FAIR Data and Interpretable AI Framework for Architectured Metamaterials

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Since the inception of the “materials genome initiative” (MGI) in 2011, rapidly developing data-driven methods are increasingly employed to complement the traditional materials science tools of experimentation, theory, and computation. While much of this early progress has been executed by individual research groups, large-scale adoption of Artificial Intelligence (AI) for materials research has been limited by a lack of sufficient datasets and frameworks. To leverage the full power of AI models to advance fundamental scientific understanding for the discovery and design of new materials, materials’ data resources should be openly shared and standardized. This project aims at filling this gap using as an exemplar the domain of mechanical metamaterials: architected, composite materials that derive superior mechanical performance, such as combined light weight and high strength, controllable fracture, extreme energy/vibration absorption, or even negative effective mass or stiffness, due to their tessellated geometrical structures. These unique properties make metamaterials enticing for applications ranging from batteries, energy harvesting, seismic protection, vibration/sound insulation, frequency filtering, wave guiding, heat management, RF telecommunication, and ultrasonic imaging.

To overcome both trial-and-error fabrication and ad-hoc testing of new metamaterial geometries, as well as the limitations of topology optimization, we will: 1) use physics-based simulations of metamaterial properties based on structure to create large Findable, Accessible, Interoperable, and Reusable (FAIR) scientific datasets covering a vast space of geometric configurations, and 2) develop a new AI framework and interpretable machine learning algorithms to enable robust discoveries with scientific data.

While the vast design space of all available metamaterial configurations cannot be exhaustively explored through experiments or even simulations, our new AI framework – Learning Refined Compositional Rules (LRCR) – provides two significant advances: 1) LRCR can rapidly find subtle yet important patterns that relate to desired properties and 2) LRCR leverages results at coarse scales to build new rules for patterns at finer and finer scales. A key aspect of this framework is the implementation of interpretable machine learning (ML) algorithms to identify classes of building blocks for the creation of novel material configurations with desired properties, while also informing practicality constraints on the ability to reliably 3D-print the new materials. Furthermore, we will make a simulation tool publicly available for other AI/ML researchers and data scientists to add to our repository, explore their own hypotheses, and verify predictions, thereby increasing the robustness of our FAIR dataset and predictions from our AI framework over time, with the help of a broad scientific community.