ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

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➢ **WEDNESDAY 2 APRIL 2014 - ROOM MA A3 30 - 16h15**

Prof. William CURTIN (EPFL, Institute of Mechanical Engineering, Lausanne, Switzerland) will present a seminar entitled :

"The Multiscale Challenges in Modeling Fracture of Metals"

Abstract:
Energy dissipation by dislocation plasticity in metals provides the resistance against crack growth that makes metals tough engineering materials. However, homogenized plasticity constitutive laws must fail at a singular crack tip, one consequence of which is that the conditions for crack growth are typically calibrated using experimental data rather than computed from fundamental mechanics. This issue, along with the size-dependence of plasticity and the need to address chemical aspects of fracture, dictates that plasticity and fracture be studied at smaller scales – from the dislocation level down to the atomistic and quantum levels. The severe challenges in simultaneously capturing the macroscopic plasticity and the nanoscale behavior at the crack tip, and doing so on time scales appropriate to real materials, are first discussed. Emerging multiscale methods for addressing some of these challenges are presented, including the Coupled Atomistic/Discrete-Dislocation (CADD) model, its extension to Quantum Mechanics, its extension from plane strain to full 3d problems, and the Coupled Discrete-Dislocation/Crystal-Plasticity model, which taken together bridge from quantum to continuum scales of plasticity. Examples of successes are shown and limitations identified. Relevant to MATHICSE interests, these advanced multiscale methods, i.e. those that go beyond the basic coupling of atomistics to a hyperelastic continuum (e.g. the Quasicontinuum model), are highly algorithmic, or recipe-based. The coupling is accomplished through ideas akin to domain decomposition but, because the different domains have different constitutive descriptions, the "boundary conditions" at the domain interfaces are non-standard and often non-local. Thus, while these methods preserve important fundamental physics and mechanics with demonstrated high and often controllable accuracy, putting such methods on a firm mathematical foundation appears to be very difficult. However, finding alternative new methods that are derived from a more-formal structure is also a huge challenge because the loss of degrees of freedom (electrons, atoms, dislocations) with increasing scale of description precludes the development of, for instance, a single energy functional from which the mechanics would emerge naturally.

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