High-Throughput Design and Analysis of Novel Ceramics for Ballistic Protection

Virtual Kick-off Meeting for ARL's *High-Throughput Materials Discovery for Extreme Conditions* Program

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Objectives

To leverage new directions in

<u>predictive modeling</u> and <u>adaptive learning</u>

for accelerated computational analysis and design of materials in extreme conditions.

The proposed application is to utilize these approaches to

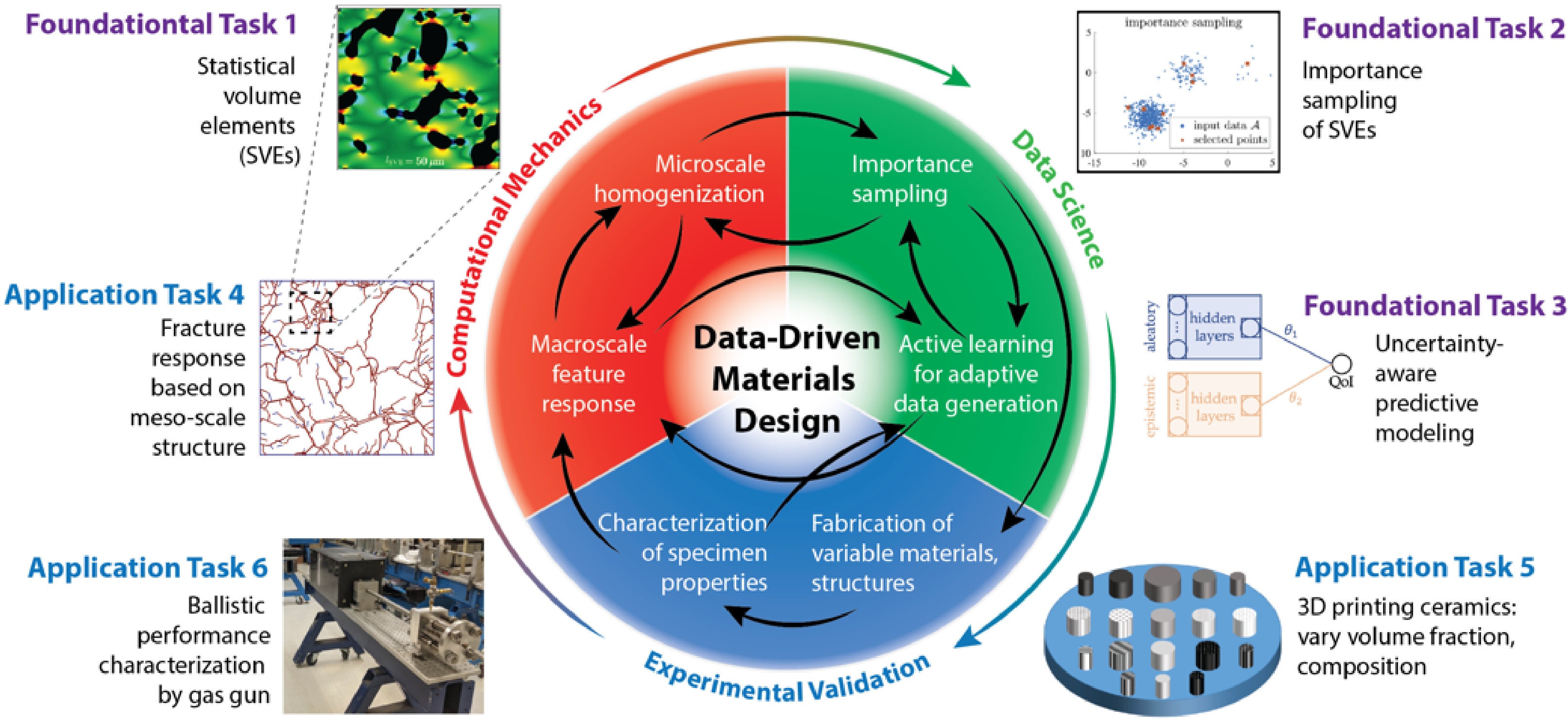
(a) determine *quantitative features of failure* in novel ceramics and

(b) *design materials* for enhanced ballistic performance, with the outlook to be additively manufactured.

Overall Technical Approach

- Foundational Research
  1. SVE Analysis
  2. Importance Sampling
  3. Uncertainty Aware Predictive Modeling
- Application Demonstrator
  4. Meso-scale Fracture Response
  5. 3D Printing of Ceramics
  6. Characterization

Application Demonstrator:
High Throughput Discovery of Novel Ceramics for Ballistics

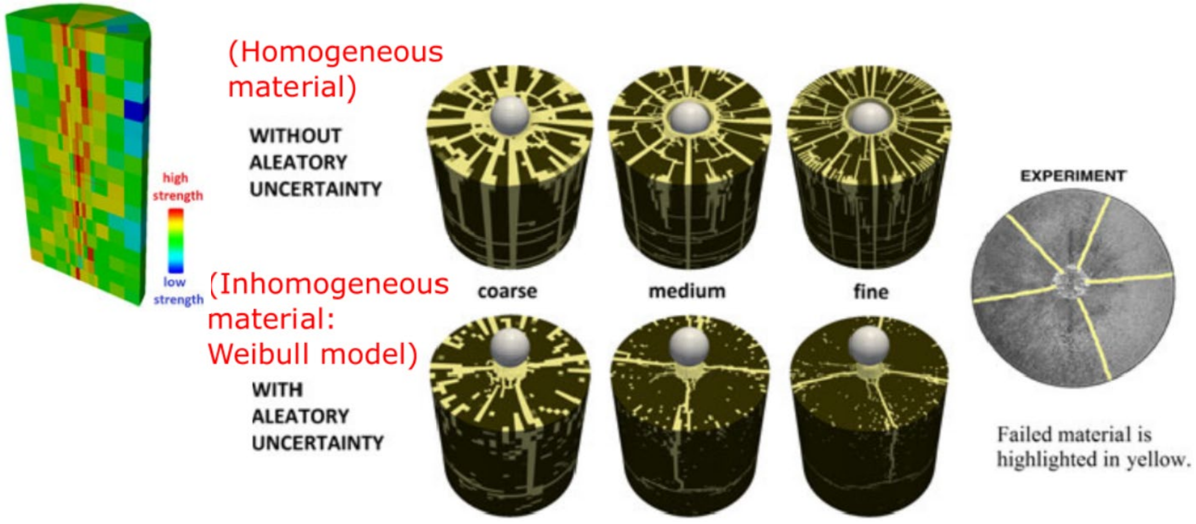


Research Plan

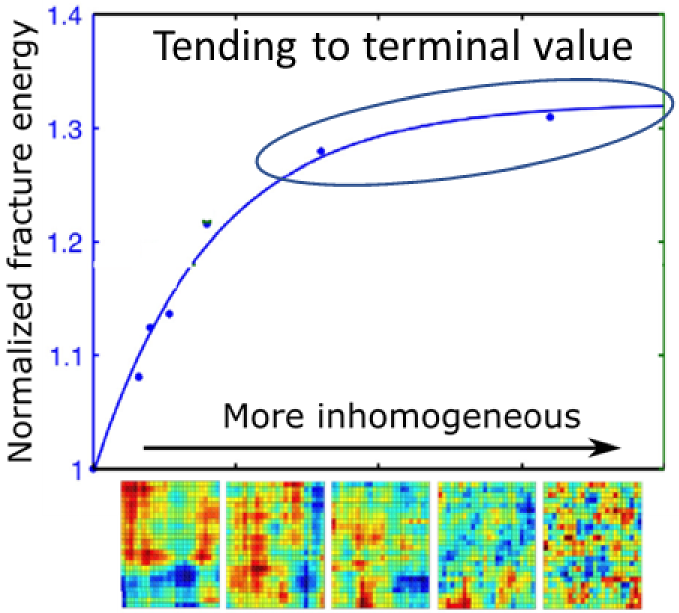
Computational Mechanics

Problems with homogeneous deterministic models

Challenge 1: Maintaining sufficient inhomogeneity

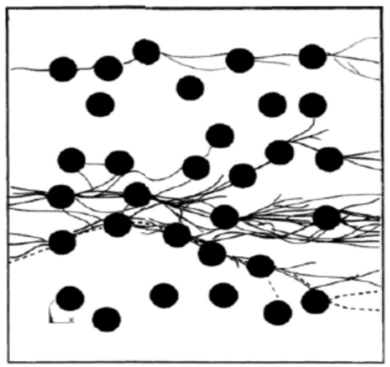


O Erik Strack, RB Leavy, and Rebecca M Brannon. Aleatory uncertainty and scale effects in computational damage models for failure and fragmentation. International Journal for Numerical Methods in Engineering, 102(3-4):468–495, 2015



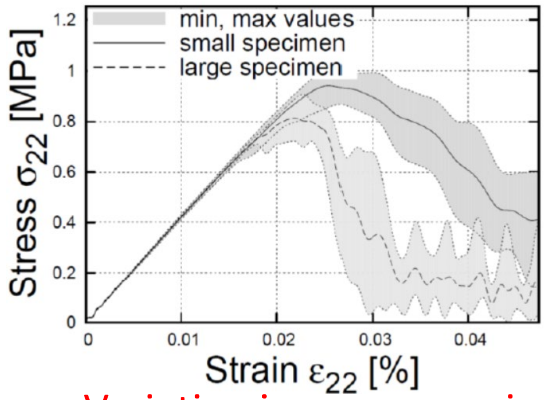
L.S. Dimas, T. Giesa, and M.J. Buehler. Coupled continuum and discrete analysis of random heterogeneous materials: Elasticity and fracture. Journal of the Mechanics and Physics of Solids, 63(1):481–490, 2014

Challenge 2: Sample-to-sample variations



A. Al-Ostaz and I. Jasiuk. Crack initiation and propagation in materials with randomly distributed holes. Engineering Fracture Mechanics, 58(5-6):395–420, 1997

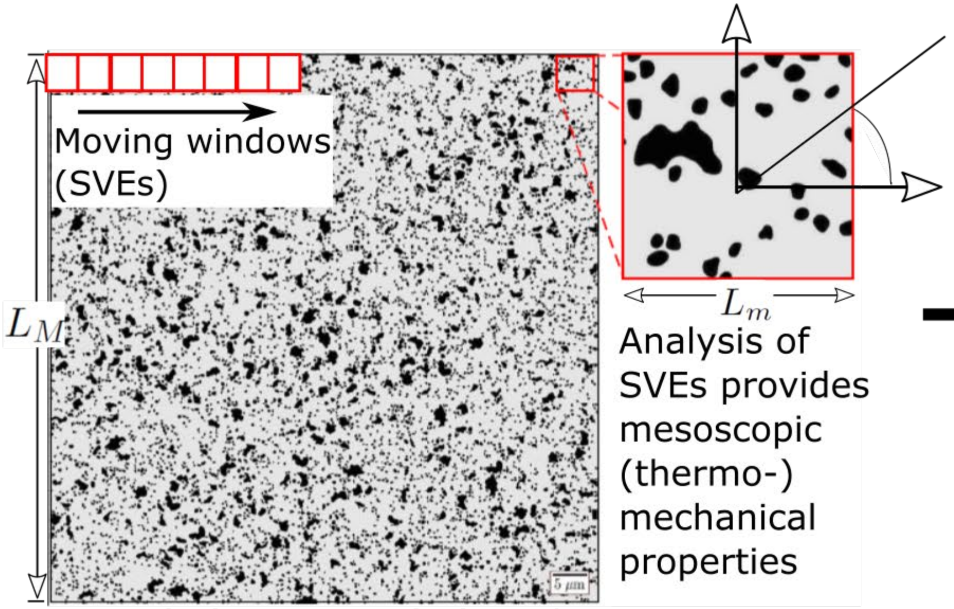
Variation in fracture pattern



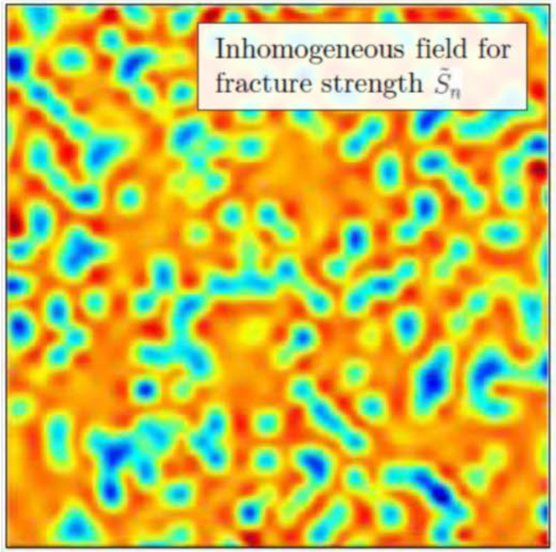
J Kozicki and J Tejchman. Effect of aggregate structure on fracture process in concrete using 2D lattice model. Archives of Mechanics, 59(4-5):365–84, 2007

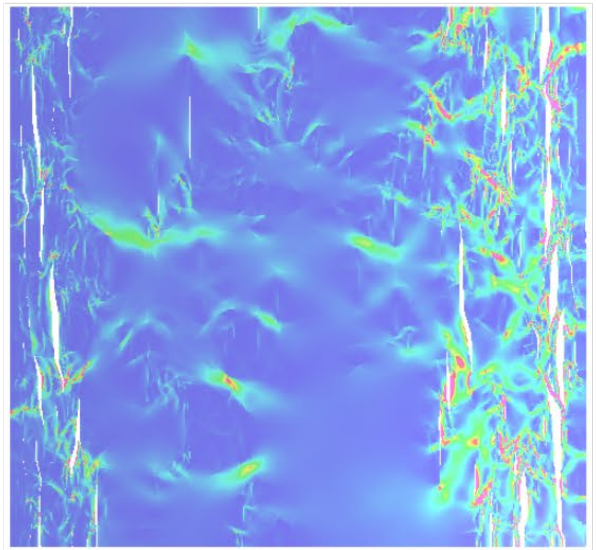
Variation in macroscopic QoIs

Related work: Homogenization using SVEs and Failure



Micro (m) to Meso (m) scale using SVEs: mesoscopic properties depend on microstructure



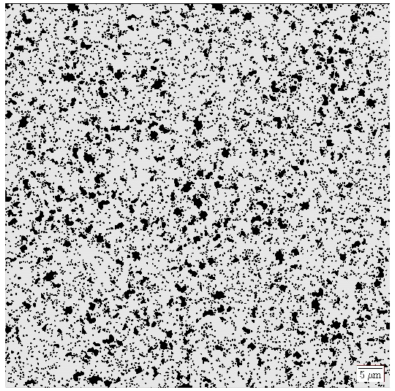


Meso (m) to Macro (M) scale: Mesoscopic material properties are realized (left) and used for fracture simulation (right)

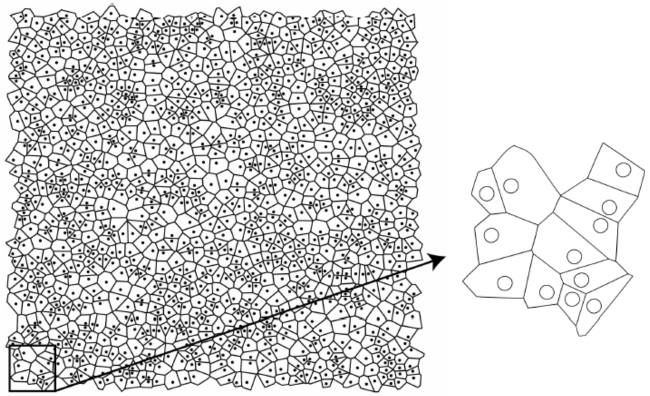
Task 1: Use of SVEs to homogenize elasticity and strength at meso-scale

- Homogenize mesoscopic elastic and fracture properties using SVEs:

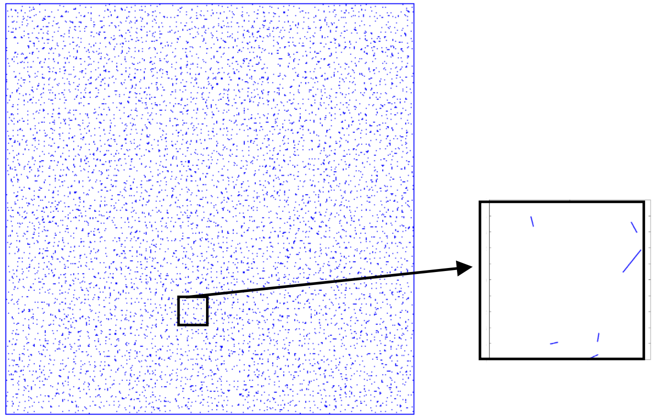
Different microstructures / SVEs



Accurate geometric modeling / (CISAMR) Soheil Soghrati (OSU)

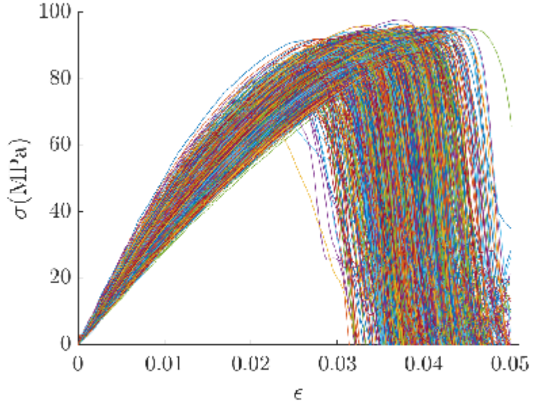


Voronoi SVEs, Katherine Acton (UST)



Microcracks & other defects

Mesoscopic elastic & fracture response is characterized

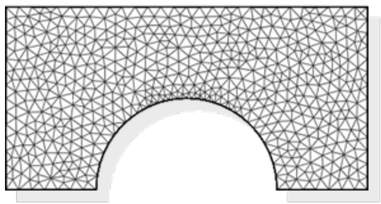


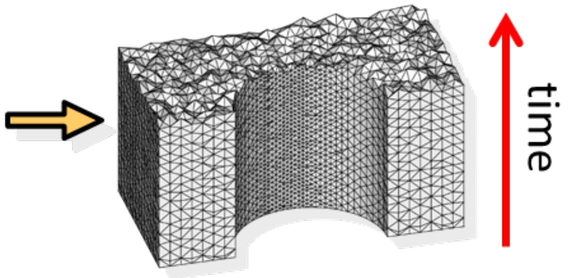
- ARL ballistic material 3D printing capabilities will be integrated in this project plan.

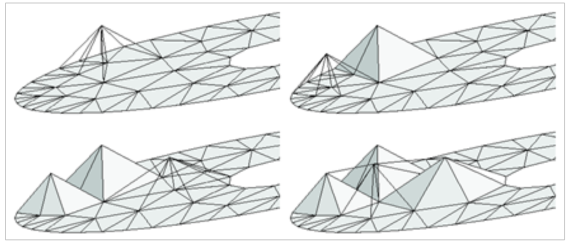
Parameter	Range of Interest
Particle composition	1:0 A:B to 0:1 A:B
Organic binder or solvent	1:0 A:B to 0:1 A:B
Particle size distribution	1:0 A:B to 0.5:0.5 A:B
Particle volume fraction	50 to 70 vol%

Task 4: Macro-scale fracture using random fields of SVE-driven properties and SML

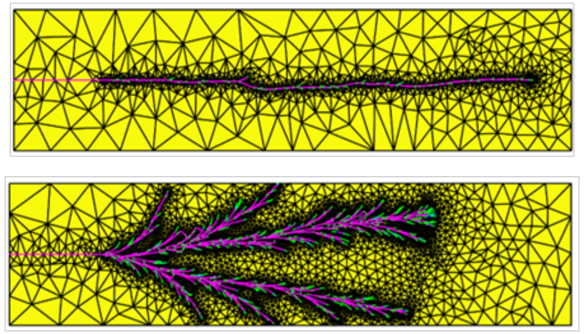
Macroscopic Fracture Simulations using asynchronous Spacetime Discontinuous Galerkin (aSDG)

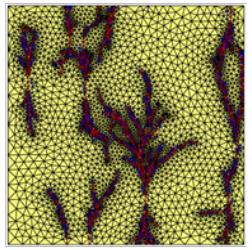






and each time only small "patch" of elements is solved





How to utilize Scientific Machine Learning (SML; Tasks 2 & 3): Substantial reduction of the number of forward simulations

- For many fragmentation analyses sufficient level of heterogeneities must be maintained in material properties:

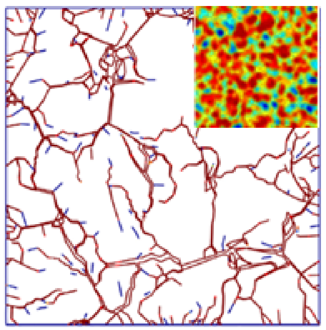
$$a(\mathbf{x},\omega) \approx \mathbb{E}[a](\mathbf{x}) + \sum_{i=1}^{n} \sqrt{\lambda_i} b_i(\mathbf{x}) Y_i(\omega)$$

Random field is represented by *n* independent random variables Y_i

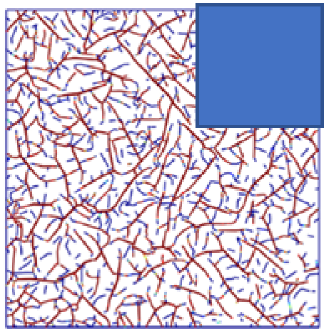
- For realistic domain sizes, 10000s of KL terms may need to be maintained!

- **Importance sampling** and **active learning** from Tasks 2, 3 is used to reduce the number of forward simulations.

Karhunen-Loever strength field



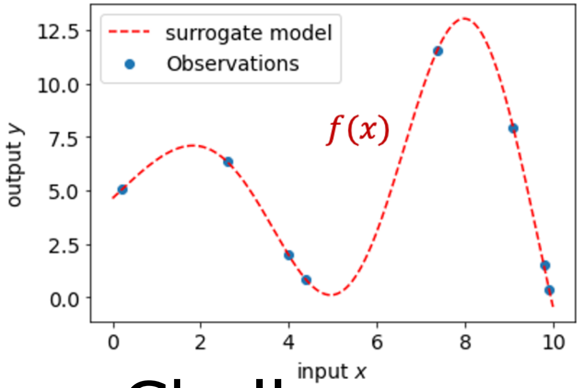
Uniform strength field

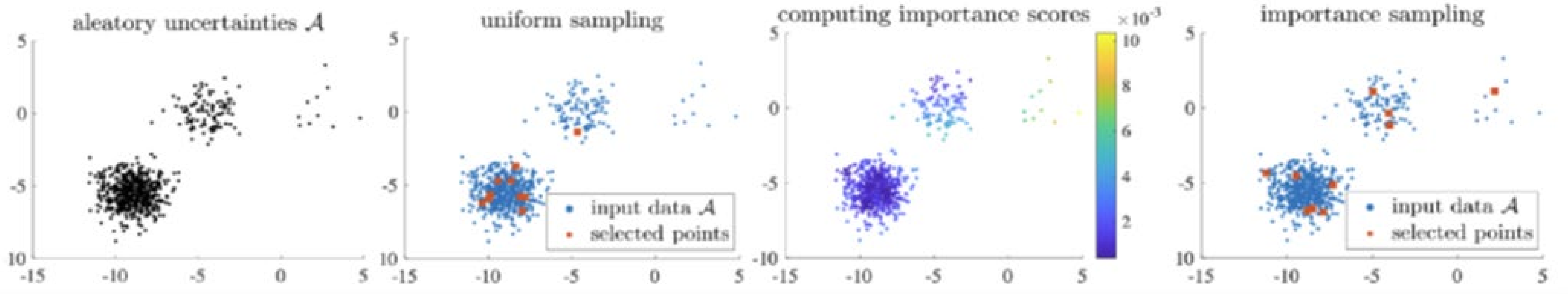


Scientific Machine Learning

Scientific Machine Learning

- Advantages
  - Build surrogate models to accelerate design/analysis of materials
  - Optimization, inverse problems, etc.



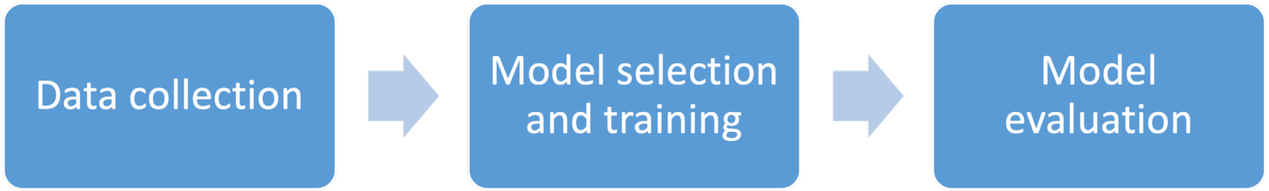


- Challenges
  - Generating data for training and testing
    - Expensive computational models, e.g., DNS
  - Incorporating various sources of uncertainty
    - Natural or physical randomness (aleatory)
    - Imperfect knowledge (epistemic)
  - Overlooking rare/extreme events: <u>Failure</u>

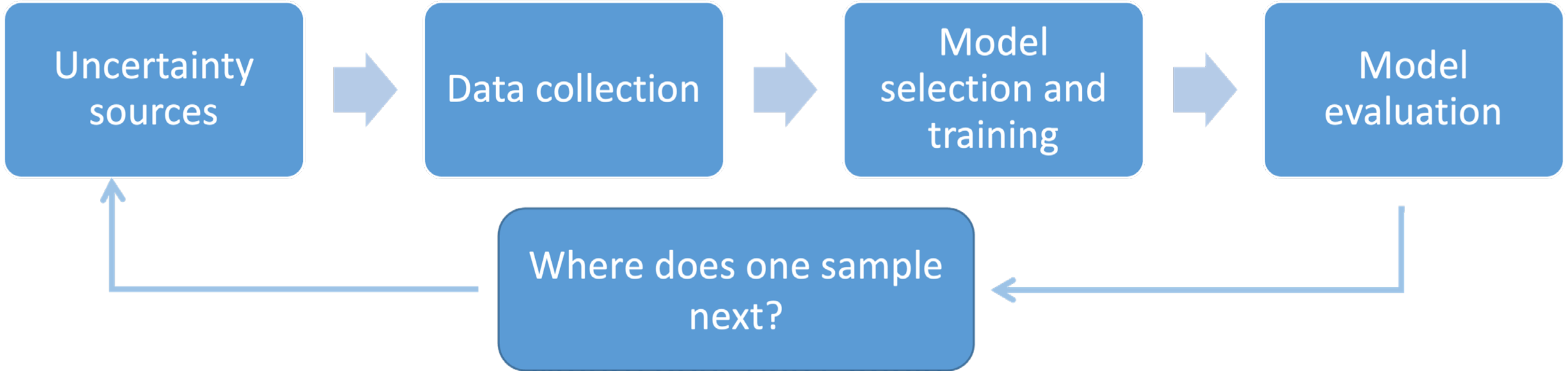
Heavy-tailed data in high-dimensional space

Overview of data science tasks

- Standard "big data" techniques are not appropriate for most *scientific and design* problems

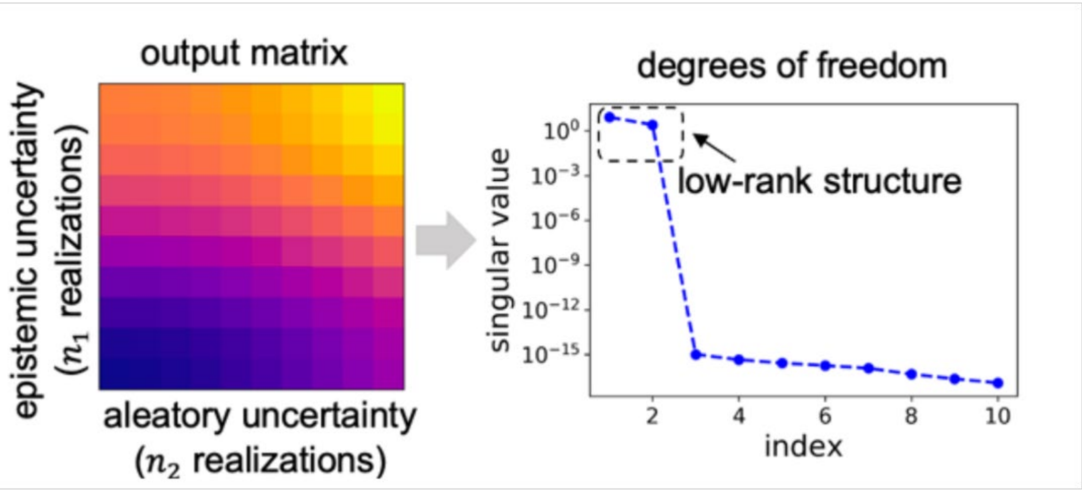


- We propose a "data-centric" approach for handling of *uncertainties* in computational models

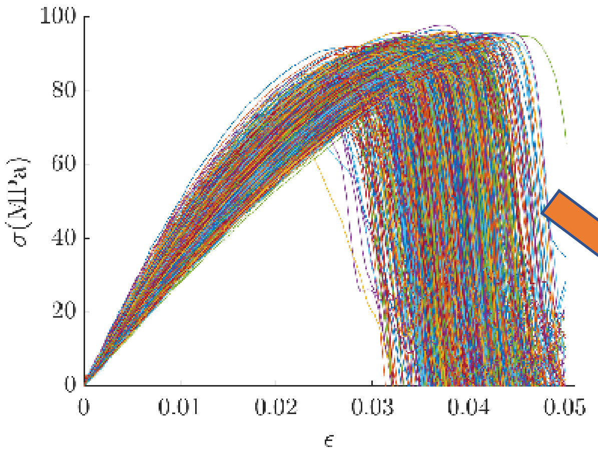


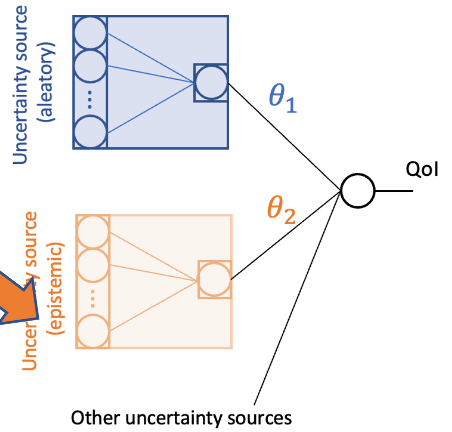
Tasks 2 and 3

- Task 2: Developing importance sampling strategies
  - Decomposing uncertainty sources in the design space to capture patterns in the output space
  - Guiding machine learning models using the underlying physics



- Task 3: Using multi-modal data for predictive modeling
  - Each uncertainty type viewed as a modality
    - Meso-scale aleatory uncertainty to be treated as epistemic in macro-scale
  - Overcoming the curse of dimensionality
  - Improved confidence intervals





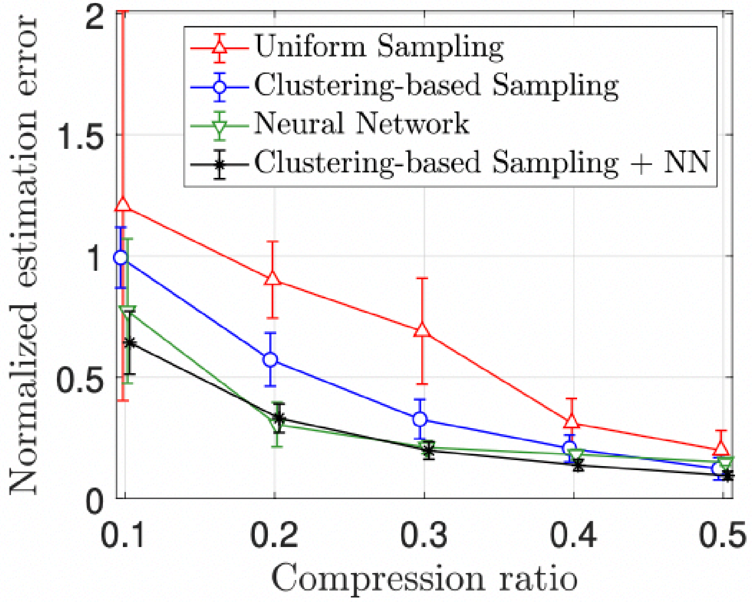
Prior work on reducing the number of simulations

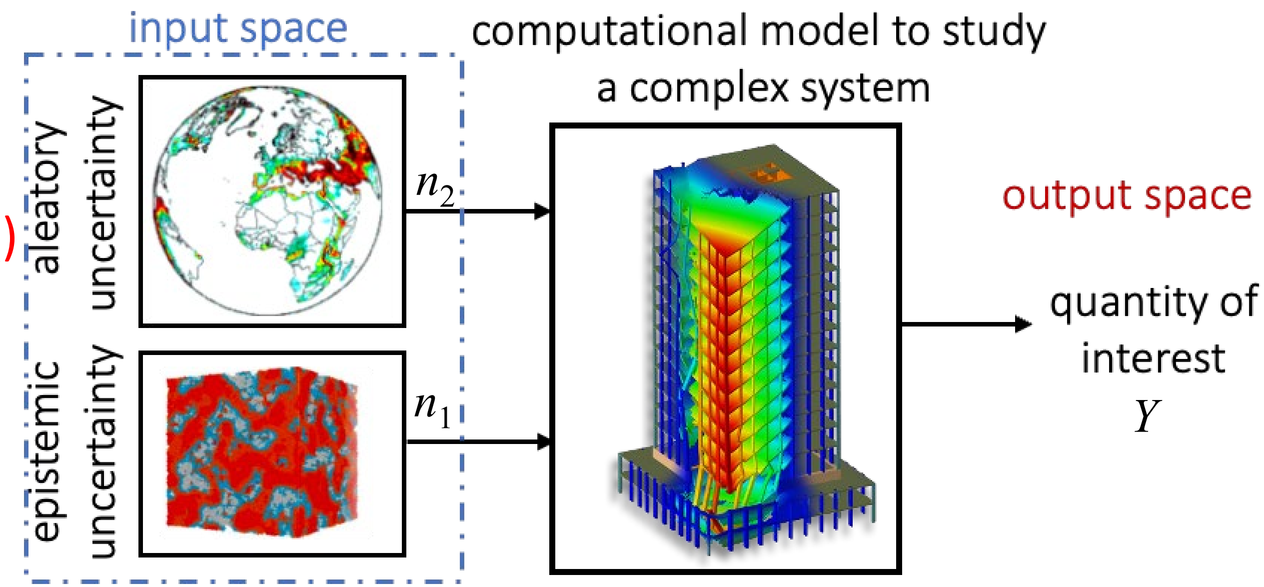
- Quantifying the impact of uncertainty in material properties and ground motion records on structural response

$$\min_{A\in\mathbb{R}^{n_1\times r},\, B\in\mathbb{R}^{r\times n_2}} \left\|\mathscr{L}\left(Y - AB\right)\right\|$$

partial observations

output matrix (n_1 X n_2)





Hariri-Ardebili, M. A., & Pourkamali-Anaraki, F. (2022). Structural uncertainty quantification with partial information. *Expert Systems with Applications*.

Fabrication, Characterization, and Validation

3D Printing of Highly Filled Materials

Existing UML/ARL collaboration with E.J. Robinette, J. La Scala, I. McAninich, et al.

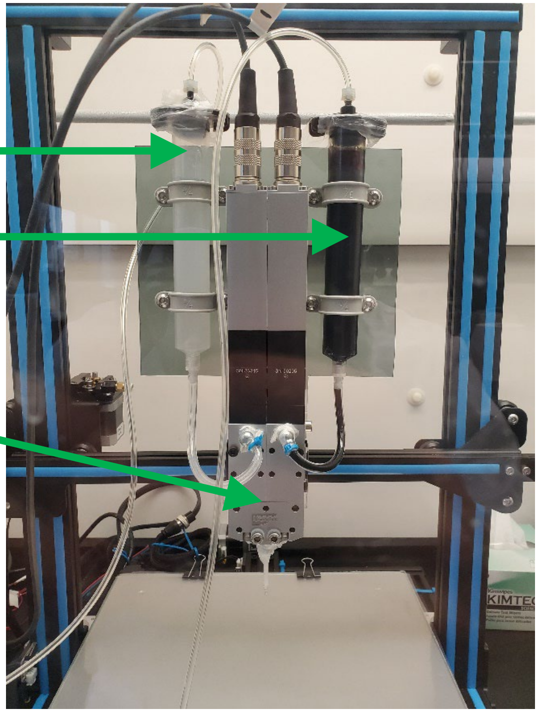
ARL: N. Ku, L. Vargas-Gonzalez
UCSD: J. Pelz, M. Myers

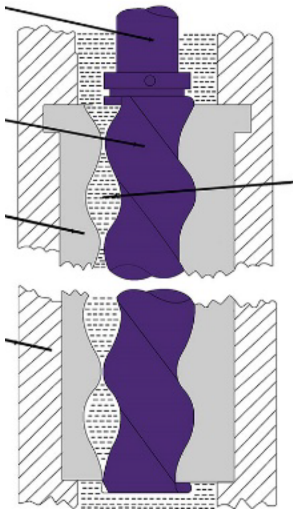
Ambient Reactive Extrusion (ARE) / Material Extrusion

Reservoir A

Reservoir B

Progressive cavity extruders





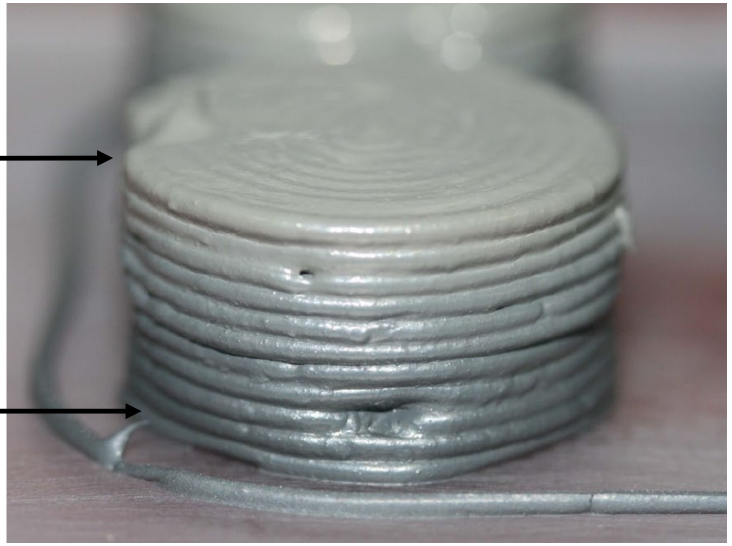
Pump viscosities
> 10^4 Pa-s

In-Line Mixing for AM of Ceramics

Silicon carbide

gradient

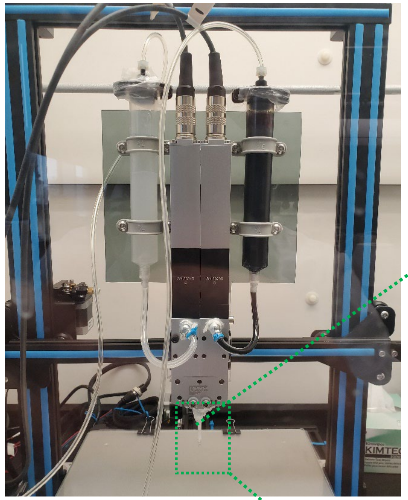
Boron carbide

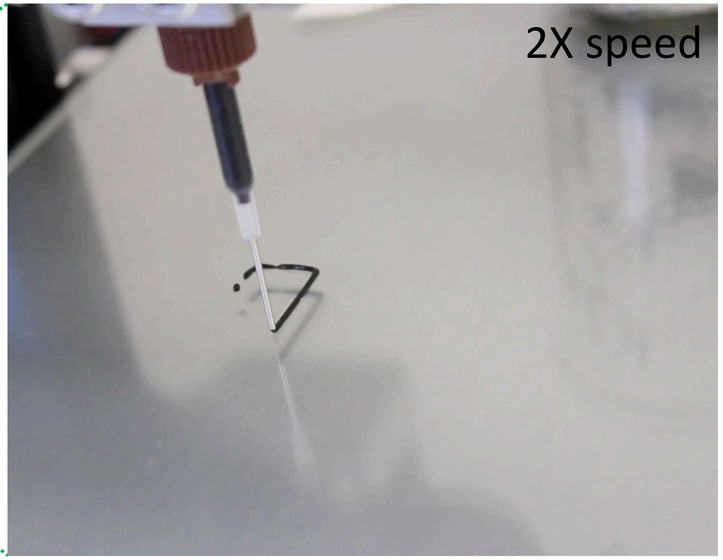


Pelz et al. *ARL-TR-8851* 2019

~50 vol% compositions printed by Direct Ink Writing

Application Demonstrator Task 5: 3D Printing Ceramics

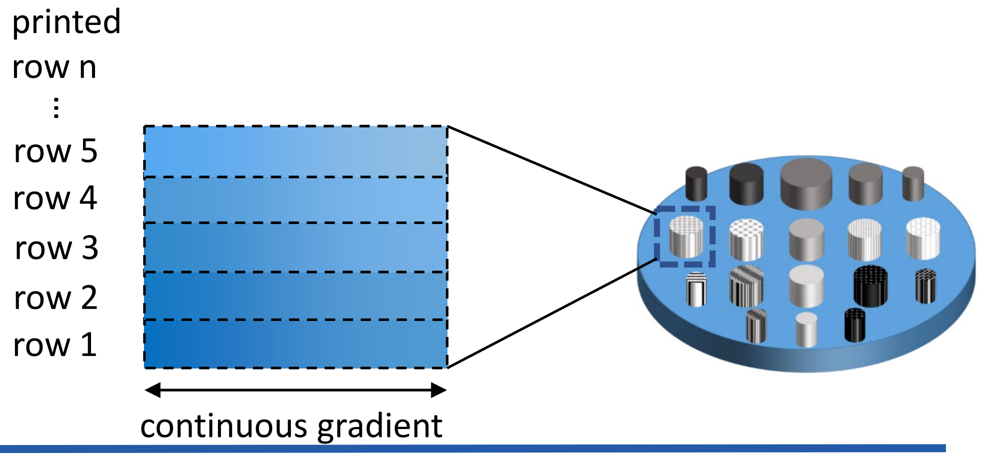




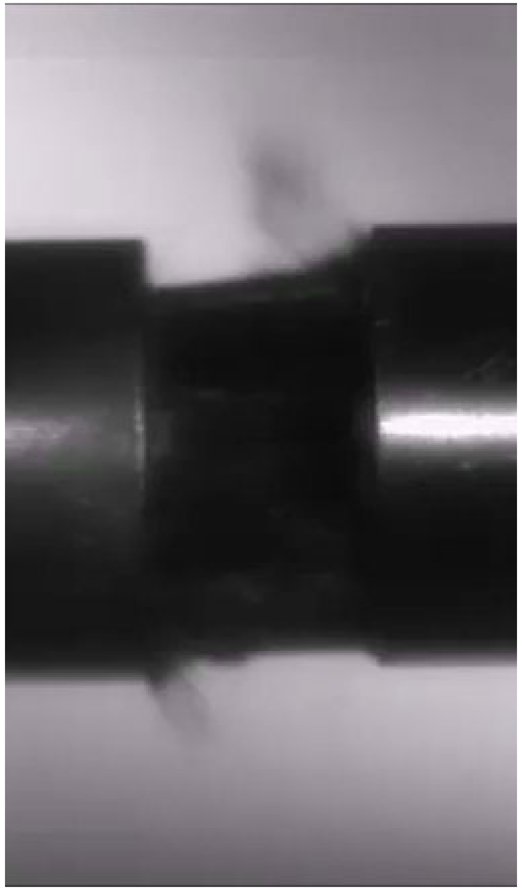
Reactive 2-part thermoset with unimodal filler (up to 40 vol%)

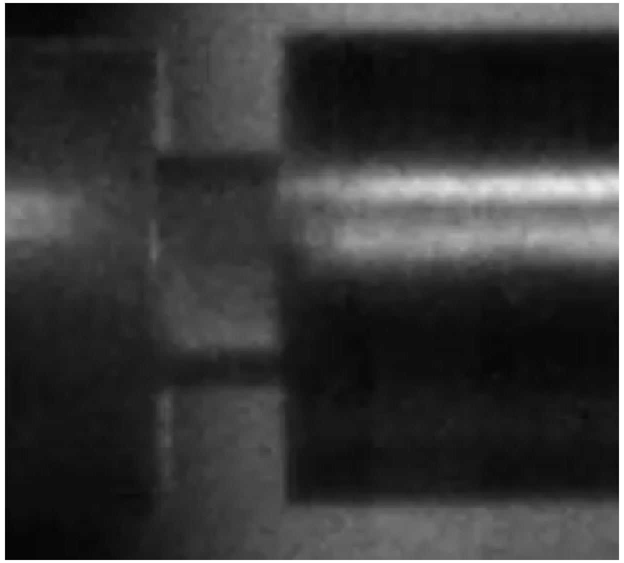
Consider the following parameters, with exact numbers determined by importance sampling

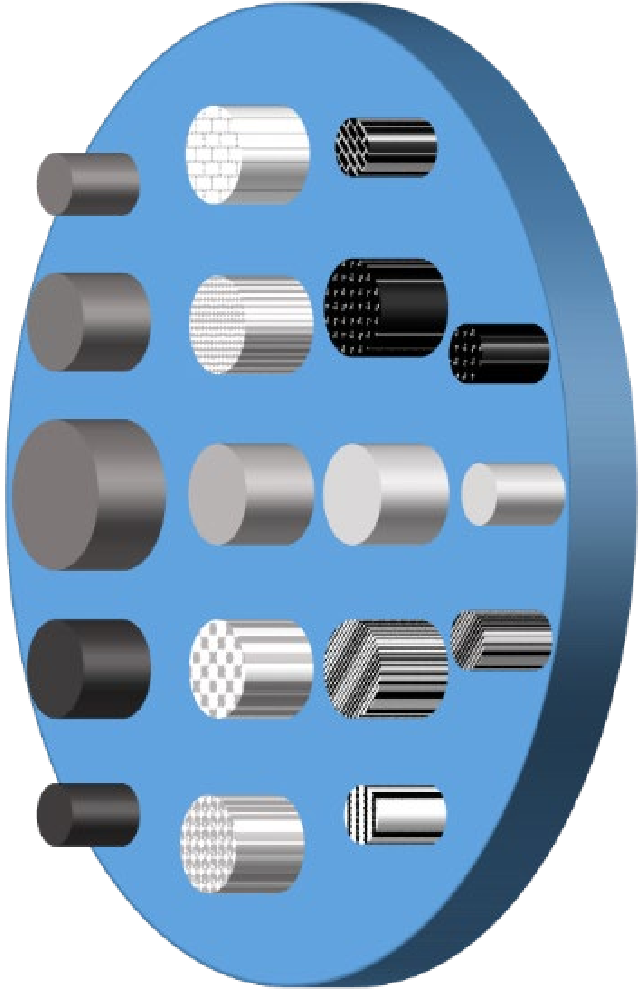
Parameter	Range of Interest
Particle composition	1:0 A:B to 0:1 A:B
Organic binder or solvent	1:0 A:B to 0:1 A:B
Particle size distribution	1:0 A:B to 0.5:0.5 A:B
Particle volume fraction	50 to 70 vol%



Application Task 6: Characterization and Validation







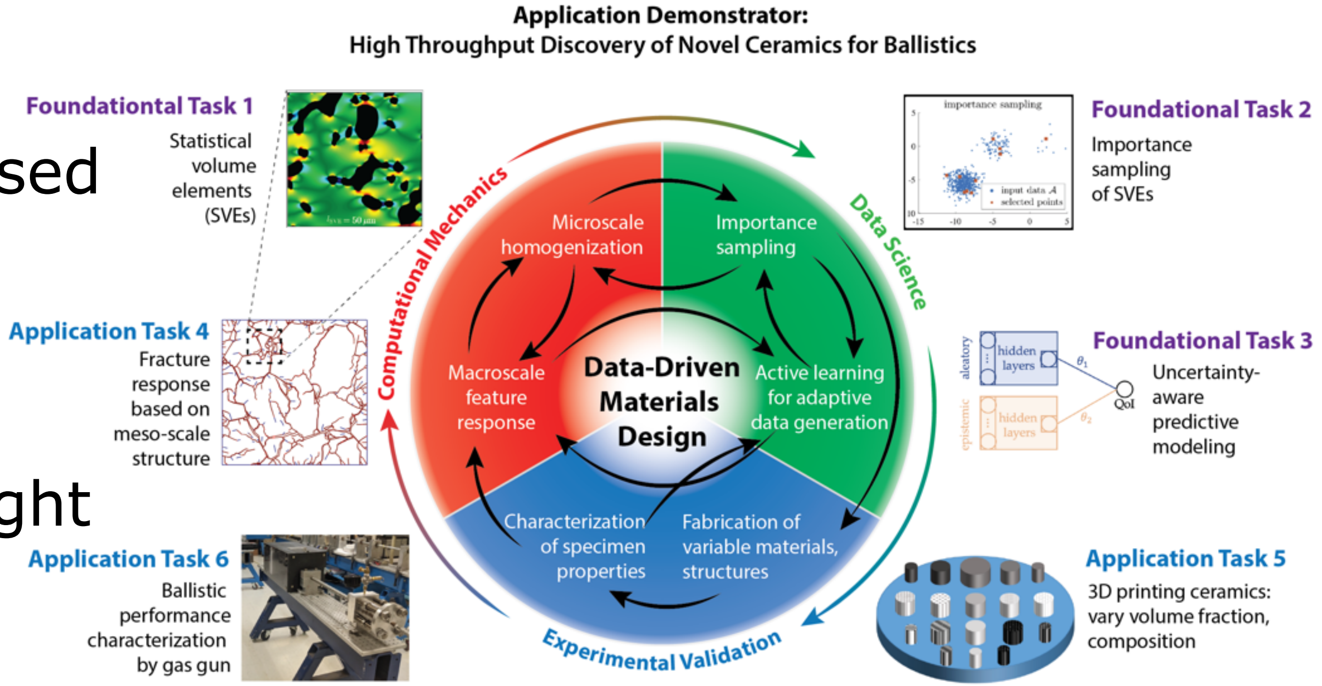
Impact: HTMDEC Program Thrusts

Short term impact on

- Thrust 1 (Material Design) in areas
  - ii. *Adaptive learning* and
  - iv. *Uncertainty quantification*, and
- Thrust 4 (ML-augmented Physics-Based Models) in areas
  - ii. *Scale-bridging considerations*, and
  - iii. *Training of ML models*.

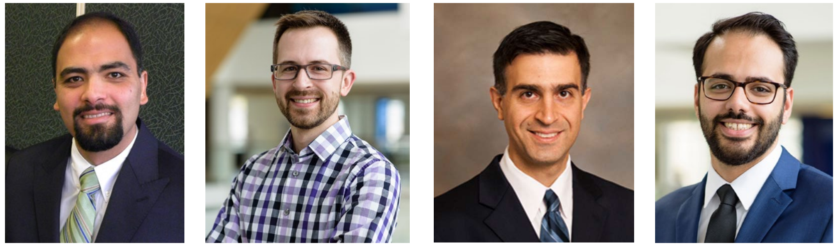
Long term, to expand results and methodology to address and gain insight in

- 1.iii. *ML/AI driven designs*,
- 4.i. *Implementation of ML-augmented physics-based models*,
- 4.v. *Developing of an overarching methodology*.



Management, Roles, and Timeline

- Ongoing
  - Material Selection (UML to seek input from ARL; Tasks 1, 2, and 5)
  - Computation SVE modeling (UTSI; Task 1)
  - Importance sampling with uncertainty (CUD; Task 2)
- Planned
  - Active learning (3)
  - Fracture modeling (4)
  - Fabrication (5)
  - Characterization (6)



Amirkhizi (PI, UML), Hansen (UML), Abedi (UTSI/UTK), Pourkamali (UML/CUD)

	Quarter 1	Quarter 2	Quarter 3	Quarter 4
Foundational Task 1: SVE-modeling of elasticity and fracture QSPRs				
Foundational Task 2: Importance sampling with uncertainty				
Foundational Task 3: Active learning for adaptive importance sampling				
Application Task 4: Macro-scale modeling for failure QoIs				
Application Task 5: Fabrication with variable micro-structure				
Application Task 6: Experimental verification of QSPRs and QoIs				

Discussion on Collaboration

- Leverage ongoing collaboration with ARL on
  - 3D printing of Ceramics (T. Plaisted, A. Rosenberger, G. Gazonas, L. Vargas-Gonzales, et al.)
  - Ambient Reactive Extrusion (E. J. Robinette, J. La Scala, I. McAninich, et al.)

- Outreach to other seedling teams, in all thrust areas

- Data management

Ceramic Properties

$E = 300$ Gpa

$\rho = 3985$ kg/m^3

$\nu = 0.27$

$T_{n,max} = 270$ Mpa