Advanced Computing for Materials and Manufacturing

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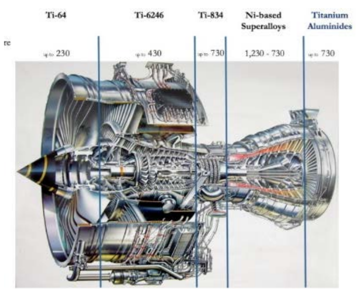
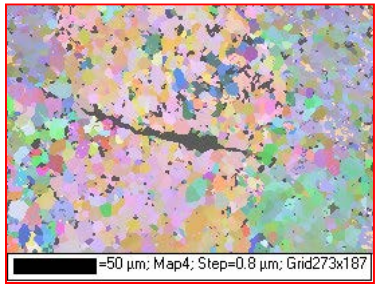
Workshop on Core Knowledge and Skills for
Effective Use of Advanced Computation and Data
Phoenix Convention Center, Phoenix, AZ
March 11, 2018

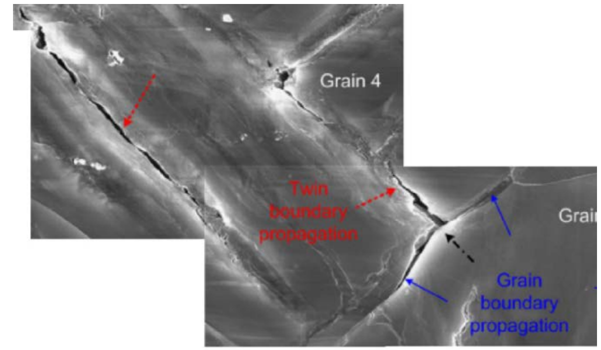
Challenges in Modeling Materials & Manufacturing: Examples

Fatigue in Titanium Alloys





Twinning in Mg Alloys

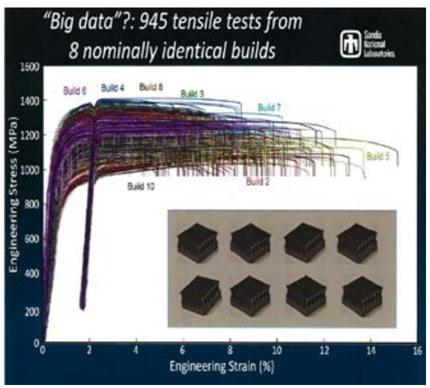


Structure-Material Problems in Additive Manufacturing

Topology Optimization

LENS, DMD

Microstructure



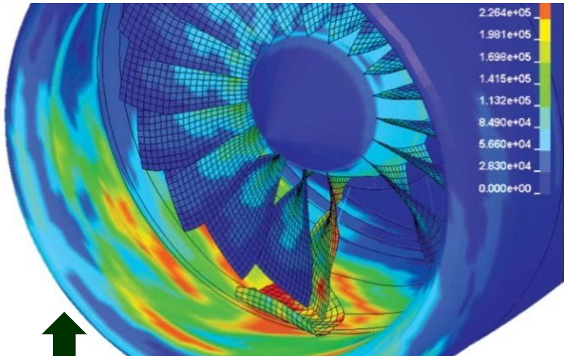
Material-Structure Modeling

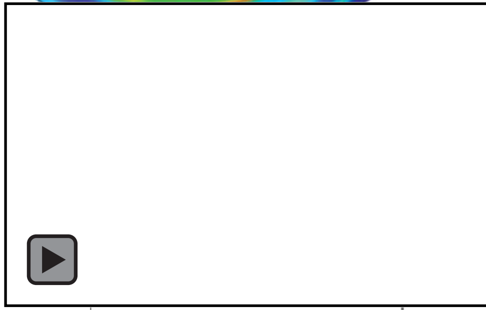
ICME & ICSME

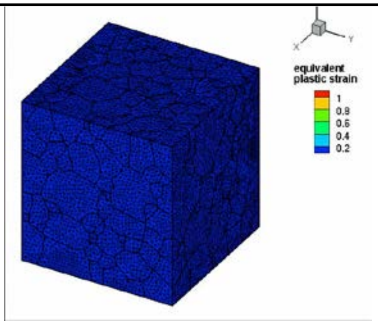
Integrated Computational Structure-Materials Engineering (ICSME) provides a Multi-Scale Framework for Structural Performance and Life

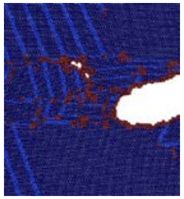
(Location-specific Material Design)

The ICME framework provides a systematic approach for effective tools coupling Computational and Experimental Materials with Computational Mechanics for predicting material behavior and life at lower scales.









Challenges in Computational Modeling at Multiple Scales

- Accurate Representation of Computational Domains at Each Scale for Modeling and Simulations of Relevant Properties and Response Functions: *RVE, SERVE, Domains and Boundary Conditions*

- Methods of Analysis and Simulation at Relevant Scales: *Accuracy and Efficiency*

- Accelerated Time Integration Methods and Multi-time Scaling

- Computational Modeling Across Scales: *Methods of Hierarchical and Concurrent Multiscaling*

Statistically Equivalent Representative Volume Element (SERVE)

Microstructural domain, for which statistical distribution functions of morphological parameters or material response functions converge to those for the entire microstructure.

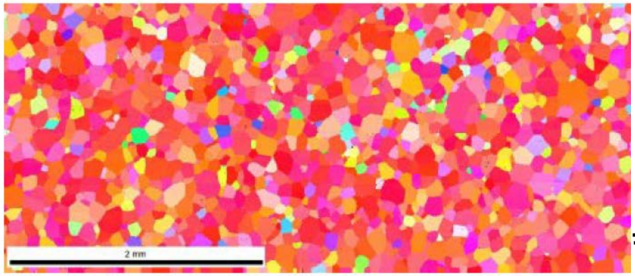
Ghosh, Swaminathan I&II (2005), McDowell, Ghosh, Kalidindi (2011), Sundararaghavan ,Zabaras (2005), Kumar, Nguyen, DeGraef , Sundararaghavan (2016), Rollett, Robert, Saylor (2006), Guo, Chawla, Jing, Torquato, Jiao (2014)

1. Microstructure-based SERVE or M-SERVE, in which morphological and crystallographic characteristics of the microstructure are the sole determinants of the SERVE domain

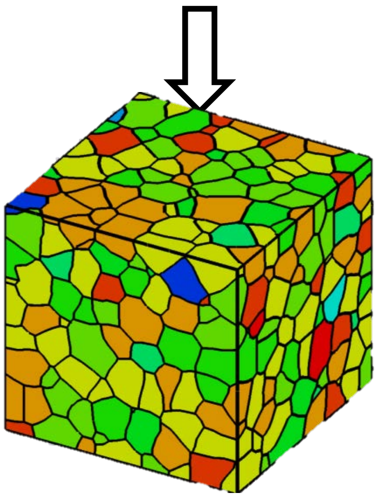
2. Property-based SERVE or M-SERVE, in which specific properties and response functions are determinants of the SERVE domain

Groeber, Ghosh, Uchic, Dimiduk I&II (2008), Niezgoda, Turner, Fullwood, Kalidindi (2010)
Bagri, Weber, Lenthe, Pollock, Woodward, Ghosh (2018), Pinz, Weber, Lenthe, Pollock, Uchic, Ghosh (2018)

M-SERVE for Ti Alloys
DREAM.3D and Beyond

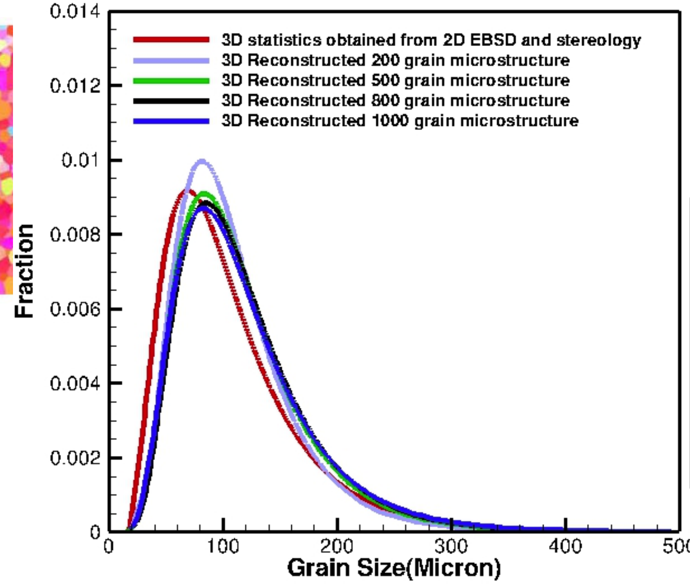


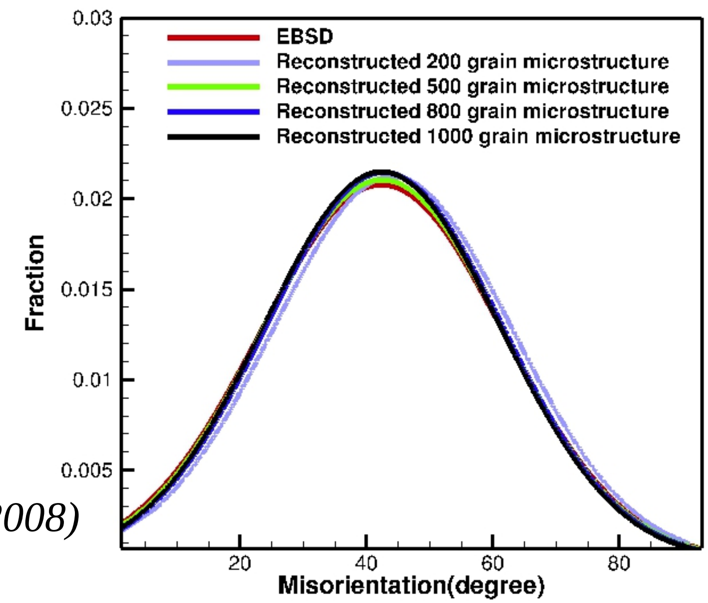
Annealed-rolled Ti-7Al EBSD scan (Courtesy of Adam Pilchak, *AFRL)*



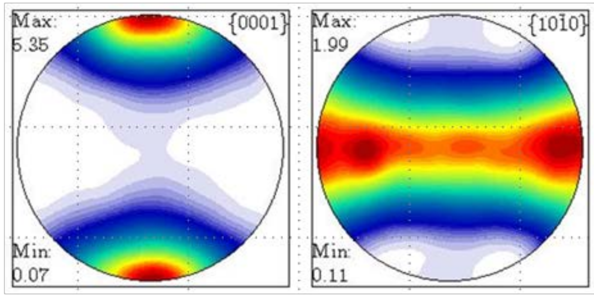
DREAM.3D

Groeber, Ghosh, Uchic, Dimiduk (2008)
Groeber, Jackson (2014)

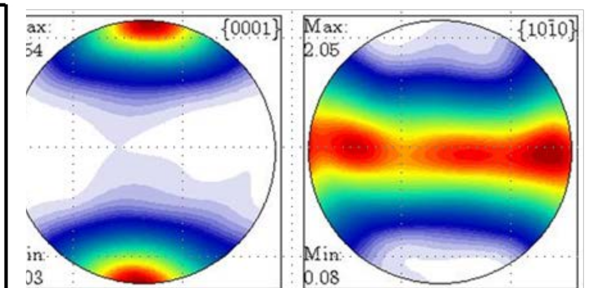




2D EBSD map

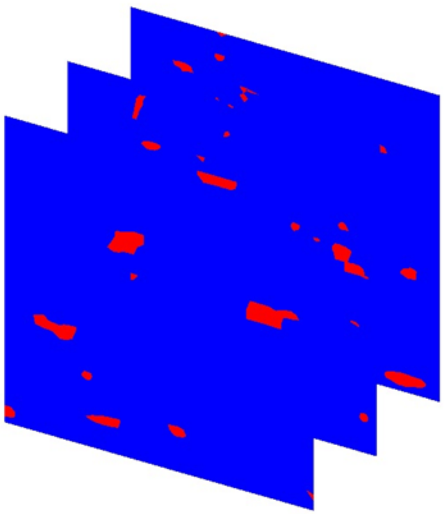


500-grain micro.



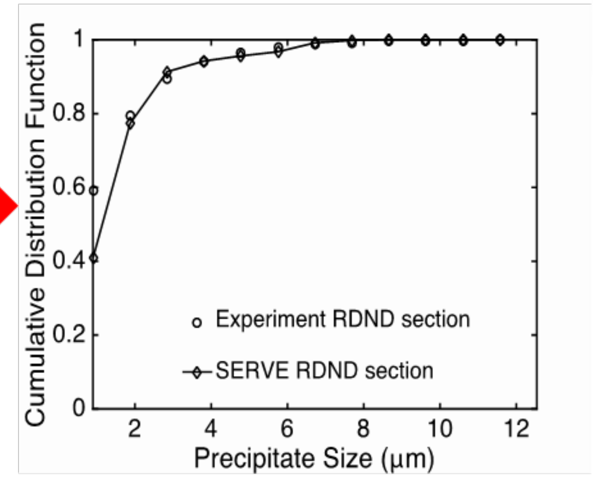
Extending M-SERVE

Al-7075 Alloys & Ni-based Superalloys



Genetic Algorithms

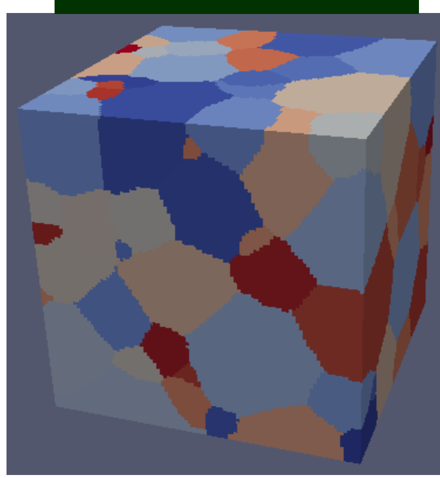
$$\text{minimize} \sum_{i=1}^{N} \left(CDF^{real} - CDF^{synthetic}\right)^2$$



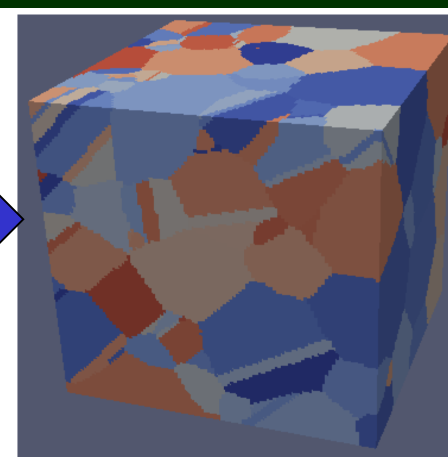
Nickel based Superalloys

Bagri, Weber, Lenthe, Pollock, Ghosh 2018

Without Twins

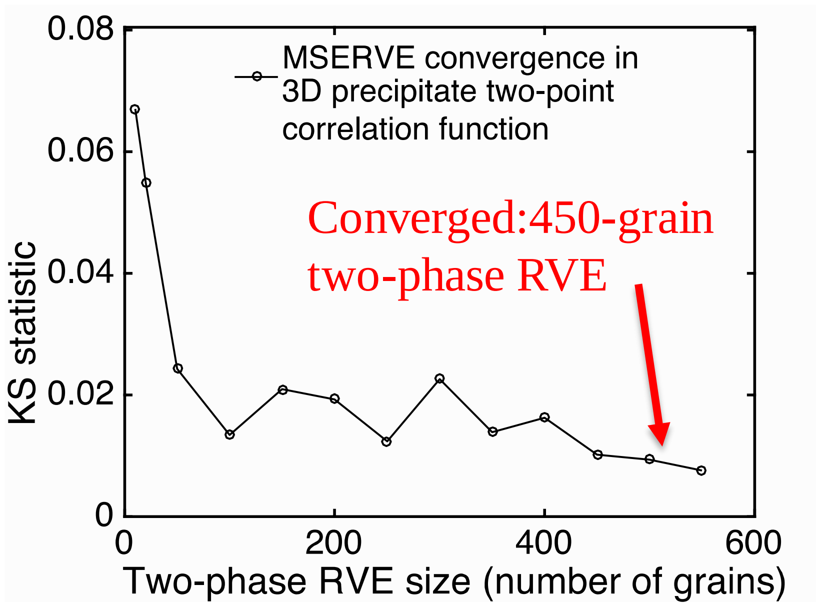


With Twins Inserted

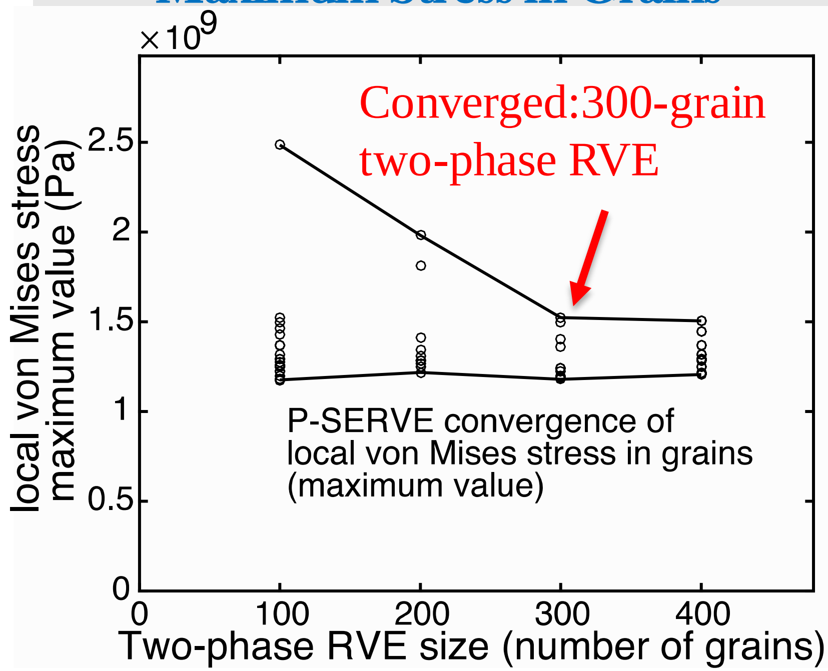


Convergence Tests for M-SERVE and P-SERVE

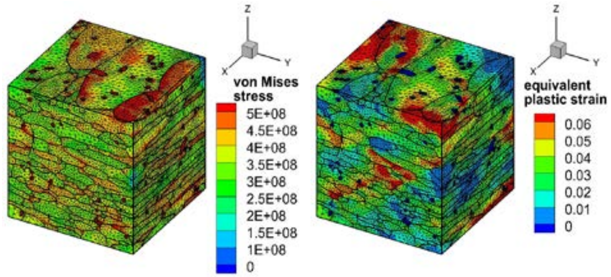
Particle two-point correlation function



Maximum Stress in Grains



Kolmogorov–Smirnov test (K–S test):
Convergence tests with error metrics



Statistically Equivalent Representative Volume Element (SERVE)

<u>RVE-based methods</u> of property determination are concerned only with the <u>size of the representative microstructural domain</u>.

- Affine transformation-based displacement boundary condition,
- Uniform traction boundary condition
- Periodic boundary condition

No consideration is given to the appropriateness of the boundary conditions applied to the RVE for solving the micromechanics.

Results in significant over-estimation of the RVE

<u>Optimally, the SERVE should</u>:

- Encompass the region required to represent essential mechanisms
- Represent boundary conditions that reflect the effect of the region exterior to the SERVE domain.

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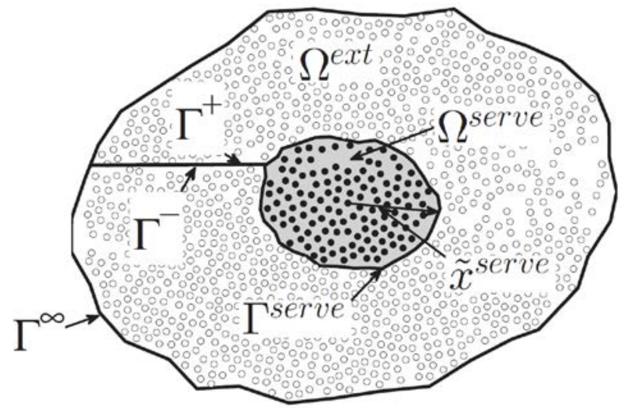
Statistically Informed Green's Function (SIGF) Approach

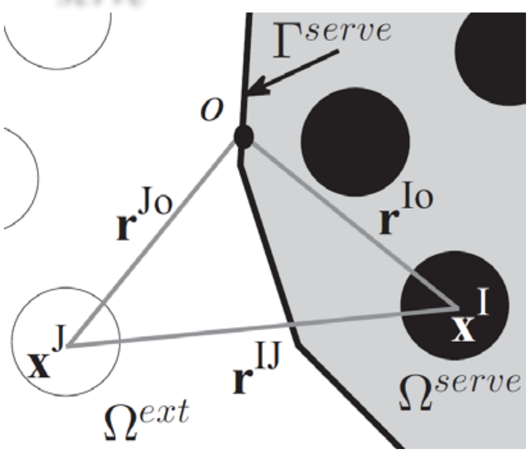
Computational Mechanics Research Laboratory — CMRL



Represent boundary conditions that reflect the effect of the region exterior to the SERVE domain.

Perturbed Displacement at x in MVE and on SERVE Boundary

Γ_{serve}

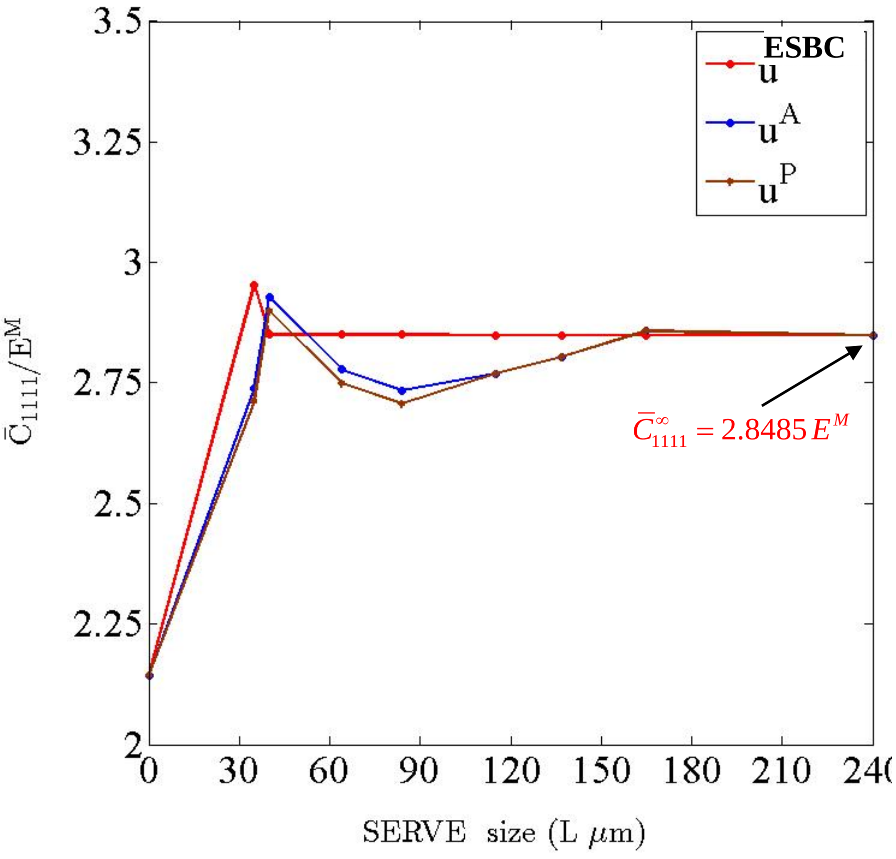


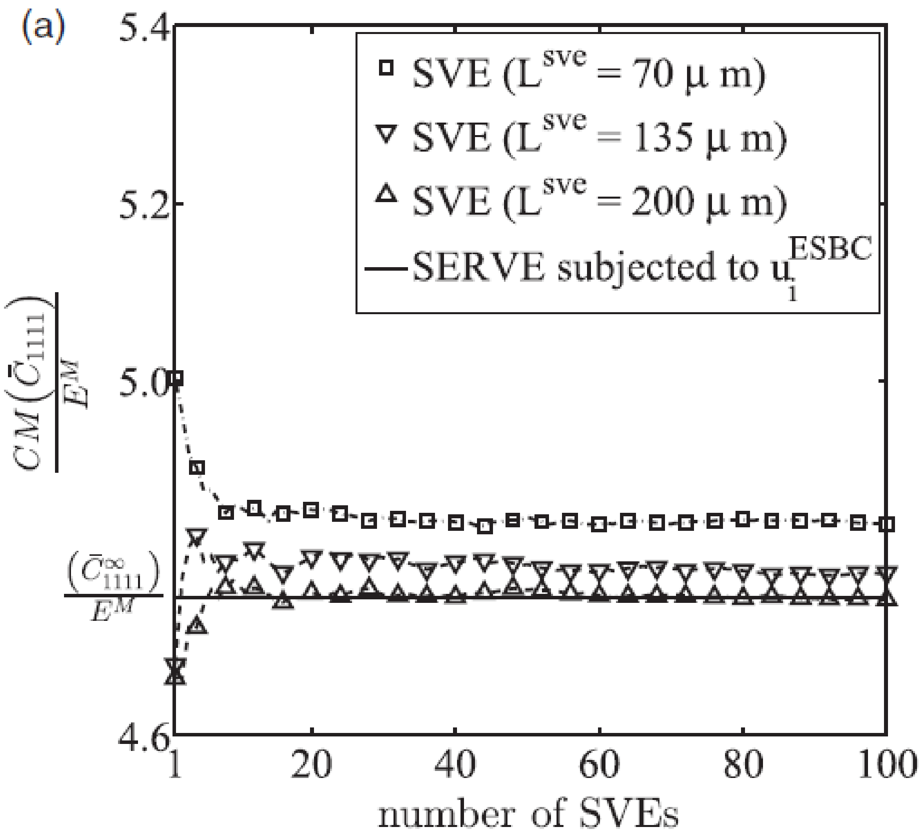
$$\boxed{u_i^*(\mathbf{x}) = \left(\int_{\Omega^{mve} \setminus \Omega_F} S_2(\mathbf{r}') L_{imn}(\mathbf{r}') A_{mnkl}(\mathbf{r}') d\Omega \right) \epsilon_{kl}^M}$$

$$A_{ijkl}(\mathbf{X}) = \left[\iota^F(\mathbf{x})(S_{ijab} + M_{ijab}) - \int_{\Omega^{mve} \setminus \Omega_F} S_2(\mathbf{r}) \hat{G}_{ijmn}(\mathbf{r}) (S_{mnpq} + M_{mnpq})^{-1} \hat{G}_{pqab}(\mathbf{r}) d\Omega \right]^{-1}$$
$$\left[\left((S_{abmn} + M_{abmn})^{-1} \int_{\Omega^{mve} \setminus \Omega_F} S_2(\mathbf{r}) \hat{G}_{mnkl}(\mathbf{r}) d\Omega \right) - \frac{1}{2}(\delta_{ak}\delta_{bl} + \delta_{al}\delta_{bk}) \right]$$

Ghosh and Kubair JMPS, (2016), Kubair, Ghosh IJSS (2017) , Kubair, Pinz, Przybyla, Ghosh J. Comp. Mat. (2018)

Homogenized Elastic Stiffness with u^A or u^P and u^{ESBC} on Γ^{serve}





SERVEs subjected to ESBCs converge for smaller volumes

Fast convergence wrt SVEs

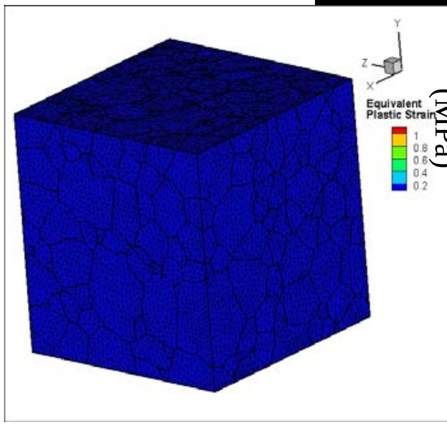
Kubair, Pinz, Przybyla, Ghosh J. Comp. Mat. (2018)

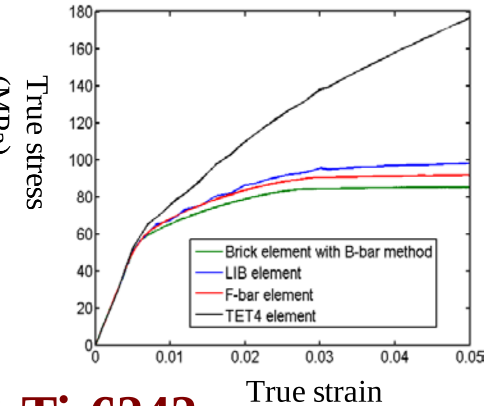
Ghosh and Kubair JMPS, (2016), Kubair, Ghosh IJSS (2017)

Methods of Analysis and Simulation at Relevant Scales: Accuracy and Efficiency

1. **Finite Element Methods: CPFEM:** ***Bronkhorst, Kalidindi, Anand (1992).*** *Kalidindi, Schoenfeld (2000), Bridier ,McDowell ,Villechaise,Mendez (2009), Mayeur, McDowell, Neu (2008), Busso , Meissonier , O´Dowd (2000), Dunne, Kiwanuka, Wilkinson (2012), Shahba ,Ghosh (2016), Venkataramani, Ghosh, Mills(2007), Roters, Eisenlohr, Hantcherli , Tjahjantoa , Bieler, Raabe (2010)*
2. **Boundary Element Methods**
3. **Fast Fourier Transform Methods** *Moulinec, Suquet (1998), Lebensohn, Kanjarla, Eisenlohr (2012) , Eisenlohr, Diehl, Lebensohn, Roters (2013)*
4. **Phase Field Methods:** *Yamanaka, Tomohiro, Takaki, Tomita, Yoshino (2009)*
5. **Peridynamics:** *Sun, Sundararaghavan (2014), Luo, Ramazani, Sundararaghavan (2018)*

Element Stabilization to Avoid Volumetric Locking in CPFEM





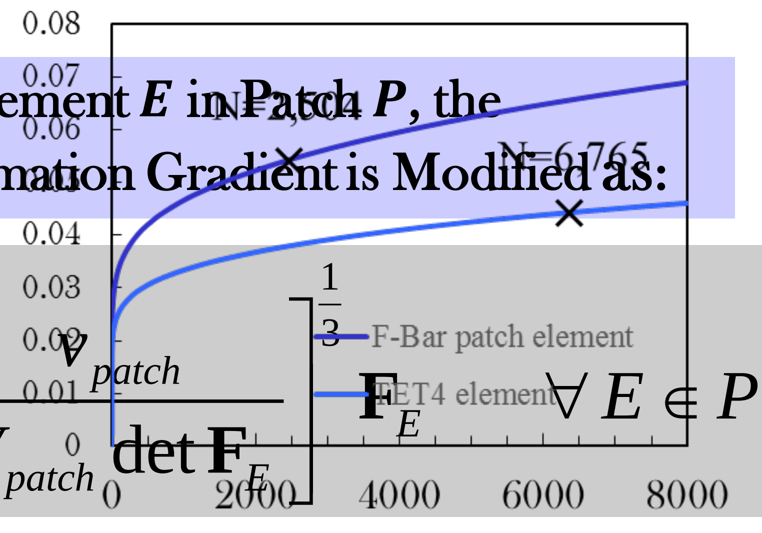
Ti-6242

$$\mathbf{F} = \mathbf{F}_{iso}\boxed{\mathbf{F}_{vol}}$$

$$\mathbf{F}_{iso} = (\det\mathbf{F})^{-\frac{1}{3}}\mathbf{F} \qquad \mathbf{F}_{vol} = (\det\mathbf{F})^{\frac{1}{3}}\mathbf{I}$$

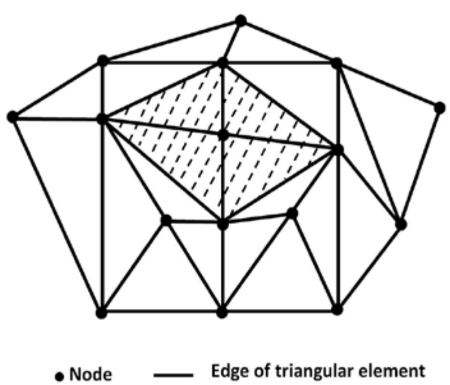
Incompressibility enforced over a non-overlapping patch of elements

For Element E in Patch P, the Deformation Gradient is Modified as:



$$\overline{\mathbf{F}}_E = \left[\frac{v_{patch}}{V_{patch}\det\mathbf{F}_E}\right]^{\frac{1}{3}}\mathbf{F}_E \quad \forall E \in P$$

F-bar Patch Method

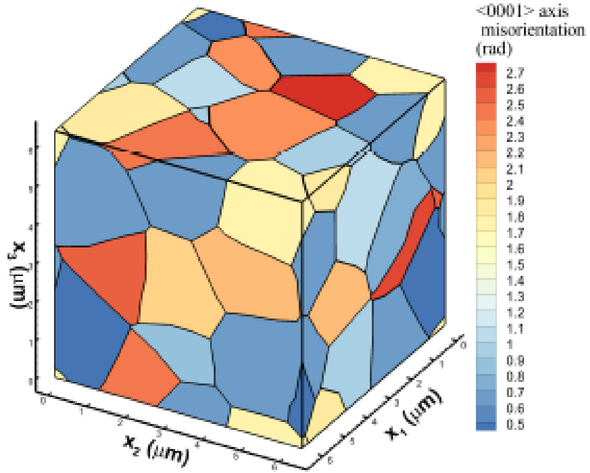


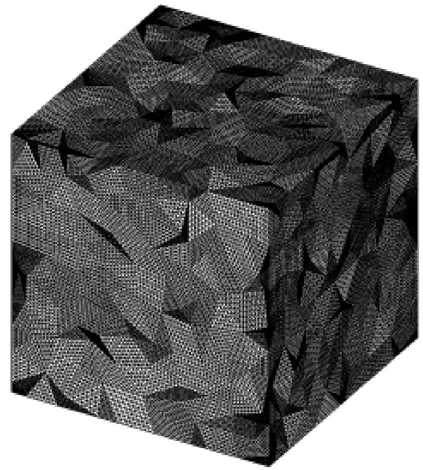
v_{patch} : deformed volume of patch

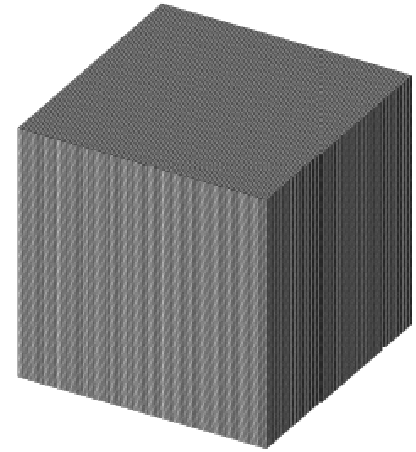
V_{patch} : reference volume of patch

Cheng, Shahba, Ghosh, Comp. Mech., 2016
de Souza Neto, Pires, Owen, IJNME 2005

Accuracy and Efficiency of CPFEM





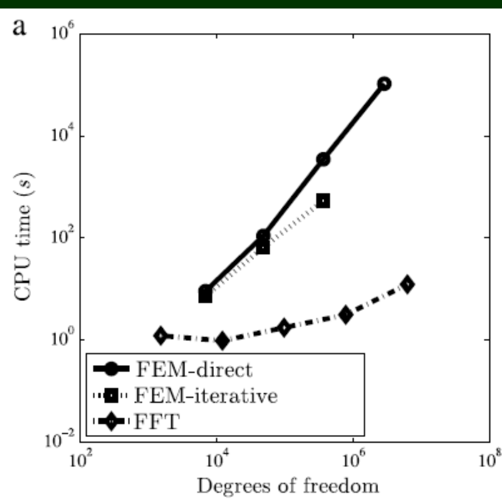


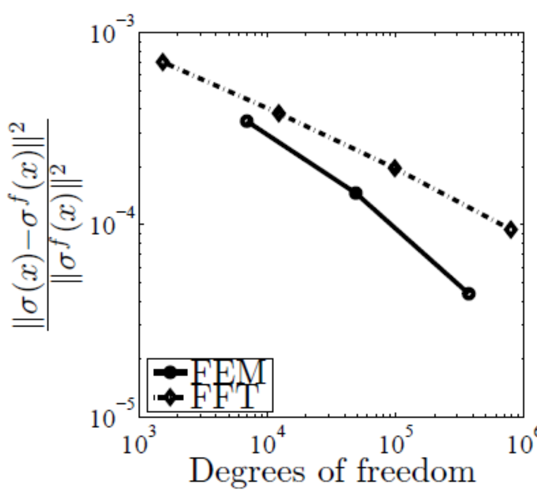
25 grains, high misorientation, Periodic BC, uniaxial load

ABAQUS STANDARD
5640192 TET Elements

FFT Code CraFT
128^3 Grid Points

(*Moulinec and Suquet,1994*)

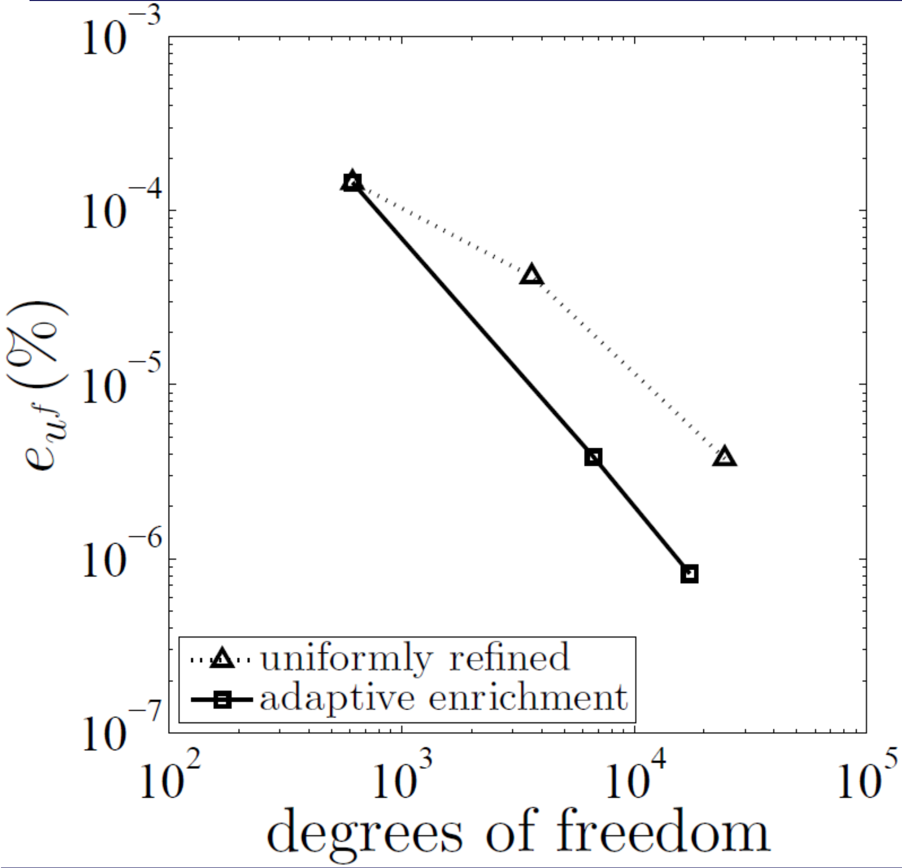


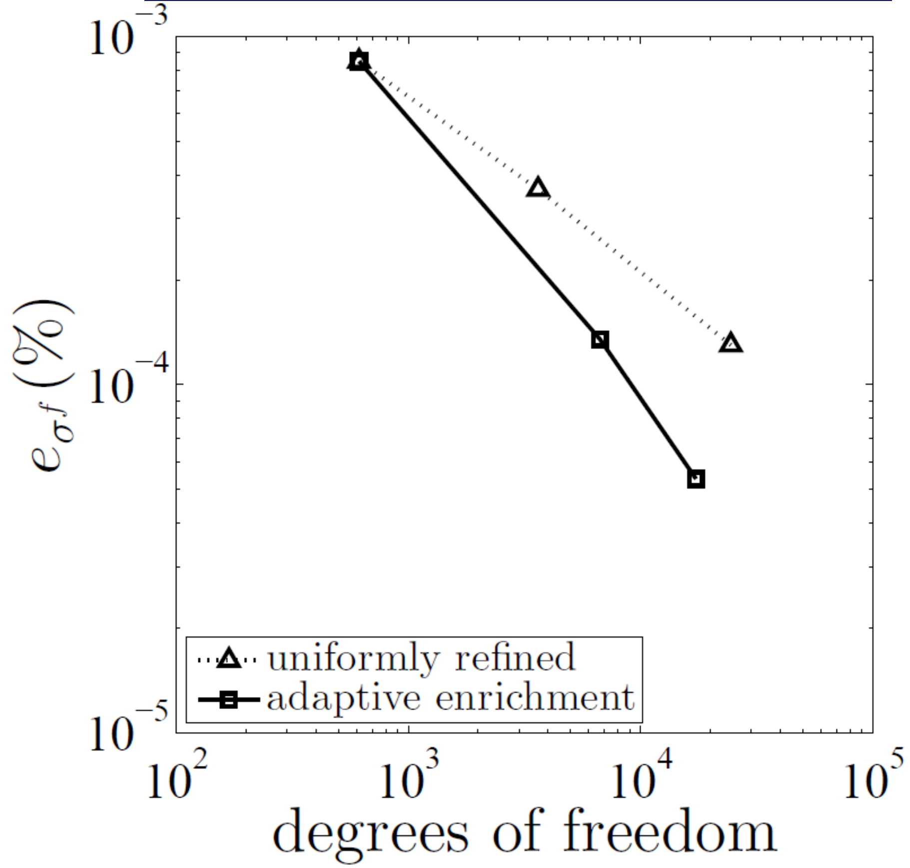


While the speed of FFT could be orders of magnitude faster, the convergence rate of the global error could slower in the presence of heterogeneities

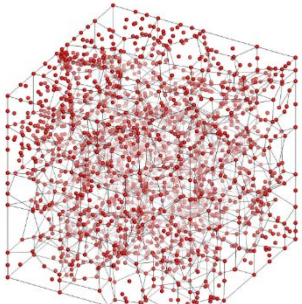
Azdoud, Cheng, Ghosh, CMAME, (2017), Azdoud, Ghosh, CMAME, (2017).

A Computationally Efficient and Accurate CPFEM-based Hierarchical Method





The adaptive method is ~ 20 faster than uniformly refined CPFEM



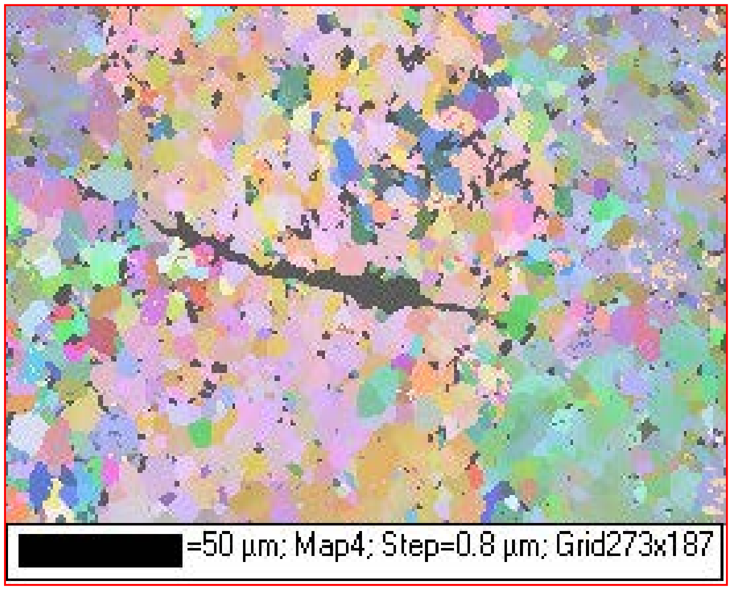
Y. Azdoud, S. Ghosh, CMAME, (2017)

Y. Azdoud, J. Cheng, S. Ghosh, CMAME, 2017

Crack Propagation

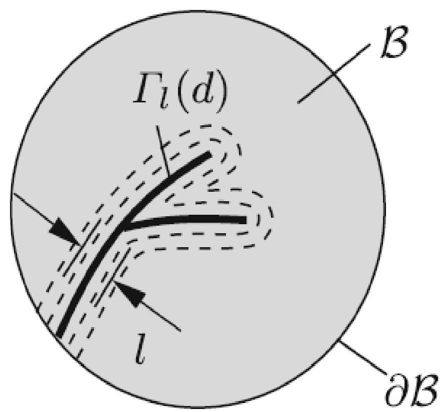
Coupling Phase-Field Modeling with CPFEM

Introduces a thermodynamic consistent plasticity-informed continuum formulation for crack propagation.

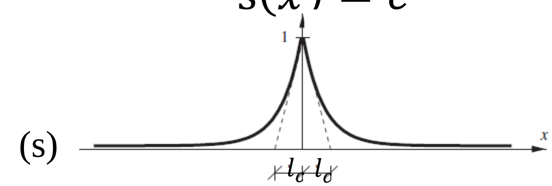


Allen-Cahn equations

Continuous Auxiliary Global Field to Approximate Sharp Crack Discontinuities.



$$s(x) = e^{-|x|/l_c}$$



Diffused crack

s is the phase field variable (order parameter):
$\boldsymbol{s} \in [\mathbf{0}, \mathbf{1}]$; $\boldsymbol{s} = \mathbf{0}$ **perfect solid;** $\boldsymbol{s} = \mathbf{1}$ **fully cracked**

Sharp crack of area Γ is regularized by a **crack surface density function** $\gamma_l(s, \nabla s)$ which measures a spatially regularized total crack surface $\Gamma_l(s)$

$$\boldsymbol{\Gamma_l(s) = \int_v \gamma_l(s, \nabla s)\, dV}$$

$$\boldsymbol{\gamma_l(s, \nabla s) = \frac{1}{2l} s^2 + \frac{l}{2} |\nabla s|^2}$$

Miehe, Hofacker, Welschinger (2010)

Challenge with Phase Field Modeling
Requires Extremely Fine Resolution

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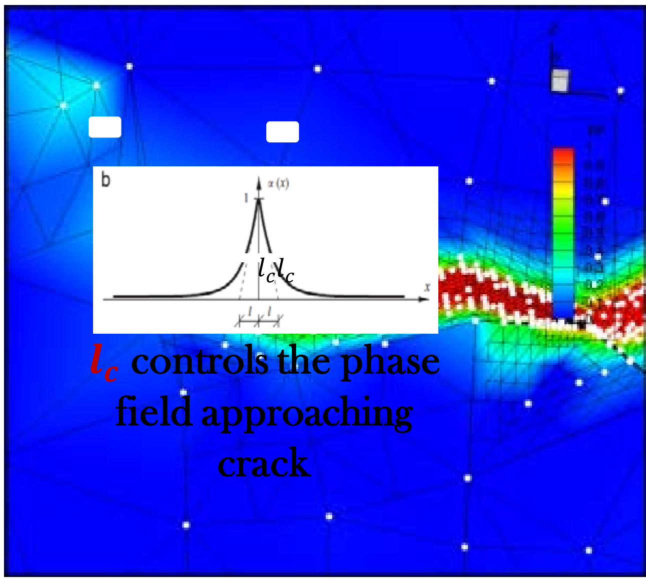
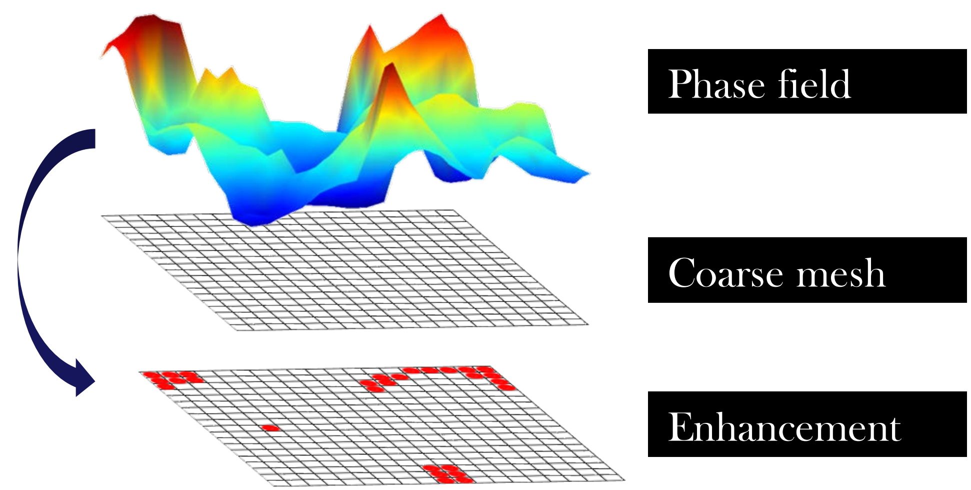
Computational Mechanics Research Laboratory CMRL

Adaptive Projection to Phase-Field Model: Wavelet-Enriched Hierarchical FEM

- *Hierarchical FE* preserves coarse mesh and adds multi-resolution shape functions
- Wavelet based Hierarchical FEM allows for optimum computation of phase field



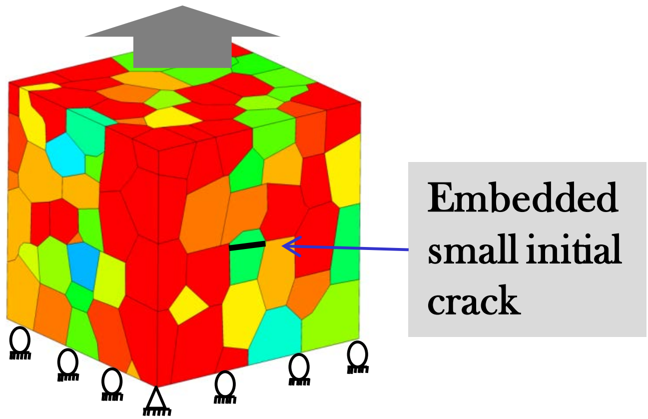
Hierarchical adaptive FEM With wavelet enhancement ~10,000 nodes are required



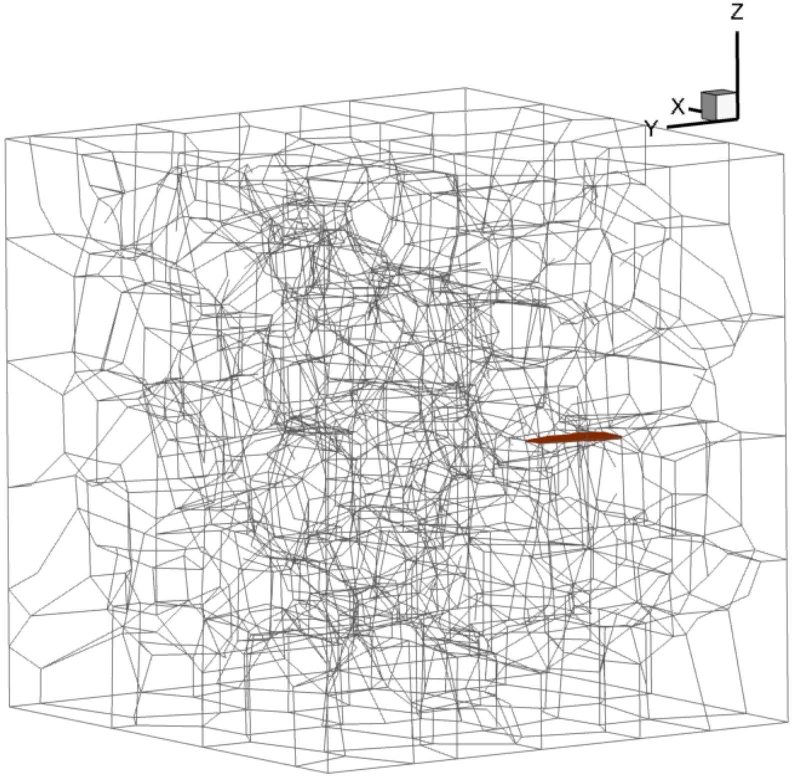
FEM with global fine mesh needs ~1,000,000 nodes

Azdoud , Ghosh, CMAME, (2017), Azdoud , Cheng, Ghosh, CMAME, (2017)

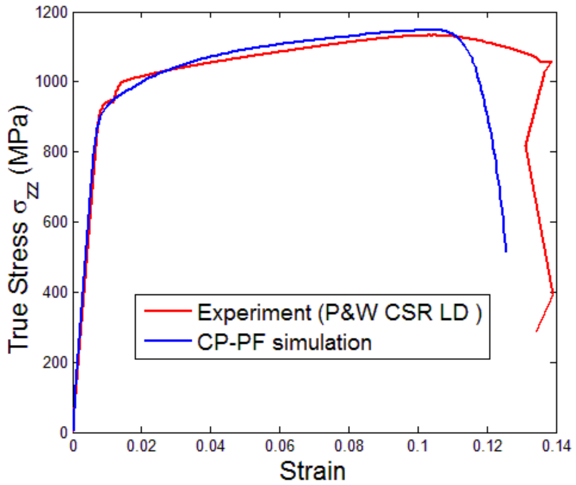
Crack Propagation in Ti-64 Microstructure using Wavelet Enriched Hierarchical FEM



Visualization of crack propagation



Macroscopic stress-strain



The same result would be obtained using conventional FEM with a fine mesh containing ~7,000,000 nodes

In the wavelet-enhanced adaptive hierarchical FEM, only ~300,000 nodes are required

Accelerated Time Integration Methods and Multi-time Scaling

1. Time Acceleration for Fatigue Modeling
2. Subcycling for Modeling Sub-Domains with Disparate Time Requirements

Wavelet Transformation Based Multi-Time Scaling Methodology *(WATMUS)*

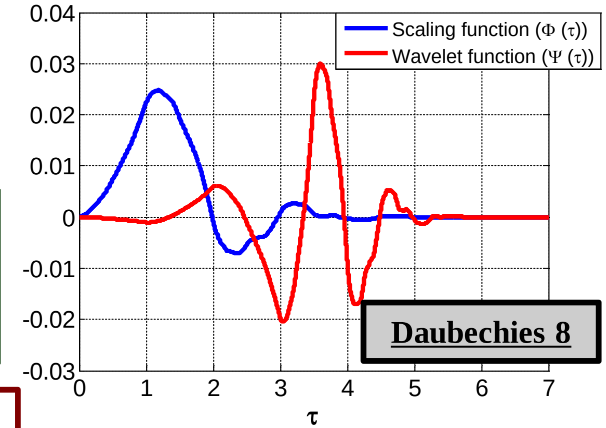
Wavelet Decomposition of Nodal Displacements

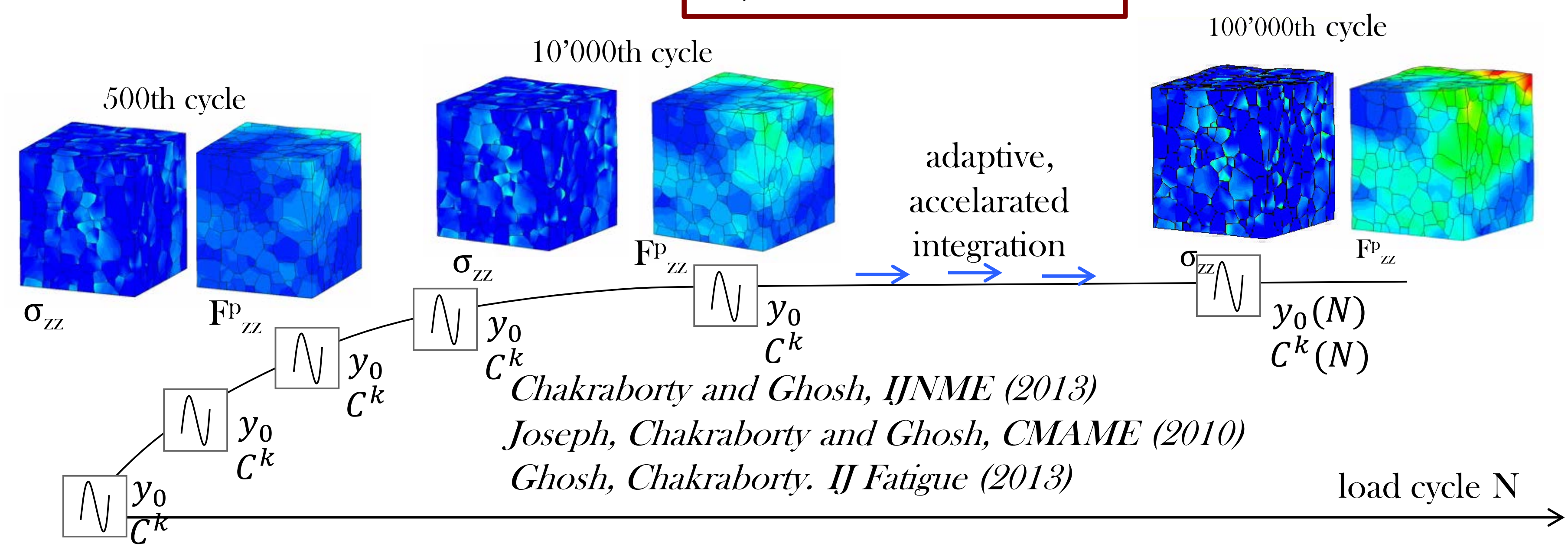
$$u(N,\tau)=\sum_k c_k(N)\psi_k(\tau)$$

Coefficients of wavelet basis
- Depends on <u>cycle</u> scale (N)
- *Independent of fine scale.*

Wavelet basis function
- Fine scale (τ) behavior
- *Independent of (N)*

$$\phi_{m,n}=2^{\frac{m}{2}}\phi(2^m\tau-n)$$

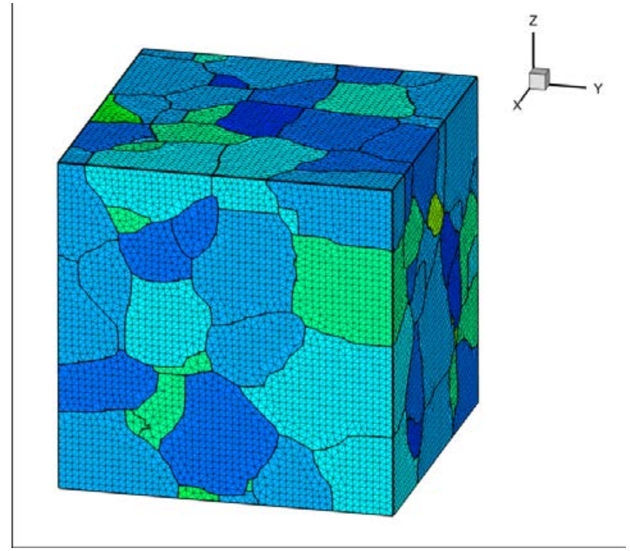




Chakraborty and Ghosh, IJNME (2013)
Joseph, Chakraborty and Ghosh, CMAME (2010)
Ghosh, Chakraborty. IJ Fatigue (2013)

Adaptive Subcycling in CPFE Simulations for Twin Evolution

- Twin bands require very high resolution FE mesh
- Twin formation intensifies time steps with localization within twin bands



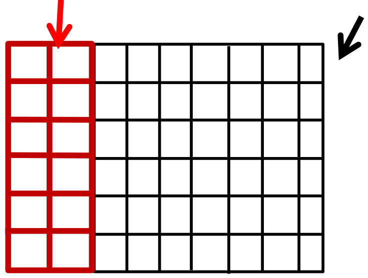
Strain localization within twin bands

97% elements can converge at $\Delta t=10s$
3% elements can converge at $\Delta t=0.03s$

1. Spatial domain decomposition
2. Solve separately using fine and coarse time steps
3. Couple and iterate

Deformation localized region (twin)

Low deformation rate region



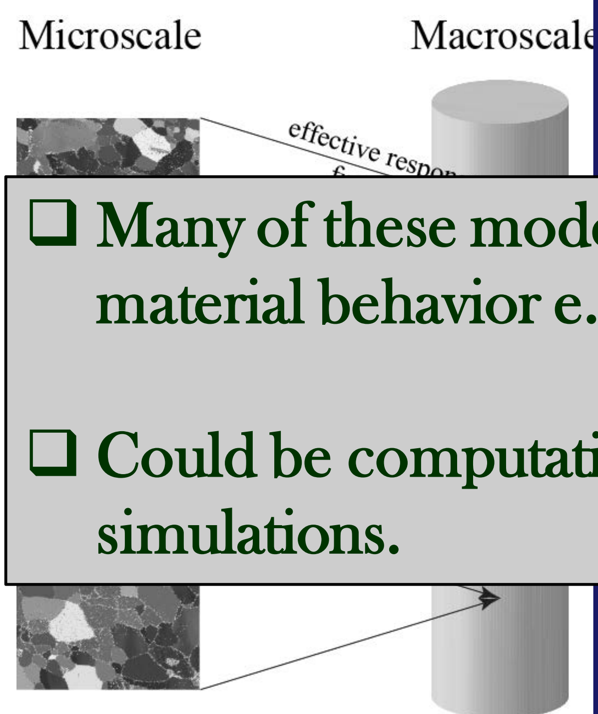
Over 1 order magnitude faster

Cheng , Ghosh, JMPS, (2017), Ghosh, Cheng, Ghosh, CM, (2017)

$$\Delta \mathbf{u} = \left(\widetilde{\mathbf{K}}^{F}_{t+\Delta t} + \mathbf{K}^{C}_{t+\Delta t}\right)^{-1} \left\{\mathbf{f}^{ext}_{t+\Delta t} - \widetilde{\mathbf{f}}^{int,F}_{t+\Delta t} - \mathbf{f}^{int,C}_{t+\Delta t}\right\}$$

$$\Delta \mathbf{u}^{corrector}_{t\to t+\Delta t} = \Delta \mathbf{u}^{trial}_{t\to t+\Delta t} + \Delta \tilde{\mathbf{u}}^{F} + \Delta \mathbf{u}$$

Hierarchical Upscaling: Homogenization Models from Micromechanical Simulations



- ❑ <u>Variational framework</u>: Ponte Castaneda (1991,1992), Hughes (1998)
- ❑ <u>Self-consistent method:</u> Kroner (1958), Budiansky and Wu (1962), Lebensohn and Tom´e (1993)

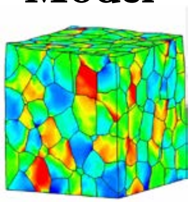
- ❑ **Many of these models are not suitable for representing complex material behavior e.g., anisotropy, path-dependent behavior etc..**
- ❑ **Could be computationally prohibitive for large-scale structural simulations.**

- ❑ <u>Reduced order models</u>: Fish, et. al. (2012), Ghosh, et. al (2007, 2009)
- ❑ <u>Distribution-Enhanced Homogenization Framework</u>: Alleman, Ghosh, Luscher, Bronkhorst, JMPS, 2015

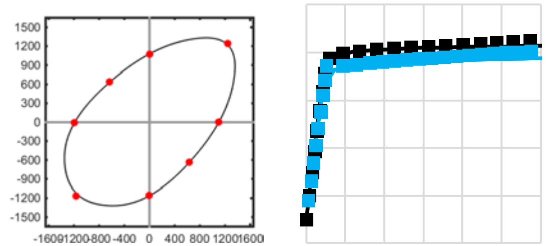
A Promising Alternative

Parametrically Homogenized Constitutive Models (PHCM)

Detailed Micromechanical Model

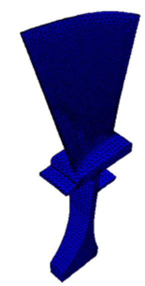


PHCM



$$\dot{\bar{\sigma}} = f(\bar{\varepsilon}, \bar{\phi}_{sv}, P_{ms}, W_p)$$

Simulations with PHCM



- ❑ Thermodynamically consistent, continuum scale, reduced order models with parametric delineation of morphological distributions
- ❑ Constitutive parameters and their evolutions expressed in terms of parameters of statistical distribution functions
- ❑ *Machine Learning* for function forms of coefficients

- ❑ Easily incorporated in commercial codes through UMAT
- ❑ Significant efficiency without loss of accuracy from physics-based models
- ❑ Direct connection to the "materials by design"

Kotha, Ozturk , Ghosh, (2018), Ozturk, Kotha, Ghosh, (2018)

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WHITING SCHOOL *of* ENGINEERING

PHCM Model and Microstructural Dependencies

Computational Mechanics Research Laboratory — CMRL

Elastic-Plastic Constitutive Equations

for Macro-modeling

Elasticity

$$\mathbf{S} = \mathbb{C}^{PHCM}(g_1, g_2, g_3) : \mathbf{E}$$

$$\mathbb{C}^{PHCM} = g_1 \mathbb{C}^{single}_{(x)} + g_2 \mathbb{C}^{single}_{(y)} + g_3 \mathbb{C}^{single}_{(z)}$$

Anisotropic Plasticity

$$\mathbf{D^p} = \dot{\gamma}_0 (Y/Y_0)^{1/m} \mathbf{N}$$

$$Y = [(|\Sigma_1| - k\Sigma_1)^a + (|\Sigma_2| - k\Sigma_2)^a + (|\Sigma_3| - k\Sigma_3)^a]^{\frac{1}{a}}$$

Transformed stress $\boldsymbol{\Sigma} = \mathbb{L}\left(\overline{OMA}^{\mu}_{ij}\right) : \mathbf{S}$

Anisotropy Tensor

Hybrid Voce Type Hardening and Grain Size Dependency

$$Y(\varepsilon_p) = Y_0(\bar{D}_\mu, \bar{D}_\sigma) + \alpha(\bar{A}_{\theta mis})\left(1 - \exp\left[-\left(\frac{\varepsilon_p}{\widetilde{\varepsilon_p}\left(\overline{OMA}^{\mu}_{ij}\right)}\right)^{0.75}\right]\right) + h_0\left(\overline{OMA}^{\mu}_{ij}, \bar{D}_\mu\right)\varepsilon_p$$

Initial Yield Strength

Hardening Modulus

Microstructural Parameters

inputs to the UMAT from EBSD scans

g_1, g_2, g_3

Texture intensity parameters

$\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$

Material symmetry axes

$\overline{OMA}^{\mu}_{ij}$

Crystallographic Orientation Measure in Material Frame

$\overline{OMA}^{\mu}_{ij}$

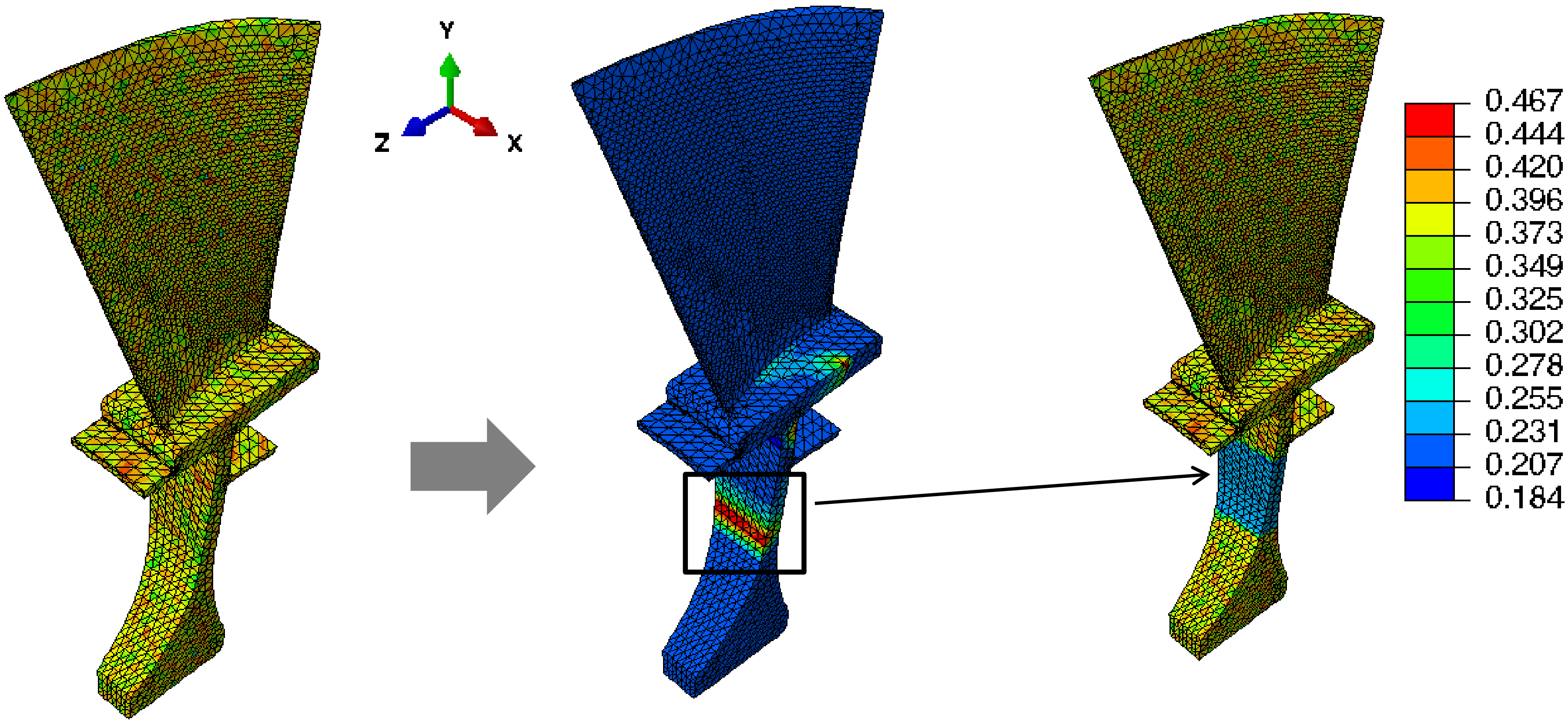
$\bar{A}_{\theta mis}$

$\bar{D}_\mu,\ \bar{D}_\sigma$

Misorientation, grain size distn.

PHCM and Material Design

Design Objective: Change the material properties in the localized band to reduce the plastic strains



Original $\overline{OMA}_{33}$ from the EBSD

Original properties leading to localized plastic strain

Modified $\overline{OMA}_{33}$ in the localized region

Summary

With unraveling of new mechanisms and defect structures in complex heterogeneous materials and structures:

- Using conventional tools are in most cases insufficient
- Need for novel methods and algorithms in Computational Mechanics and Computational Materials Science is becoming more meaningful.
- Better methods of reaching large audiences with these tools