

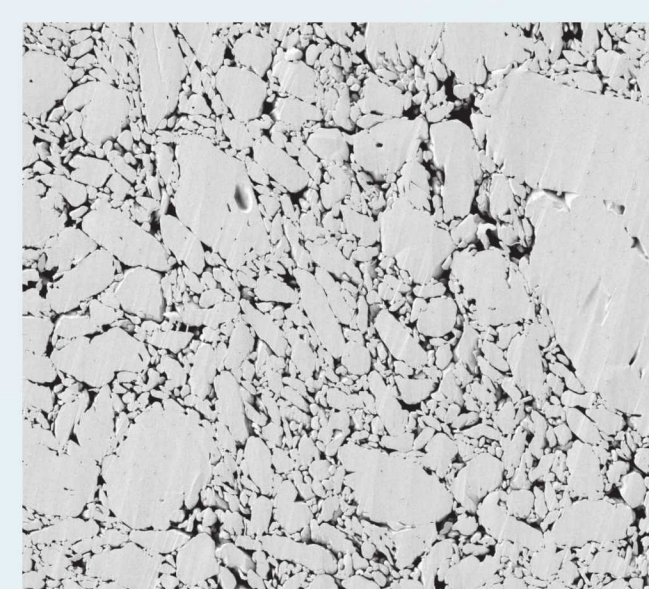
# DATA ANALYSIS OF HETEROGENEOUS MATERIAL MICROSTRUCTURES

## applications to energetic materials and polymer foams

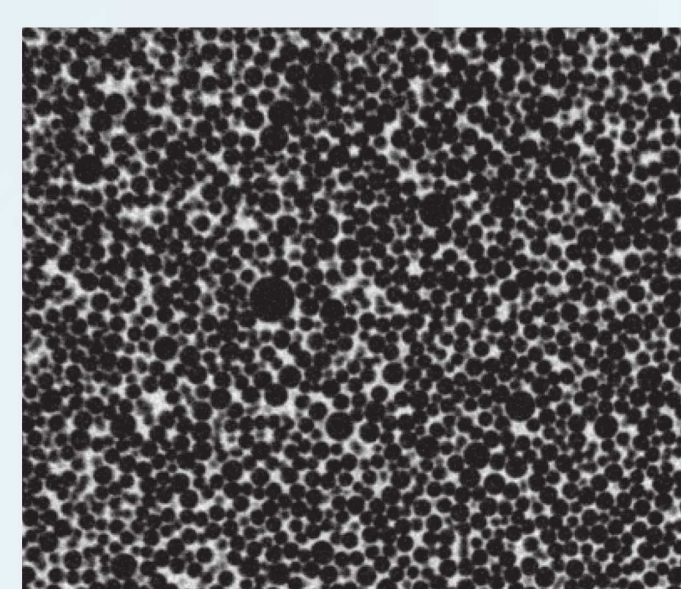
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### HETEROGENEOUS MATERIALS

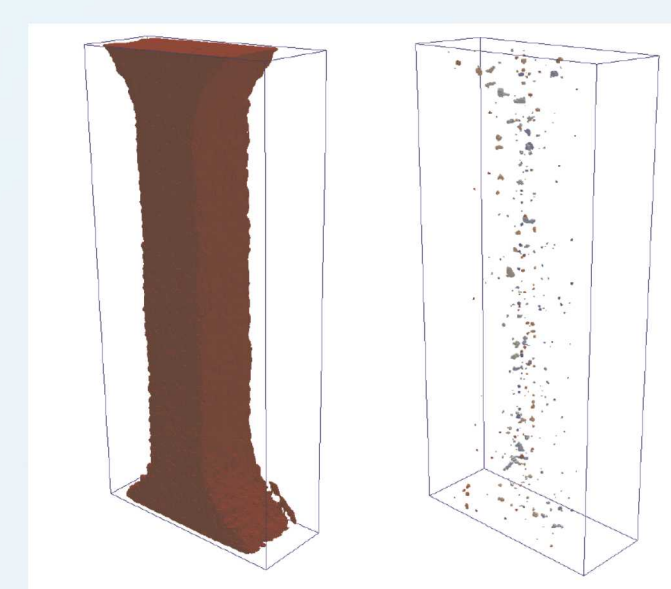
- Many Sandia mission-critical technologies rely on materials with complex, process-dependent microstructures:



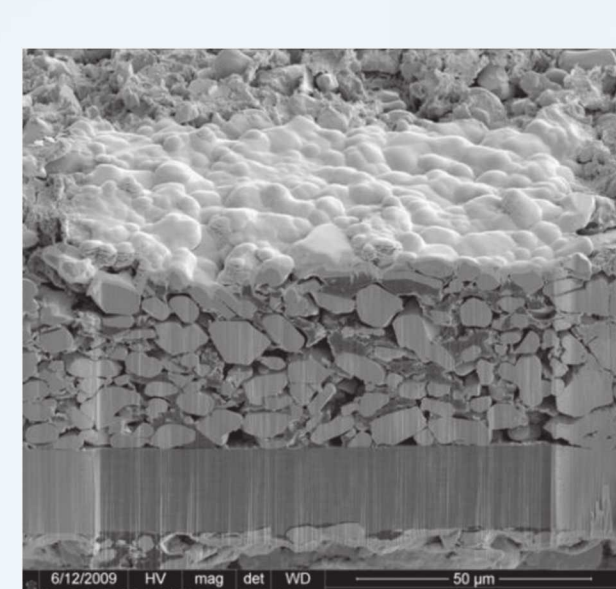
*Energetic materials*  
(explosives, pyrotechnics, propellants)



*Polymer foams*  
(compression pads, shipping container foams)



*Additively manufactured components*

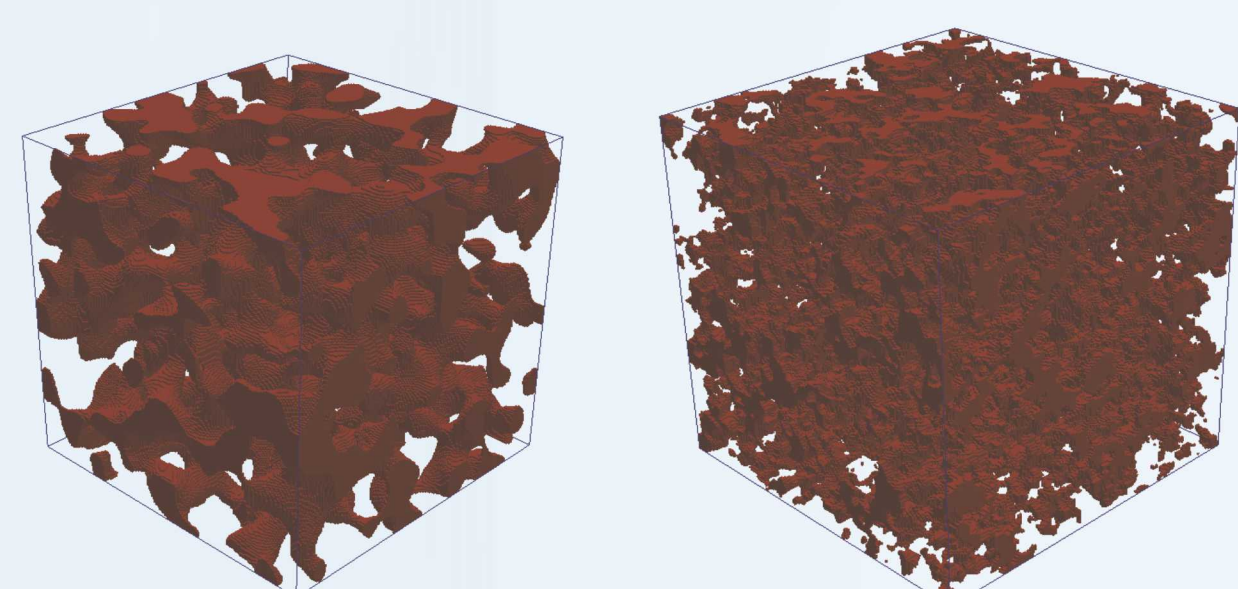


*Battery electrodes<sup>1</sup>*

- Goal: quantify/understand microstructure
  - Build process-structure-property relationships
  - Inform homogenized continuum models

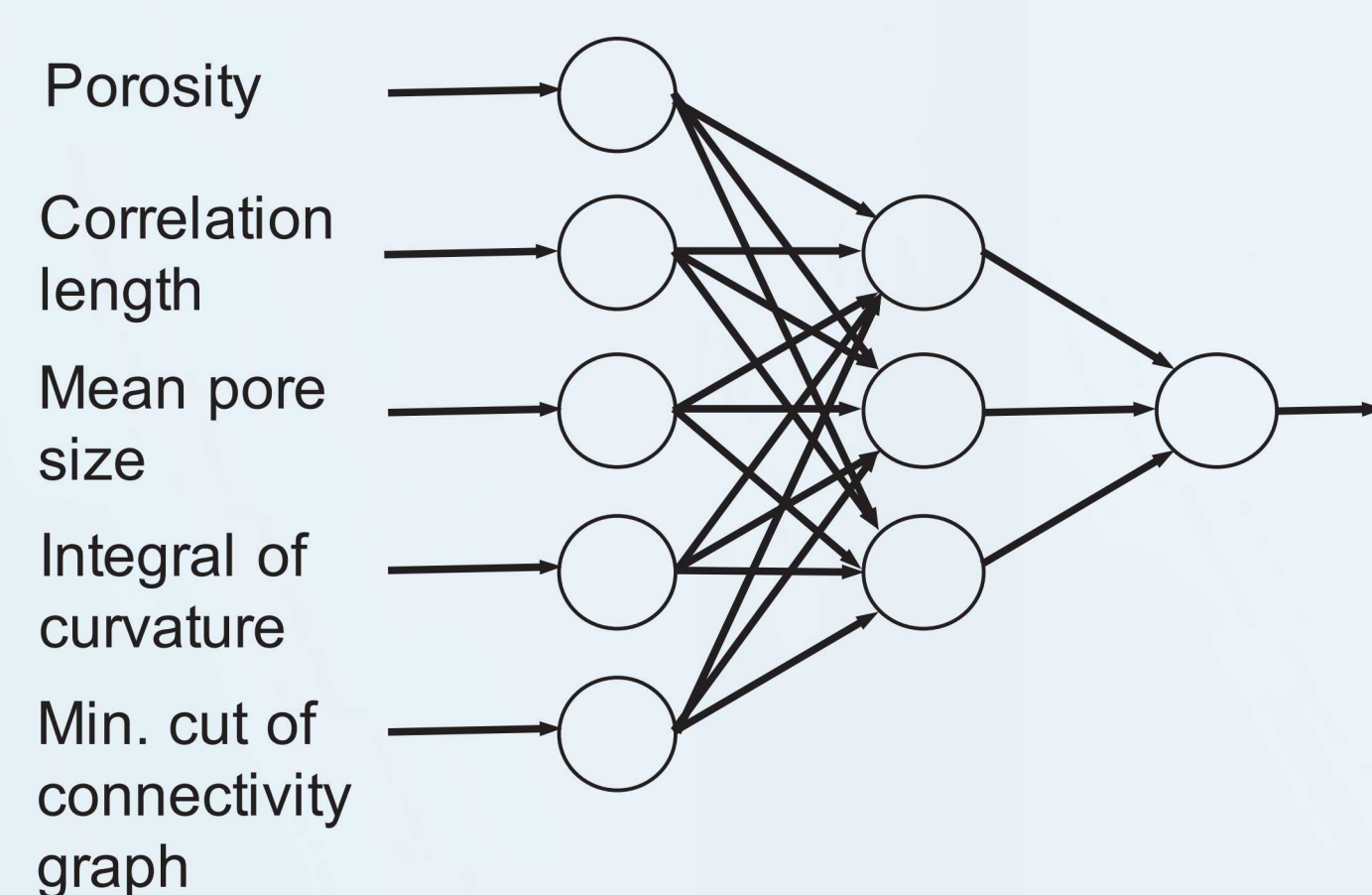
### MICROSTRUCTURE ANALYSIS: CORNING CRADA

- Proof of concept and development of analysis tools
- Generate large ensemble of microstructures (>1000), use direct numerical simulation to obtain effective property of interest:

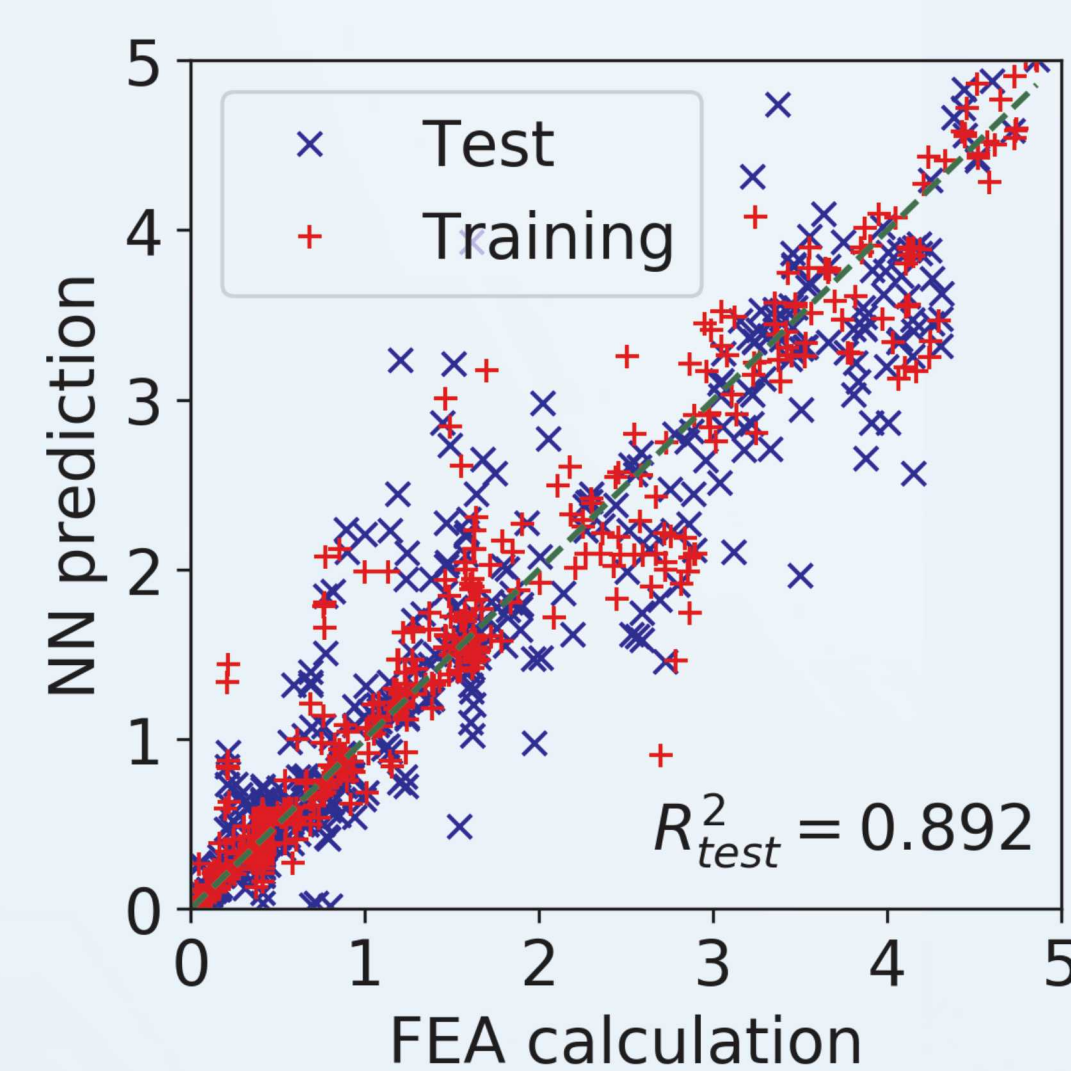


- Compute various structural metrics:
  - Porosity, specific surface area, spatial correlations, topology, pore size/shape distributions, local geometry (e.g. curvature), ...
- Machine learning model (neural network) for regression: can we predict effective properties based on structural metrics?

Input: structural metrics



Output: effective property (for training, computed numerically)

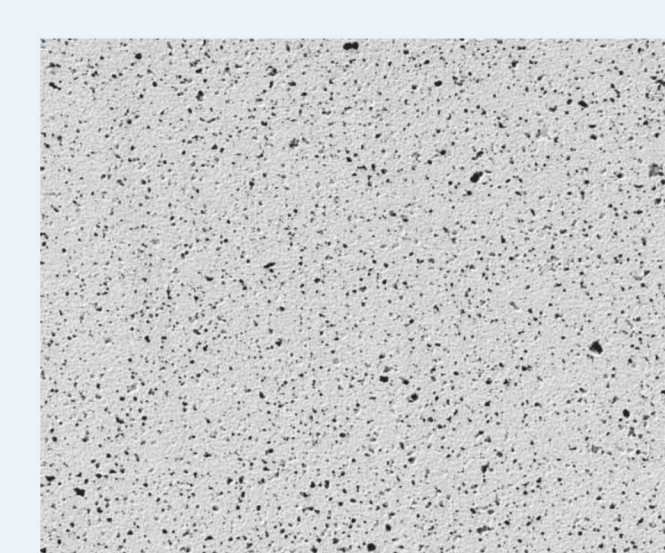


- Summary
  - Structural metrics can predict physical properties of interest
  - Machine learning models are effective with sufficient data, but can also identify relevant features

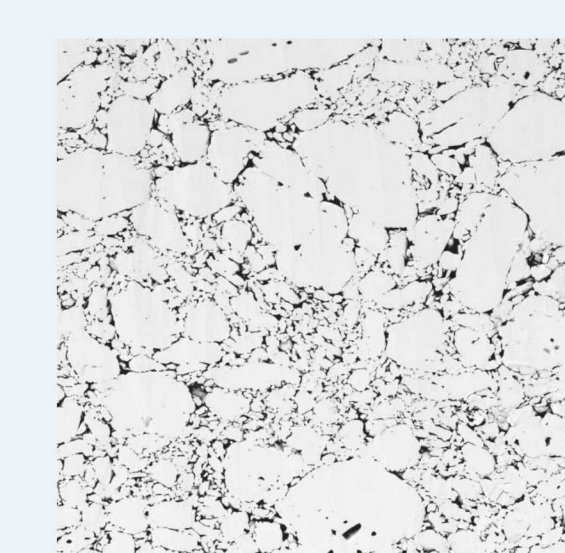
### APPLICATION TO ENERGETIC MATERIALS

- Goal: relate microstructure to shock detonation response
  - Current ES LDRD (PI: Yarrington)
  - Same material: triaminotrinitrobenzene (TATB), two different initial particle types (UF and Nano), pressed to various densities (%TMD)

Microscopy imaging of structures

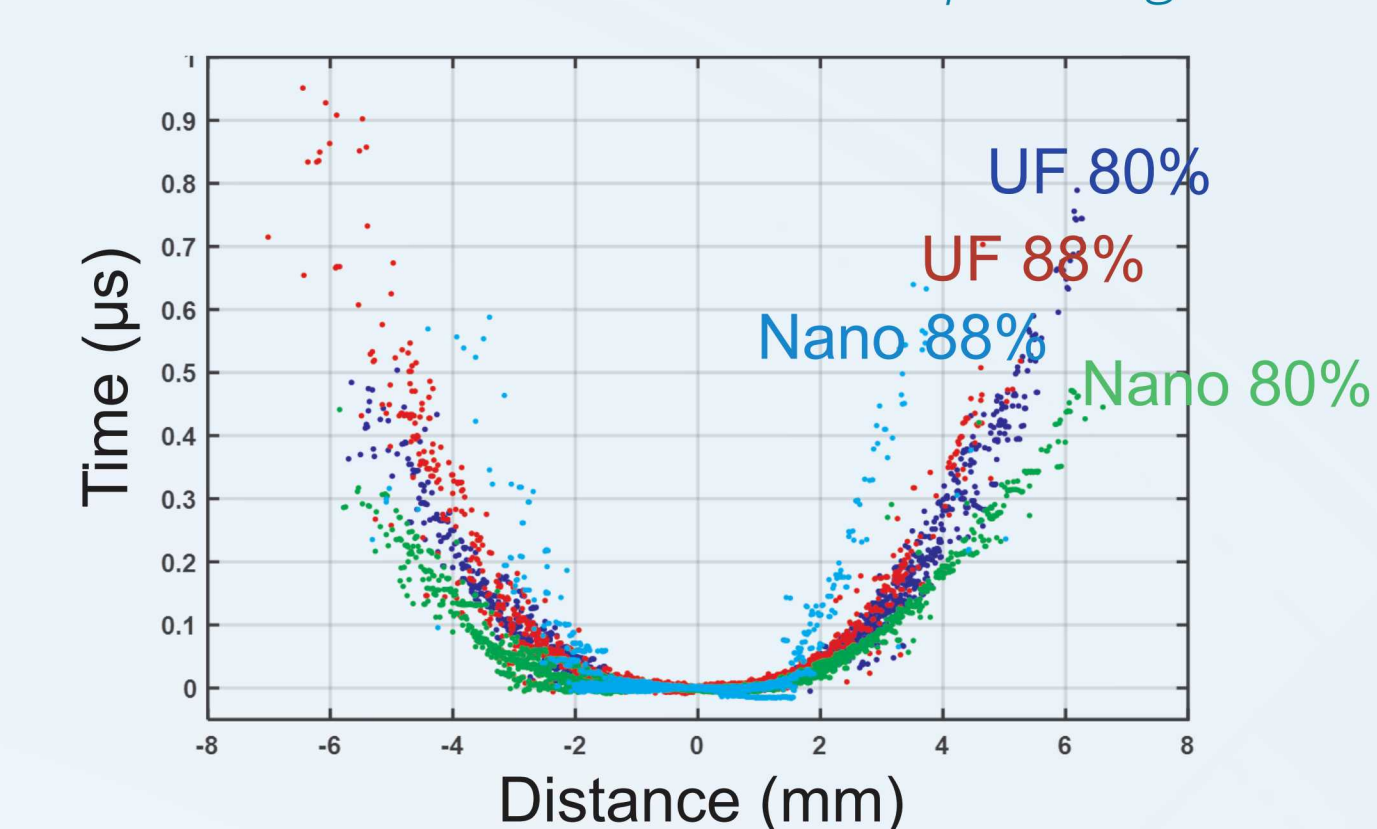


TATB Nano 88% TMD

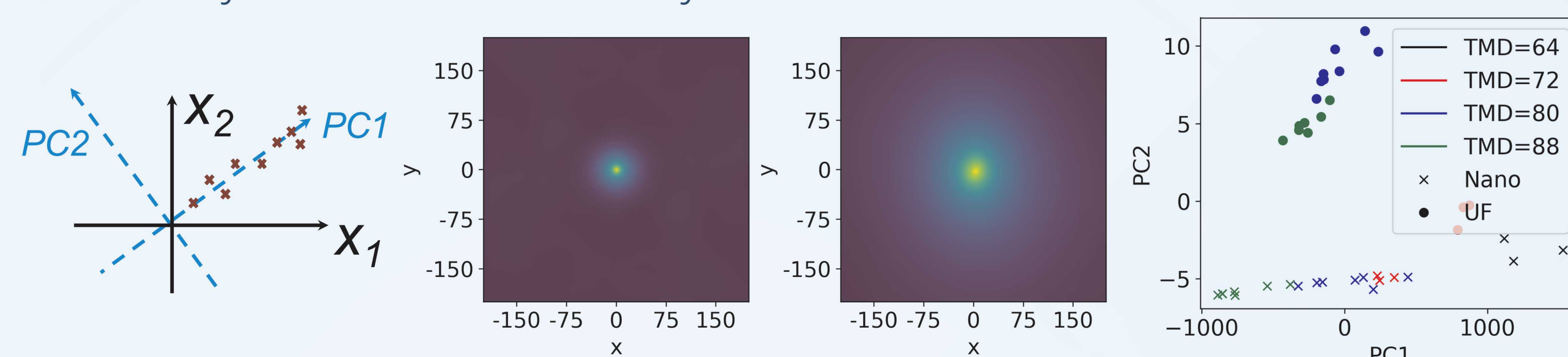


TATB UF 88% TMD

Measured detonation wave spreading



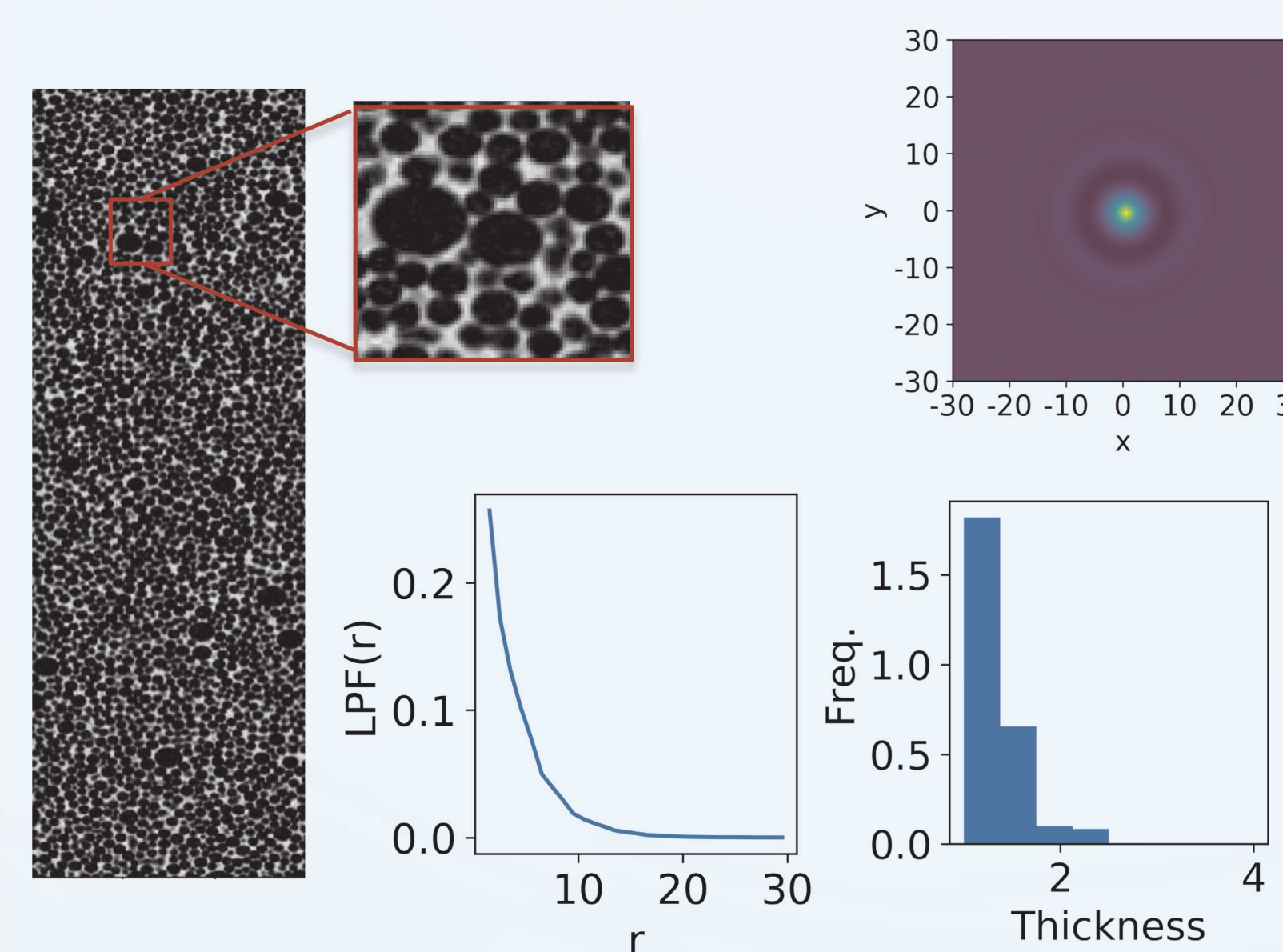
- Two-point correlation functions + principal components analysis for dimensionality reduction<sup>2,3</sup>:



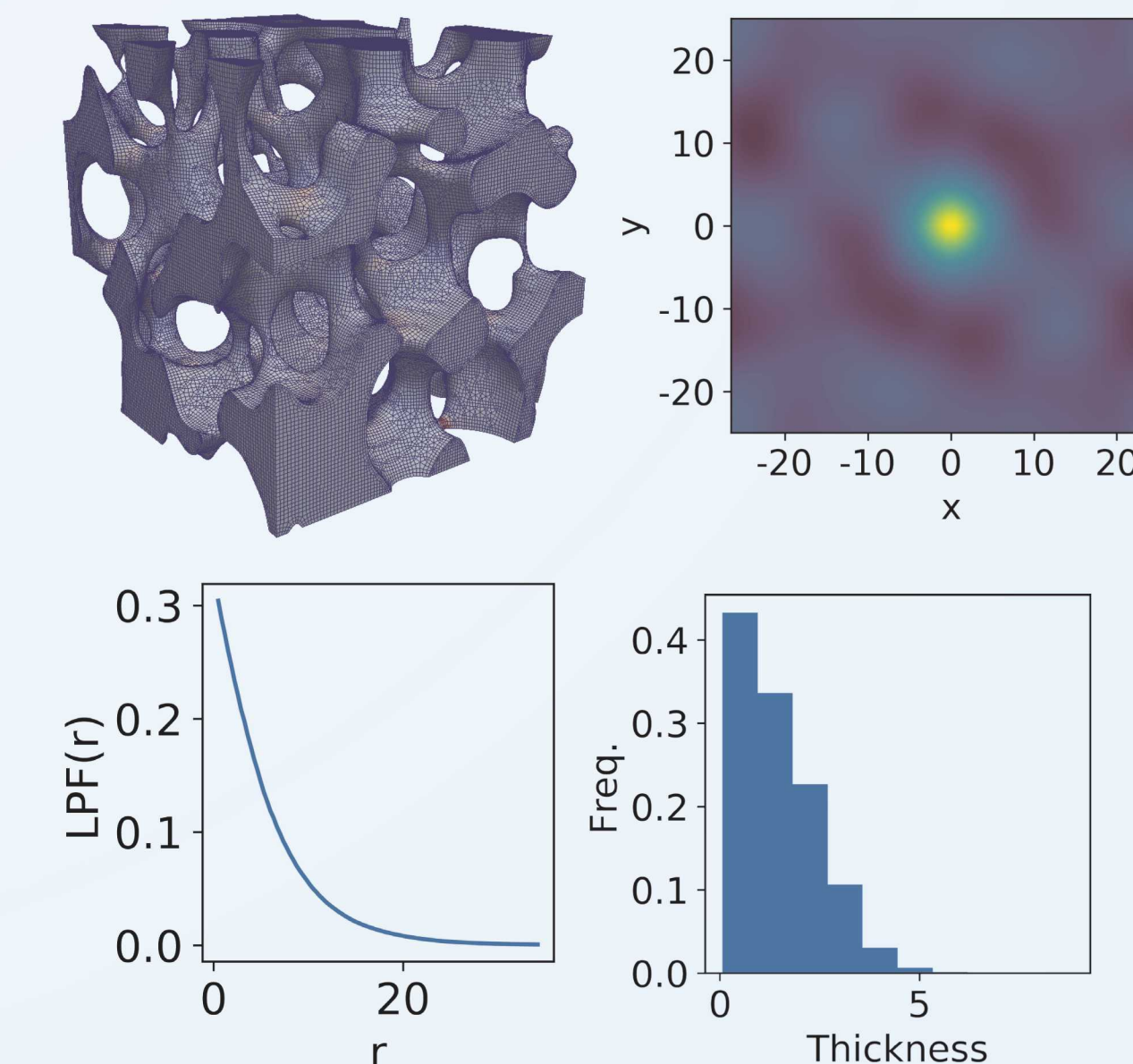
### APPLICATION TO POLYMER FOAMS

- Current ES LDRD (PI: Kramer)
- Goals:
  - understand polymer foam deformation mechanisms
  - inform macroscale foam models for various polymers, densities, temperatures

Micro-computed tomography (CT):  
3D foam structure under varying loads



FEA simulation of explicit microstructure



- Future work
  - Apply statistical metrics and dimensionality reduction across various polymers, densities, microstructures and load conditions
  - Machine learning-based constitutive models: relate strain paths to stress states based on microscale simulations

#### References

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- Latypov, M. I., & Kalidindi, S. R. (2017). Data-driven reduced order models for effective yield strength and partitioning of strain in multiphase materials. *Journal of Computational Physics*, 346, 242-261.