Mechanical Engineering Doctoral Defense

Physics-Based and Data-Driven Models for Microstructure-Sensitive Material Failure Prediction

School for Engineering of Matter, Transport and Energy

Changyu Meng

Advisor: Yongming Liu

Abstract

The relationships between the properties of materials and their microstructures have been a central topic in materials science. The microstructure-property mapping and numerical failure prediction are critical for integrated computational material engineering (ICME). However, the bottleneck of ICME is the lack of a clear understanding of the failure mechanism as well as an efficient computational framework. To resolve these issues, research is performed on developing novel physics-based and data-driven numerical methods to reveal the failure mechanism of materials in microstructure-sensitive applications.

First, to explore the damage mechanism of microstructure-sensitive materials in general loading cases, a nonlocal lattice particle model (LPM) is adopted because of its intrinsic ability to handle the discontinuity. However, the original form of LPM is unsuitable for simulating nonlinear behavior involving tensor calculation. Therefore, a damage-augmented LPM (DLPM) is proposed by introducing the concept of interchangeability and bond/particle-based damage criteria. The proposed DLPM successfully handles the damage accumulation behavior in general material systems under static and fatigue loading cases.

Then, the study is focused on developing an efficient physics-based data-driven computational framework. A data-driven model is proposed to improve the efficiency of a finite element analysis neural network (FEA-Net). The proposed model, i.e., MFEA-Net, aims to learn a more powerful smoother in a multigrid context. The learned smoothers have good generalization properties, and the resulted MFEA-Net has linear computational complexity. The framework has been applied to efficiently predict the thermal and elastic behavior of composites with various microstructural fields.

Finally, the fatigue behavior of additively manufactured (AM) Ti64 alloy is analyzed both experimentally and numerically. The fatigue experiments show the fatigue life is related with the contour process parameters, which can result in different pore defects, surface roughness, and grain structures. The fractography and grain structures are closely observed using scanning electron microscope. The sample geometry and defect/crack morphology are characterized through micro computed tomography (CT). After processing the pixel-level CT data, the fatigue crack initiation and growth behavior are numerically simulated using MFEA-Net and DLPM. The experiments and simulation result.

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Zoom Link: https://asu.zoom.us/j/3208330225