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Atomistic-continuum coupling for dynamic crack propagation

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ABSTRACT

1 Introduction

The most classical engineering approach to describe crack initiation and propagation is Linear Elastic Fracture Mechanics. More recently, the conventional finite element framework has been extended to allow for crack initiation and propagation at arbitrary locations, and in arbitrary directions. Indeed, the eXtended Finite Element Method, which exploits the partition-of-unity property of finite element shape functions allows enrichments such that cracks can be incompatible with the underlying discretization, and remeshing is no longer needed [1].

Another approach is to describe the crack tip with an atomistic model, so that we have a two-scale numerical model. At the microscopic scale, different choices are possible : Either a classical molecular description, which employs Molecular Dynamics, or one that takes its point of departure in quantum mechanics. The latter approach is physically the most meaningful : The Schrödinger equation is solved as a function of the electronic configuration, and methods such Density Functional Theory are used to make the bridge to the next higher scale [2]. A major inconvenience of the approach are the high numerical costs, which currently seems prohibiting. In classical molecular modeling interatomic forces are derived from a potential, which can be viewed as the constitutive equation at this level. Various analytical expressions for interatomic potentials have been proposed, such as the Lennard-Jones and Morse potentials, while others are derived from experiments and have been tabulated, among them the Embedded Atom Method [3]. The latter are somewhat harder to utilize in computations, but they give a better description of metallic bonds. In this contribution we will use a Molecular Dynamics approach to model the crack tip and we will choose the potentials depending on the material.

2 Coupling models

The coupling of the Molecular Dynamics and continuum descriptions is the major goal of this contribution. We have, on one hand, « far » from the crack tip, a classical continuum formulation, and on the other hand, near the crack tip, a discrete atomistic grid. In order to obtain an efficient global formulation, a large scale difference has to be bridged between the two zones : The characteristic parameters (space and time) at the atomic level are much smaller than those in the finite element formulation. We also need to couple two models that describe the same physical reality, but rely on radically different tools : In the (extended) finite element part, classical quantities are used such as stress and strain, but at the atomic level, only quantities like displacements and bonding energies make sense.

Some multi-scale methods that are in principle capable of bridging the scales and the models used have been reviewed in [4]. In this contribution we have chosen for a weak coupling between the two models, as the one proposed in [5]. This coupling implies an energy coupling and its major advantage is that it relies on the transfer of energy, the only quantity that is extrinsic to the modelling. In practice, the extended finite element equations are written in a weak format and coupled through a partition of energy to the atomistic description, so that the energy is distributed between both models.

3 Coupling material properties

The coupling method proposed before can only give satisfactory results if in both domains the same material is described. This means that we have to choose the model parameters such that they result in a behaviour that is globally consistent. To this end we have upscaled the material properties from the atomic level to the continuum scale assuming linearity, homogeneity and …, while exploiting the Cauchy-Born rule [6]. Thus, material properties such as Young's modulus and Poisson's ratio, used at the macro scale, have been obtained from the nano behaviour. This is another step, essential for building a consistent coupling scheme.

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