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The multifaceted nature of uncertainty in structure-property linkage with crystal plasticity finite element model

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Sandia National Laboratories

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TMS 2023 Annual Meeting & Exhibition

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Acknowledgment

Joint works with

- Pieterjan Robbe (SNL)
- Tim Wildey (SNL)
- David Montes de Oca Zapiain (SNL)
- Hojun Lim (SNL)

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Introduction

Uncertainty is ubiquitous in microstructures and structure-property linkage with ICME models.

Sources of uncertainty:

- aleatory uncertainty (irreducible):
  - natural randomness of microstructures
- epistemic uncertainty (reducible):
  - numerical approximation in numerical solvers
  - model-form error, e.g. lack of modeling for internal state variables
  - model discrepancy – disagreement between experiment and computation
  - plasticity constitutive modeling assumptions
  - mesh discretization

UQ in CPFEM: why is it interesting?

- stochastic: RVE
- deterministic: RVE, constitutive models, solvers

(1) High-throughput model calibration under microstructure-induced uncertainty

(joint work w/ Hojun Lim)

Reference

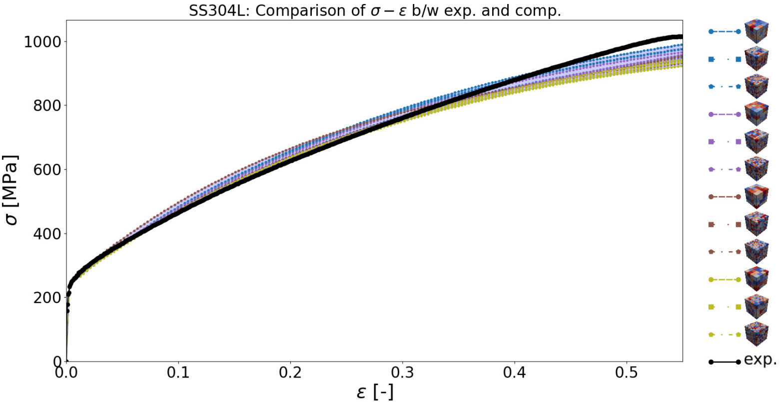
Anh Tran and Hojun Lim (2023). "An asynchronous parallel high-throughput model calibration framework for crystal plasticity finite element constitutive models". In: *Computational Mechanics* (accepted)

Summary:

- calibrate constitutive model parameters in a high-throughput manner
- run *concurrently* more than 20 CPFEM simulations on HPC with scheduler
- using an asynchronous parallel Bayesian optimization workflow (Anh Tran et al. (2022). "aphBO-2GP-3B: a budgeted asynchronous parallel multi-acquisition functions for constrained Bayesian optimization on high-performing computing architecture". In: *Structural and Multidisciplinary Optimization* 65.4, pp. 1–45)
- loss function is a weighted Sobolev norm to account for hardening
- optimize under (microstructure-induced) uncertainty: average loss by Monte Carlo estimator over an ensemble of RVEs
- demonstrate on (1) SS304L, (2) Tantalum, (3) Cantor high-entropy alloy

(1) High-throughput model calibration under microstructure-induced uncertainty

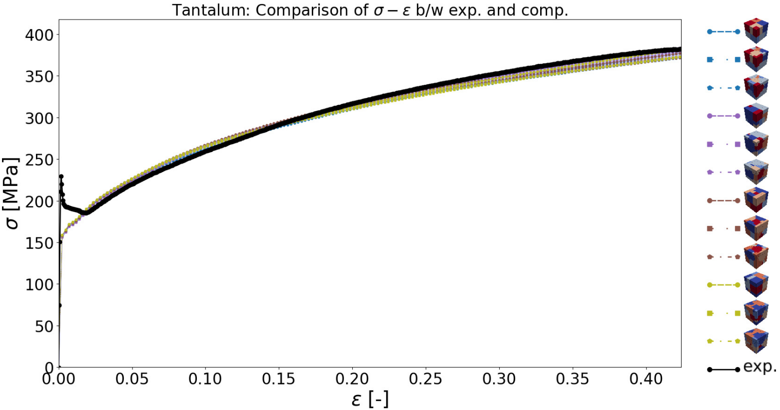
(joint work w/ Hojun Lim)



Comparison of homogenized materials properties between experimental data and computational results for SS304L across different mesh resolutions and for different SERVEs. ☐ material variability. ●: experimental data.

(1) High-throughput model calibration under microstructure-induced uncertainty

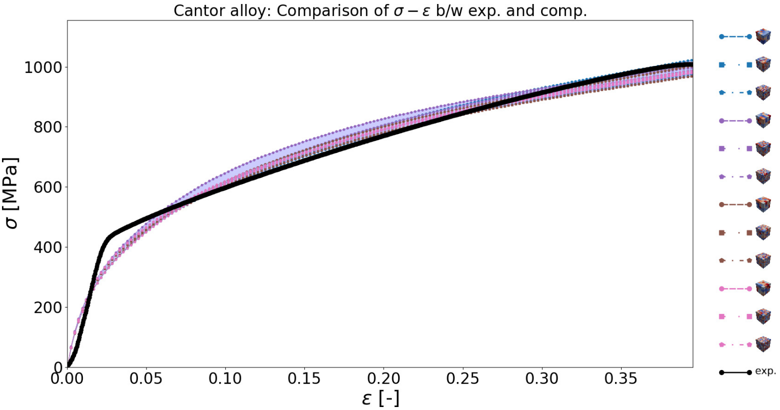
(joint work w/ Hojun Lim)



Comparison of homogenized materials properties between experimental data and computational results for Tantalum across different mesh resolutions and for different SERVEs. ☐ material variability. ●: experimental data.

(1) High-throughput model calibration under microstructure-induced uncertainty

(joint work w/ Hojun Lim)



Comparison of homogenized materials properties between experimental data and computational results for Cantor high-entropy alloy across different mesh resolutions and for different SERVEs. ☐ material variability. ●: experimental data.

(2) UQ of constitutive models

(joint work w/ Tim Wildey, Hojun Lim)

Reference

Anh Tran, Tim Wildey, and Hojun Lim (2022). "Microstructure-sensitive uncertainty quantification for crystal plasticity finite element constitutive models using stochastic collocation method". In: *Frontiers in Materials* 9, pp. 1–20

Summary:

- quantify uncertainty of homogenized σ_Y/ε_Y (initial yield) induced by uncertain constitutive model parameters by stochastic collocation method (Xiu and Karniadakis 2002) (polynomial chaos expansion + sparse grid)
- apply on fcc Cu (phenom model w/o twinning), hcp Mg (phenom model w/ twinning), and bcc W (dislocation-density-based)
- global sensitivity analysis using Sobol' indices

(2) UQ of constitutive models

(joint work w/ Tim Wildey, Hojun Lim)

DAKOTA

Explore and predict with confidence

- uncertainty quantification
- sensitivity analysis

DAMASK

Düsseldorf Advanced Material Simulation Kit

PETSc TAO

- crystal plasticity finite element
- spectral solver via PETSc

DREAM.3D

BlueQuartz Edition

- representative volume element
- grain geometries + orientations

(2) UQ of constitutive models

(joint work w/ Tim Wildey, Hojun Lim)

Generalized polynomial chaos expansion

Dongbin Xiu and George Em Karniadakis (2002). "The Wiener–Askey polynomial chaos for stochastic differential equations". In: *SIAM Journal on Scientific Computing* 24.2, pp. 619–644

The second-order random process $f(\theta)$ can be represented as

$$\begin{aligned} f(\theta) &= c_0 I_0 + \textstyle\sum_{i_1=1}^{\infty} c_{i_1} I_1(\xi_{i_1}(\theta)) \\ &+ \textstyle\sum_{i_1=1}^{\infty} \sum_{i_2=1}^{\infty} c_{i_1 i_2} I_2(\xi_{i_1}(\theta), \xi_{i_2}(\theta)) \\ &+ \textstyle\sum_{i_1=1}^{\infty} \sum_{i_2=1}^{\infty} \sum_{i_3=1}^{\infty} c_{i_1 i_2 i_3} I_3(\xi_{i_1}(\theta), \xi_{i_2}(\theta), \xi_{i_3}(\theta)) + \cdots , \end{aligned} \tag{1}$$

- $I_n(\xi_{i_1}, \cdots, \xi_{i_n})$: the Wiener-Askey polynomial chaos of order n in terms of the random vector $\boldsymbol{\xi} = (\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_n})$
- c's are polynomial chaos expansion coefficients

(2) UQ of constitutive models

(joint work w/ Tim Wildey, Hojun Lim)

Without loss of generality, we can rewrite the previous equation as

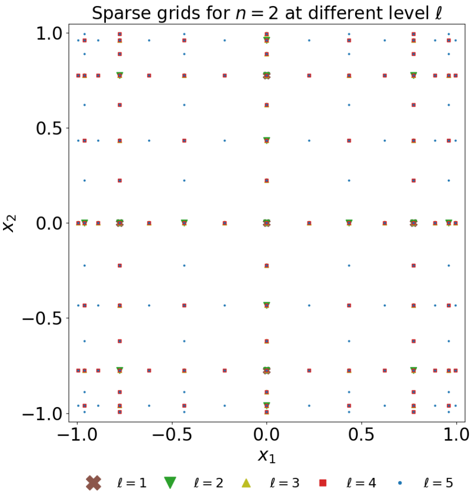
$$f(\theta) = \sum_{j=0}^{\infty} \widehat{f}_j \boldsymbol{\Phi}_j(\boldsymbol{\xi}(\boldsymbol{\theta})), \tag{2}$$

- there is a one-to-one correspondence between the function $I_n(\xi_{i_1}, \cdots, \xi_{i_n})$ and $\boldsymbol{\Phi}_j(\boldsymbol{\xi})$
- $\boldsymbol{\Phi}_j(\boldsymbol{\xi}(\theta))$ are orthogonal polynomials in terms of $\boldsymbol{\xi} := \{\xi_i(\theta)\}_{i=1}^{d}$,
- coefficients are determined by projection, exploiting the fact that $\{\boldsymbol{\Phi}_j\}$ is an orthogonal basis (problem: $\boldsymbol{\xi}$ may be high-dimensional)

$$\widehat{f}_j = \frac{\langle f, \boldsymbol{\Phi}_j \rangle}{\langle \boldsymbol{\Phi}_j, \boldsymbol{\Phi}_j \rangle}. \tag{3}$$

(2) UQ of constitutive models

(joint work w/ Tim Wildey, Hojun Lim)



Comparison of 2D Smolyak nested sparse grids at various level ℓ, $1 \leq \ell \leq 5$, with the number of abscissas varies at 5, 17, 49, 97, 161, respectively, using Gaussian abscissas for quadrature.

(2) UQ of constitutive models

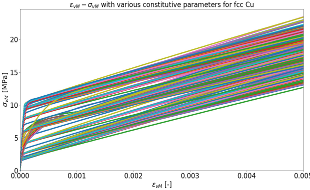
(joint work w/ Tim Wildey, Hojun Lim)

Table: The number of collocation points used by sparse grid and full tensor grid.

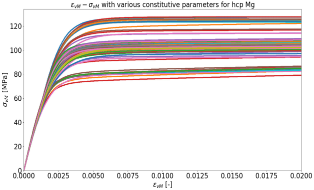
Level ℓ	$n=5$ sparse	$n=5$ full	$n=7$ sparse	$n=7$ full	$n=16$ sparse	$n=16$ full
0	1	1	1	1	1	1
1	11	243	15	2187	33	4.3e+7
2	71	16807	127	823543	577	3.3e+13
3	351	759375	799	170859375	7105	6.5e+18
4	1391	28629151	4047	27512614111	68865	7.2e+23
5	4623	992436543	17263	3938980639167	556801	6.1e+28

(2) UQ of constitutive models

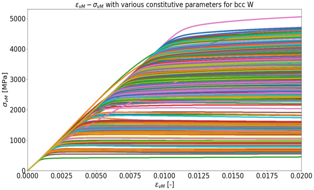
(joint work w/ Tim Wildey, Hojun Lim)



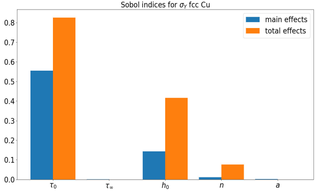
fcc Cu



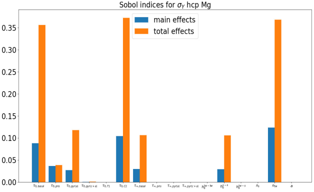
hcp Mg



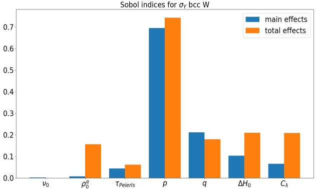
bcc W



Sobol' indices for σ_Y for fcc Cu.



Sobol' indices for σ_Y for hcp Mg.



Sobol' indices for σ_Y for bcc W.

(3) Multi-fidelity UQ for CPFEM

(joint work w/ Pieterjan Robbe, Hojun Lim)

Reference

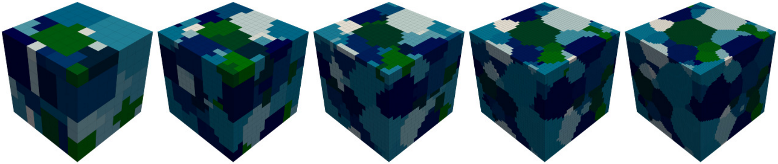
Anh Tran, Pieterjan Robbe, and Hojun Lim (2023). "Multi-fidelity microstructure-induced uncertainty quantification by advanced Monte Carlo methods". In: *Materialia* 27, p. 101705

Summary:

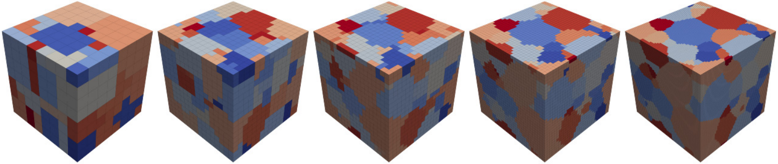
- treat statistically equivalent RVEs (SERVEs) as i.i.d. Monte Carlo samples
- use multi-level Monte Carlo (MLMC) (1-d) and multi-index Monte Carlo (MIMC) (multi-d) to adaptively estimate effective materials property at various levels of fidelity
- MIMC is a generalization of MLMC in multi-dimensional spaces
- fidelity: mesh resolutions and constitutive models

(3) Multi-fidelity UQ for CPFEM

(joint work w/ Pieterjan Robbe, Hojun Lim)



(a) 8^3: DDB. (b) 16^3: DDB. (c) 20^3: DDB. (d) 32^3: DDB. (e) 64^3: DDB.



(f) 8^3: Phen. (g) 16^3: Phen. (h) 20^3: Phen. (i) 32^3: Phen. (j) 64^3: Phen.

Adaptive sampling SERVEs with multiple mesh resolutions and multiple constitutive model using MLMC and MIMC. Top row: dislocation-density-based; Bottom row: phenomenological. Left to right: coarse to fine

(3) Multi-fidelity UQ for CPFEM

(joint work w/ Pieterjan Robbe, Hojun Lim)

References

Michael B Giles (2015). “Multilevel Monte Carlo methods”. In: *Acta Numerica* 24, pp. 259–328; Abdul-Lateef Haji-Ali, Fabio Nobile, and Raúl Tempone (2016). “Multi-index Monte Carlo: when sparsity meets sampling”. In: *Numerische Mathematik* 132.4, pp. 767–806

Multi-level Monte Carlo in the nutshell:

$$\mathbb{E}\left[Q_L(\omega)\right] = \sum_{\ell=1}^{L} \mathbb{E}\left[Q_\ell(\omega) - Q_{\ell-1}(\omega)\right] + \mathbb{E}\left[Q_0(\omega)\right] = \sum_{\ell=0}^{L} \mathbb{E}\left[\Delta Q_\ell(\omega)\right], \quad (4)$$

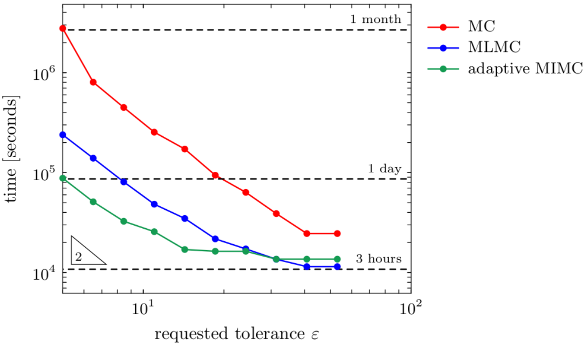
where ω is a RVE realization.

Goal: efficiently estimate homogenized material properties

- by a multi-fidelity approach, exploiting cost-accuracy trade-off
- Equation 4 can evaluate homogenized property of fine mesh with a series of coarser meshes
- by a telescoping sum: Q_L = fine mesh; $Q_\ell (1 \leq \ell \leq L)$: series of coarsening meshes
- $\mathbb{E}\left[\cdot\right]$ to average over a microstructure ensemble (multiple ω) and account for aleatory uncertainty

(3) Multi-fidelity UQ for CPFEM

(joint work w/ Pieterjan Robbe, Hojun Lim)



Yield strength σ_Y: MLMC is $\sim 11.6\times$ faster compared to MC, adaptive MIMC is $\sim 2.7\times$ faster compared to MLMC. Overall speedup $\sim 31.5\times$.

(4) Stochastic inverse problems in structure-property

(joint work w/ Tim Wildey)

Reference

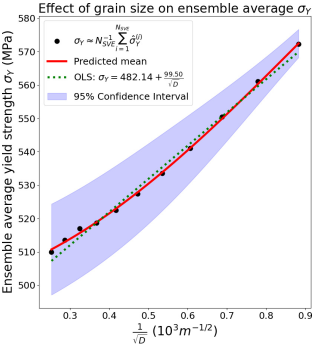
Anh Tran and Tim Wildey (2020). "Solving stochastic inverse problems for property-structure linkages using data-consistent inversion and machine learning". In: *JOM* 73, pp. 72–89

Summary:

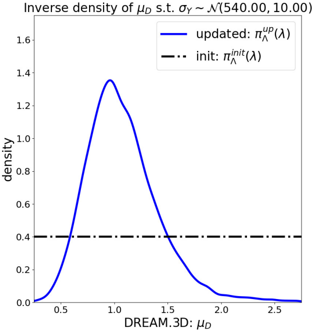
- Problem statement: given (1) a target distribution of QoIs associated with materials properties (e.g. σ_Y) and (2) a structure-property forward model (CPFEM or a ML model, e.g. GPR), infer a distribution of microstructure features, such that the push-forward distribution is consistent with the target distribution of QoIs
- using a stochastic inverse method (T Butler, J Jakeman, and T Wildey (2018a). "Combining push-forward measures and Bayes' rule to construct consistent solutions to stochastic inverse problems". In: *SIAM Journal on Scientific Computing* 40.2, A984–A1011; T Butler, J Jakeman, and T Wildey (2018b). "Convergence of Probability Densities Using Approximate Models for Forward and Inverse Problems in Uncertainty Quantification". In: *SIAM Journal on Scientific Computing* 40.5, A3523–A3548)
- example:
  - given a deterministic Hall-Petch relationship
  - given a distribution of σ_Y
  - solve for distribution of grain size D

(4) Stochastic inverse problems in structure-property

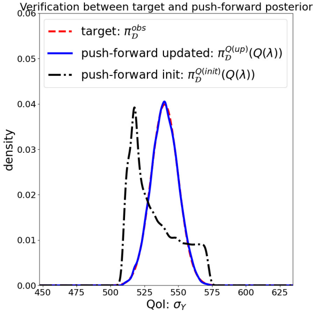
(joint work w/ Tim Wildey)



Hall-Petch by OLS and GPR.



Uniform *prior* and updated *posterior*.



Matching target pdf with push-forward *posterior*.

$$\pi_\Lambda^{\text{up}}(\lambda) = \pi_\Lambda^{\text{init}}(\lambda) \frac{\pi_\mathcal{D}^{\text{obs}}(Q(\lambda))}{\pi_\mathcal{D}^{Q(\text{init})}(Q(\lambda))}, \quad \lambda \in \Lambda.$$

(5) Proper orthogonal decomposition ROM

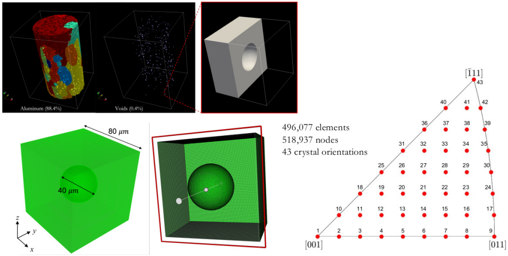
(joint work w/ David Montes de Oca Zapiain, Hojun Lim)

Reference

Wednesday AM | March 22, 2023
Cobalt 502B | Hilton
9:30 AM
Development of Structure-property Linkages for Damage in Crystalline Microstructures Using Bayesian Inference and Unsupervised Learning:
David Montes de Oca Zapiain[1] ; Anh Tran[1]; Hojun Lim[1]; [1] Sandia National Labs

(5) Proper orthogonal decomposition ROM

(joint work w/ David Montes de Oca Zapiain, Hojun Lim)



Capturing effects of voids using CPFEM.

Summary:

- investigate anisotropic effect of spherical void in a single crystal cube
- current stage: vary t; next stage: vary Euler angles $(t, \rho_1, \Phi, \rho_2)$
- QoIs: full-field von Mises σ, equivalent plastic strain, stress triaxiality at various times t
- develop a parametric reduced-order model using proper-orthogonal decomposition (SVD-based) method
- interpolate coefficients using GP

(5) Proper orthogonal decomposition ROM

(joint work w/ David Montes de Oca Zapiain, Hojun Lim)

SciML - $(\rho_1, \Phi, \rho_2) = (145, 90, 45)$
EQPS

CPFEM - $(\rho_1, \Phi, \rho_2) = (145, 90, 45)$
EQPS

POD

σ_{vM}

POD

σ_{vM}

POD

POD

(5) Proper orthogonal decomposition ROM

(joint work w/ David Montes de Oca Zapiain, Hojun Lim)

SciML - $(\rho_1, \Phi, \rho_2) = (135, 90, 90)$
EQPS

CPFEM - $(\rho_1, \Phi, \rho_2) = (135, 90, 90)$
EQPS

POD

σ_{vM}

POD

σ_{vM}

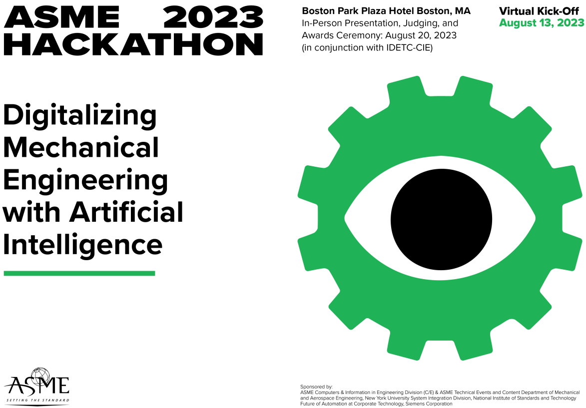
POD

POD

Conclusion

In this talk:

- we cover 5 different topics of UQ for CPFEM in ICME context
  1. high-throughput model calibration with Bayesian optimization
  2. UQ of constitutive models in CPFEM
  3. MIMC/MLMC for multi-fidelity UQ of CPFEM
  4. stochastic inverse from property to structures
  5. parametric ROM for CPFEM
- we analyze why that structure-property may be more vulnerable to uncertainty than process-structure (due to aleatory uncertainty),
- both aleatory and epistemic uncertainty are important and needed to be quantified for a robust and reliable ICME prediction.



- a hybrid (complete virtual possible / optional on-site @ Boston) hackathon event
- featuring exascale materials design with monetary prizes
- students and postdocs are welcome
- Google “asme hackathon”

Thank you for listening.

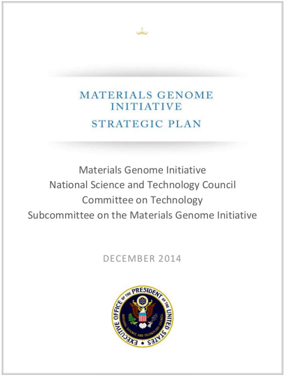
References

- Anh Tran and Hojun Lim (2023). "An asynchronous parallel high-throughput model calibration framework for crystal plasticity finite element constitutive models". In: *Computational Mechanics*
- Anh Tran, Pieterjan Robbe, and Hojun Lim (2023). "Multi-fidelity microstructure-induced uncertainty quantification by advanced Monte Carlo methods". In: *Materialia* 27, p. 101705
- Anh Tran, Tim Wildey, and Hojun Lim (2022). "Microstructure-sensitive uncertainty quantification for crystal plasticity finite element constitutive models using stochastic collocation method". In: *Frontiers in Materials* 9, pp. 1–20
- Anh Tran and Tim Wildey (2020). "Solving stochastic inverse problems for property-structure linkages using data-consistent inversion and machine learning". In: *JOM* 73, pp. 72–89

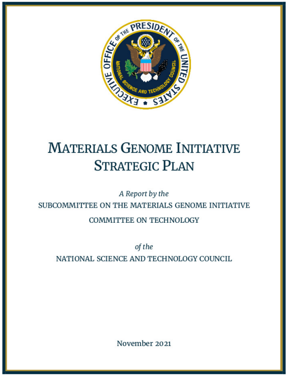
Thank you for listening.

Beyond forward ICME models: MGI as inverse problems (2010s)

US NSTC 2011



Holdren et al. 2014

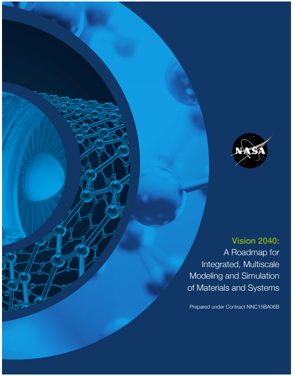


Lander et al. 2021

Beyond forward ICME models: MGI as inverse problems (MGI in 2020s)

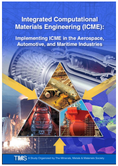
Pablo et al. 2019

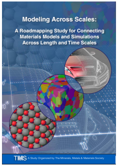
Christodoulou et al. 2021

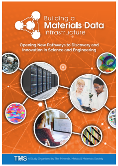


Liu et al. 2018

TMS Studies


Integrated Computational Materials Engineering (ICME):
Implementing ICME in the Aerospace, Automotive, and Maritime Industries
TMS A Study Organized by The Minerals, Metals & Materials Society


Modeling Across Scales:
A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales
TMS A Study Organized by The Minerals, Metals & Materials Society


Building a Materials Data Infrastructure
Opening New Pathways to Discovery and Innovation in Science and Engineering
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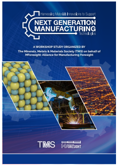
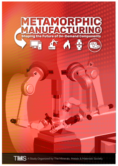
ADVANCED COMPUTATION AND DATA IN MATERIALS AND MANUFACTURING:
CORE KNOWLEDGE GAPS AND OPPORTUNITIES
TMS A Study Organized by The Minerals, Metals & Materials Society


Harnessing Materials Innovations to Support
NEXT GENERATION MANUFACTURING Technologies
A WORKSHOP STUDY ORGANIZED BY
The Minerals, Metals & Materials Society (TMS) on behalf of MForesight: Alliance for Manufacturing Foresight
TMS
MFORESIGHT


METAMORPHIC MANUFACTURING
Shaping the Future of On-Demand Components
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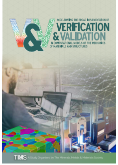
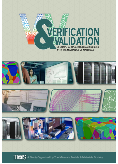
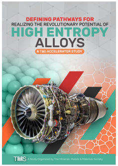
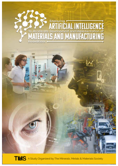
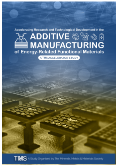

ACCELERATING THE BROAD IMPLEMENTATION OF
V&V
VERIFICATION & VALIDATION
IN COMPUTATIONAL MODELS OF THE MECHANICS OF MATERIALS AND STRUCTURES
TMS A Study Organized by The Minerals, Metals & Materials Society


V&V
VERIFICATION & VALIDATION
OF COMPUTATIONAL MODELS ASSOCIATED WITH THE MECHANICS OF MATERIALS
TMS A Study Organized by The Minerals, Metals & Materials Society

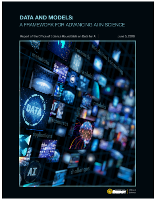

CREATING THE NEXT-GENERATION
MATERIALS GENOME INITIATIVE WORKFORCE
TMS A Study Organized by The Minerals, Metals & Materials Society


DEFINING PATHWAYS FOR
REALIZING THE REVOLUTIONARY POTENTIAL OF
HIGH ENTROPY ALLOYS
A TMS ACCELERATOR STUDY
TMS A Study Organized by The Minerals, Metals & Materials Society

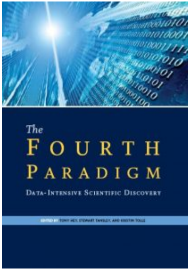

Employing
ARTIFICIAL INTELLIGENCE
to Accelerate Development and Implementation of
MATERIALS AND MANUFACTURING
Innovations
TMS A Study Organized by The Minerals, Metals & Materials Society


Accelerating Research and Technological Development in the
ADDITIVE MANUFACTURING
of Energy-Related Functional Materials
A TMS ACCELERATOR STUDY
TMS A Study Organized by The Minerals, Metals & Materials Society

DOE Office of Science / ASCR-BES-FES



Beyond forward ICME models: MGI as inverse problems



The Fourth Paradigm: Data-Intensive Scientific Discovery Hey, Tansley, Tolle, et al. 2009.

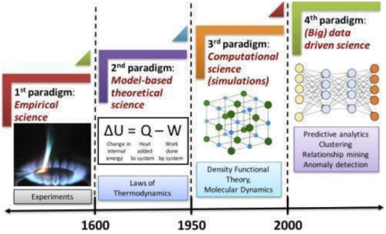


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

The four paradigms of science: empirical, theoretical, computational, and AI. Agrawal and Choudhary 2016.

- ICME is the 3rd paradigm,
- AI is the 4th paradigm,
- Is SciML the 5th?

Beyond forward ICME models: MGI as inverse problems

Challenges:

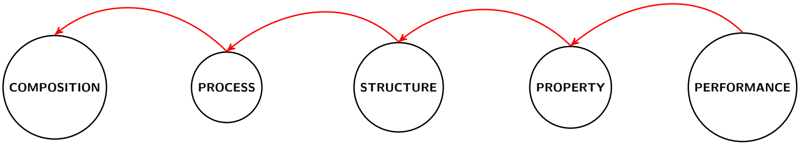
- optimization under (microstructure-induced) uncertainty
- small (sparse) + noisy datasets, high-dimensional
- high computational cost for ICME models → sample-efficient

Goals:

- traditional approach: 20+ years
- accelerate materials design by "2× at a fraction of the cost" (original)

Accelerators:

- ICME: experimental[2] → computational[3]
- ML/AI: computational[3] → ML[4]



Process-structure-property relationship

Nature of inverse problems

The nature of the input, i.e. deterministic or stochastic, determines the methodology for solving the inverse problem in PSPP.

- for deterministic variables in process→composition, process→structure: Bayesian optimization (or any other optimization methods)
- for stochastic variables (typically affiliated with microstructure), such as grain size distribution, orientation distribution, in structure→property: Bayesian inference is more appropriate to infer a distribution of features