NC STATE UNIVERSITY

CCEE Structures & Mechanics Seminar – Wed. October 21st @ 3pm

Zoom link: https://ncsu.zoom.us/j/97052779798

A modeling framework for coupled plasticity and chemical diffusion with application to material degradation

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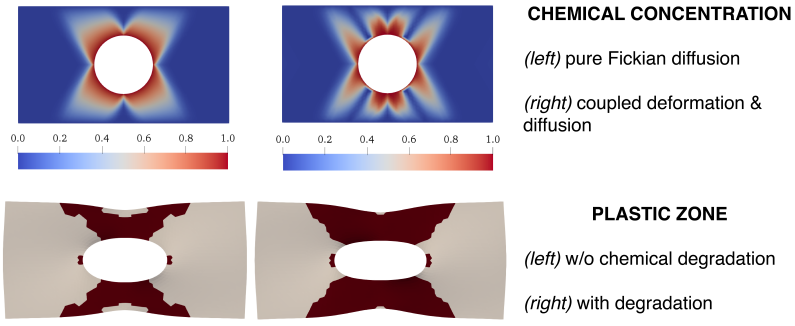
Abstract: Multi-physics modeling is essential to many modern engineering problems ranging from moisture ingress in cementitious materials, ion transport in batteries, hydrogen diffusion in metals, and soil consolidation. This presentation details a modeling framework for studying the response of plastically deformable materials due to the presence and transport of a chemical species. The constitutive model incorporates experimental results from the literature to capture the elastic and plastic material property evolution coupled with chemical diffusion. Since the mathematical model is not amenable to analytical solutions, a robust computational framework will be presented for solving the resulting coupled partial differential equations. I will establish the need to obtain non-negative concentrations for the diffusant, which is not the case with many popular numerical formulations. These unphysical violations will be particularly predominant when the diffusion process is anisotropic. The proposed computational framework employs an optimization-based numerical scheme that preserves physical constraints (e.g., non-negative concentrations) and mathematical properties (e.g., maximum principles). Representative numerical examples are provided to glean the underlying physics of degrading elastoplastic solids due to chemical transport; for example, how plastic zones evolve via material degradation. The talk will conclude by highlighting planned efforts to extend this unique framework for modeling the inverse of degradation (i.e., healing) in heterogeneous materials along with a discussion of related outstanding problems.



Bio: Professor Kalyana Nakshatrala is an associate professor in the Department of Civil and Environmental Engineering with a courtesy appointment in Mechanical Engineering at the University of Houston (UH). In 2019, he was a faculty associate at the California Institute of Technology. Before becoming a faculty member, he was a postdoctoral research associate at the University of Illinois at Urbana-Champaign (UIUC) in collaboration with Los Alamos and Pacific Northwest National Laboratories. Nakshatrala received his Ph.D. in Civil Engineering with a certificate in Computational Science and Engineering along with two M.S. degrees, one in structural engineering and the other in applied mathematics, from UIUC. He obtained his bachelor's degree in Civil Engineering from the Indian Institute of Technology-Madras. Professor Nakshatrala is devoted to student mentorship and had a recent PhD advisee win first prize at the 2018 Engineering Mechanics Institute (EMI) Conference and another doctoral student win the 2016 Robert J. Melosh Medal, an international award given to the best student paper in Computational Mechanics. He has also been recognized for his dedication to teaching, including the 2019 Kittinger Teaching Excellence Award—the highest teaching honor conferred by the Cullen College of Engineering at UH. He remains active in the academic community as an associate editor for the ASCE *Journal of Engineering Mechanics* and serves on the early career research board for IOPScience's *Multifunctional Materials*.