Graduate Student Research Seminar

Spring 2025

Multiscale Materials Modelling & VVUQ

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Advisor: Enrique Martinez Saez

Monday, September 8th

3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Materials modeling is growing in popularity among scientists and engineers for the capability of predicting material behavior without the need for costly experimental equipment. Current research within the field of materials modeling has turned attention towards multi-scale data driven approaches to simulate material deformation mechanisms from the microscale to the macroscale. This involves fitting simulated behavior to a constitutive model, which can be deployed at larger scales; however, the validity of the fitting procedure is not frequently called into question. The application of methods with the goal of verification, validation, and uncertainty quantification attempts to address the systemic uncertainty of materials models originating from a number of sources, including parameter uncertainty, model inadequacy, and in the case of stochastic models, residual variability. As information is passed between scales, adequate calibration procedures should be conducted that aim to reduce parameter uncertainty associated with conducting computational studies. Discrete dislocation dynamics simulations shall be calibrated to best match the underlying defect behaviors evident in atomistic molecular dynamics simulations. Verification of the physical mechanisms observed shall be made and validation of model agreement shall be obtained with accompanied uncertainty quantification. The dislocation core size is calibrated to validate the agreement of the critical resolved shear stress between models. This is followed by the calibration of drag parameters and line tension approximations to validate the agreement of the thermal activation rate between models. The calibrated mesoscale model will be utilized to generate single-crystal plasticity models that will be extrapolated to polycrystalline materials. The polycrystalline models are applied to FEA simulations to verify the agreement of the multi-scale modeling approach with experimentally observed results. Added complexities from alloy systems are addressed, and analytical stochastic models describing the thermally activated deformation behavior are formulated.

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