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Uncertainty in the Definition and Calibration of Multiscale Material Models

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Multiscale VVUQ

- Individual model VVUQ – single model focusing on single length and/or time scales → historical focus
- Multiscale model VVUQ – single model or coupled set of models comprising a simulation operating over multiple length/time scales in concurrent or hierarchical manner → needs attention
- Multiphysics model VVUQ – ensuring that the implementation of a modeling framework spanning multiple physical phenomena is mathematically and physically consistent → virgin territory

See: Panchal, J.H., Kalidindi, S.R., and McDowell, D.L., Computer-Aided Design, Vol. 45, No. 1, 2013, pp. 4–25.

HMMs vs CMMs

- Hierarchical Multiscale Model – one way
  - Uncertainties in model form, initial values, parameters, choice of scales to bridge
  - Typically operates from bottom-up, but model calibration involves combination of bottom-up and top-down information
- Concurrent Multiscale Model – two way
  - Uncertainties in model form relate to the way the model form is structured to achieve concurrency
  - Often practically limited to coarse-graining (e.g., same model form, but different DOF) or reduced order models

Note:

- Intrusive or embedded UQ methods are attractive for CMMs

Uncertainty: Amount of Data/Info

- "Plentiful" Data:
  - Fusion of large scale experiments (e.g., synchrotron tomography) with models
  - Large scale parametric computational runs across a range of random samples/instantiations of microstructures
  - Plentiful data to support training/calibration, and validation

- "Small" Data:
  - Limited number of sensors/measurements
  - Limited number of experiments or expensive simulations
  - More common scenario in materials design and development

UQ is useful for each case:

- Plentiful – UQUP, statistical learning algorithms that track uncertainty
- Small – algorithmic decision support to guide choice of next experiment or simulation

Uncertainty in a Microstructure-Sensitive Extreme Value Fatigue Design Framework

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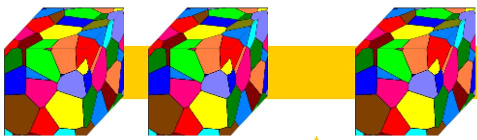
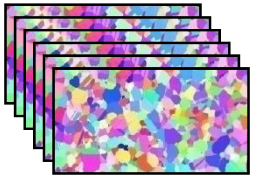
1. Generate multiple SVEs based on predefined distributions of key microstructure attributes

$$\Omega_1, \Omega_1, \cdots, \Omega_n$$

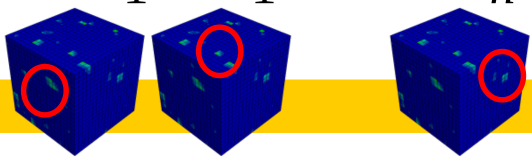


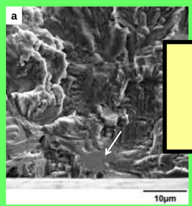


Groeber et al. 2007, IN100

2. Identify EV response of SVEs via simulation

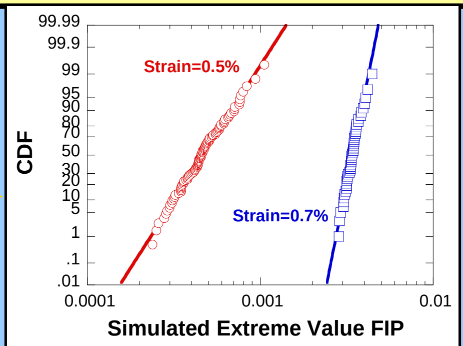
$$\Omega_1, \Omega_1, \cdots, \Omega_n$$



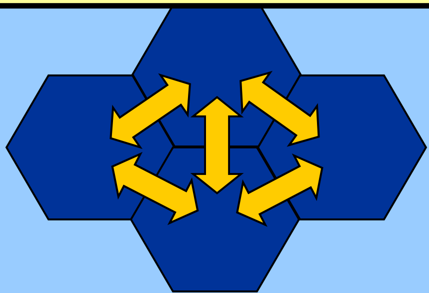


Experimental Calibration/Validation

3. Characterize EV distributions of key response parameters



4. Characterize correlated microstructure attributes coincident with the EV response (EV marked correlation functions)



5. Identify extreme value correlated attributes key to response and rank microstructures

6(a). Iterate materials design

6(b). Select top candidates for experimental evaluation

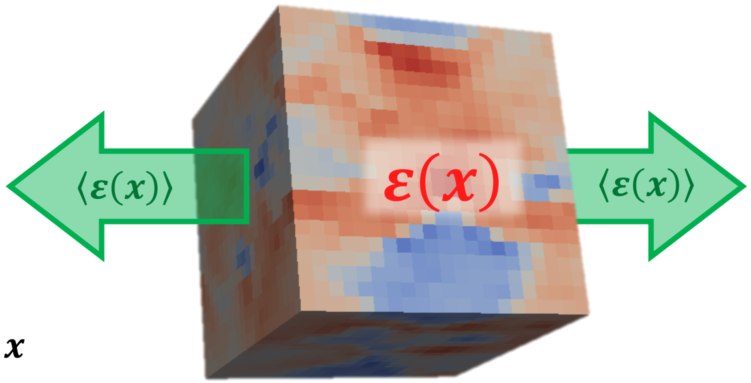
C. Przybyla, GT, 2010

Gap: Sufficiently Accurate High Throughput Inverse Modeling

The **Materials Knowledge System** (MKS) is a localization technique to determine local response (eg. ε_{11}) given macroscopic applied condition

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{a}(\boldsymbol{x})\langle\boldsymbol{\varepsilon}(\boldsymbol{x})\rangle$$

- $\boldsymbol{a}(x)$: 4th rank localization tensor at spatial location $\boldsymbol{x}$
- $\langle\ \ \rangle$: ensemble average over RVE



MKS

Now expand $\boldsymbol{a}(\boldsymbol{x})$:

$$\boldsymbol{\varepsilon}(x) = \left(\boldsymbol{I} - \int_R \int_H \boldsymbol{\alpha}(r,n) m(x+r,n)\, dn\, dr + \int_R \int_R \int_H \int_H \tilde{\boldsymbol{\alpha}}(r,r',n,n') m(x+r,n) m(x+r+r',n')\, dn\, dn'\, dr\, dr' - \cdots\right)\langle\boldsymbol{\varepsilon}(x)\rangle$$

Microstructure function:

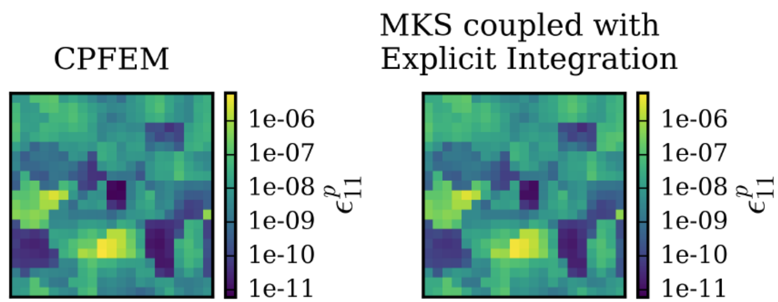
$$m(x,n) = \sum_L \sum_s M_s^L Q_L(n) X_s(x)$$

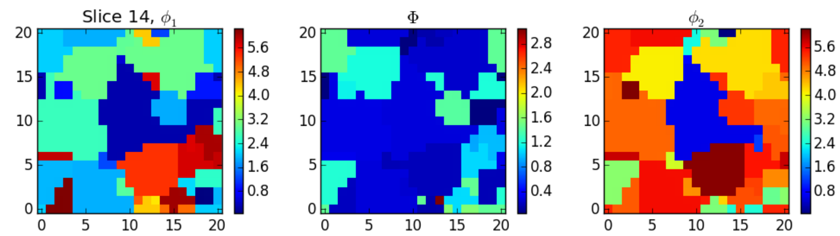
Influence function:

$$\boldsymbol{\alpha}(r,n) = \sum_L \sum_t \boldsymbol{A}_t^L Q_L(n) \chi_t(r)$$

$Q_L(n)$: orthonormal Fourier basis
$X_s(x)$: indicator basis

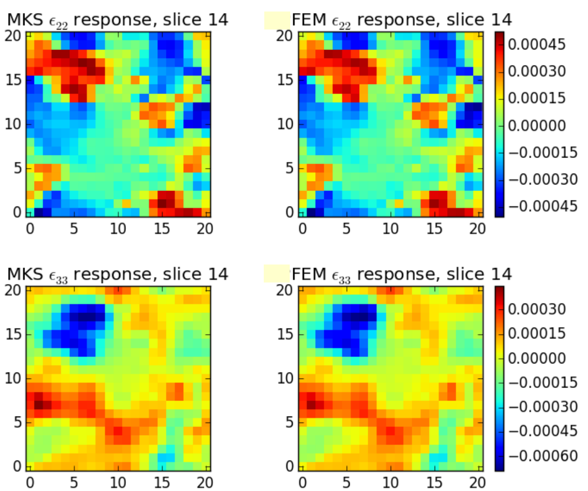
Kalidindi (2012), Adams (2012), Kröner (1986), Yabansu (2014)





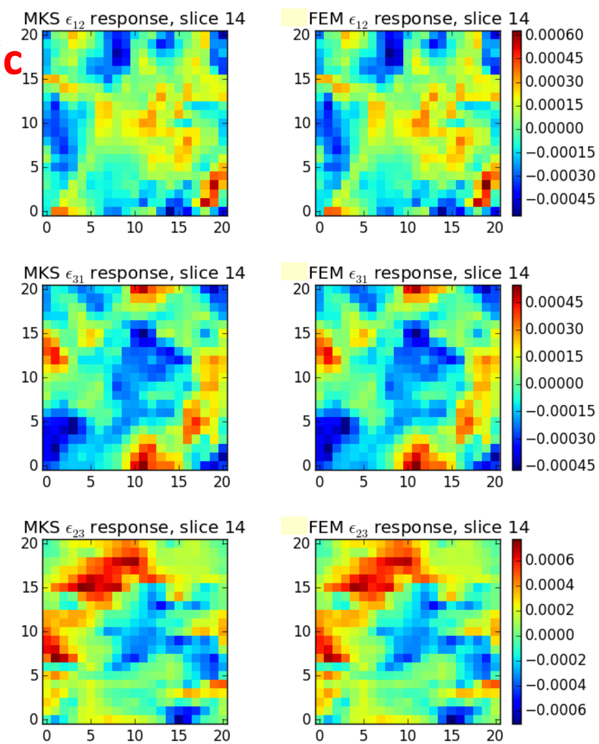
MKS prediction of ε tensor for basal textured α-Ti:

Epistemic approx. error



ε_{22} mean error: 0.20%
ε_{22} max error: 1.2%

ε_{33} mean error: 0.22%
ε_{33} max error: 1.3%



ε_{12} mean error: 0.35%
ε_{12} max error: 2.1%

ε_{13} mean error: 0.29%
ε_{13} max error: 3.2%

ε_{23} mean error: 0.29%
ε_{23} max error: 1.8%

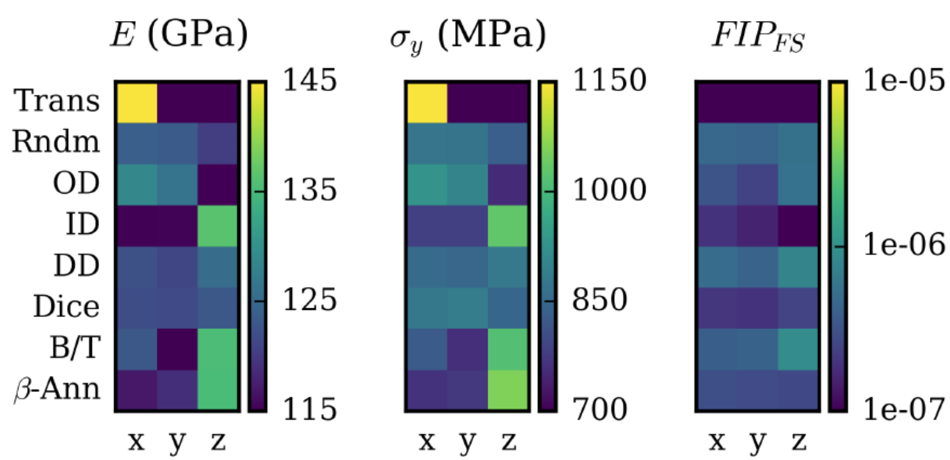
Recent NSF CMMI-1333083 GOALI with S. Kalidindi (GT) and D. Shih (Boeing)

Design Problem for Multiple Props, Ti64

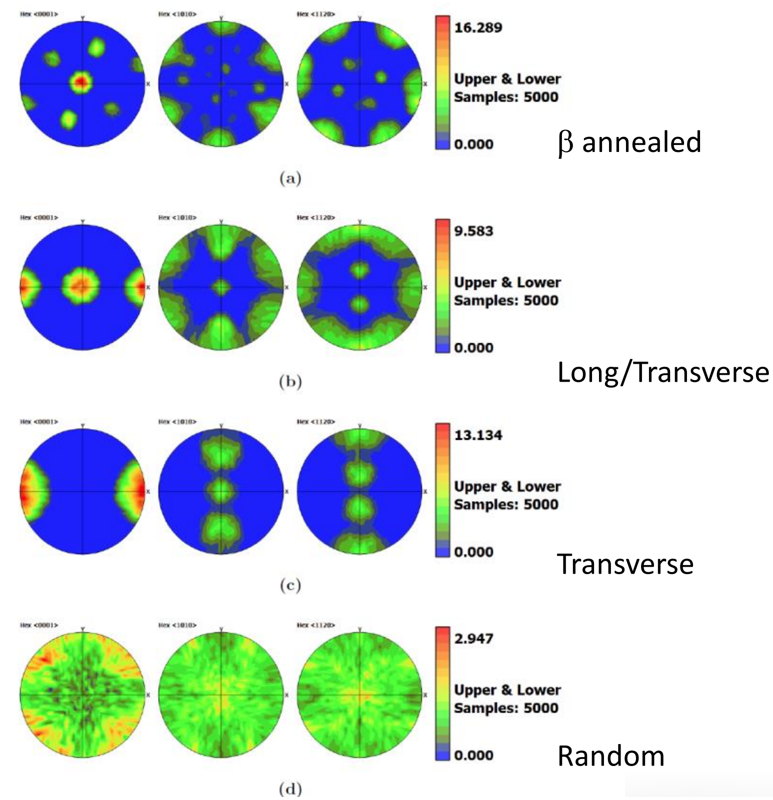
Priddy, M.W., Paulson, N.H., Kalidindi, S.R., and McDowell, D.L., International Journal of Fatigue, Vol. 104, 2017, pp. 231-242.

Multiple design objectives include elastic stiffness, directional yield strength and HCF resistance.

$$(E),\ (\sigma_y),\ \text{and}\ FIP_{FS}$$

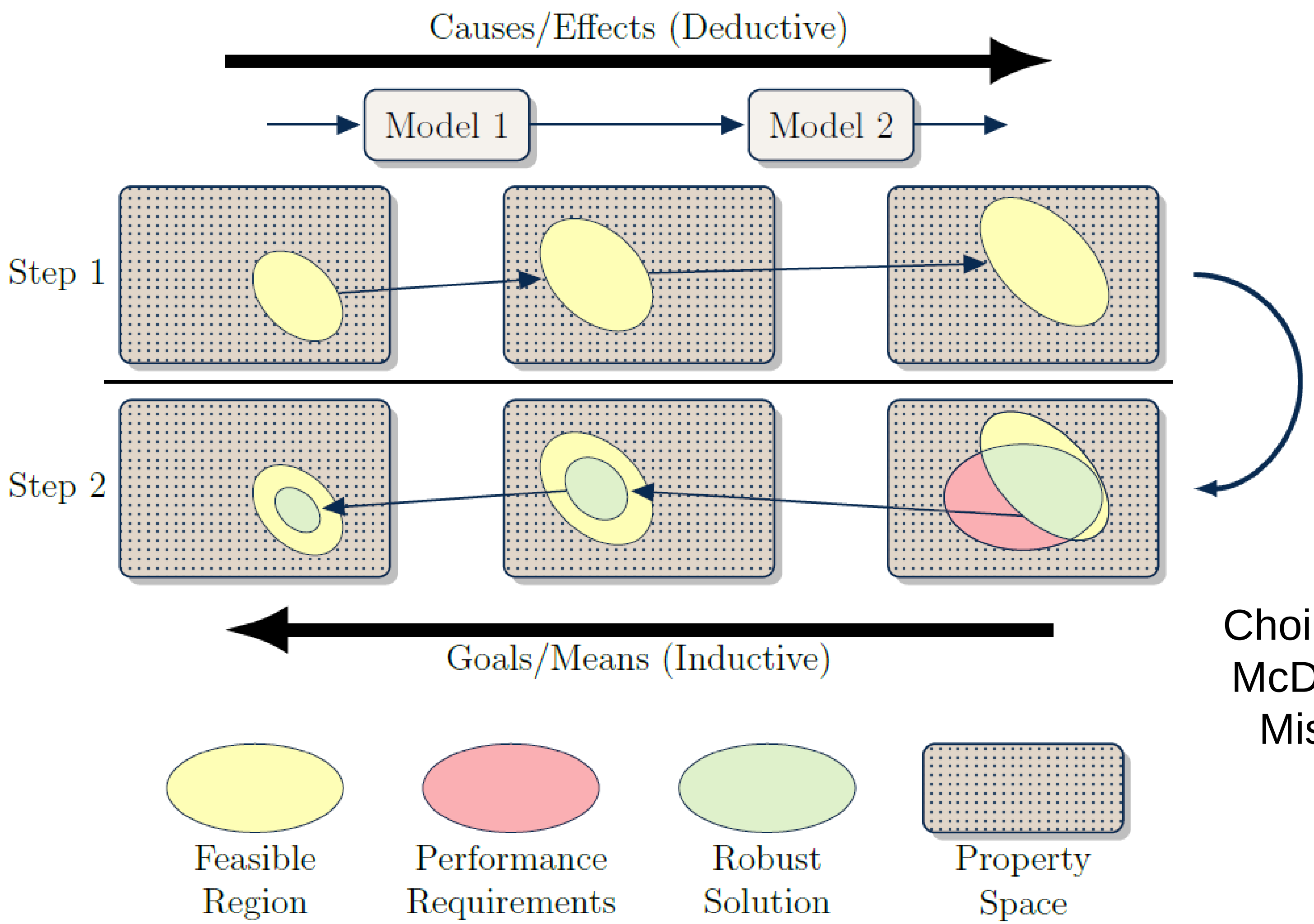


Mean (E, σ_y) *and* FIP_{FS} for 0.10 probability level for each of 8 textures and three orthogonal uniaxial loading conditions.



Kern, P.C., Priddy, M.W., Ellis, B.D., and McDowell, D.L., "pyDEM: A Generalized Implementation of the Inductive Design Exploration Method," Materials & Design, Vol. 134, 2017, pp. 293-300.

P. C. Kern, M. W. Priddy, B. D. Ellis, D.L. McDowell, pydem 1.0.0, 2017: https://github.com/materialsinnovation/pydem



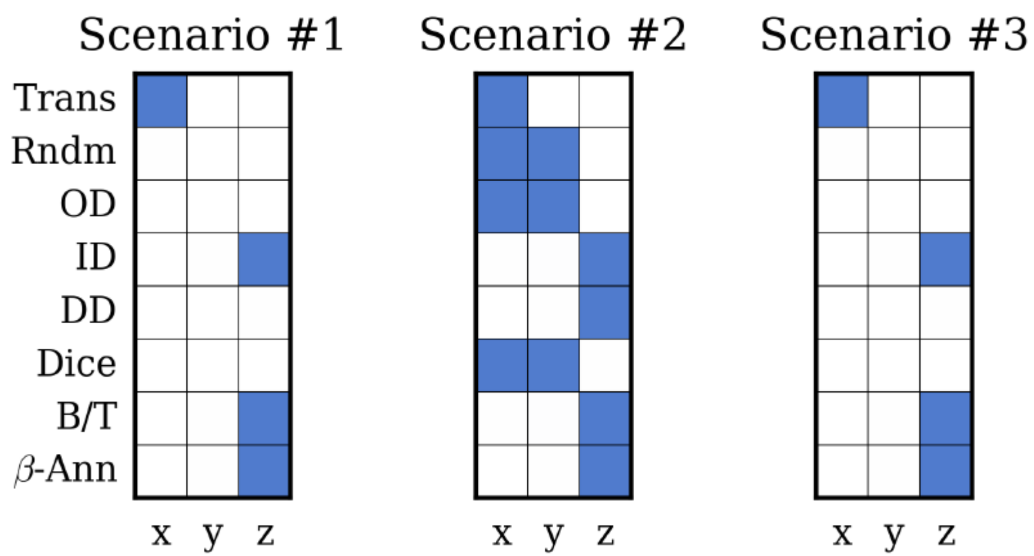
Choi, 2005; Choi, McDowell, Allen, Mistree, 2008

Texture Design Problem

Table 6.3: Texture IDEM Design Requirements

Scenario	E (mean)	σ_y (mean)	FIP_{FS}
#1	> 130 GPa	–	$< 5 \times 10^{-6}$
#2	–	> 900 MPa	$< 5 \times 10^{-6}$
#3	> 130 GPa	> 900 MPa	$< 5 \times 10^{-6}$

Max FIP_{FS} at 10% cumulative probability



Priddy PhD Thesis, 2016

Two-dimensional representation of the feasible space for each of the design space for each design scenario applied to each of the 8 textures and 3 loading directions. Blue boxes indicate satisfaction of the performance requirements.