Machine Learning Driven Material Performance Prediction

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Center for Applied Scientific Computing

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Lawrence Livermore National Laboratory

My background

Brian Gallagher

FOLLOW

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Verified email at llnl.gov - Homepage

Scientific Machine Learning   Data Mining   Statistical Relational Learning   Network Analysis

TITLE	CITED BY	YEAR
Predicting compressive strength of consolidated molecular solids using computer vision and deep learning B Gallagher, M Rever, D Loveland, TN Mundhenk, B Beauchamp, ... Materials & Design 190, 108541	13	2020
Nanomaterial synthesis insights from machine learning of scientific articles by extracting, structuring, and visualizing knowledge AM Hiszpanski, B Gallagher, K Chellappan, P Li, S Liu, H Kim, J Han, ... Journal of chemical information and modeling 60 (6), 2876-2887	12	2020
Reliable and explainable machine-learning methods for accelerated material discovery B Kailkhura, B Gallagher, S Kim, A Hiszpanski, TYJ Han npj Computational Materials 5 (1), 1-9	38	2019

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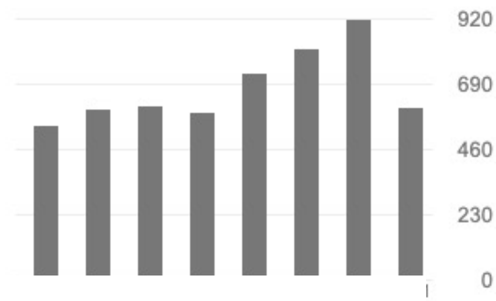
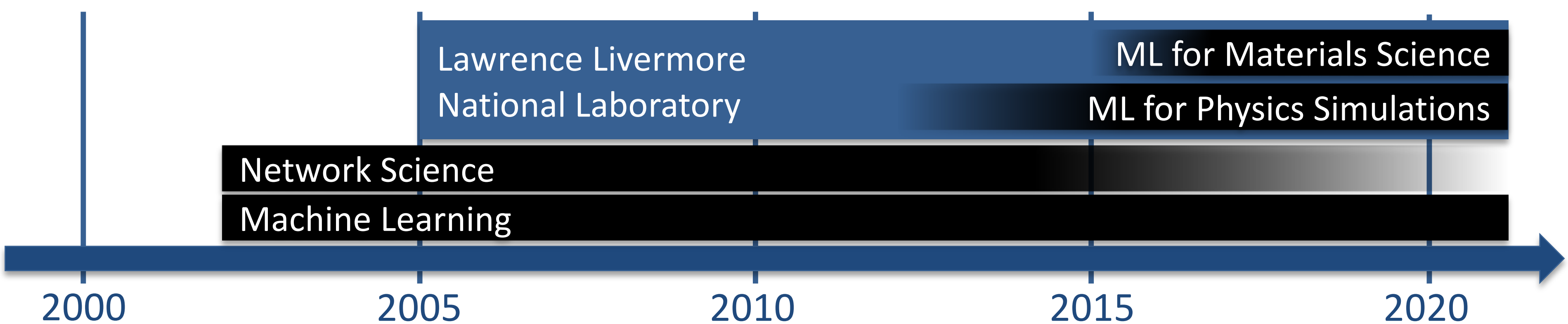
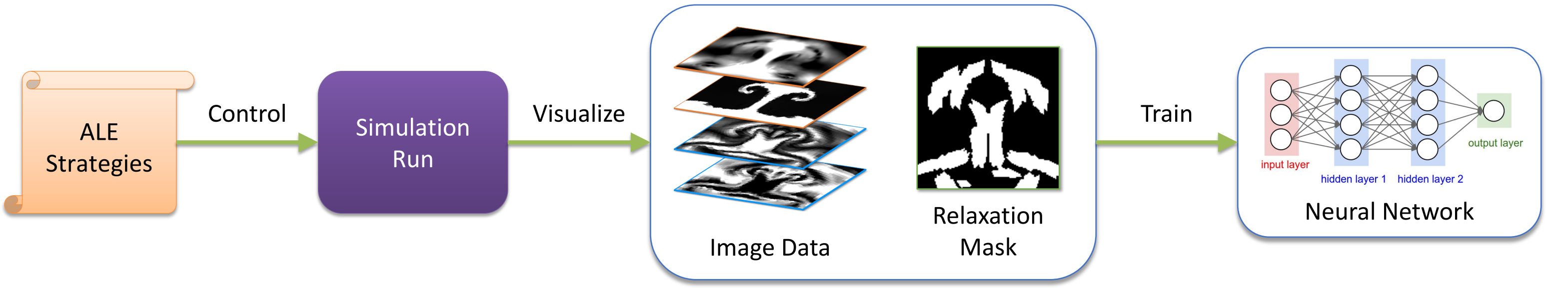




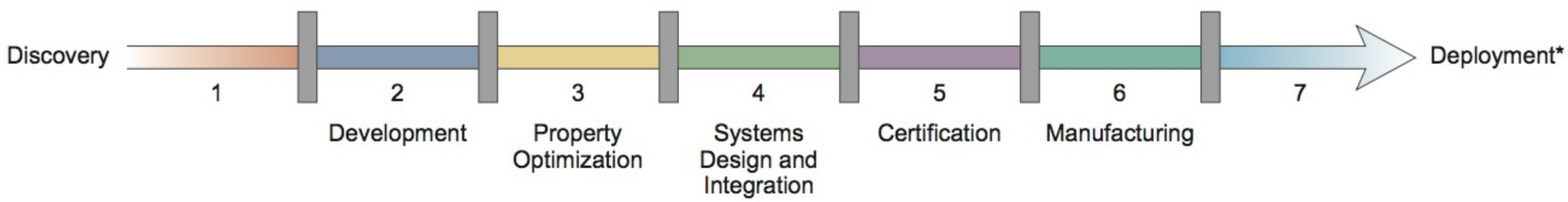
Scientific Machine Learning Applications

- ML-driven physics simulations (2012 -)



  - *Jiang et al., A Supervised Learning Framework for Arbitrary Lagrangian-Eulerian Simulations. ICMLA 2016.*
  - *Jiang et al., A deep learning framework for mesh relaxation in arbitrary Lagrangian-Eulerian simulations. SPIE 2019.*
  - *Jiang et al., Exploiting Spark for HPC Simulation Data: Taming the Ephemeral Data Explosion. HPC Asia 2020.*

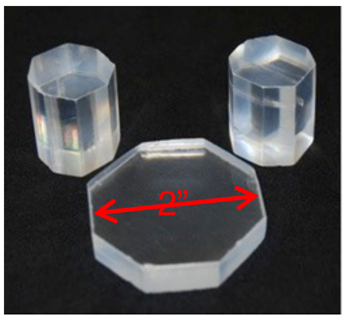
- ML-driven materials discovery & development (2015 -)



  - *Kailkhura et al., Reliable and explainable machine-learning methods for accelerated material discovery. npj Computational Materials 2019.*
  - *Hiszpanski et al., Nanomaterials Synthesis Insights from Machine Learning of Scientific Articles by Extracting, Structuring, and Visualizing Knowledge. Journal of Chemical Information and Modeling 2020.*
  - *Gallagher et al., Predicting Compressive Strength of Consolidated Molecular Solids Using Computer Vision and Deep Learning. Materials & Design 2020.*

Machine Learning for Materials Science

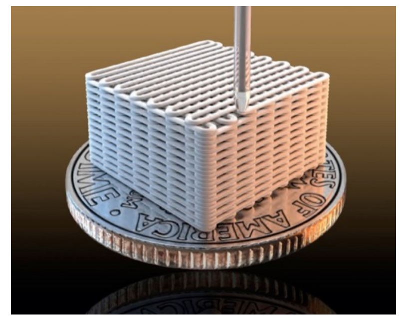
Success of LLNL and partner missions requires timely development and deployment of diverse materials



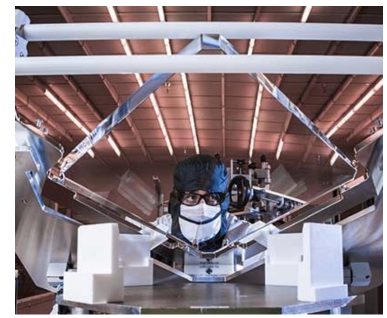
Plastic scintillators

Energetic Materials

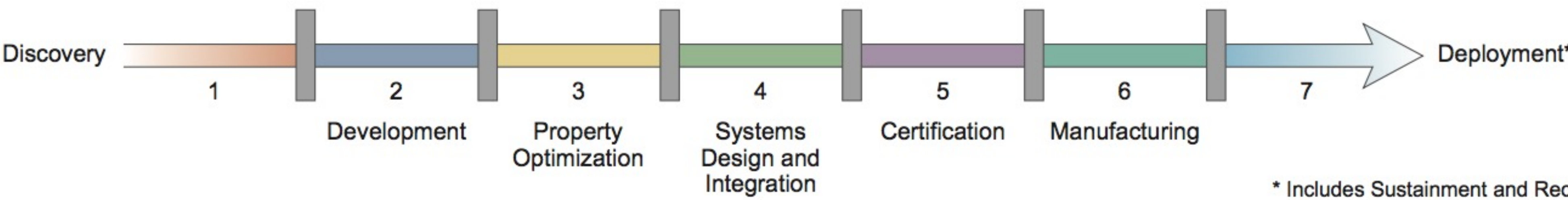
Porous Materials



AM components

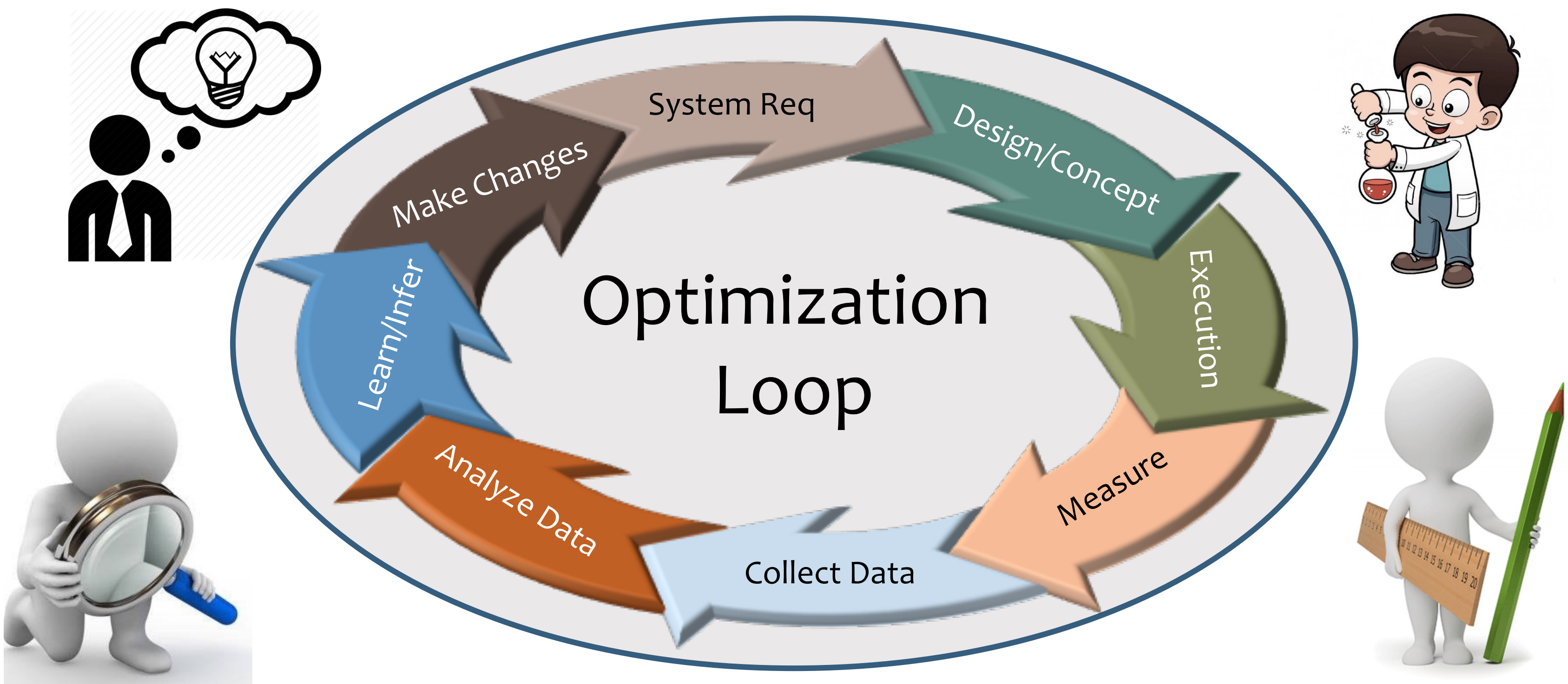


Optical Materials



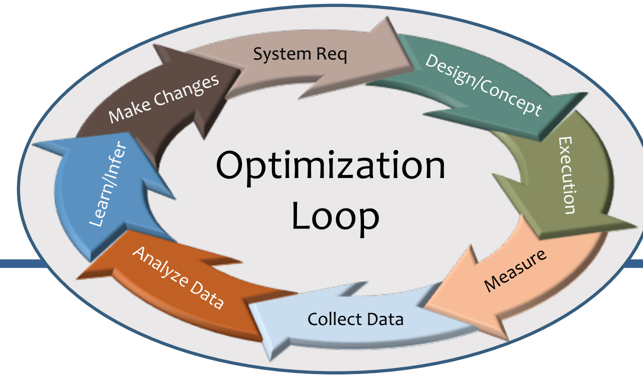
* Includes Sustainment and Recovery

Materials discovery, development and deployment requires many iterations

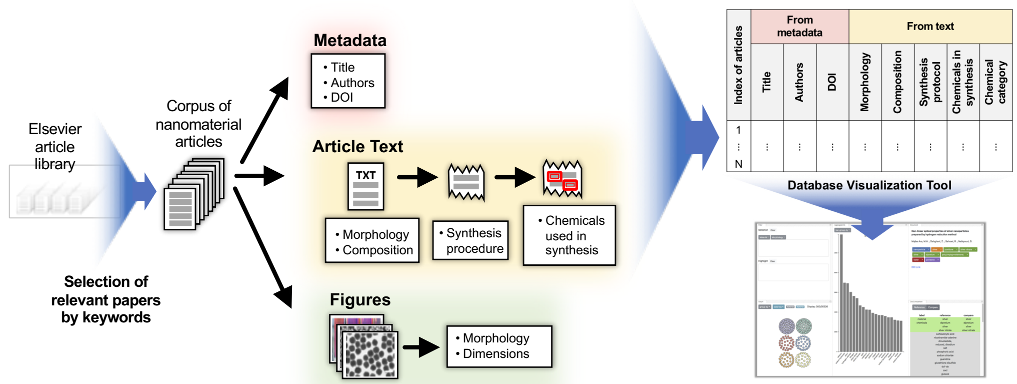


Two ways to help: (1) reducing the number of iterations and/or
(2) reducing time per iteration

Optimizing the optimization loop



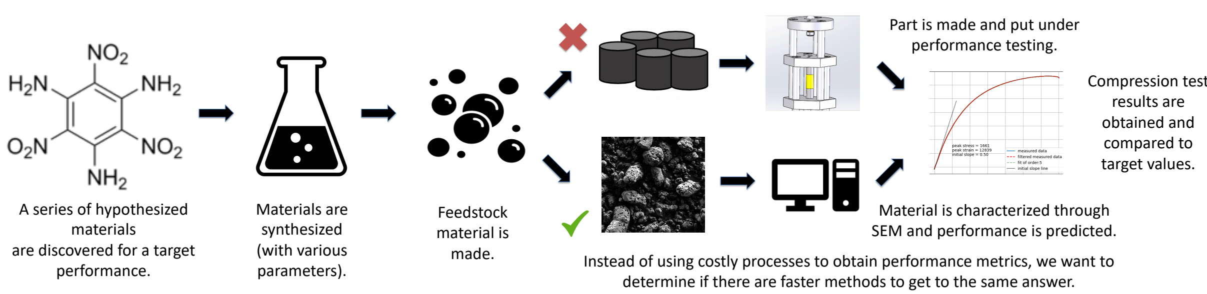
1. Automated data collection



- Inform synthesis protocol
- **Reduce iterations** required to synthesize new materials

Hiszpanski et al., Nanomaterials Synthesis Insights from Machine Learning of Scientific Articles by Extracting, Structuring, and Visualizing Knowledge. Journal of Chemical Information and Modeling 2020.

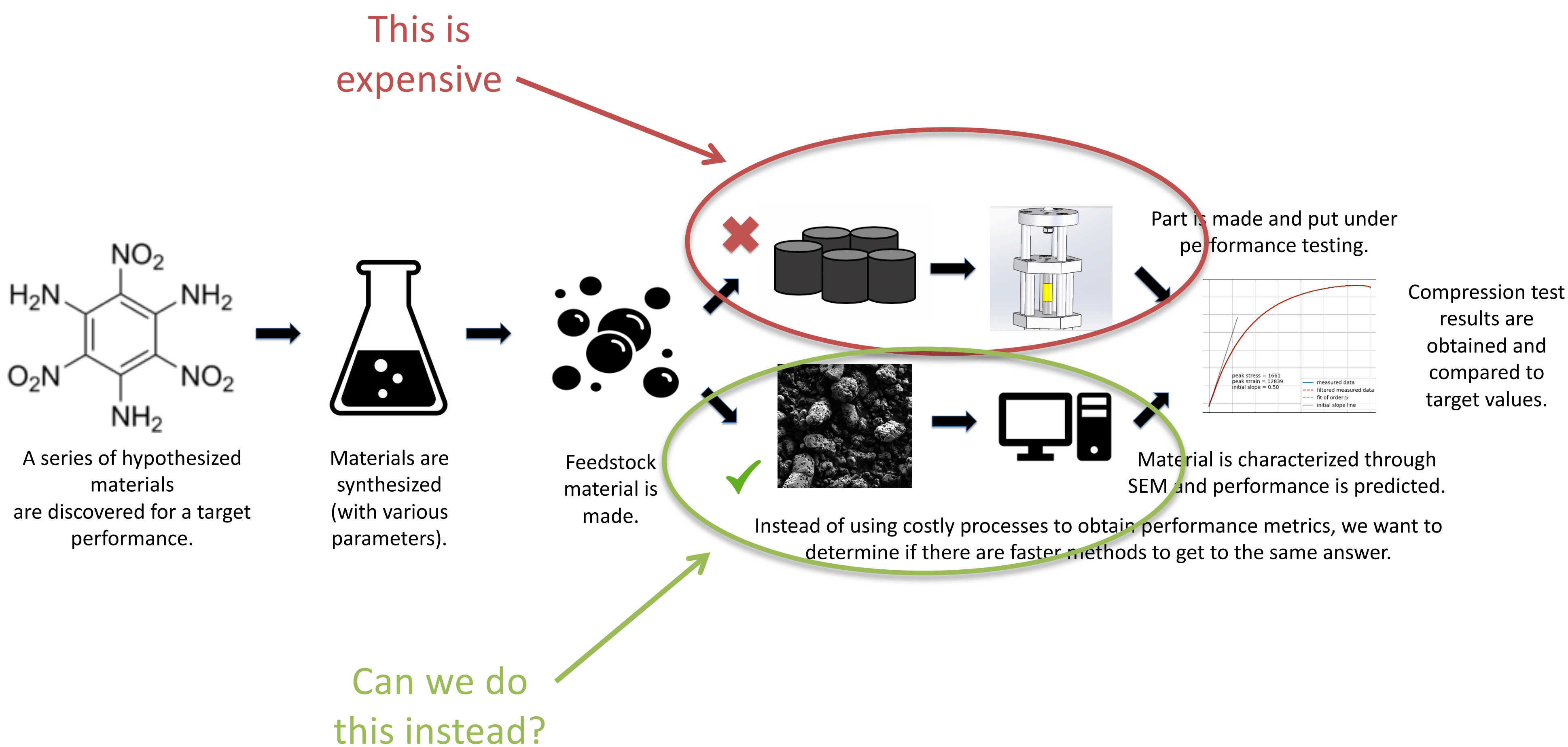
2. Materials performance prediction



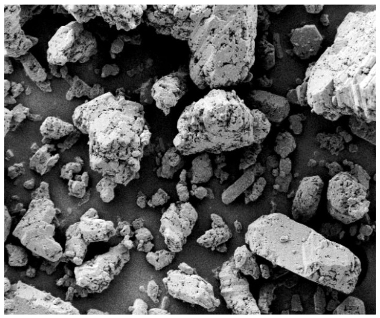
- Identify candidate materials
- **Shorten iteration time** by eliminating costly performance testing

Gallagher et al., Predicting Compressive Strength of Consolidated Molecular Solids Using Computer Vision and Deep Learning. Materials & Design 2020.

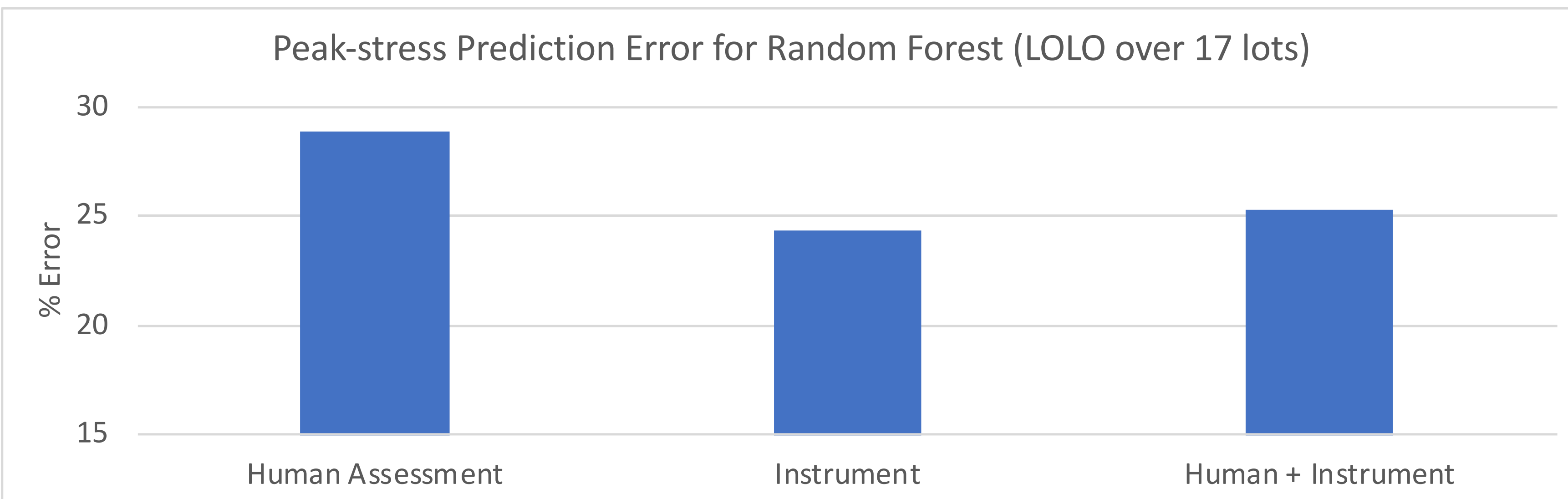
Using Machine Learning to Predict Material Performance



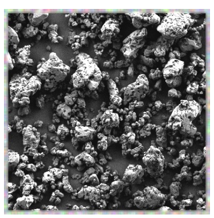
Performance baselines: human assessment & instrument measurements

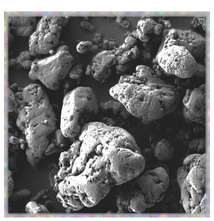


Material Attributes:	Analytical Tools
• crystal structure	XRD
• particle size	**SEM**, PSD
• morphology	**SEM**
• surface area	**SEM**, BET
• voids	**SEM, CT**
• surface texture	**SEM**
• aggregation	**SEM**
• density	pycnometry
• purity	HPLC

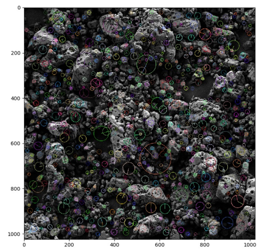


Approaches: “Traditional” Computer Vision + ML vs. End-to-end Deep Learning

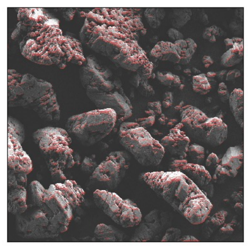




Bag of Visual Words (BoVW)



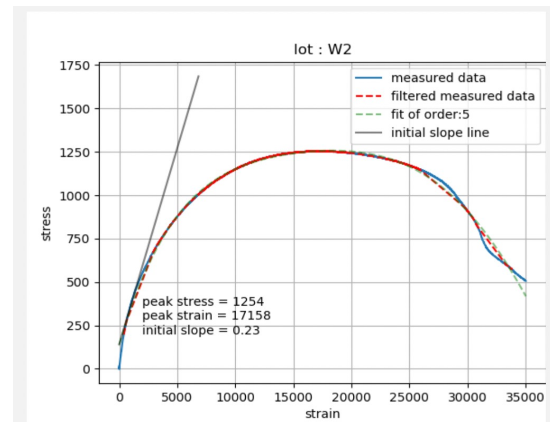
Binarized Statistical Image Features (BSIF)



local shape

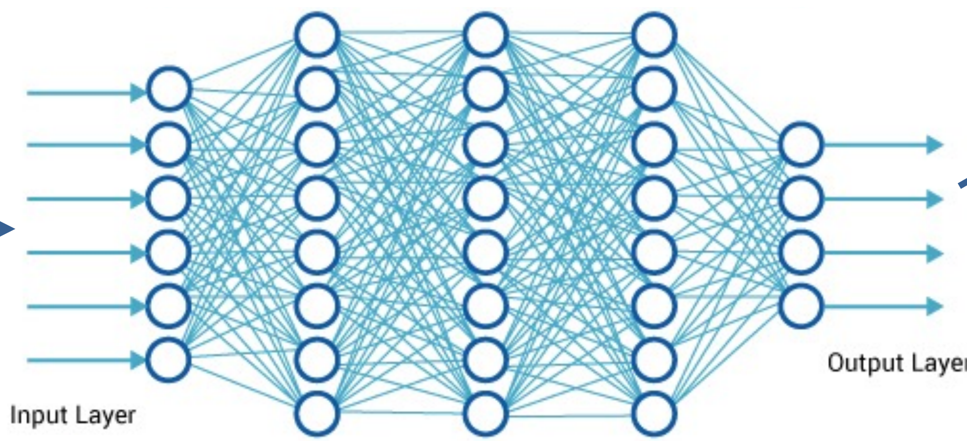
image texture

Random Forest



mechanical property

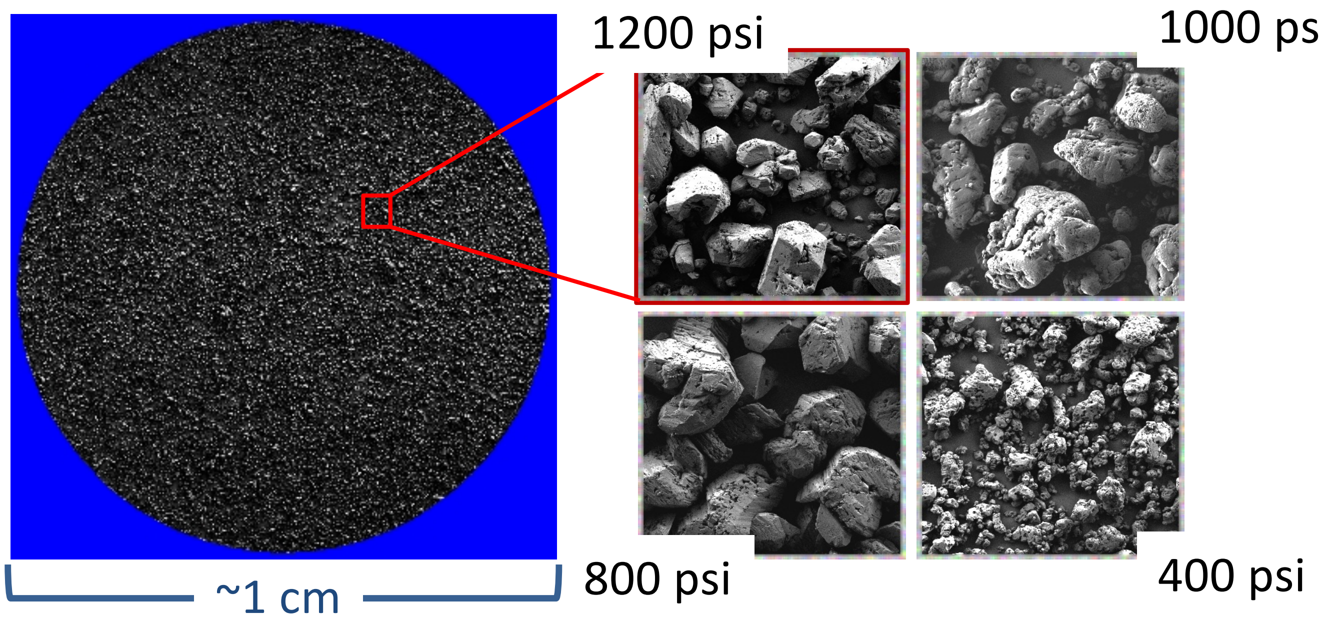
DenseNet 121 (ImageNet pre-trained)



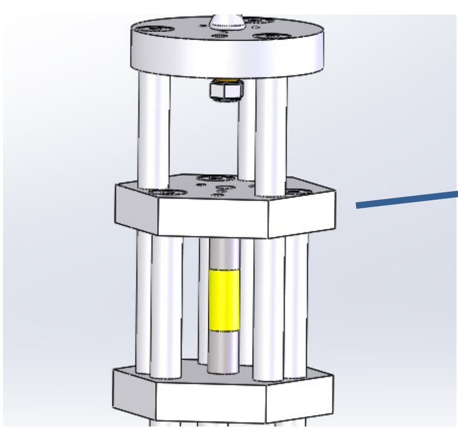
Sample preparation and data collection

30 lots of material

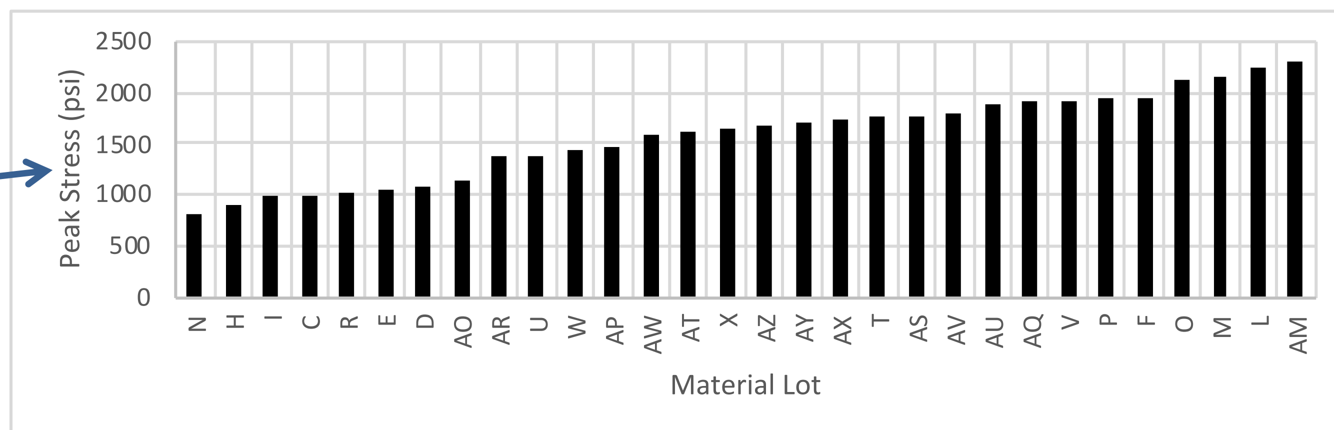
~1000 scanning electron microscope (SEM) images per lot



2 material samples per lot

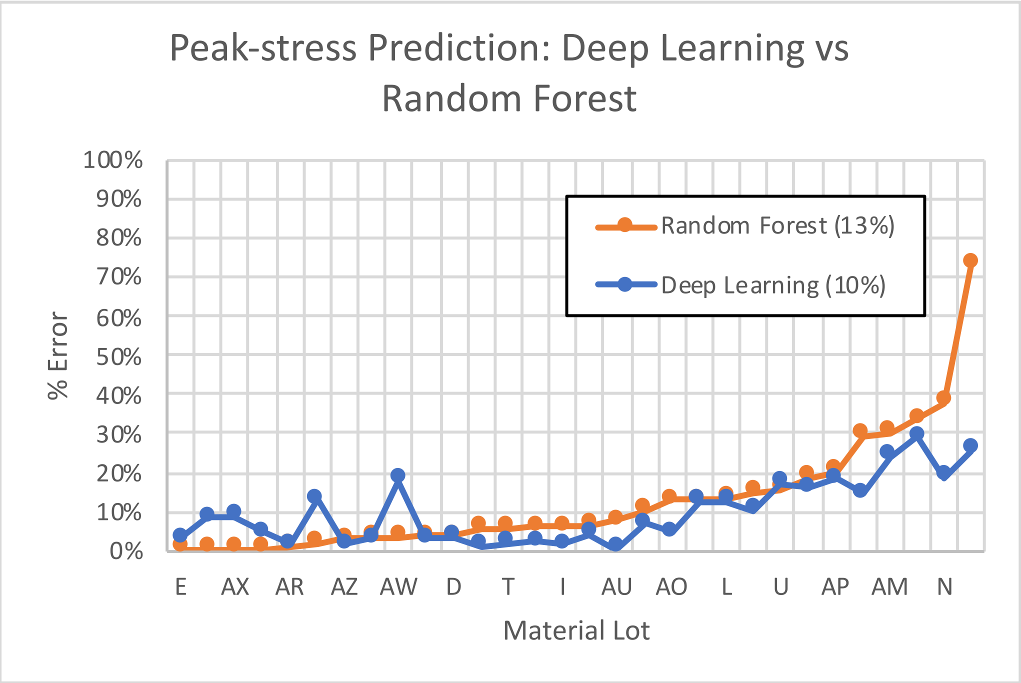


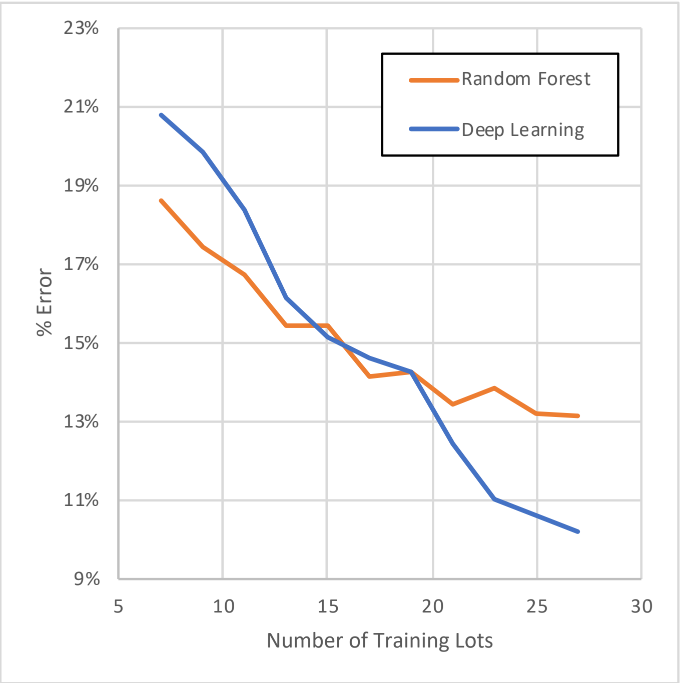
compression test



Experimental Setup & Results

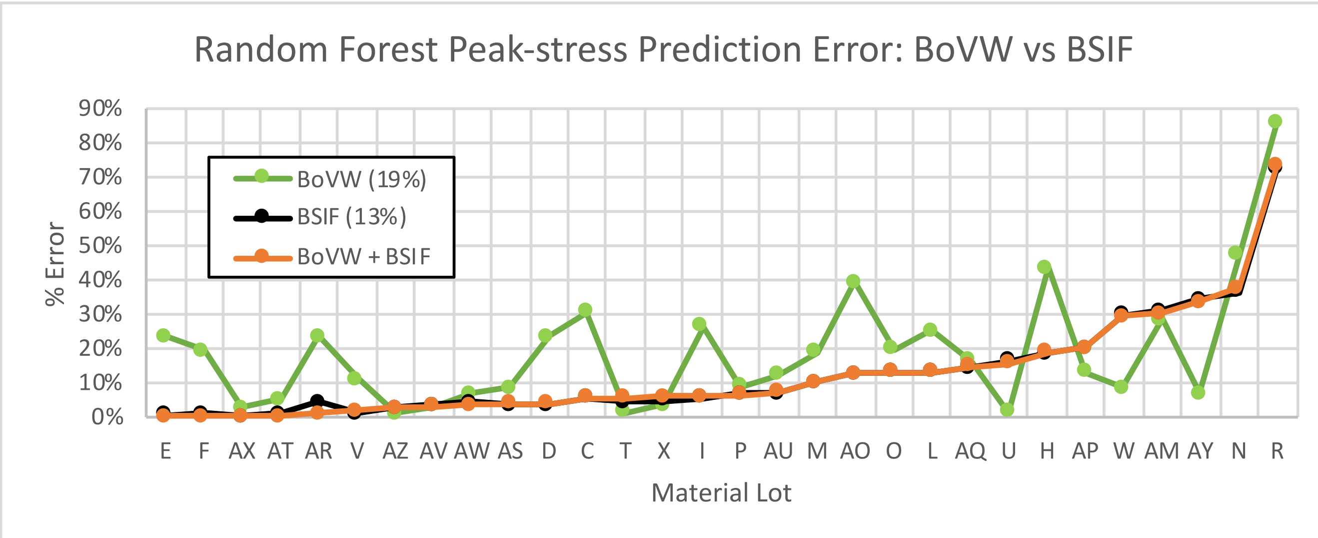
- Regression (predict scalar peak-stress)
- Goal is generalization to unseen lots
  - Leave out an entire lot for evaluation
  - Lot classification is a much easier problem



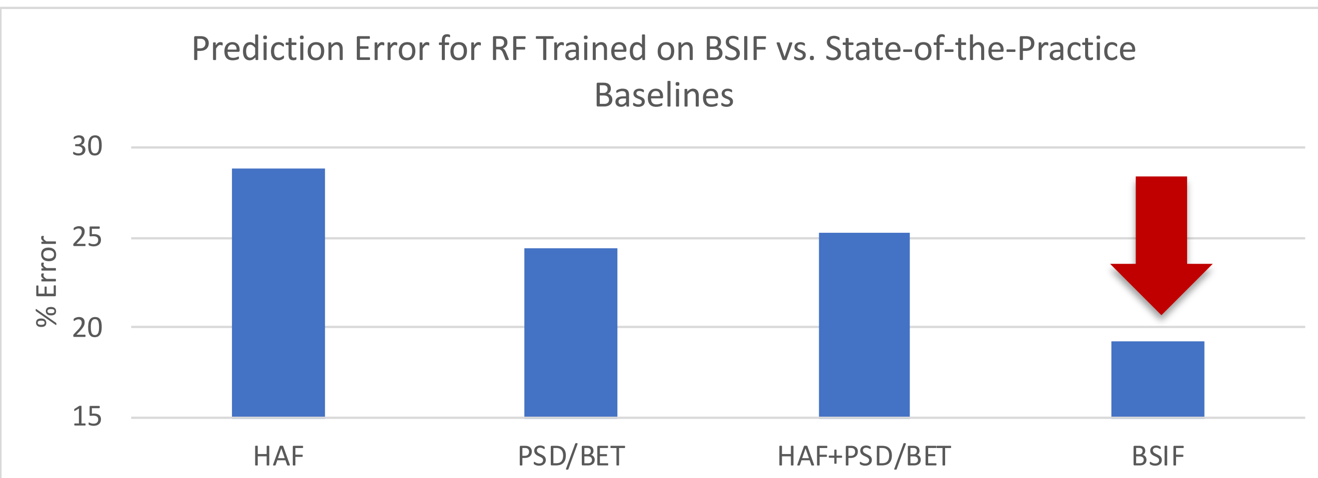


Explaining the results to a Materials Scientist

Part I



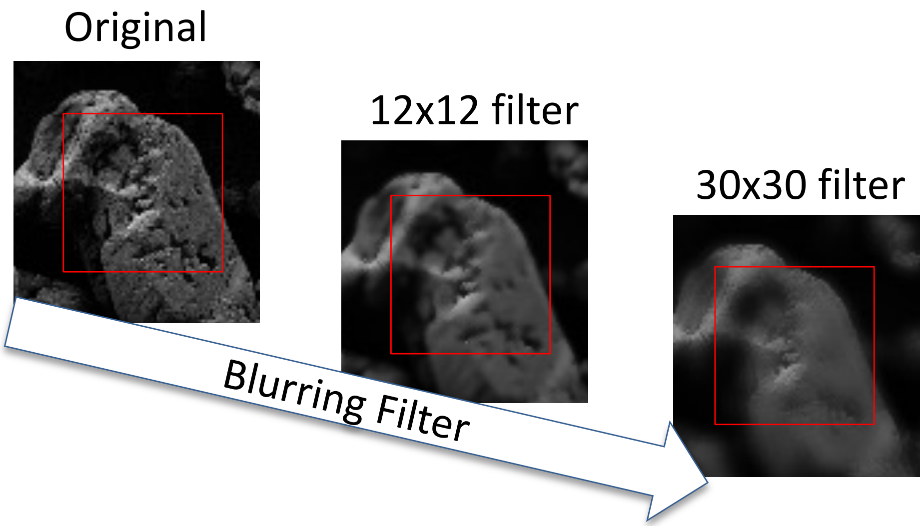
First: texture (BSIF) is more predictive of performance than local shape (BoVW).

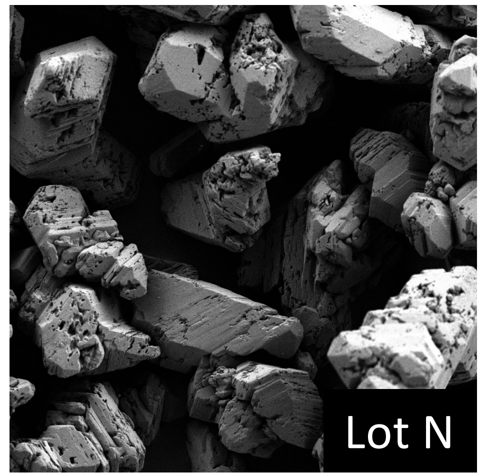


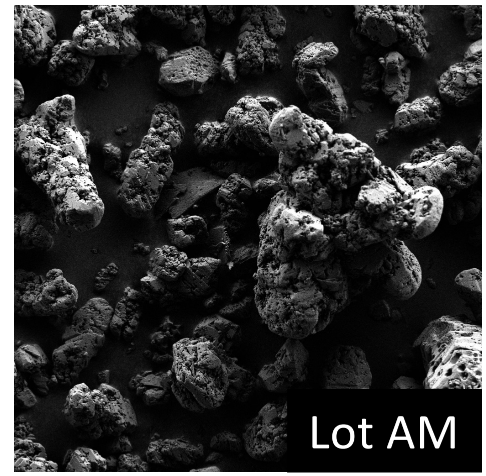
Second: BSIF is capturing something that current approaches do not.

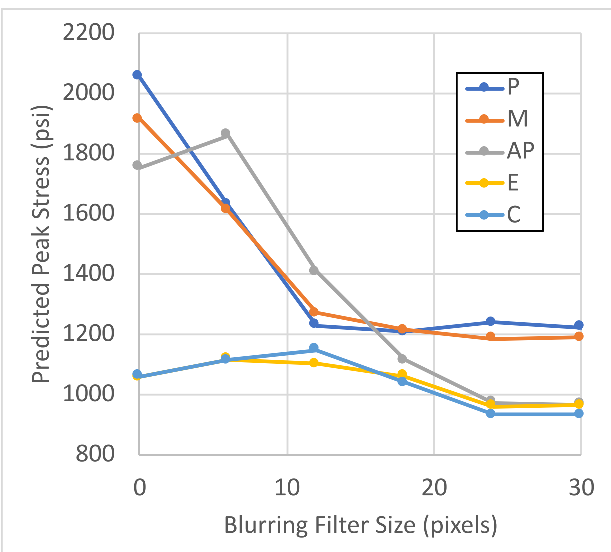
Explaining the results to a Materials Scientist

Part II



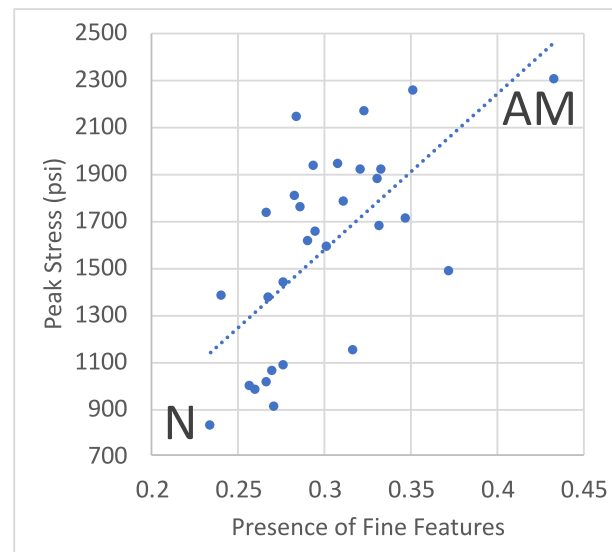






1. Our models rely on fine crystal attributes (pores and defects) smaller than 12x12 pixels (~3x3 µm).

2. Differences in these fine crystal attributes correlate with real performance differences in material lots.



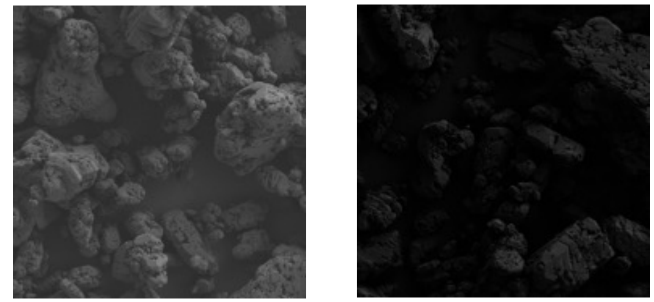
Conclusions: Material Performance Prediction

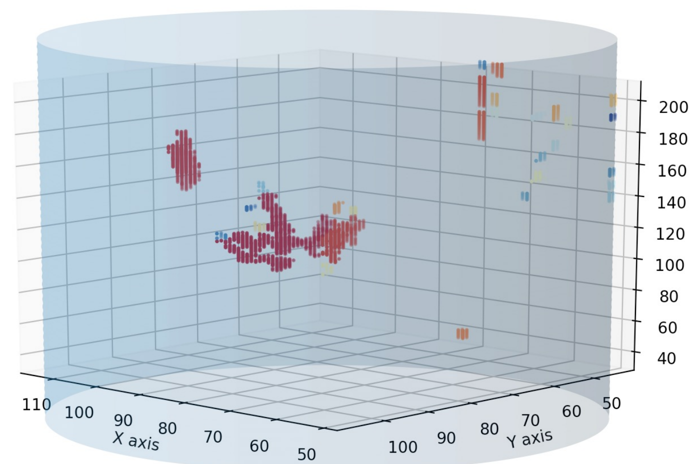
- Computer Vision/ML approach yields 24% improvement
- Synthesizing more material lots improves performance
  - Trend expected to continue in the short term
- Deep Learning is the more powerful (lower bias) method
  - The more powerful method is not always the best.
    - Don't underestimate variance!
    - Don't underestimate robustness and usability!
- Fine crystal attributes are strong indicators of material strength
  - Not adequately captured by current instruments or human assessment

Gallagher et al., Predicting Compressive Strength of Consolidated Molecular Solids Using Computer Vision and Deep Learning. Materials & Design 2020.

Material Performance Prediction: Ongoing Work

- Real-world data acquisition conditions
  - SEM filament change *(Zhong)*
- Material defect detection
  - Detect, classify, and quantify CT anomalies *(Loveland)*
- Uncertainty quantification
  - Bayesian neural networks, deep ensembles, and uncertainty calibration *(Zhang, Kailhura)*
- Explainable deep learning
  - GAN-based image editing *(Liu, Zhang, Kailkhura)*
  - *Texture-based explanation (Mundhenk)*


Acquisition conditions affect images



Defect identification in 3D CT data

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