AI-Based Knowledge Systems for Supporting Materials-Manufacturing Innovations

Surya R. Kalidindi

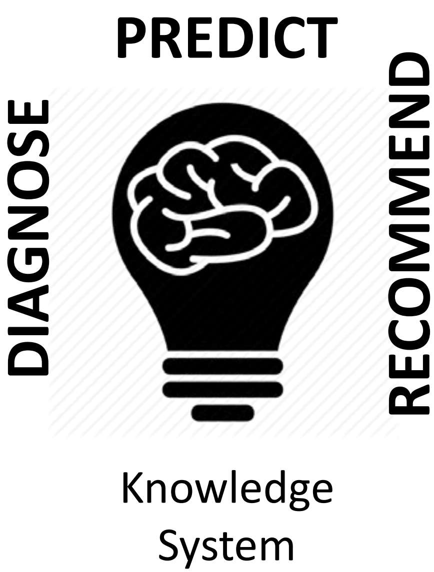
Funding: DoD, NIST

MINED

Georgia Tech

CREATING THE NEXT

AI-Based Materials Knowledge Systems (MKS)



- Specifically designed to <u>support</u> accelerated discovery, development, and deployment of new/improved materials in advanced technologies
- Main Functions: Diagnose, Predict, Recommend
- Expressed as a library of Process-Structure-Property (PSP) linkages covering all materials classes and all relevant material structure length scales (and relevant time scales)
- Formulated on a rigorous Bayesian statistical framework that accounts for the uncertainty of the curated knowledge
- Continuously ingests a variety of information from disparate sources and dynamically evolves
- Highly efficient both in front-end (user-facing) and in the back-end (knowledge update) computations

PSP Linkages Over a Hierarchy of Material Structure Scales

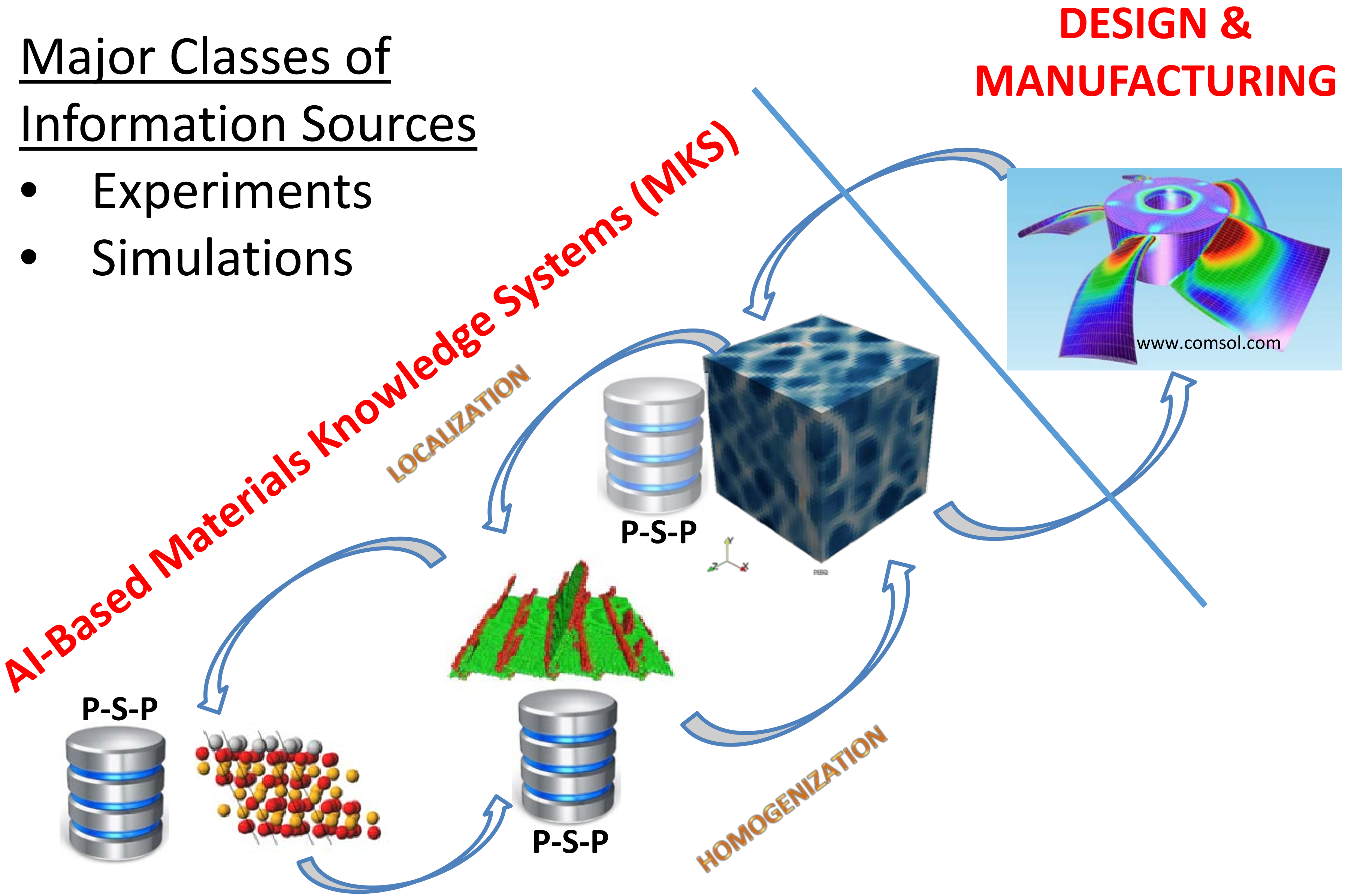
Process	Structure	Property
• Thermo-mechanical (T(t), **L**(t), **σ**(t), $\dot{c}$(t), …) • Placement of Specific Defects (e.g., grain/phase boundaries, $g, \Delta g, n$) • Placement of chemical species ($c_i, V, p, \boldsymbol{x}_n, \ldots$)	• Microstructure • Dislocation/defect structure • Interface atomic structure • Atomic structure with defects, disorder, etc. • Electron density field	• Young's Modulus • Yield Strength • Fatigue Strength • Conductivity • Permeability • Critical Resolved Shear Strength • Grain Boundary Energy • Vacancy Formation Energy

- Process and Property variables have rigorous mathematical definitions
- Critical Need: A framework for high-value low-dimensional representations of the material structure (minimal information loss with maximum recoverability) that is broadly applicable to various material classes at different length scales.

AI-Based Materials Knowledge Systems
(knowledge integration as opposed to tool integration)

Major Classes of Information Sources

- Experiments
- Simulations



Stochastic Framework for MKS

- Property: $P \in \mathcal{R}; p(P) = \mathcal{N}\left(P \middle| \bar{P}, \sigma_p^2\right)$

- Material (Hierarchical) Structure: $\boldsymbol{\mu} \in \boldsymbol{\mathcal{M}}$; $p(\boldsymbol{\mu}) = \mathcal{N}\left(\boldsymbol{\mu} \middle| \bar{\boldsymbol{\mu}}, \boldsymbol{\Sigma}_{\boldsymbol{\mu}}\right)$

- Process: $\boldsymbol{\mathcal{P}} \in \mathcal{R}^n; p(\boldsymbol{\mathcal{P}}) = \mathcal{N}\left(\boldsymbol{\mathcal{P}} \middle| \bar{\boldsymbol{\mathcal{P}}}, \boldsymbol{\Sigma}_{\boldsymbol{\mathcal{P}}}\right)$

- Governing Physics: expressed as field (differential) equations and material constitutive laws or equivalently as Green's functions

$$\boldsymbol{\varphi} \in \boldsymbol{\Phi}; p(\boldsymbol{\varphi}) = \mathcal{N}\left(\boldsymbol{\varphi} \middle| \bar{\boldsymbol{\varphi}}, \boldsymbol{\Sigma}_{\boldsymbol{\varphi}}\right)$$

- Physics-Based Simulations: $p\left(P \middle| \boldsymbol{\mu}, \boldsymbol{\varphi}, \boldsymbol{\Sigma}_{\boldsymbol{\mu}}, \boldsymbol{\Sigma}_{\boldsymbol{\varphi}}\right)$ and $p\left(\boldsymbol{\mu} \middle| \boldsymbol{\mathcal{P}}, \boldsymbol{\varphi}, \boldsymbol{\Sigma}_{\boldsymbol{\mathcal{P}}}, \boldsymbol{\Sigma}_{\boldsymbol{\varphi}}\right)$ - machine learning has opened new avenues for sampling these distributions within practical computational budgets

- Physical Experiments (typically small datasets): $p\left(P \middle| \boldsymbol{\mu}, \boldsymbol{\Sigma}_{\boldsymbol{\mu}}, \boldsymbol{\varphi}^*\right)$ and $p\left(\boldsymbol{\mu} \middle| \boldsymbol{\mathcal{P}}, \boldsymbol{\Sigma}_{\boldsymbol{\mathcal{P}}}, \boldsymbol{\varphi}^*\right)$; $\boldsymbol{\varphi}^*$= undetermined governing physics

Bayesian Update of Governing Physics

(a formal framework for uncovering new physics)

$$p\left(\boldsymbol{\varphi}\middle|\boldsymbol{E},\boldsymbol{\Sigma}_{\boldsymbol{E}}\right) \propto \underbrace{p\left(\boldsymbol{E}\middle|\boldsymbol{\varphi},\boldsymbol{\Sigma}_{\boldsymbol{E}}\right)} p(\boldsymbol{\varphi})$$

<u>Sequential Design of Physical Experiments</u>

Decide on the next experiment that is likely to produce the largest information gain in updating the governing physics.

<u>Physics-Based Models</u>

Build Gaussian Process models trained to simulation datasets produced by executing physics-based models by adaptive sampling of input domain for maximizing fidelity of extracted GP.

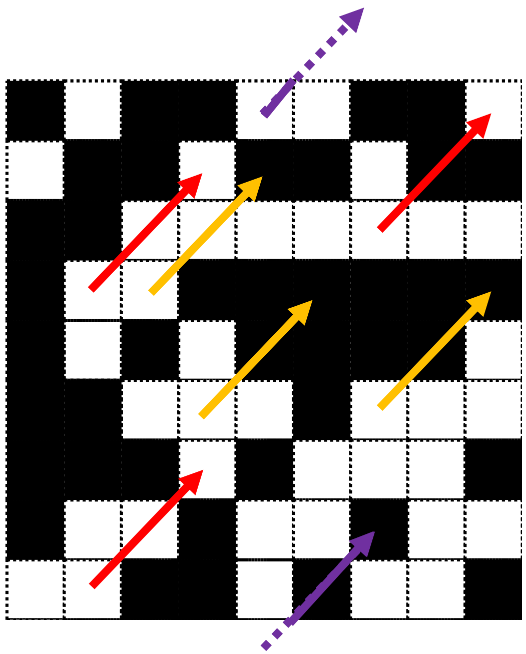
Process-Structure: $p\left(\boldsymbol{\mu}\middle|\boldsymbol{\mathcal{P}},\boldsymbol{\varphi},\boldsymbol{\Sigma}_{\boldsymbol{\mathcal{P}}},\boldsymbol{\Sigma}_{\boldsymbol{\varphi}}\right)$

Structure-Property: $p\left(P\middle|\boldsymbol{\mu},\boldsymbol{\varphi},\boldsymbol{\Sigma}_{\boldsymbol{\mu}},\boldsymbol{\Sigma}_{\boldsymbol{\varphi}}\right)$

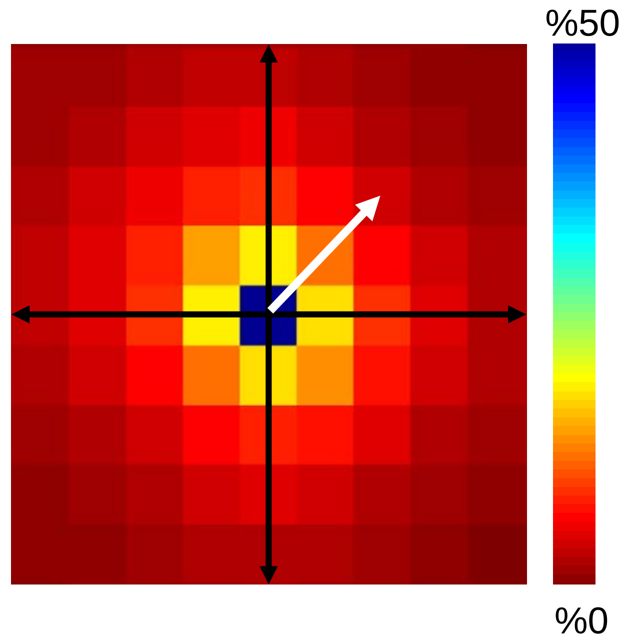
Foundational framework for Materials Knowledge Systems: Diagnose, Predict, Recommend

Structure Quantification: n-Point Spatial Correlations

- Spatial correlations capture all of the salient measures of the microstructure
- Allow efficient computations using discrete Fourier transforms (DFTs)



$$f_r^{hh'} = \frac{\#\,Trials\ Successful}{\#\,Trials\ Attempted}$$

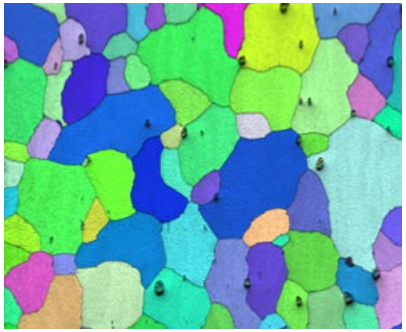


Complete Set of $f_r^{hh'}$ for all possible r

$$f_{\boldsymbol{r}}^{np} = \frac{1}{S_{\boldsymbol{r}}}\frac{1}{J}\sum_{\boldsymbol{s}}\sum_{j=1}^{J} {}^{(j)}m_{\boldsymbol{s}}^{n}\ {}^{(j)}m_{\boldsymbol{s}+\boldsymbol{r}}^{p}$$

S. R. Kalidindi, “Hierarchical Materials Informatics”, Butterworth Heinemann, 2015.

Polycrystal Microstructures



$$m(g,\boldsymbol{x}) \approx \sum_{L}^{\tilde{L}} \sum_{\boldsymbol{s}}^{\boldsymbol{S}} M_{\boldsymbol{s}}^{L} T_L(g) \chi_{\boldsymbol{s}}(\boldsymbol{x})$$

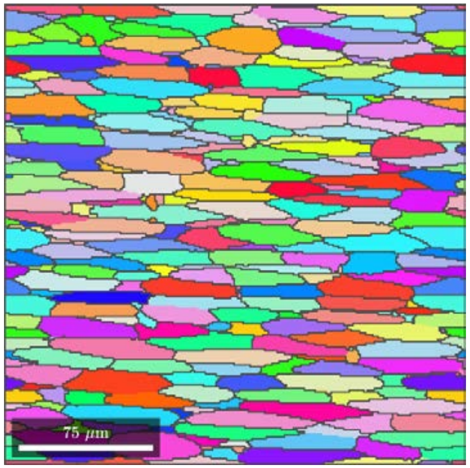
$$f(g,g'|\boldsymbol{r}) \approx \sum_{L}^{\tilde{L}} \sum_{K}^{\tilde{L}} \sum_{\boldsymbol{t}}^{\boldsymbol{S}} F_{\boldsymbol{t}}^{LK} T_L(g) T_K(g') \chi_{\boldsymbol{t}}(\boldsymbol{r})$$

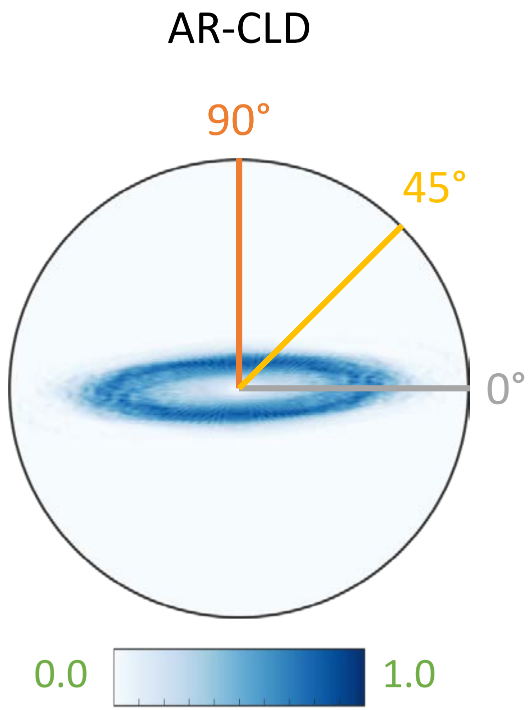
$$f(g,g'|\boldsymbol{r}) = \frac{1}{Vol(\Omega_{\boldsymbol{r}})} \int_{\Omega_{\boldsymbol{r}}} m(g,\boldsymbol{x}) m(g',\boldsymbol{x}+\boldsymbol{r}) d\boldsymbol{x}$$

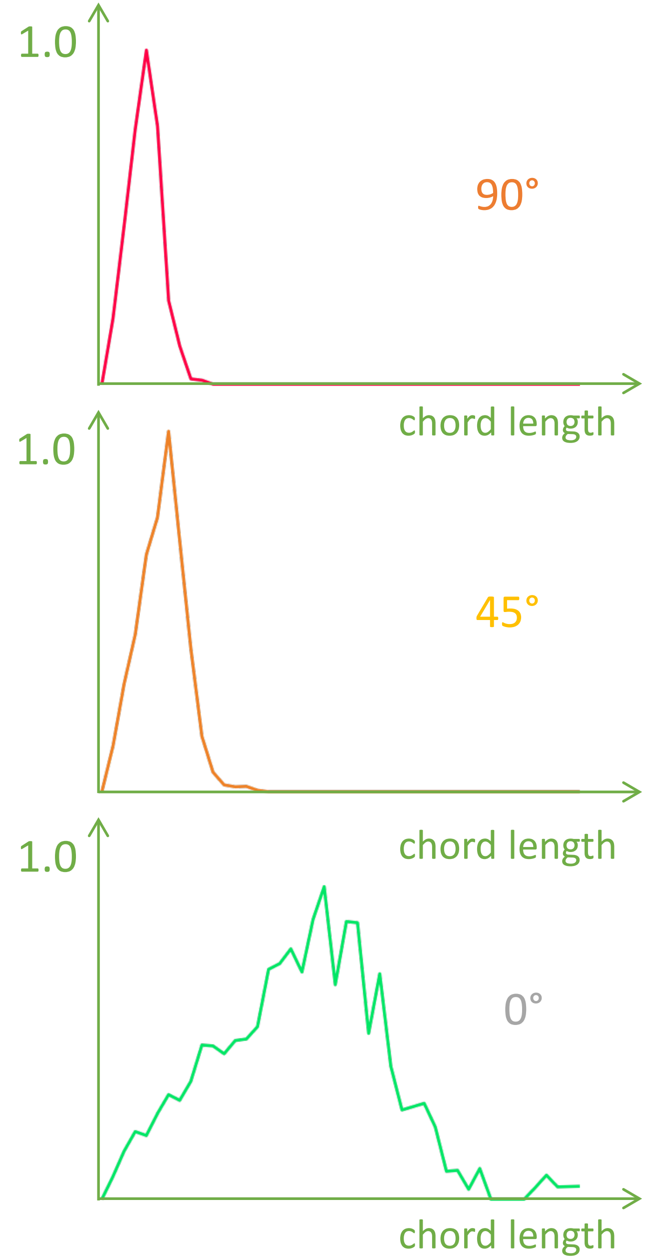
$$F_{\boldsymbol{t}}^{LK} = \frac{1}{|\boldsymbol{S}_{\boldsymbol{t}}|} \sum_{\boldsymbol{s}}^{\boldsymbol{S}_{\boldsymbol{t}}} \boldsymbol{M}_{\boldsymbol{s}}^{L} \boldsymbol{M}_{\boldsymbol{s}+\boldsymbol{t}}^{K}$$

Angularly Resolved Chord-Length Distirbution

Microstructure







AR-CLD: Captures the probability of a randomly selected pixel belonging to a chord of specified length in a specified direction.

Quantification of Atomic Structures

Input:
atomic coordinates
Lattice Dimensions
(From atomistic file formats)

→

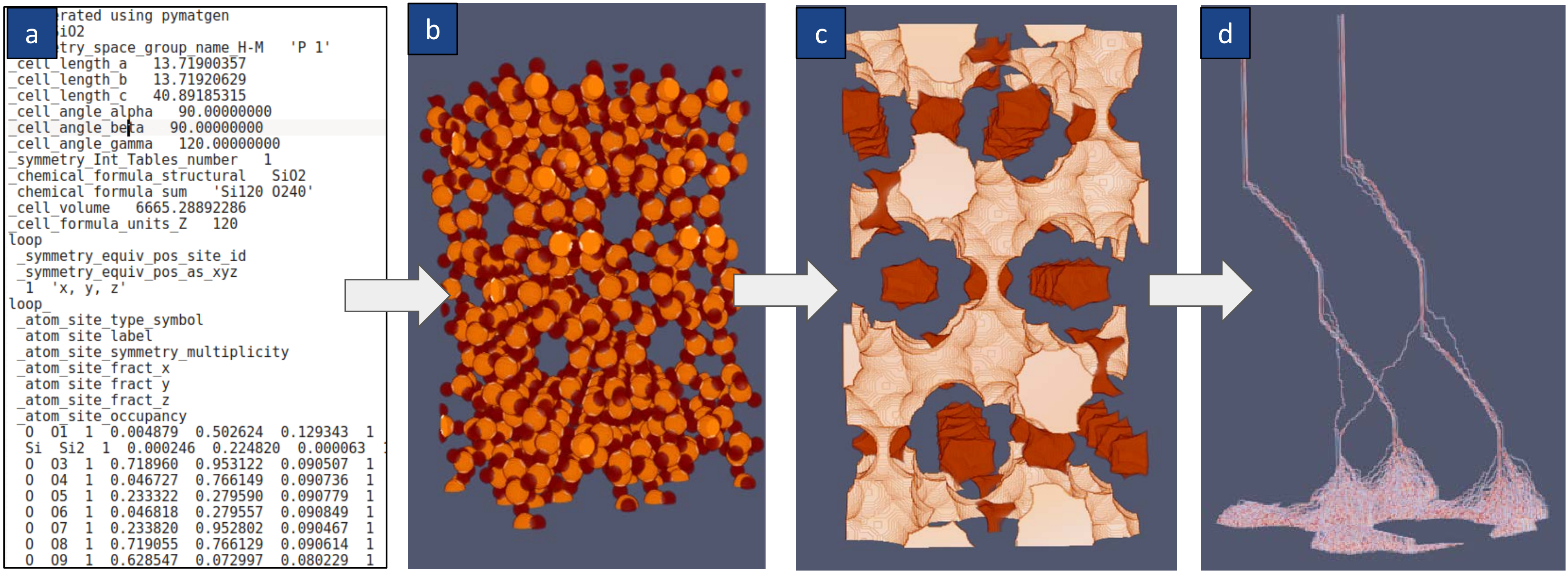
Generate grid representation of the Molecular Structure

→

Compute the pore region that can be accessed by a probe molecule

→

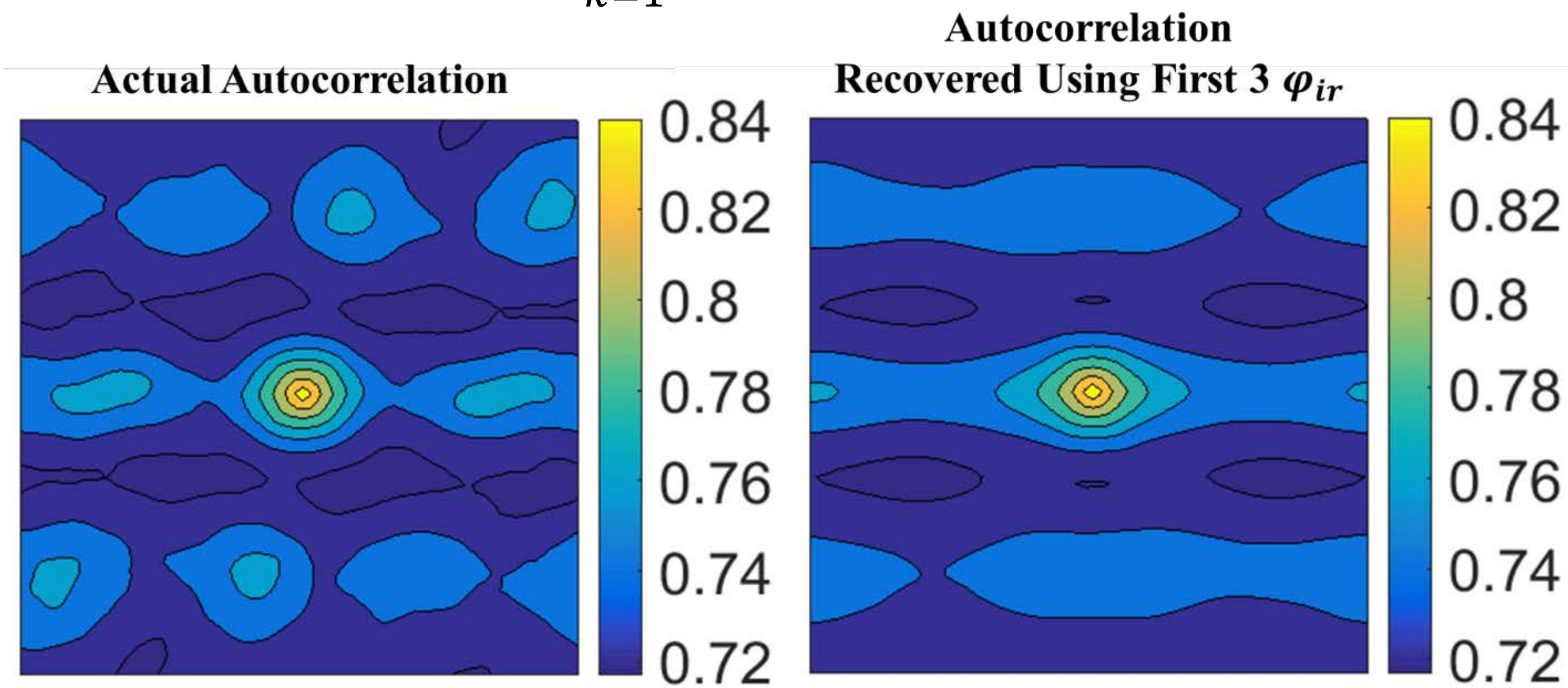
Compute pore characteristics:
Accessible Volume,
PLD, LCD,
Accessible Paths,
Tortuosity



Define features of interest in a rigorous statistical framework → **Feature Engineering**

Low-Dimensional Representations of material structure distributions Using PCA

$$f_r^{(j)} \approx \sum_{k=1}^{\tilde{R}} \alpha_k^{(j)} \varphi_{kr} + \bar{f}_r$$

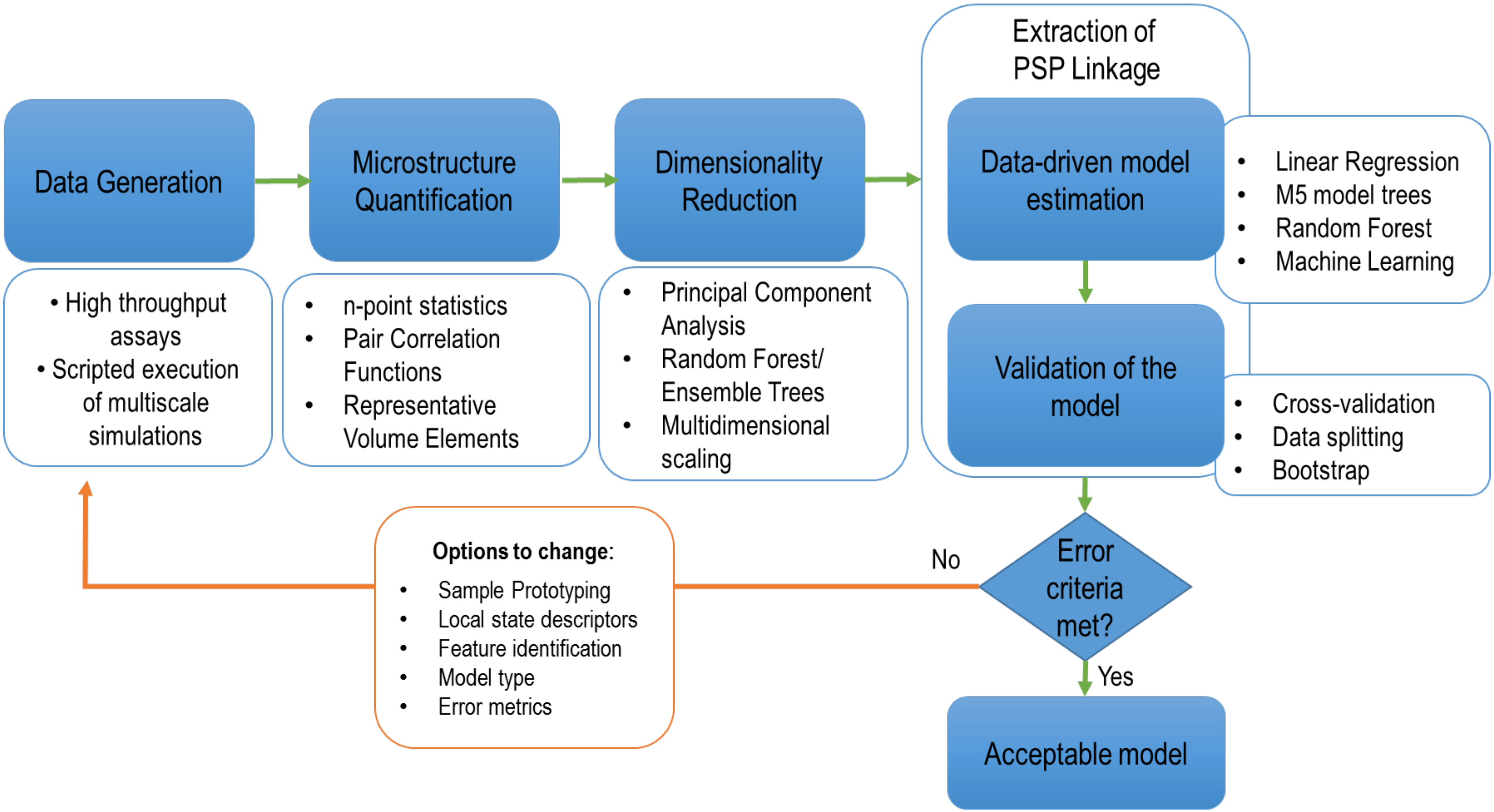


$$\widehat{f_r} = \overline{f_r} + 7.95\varphi_{1r} + 0.46\varphi_{2r} + 0.78\varphi_{3r}$$

Microstructure ($\boldsymbol{\mu}$) = (7.95, 0.46, 0.78)

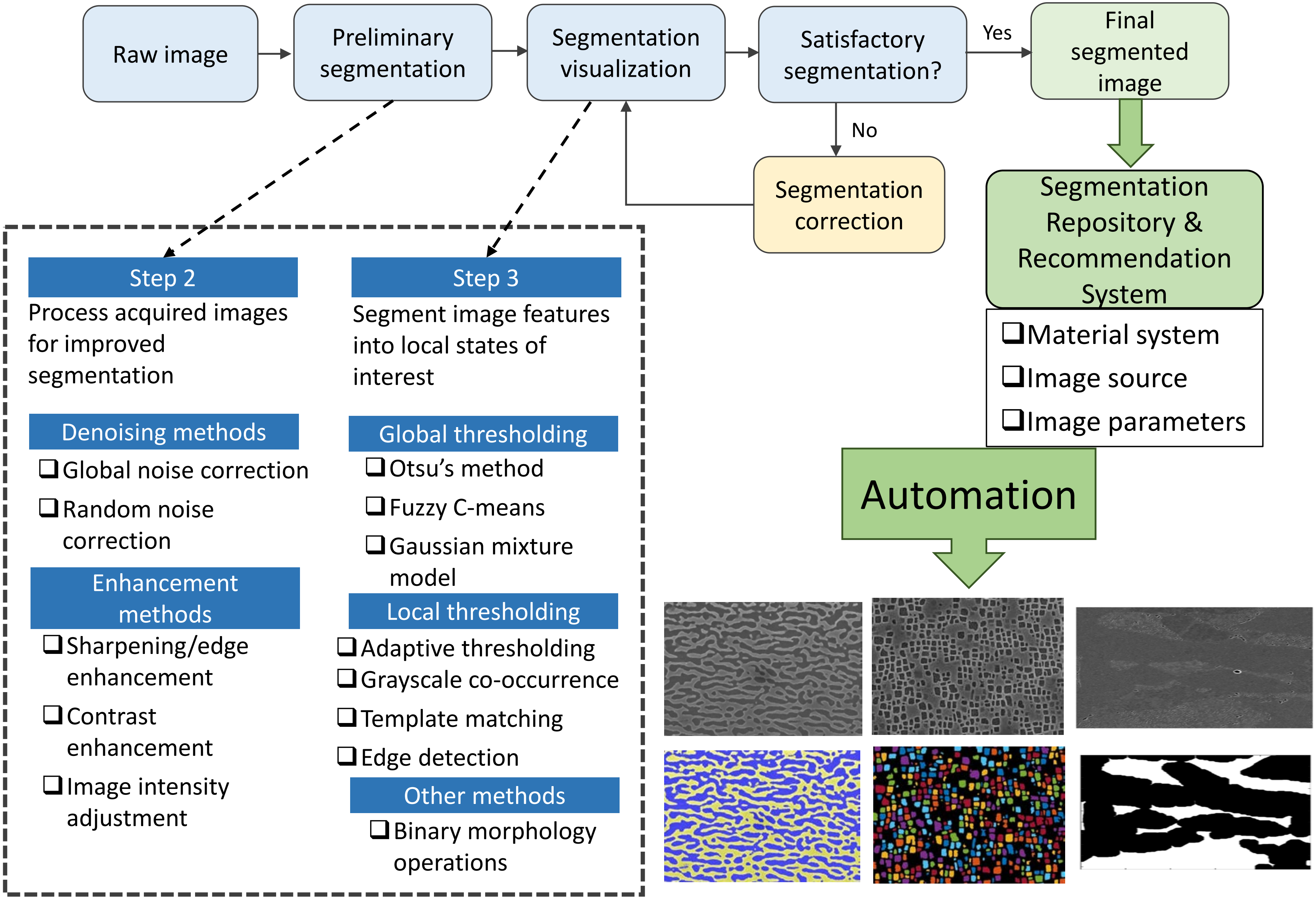
S. R. Kalidindi, "Hierarchical Materials Informatics", Butterworth Heinemann, 2015.

Templated Workflows for Extracting PSP Linkages



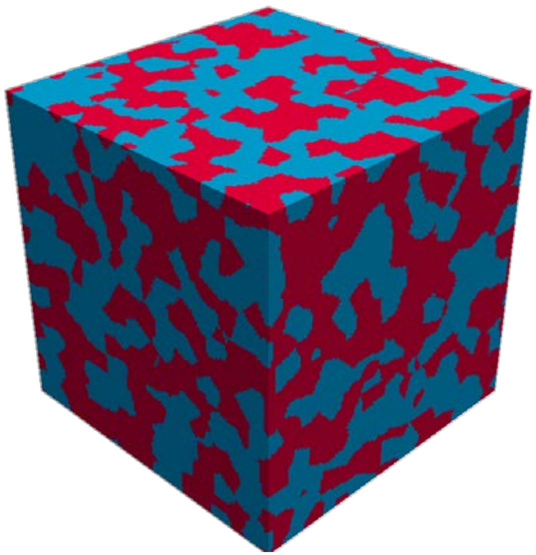
PyMKS (www.pymks.org) ~ 4000 downloads in last 12 months
https://github.com/ahmetcecen/MATLAB-Spatial-Correlation-Toolbox

Image Analyses Workflow



MKS Homogenization for Multiphase Plasticity

Latypov and Kalidindi, *Journal of Computational Physics*, **346**, pp. 242–261, 2017
Latypov et al., *Computer Methods in Applied Mechanics and Engineering*, **346**, pp. 180-196, 2019



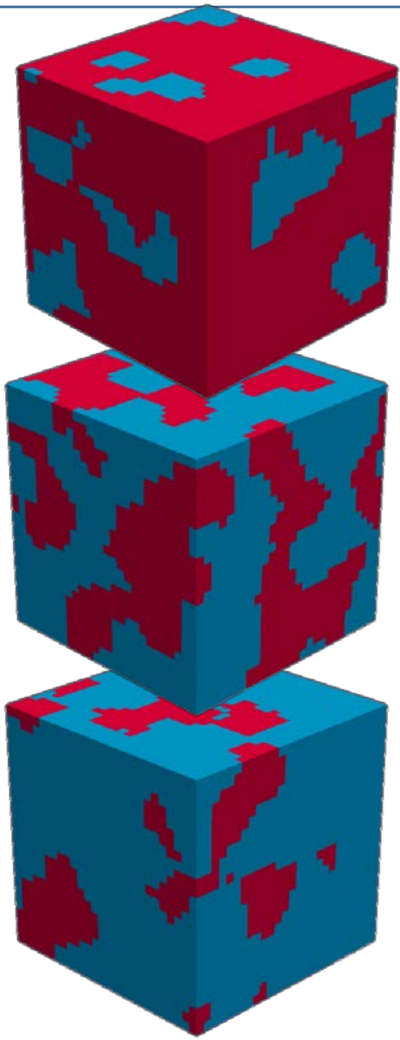
- **MKS Homogenization Framework**
- **Effective Yield Strength**
- **Partitioning of the imposed strains among the microscale constituents**
- **Single database for a broad range of contrasts**

$$\begin{pmatrix} L_{11} & 0.0 & 0.0 \\ 0.0 & -L_{11}/2 & 0.0 \\ 0.0 & 0.0 & -L_{11}/2 \end{pmatrix}$$

Isotropic perfectly-plastic
YS2:YS1 = **2**:1 … **10**:1

Prediction of Composite Stress-Strain Responses

Inputs

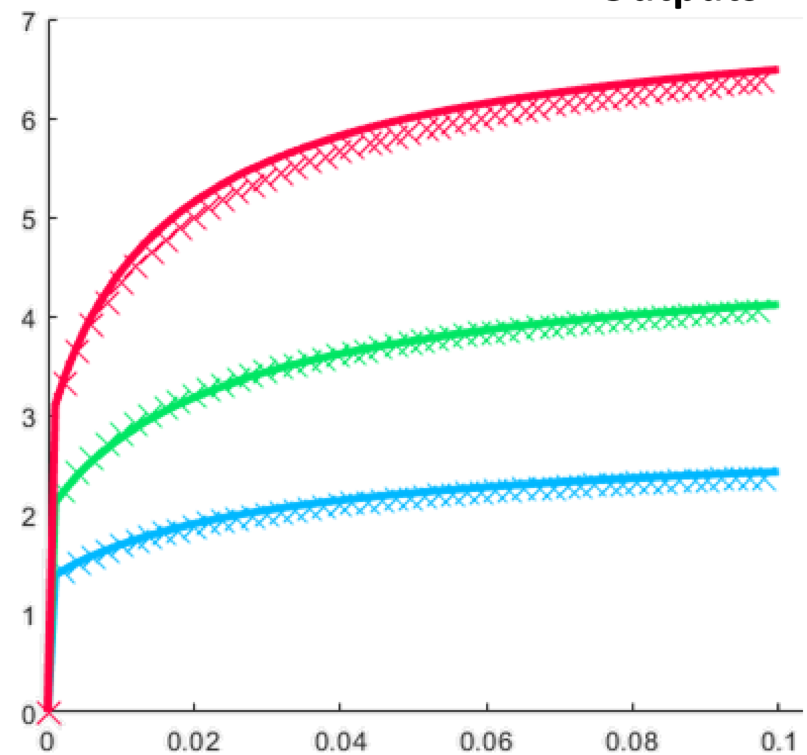


$$\dot{g_\alpha} = h_\alpha(g)\dot{\epsilon_\alpha}$$
$$\dot{g_\beta} = h_\beta(g)\dot{\epsilon_\beta}$$

User-specified hardening laws for each phase

3-D Microstructure

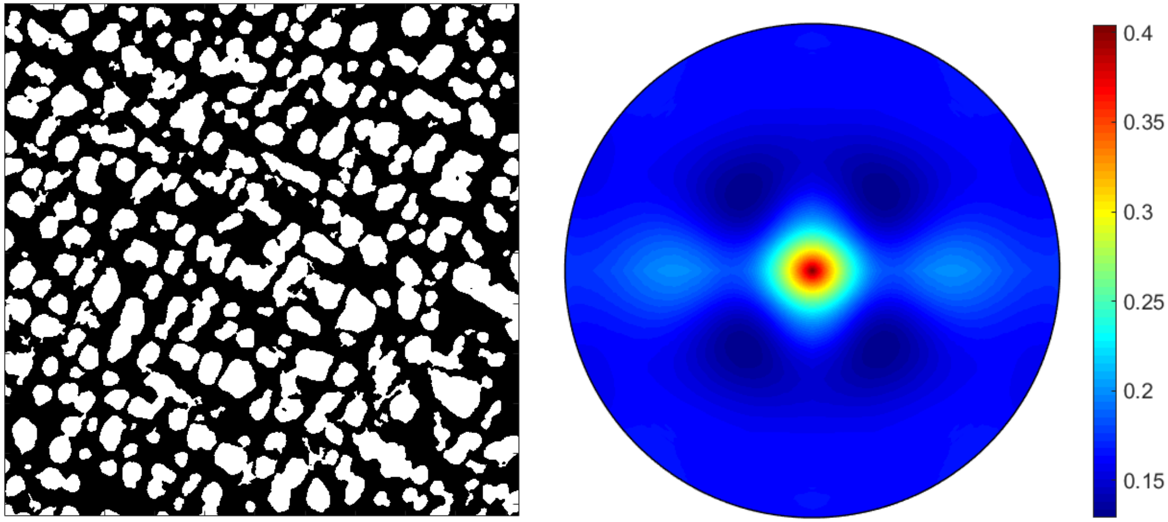
Outputs



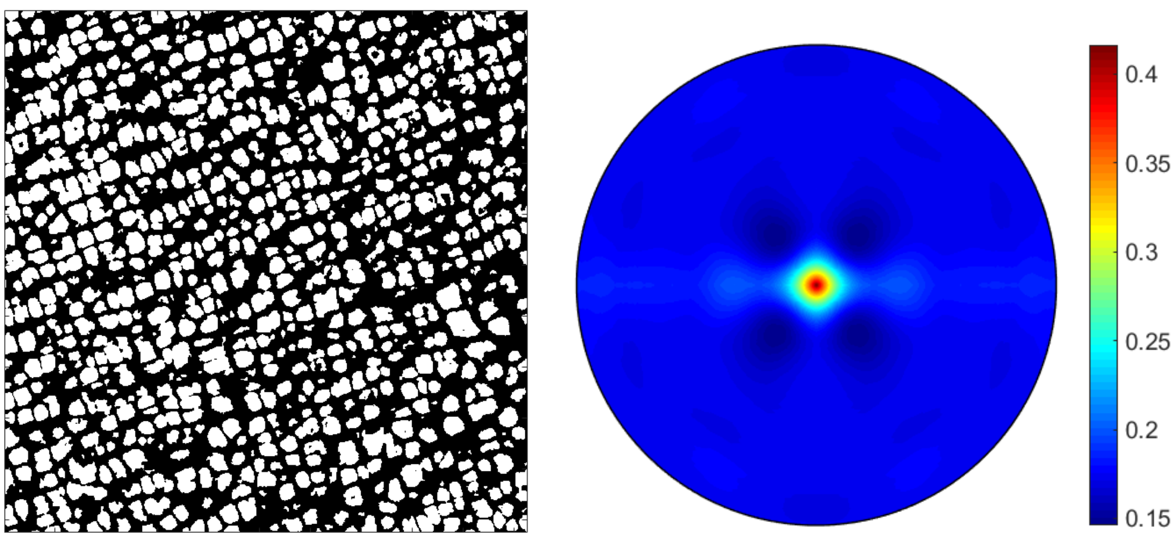
CPU Time	MKS	**0.5 s**
	FEM	up to ~24 hrs

Process-Structure Linkages in Superalloys

Sample 25



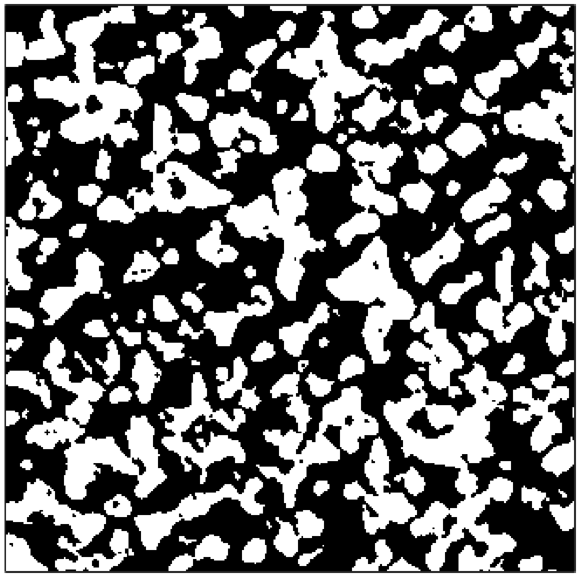
Sample 3

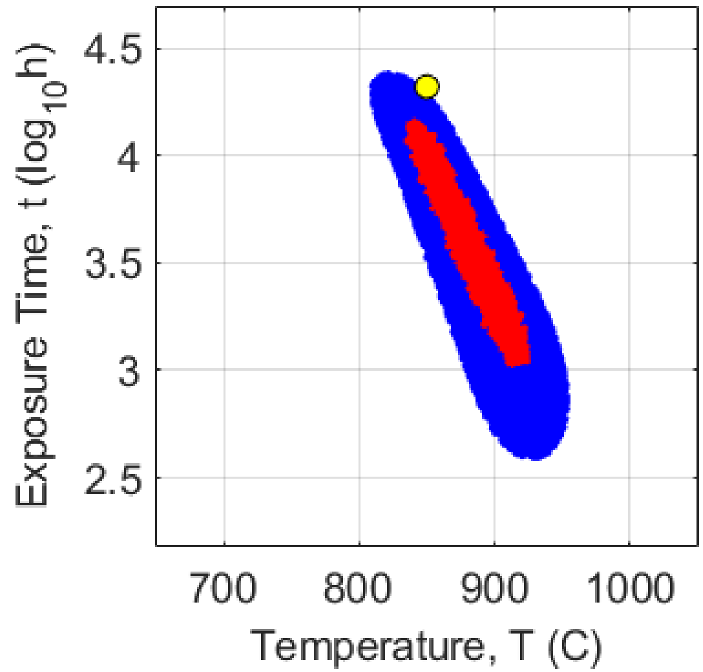


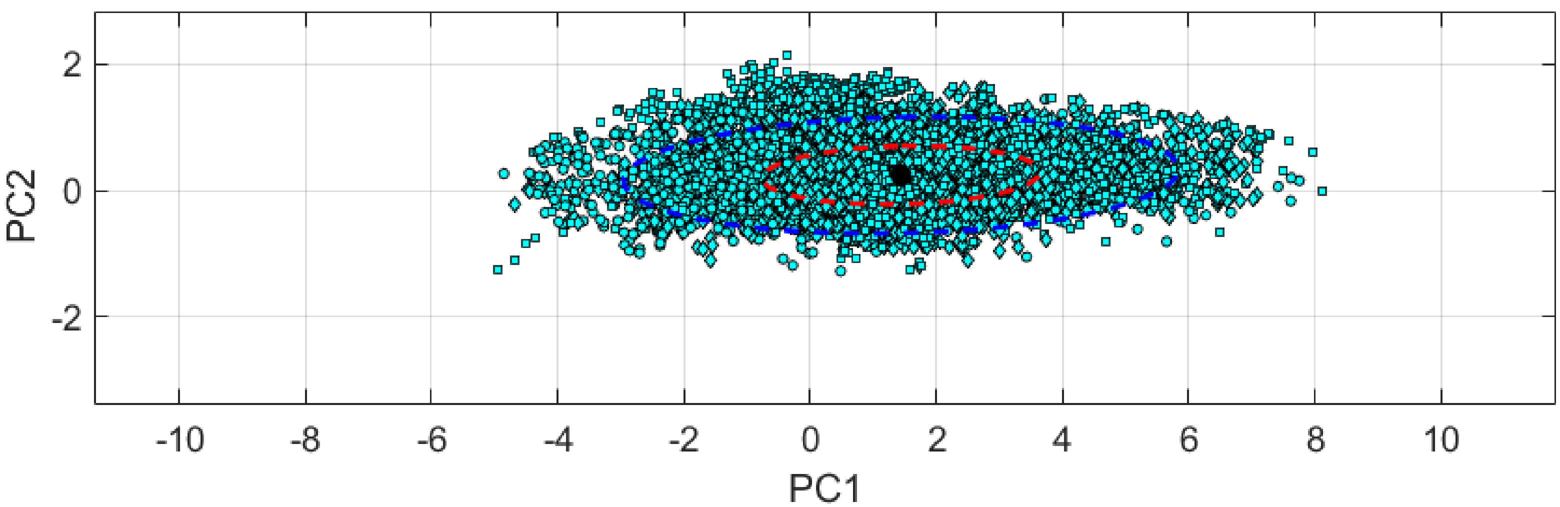
Sample index	Temperature (C)	Time (scaled)
1	700	0.40
2	700	0.52
3	700	0.72
4	700	0.95
5	750	0.70
6	750	1.00
7	800	0.25
8	800	0.49
9	800	0.70
10	800	0.89
11	800	0.97
12	850	0.24
13	850	0.39
14	850	0.59
15	850	0.90
16	900	0.22
17	900	0.23
18	900	0.45
19	900	0.69
20	900	0.91
21	900	0.97
22	950	0.00
23	950	0.47
24	950	0.73
25	1000	0.36
26	1000	0.48
27	1000	0.70

Process-Structure Linkages in Superalloys: Inverse Solutions Using MCMC Sampling

Unknown Sample

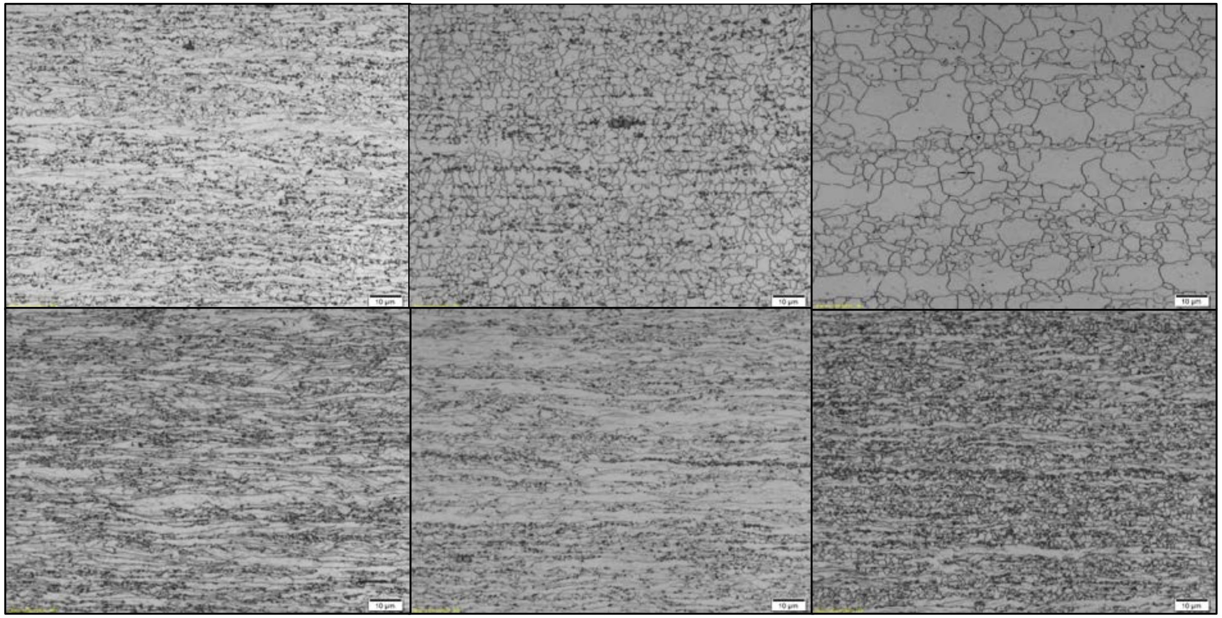






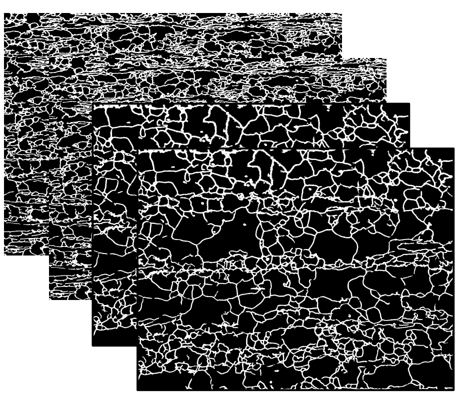
Correlation of Images to Properties

Optical Images of Steel Samples

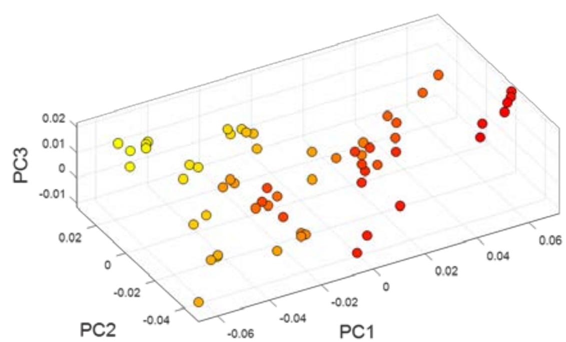


#	ID	Average Rp0.2/ Mpa	Average Rm/ Mpa
1	T414	641.7575	696.31
2	T415	586.542	660.74
3	T416	602.3725	674.29
4	T417	536.0675	612.84
5	T418	511.0605	602.14
6	T419	766.784	796.88
7	T420	700.0695	744.43
8	T421	684.925	734.82
9	T422	649.955	705.84
10	T423	648.257	705.37
11	T424	601.227	666.12
12	T433	606.2115	672.81
13	T425	594.326	661.46
14	T426	583.0125	658.73
15	T427	574.538	656.16
16	T428	862.9575	877.12
17	T429	676.478	720.55
18	T430	669.9825	731.06
19	T431	646.828	726.19
20	T432	933.7515	944.85

Image Segmentation

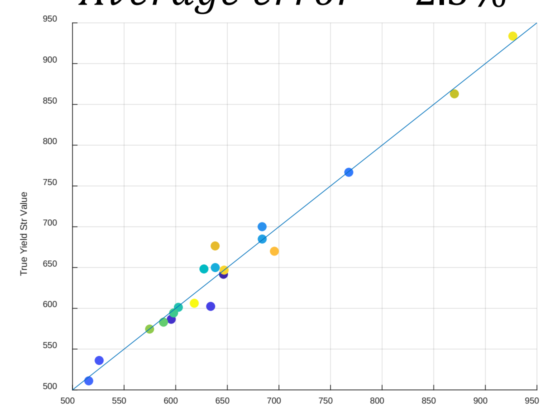


Reduced-Order Microstructure Representation

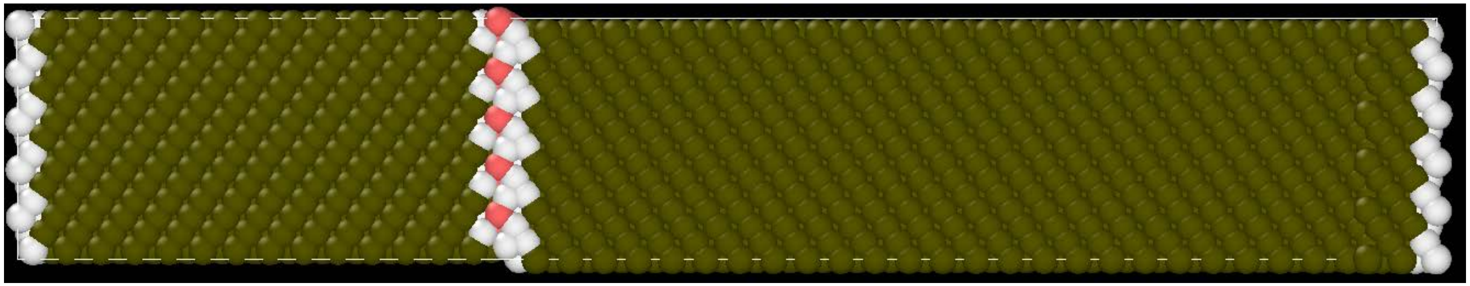


Reduced-Order Model

$Average\ error = 2.5\%$



atomMKS: Application to Grain Boundary Structures



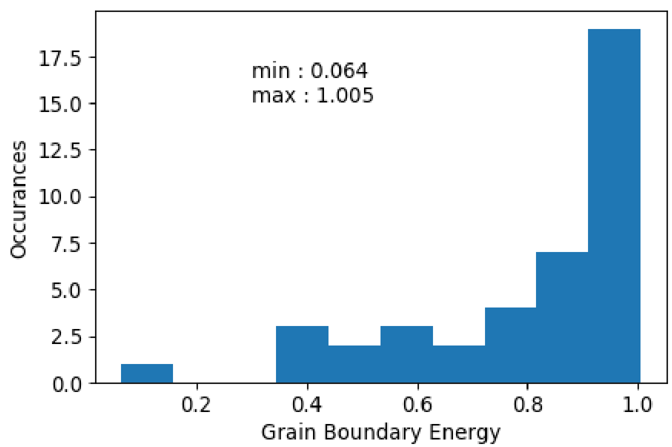
✓	Other	910	5.6%	0
✓	FCC	15275	93.6%	1
✓	HCP	130	0.8%	2
✓	BCC	0	0.0%	3
✓	ICO	0	0.0%	4

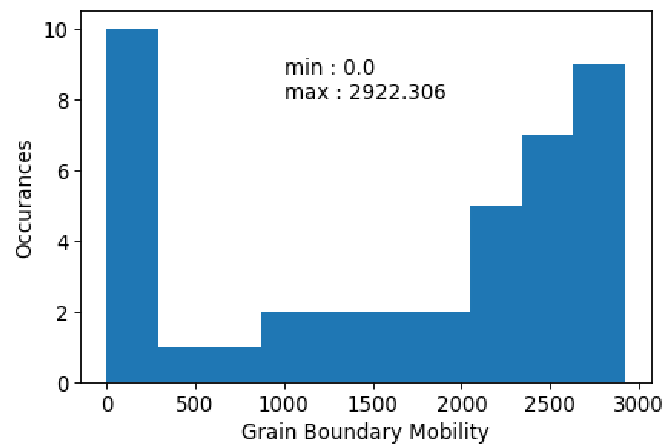
Grain boundary atoms identified using Common Neighbour Analysis. Atoms other than FCC constitute grain boundary.

Material: Ni (FCC)
Properties of Interest:

- Grain Boundary Energy
- Mobility

41 types of sigma-3 Grain Boundaries and associated property values provided.

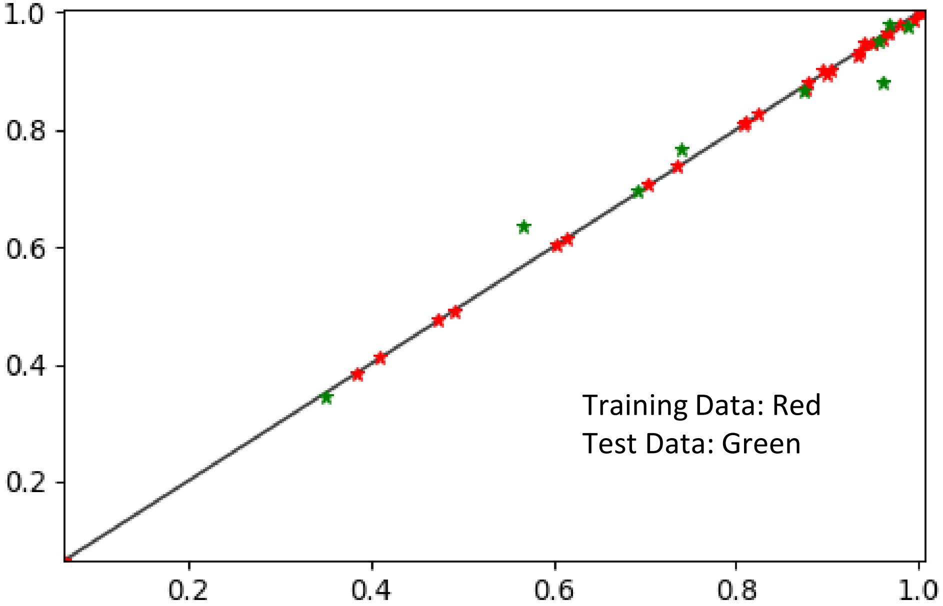




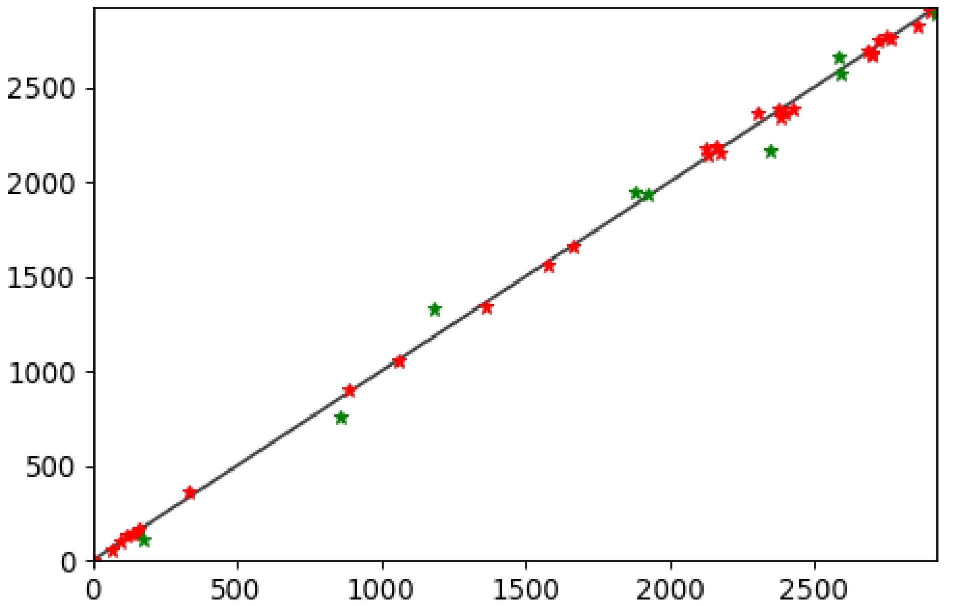
Collaboration with Prof. Fadi Abdeljawad, Clemson University

atomMKS: Reduced-order Models Using Ridge-Regression on PC Scores

Grain Boundary Energy



Grain Boundary Mobility

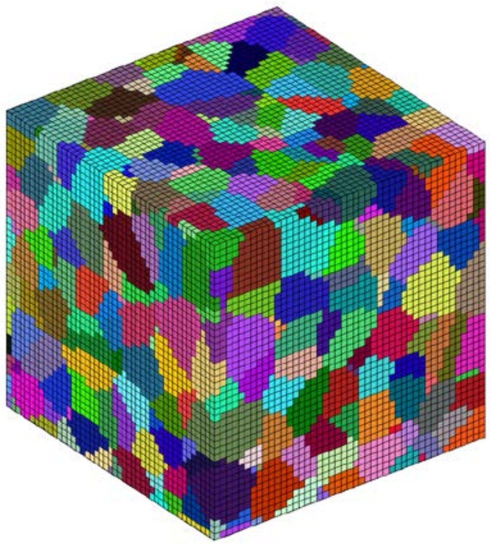


RMS Error: 0.037 J/m^2

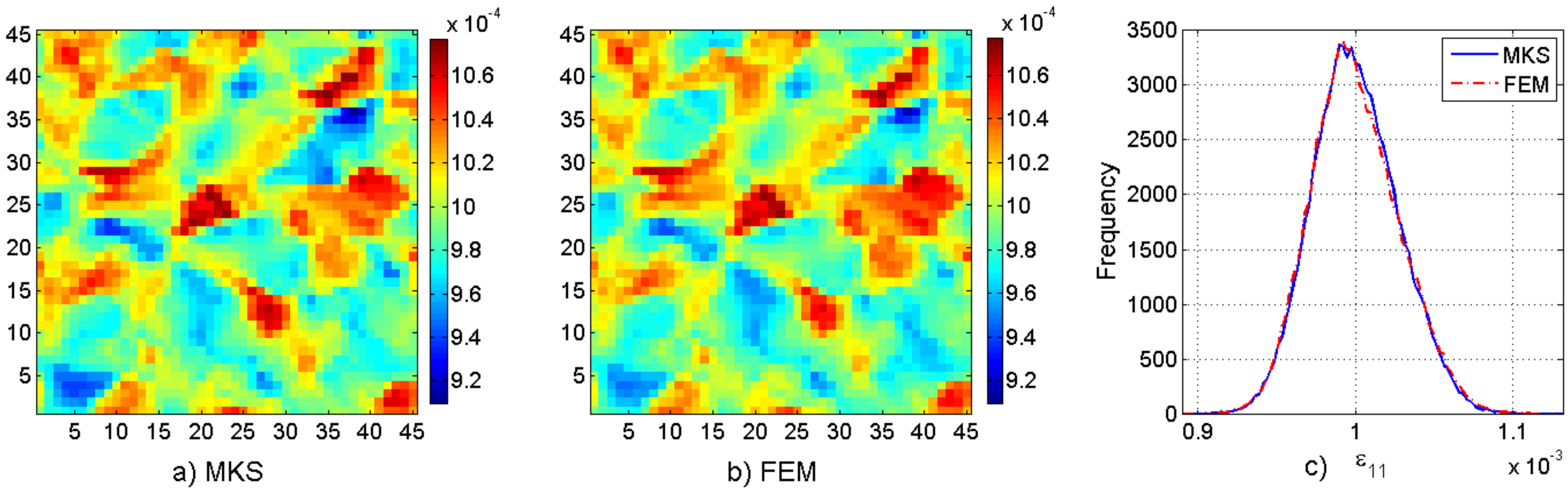
RMS error: 96.39 m/(s GPa)

Stress Fields in Polycrystals

Yabansu and Kalidindi, *Acta Materialia*, **94**, pp. 26–35, 2015



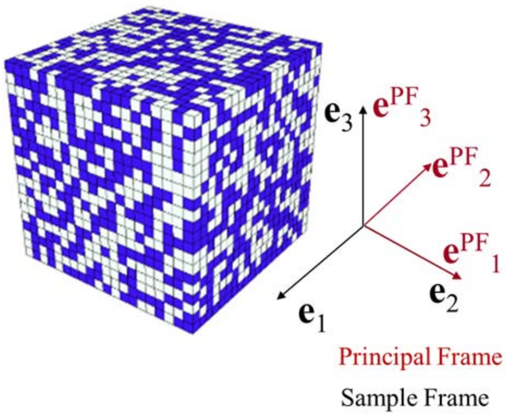
- 45 x 45 x 45 Microstructure. Each color represents a distinct crystal lattice orientation randomly selected from cubic FZ.
- FEM prediction: 3 minutes with 16 processors on a supercomputer
- MKS prediction: 30 seconds with only 1 processor on a standard desktop computer

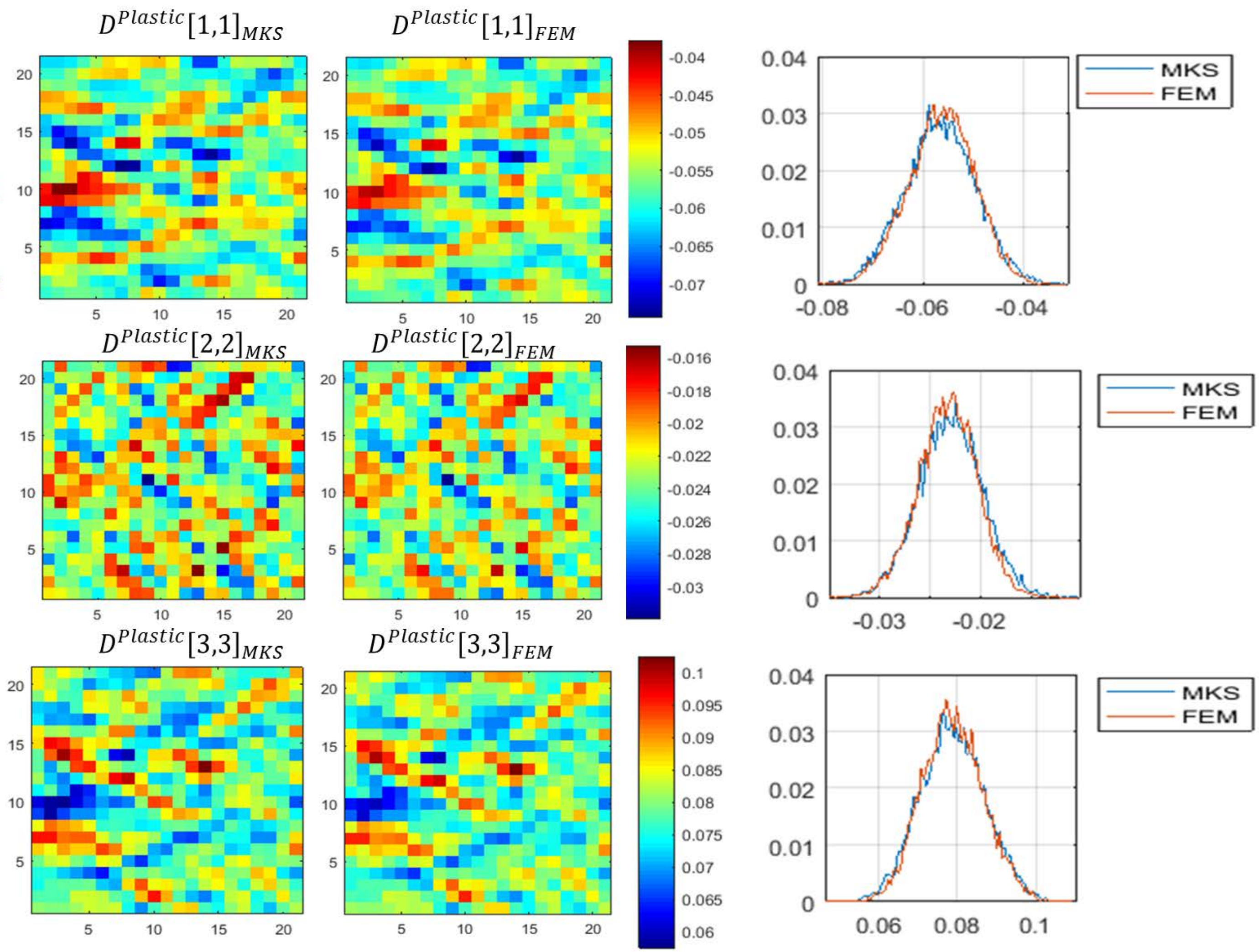


a) MKS b) FEM c)

Plastic Strain Rates in Two-Phase Composites

Montes De Oca Zapiain et al., *Acta Materialia,* 2017





For a 43X43X43 RVE the FEM analysis required 15 hours on a one 2.4 GHz AMD processor node in the Georgia Tech super computer cluster, while the MKS predictions were obtained in 306.5 seconds on the same resource.

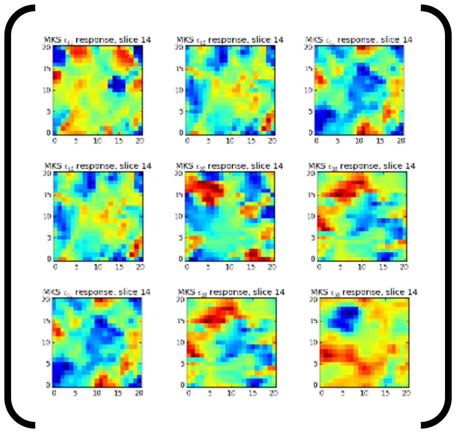
Ranking for Fatigue Performance

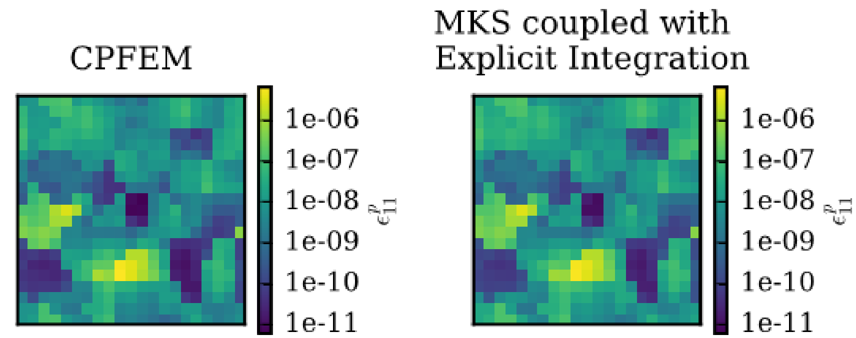
Paulson, Priddy, McDowell, Kalidindi, Materials and Design, 154, 2018

Predict $\boldsymbol{\varepsilon}_{total}$ using MKS localization

$\boldsymbol{\varepsilon}_{total} \rightarrow$

0.5% applied strain amplitude



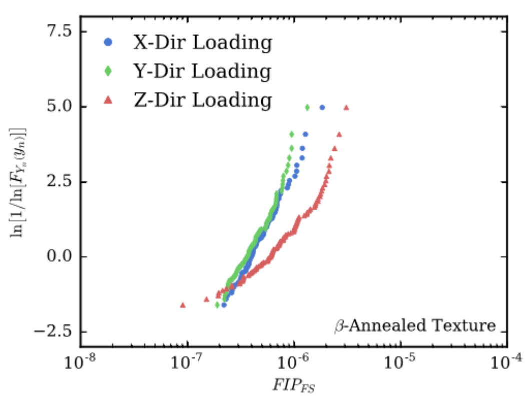


Estimate $\boldsymbol{\varepsilon}_{plastic}$ $\mathbf{(post-analyses)}$

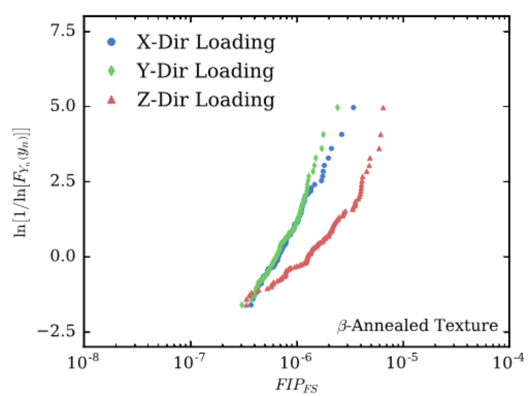
Construct distribution of extreme fatigue indicator parameters (FIPs)

$$FIP_{FS} = \frac{\Delta\gamma^{p}_{max}}{2}\left(1 + k\frac{\sigma^{n}_{max}}{\sigma_{y}}\right)$$

MKS + Explicit Integration



CPFEM



New protocol is **40X faster** than traditional protocols for ranking new microstructures for fatigue resistance

High-Throughput “Autonomous” Experiments

Macroscale

- Current protocols for materials testing need significant amounts of material produced with a consistent processing history.
- Standardized testing (e.g., tension tests) require significant effort in making samples.
- Current protocols are not suitable for rapid screening of the extremely large materials design space (this is the product space that includes all chemical compositions and process histories of interest).

Microscale

- A extremely large amount of experimental data is needed to calibrate multiscale materials constitutive models.
- Current protocols require sophisticated equipment, incur significant time and cost, and produce only limited amount of data.

Critically need high throughput, cost-effective, protocols for multiresolution mechanical measurements at different material structure/length scales.

Spherical nanoindentation stress-strain curves

$$P = \frac{4}{3} E_{eff} R_{eff}^{\frac{1}{2}} h_e^{\frac{3}{2}}$$

$$S = \frac{dP}{dh_e} = 2aE_{eff}$$

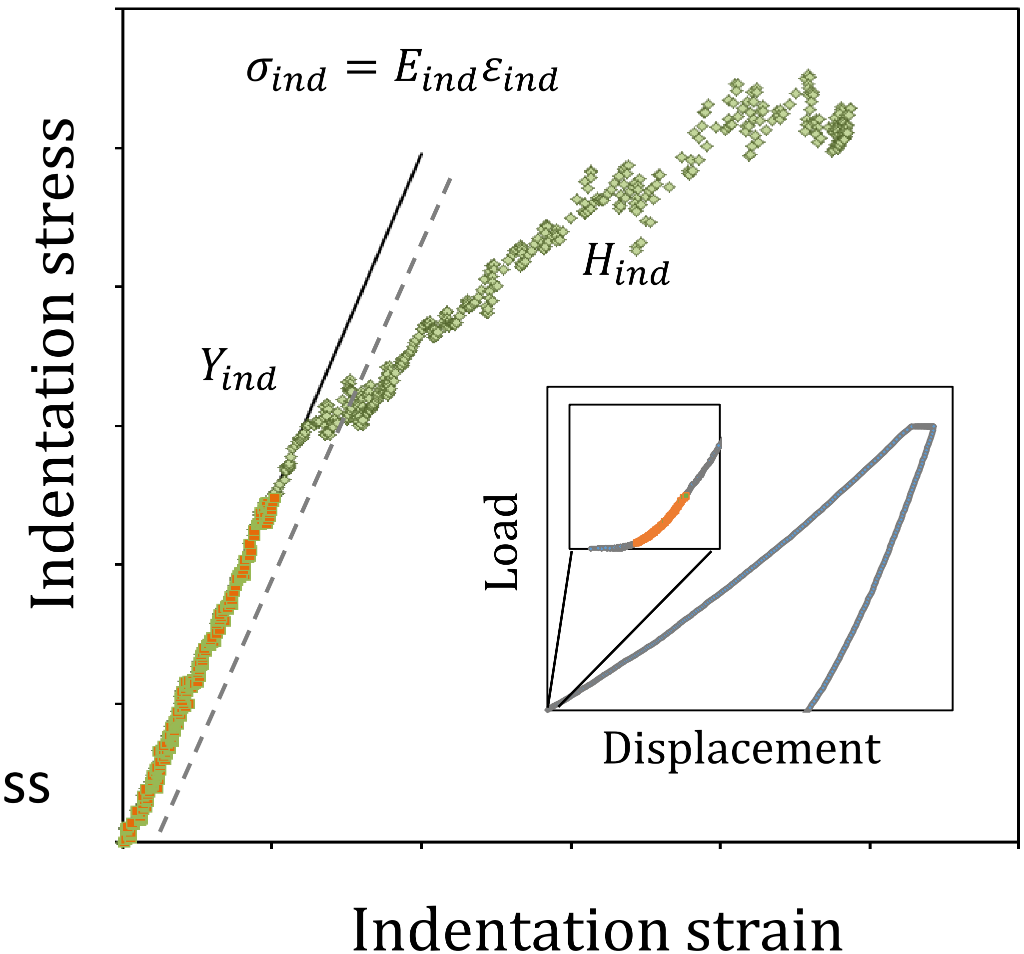
$$\sigma_{ind} = \frac{P}{\pi a^2}$$

$$\varepsilon_{ind} = \frac{4}{3\pi}\frac{h}{a}$$

S: elastic unloading stiffness

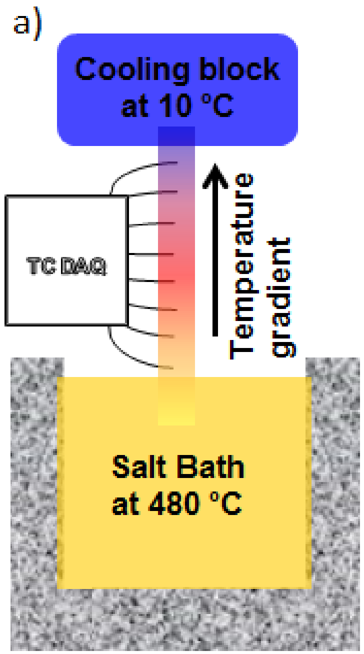
σ_{ind}: indentation stress

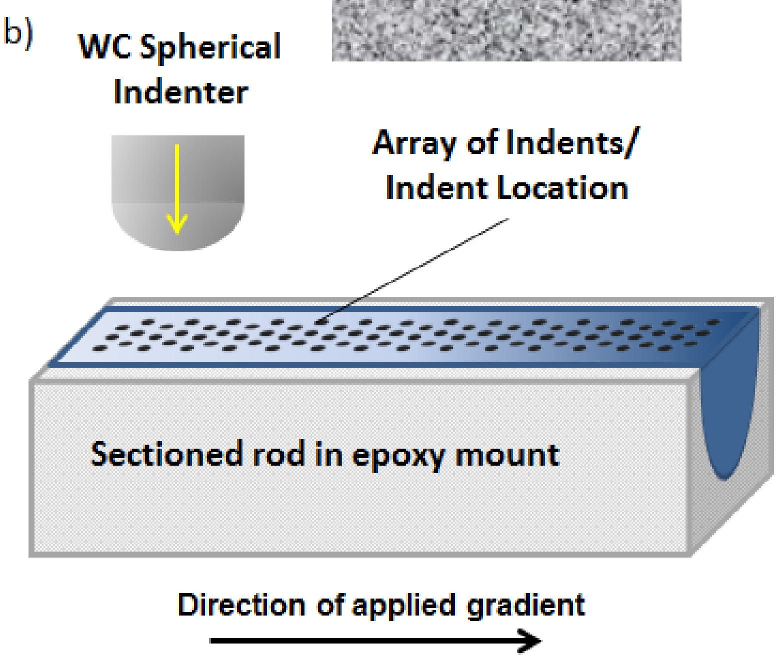
ε_{ind}: indentation strain

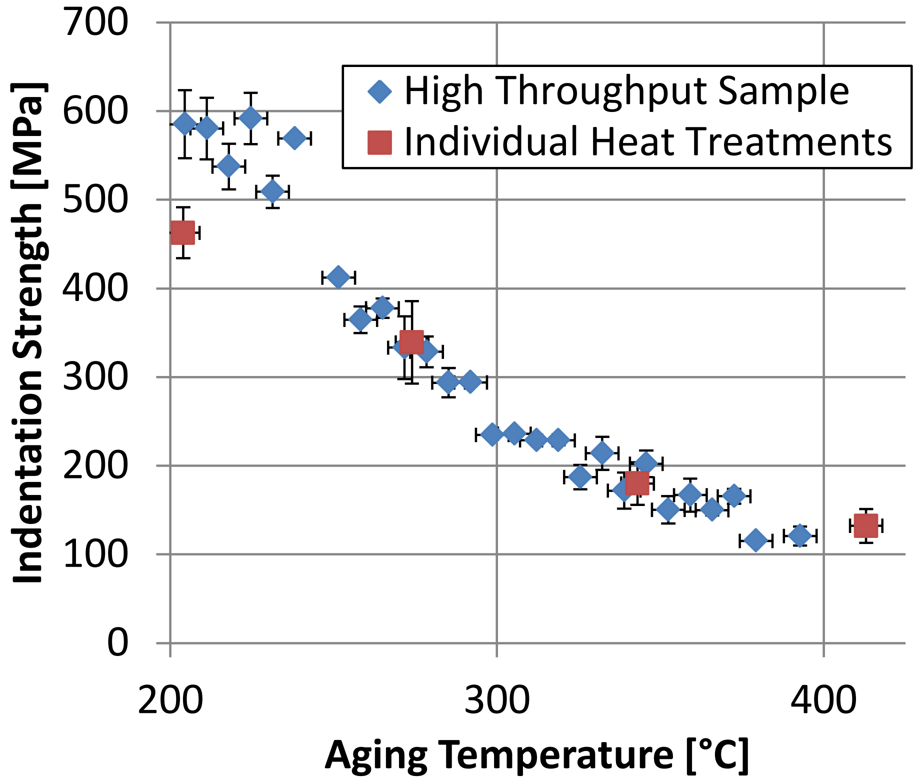


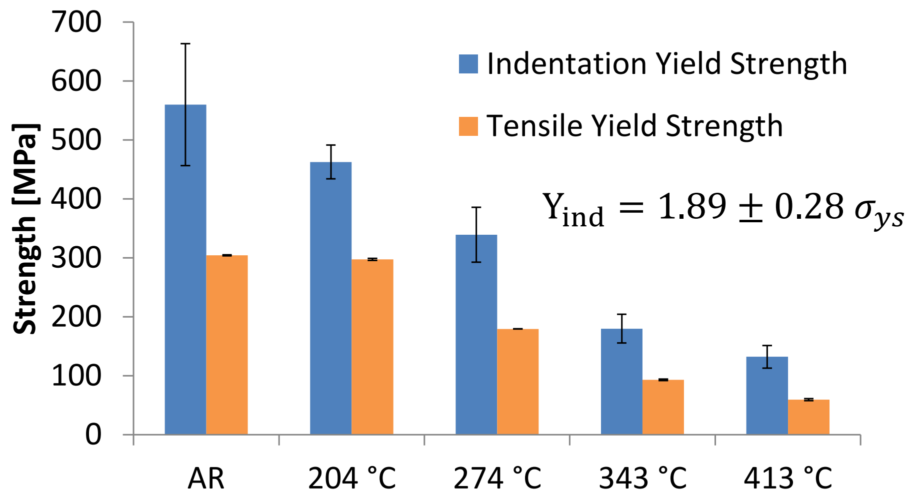
S.R. Kalidindi and S. Pathak. Acta Mat., 2008.

Applications to Rapid Screening of Process Space

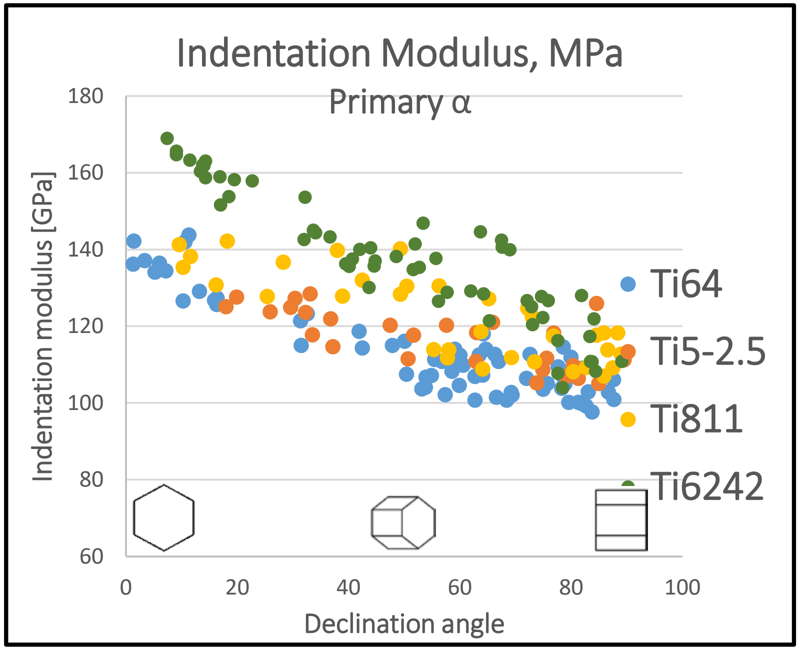


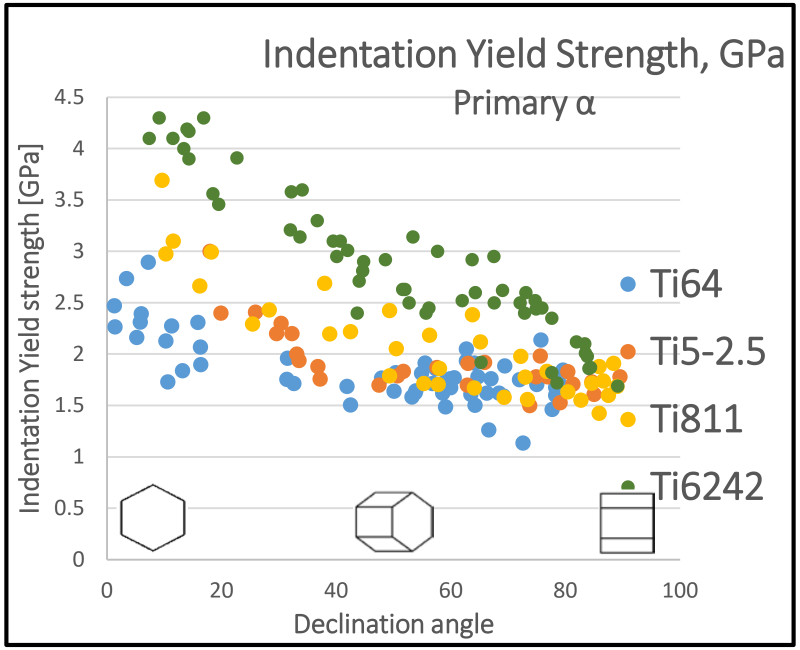






Orientation Dependence of Indentation Properties of primary α in Ti alloys

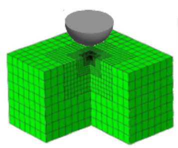




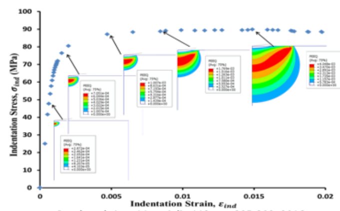
Estimation of Intrinsic Single Crystal Properties from Indentation Measurements

Step 1.

FEM Prediction of Indentation Property*

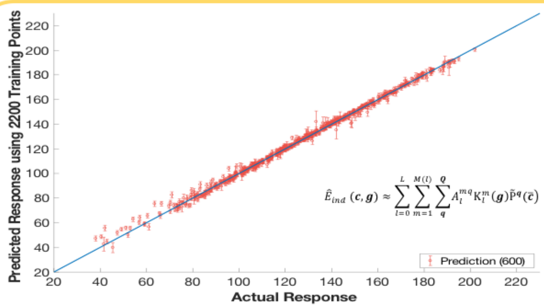


*For a given set of crystal level properties

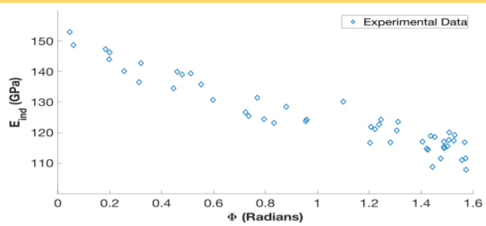


Patel et al. Acta Materialia 112, pp. 295-302, 2016.

High Fidelity Surrogate Model



Experimental Measurements

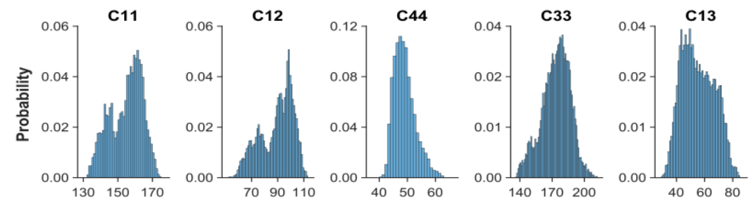


Weaver et al., *Acta Materialia*, 117, pp. 23-34, 2016.

Step 2.

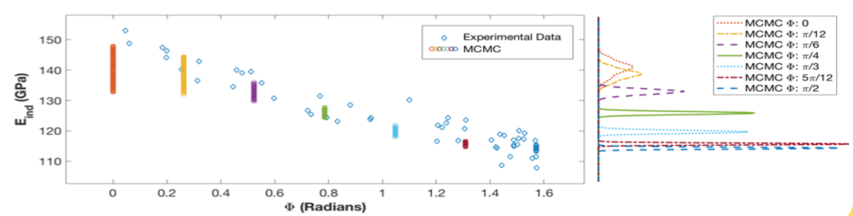
Estimation of Crystal Level Properties with Critical Evaluation of Uncertainty (e.g. Elastic Constants for CP-Ti)

1. Identify estimations with high confidence



	C11	C12	C44	C33	C13
MAP (GPa)	161.5	98.5	47.5	179.5	49.5
Mean (GPa)	154.9	89.3	49.0	173.7	55.3
STDEV	9.3	12.6	3.8	13.2	11.5

2. Identify areas which reflect high uncertainty



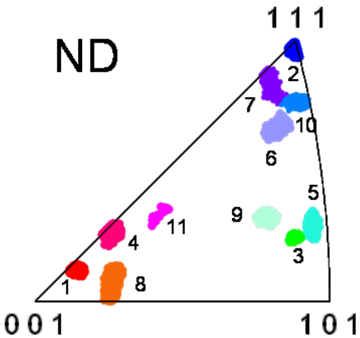
Estimation of CRSS Values in BCC Polycrystal Samples

As-cast Fe3%Si

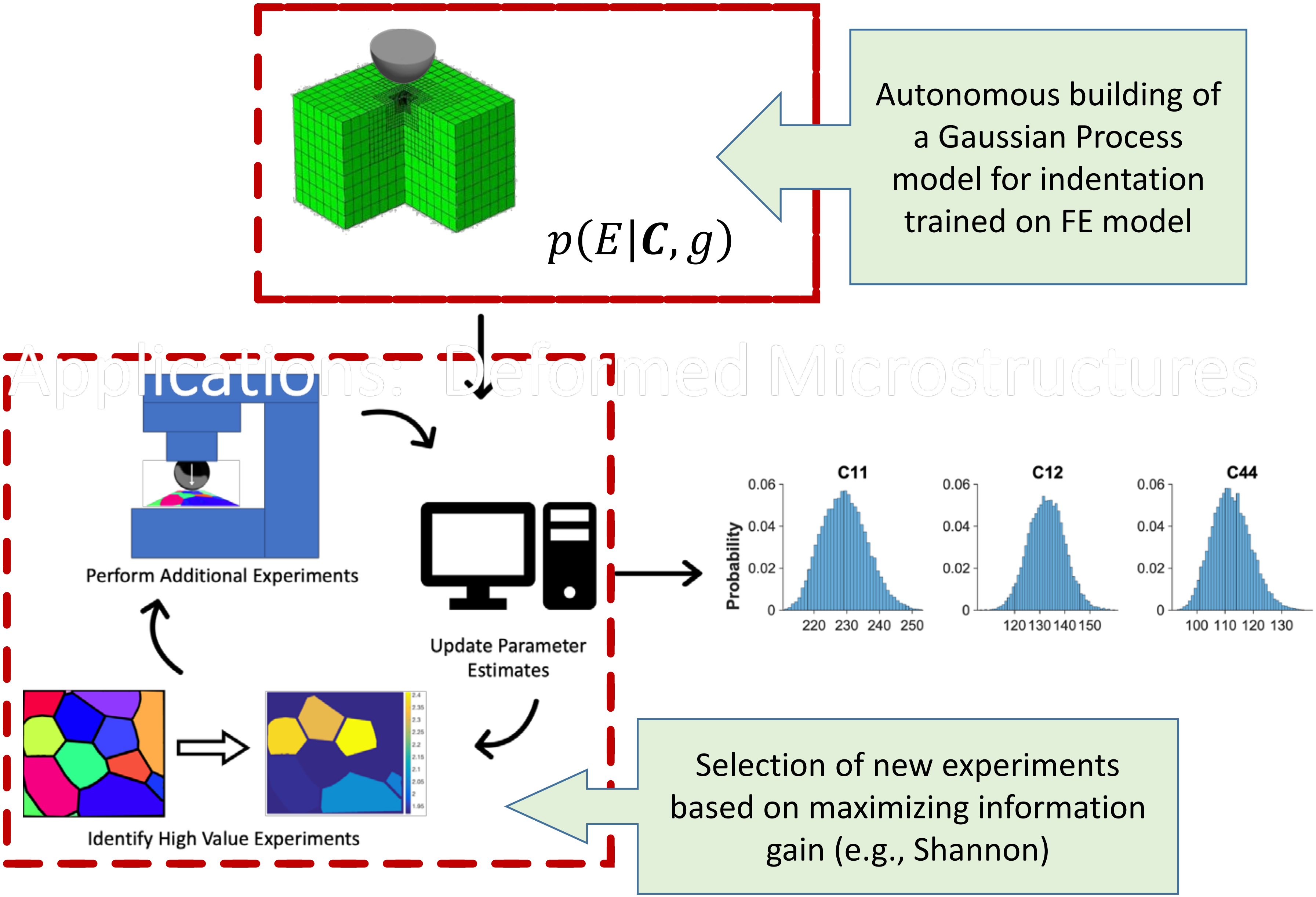
Orientation ($\varphi_1, \Phi, \varphi_2$)	**Experimental#** Y_{ind} **(GPa)**
339.8, 54.4, 46.1	1.13 ± 0.04
103.7, 121.6, 49.9	1.12 ± 0.02
232.5, 53.1, 324.0	1.12 ± 0.16
83.2, 125.4, 30.4	1.10 ± 0.02
3.0, 41.3, 76.4	1.09 ± 0.04
194.7, 79.7, 317	1.07 ± 0.01
50.0, 38.1, 250.1	1.06 ± 0.02
114.2, 85, 173.5	0.85 ± 0.04
170.0, 102.6, 357.9	0.91 ± 0.06
163.6, 78.8, 168	0.93 ± 0.04
259.9, 238.0, 145.8	1.0 ± 0.06

$$Y_{ind}(s, \Phi, \varphi_2) = s \sum_{l=0}^{\infty} \sum_{m=1}^{M(l)} A_l^m \dot{K}_l^m (\Phi, \varphi_2)$$

	s (MPa)
Literature	146.12 to 161
Model Prediction	155.4 ± 3.5



Sequential Design of Experiments



HT Ductility Screening Using Small Punch Tests

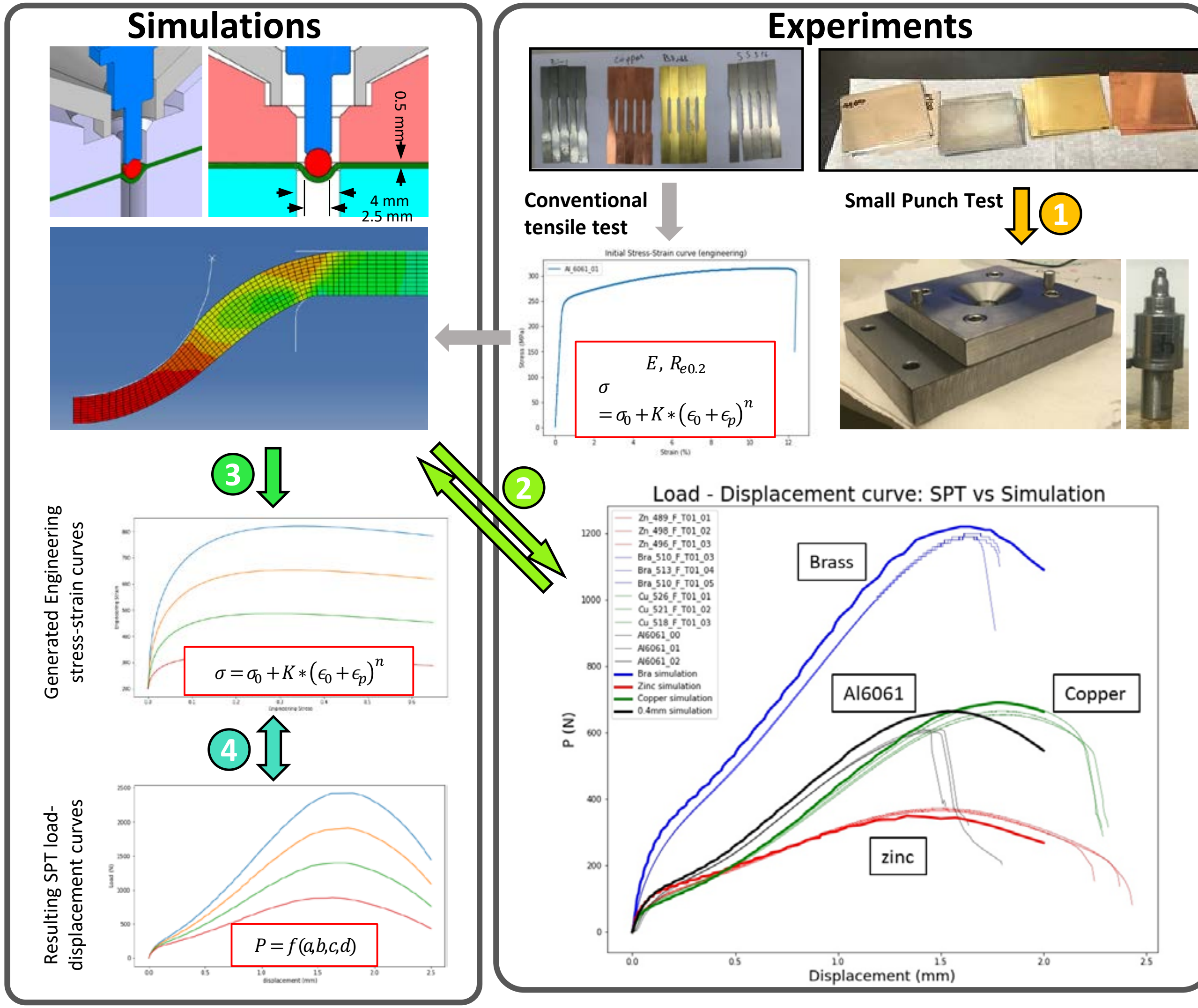
1
- Design of an experimental Small Punch Test setup

2
- Calibration of a numerical (FE) model with experimental measurements on a variety of different metals

3
- Generation of SPT data over a wide range of hypothetical material property sets using the numerical model

4
- Building correlations between Tensile properties $(\sigma_0, K, \epsilon_0, n)$ and SPT curves parameters (a,b,c,d)
- Develop inverse solution methodology for estimating $(\sigma_0, K, \epsilon_0, n)$ from measured (a,b,c,d)

5
- Development of an optimized apparatus for high speed testing: automation and parallelization



Summary Statements

- A physics-centered Bayesian framework can serve as a foundational element in the design and build of AI-based materials knowledge systems that can provide objective decision support in all aspects of materials innovation.
- High-throughput experimental and computational protocols are critically needed to generate the data needed to feed the envisioned knowledge systems.