RESEARCH STATEMENT – JOBIN KOLLIYIL JOY

Research in the mechanics of materials plays a vital role in advancing manufacturing processes by enabling a deeper understanding of material behavior under extreme conditions. A key objective in this area is the development of innovative materials and design methodologies that improve structural integrity, support sustainable practices, and facilitate next-generation manufacturing techniques across critical industries such as aerospace, energy, and biomedical engineering. Future progress in this direction increasingly relies on the integration of computational modeling, advanced experimental characterization, data-driven methods, and uncertainty quantification to optimize the performance, durability, and reliability of materials in high-performance applications.

Building on this need, my research focuses on improving the predictability and control of material behavior during processing through the development of physics-based and data-driven models. A key aspect of my approach is the integration of computational simulations with experimental validation to develop robust, high-fidelity predictive frameworks. I draw on my expertise in process modeling, finite element analysis (FEA), crystal plasticity, machine learning, probabilistic methods, and experimental design to investigate material behavior across multiple length scales (see Figure 1). By combining these approaches with optimally designed experiments and advanced characterization methods, I aim to develop predictive capabilities for the critical mechanisms driving microstructure evolution and failure. This integrated methodology bridges the gap between fundamental materials science and real-world challenges in manufacturing and structural qualification. I also see an emerging opportunity to incorporate mechanics-aware AI agents as tools that connect simulation, experimental data, literature knowledge, and uncertainty estimates within scientifically constrained, human-supervised research workflows. My long-term vision is to establish a synergistic, micromechanics-informed strategy for rapid material design and qualification that leverages data-driven modeling, uncertainty quantification, and targeted experimentation. In the following sections, I outline my research plan to advance these components, their integration into a unified framework, and potential directions for future work.

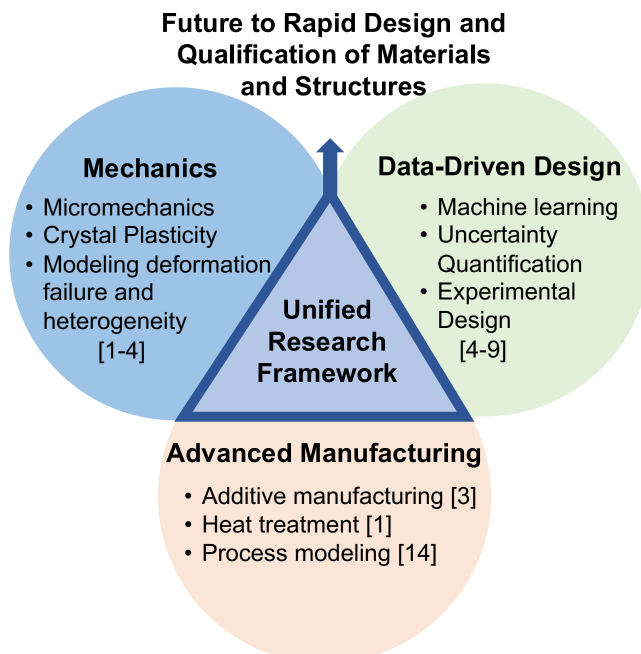

Figure 1: A synergistic strategy for rapid material qualification through Micromechanics, data-driven machine learning models, probabilistic quantification, and integrated experimentation.

Solving complex engineering problems requires an interdisciplinary approach. My research vision aligns with collaborative efforts that bring together experts in materials science, mechanical engineering, manufacturing, and computational modeling. I seek to establish partnerships with industry and national laboratories to apply my research to real-world challenges, including the development of high-performance alloys for aerospace applications, bio-inspired materials for medical devices, and next-generation structural materials for energy systems.

Micromechanical modeling for next generation materials:

Microstructures serve as a physical record of a material's processing history. Micromechanical modeling aims to quantitatively capture the complex relationships between microstructural characteristics and macroscopic material response, thereby providing a rigorous framework for the design and optimization of advanced structural materials. The micromechanical modeling framework[1] I developed for NiTiHf shape memory alloys (SMAs) exemplifies my broader research theme of a unified framework—integrating microstructural insights from experimental techniques such as transmission electron microscopy and differential scanning calorimetry with FEA and uncertainty quantification. This integrated approach enables predictive assessment of material behavior, including quantification of variability arising from microstructural heterogeneity and processing conditions.

Micromechanical approaches have become increasingly relevant with advanced manufacturing methods like additive manufacturing (AM), which create complex, non-equilibrium microstructures. AM steels, for example, often outperform wrought counterparts due to hierarchical microstructures with dense dislocation networks and fine grains[10]. Crystal plasticity models effectively capture these dislocation dynamics and offer physics-based insights into their mechanical behavior. In my recent work[3], we demonstrated the capability of crystal plasticity framework to predict the improved strength of AM steels (see Figure 2).

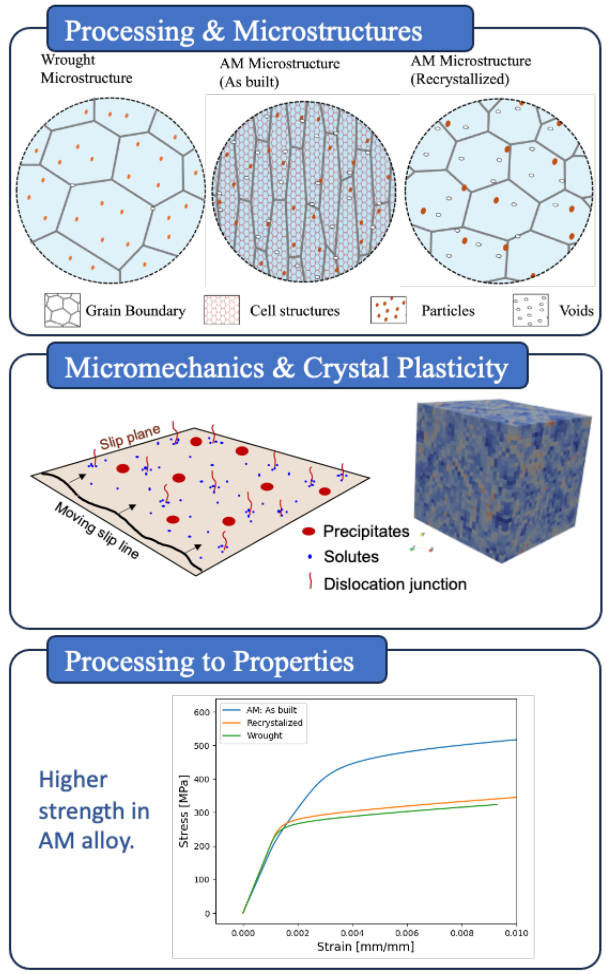

Figure 2: Processing conditions critically influence the evolution of material microstructures, including grain morphology, phase distribution, and dislocation structures. Micromechanical modeling bridges these microstructural features with macroscopic behavior, enabling accurate prediction of mechanical response and accelerating materials development for advanced manufacturing applications

Recent advances in powder metallurgy and additive manufacturing have enabled the design of complex, heterogeneous microstructures through the incorporation of secondary phases such as oxides, carbides, and high-entropy alloys[11,12]. These microstructures offer enhanced strength, ductility, and thermal stability, creating new opportunities for materials innovation. To capitalize on these opportunities, my research will focus on developing predictive, multiscale micromechanical modeling frameworks that link microstructural features—such as grains, inclusions, and dislocation networks—to macroscopic behavior. Using crystal plasticity finite element methods (CPFEM) and representative volume elements (RVEs) informed by experimental data, I aim to simulate texture evolution, damage accumulation, and performance under extreme loading conditions. A key goal is to capture the effects of processing-induced heterogeneity on deformation, fatigue, and failure, ultimately enabling the design and qualification of next-generation structural materials. This work will be grounded in close collaboration with experimentalists to ensure model accuracy and relevance.

Data-driven approaches for accelerated material development

Architected microstructures produced through advanced manufacturing demand high-fidelity simulations to accurately predict and optimize material behavior. While CPFEMs provide valuable physical insight, their high computational cost poses challenges for large-scale studies such as microstructure optimization and materials discovery. To overcome this limitation, my research integrates machine learning (ML) with micromechanical modeling to accelerate simulations while preserving physical accuracy. This hybrid approach enables efficient exploration of structure–property relationships and supports the rapid development of advanced materials.

Surrogate modeling, dimensionality reduction, and physics-informed ML approaches are leveraged to enable rapid prediction of material response, identification of critical microstructural features, and exploration of high-dimensional process-structure-property relationships (see Figure 3). These tools enhance our ability to navigate vast material and process design spaces, providing critical insights for optimizing the performance and manufacturability. In my doctoral research[4,13], I investigated the integration of machine learning techniques and faster computational tools based on Fast Fourier Transform (FFT) on micromechanical modeling to predict the hysteresis behavior of SMAs. Building on this foundation, I aim to advance the unified micromechanical modeling framework by coupling machine learning models with experimental data and uncertainty quantification, enabling the development of adaptive and robust predictive tools for material behavior across a range of processing and service conditions.

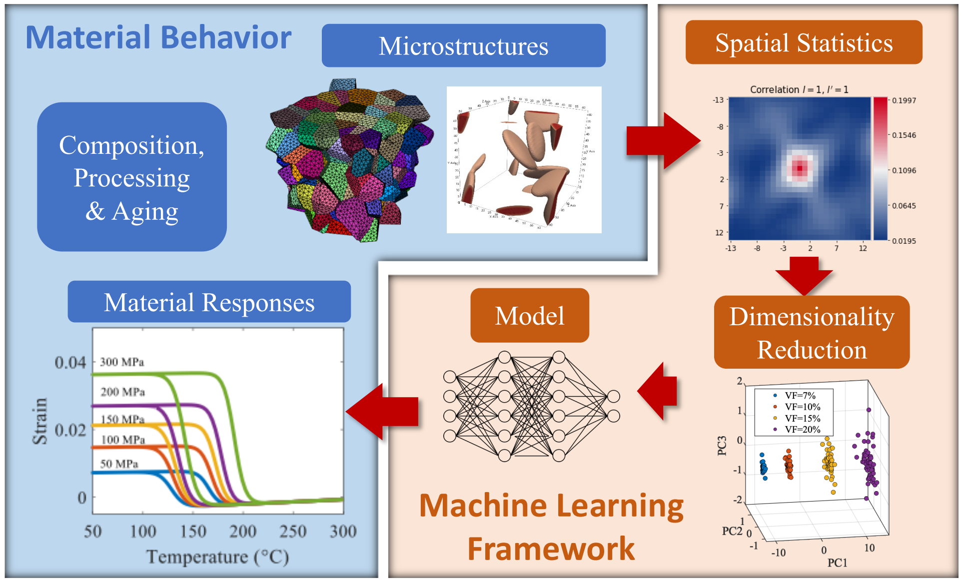

Figure 3: Machine learning framework for rapid prediction of material response, enabling accelerated design, optimization, and deployment of next-generation materials.

Looking ahead, I expect AI agents to become useful supporting tools in computational mechanics and materials research. In my group, I would be interested in selectively using mechanics-aware agents to help integrate simulation databases, experimental observations, and uncertainty estimates for tasks such as design exploration, experiment planning, and model calibration. Any such use will remain grounded in mechanics-based constraints, verification checks, and human oversight, with the primary emphasis continuing to be on rigorous physical modeling, experimental validation, and interpretable scientific insight.

Going forward, I aim to advance the unified framework by coupling machine learning (ML) surrogates with experimental data streams and uncertainty quantification (UQ) pipelines to develop adaptive, robust predictive tools that generalize across a wide range of processing and service conditions. The outcome of this research will be the development of AI-driven, micromechanics-informed design frameworks that enable the discovery and qualification of sustainable materials tailored for both mechanical performance and environmental goals. These tools will streamline materials discovery, reduce waste and energy consumption, and shorten qualification timelines, thereby supporting efficient manufacturing in aerospace, energy, and biomedical sectors. More broadly, this work aligns with national priorities in clean energy and sustainable innovation, while also opening pathways for external funding and industry collaboration.

Uncertainty quantification, experimental design and reliability prediction

As demonstrated in our previous work on SMAs[6], a Bayesian optimal experimental design can effectively integrate experiments, modeling, and uncertainty quantification (UQ) to reduce the number of tests required for material discovery. At the core of this integration is the UQ, which provides a rigorous foundation for translating heterogeneous experimental data into reliable material models. By explicitly modeling uncertainty in parameters obtained from different characterization techniques, this approach enables high-confidence predictions—even in data-scarce environments. This capability is particularly impactful for micromechanical modeling using CPFEM and RVEs, which depend on well-calibrated inputs to simulate material behavior under realistic conditions. The synergy between integrated experimental data, high-fidelity modeling, and UQ forms a powerful framework for materials design (see Figure 4). This is especially valuable in aerospace and energy applications, where even small deviations in performance can have critical consequences. By developing methods that not only predict material behavior but also quantify the confidence in those predictions, my research aims to deliver robust, scalable, and trustworthy solutions for next-generation manufacturing technologies.

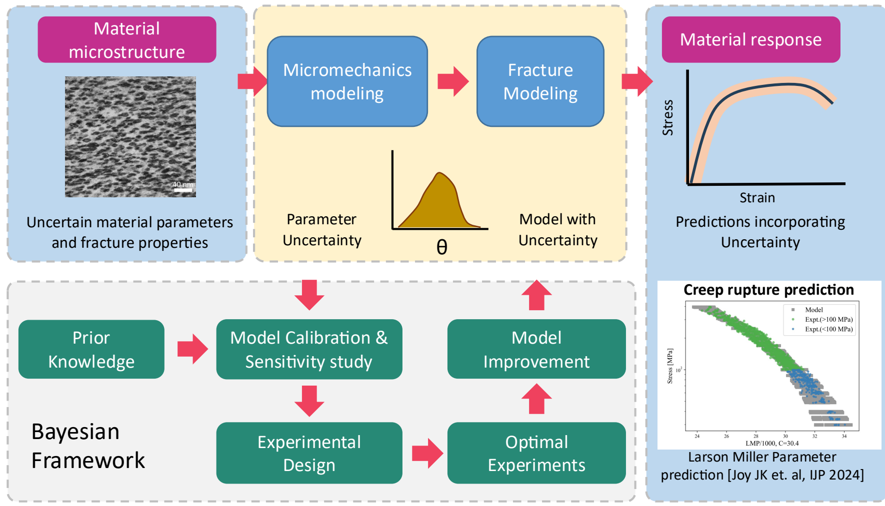

Figure 4: Bayesian-based material design framework that integrates model calibration, optimal experimental design, and predictive modeling. By accounting for model uncertainty and variability, it enables robust prediction of material response and fracture behavior with quantified confidence intervals, supporting reliability and accelerated material qualification.

A key component of the unified framework I aim to develop is the integration of multiscale material characterization with experimental design guided by UQ. While experimental techniques such as tensile testing, nanoindentation, and microstructural analysis offer valuable insights across different scales, they are often applied in isolation. This fragmented approach limits the development of consistent structure–property relationships, especially for complex behaviors like creep, fatigue, and fracture in heterogeneous materials. My research will address this gap by designing integrated characterization strategies that connect diverse experimental methods through shared descriptors and modeling frameworks. For instance, in my recent work[8,9], we demonstrated that strain rate jump tests of nanoindentation, when coupled with a minimum of two bulk creep tests, can be used to accurately predict creep rupture life in steel alloys—highlighting how a unified framework can accelerate material qualification while reducing costs.

Research outlook

My research program will operate at the intersection of computational solid mechanics, advanced manufacturing, and data-driven materials design. Key areas for near-term development include: (i) multiscale crystal plasticity frameworks for AM and powder-processed alloys; (ii) physics-informed machine learning models, with selective use of mechanics-aware AI agents as supporting tools for rapid structure–property prediction, inverse design, and closed-loop computational/experimental workflows; and (iii) Bayesian experimental design protocols for accelerated qualification of structural materials. Underpinning these thrusts is a commitment to open, reproducible computational tools that the research community can build upon.

I intend to pursue research funding through national and international agencies, including Science and Engineering Research Board (SERB), Department of Science and Technology (DST), and Defence Research and Development Organisation (DRDO), as well as through collaborative engagements with industry partners in the aerospace, energy, and biomedical sectors. By aligning the research agenda with national and global priorities—such as sustainable manufacturing, materials by design, and digital engineering—my group aims to make impactful contributions to both foundational science and real-world applications. At Indian Institute of Technology Madras, I am particularly excited about the opportunity to engage with its interdisciplinary research ecosystem, leveraging complementary expertise across departments and research centers. A core part of my academic vision is to mentor and train the next generation of engineers and scientists through integrative research that combines computational modeling, experimental validation, and data-driven approaches, equipping them to address future challenges in materials and manufacturing.

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