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Efficient Propagation/Quantification of Uncertainty from CALPHAD to Multi-Physics Phase Field Microstructure Simulations

(and some machine learning)

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Outline

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- Introduction to Uncertainty Propagation
- Case 1: Microstructure Evolution in the Solid State: Thermoelectrics
- Case 2: Microstructure Evolution during Additive Manufacturing
- Summary and Conclusions

Overview of Bayesian Uncertainty Quantification and Propagation

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- UQ:
  - Inverse problem in uncertainty analysis: determine the parameterization of your models when confronted with experimental data (or any other approximation to the ground truth)
- UP:
  - Forward problem in uncertainty analysis: propagate uncertainty in model parameters, simulation conditions forward through a model or through a model chain
- Within a Bayesian framework that provides principled way for updating knowledge

Overview of Bayesian Uncertainty Quantification and Propagation

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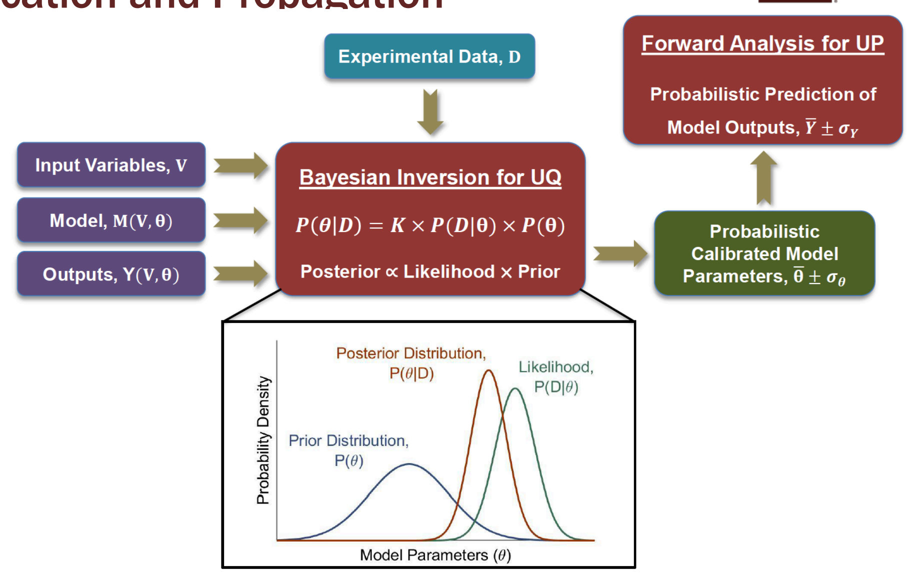

Motivation: Uncertainty Quantification (Simulation V&V)

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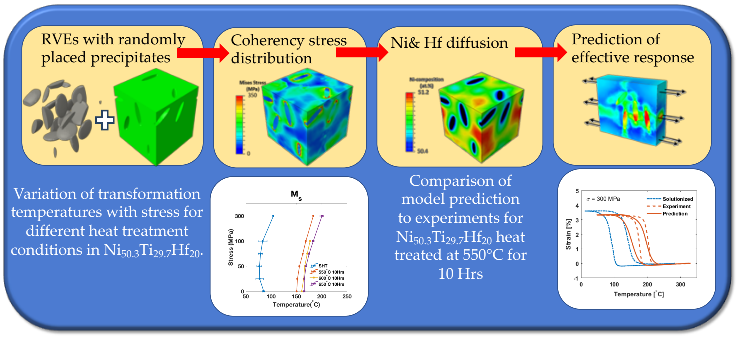

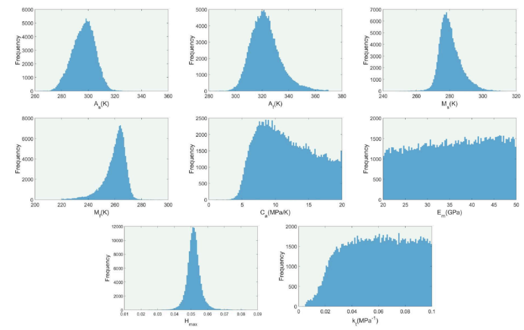

Motivation: Uncertainty Propagation (Simulation V&V)

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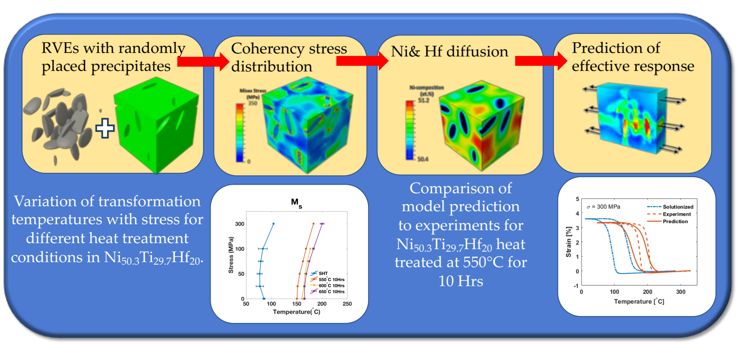
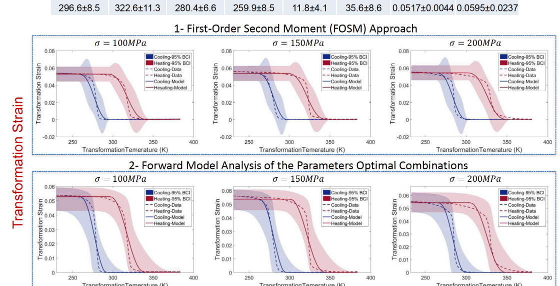


Calibrated Model Parameters

A_s (K)	A_f (K)	M_s (K)	M_f (K)	C_a ($\frac{MPa}{K}$)	E_m (GPa)	H_{max}	$k_t (MPa^{-1})$
296.6±8.5	322.6±11.3	280.4±6.6	259.9±8.5	11.8±4.1	35.6±8.6	0.0517±0.0044	0.0595±0.0237



Implementation of Uncertainty Quantification (and Propagation)

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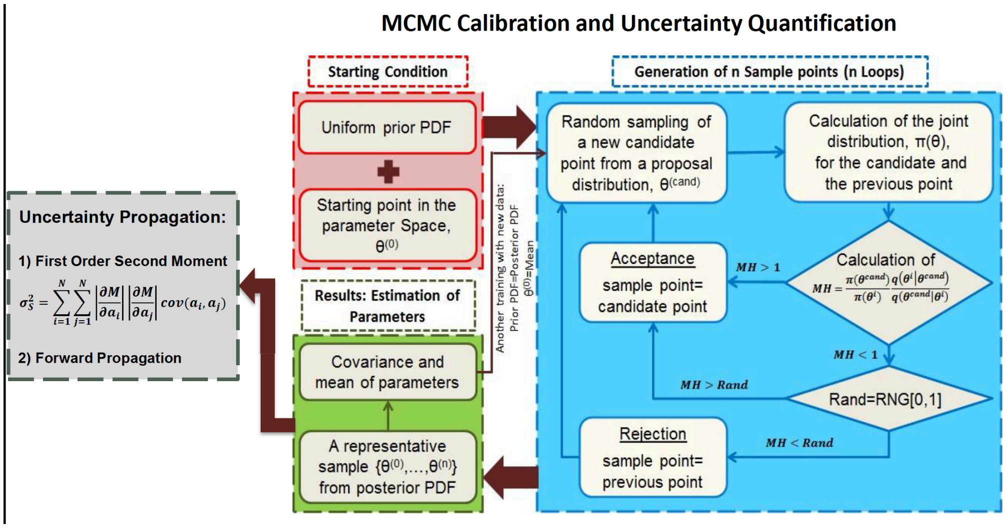

Approaches to Bayesian Uncertainty Propagation

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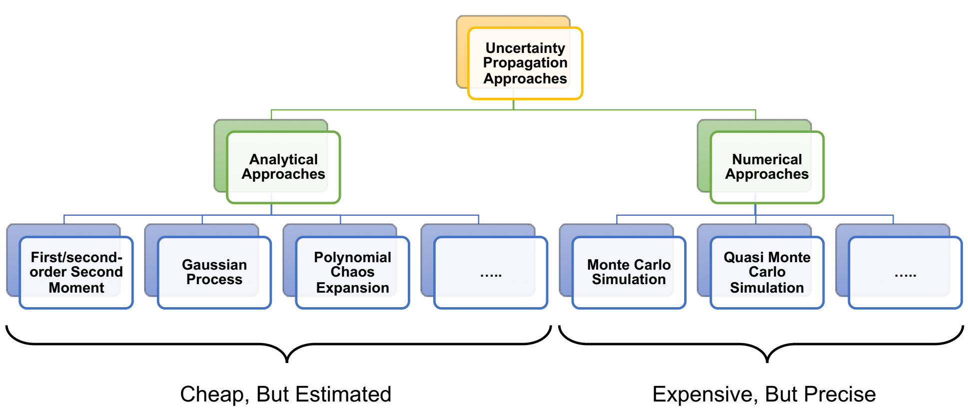
Uncertainty Propagation is a forward analysis which is usually referred to the process of passing uncertainties from the model parameters to predictions or across a chain of multi-scale models.



System-Level Uncertainty Propagation

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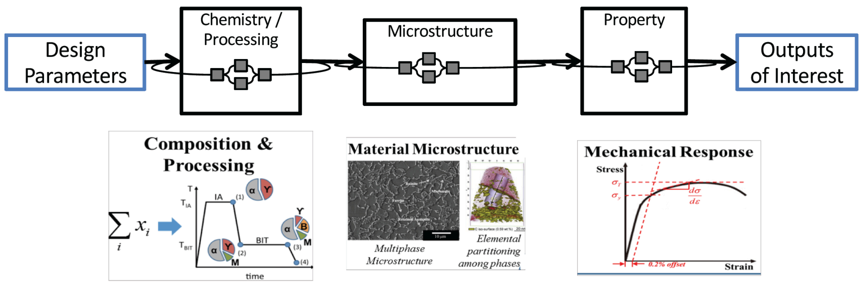
- System-level uncertainty analysis/propagation may be cumbersome due to factors that result in inadequate integration of models.
  - Models are computationally expensive
  - Model chains are difficult to integrate seamlessly
  - Model outputs may not be regular or continuous



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Solid-Solid Phase Transformations in Thermoelectrics

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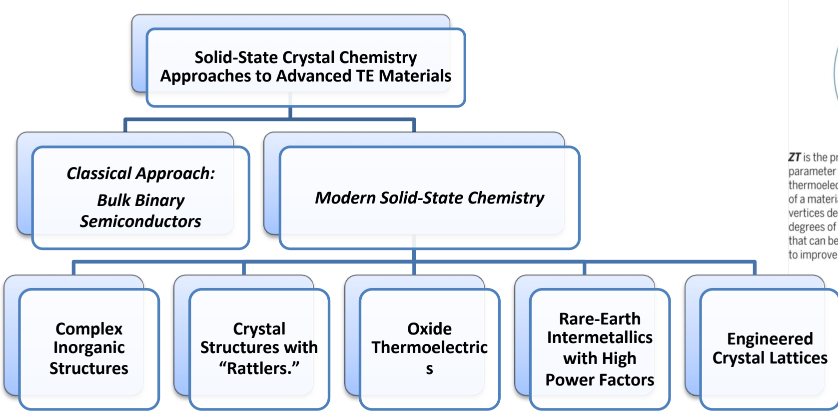
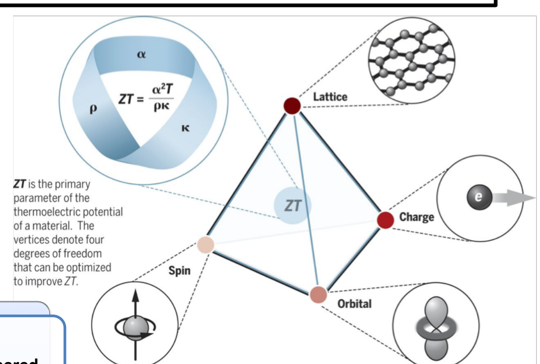
Challenges:

- Phase field models are complex, computationally expensive, involving coupled, non-linear physical phenomena
- Moreover, the dimensionality of the input parameter space is high
- Finally, the output space may be very complex and non-linear
- **Question:**
  - **How does one propagate uncertainty efficiently through such complex models?**

Motivation: Microstructural design of Thermoelectric Materials

A key factor in TE technologies is the development of high-performance TE materials.
- Either completely new materials or
- Through more ingenious materials engineering of existing materials.





Process-structure-property-performance

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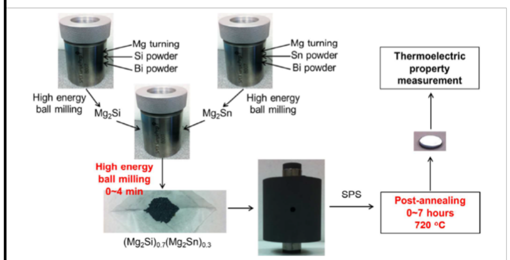
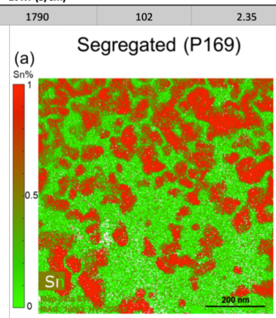
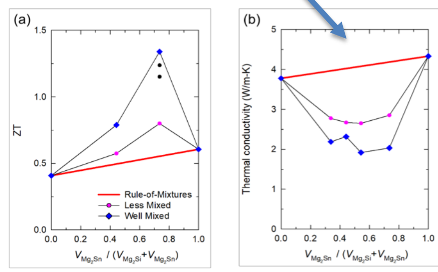
Strategy: Minimizing Thermal Conductivity

- Mass fluctuation scattering
- Scattering phonons in different frequency ranges

Electrical conductivity at RT (S/cm)	Density (%)	Carrier (10^{20} cm^{-3})
1790	102	2.35







Process → Structure → Property/Performance

Experimental evidence of phase dissolution in $Mg_2Si_xSn_{1-x}$

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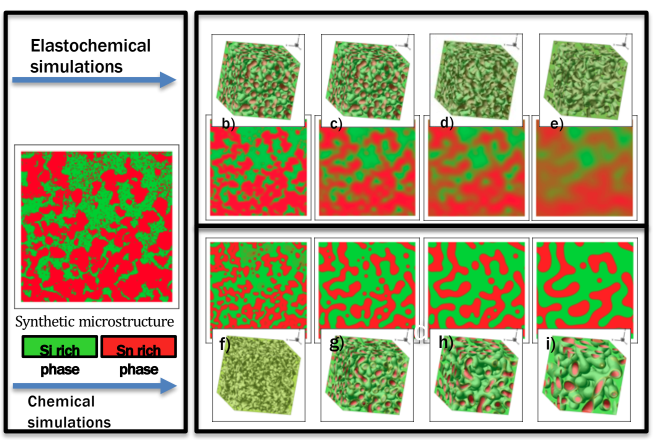
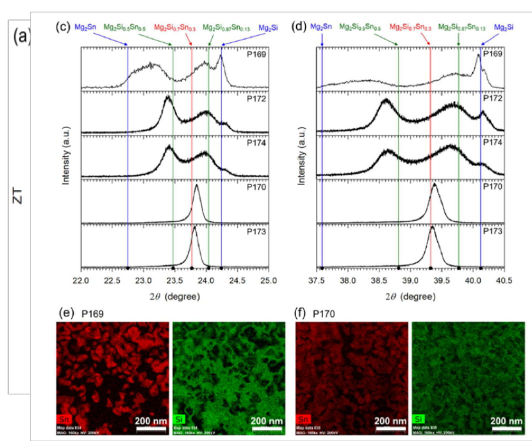
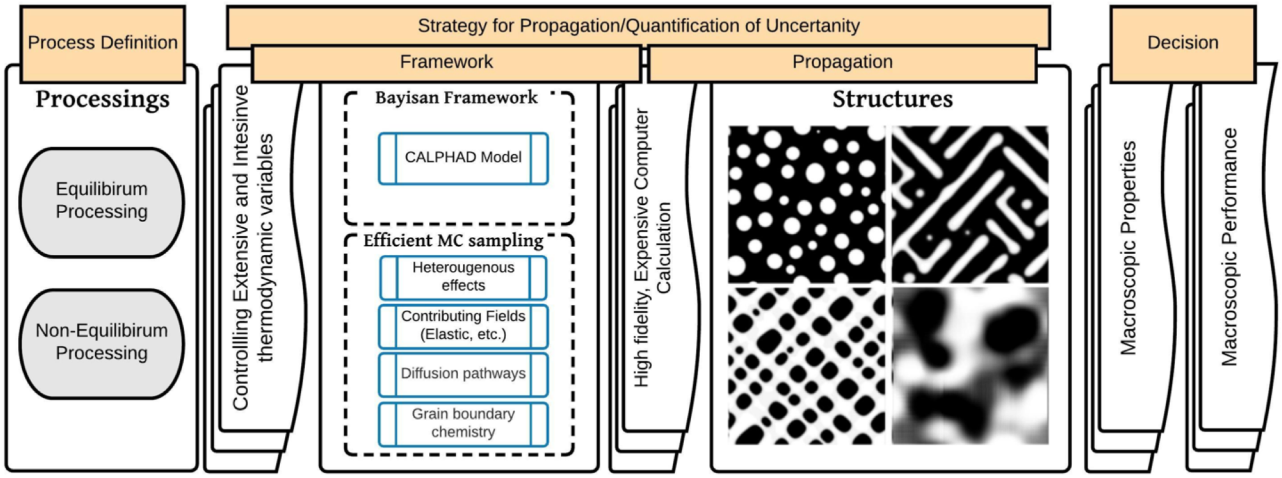




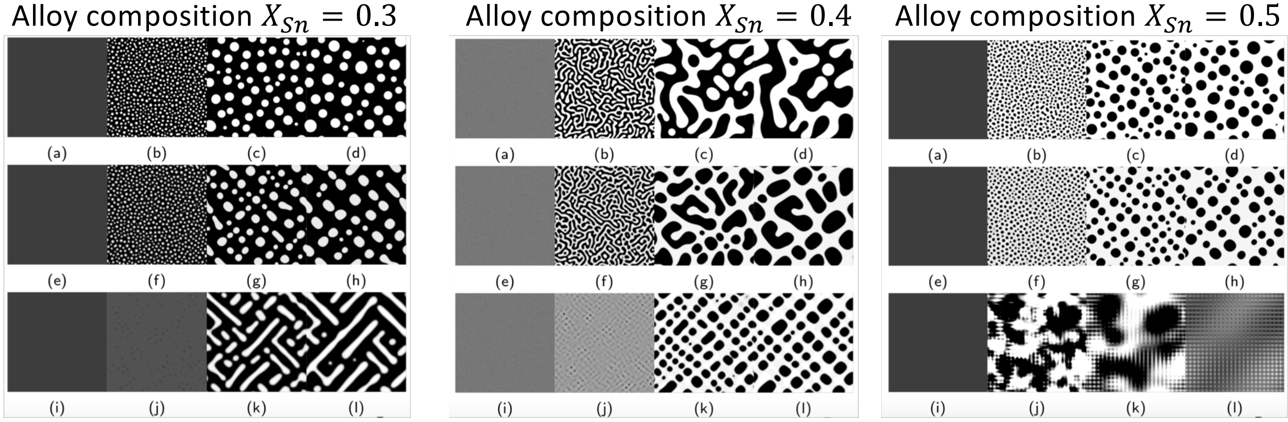
Structure → Property/Performance

Our strategy for investigating/altering composition and structure space



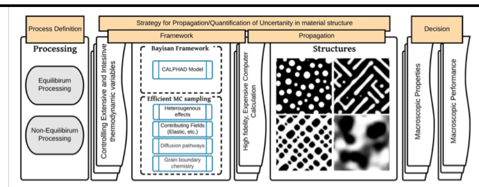
Is it only the mass scattering effect?
The impact of lattice strain on the nanostructure

Alloy composition $X_{Sn} = 0.3$ | Alloy composition $X_{Sn} = 0.4$ | Alloy composition $X_{Sn} = 0.5$



Figures description:
Evolution of the microstructure under different lattice strain conditions.

- First row: $\varepsilon^T = 0.001$, second row: $\varepsilon^T = 0.008$, and third row: $\varepsilon^T = 0.014$.



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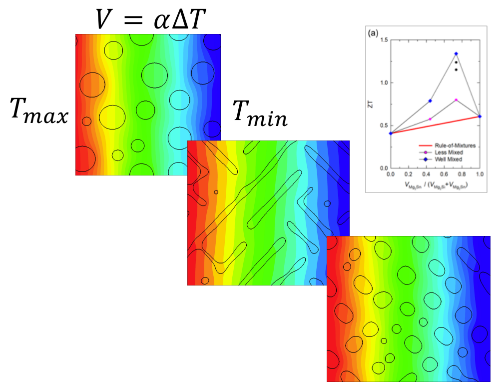
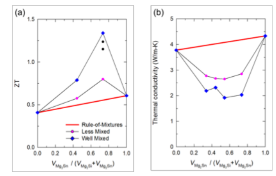
Structure → Property/Performance





Overall Bayesian Framework for UQ/UP

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First Step: UQ/UP over CALPHAD Model

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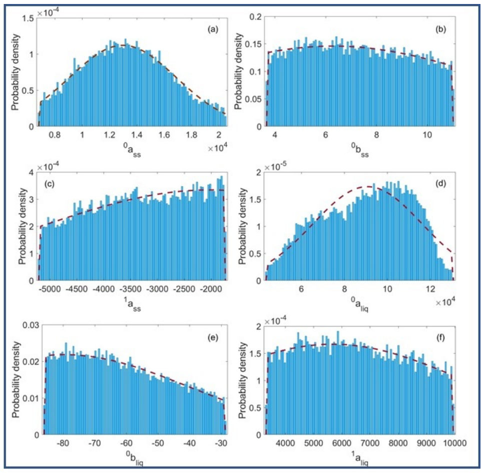
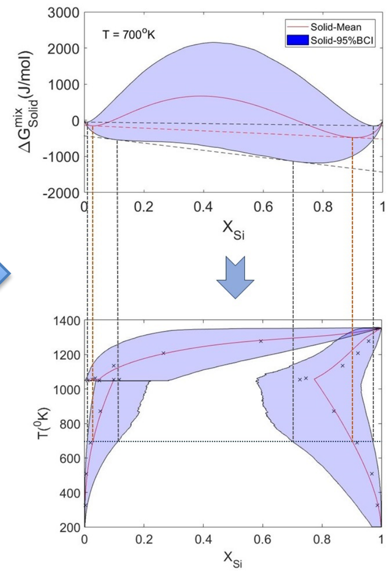
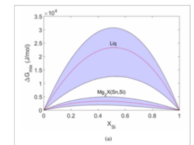
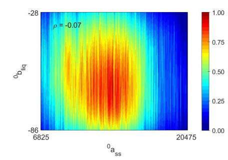






Joint frequency distribution between a selected pair of parameters



General Overview:

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Process space → Structure space → Property space

Model	Sub-model	Parameter	graph	Unit	PDF form	μ	std	Lower Bound	Upper Bound
Phase-field Model Inputs	CALPHAD Model inputs	$^0a_{ss}$		$J.mol^{-1}$		12975.13	3884.57	6824.89	20474.69
		$^0b_{ss}$		$J.mol^{-1}$		6.28	6.24	3.67	11.02
		$^1a_{ss}$		$J.mol^{-1}$		-2027.82	3109.07	-5208.34	-1736.11
		$^0a_{liq}$		$J.mol^{-1}$		90748.41	25283.62	43550.19	130650.57
		$^0b_{liq}$		$J.mol^{-1}$		-79.59	38.83	-86.03	-28.68
		$^1a_{liq}$		$J.mol^{-1}$		5670.01	4636.98	3314.80	9944.41
		Initial Composition		mol	Uniform	-	-	0.3	0.5
		SFTS (ϵ^T)		-	Uniform	0	0.02	-0.02	+0.02
		$C_{11}\ Mg_2Sn$		GPa	Normal	77.1471	5.9155	68.3000	83.7100
		$C_{12}\ Mg_2Sn$		GPa	Normal	26.9833	7.2103	17.6800	39.7900
		$C_{44}\ Mg_2Sn$		GPa	Normal	30.7158	7.7791	16.0300	41.9400
		$C_{11}\ Mg_2Si$		GPa	Normal	120.2873	3.4141	114.0700	126.0000
		$C_{12}\ Mg_2Si$		GPa	Normal	22.5536	1.9625	19.5600	26.0000
		$C_{44}\ Mg_2Si$		GPa	Normal	46.9955	6.2219	33.3200	58.2000
		Interface mobility (M)		$m^2s^{-1}.J^{-1}$	Uniform	-	-	$10^{-14}/(RT)$	$10^{-16}/(RT)$
		Gradient energy Coefficient (κ)		$J.m^{-2}$	Uniform	-	-	2.0×10^{-26}	2.0×10^{-24}
		Molar volume ($V_m^{Mg_2Si}$)		$m^3.mol^{-1}$	Normal	5.96×10^{-05}	3.19×10^{-06}	-	-
		Molar volume ($V_m^{Mg_2Sn}$)		$m^3.mol^{-1}$	Normal	4.99×10^{-05}	3.57×10^{-06}	-	-

Specification of Input Parameter Uncertainty in Phase-field Approach

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Thermodynamic stat

$F^{tot}(c, \epsilon, \nabla c) =$

$f^i(c_i, T) = \sum_i c_i G_i^0 + RT \sum_i c_i ln(c_i) +$

CALPHAD energy form

f^{inte}

$^0a_{ss}$ $J.mol^{-1}$

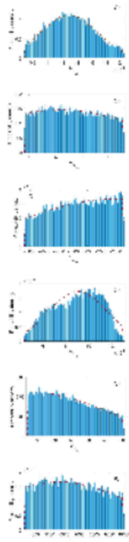
$^0b_{ss}$ $J.mol^{-1}$

$^1a_{ss}$ $J.mol^{-1}$

$^0a_{liq}$ $J.mol^{-1}$

$^0b_{liq}$ $J.mol^{-1}$

$^1a_{liq}$ $J.mol^{-1}$



orm	μ	std	Lower Bound	Upper Bound
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	90748.41	25283.62	43550.19	130650.57
	-79.59	38.83	-86.03	-28.68
	5670.01	4636.98	3314.80	9944.41
rm	-	-	0.3	0.5
rm	0	0.02	-0.02	+0.02
nal	77.1471	5.9155	68.3000	83.7100
nal	26.9833	7.2103	17.6800	39.7900
nal	30.7158	7.7791	16.0300	41.9400
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nal	5.96×10^{-05}	3.19×10^{-06}	-	-
nal	4.99×10^{-05}	3.57×10^{-06}	-	-

Efficient Sampling

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- Our posterior information includes:
  - marginal probability densities — $f_{\mathbf{X}_i}(\mathbf{x}_i)$
  - pairwise correlation estimates — $R \in [-1, 1]^{d \times d}$
- First sample from independent, identically distributed normal random vectors

$$\mathbf{G}_1, \mathbf{G}_2, \ldots, \mathbf{G}_n \text{ i.i.d.} \sim \mathcal{N}(\mathbf{0}, R)$$

- Pass through a Gaussian copula $\{\mathbf{u}_i = \Phi(\mathbf{g}_i)\}_{i=1}^n$

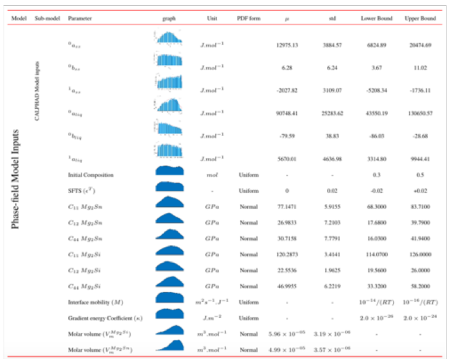
  Creates uniform samples while preserving correlation

- Use marginal cumulative distributions for inverse transform $F_{\mathbf{X}_i}^{-1}(\mathbf{u}_i)$

  Creates samples from correct marginal distributions while still preserving defined correlations

General Overview:

Process space → Structure space → Property space



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		Molar volume ($V_m^{Mg_2Si}$)		$m^3.mol^{-1}$	Normal	5.96×10^{-05}	3.19×10^{-06}	-	-
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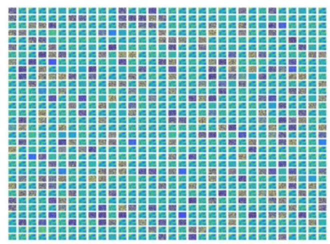

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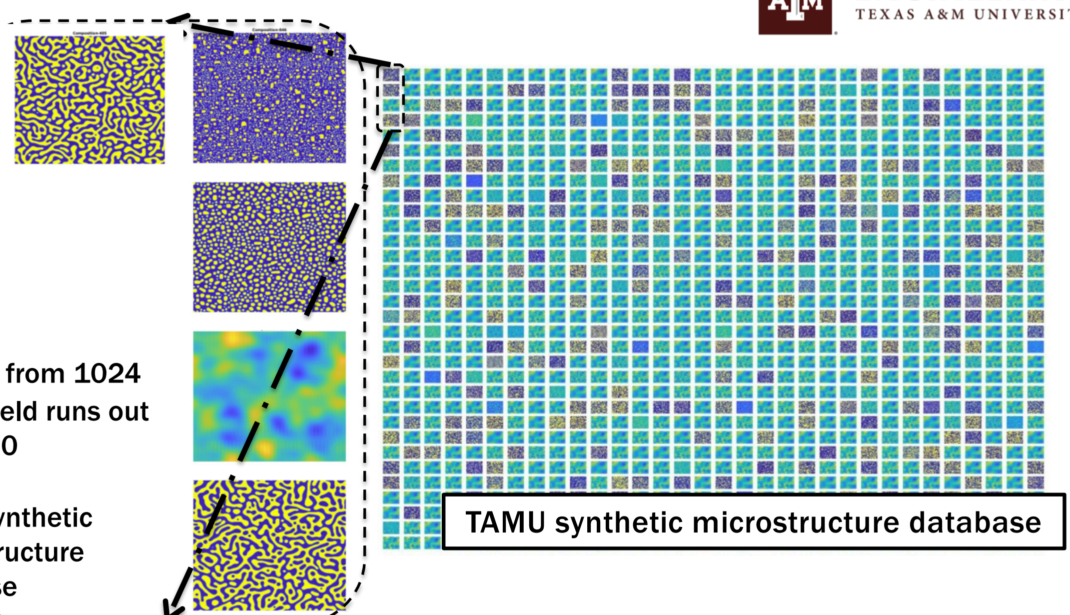
Microstructure mosaic from High-throughput phase-field calculations



- Created from 1024 phase-field runs out of 10000
- TAMU synthetic microstructure database

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		Molar volume ($V_m^{Mg_2Si}$)		$m^3.mol^{-1}$	Normal	5.96×10^{-05}	3.19×10^{-06}	-	-
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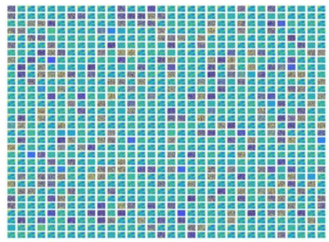

Target variables	Likelihood kernel	μ	std	Min.	Max.
C^α		0.4887	0.34	0.3112	0.9219
C^β		0.3626	0.24	0.0884	0.5089
Char. Length		-	-	0	7.0000e-07
Volume fraction		0.12	1.86	0	1.0
Roundness		0.96	0.32	0	1.5
Cubicness_1		1.15	0.38	0	2.8284
Cubicness_2		0.97	0.38	0	1.6499
$\bar{\mu}_{chem}$		-310.48	-1.98	-955.75	1273.38
$\bar{\mu}_{elas}$		-0.03	-2.14	-0.33	0.1302
$\bar{\mu}_{int}$		-	-	-	9.6552e-07

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How to propagate uncertainty in the microstructure space?

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Target variables	Likelihood kernel	μ	std	Min.	Max.
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C^β		0.3626	0.24	0.0884	0.5089
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Cubicness_1		1.15	0.38	0	2.8284
Cubicness_2		0.97	0.38	0	1.6499
$\bar{\mu}_{chem}$		-310.48	-1.98	-955.75	1273.38
$\bar{\mu}_{elas}$		-0.03	-2.14	-0.33	0.1302
$\bar{\mu}_{int}$		-	-	-	9.6552e-07

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How to propagate uncertainty in the microstructure space?

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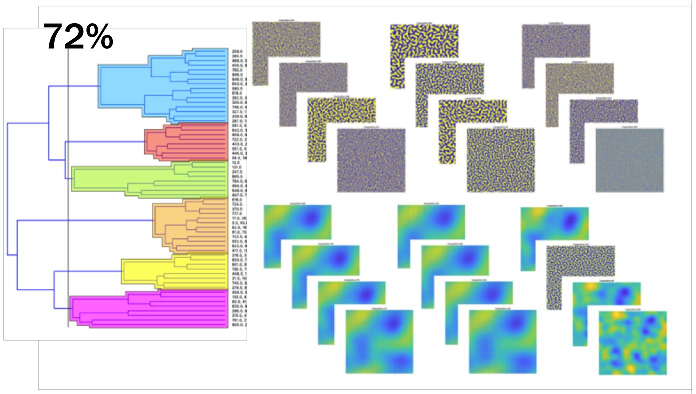

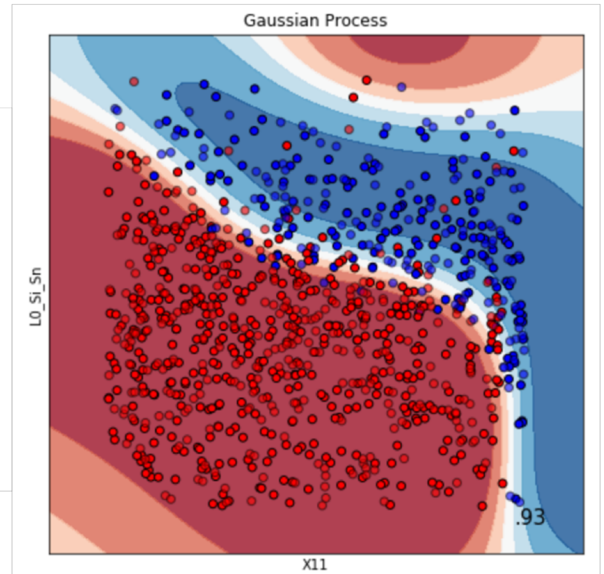

Next Step: Efficient Uncertainty Propagation

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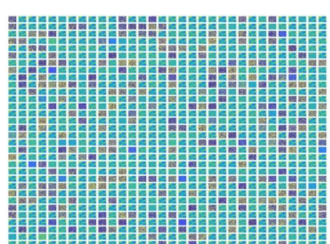
Process space → Structure space → Property space

By Efficiently Sampling this

Model	Sub-model	Parameter	graph	Unit	PDF form	μ	std	Lower Bound	Upper Bound
Phase-field Model Inputs	CALPHAD Model inputs	$^0a_{ss}$		$J.mol^{-1}$		12975.13	3884.57	6824.89	20474.69
		$^0b_{ss}$		$J.mol^{-1}$		6.28	6.24	3.67	11.02
		$^1a_{ss}$		$J.mol^{-1}$		-2027.82	3109.07	-5208.34	-1736.11
		$^0a_{liq}$		$J.mol^{-1}$		90748.41	25283.62	43550.19	130650.57
		$^0b_{liq}$		$J.mol^{-1}$		-79.59	38.83	-86.03	-28.68
		$^1a_{liq}$		$J.mol^{-1}$		5670.01	4636.98	3314.80	9944.41
		Initial Composition		mol	Uniform	-	-	0.3	0.5
		SFTS (ϵ^T)		-	Uniform	0	0.02	-0.02	+0.02
		C_{11} Mg_2Sn		GPa	Normal	77.1471	5.9155	68.3000	83.7100
		C_{12} Mg_2Sn		GPa	Normal	26.9833	7.2103	17.6800	39.7900
		C_{44} Mg_2Sn		GPa	Normal	30.7158	7.7791	16.0300	41.9400
		C_{11} Mg_2Si		GPa	Normal	120.2873	3.4141	114.0700	126.0000
		C_{12} Mg_2Si		GPa	Normal	22.5536	1.9625	19.5600	26.0000
		C_{44} Mg_2Si		GPa	Normal	46.9955	6.2219	33.3200	58.2000
		Interface mobility (M)		$m^2s^{-1}.J^{-1}$	Uniform	-	-	$10^{-14}/(RT)$	$10^{-16}/(RT)$
		Gradient energy Coefficient (κ)		$J.m^{-2}$	Uniform	-	-	2.0×10^{-26}	2.0×10^{-24}
		Molar volume ($V_m^{Mg_2Si}$)		$m^3.mol^{-1}$	Normal	5.96×10^{-05}	3.19×10^{-06}	-	-
		Molar volume ($V_m^{Mg_2Sn}$)		$m^3.mol^{-1}$	Normal	4.99×10^{-05}	3.57×10^{-06}	-	-



How do we get this?

Target variables	Likelihood kernel	μ	std	Min.	Max.
C^α		0.4887	0.34	0.3112	0.9219
C^β		0.3626	0.24	0.0884	0.5089
Char. Length		-	-	0	7.0000e-07
Volume fraction		0.12	1.86	0	1.0
Roundness		0.96	0.32	0	1.5
Cubicness_1		1.15	0.38	0	2.8284
Cubicness_2		0.97	0.38	0	1.6499
$\bar{\mu}_{chem}$		-310.48	-1.98	-955.75	1273.38
$\bar{\mu}_{elas}$		-0.03	-2.14	-0.33	0.1302
$\bar{\mu}_{int}$		-	-	-	9.6552e-07

Challenge: Sampling Issues

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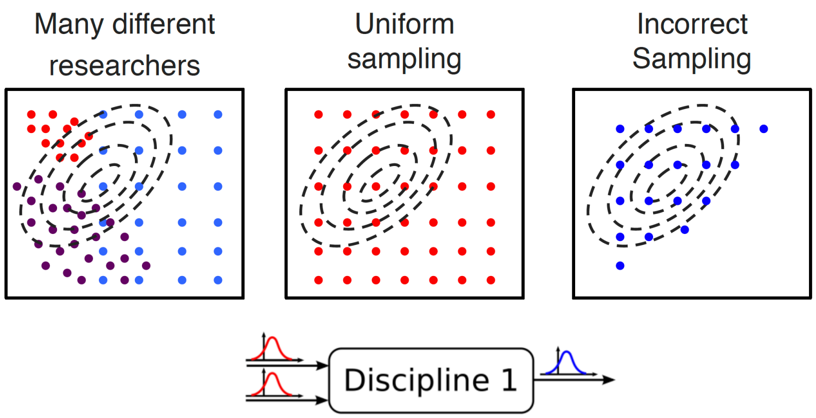

Need: A method for reusing previously propagated sample points through expensive computational models or experiments even if those samples were not drawn from the desired input distribution.

Challenge: Sampling Issues

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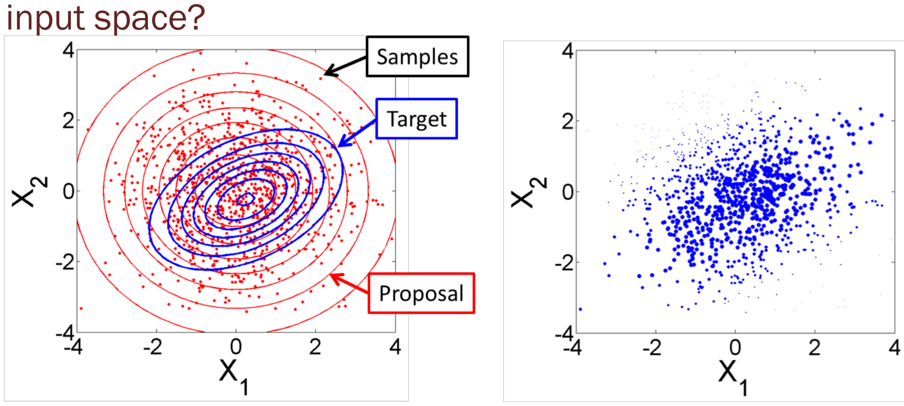
- Is there a way to ‘smartly’ sampling the input space in such a way that we can attain a target distribution from sparse efficient sampling over the input space?



Approach 1: Probability Measure Optimized Importance Weights

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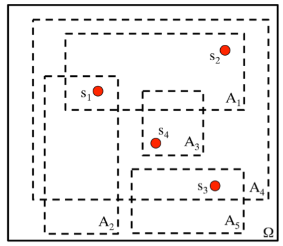
Given a set of input samples and a desired target input probability measure:

- Construct a set of subsets of the sample space.
- Create a row vector for each subset with a one or zero entry if a given sample is in the subset or not. Create a matrix from the set of row vectors.
- Create a column vector with entries equal to the probability of a sample occurring in a given subset according to the target measure.
- Solve for importance weights using least squares.



$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} \mathbb{P}(A_1) \\ \mathbb{P}(A_2) \\ \mathbb{P}(A_3) \\ \mathbb{P}(A_4) \\ \mathbb{P}(A_5) \end{bmatrix}$$

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Approach 1: Probability Measure Optimized Importance Weights. Benchmark: Johnson-Cook Model

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$$\sigma = [A + B(\epsilon_{pl})^n] \cdot \left[1 + C \ln\left(\frac{\dot{\epsilon_{pl}}}{\dot{\epsilon_o}}\right)\right] \cdot \left[1 - \left(\frac{T - T_o}{T_m - T_o}\right)^m\right]$$

Material Coefficient	Units	Target Distribution	Proposal Distribution
A	[MPa]	$\mathcal{N}(\mu = 775, \sigma^2 = 50)$	$\mathcal{U}[595, 955]$
B	[MPa]	$\mathcal{N}(\mu = 600, \sigma^2 = 100)$	$\mathcal{U}[350, 850]$
C	[-]	$\mathcal{N}(\mu = 0.025, \sigma^2 = 0.0025)$	$\mathcal{U}[0.0005'0.005]$
n	[-]	$\mathcal{N}(\mu = 0.38, \sigma^2 = 0.025)$	$\mathcal{U}[0.3, 0.45]$
m	[-]	$\mathcal{N}(\mu = 0.98, \sigma^2 = 0.01)$	$\mathcal{U}[0.95, 1.01]$

Material Parameters	Units	Selected Value
Effective plastic strain (ϵ_{pl})	[-]	0.08
Plastic strain rate ($\dot{\epsilon_{pl}}$)	[s^{-1}]	500
Reference strain rate ($\dot{\epsilon_o}$)	[s^{-1}]	1
Current Temperature (T)	[°c]	600
Room Temperature (T_o)	[°c]	22
Melting Temperature (T_m)	[°c]	1632

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Approach 1: Probability Measure Optimized Importance Weights. Benchmark: Johnson-Cook Model

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$$\sigma = [A + B(\epsilon_{pl})^n] \cdot \left[1 + C \ln\left(\frac{\dot{\epsilon_{pl}}}{\dot{\epsilon_o}}\right)\right] \cdot \left[1 - \left(\frac{T - T_o}{T_m - T_o}\right)^m\right]$$

Material Coefficient	Units	Target Distribution	Proposal Distribution
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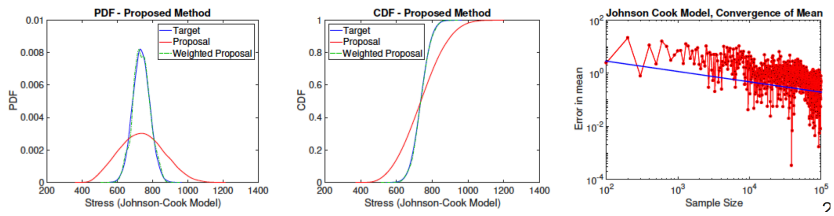
m	[-]	$\mathcal{N}(\mu = 0.98, \sigma^2 = 0.01)$	$\mathcal{U}[0.95, 1.01]$

Results shown with 100,000 proposal samples



Approach 2: Ordered Monte Carlo

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- Monte Carlo approaches to UP require ~1x10^6 evaluations to converge
- Key idea: *all samples are useful* ***on average***
- Thus, there are some samples that are more useful than others

Proposed Approach: Reordered MC Sampling

1. Generate planned sample set.
2. Construct ECDF of planned sample set
3. Find sample that, when removed from the planned sample set, results in the smallest change (L_2 sense) in the ECDF of the planned sample set.
4. Propagate this sample through the computational model.
5. Remove this sample from the planned sample set.
6. Return to Step 3.

Approach 2: Ordered Monte Carlo

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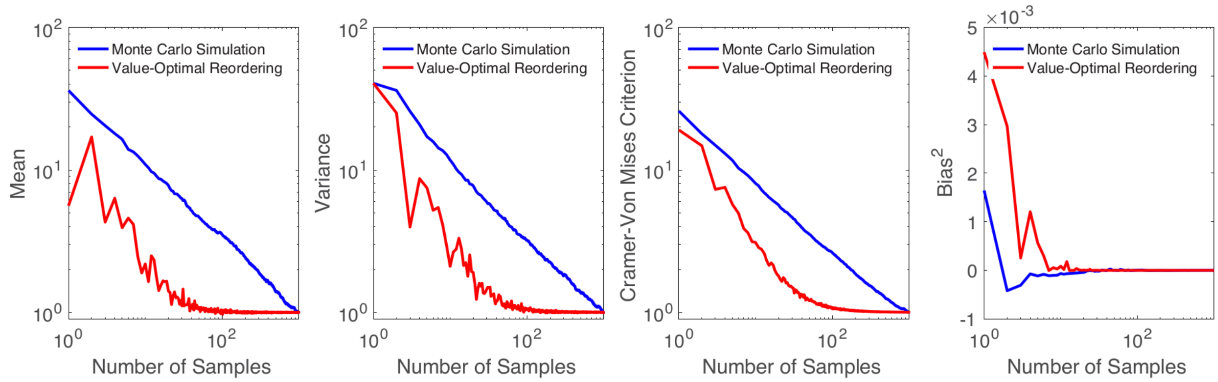

Next Step: Apply Advanced UP and test against PF Dataset (as Ground Truth)

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Process space → Structure space → Property space

Model	Sub-model	Parameter	graph	Unit	PDF form	μ	std	Lower Bound	Upper Bound
Phase-field Model Inputs	CALPHAD Model inputs	${}^{0}a_{ss}$		$J.mol^{-1}$		12975.13	3884.57	6824.89	20474.69
		${}^{0}b_{ss}$		$J.mol^{-1}$		6.28	6.24	3.67	11.02
		${}^{1}a_{ss}$		$J.mol^{-1}$		-2027.82	3109.07	-5208.34	-1736.11
		${}^{0}a_{liq}$		$J.mol^{-1}$		90748.41	25283.62	43550.19	130650.57
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		${}^{1}a_{liq}$		$J.mol^{-1}$		5670.01	4636.98	3314.80	9944.41
		Initial Composition		mol	Uniform	-	-	0.3	0.5
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		$C_{11}\ Mg_2Sn$		GPa	Normal	77.1471	5.9155	68.3000	83.7100
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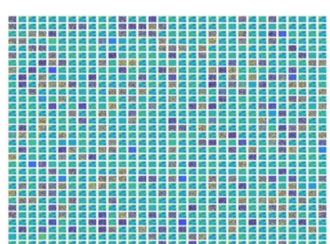
		Interface mobility (M)		$m^2s^{-1}.J^{-1}$	Uniform	-	-	$10^{-14}/(RT)$	$10^{-16}/(RT)$
		Gradient energy Coefficient (κ)		$J.m^{-2}$	Uniform	-	-	2.0×10^{-26}	2.0×10^{-24}
		Molar volume ($V_m^{Mg_2Si}$)		$m^3.mol^{-1}$	Normal	5.96×10^{-05}	3.19×10^{-06}	-	-
		Molar volume ($V_m^{Mg_2Sn}$)		$m^3.mol^{-1}$	Normal	4.99×10^{-05}	3.57×10^{-06}	-	-



Target variables	Likelihood kernel	μ	std	Min.	Max.
C^{α}		0.4887	0.34	0.3112	0.9219
C^{β}		0.3626	0.24	0.0884	0.5089
Char. Length		-	-	0	7.0000e-07
Volume fraction		0.12	1.86	0	1.0
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$\bar{\mu}_{int}$		-	-	-	9.6552e-07

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UP in Phase Field Models for Additive Manufacturing

Pejman Honarmandi[1], Vahid Attari[1], Isaac Benson[2], Douglas Allaire[2] and,
Mohammed Mahmoud[3], Alaa Elwany[3], Supriyo Ghosh[1], Kubra Karayagiz[1],
Raymundo Arroyave,[1,2,3]

[1]Department of Materials Science and Engineering, Texas A&M University
[2]Department of Mechanical Engineering, Texas A&M University
[3]Department of Industrial and Systems Engineering, Texas A&M University

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Challenges:

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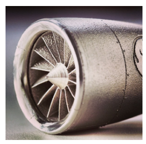
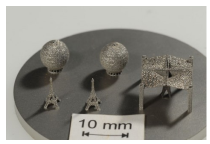
- Simulations in materials may be the result of a complex chain of models
- Each model is computationally expensive
- Some model outputs are observable, some aren't.
- Moreover, the experimental information necessary to validate/calibrate models is scarce
- **Question:**
  - **How does one calibrate multiple models in a model chain with incomplete information?**

Motivation

Selective Laser Melting (SLM)

Applications:

- Mostly in dental and aerospace industry



Advantages:

- Fabrication of complex geometries
- Fully dense parts
- Near-net-shape production
- No need for part-specific tooling
- Minimum waste of material

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Motivation

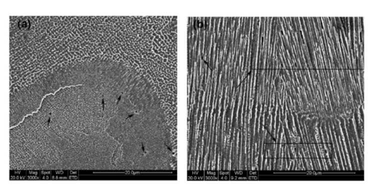
Challenges

Part quality

- Micro-cracks
- Delamination
- Balling effect
- Porosity
- Swelling

Variability

- Microstructure
- Mechanical properties
- *Swelling*



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Framework

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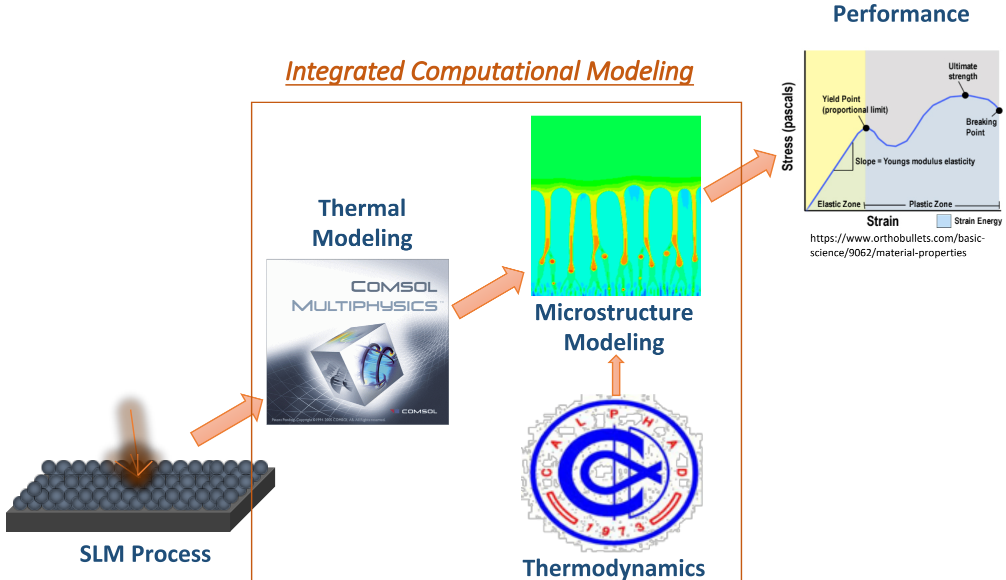

Framework

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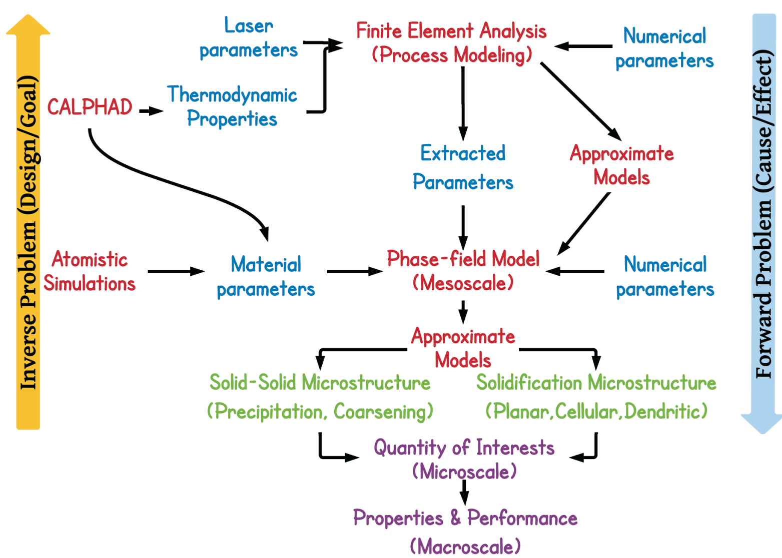

Coupling of Models

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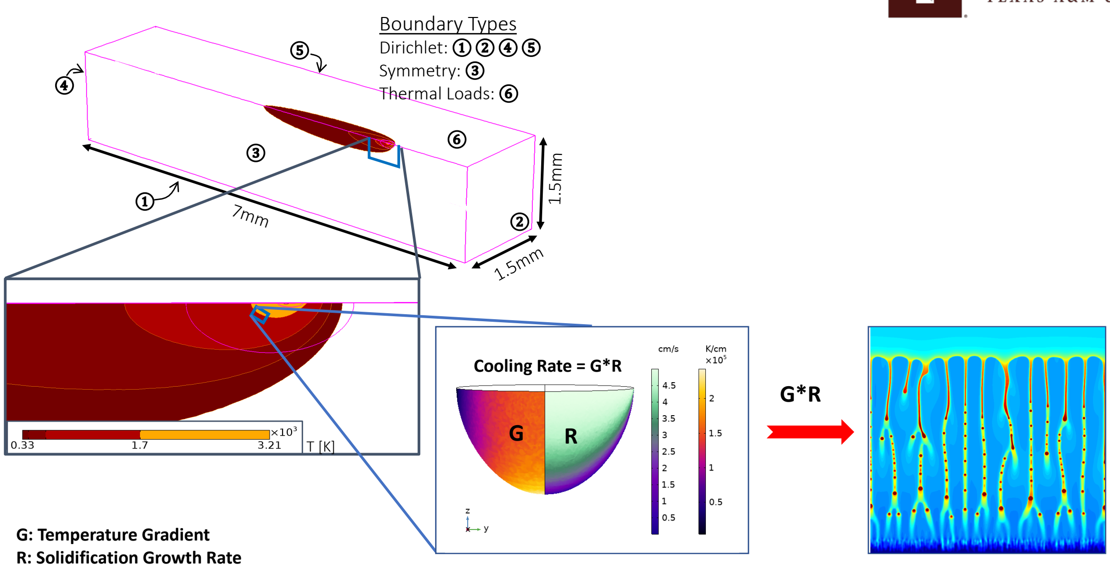

G: Temperature Gradient
R: Solidification Growth Rate

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Application to AM of Ni-Nb

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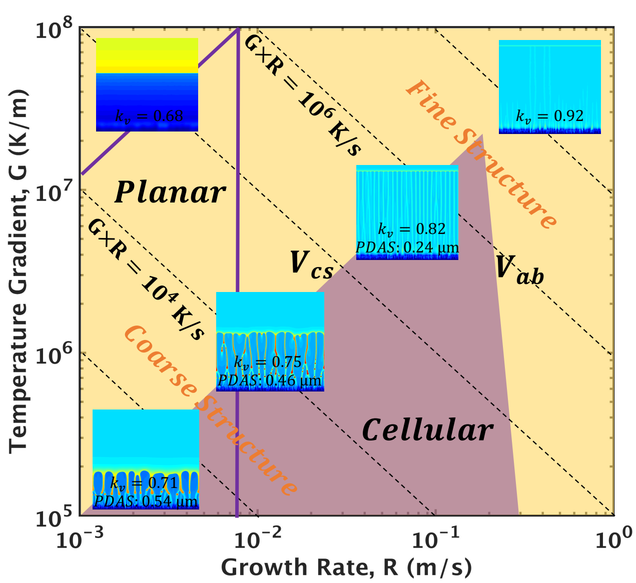

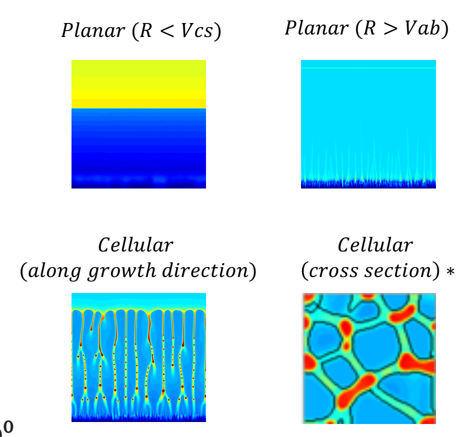

* thanks to Xueqin Huang

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Effect of Process Parameters on Thermal Output

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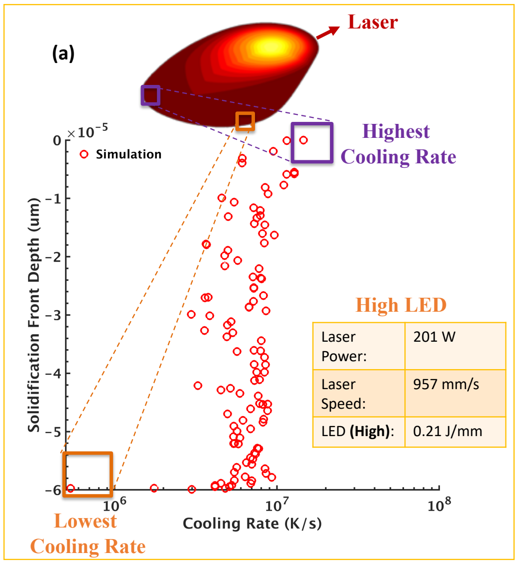
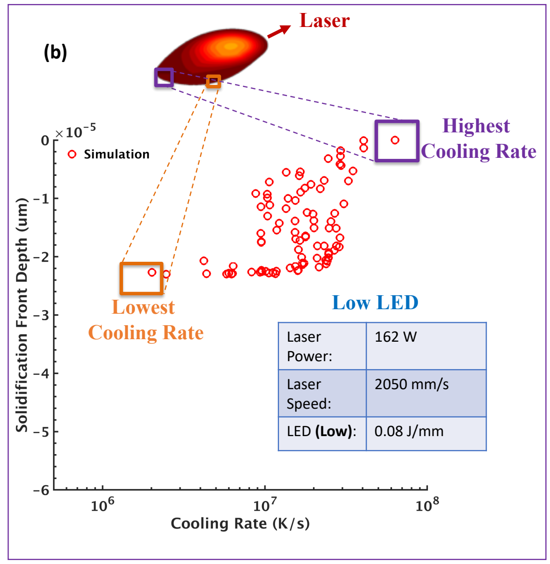


Laser Power:	201 W
Laser Speed:	957 mm/s
LED **(High)**:	0.21 J/mm



Laser Power:	162 W
Laser Speed:	2050 mm/s
LED **(Low)**:	0.08 J/mm

Effect of Process Parameters on Microstructure

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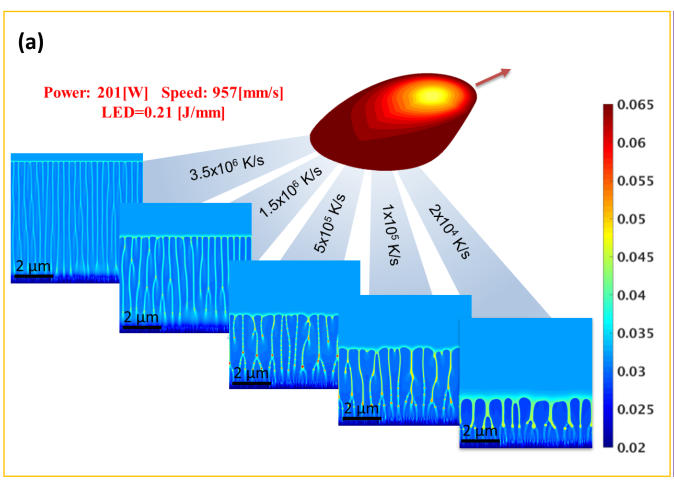
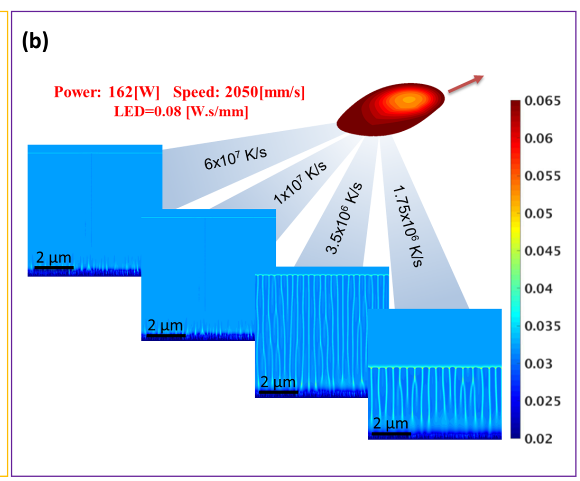
High LED



Low LED



Experimental Validation

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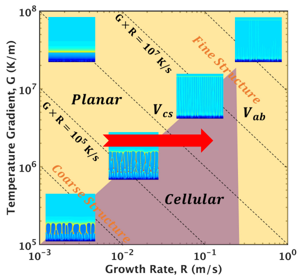
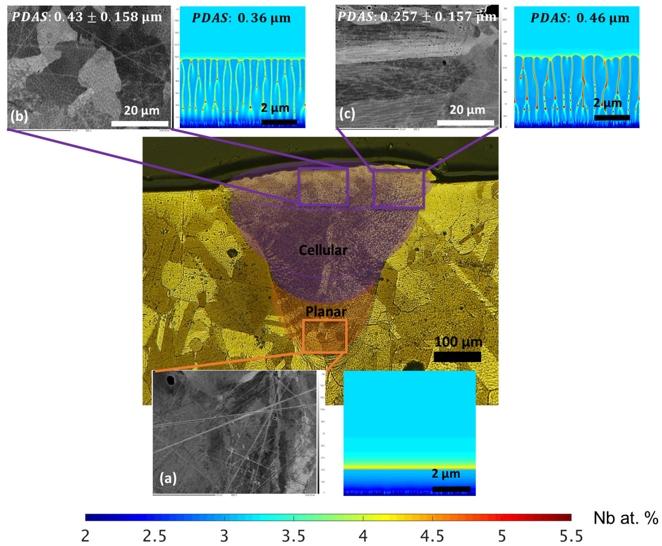
High LED

Laser Power:	122 W
Laser Speed:	50 mm/s
LED:	2.44 J/mm





Experimental Validation

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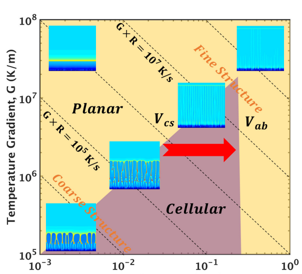
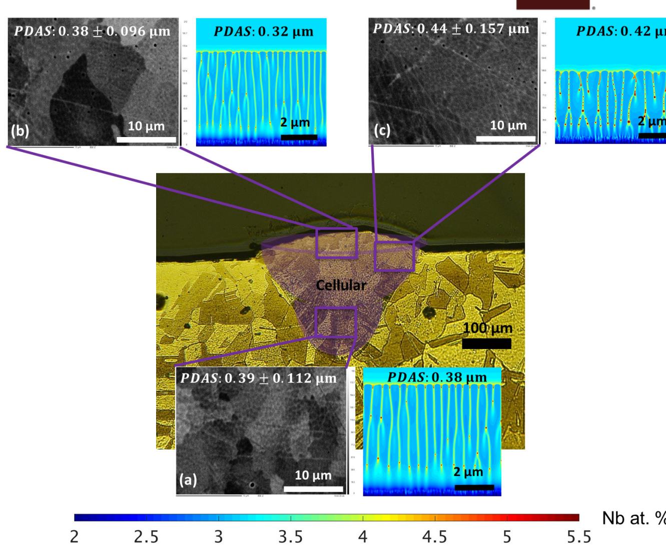
Medium LED

Laser Power:	122 W
Laser Speed:	50 mm/s
LED:	2.44 J/mm





Experimental Validation

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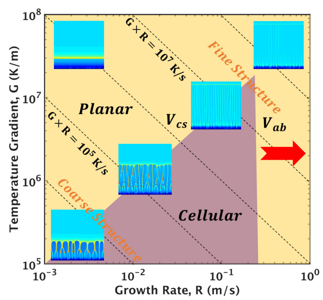
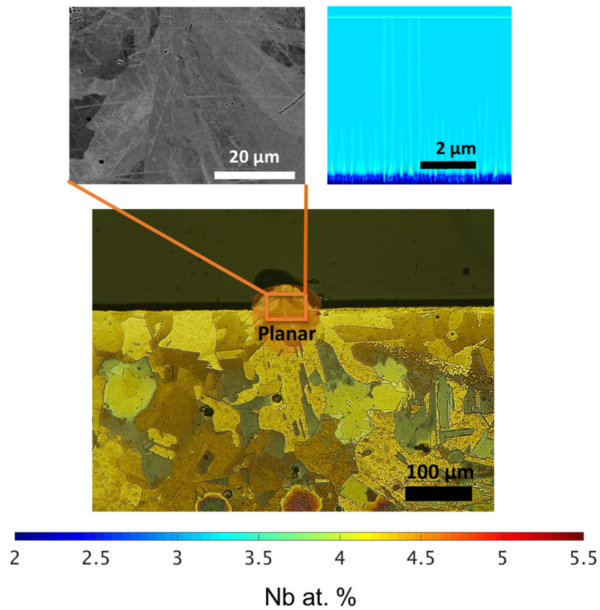
Low LED

Laser Power:	162 W
Laser Speed:	957 mm/s
LED (LOW):	0.169 J/mm





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How do we Calibrate the PFM?

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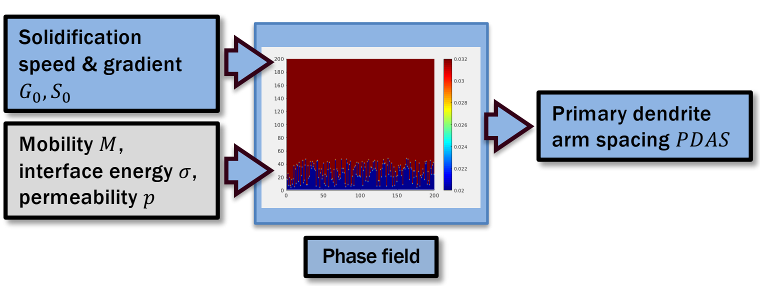
- We need physical observations to calibrate the model



- But S and G are unobservable

index	S (mm/s)	G (K/m)	PDAS (um)
1	1[illegible]	8.83[illegible]06	0.365
2	515	1.[illegible]E+07	0.350
3	602	[illegible]09E+07	0.290
4	238	[illegible]3E+06	0.316
...	...	...	...
11	1[illegible]	1.18[illegible]07	0.415

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Experimental Observations

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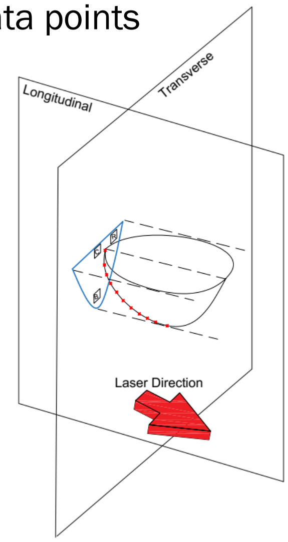
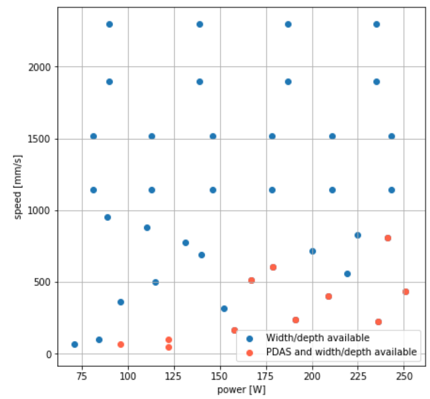
- 11 data points





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Experimental Observations for FE Model

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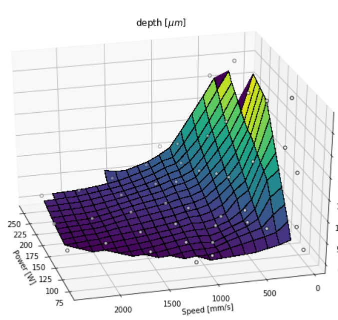
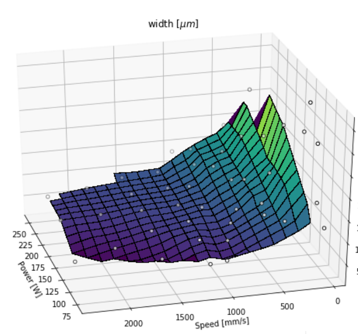
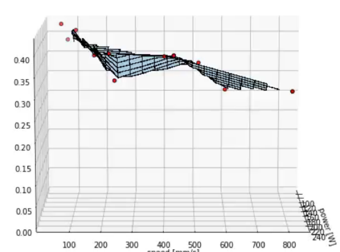
44 data points (power, speed, width, depth)







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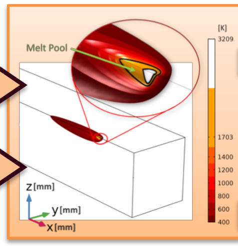
Multi-Level Calibration

- We couple two models and calibrate them together

Power P, speed v

Conductivity $K_S, K_L, K_{Lz}, K_V, K_{Vz}$, Absorptivity A_0, A_{max}



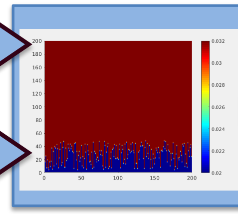
FE Model

Melt pool dimensions W, D, L

Temperature field $T(x, y, z, t)$

Solidification gradient G_0

Mobility M, interface energy σ, permeability p



Phase field

Primary dendrite arm spacing $PDAS$

Emulation (Surrogate Modeling)

- We replace the computationally-heavy models with fast emulators

Power P, speed v

Conductivity $K_S, K_L, K_{Lz}, K_V, K_{Vz}$, Absorptivity A_0, A_{max}

θ_1

M_1

FE Model

Melt pool dimensions W, D, L

Temperature field $T(x, y, z, t)$

Solidification gradient G_0

Mobility M, interface energy σ, permeability p

θ_2

M_2

Phase field

Primary dendrite arm spacing $PDAS$

Bayesian Estimation

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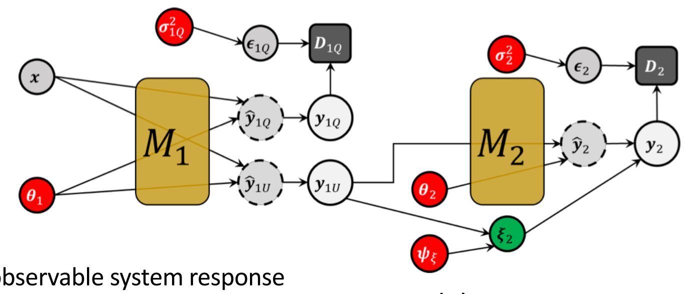
We construct a network of variables and use a Bayesian updating scheme to estimate the model parameters.



Model 1

- $\boldsymbol{y}_{1Q}$: observable system response
- $\boldsymbol{D}_{1Q}$: experimental data for $\boldsymbol{y}_{1Q}$
- $\boldsymbol{y}_{1U}$: unobservable system response

Model 2

- $\boldsymbol{y}_2$: observable system response
- $\boldsymbol{D}_2$: experimental data for $\boldsymbol{y}_2$
- $\boldsymbol{\xi}_2$: auxiliary variable correcting for $\hat{\boldsymbol{y}}_{1U}$

Bayesian Estimation

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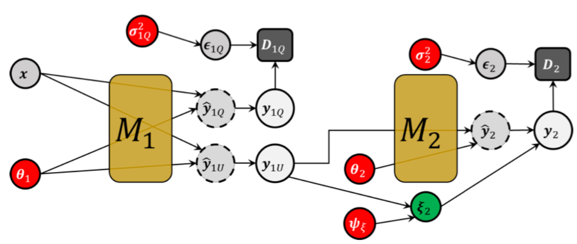
We construct a network of variables and use a Bayesian updating scheme to estimate the model parameters.

$$\boldsymbol{y}_1 = \begin{pmatrix} y_{1Q} \\ y_{1U} \end{pmatrix} = \begin{pmatrix} \hat{y}_{1Q}(x, \theta_1) + \boldsymbol{\epsilon} \\ \hat{y}_{1U}(x, \theta_1) + \boldsymbol{\epsilon} \end{pmatrix},$$

$$y_2 = \hat{y}_2(y_{1U}, \theta_2) + \xi_2(y_{1U}) + \boldsymbol{\epsilon}.$$

$$f(\mathcal{U}) = \pi(\theta_1) \cdot \pi(\theta_2) \cdot \pi(r_\xi) \cdot \pi\left(\sigma_\xi^2\right) \cdot p\left(\boldsymbol{D}_{1Q} | y_{1Q}\right) \cdot p\left(\boldsymbol{D}_2 | y_2\right)$$



Preliminary Results

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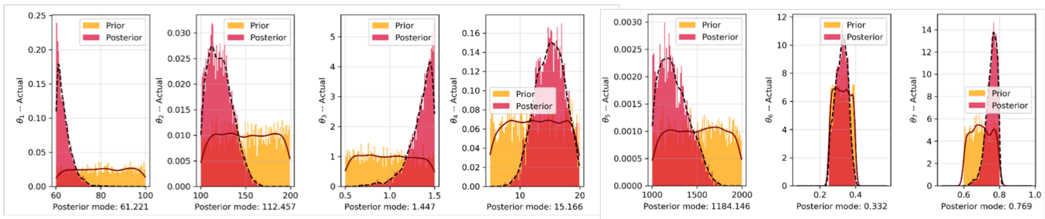
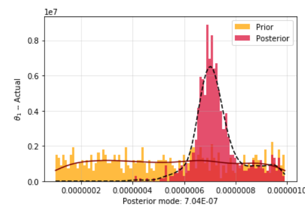
- Calibration parameters are estimated using the posterior distribution.
- Model 1 has seven calibration parameters ($\theta_1, \ldots, \theta_7$):

  1. K_S
  2. K_L
  3. K_{Lz}
  4. K_V
  5. K_{Vz}
  6. A_{bulk}
  7. A_{max}



- Model 2 has one calibration parameter:
  1. σ (interfacial energy)



Results (Ct'd)

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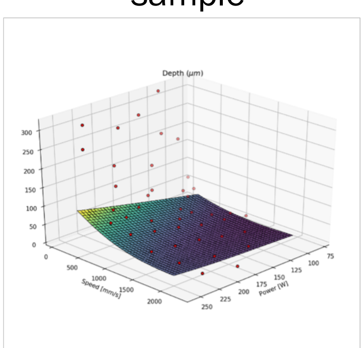
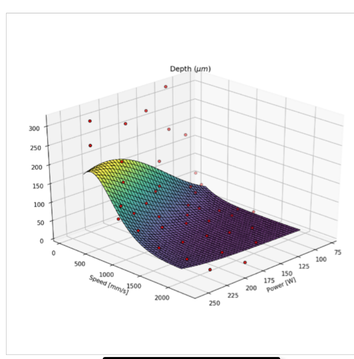
- Calibrated response surface for each output
  - sample



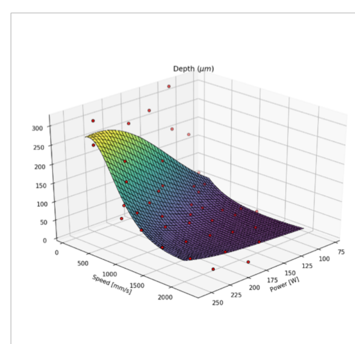
Emulator response

\+



Discrepancy

=



Final estimate

Results (Ct'd)

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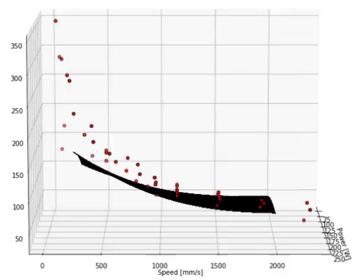
- Calibrated response surface for the FE model
  - sample

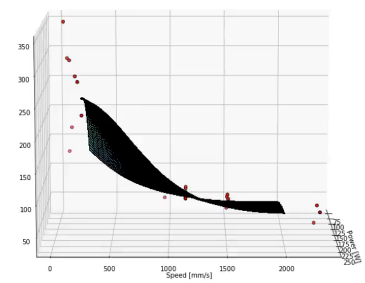
Melt pool width predictions

MAPE = (36.2 μm) 21.1%



Response with calibrated parameters

MAPE = (18.6 μm) 12.1%



Response corrected using discrepancy function

Results (Ct'd)

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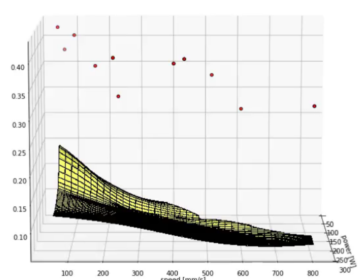
- Calibrated response surface for the PF model

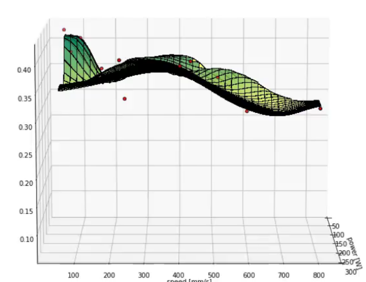
PDAS predictions

MAPE = (0.260 μm) 71.6%



Response with calibrated parameters

MAPE = (0.020 μm) 5.8%



Response corrected using discrepancy function

Results (Ct'd)

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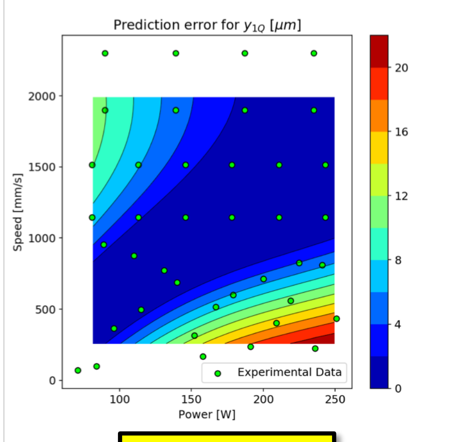
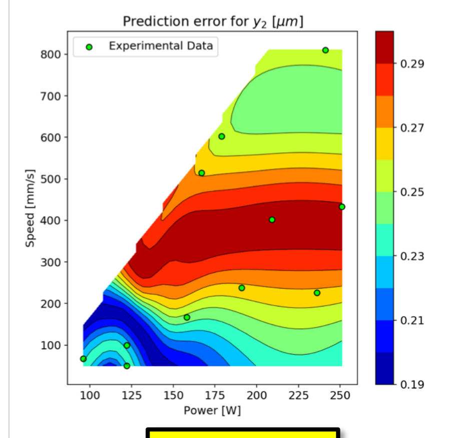
- Can we identify areas of missing physics from each model?



Melt pool width predictions



PDAS predictions

Summary

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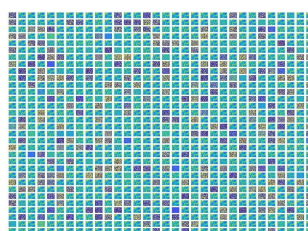
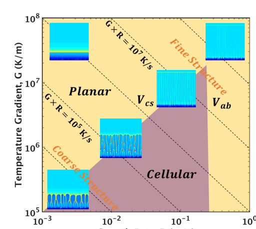
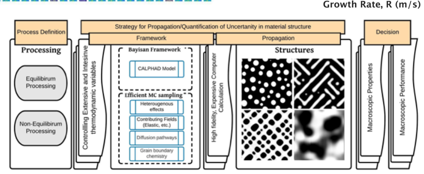
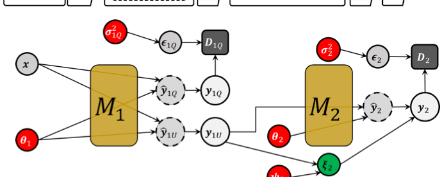
- UQ/UP is a central challenge to materials modeling and simulation-assisted materials design
- We have carried out massive HT phase field models to explore UP approaches in materials modeling
- Novel approaches to UP are being explored to make the process more efficient and practical
- UQ/UP through Bayesian Networks may be a promising approach when attempting simultaneous calibration of models along a complex model chain









THANKS