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## **Computational Mechanics and Artificial Intelligence Lab**

My research group's focus is bridging the principles of computational mechanics for solids with advanced machine learning to address significant engineering challenges such as sustainable manufacturing and innovative materials modeling. We are utilizing state-of-the-art ML techniques like interpretable, geometric deep learning, generative AI, and reinforcement learning, all while ensuring adherence to fundamental physical laws.

Machine Learning-Based Metamodels: Developing Models of Models ------



**Objective:** Efficiently predict the behavior of novel materials and systems without the need for new individualized models for each application.

•Neural network-based models that are deeply rooted in classical mechanics theory and physical principles.

•Rigorous validation for trustworthiness (precision, robustness, interpretability).

**Topics:** Universal neural network metamodels for pressuredependent plasticity for more details, neural network models for  $\beta$ -HMX energetic materials based on molecular dynamics.

## Mechanics in Non-Euclidean Domains with Geometric Learning ------

**Objective:** Geometric learning on manifolds and graphs for nuanced understanding and representation of material behaviors.

•Creation and utilization of non-Euclidean, graph-based material descriptors.

•Description of phenomena at the microscale as graphs, facilitating the connection of behaviors across scales.

**Topics:** Graph descriptors for polycrystals, graph representation of plastic rearrangement and localization.



## Generative AI for Design of Digital Twins and Synthetic Datasets -----

Original Database





**Objective:** Leveraging cutting-edge capabilities of generative AI for designing materials with targeted properties and behaviors •Digital twins and synthetic datasets for complex material systems (granular assembles, architected materials, metamaterials).

•Addressing prevalent challenges of limited data availability in engineering applications.

**Topics:** Targeted microstructure design for behavior and topology digital twins, mass generation of granular synthetic datasets.