Speaker: Franz Bamer

Titel: Molecular Mechanics of Disordered Solids: an overview

Abstract: Disordered solids are ubiquitous in engineering and everyday use. Although research has made considerable progress in the last decades, our understanding of the mechanics of these materials is, at best, in an embryonic state. Since the nature of disorder complicates the realization of physically meaningful continuum-mechanical models, particle-based molecular descriptions provide a powerful, yet expensive, alternative. In this contribution, we present the numerical realization of classical molecular dynamics in a nutshell, including the concept of the potential energy landscape of disordered solids. In particular, this concerns computationally expensive algorithms necessary to numerically generate disordered materials, considering their thermodynamic properties and structural identification, and we discuss some intriguing phenomena that are, to date, mostly ignored when applying models based on continuum-mechanical frameworks. To overcome the downside of such formulations, we present an outline of model order reduction strategies that we think can be embedded into the framework of the theory of disordered solids. The goal is to find an effective method for a slowly driven mechanical system with abrupt, highly nonlinear disturbances.