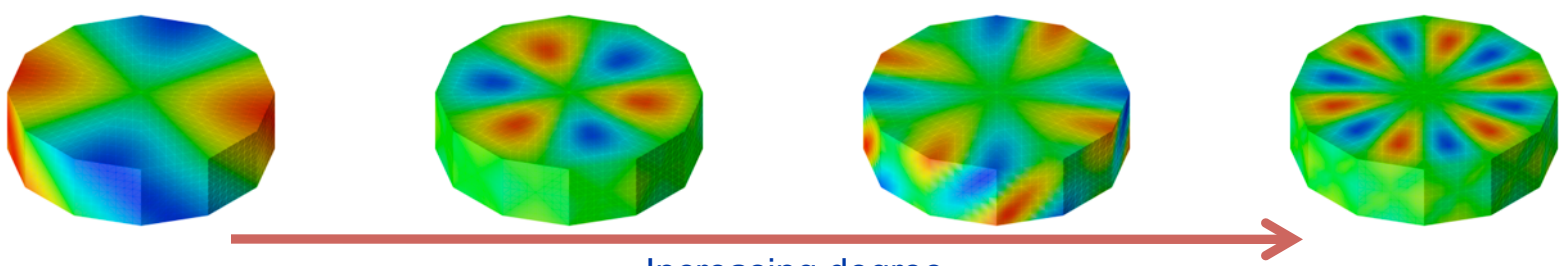
$$\int \nabla u \nabla \phi = \lambda \int u \phi, \ \forall \phi$$

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



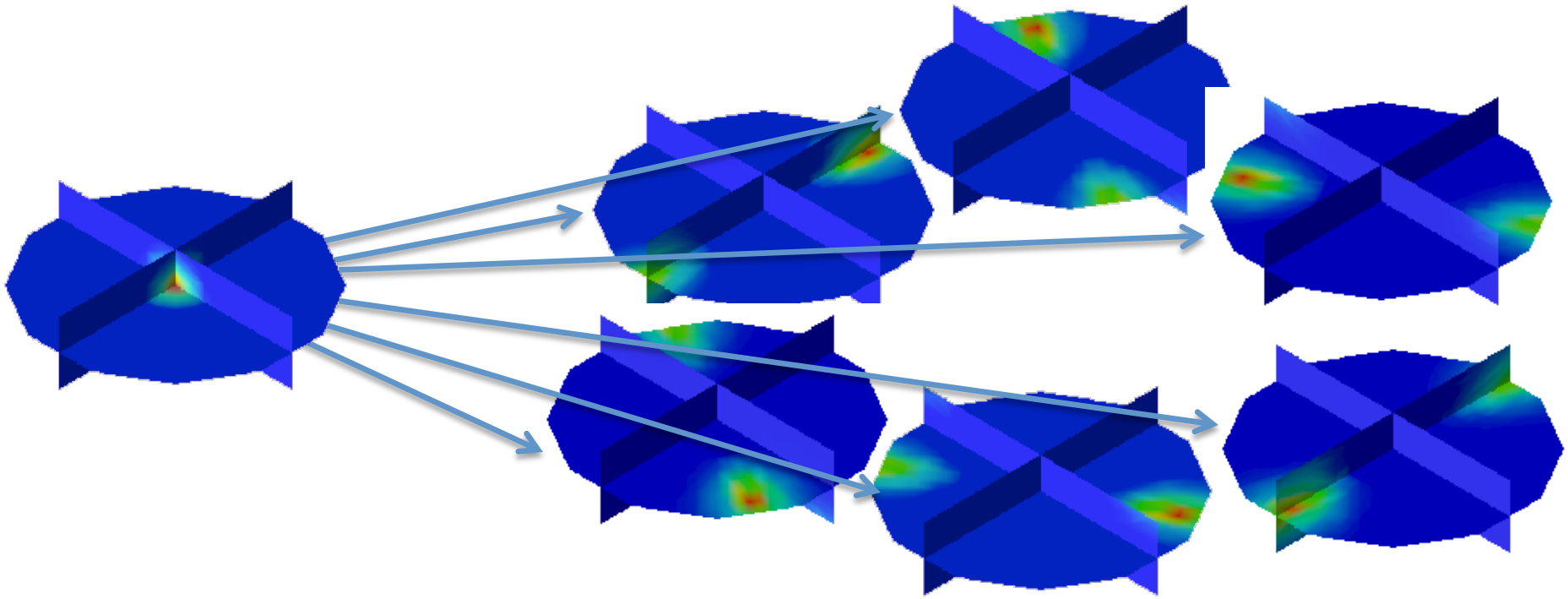


Twinning operators amount to non-local source/sink relationships

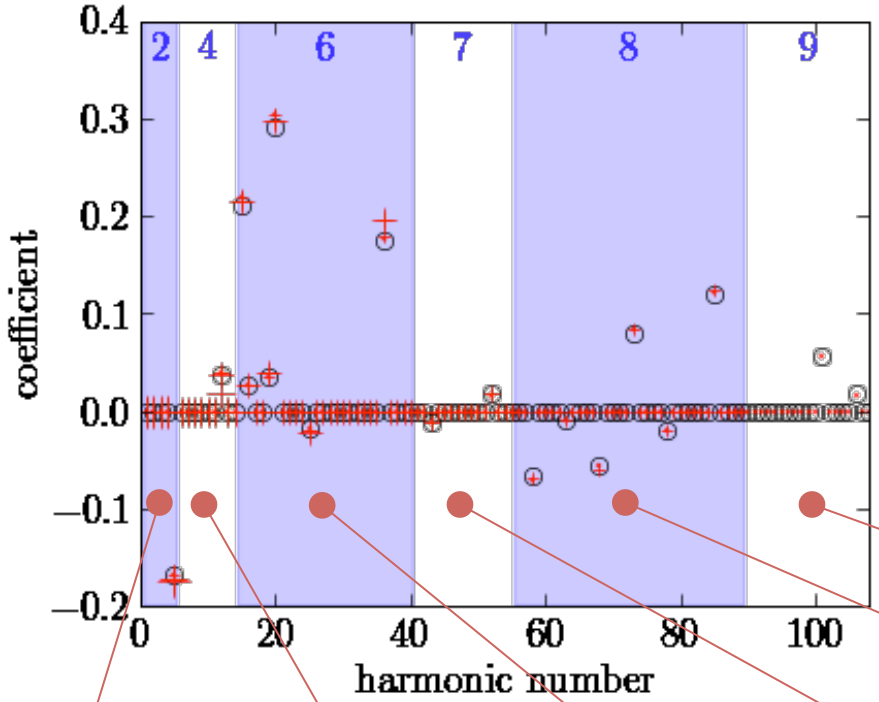
- Twinning operators involve the construction of modified 2-form "mass" (L-2 inner product) matrices:

$$\bar{f} \cdot (L_{\mathrm{t}}\bar{g}) = \int_{\mathcal{R}} f(\mathbf{r}) g(\mathbf{r}\mathbf{r}_{\mathrm{t}}) \mathrm{d}\mu$$

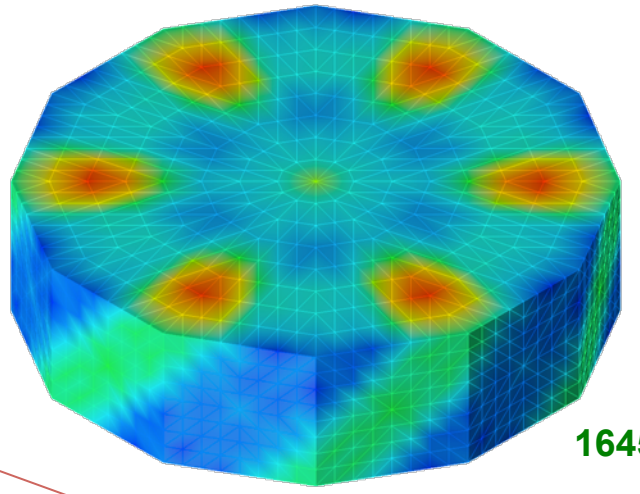
- Example: image of Gaussian at the origin under six twinning operators



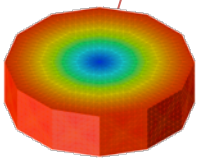
Uniaxial deformation to 25% strain illustrates convergence

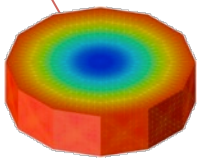


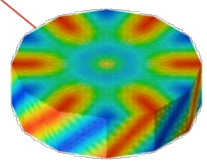
Direct evolution with full DOF:

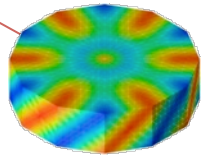


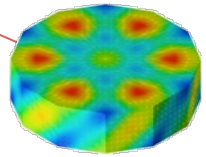
1645.63

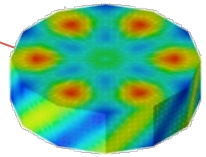










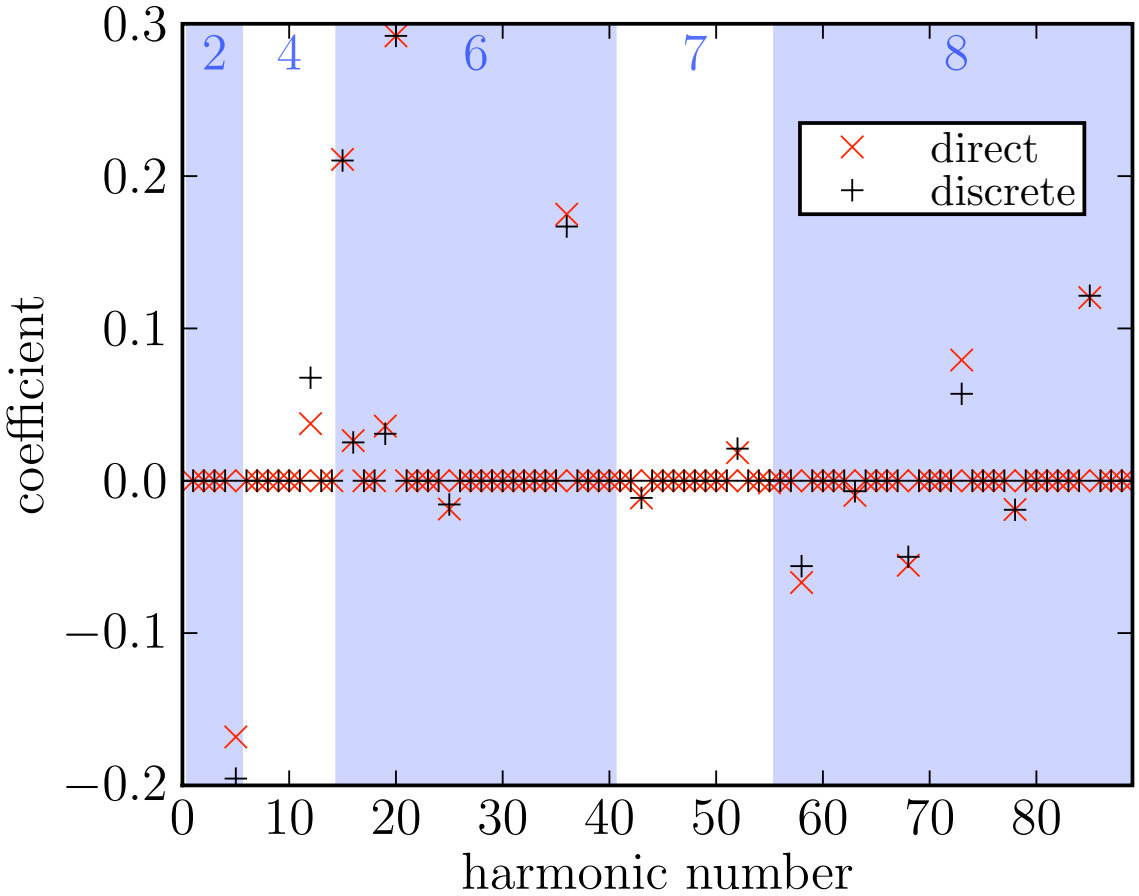


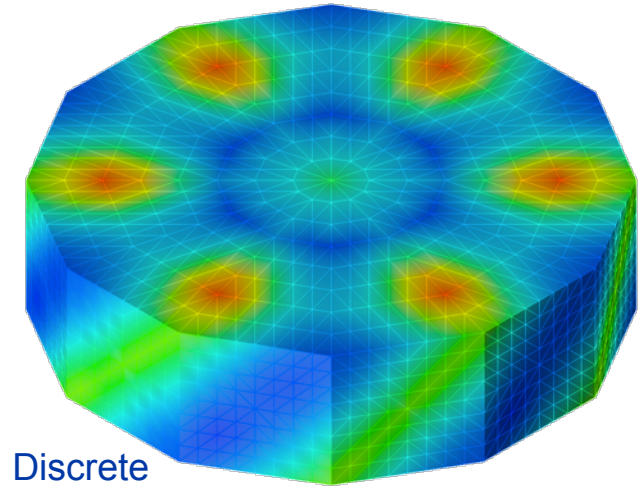
0.468057	0.466554	0.234315	0.233312	0.160327	0.149172
1627.46	1635.77	1624.98	1624.75	1641.73	1644.25

L_2 norm of difference with direct evolution

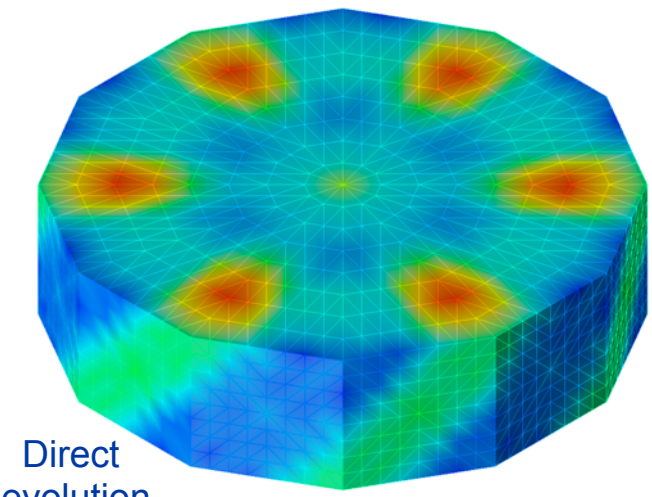
strength measure (MPa)

Discrete aggregate results agree with direct continuous evolution methods



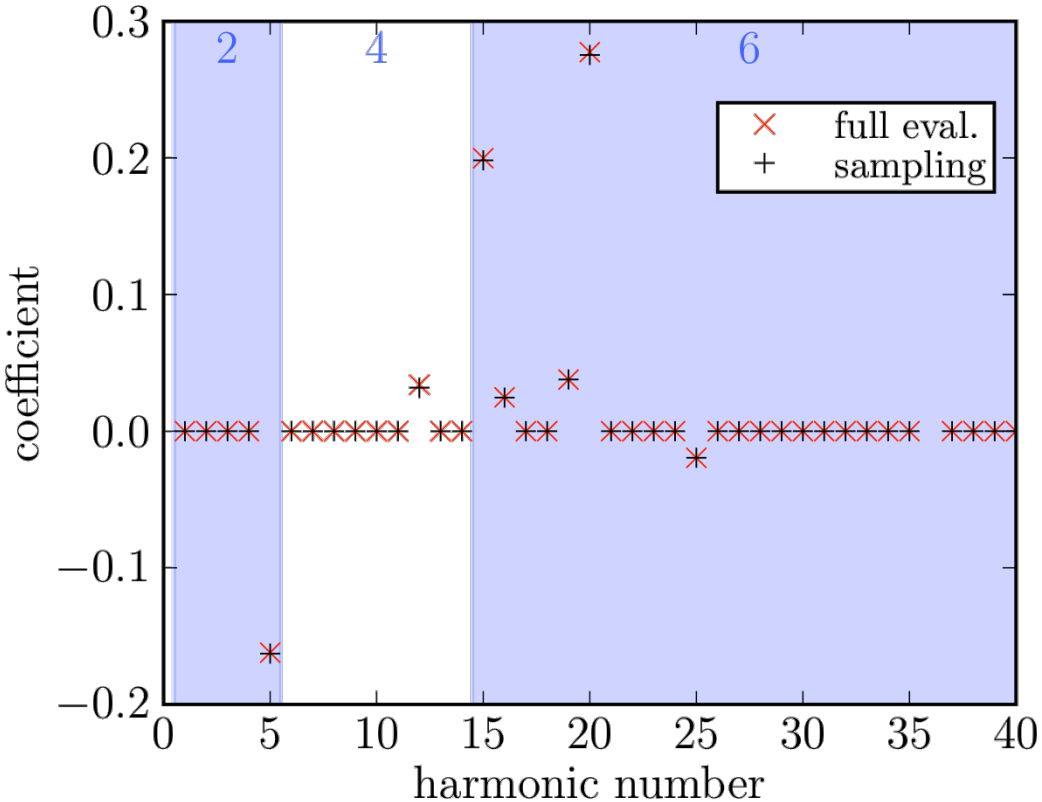


Discrete aggregate



Direct evolution

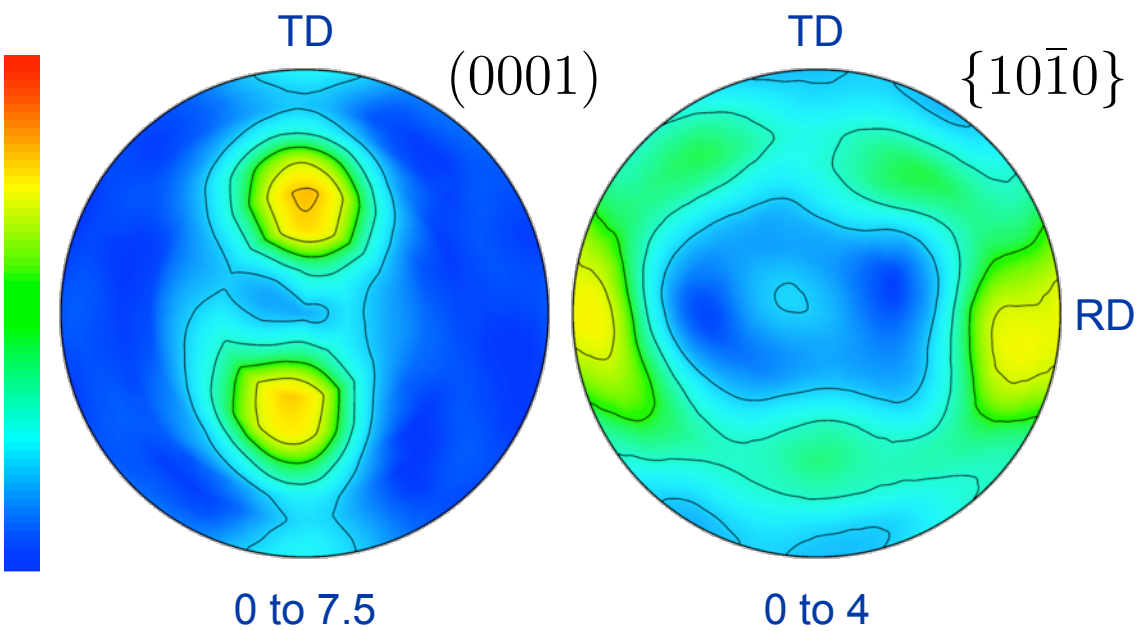
Even under monotonic loading, sampling provides benefit

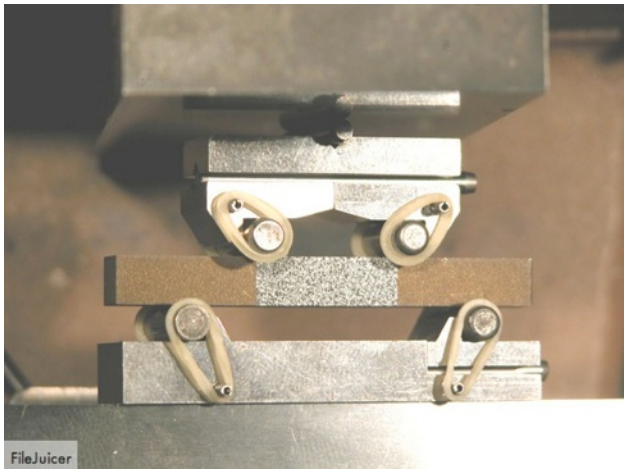


Evaluation fraction < 0.1

Example application – four-point bend of textured titanium

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

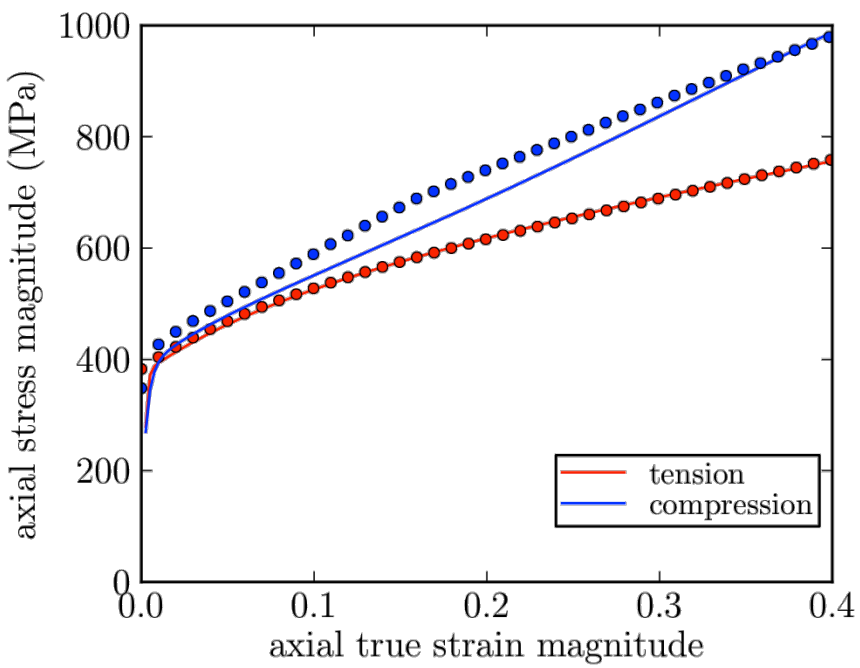


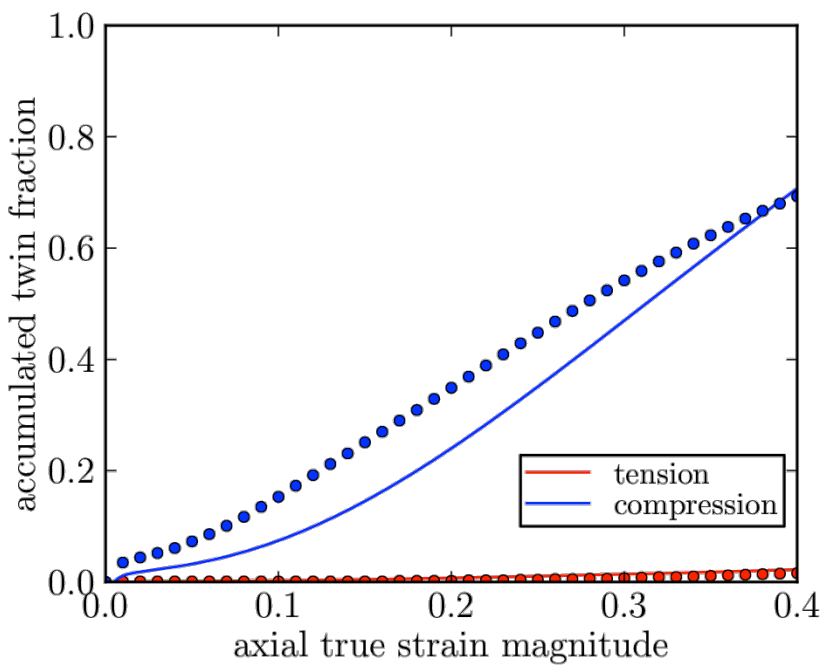


Nixon, Lebensohn, Cazacu, & Liu, *Acta Mat.*, 2010

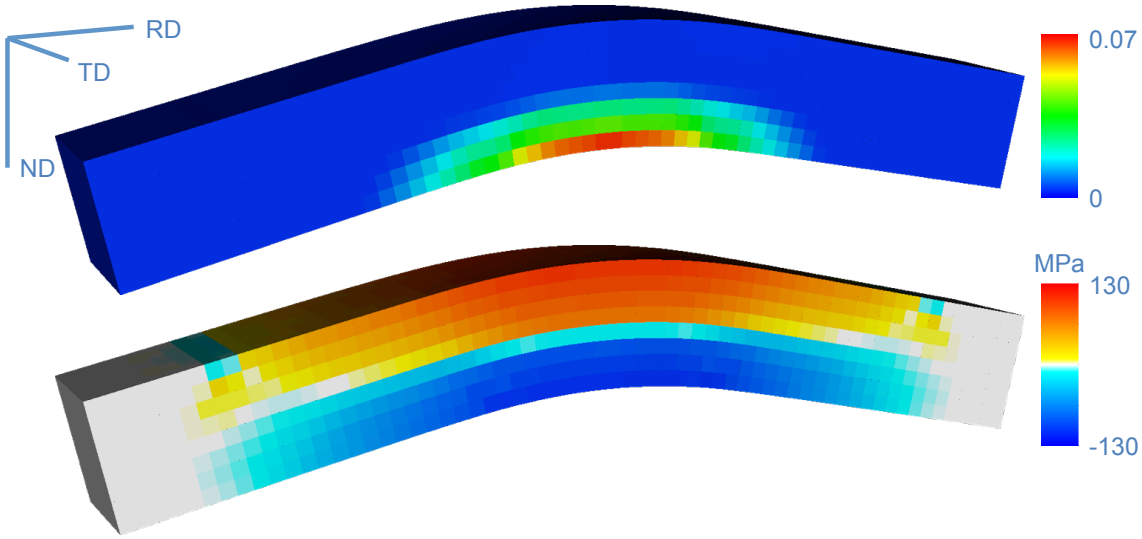
Harmonic-based scheme captures salient features of the response

- 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





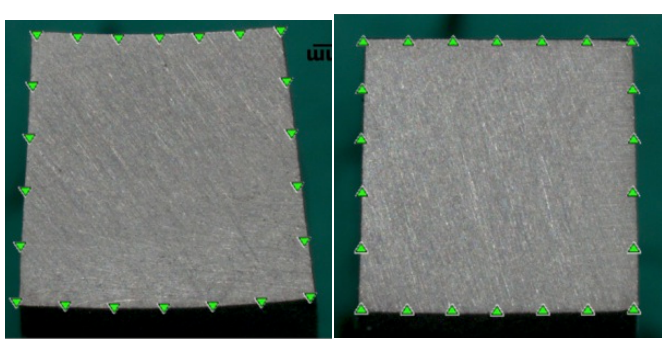
Four-point bend results demonstrate utility in component-scale simulations

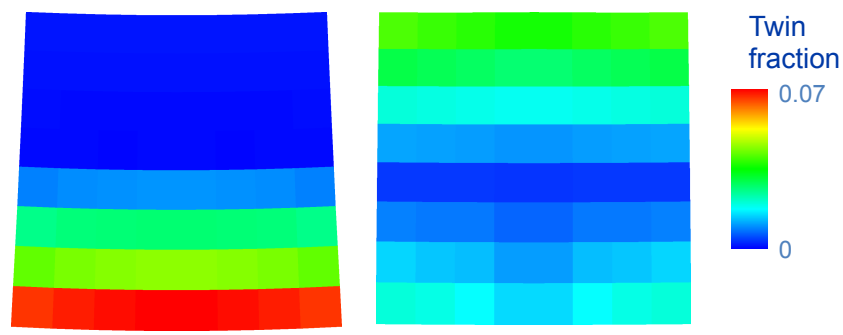


Twin fraction: tension-compression asymmetry

Axial stress

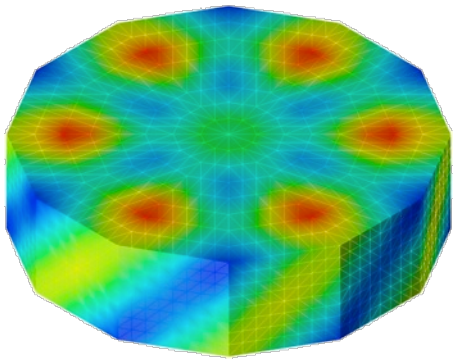
Shape of cross-sections for two different bend orientations – agree with published results (Knezevic *et al.*, *Mat. Sci. Eng. A*, 2013)





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?



$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = \int_{\mathcal{R}} \rho \mathbf{v} \cdot \nabla H_i \mathrm{d}\mu + \int_{\mathcal{R}} \Theta H_i \mathrm{d}\mu$$

$$\rho = \sum_i c_i H_i$$