SAND2017-XXXXC

SAND2017-12923C

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Uncertainty Quantification and Data Science in Materials Applications

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LDRD

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Acknowledgements

With thanks to:

- Brad Boyce, Bradley Jared, Allen Roach, Stephen Foiles
- Jonathan Madison, John Mitchell, Dan Bolintineanu
- Bart van Bloemen Waanders, Tom Seidl, Tim Wildey
- Joe Bishop, Kyle Johnson
- Brian Adams, Mike Eldred, Jim Stewart
- Tim Trucano, Marty Pilch, Bill Oberkampf
- Prof. Yan Wang and Prof. Dave McDowell, Joel Blumer and Aaron Tallman
- …and many others

Data Science

- Wikipedia Definition:

Data science is an **interdisciplinary field about processes and systems to extract knowledge or insights from data in various forms**, either structured or unstructured, similar to data mining.

Data science employs techniques and theories **drawn from many fields** within the broad areas of mathematics, statistics, operations research, information science, and computer science, including signal processing, probability models, machine learning, statistical learning, data mining, database, data engineering, pattern recognition and learning, visualization, predictive analytics, uncertainty modeling, data warehousing, data compression, computer programming, artificial intelligence, and high performance computing.

[https://en.wikipedia.org/wiki/Data_science]

Uncertainty Quantification (UQ)

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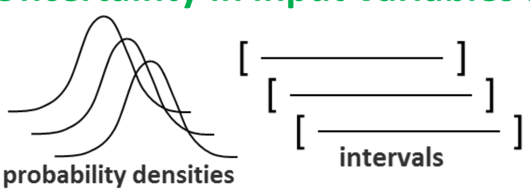
Goal: Account for natural variability and state-of-knowledge uncertainties affecting computational models.

Why? Uncertainty-aware predictions support risk-informed decision making, model validation, and robust design.

Forward UQ: propagate uncertainties to put error bars on simulation predictions

Uncertainty in input variables *u*



physical parameters / properties, initial/boundary conditions, numerical accuracy, geometry, data

Simulation Model *s(u)*

Statistics or intervals on output *s(u)*

Observations: experimental or upstream model

Inference / Inverse UQ: characterize parameter uncertainty from observations

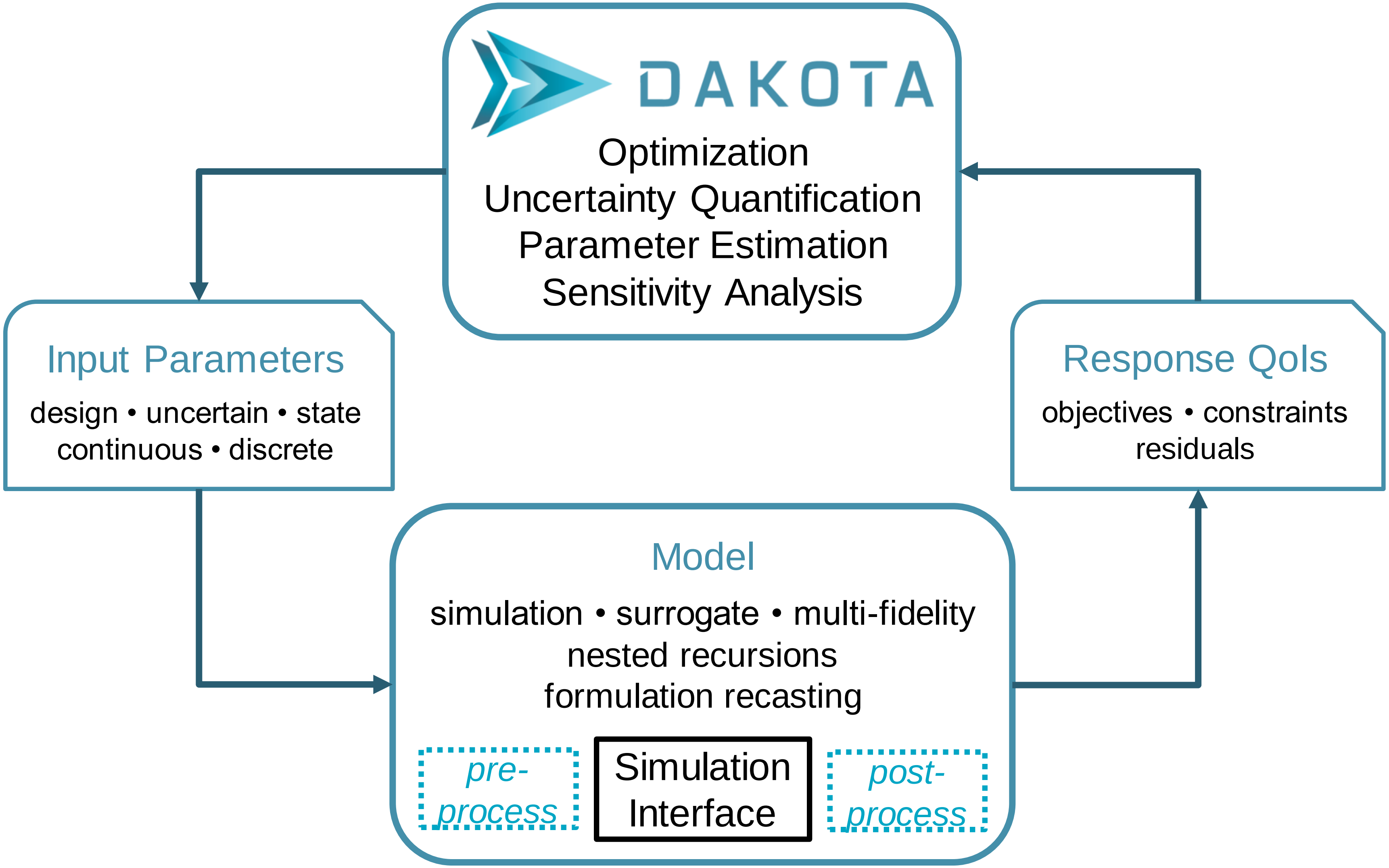
Data Science vs. UQ in Materials Modeling

- Data science seeks to provide analysis and linkages such as process-structure-property mappings
- Uncertainty quantification methods seek to propagate input uncertainties through simulation models to understand resulting output uncertainties.

- BOTH have a focus on multi-scale

This talk will address:

1. UQ Methods
2. Data Science examples
3. Closing thoughts



Available at https://dakota.sandia.gov

Uncertainty Quantification Methods

- Monte Carlo sampling:
  - LHS, Quasi MC, Design of Experiments, Adaptive Sampling
- Local and global reliability
  - Employ optimization to efficiently determine failure probabilities
- Polynomial chaos expansions / stochastic collocation
  - Large research investment, adaptive sparse grids, compressive sensing
- Mixed aleatory-epistemic approaches
  - Regulatory Requirements, "uncertainty on uncertainties"
- Surrogate Models: Gaussian processes, PCE, splines, etc.

We focus on UQ methods that are as efficient and accurate as possible assuming simulations are very costly.

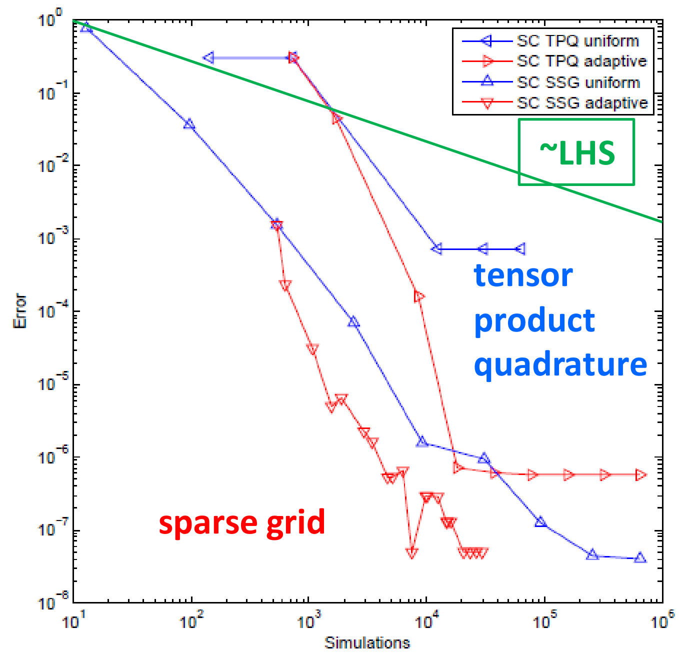
Dakota: State-of-the-Art UQ R&D

- Continual advanced algorithm R&D to tackle computational challenges (particularly in SNL's national security mission):
  - Severely constrained simulation budgets
  - High-dimensional parameter spaces
  - Nonsmooth or unreliable quantities of interest

- Notable active areas:
  - Multi-level, multi-fidelity UQ (and optimization)
  - Bayesian inference
  - Dimension reduction and surrogate modeling
  - Random field modeling
  - Discrepancy modeling

Stochastic Expansions: What Are They?

- General-purpose UQ methods that build UQ-tailored polynomial approximations of the output responses
- Perform particularly well for smooth model responses
- Resulting convergence of statistics can be considerably faster than sampling methods
- Two categories
  - Polynomial Chaos: specify the type of orthogonal polynomials and coefficient estimation scheme
  - Stochastic Collocation: specify the type of polynomial basis and the points at which the response will be interpolated

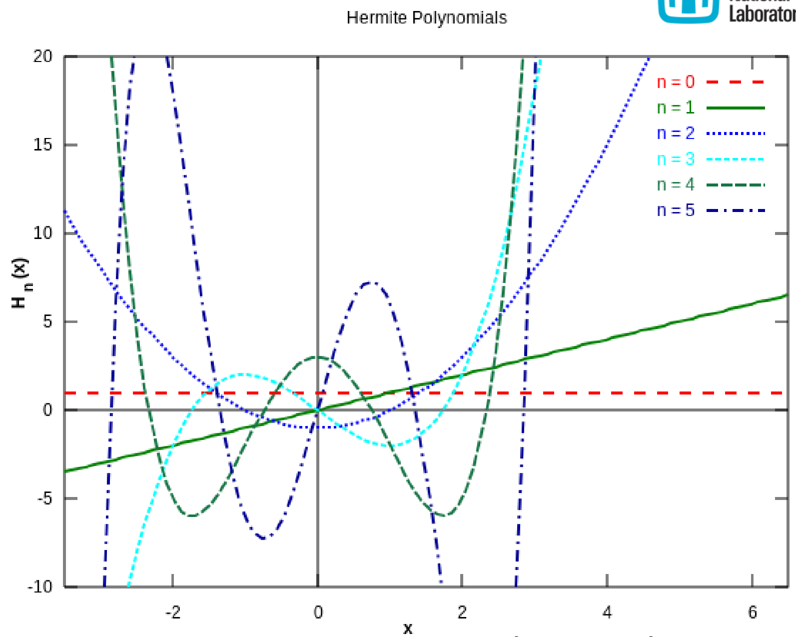


Polynomial Chaos: How Does It Work?

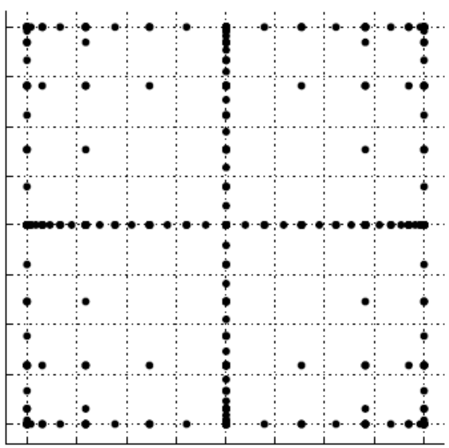
- Uses an orthogonal polynomial basis $\Psi_j(\xi)$, e.g., Hermite polynomials orthogonal w.r.t. normal density
- Evaluates the model in a strategic way (sampling, quadrature, sparse grids, cubature)…
- …to efficiently approximate the coefficients of an orthogonal polynomial approximation of the response

$$R = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\boldsymbol{\xi})$$

$$\alpha_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j^2 \rangle} = \frac{1}{\langle \Psi_j^2 \rangle} \int_{\Omega} R \, \Psi_j \, \varrho(\boldsymbol{\xi}) \, d\boldsymbol{\xi}$$



Hermite Polynomials


Sparse Grid

Why is polynomial chaos not used more in materials science?

- Possible reasons:
  - Non-smooth responses. This is not a showstopper, but the accuracy of the expansion degrades around discontinuities
  - The stochastic nature of some of the simulations. That is, we are not trying to approximation a deterministic input→output mapping.
  - Lack of software to calculate the polynomial terms and their coefficients
    - There are a number of toolkits available now
  - Lack of familiarity, coupled with the fact that everyone knows Monte Carlo sampling

Adaptive Basis Selection: Compressed Sensing in High Dimensions

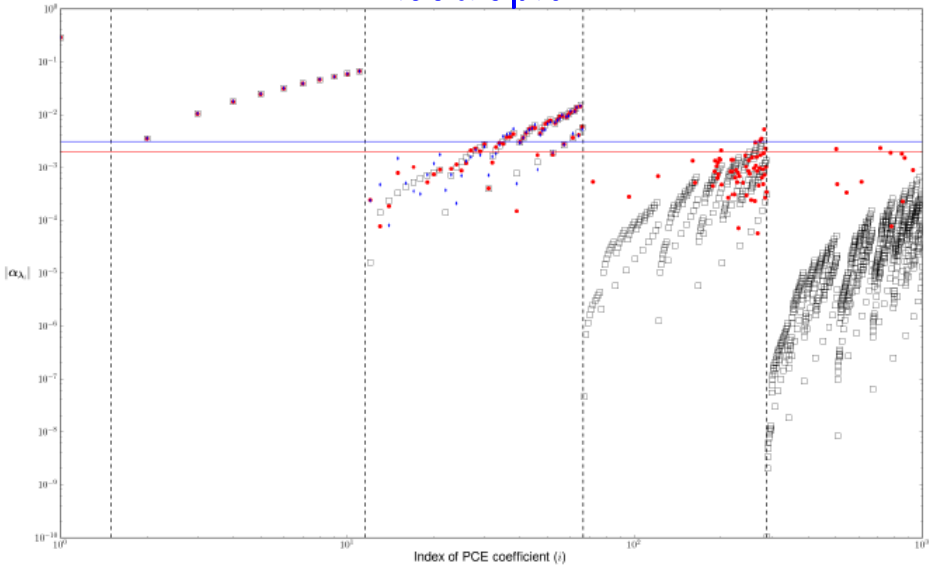
In high dimensions, we may only be able to consider a 2nd or 3rd degree total-order basis

p	3	4	5
$\mathcal{A}_{3,1}^{40}$	$12,341$	$135,751$	$1,221,759$

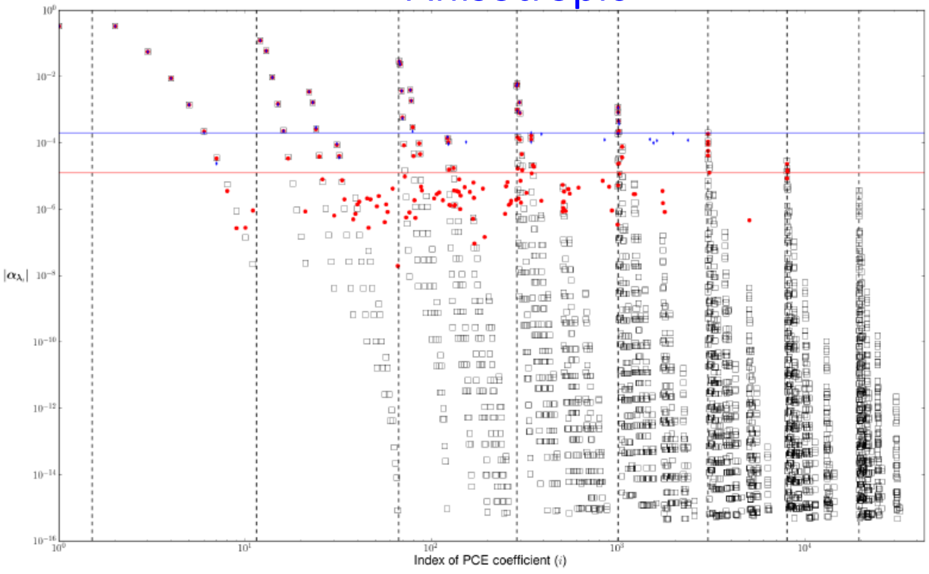
What if the function is anisotropic and important coefficients correspond to p > 3?

We seek algorithms that can adaptively determine an effective basis → *expanding front*

Isotropic



Anisotropic



Bayesian Calibration

- **Goal of Bayesian methods: Obtain statistical characterization of parameters consistent with data and its associated uncertainty**
- Generate posterior distributions on model parameters, given
  - Experimental data
  - A prior distribution on model parameters
  - A presumed probabilistic relationship between experimental data and model output that can be defined by a likelihood function

$$\pi(\theta \mid d) \propto \pi(\theta) L(d \mid \theta)$$

Posterior distribution

Model parameters

Observed Data

Prior parameter distribution

Likelihood function which Incorporates the model

Bayesian Calibration

- Experimental data = Model output + error

$$d_i(\mathbf{x}_i) = M(\boldsymbol{\theta}, \mathbf{x}_i) + \varepsilon_i$$

- If we assume error terms are independent, zero mean Gaussian random variables with variance σ^2, the likelihood is:

$$L(\boldsymbol{\theta}) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \mathbf{exp}\left[-\frac{(d_i(\mathbf{x}_i) - M(\boldsymbol{\theta}, \mathbf{x}_i))^2}{2\sigma^2} \right]$$

- How do we obtain the posterior?
  - We use a technique called Markov Chain Monte Carlo (MCMC)
  - In MCMC, the idea is to *generate a sampling density that is approximately equal to the posterior.*
  - MCMC algorithms are computationally expensive: Typically requires $O(10^4) – O(10^5)$ samples → prohibitive for high fidelity models

Bayesian Calibration

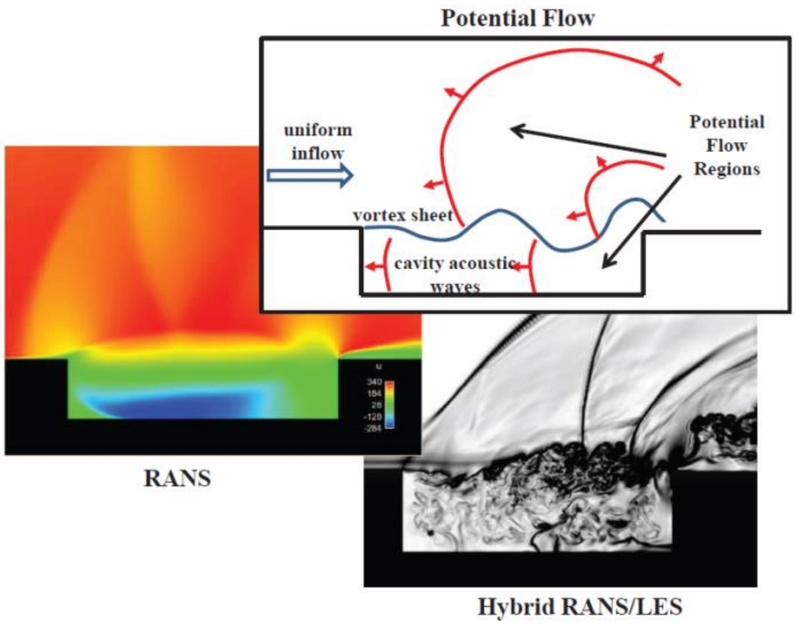
- Efficient methods for MCMC
  - Surrogate models, PCE. Adapt the emulator in regions of high likelihood
  - DRAM algorithms: Adapt the proposal covariance based on the accepted samples. Precondition the proposal covariance by the inverse of the Hessian of the posterior.
  - Hybrid MCMC: introduce an auxiliary momentum vector and implement Hamiltonian dynamics, so the potential energy function is the target density.
- Problems:
  - Bayesian analysis is conceptually attractive
  - **But it is difficult to obtain good posteriors**
  - MCMC algorithms are very expensive, need a good "mixing" of the chains, easy to get garbage posteriors and not realize it, results are highly dependent on assumptions made about process variance

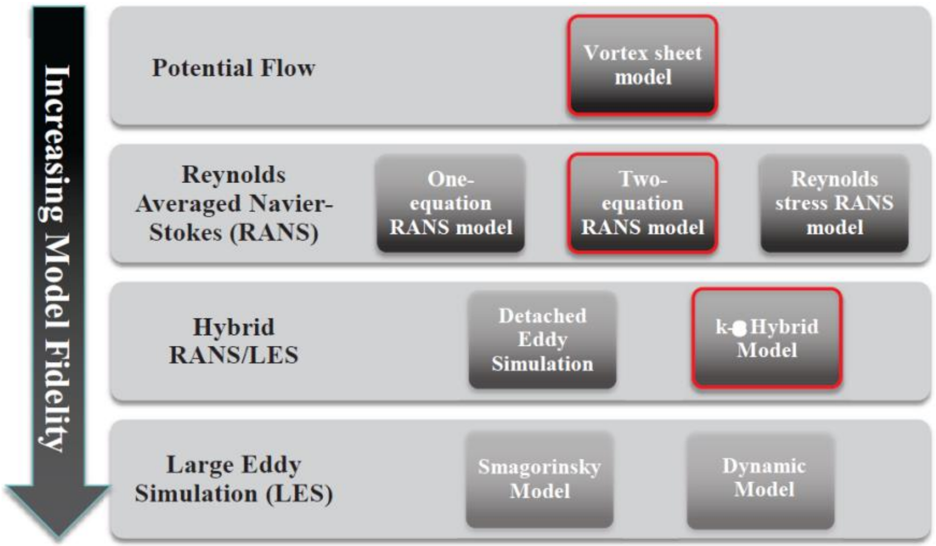
Multi-fidelity

Discrete model choices for same physics

- A clear hierarchy of fidelity (low to high)
- The model inputs and outputs are the same

Horizontal Axis Wind Turbine | *Vertical Axis Wind Turbine*





Multifidelity UQ using Stochastic Expansions

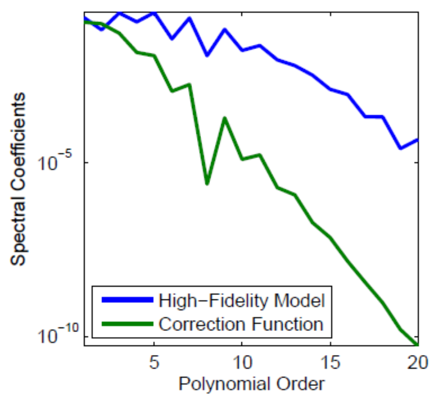
- High-fidelity simulations (e.g., RANS, LES) can be prohibitive for use in UQ
- Low fidelity “design” codes often exist that are predictive of basic trends
- Can we leverage LF codes w/i HF UQ in a rigorous manner? → global approxs. of model discrepancy

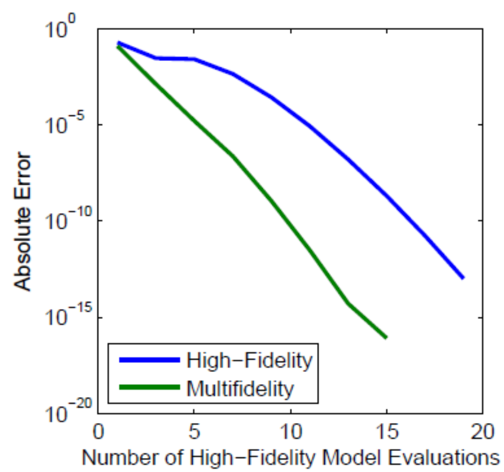
$$\hat{f_{hi}}(\xi) = \sum_{j=1}^{N_{lo}} f_{lo}(\xi_j) L_j(\xi) + \sum_{j=1}^{N_{hi}} \Delta f(\xi_j) L_j(\xi)$$

$N_{lo} >> N_{hi}$

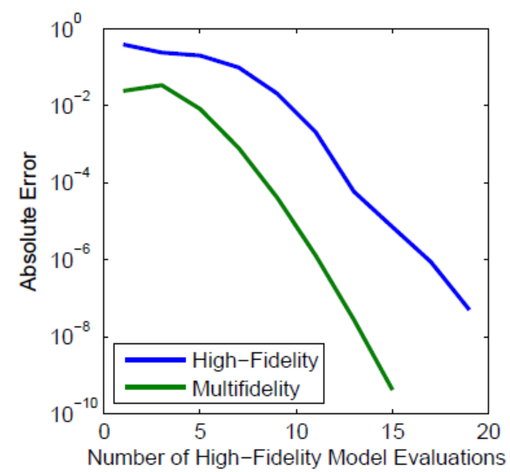
$$R_{\text{high}}(\xi) = e^{-0.05\xi^2}\cos 0.5\xi - \underbrace{0.5e^{-0.02(\xi-5)^2}}_{\text{discrepancy}}$$

$$R_{\text{low}}(\xi) = e^{-0.05\xi^2}\cos 0.5\xi,$$





(a) Error in mean



(b) Error in standard deviation

Low fidelity

CACTUS: Code for Axial and Crossflow TUrbine Simulation

High fidelity: DG formulation for LES

Full Computational Fluid Dynamics/

Fluid-Structure Interaction

Multi-level Monte Carlo

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Monte Carlo estimator: $\hat{Q} = \frac{1}{N}\sum_{i=1}^{N} Q_i$ → analytic variance $Var[\hat{Q}] = \frac{\sigma_Q^2}{N}$

Geometrical MLMC – targeting discretization levels

Multilevel Monte Carlo estimator

$$\hat{Q}_M^{\mathrm{ML}} \stackrel{\mathrm{def}}{=} \sum_{\ell=0}^{L} \hat{Y}_{\ell,N_\ell}^{\mathrm{MC}} = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left(Q_{M_\ell}^{(i)} - Q_{M_{\ell-1}}^{(i)} \right)$$

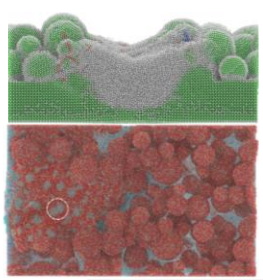
$$\left. \begin{aligned} \mathcal{C}(\hat{Q}_M^{ML}) &= \sum_{\ell=0}^{L} N_\ell \mathcal{C}_\ell \\ \sum_{\ell=0}^{L} N_\ell^{-1} \mathbb{V}ar\left(Y_\ell\right) &= \varepsilon^2/2 \end{aligned} \right\} \xrightarrow{\textit{Lagrange multipliers}} \boxed{N_\ell = \frac{2}{\varepsilon^2} \left[\sum_{k=0}^{L} \left(\mathbb{V}ar\left(Y_k\right) \mathcal{C}_k \right)^{1/2} \right] \sqrt{\frac{\mathbb{V}ar\left(Y_\ell\right)}{\mathcal{C}_\ell}}}$$

[Giles, 2008]

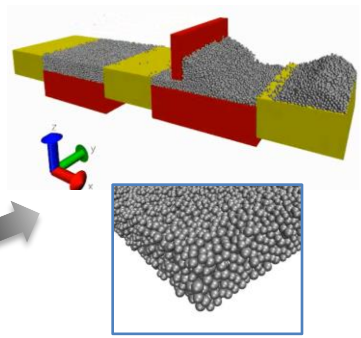
Additive Manufacturing Modeling

Codes
LAMMPS, SPPARKS,
Sierra/Aria, Sierra/Adagio

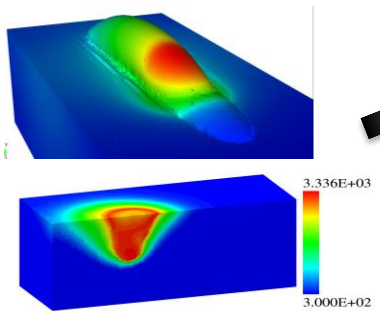
Powder Behavior
Mark Wilson



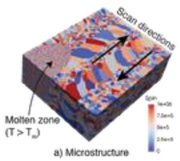
Powder Spreading
Dan Bolintineanu



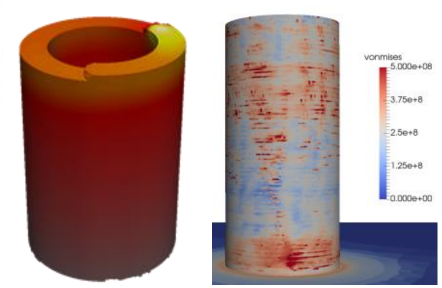
Mesoscale Thermal Behavior Mario Martinez & Brad Trembacki



Mesoscale Texture/Solid Mechanics/CX
Judy Brown, Theron Rodgers and Kurtis Ford



Part Scale Thermal & Solid Mechanics
Kyle Johnson, Kurtis Ford & Joe Bishop



Part Scale Microstructure
Theron Rodgers

10^{-6} 10^{-3} 1

Length Scale (m)

Data Science

Data Science in Born Qualified

1. Statistical Analysis Techniques of both Process Data and Coupon/Part Data
2. Microstructural Analysis
3. Design of Experiments
4. Surrogate models
5. Data management/archiving and dimension reduction methods
6. Optimization: control, design of parts and processes, experimental design

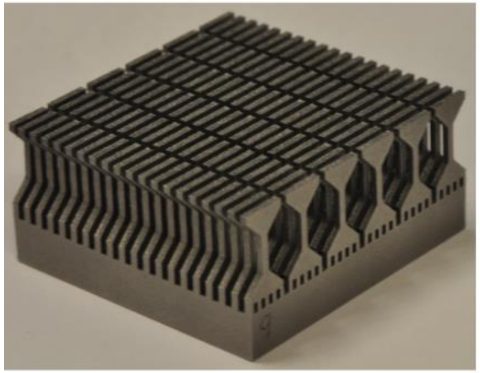
→

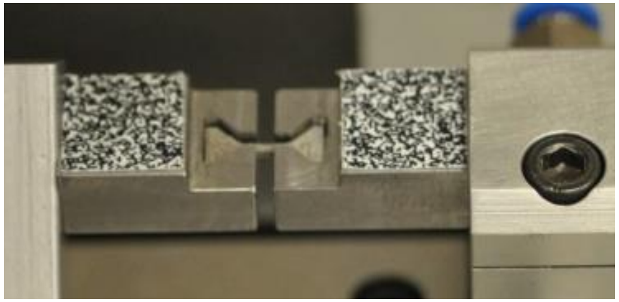
- Process Development and Control (LENS, Powder Bed, Direct Write)
- Prototype Evaluation (Three exemplars)
- Predict Performance

Goal is to change the change the engineering design and qualification paradigm for component design and manufacturing

120 Dogbone Specimens

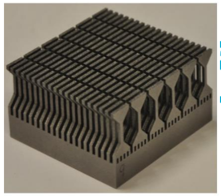
- Array of 120 tensile bars of 17-4PH stainless steel made on powder bed machine
- Focus on high-throughput tensile testing
- More details in *Journal of Materials Processing Technology*, including differences in Weibull distributions with small sample numbers vs. full set of 109 samples.



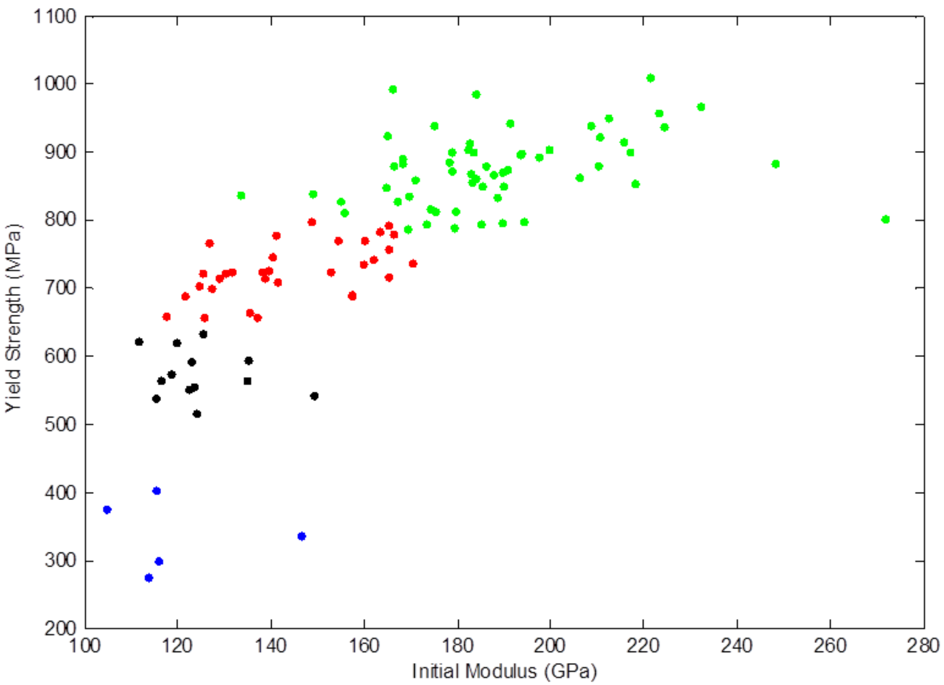


Salzbrenner, B. C., J. M. Rodelas, J. D. Madison, B. H. Jared, L. P. Swiler, Y. Shen, and B. L. Boyce. "High-Throughput Stochastic Tensile Performance of Additively Manufactured Stainless Steel." *Journal of Materials Processing Technology*, Vol. 241, pp.1-12, March 2017.

Cluster Analysis

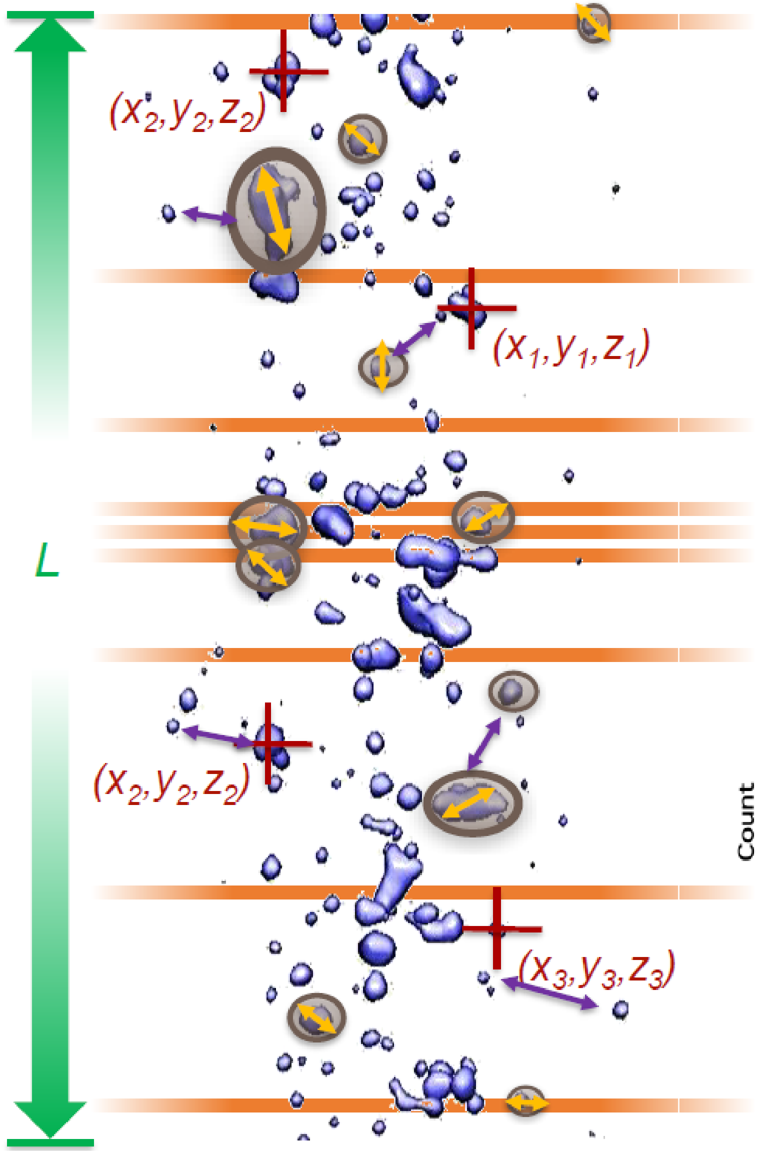


- 15 attributes were measured, including density, mass, dimensions, initial and unloading modulus, yield and tensile strength, ductility
- Correlation matrix shows less correlation than expected
- Performed k-means clustering on the data set.
- Successful grouping into four clusters, some identification of clusters with build position

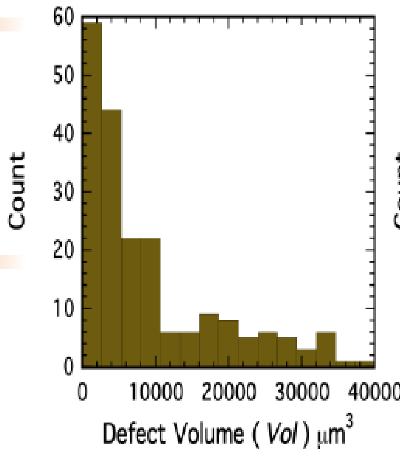


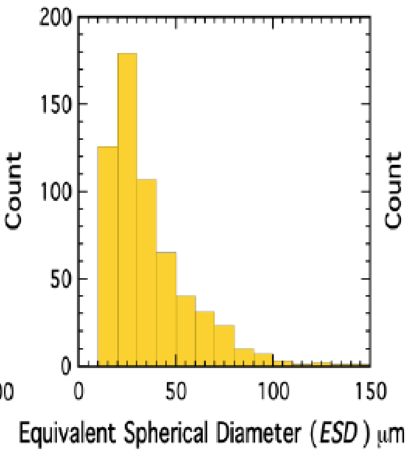
	A	B	C	D	E	F
1	3	3	3	3	3	3
2	3	3	3	3	3	2
3	3	3	3	3	3	3
4	3	3	3	3	3	3
5	3	3	3	3	3	3
6	3	3	4	3	3	3
7	3	3	3	3	3	1
8	3	3	3	3	3	1
9	3	1	1	1	4	3
10	3	1	4	3	4	1
11	3	1	1	1	1	3
12	1	1	2	1	2	3
13	3	1	4	1	1	3
14	1	3	4	4	4	3
15	1	1	1	1	1	
16	3	1	4	2	1	
17	3	1	2	4	1	
18	3	3	4	1	1	
19	1	4	1	4	1	

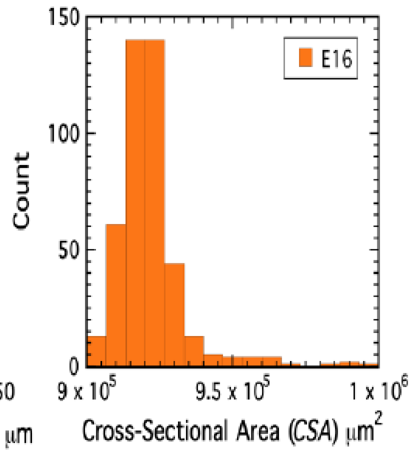
Defect Characterization



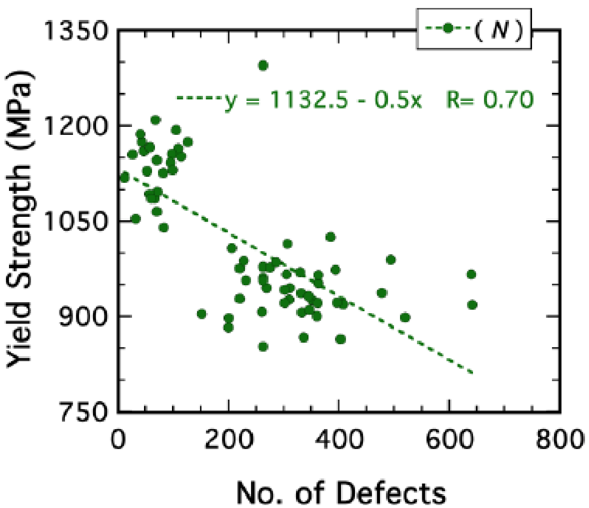
- Total Volume of Defects (V_{tot})
- Pore Volume Fraction (V_{fract})
- Spatial Location of Pores (*x, y, z*)
- Total Number of Defects (*N*)
- Total Defects/Length (*N/L*)
- Average Defect Volume ($V_{avg.}$)*
- Average Equivalent Spherical Diameter ($ESD_{avg.}$)*
- Average Cross-Sectional Area ($CSA_{avg.}$)*
- Average Nearest Neighbor Distance ($NND_{avg.}$)*

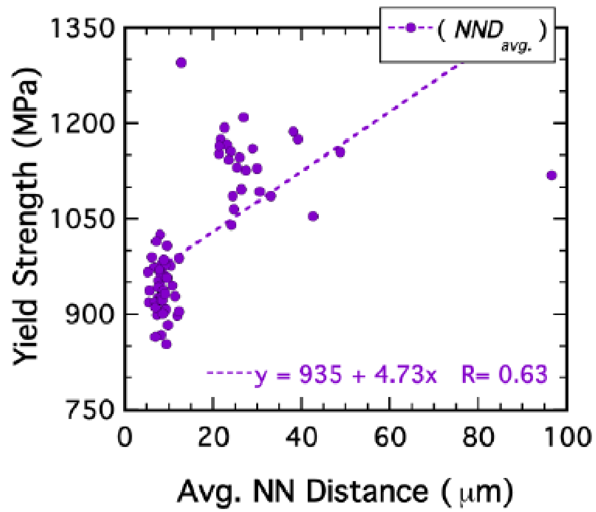


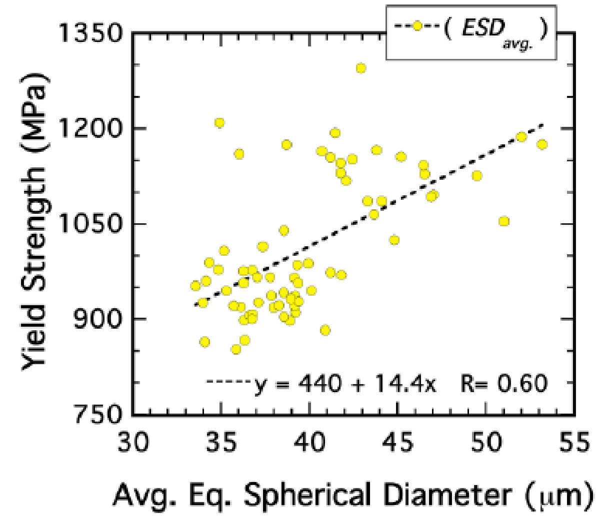


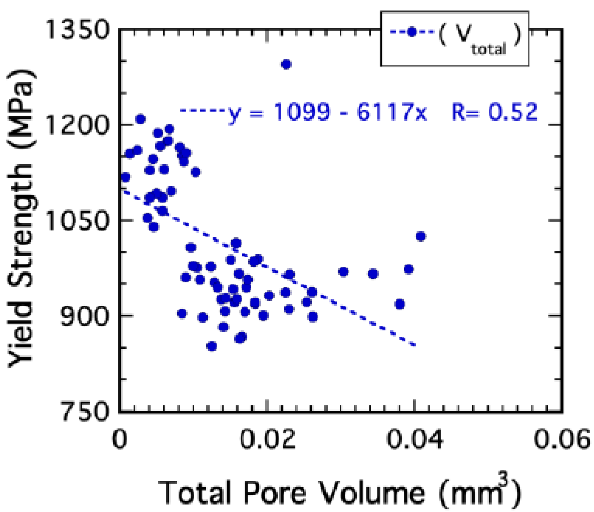


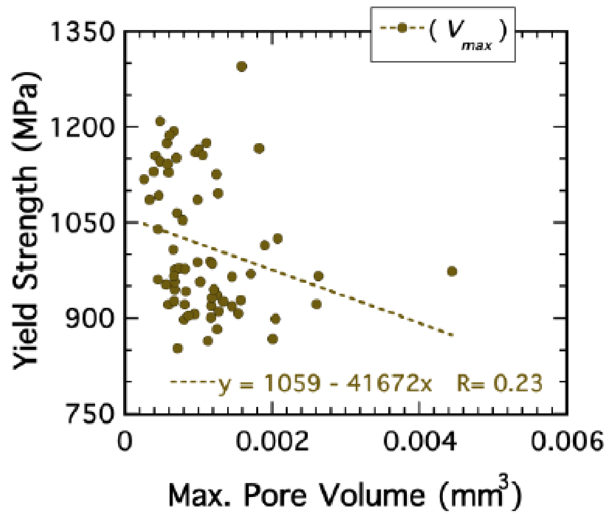
Individual Correlations with YS







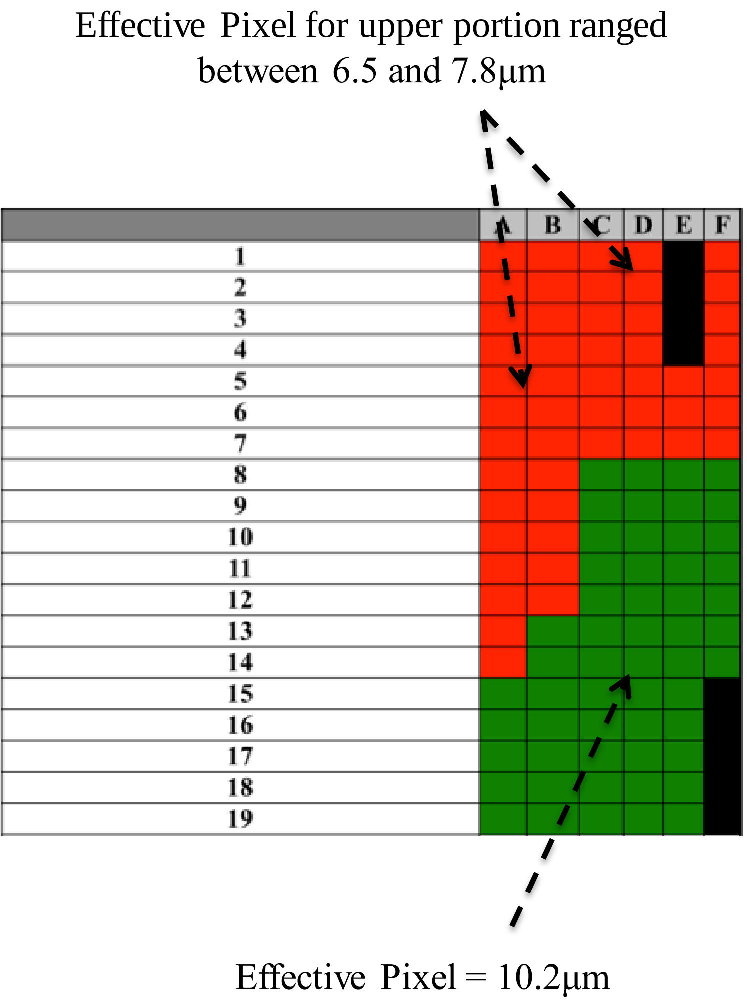




In relation to Y.S.

Measure	R value	R^2
No. of Defects	-0.705	0.50
Avg. NN Distance (mm)	0.631	0.40
Avg. ESD (mm)	0.601	0.36
Max CSA Redux (mm^2)	-0.581	0.38
Total Pore Volume (mm^3)	-0.518	0.27
Avg. Defect Vol. (mm^3)	0.500	0.25
Max CSA Redux (%)	-0.486	0.24
Maximum Pore Size	-0.257	0.07

Two-point correlation

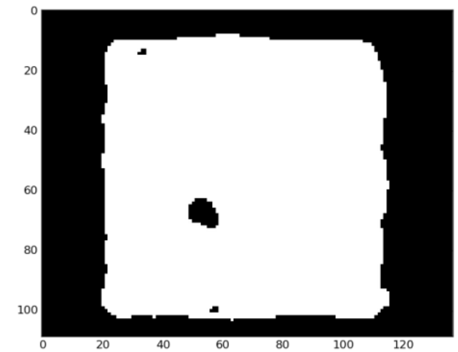


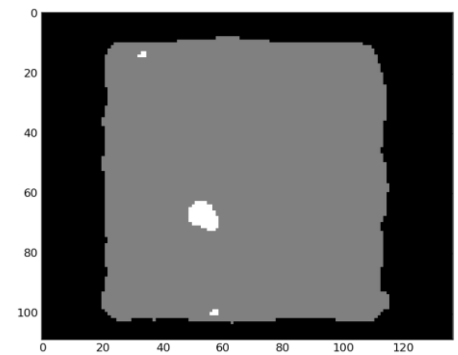
- Started with lower portion of the build plate to use a consistent voxel size
- Used Dan Bolintineanu's PyMu software which is similar to PyMKS: Python library to perform statistical analysis of microstructures
- Each dogbone has a different number of tiff images, sometimes a different number of X-Y voxels

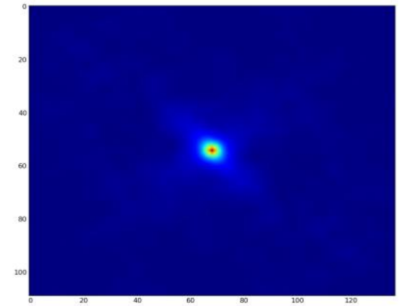
2-point statistics

- Approach:
  - Filter the data to find the minimum domain size
  - Create mask by setting exterior to -1 with connected components algorithm. Exterior is -1, pore is 1, solid is 0
  - Take s2 (using normalized cross correlation)
  - Crop s2 to minimum domain size
  - Flatten s2, stack into PCA matrix
  - Perform SVD on PCA matrix

  - PCA matrix is 44 rows x 1.7M columns
  - Poor results: not seeing 2-3 principal components. It requires 32 components to account for 90% of the variance.







High-throughput tests

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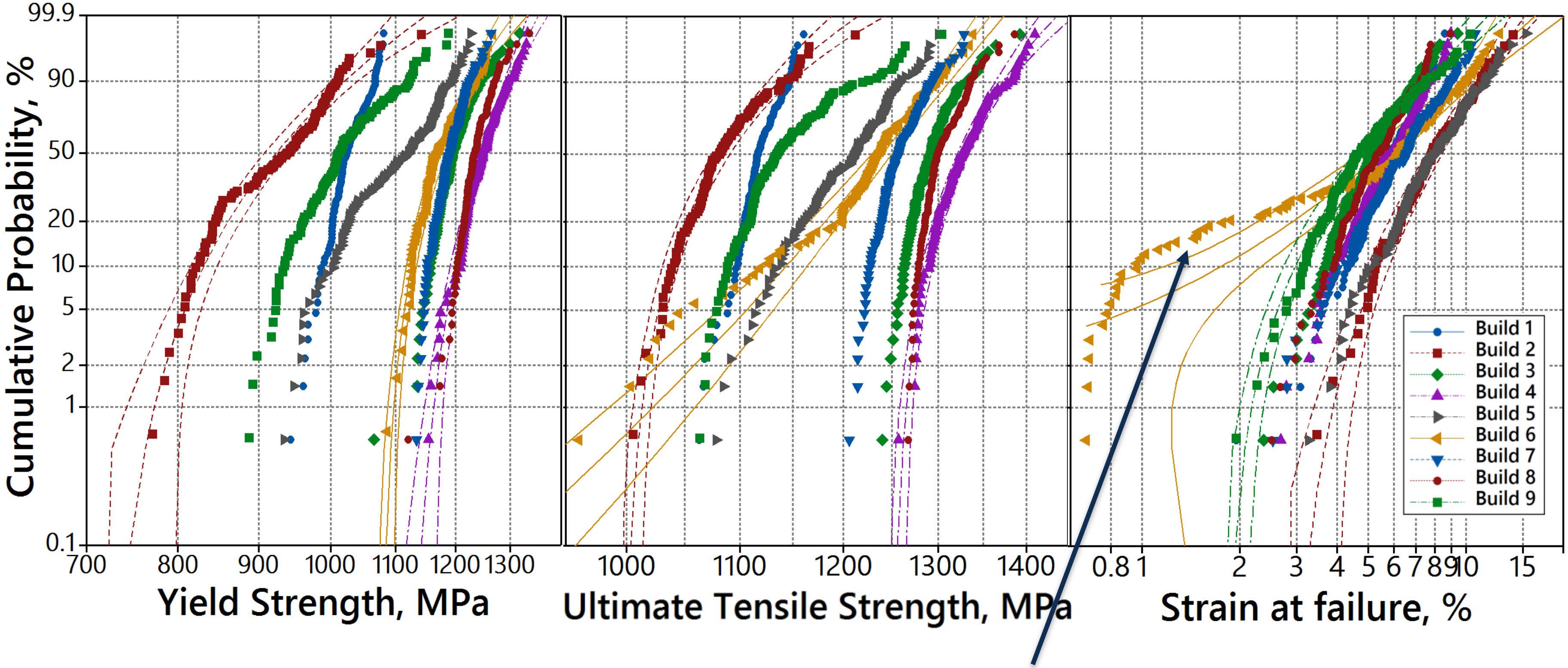
- Tested 9 builds, each one with 6 columns by 20 rows of tensile bars, 1065 specimens
- Produced with same build file on nominally identical Concept Laser Mlab printers



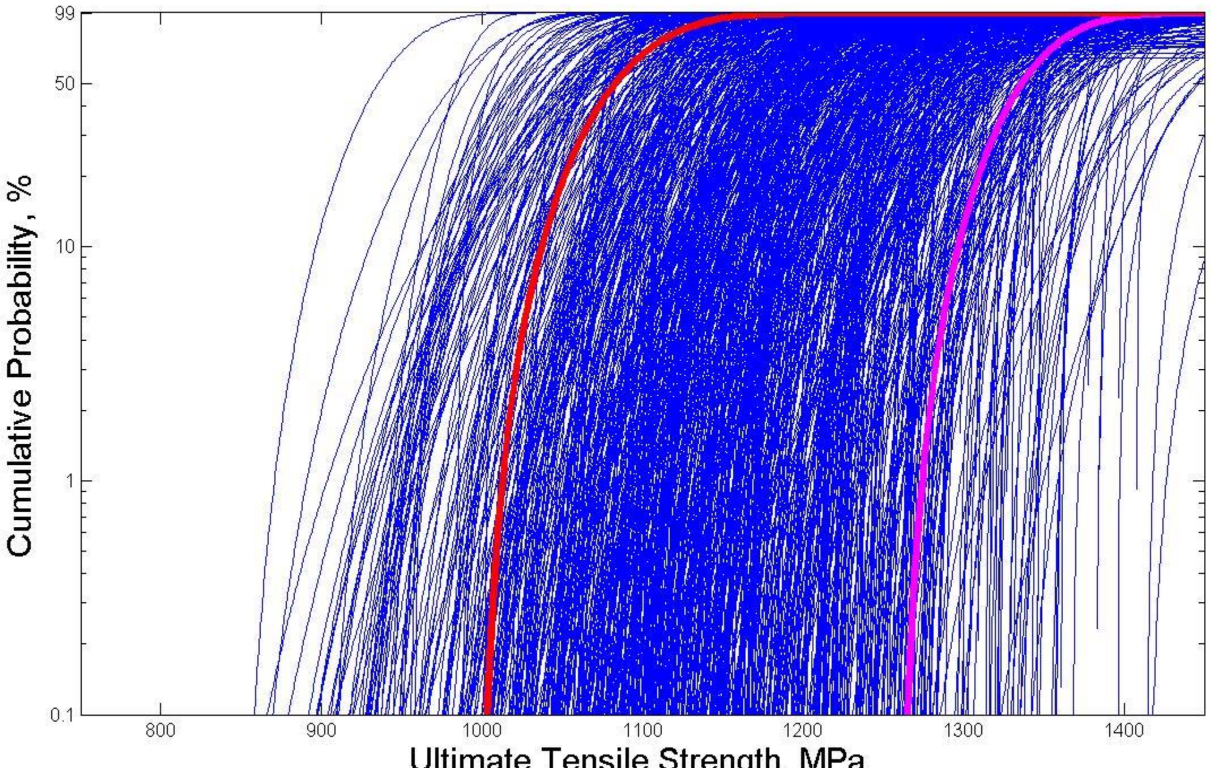
- Build 6 contained 25 instances of failure strains below 1.95% whereas the other eight builds all exhibited values above 1.95%. The loss of ultimate strength was caused by the low ductility.

Boyce, B. L., Salzbrenner, B. C., Rodelas, J. M., Swiler, L. P., Madison, J. D., Jared, B. H. and Shen, Y.-L. (2017), "Extreme-Value Statistics Reveal Rare Failure-Critical Defects in Additive Manufacturing". *Advanced Engineering Materials*. 1700102. doi:10.1002/adem.201700102

Epistemic Treatment of Build-to-Build Variation

$$P = 1 - e^{\left[-\left(\frac{(\alpha-\gamma)}{(\eta-\gamma)}\right)^{\beta}\right]}$$

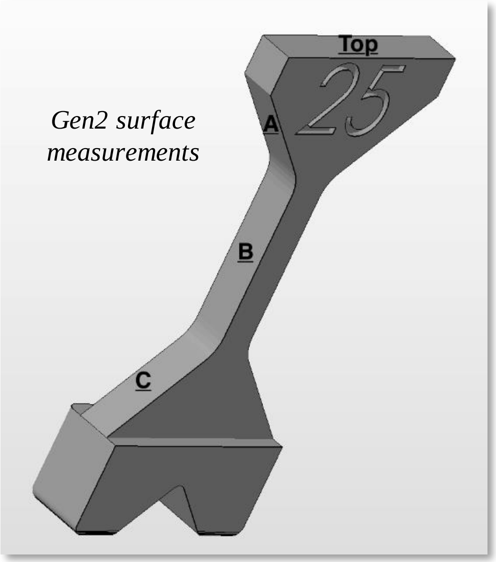
Removing Build 6, we have eight values of the 3 Weibull parameters (β, η, γ). Treating this as a multivariate normal, we drew 1000 realizations of the 3 Weibull parameters. Builds 2 and 4, the bounding cases, are colored in red and magenta, respectively.



316L Stainless Steel Process Sensitivity

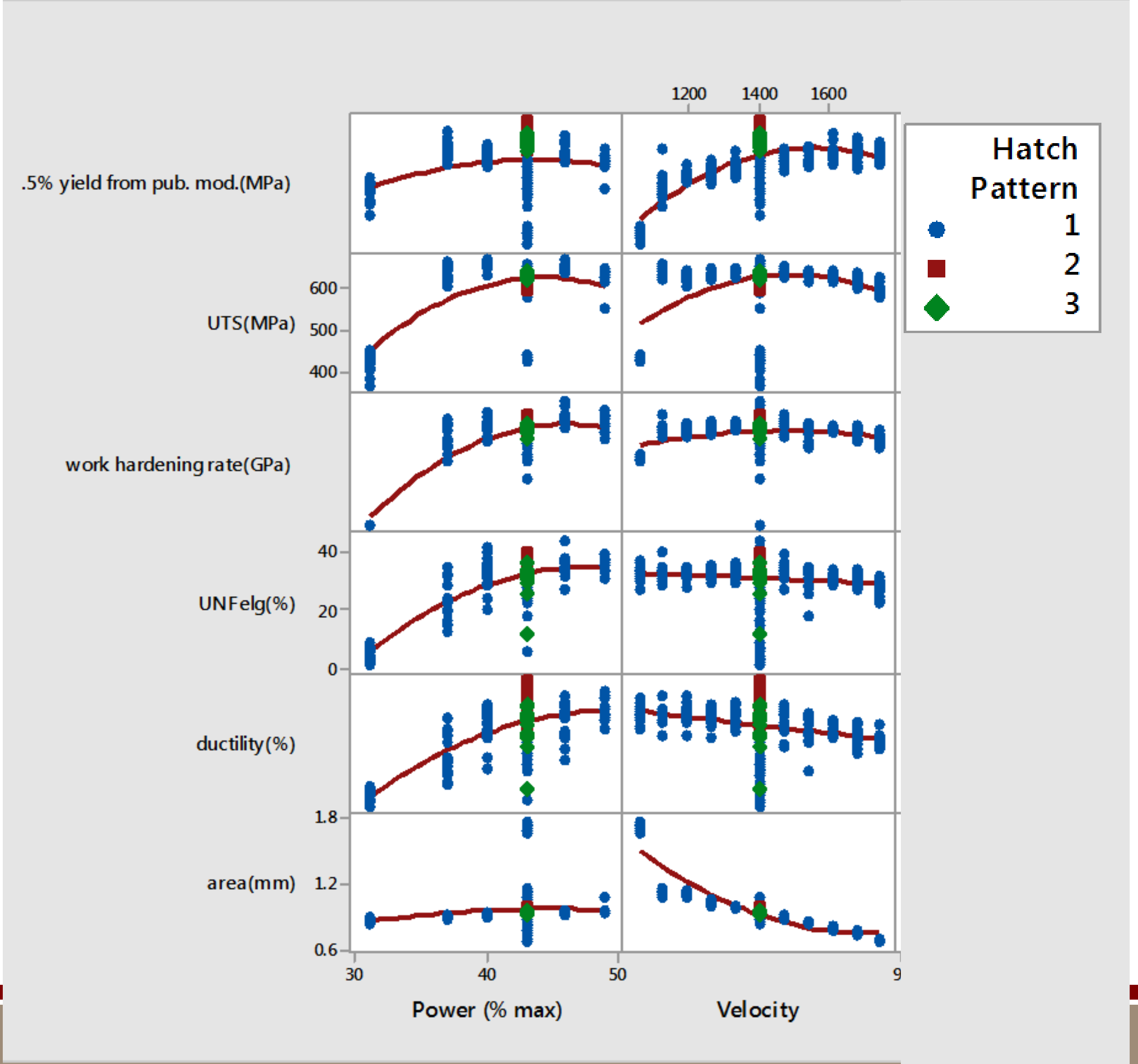
- Process variables
  - Vary individually
  - printed: power, velocity, hatch spacing, scan strategy
  - planned: focus, layer thickness, O_2 level, powder recycling
- Measurements
  - top surface distortion (after EDM)
  - surface finish (top, side, angles)
  - Archimedes density
  - CT
  - resonance testing
  - tensile testing
  - metallography, fractography
- Leveraging tools to quantify relationships
  - how well can process changes be identified?

316L SS samples w/varying laser power



Statistical Analysis of Experiments on ProX200 Machine at SNL

- Hatch pattern 1 is hexagonal, 2 is mesh, 3 is normal.
- The red line is a best fit quadratic function,
- Power is best correlated with UTS, work hardening, UNFelg, ductility
- Velocity is correlated with area

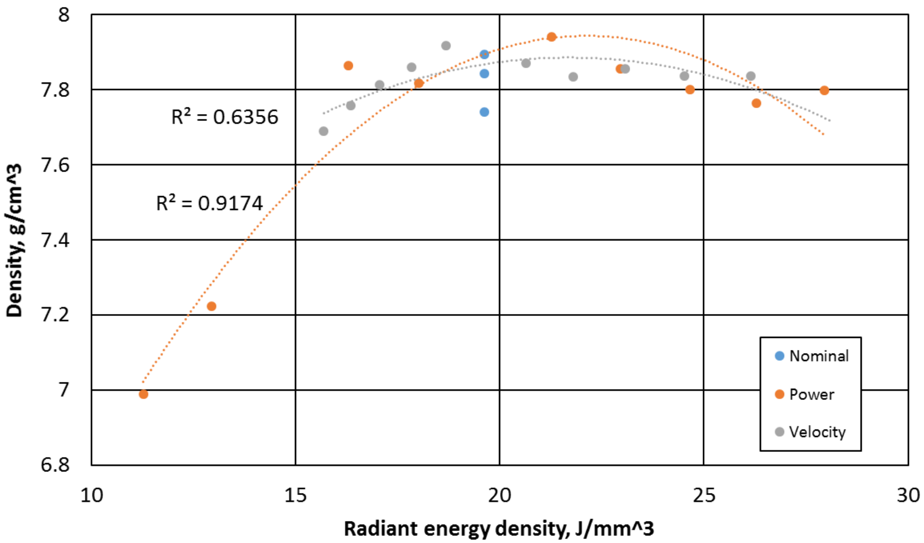


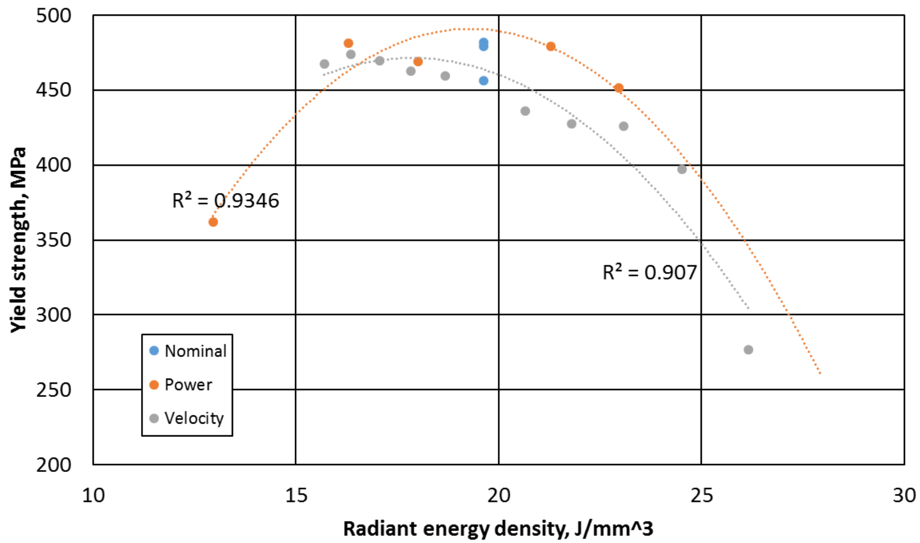
Statistical Analysis of Experiments on ProX200 Machine at SNL

	.5% yield from pub. mod.(MPa)	*.5% yield from unloading mod.(MPa)*	*unloading modulus(GPa)*	*UTS(MPa)*	*work hardening rate(GPa)*	*UNFelg (%)*	*ductility (%)*	*area (mm)*	*Power (% max)*
.5% yield from pub. mod.(MPa)	1.00								
.5% yield from unloading mod.(MPa)	0.99	1.00							
unloadingmodulus(GPa)	0.74	0.72	1.00						
UTS(MPa)	0.52	0.79	0.83	1.00					
work hardening rate(GPa)	0.61	0.56	0.56	0.75	1.00				
UNFelg(%)	0.28	0.27	0.24	0.58	0.80	1.00			
ductility(%)	0.18	0.11	0.12	0.45	0.70	0.91	1.00		
area(mm)	-0.48	-0.75	-0.63	-0.50	-0.14	0.09	0.22	1.00	
Power (% max)	0.19	0.23	0.19	0.51	0.68	0.74	0.68	0.10	1.00
Velocity	0.40	0.59	0.38	0.27	0.09	-0.08	-0.24	-0.84	0.00
Hatch Pattern	0.21	0.26	0.15	0.06	0.07	0.06	0.07	-0.02	0.05
Density	0.22	0.27	0.38	0.68	0.74	0.72	0.62	0.18	0.74

- Scan velocity was most strongly negatively correlated with area of the dogbone. As the velocity increases, the area decreases.
- Power was strongly positively correlated with the work hardening rate, UNFelg, and ductility.
- Power and density were strongly correlated, but power was not particularly correlated with the yield strength numbers.

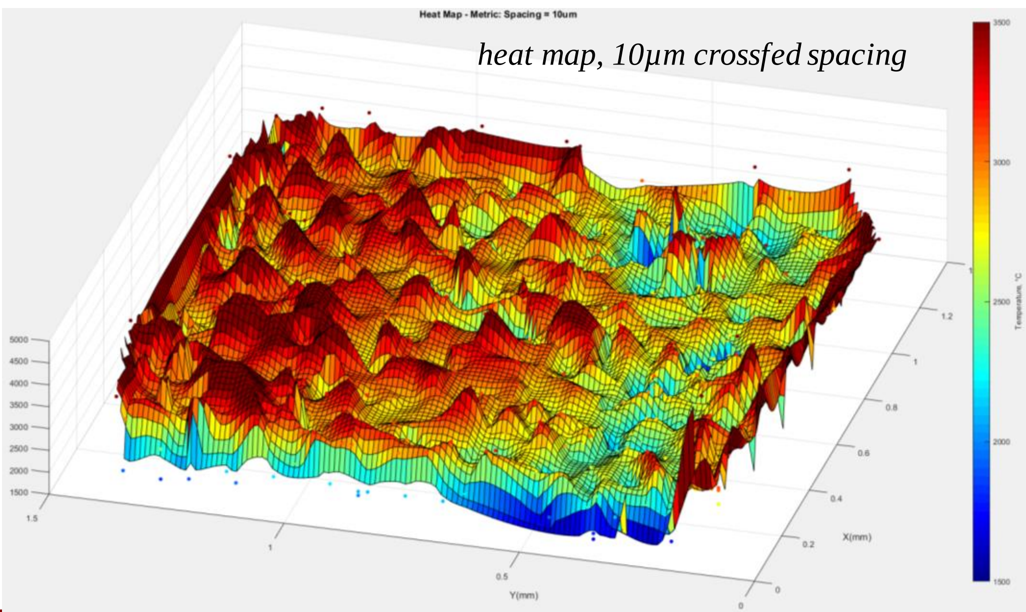
316L Process Impacts

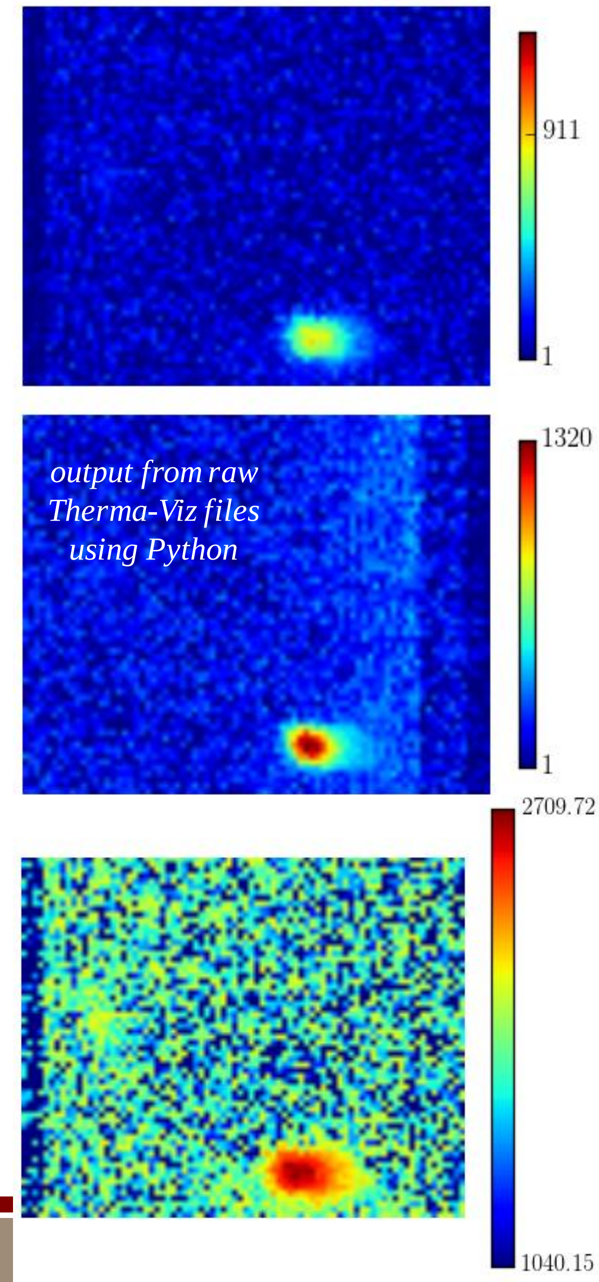




Therma-Viz Data Analysis

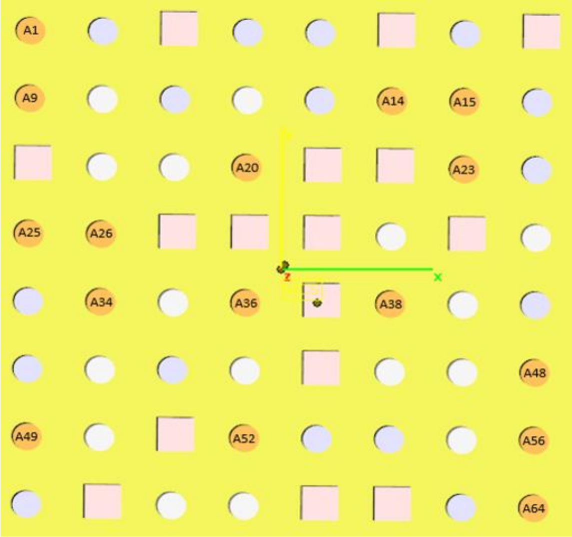
- Melt pool metrics
  - peak temperature
  - centroid location
  - area, length, width
- Need capability to analyze 100K images, overcome the relative temperature issue





Use of spatial process to correlate material properties

- On one build plate, different specimens were constructed for testing of tensile properties, impact, and hardness
- Since the specimens were at different locations on the plate and also at different locations across builds, we constructed a Gaussian process (GPs) for each property as a function of (X,Y).
- Sampling the GPs on a regular grid then gave a comparable set of points at which to correlate the properties



Example Build Plate

	Tensile strength (MPa)	0.2% Yield Strength (MPa)	Charpy Impact	Hardness HV_500
Tensile strength (MPa)	1.00			
0.2% Yield Strength (MPa)	0.97	1.00		
Charpy Impact	0.32	0.32	1.00	
Hardness HV_500	0.40	0.45	0.17	1.00

Examples of Data Analysis

- Correlation of material properties (yield strength, tensile strength, ductility) to pore information from CT (number of pores, size or volume of pores, etc.)
- Models predicting yield strength as a function of other variables, pore data.
- Spatial variability of data across the build plate
- Spatial variability within a dogbone
- Process maps: laser power -> melt pool properties -> material properties
- Relationship of surface finish to laser power
- ETC.

Verification and validation for Integrated Computational Materials Engineering (ICME)

Do you know how good (or bad) your modeling and simulation is?

- Perform due diligence and communicate frankly about assumptions, approximations, and limitations affecting simulation credibility.

Nothing against ostriches, of course

Elephants in the Room

- We need to make better use of experimental data.
  - We tend to only use experimental data for calibration of a particular subset of parameters
  - Bayesian calibration only implicitly incorporates uncertainty in the experiments in the predictions. Ideally, we would use statistical mixture models which give equal weighting to experiments and simulations in predictions
- Where are the benchmark tests for V&V of multiscale materials models?
  - Verification: what is the analog to manufactured or analytic solutions of PDEs? What constitutes a strong test that a code must always pass?
  - Validation: What are multi-scale experiments used for comparison? Is the validation comparison always at the system level (e.g. stress-strain relationships) or can we validate intermediate quantities such as number of pores in an AM material?

Benchmark tests for multiscale materials modeling

- http://www.altairhyperworks.com/product/Multiscale-Designer
  - Multiscale Designer is an efficient tool for development and simulation of multiscale material models of … heterogeneous materials. Multiscale Designer - Mechanical has been validated against more than 50 benchmark problems at the coupon and component levels with various composite product forms.

- R. E. Miller and E. B. Tadmor. "A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods." *Modelling and Simulation in Materials Science and Engineering,* Volume 17, Number 5. 2009 IOP Publishing Ltd.
  - "Truth" or "Gold Standard" is atomistic simulation. Is this always correct?

- Is the ICME community developing standards?
  - ASME, *V&V 10-2006 Guide for Verification and Validation in Computational Solid Mechanics*, American Society of Mechanical Engineers (2006).

Closing thoughts

There are a number of efficient forward UQ propagation methods that may be used for multi-scale materials models

- Sampling, stochastic expansions
- Surrogates, meta-models
- Multi-fidelity approaches, multi-physics, multi-scale
- Research emphasizes scalability and exploitation of structure

Calibration is a big part of UQ, and may be used at various scales

- Challenges and opportunities with Bayesian calibration
- More careful use of experimental data

Data Science

- Additive technologies make it easy to generate lots of data
- Processing the data and identifying generalizable relationships still a challenge
- Much of the data science for materials involves experimental design and statistical characterization, but not necessarily simulation UQ

Extra slides