AAE 590X MesoScale Failure In Aerospace Materials

T-Th 9-10:15 ARMS 1021 Instructor: Vikas Tomar Spring 2010

Description

The primary focus of the proposed course is on correlating recently developed solid mechanics theories for modeling material failure with the atomistic modeling descriptions in materials of interest to aerospace industry e.g. metals such as aluminum, ceramics such as silicon carbide based composites, and polymer matrix composites. Modeling and experiments into development and characterization of new materials require analyses at a primary dominating length scale of a few micrometers and a primary dominating timescale of few seconds. Such length scale and time scale are covered in the realm of "mesoscale" analyses that bridge nanoscale and continuum studies. While quantum mechanical and atomistic models of nanoscale material failure can provide qualitative performance or mechanistic information on behavior of a dominating fraction of material morphology, they cannot be used to derive a quantitative material characterization information for direct use by experimentalists or designers. On the other hand, high scale computational methods such as finite element and boundary element methods can provide enough length and time scale resolution for solving engineering problems. However, such methods use material models and theories which have become increasingly complex while not providing a comprehensive material behavior description at the same time. These theories need to be fitted to existing material data to get the values of constants. Therefore, the extrapolation of these theories for unexplored domains is questionable.

This course focuses on an in depth study of new approaches that have come recently in light to bridge the gap between the atomistic mechanics of materials and the continuum mechanics of materials. The focus of presentation is on how atomistic model information on mechanics of materials can be linked to continuum information and experiments related to mechanics of materials at realistic timescale and length scale. The audiences of the course are first and second year graduates students as well as senior undergraduates with interest in solving solid mechanics problems related to complex materials with dominant microstructural features at mesoscale (~few μm).

The course will cover the following contents in the order given below (15 weeks):

1. Atomic Scale Analyses Based on classical Molecular dynamics (MD) and Monte Carlo (MC) based schemes to Analyze Failure in Mechanics of Materials; (4 weeks)
    a. Focus during this section is on developing an in-depth understanding of how atomic scale studies based on MD and MC have been used to analyze material failure in cases such as nanocomposites and nanostructured materials along with a highlight of the need for improvements.
2. Multiscale modeling approaches in mechanics of materials; (4 weeks)
    a. After an in-depth study of atomistic mechanics of materials, here numerical models focusing on presenting an equivalent continuum/coarse grained information of atomistic models will be discussed.
3. Introduction to prominent mesoscale modeling schemes in mechanics of materials: (7 weeks)
    a. After discussing the equivalent continuum type models the focus will turn on to a study of failure using schemes that aim to bypass an atomistic-continuum coupling by defining specific phenomenological models that try to capture atomistic information while presenting a continuum information, e.g. dislocation dynamics, peridynamics, micromorphic theory etc.

Evaluation:

The focus of course is on in-depth study of mesoscale failure with primary objective being mechanics of materials and failure information. Each of the three sections discussed above will have one class project. Besides the class project there will be bi-weekly analytical homeworks or survey assignments.

Learning Goal:

By the end of course students are expected to understand:

1. How atomistic mechanics of materials can be used to solve nano- and meso- level failure. What care should be taken in extrapolating the simulation outcomes to unknown territories.
2. To what extent the state of the art in Multiscale modeling can be used to solve real physical material failure problems.
3. What are the fundamental developments that are needed to be brought out to understand and quantify failure correctly in new materials with complex microstructures and dominating length scale of a few micrometers.