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Sensitivity of Void Mediated Failure to Geometric Design Features of Porous Metals

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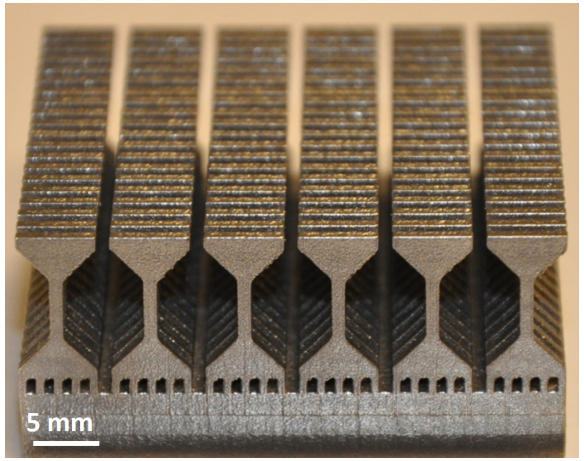
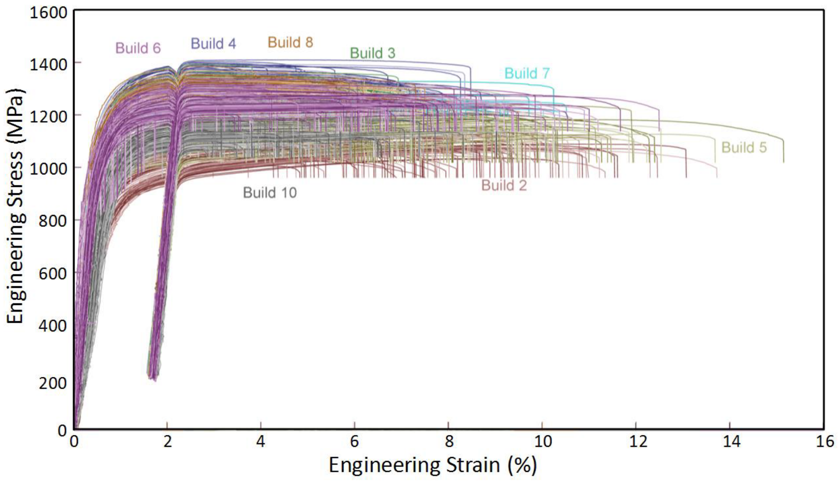
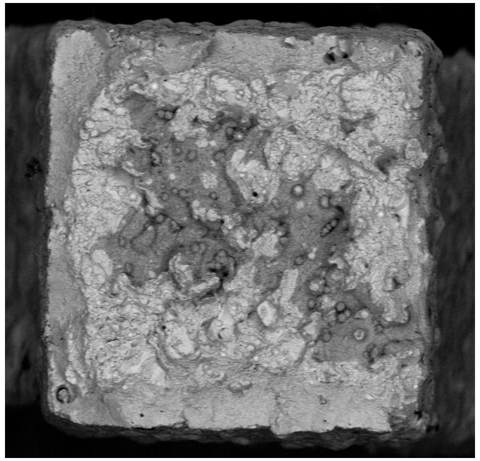
Susceptibility of Additive Manufacturing Processes to Variable Performance

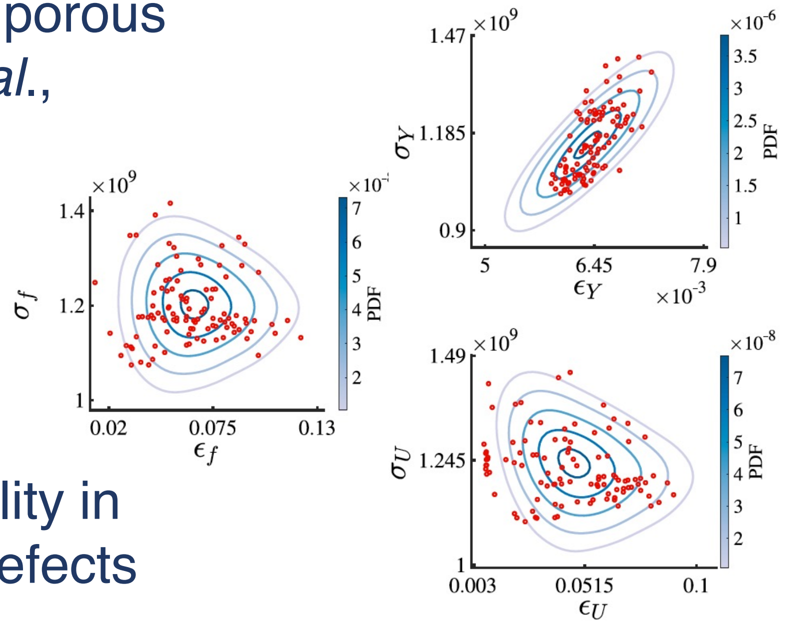
- Metal additive manufacturing (AM) is a relatively recent and now widespread manufacturing process:
  - ✓ Enables new levels of geometric complexity in design
  - ✗ Imprecise control of internal porosity, surface roughness, and conformity to designed geometry.
- There is a need to characterize the errors introduced by such processes and the propagation of such errors through numerical predictions.
- In our context, we see large variability in the mechanical responses due to manufacturing-induced defects and geometric deviation from the design targets.







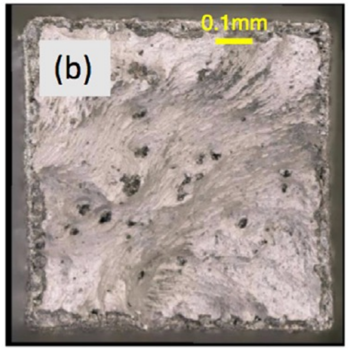
Effect of Manufacturing-Induced Porosity on Stress Concentrations

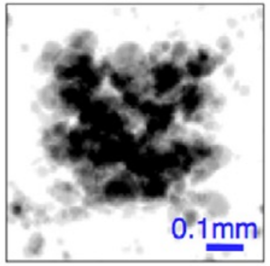


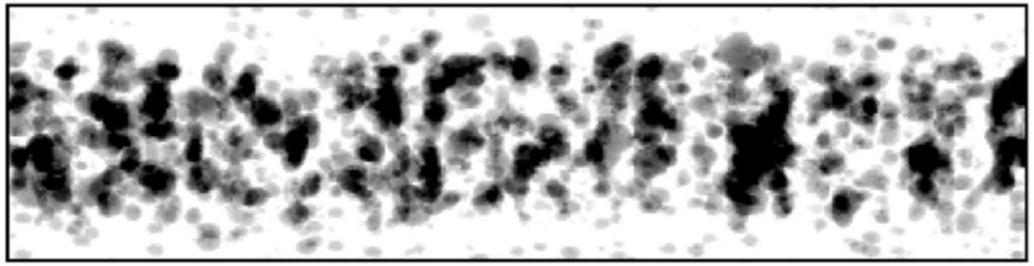
- **Previous work** [Khalil *et al.*, CMAME, 2021]: Developed a model of porous metal deformation and failure tuned to experimental data [Boyce *et al.*, AEM, 2017]:
  - Karhunen-Loève expansion (KLE) used to model to the experimentally-observed, AM-induced explicit porosity
    - Facilitated by the availability of new high-resolution data acquisition techniques
  - Bayesian techniques were used to represent the observed variability in mechanical responses due to porosity and other microstructural defects
- **Objective:** Investigate how stress concentrations due to geometric design features interact with AM-induced porosity
  - Quantify the probability of unexpected failure using statistical models based on a large sample (~10k) of the porosity realizations
  - Utilize the previously calibrated model along with porosity KLE model
  - To establish quantitative relationships between geometric and material defects, we focus on a double U-notched specimen, a test geometry commonly

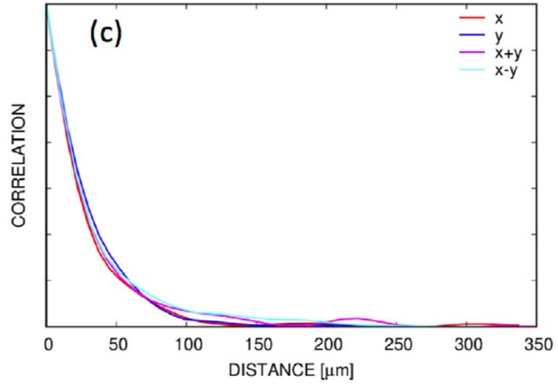
Explicit Characterization of Porosity in AM Materials – CT Scans

- In order to study the interplay of geometric design features and explicitly modeled pores arising from additive manufacturing, a generative model for the explicit porosity is needed:
  - Consistent with statistical properties of porosity process
    - Available 3-dimensional CT scans, at 7.5 μm resolution, of (~40) 17-4PH stainless steel dogbone-shaped test samples, at 0.75 mm x 0.75 x mm x 4 mm (interior dimensions)
    - Reveal widely varying and pervasive porosity: mean porosity of 0.008 (varying sample-to-sample by ~ 60%) and spatial correlation length of 50 μm.
  - Needed to generate a large set of porosity realizations for subsequent statistical analysis









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- The explicit characterization of porosity in AM materials for subsequent uncertainty propagation necessitates a stochastic description:
  - Various computational approaches are available: [Quibler, J. Colloid Interface Sci., 1984], [Adler *et al*., Int. J. Multiph. Flow., 1990], [Yeong and Torquato, Phys. Rev. , 1998]
- Alternative strategy: Karhunen-Loève expansions
  - Reduced order models of stochastic process, α, with finite variance
  - Spectral decomposition of correlation function: analogous to Fourier series expansion
  - Optimal in L^2 sense of capturing variance/energy of target process
  - Proposed for 2-D porosity process by Ilango et al. [Prob. Eng. Mech., 2013], extended to 3-D by Khalil et al. [CMAME, 2021]

$$\alpha(x) = \sum_{i=1}^{L} a_i \sqrt{\lambda_i}\, \psi_i(x)$$

  - Eigenvalues, λ_i, and eigenfunctions, $\psi_i(x)$, are obtained by solving the homogeneous Fredholm integral equation of the second kind:

$$\int R_{\alpha\alpha}(x_1, x_2)\, \psi_i(x_1)\, dx_1 = \sqrt{\lambda_i}\, \psi_i(x_2)$$

  - Eigenvalues and eigenfunctions only available analytically for limited family of correlation functions $R_{\alpha\alpha}$

Explicit Characterization of Porosity in AM Materials – Karhunen-Loève Expansions

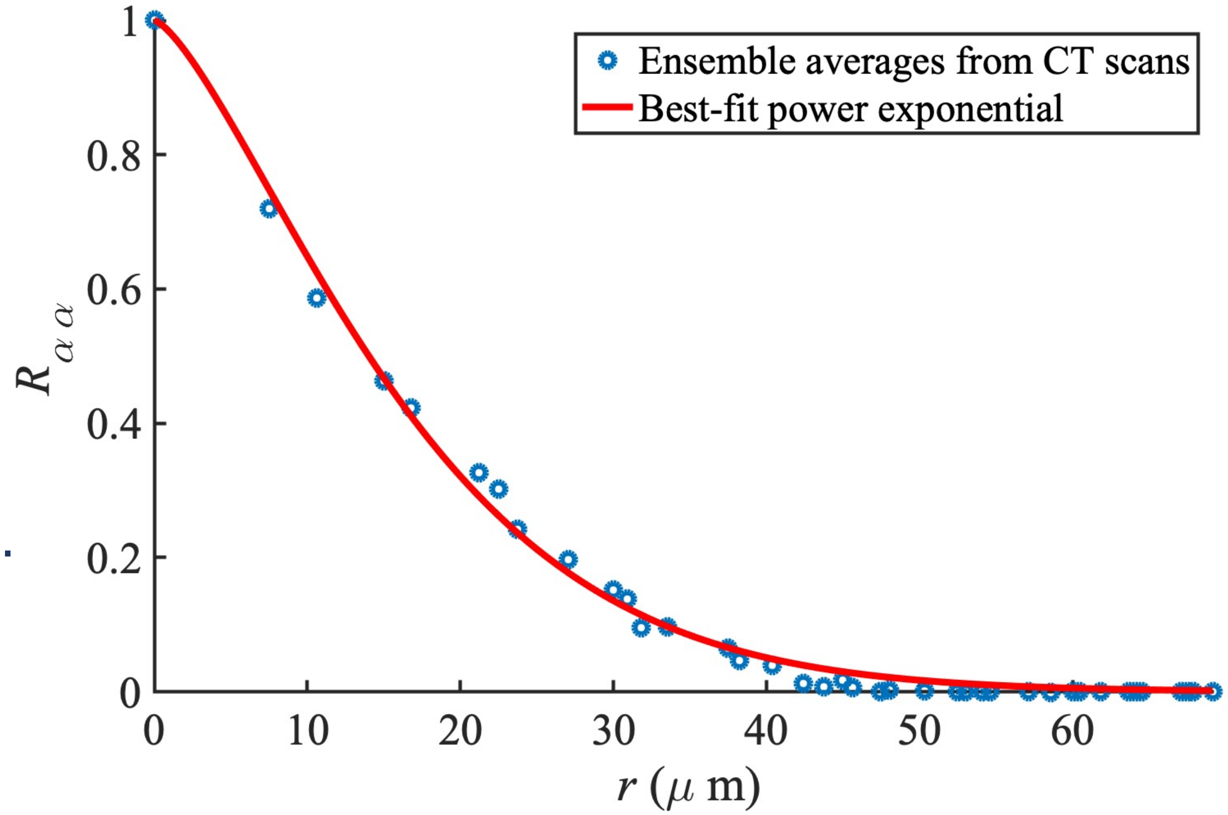
- We need to fully describe the correlation function $R_{\alpha\alpha}$
- Having performed an extensive analysis, we see strong evidence that the binary random process modeling porosity is homogeneous and isotropic
- Therefore, we need only capture a two-point correlation function from available data

- We fit the data to the widely-used power-exponential correlation function

$$R(x_1, x_2) = R_{\alpha\alpha}(r) = e^{-(r/\kappa)^{\rho}}$$

$$r = [x_1 - x_2]$$

- Least-squares regression provides $\kappa = 18\ \mu\mathrm{m}$ and $\rho = 1.4$
- Eigenvalues and eigenfunctions not available analytically for this choice of $\{\kappa, \rho\}$. Estimates obtained numerically on a discretized mesh used for subsequent FEM simulations (L ≅10k modes)
- Details in [Khalil *et al*., CMAME, 2021]



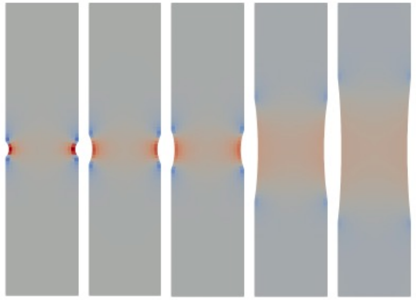
Computational Model

- The numerical model used in numerical experiments is based. On the isothermal variant of the Bammann-Chiesa-Johnson (BCJ) viscoplastic damage model
- This results in a hierarchical modeling approach, or a two-level model:
  - Pores above a given size threshold represented explicitly in the finite element meshes, simulated using KLE
  - Sub-threshold pores are modeled with an initial damage field as facilitated by the BCJ model
- The model was previously calibrated [Khalil *et al.*, CMAME, 2021]
  - Stress-strain experimental data on AM 17-4 PH stainless steel tension specimens loaded to failure
  - Modeling error was partially captured using novel Bayesian embedded-error techniques

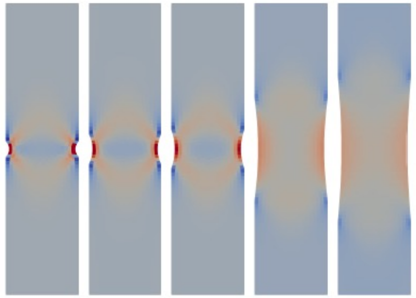
Parameter		Value
Young's modulus (GPa)	E	240
Poisson's ratio	v	0.27
Yield strength (MPa)	Y	600
Initial void size (μm^3)	ν_0	0.1
Initial void density (μm^{-3})	η_0	0.001
Flow exponent	n	10
Damage exponent	m	2
Flow coefficient	f	10
Isotropic dynamic recovery	R	4
Isotropic hardening (GPa)	H	5
Initial hardening (MPa)	κ_0	460
Shear nucleation	N_1	10
Triaxiality nucleation	N_3	13
Maximum damage	$\phi_{\max}$	0.5

Model Geometry

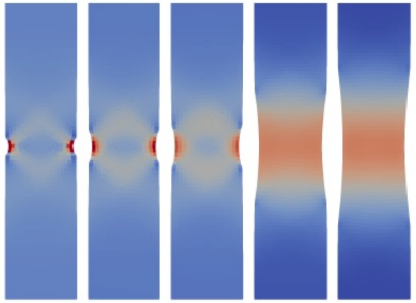
- Double U-notched tension specimen
  - Common geometry for mechanical tests
  - Allows us to investigate the effects of stress concentration with a few geometric parameters, namely the notch depth D and notch radius R
  - Specimen dimension were fixed at 1x1x4 mm^3, as was element size (~0.05 mm).
  - R varied over the range 0.05-15 mm, D over 0.15-0.45 mm
  - Simulations without explicit pores for R = 0.15, 0.45, 0.75, 5.0, 10.0 mm at 4.7% strain, left to right



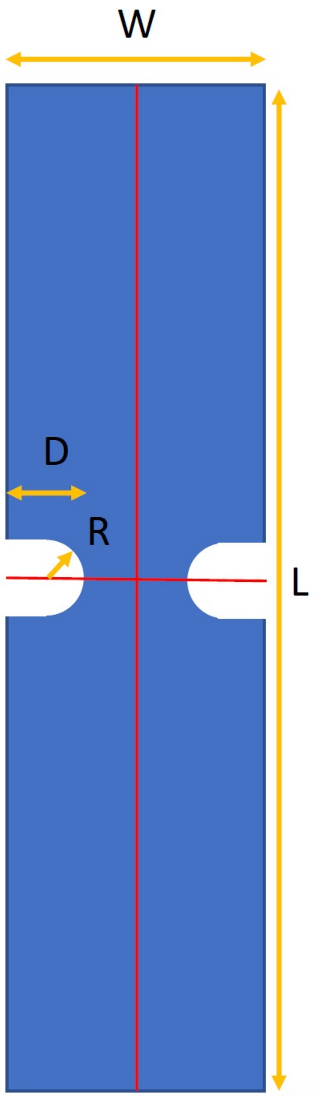
Pressure



Von Mises stress



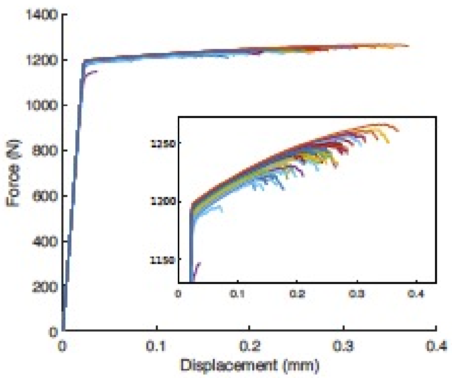
Damage



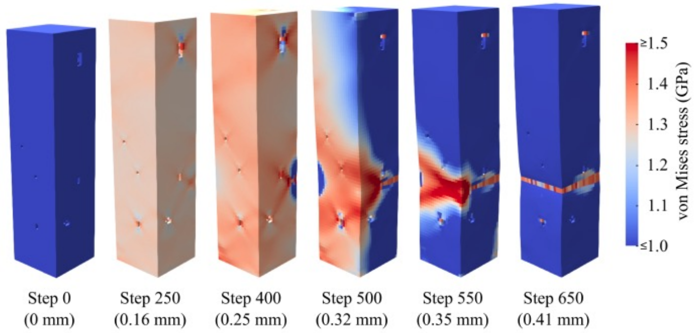
- Notch radius largely determines the height of the potential localization zone and the acuteness of the stress concentration
- Notch depth influences the width of the potential localization zone

Plasticity-Damage-Porosity Simulations: Rectangular Specimen

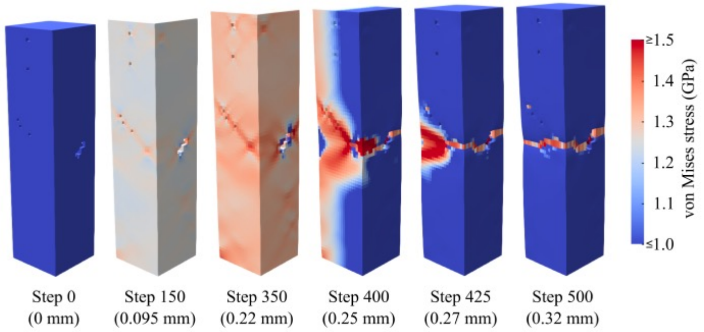
- Simulations of tensile loading: Baseline effect of pores without stress concentrations, we ran 10,000 explicit porosity realizations of the nominal geometry without the double U-notch
- Little variability is observed in elastic regime. For plastic response, some variation in yield and hardening, but the dominant variability is in failure strain



Force-displacement curves for 50 realizations



Evolution of the von Mises stress field, 2nd realization



Evolution of the von Mises stress field, 6th realization

- Showing above failure modes for a realization that fails at the largest concentrations of pores and one that does not: stress fields are qualitatively similar from one realization to the next.
- Previously [Khalil *et al*., CMAME, 2021], we explored yield strength, ultimate strength and several quantities related to failure
- Currently, we are interested in modeling failure location

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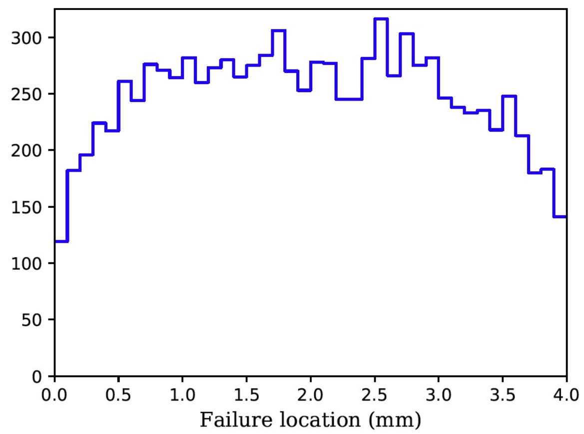
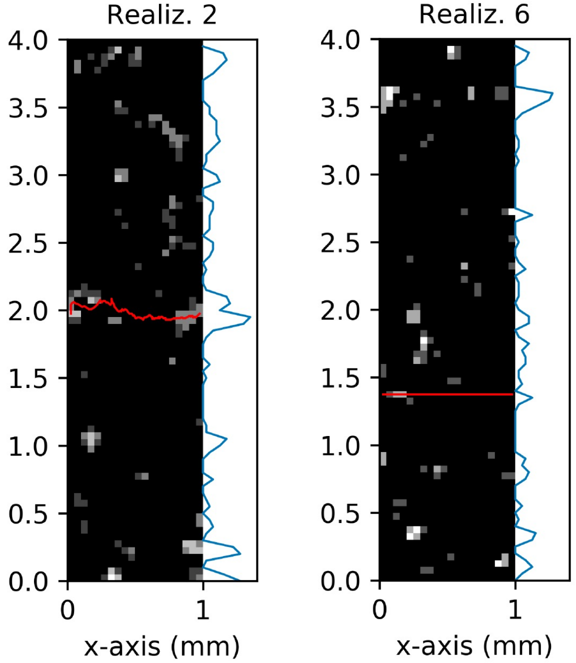
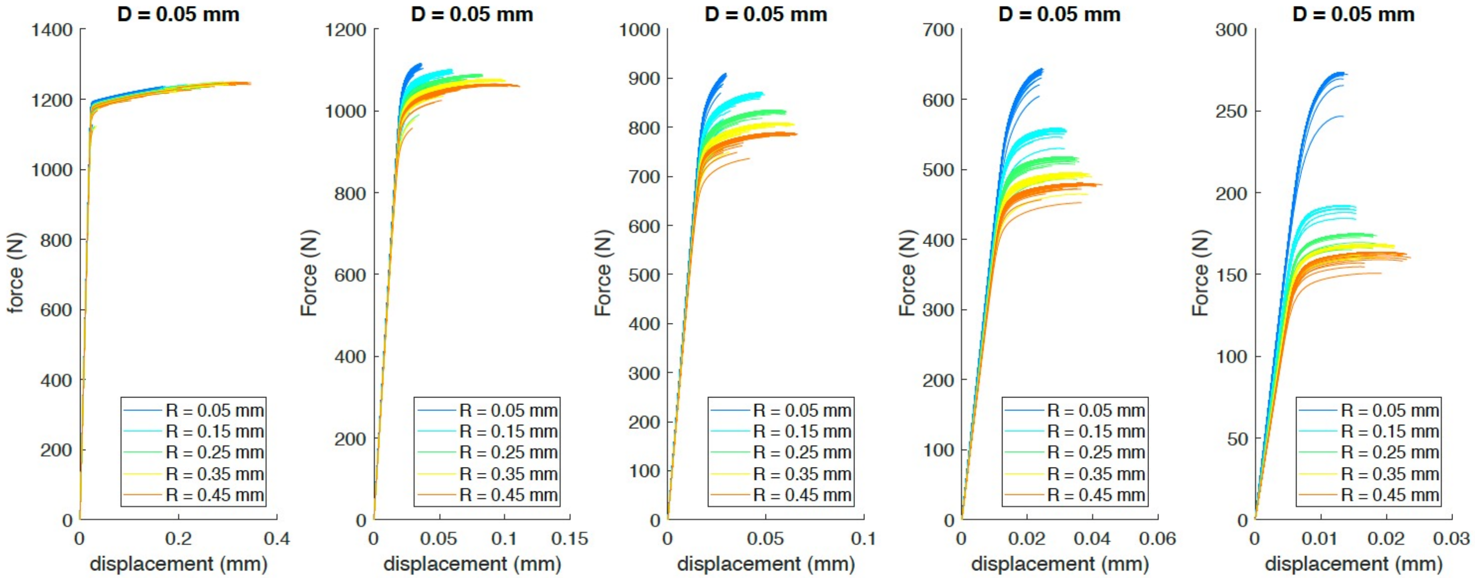
- The histogram of 10,000 simulated failure locations suggests a nearly uniform distribution in failure location across the specimens with slight but apparent boundary effects
- Failure surface and explicit pores for the two previously-selected realizations:
  - Little to suggest a simple mechanistic explanation for why one realization fails where pore concentration is high, and the other does not
- While individual specimens are seen to fail near large pores, in regions with multiple pores, or where pores are adjacent to the specimen surface, detailed statistical analysis reveals that none of these observations have significant explanatory power on the failure location:
  - Correlation coefficient of the location of the largest void and failure was only 0.26
- Difficulty in devising a simple mechanistic predictor of failure location motivates the statistical treatment and modeling





Plasticity-Damage-Porosity Simulations: Notched Specimen

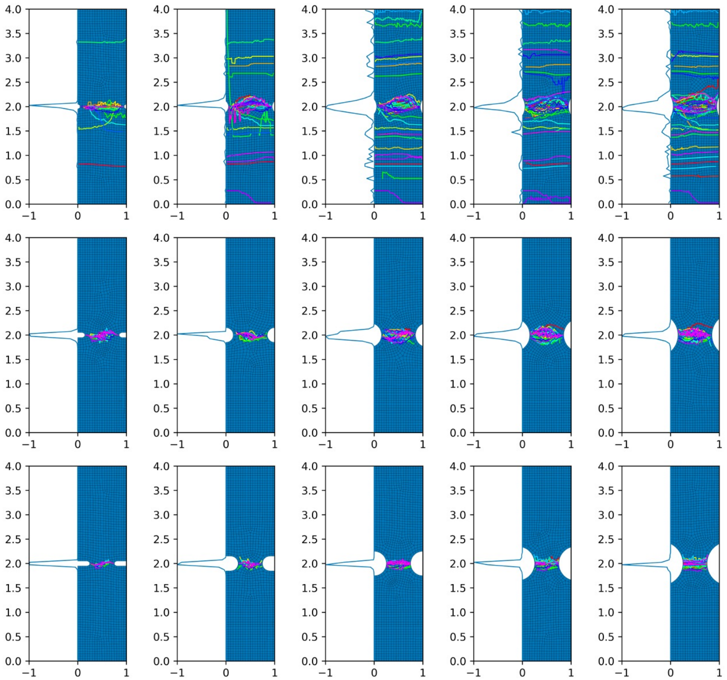
- Tensile loading simulations were conducted for each choice of geometry parameters, repeated across 1000 realizations of the explicit porosity
- Force-displacement curves for select realizations:

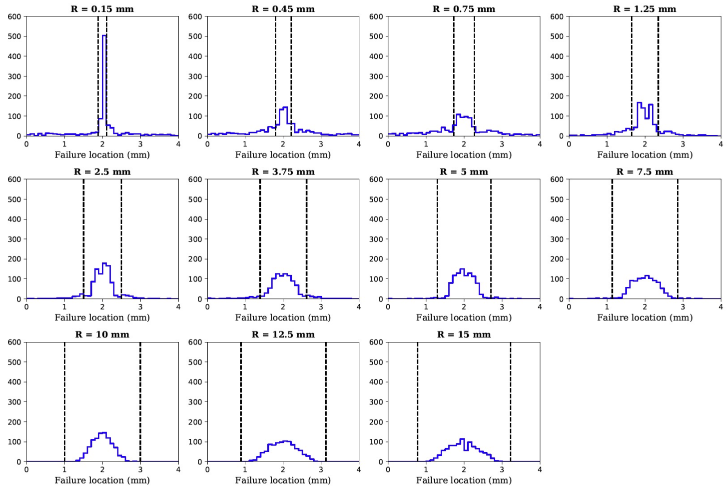


- Key observations:
  - Little variability in the shallowest notch case, most variability in the failure strain
  - Decreasing notch radius leads to earlier onset of failure
  - Increasing notch depth leads to more rapid damage evolution
  - Specimens with sharper notches also experience an apparent delay in the onset of yield

Plasticity-Damage-Porosity Simulations: Notched Specimen

- Ensemble of failure surfaces for various geometries:
  - For most, the distribution of failure is centered at the mid-plane with a roughly lenticular locus
  - Beyond that region, failures seem uniformly scattered
  - Only the shallowest notches had a significant likelihood of failure outside the vicinity of the notch
- The histogram of 1,000 simulated failure locations:
  - The distribution is narrow and peaked for the narrow notches and correspondingly broad for the wide notches
  - For the narrowest notches there is a significant background distribution of failures outside the notch
  - For intermediate notch widths, we see either one central peak superimposed on a fairly uniform background or a tri-modal distribution
  - For the widest notches, bell-shaped distributions





Statistical Models of Failure Locations: Beta Mixture Models

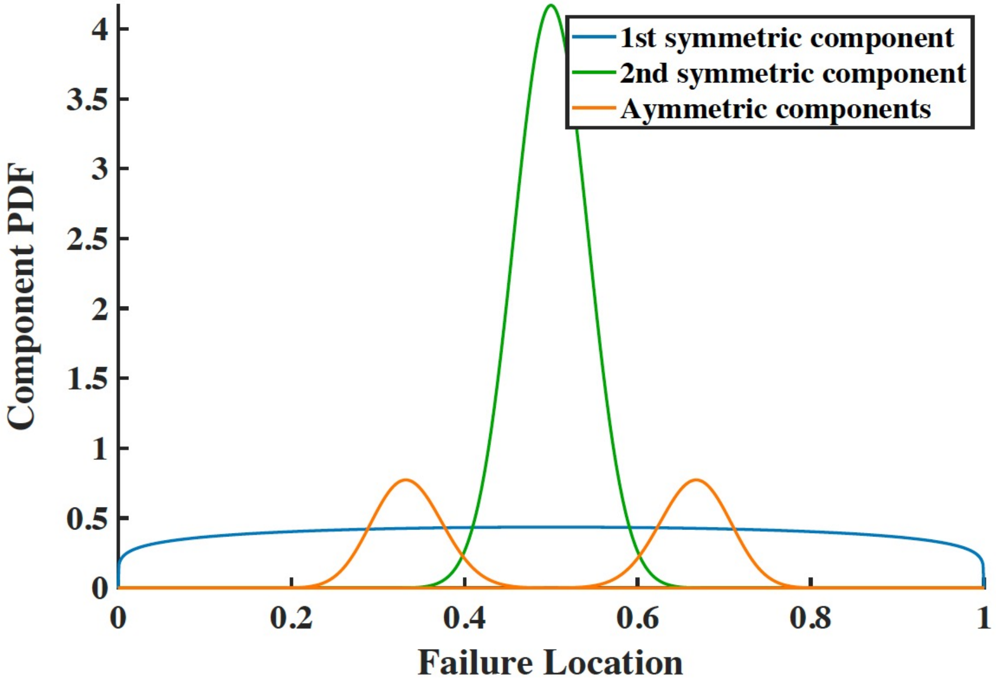
- Objective: Develop statistical models for a probabilistic characterization of failure location
- Reduce the three-dimensional failure location to a one-dimensional variable representing the axial location of the centroid of the failure region to enable robust statistical analysis
- Idea: Utilize finite mixture models:
  - ✗ Gaussian mixture models have components that are symmetric and of infinite support
  - ✓ Beta mixture models (BMMs) rely on beta components (of finite support) and can capture various non-Gaussian trends more effectively

$$f(z\,;\mathbf{W},\mathbf{A},\mathbf{B}) = \sum_{k=1}^{K} w_k \,\mathrm{Beta}(z\,;a_k,b_k)\ ,$$

$$\mathbf{W} = \{w_1,\dots,w_K\},\ \mathbf{A} = \{\mathbf{a}_1,\dots,\mathbf{a}_K\},\ \mathbf{B} = \{\mathbf{b}_1,\dots,\mathbf{b}_K\}$$

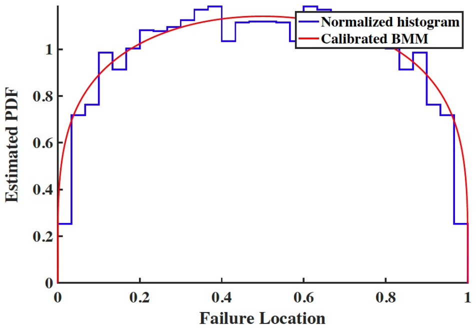
$$\mathrm{Beta}(z;a,b) = \frac{1}{\mathrm{beta}(a,b)} z^{a-1}(1-z)^{b-1},\ a,b>0\ ,$$

$$\{\mathbf{W},\mathbf{A},\mathbf{B}\}_{\mathrm{MLE}} = \underset{\mathbf{W},\mathbf{A},\mathbf{B}}{\arg\max} \sum_{j=1}^{n} \log f(z_j\,;\mathbf{W},\mathbf{A},\mathbf{B})\ ,$$

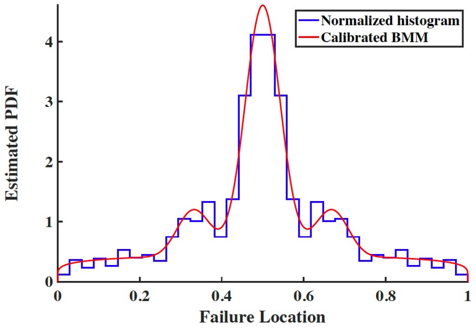


Statistical Models of Failure Locations – Fitted BMMs

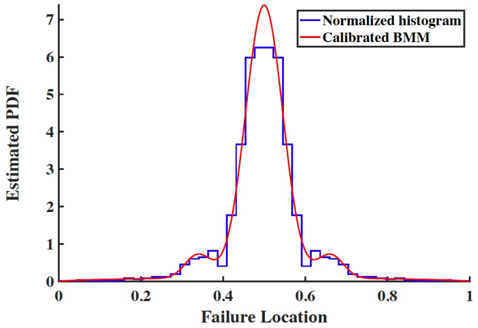
- A practical issue with finite mixture models relates to the choice of number of components, K:
  - Information-theoretic approaches: Akaike and Bayesian information criteria (AIC, BIC)
  - Cross-validation
  - Bayesian: Bayesian model evidence
- AIC was used to provide initial values for K, ranging from 1 to 5 components
- For interpretability, and with small loss in data-fit, we decided to “fix” the number of components across the different geometries to one of three choices (with AIC used in final selection):
  - One symmetric component (no notch geometry)
  - Two symmetric components
  - Two symmetric components and two asymmetric/mirrored components
- AIC-selected BMMs superimposed over the histogram of failure locations for various notch radii:



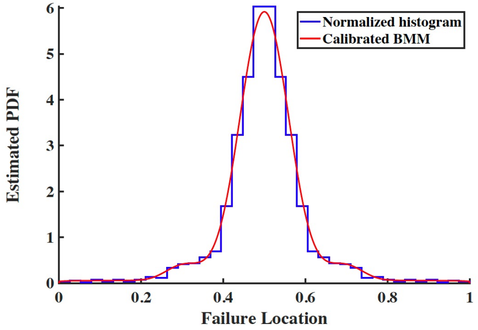
No notch



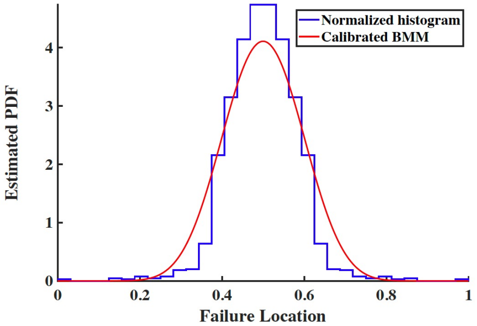
$R = 0.75$ mm



$R = 2.5$ mm



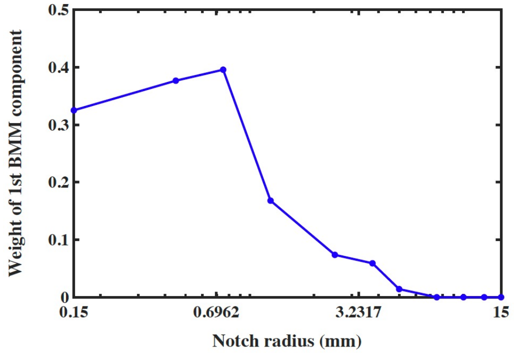
$R = 3.75$ mm

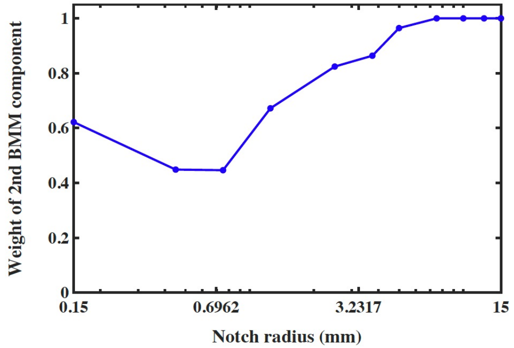


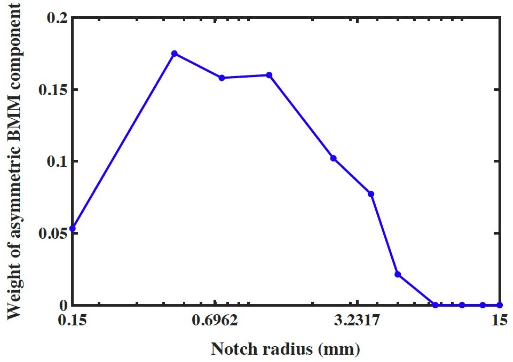
$R = 7.5$ mm

Statistical Models of Failure Locations – Physical Interpretation

- Question: What is the likelihood of porosity-induced failure outside the notch region as a function of the stress intensities induced by the geometric features?
- The four BMM components intend to capture:
  - A narrow, central peaked distribution: high-triaxiality stress concentration
  - A broad, nearly uniform distribution: porosity-induced homogeneous stress concentrations
  - Two mirrored off-center peaks near the notch edges: shear-dominant stress concentrations
- The weights (probabilities) of the BMM components capture the relative importance of the three mechanisms in specimen failure
- Key observations:
  - As the notch broadens, more certainty that the specimen will fail within the notch
  - Stress concentrations at the notch edges are significant drivers for all but the sharpest notch
  - For smaller notches, that failures occur with significant frequency outside the notch







Summary

- Statistical study to investigate how a background, uniform porosity interacts with stress concentrations due to as-designed, nominal geometry in a ductile additively-manufactured metal
- The U-notched tension specimen allows us to study the effects of stress concentration with a few geometric parameters
- AM-induced explicit porosity is model and propagated using reduced-order stochastic process models
- Synthetic realizations for failure location used in constructing interpretable beta mixture models:
- Two asymptotic regimes:
  - Small notches: A significant fraction of the failures are outside the stress concentration region due to intrinsic stress
  - Large notches: All failures occur in the notch region and the distribution of failure locations appears insensitive to geometry for specimens with well-separated geometric and material length scales
- Intermediate regime: multi-modal distributions arise associated with the primary stress concentration at the notch root as well as secondary stress concentrations at the notch edges
- Currently, we are proceeding with a feasibility study of constructing deep neural network surrogates to capture the mapping from 3-D explicit porosity realizations to 3-D damage fields