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The construction and application of an atomistic **J**-integral via Hardy estimates of continuum fields

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ABSTRACT

In this work we apply a Lagrangian kernel-based estimator of continuum fields to atomic data in order to estimate the **J**-integral for the analysis of cracks and dislocations. We show that this method has the properties of: consistency between the energy, stress and deformation fields; path independence of the contour integrals of the Eshelby stress; and excellent correlation with linear elastic fracture mechanics theory for appropriately constructed simulations. We discuss the appropriate reference configuration and reference energy for this type of analysis. Lastly, we use canonical examples to demonstrate that the proposed method is a direct and rational approach for estimating the configurational forces on atomic defects.

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1. Introduction

At the macro-scale, Eshelbian mechanics has found myriad applications ranging from the analysis of defects to the modeling of the dynamics of phase boundaries (Gurtin, 2000). With the advent of nanoscience and nanotechnology, there is strong motivation to extend its application to the nanoscale where issues of dissipation, compatibility, and isotropy are of both scientific and practical interest. For example, with an accurate measure of the atomic configurational forces we can construct traction-separation laws for macroscale closures of fracture problems and estimate resistance limits for defects propagating in complex environments, e.g. composed of clusters and aggregates of defects and dislocations, via simulation.

Eshelby's seminal work (Eshelby, 1951, 1975) lead to Rice's well-known **J**-integral (Rice, 1968) of fracture mechanics and can be connected to Peach and Koehler's work (Peach and Koehler, 1950) on the force on dislocations. The **J**-integral is a path independent contour or surface integral (in 2- or 3-dimensions, respectively) that evaluates the energetic driving force that acts to propagate an existing defect in a continuous medium. The **J**-integral is commonly used in numerical simulations of continuum mechanical deformation, such as the finite element method, to indicate when a critical loading state has been achieved that will result in crack growth. In the context of dislocations and linear elasticity, the **J**-integral represents the force to move a dislocation through the material in which it is embedded. For both cracks and dislocations, the **J**-integral force is ultimately due to applied loads and interactions with other defects.

The use of molecular simulation methods to develop insight on mechanisms of fracture in materials has spawned numerous efforts to develop an "atomic-scale" **J**-integral, i.e. one estimated directly from atomistic information. The first such effort (known to the authors) is that of Inoue et al. (1994, 1995), who combined potential energy, the per-atom contribution to the virial and an estimate of the displacement gradient at an atom for designated atoms comprising a loop around a crack tip to calculate the "H-sum" parameter, an approximation for **J**. While the authors claim that this H-sum is path independent, their work clearly shows significant non-zero values of H for a closed path that does not enclose a crack tip.

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Nakatani et al. (1998, 2000) attempted to avoid the difficulties that plague the calculation a contour integral by using a domain integral approach where atomic contributions to **J** are weighted spatially according to each atom's position within an annular region surrounding a crack tip. They examined how their estimate of **J** depended on the geometric features of the annular region. This work is interesting in two regards. First, the authors explicitly comment that an unloaded, uncracked system must be used to define a reference state with regard to strain energy density, with the exception of atoms at free surfaces where the reference energy is given by the surface energy. With regard to stress, they ascertain that the bulk lattice provides the appropriate reference value for every atom; whereas for energy, two different reference states are used. Second, Nakatani et al. show that their measurement of **J** agrees with the theoretical solution provided from linear elastic fracture mechanics (LEFM) only for small values of stress intensity factor, whereas for large deformation, deviation from the LEFM value occurs due to geometric non-linearity. Both of these issues will be addressed later in this article. Jin and Yuan (2005) and Khare et al. (2007) have also used a domain integral approach for calculating an atomistic **J**-integral, where differences from the Nakatani et al. formulation are due to how strain energy density is calculated.

Xu et al. (2004) presented calculations of **J** using an energy release rate form, i.e. energy per unit area created during crack advance, in order to estimate a critical value for the ductile fracture of a nickel crystal. Although fundamental in their approach, Xu et al. did not examine whether their metric is consistent with LEFM, nor with the contour-based methods that they cite, e.g. Inoue et al. (1994). In addition, this approach is limited to defects that can propagate stably due to the need to make a finite difference approximation of the change in potential energy with respect to a (finite) change in crack length. As a consequence, it is clearly limited to estimating the critical value of **J**. No quantification of the driving force is possible prior to crack length extension. Also, it becomes complex in its application in the context of isolating the **J** of an individual defect in a group of defects, unlike contour based methods. In an attempt to use both atomistic and continuum simulation methods to characterize the fracture of a graphene sheet, Tsai et al. (2010) have recently shown that calculation of such a strain energy release rate displays better agreement with a continuum model of fracture than using atomistic-based stress fields to directly estimate an appropriate stress intensity factor. For the latter method, these authors show that the near-tip stress fields display non-local behavior, making a quantitative estimate of stress intensity factor unreliable. However, calculations of energy release rate using both global and local techniques are in agreement with estimates made from their continuum model.

Finally, Choi and Kim (2007) combined atomistics with anisotropic linear elasticity, a hybrid definition of atomic-scale deformation gradient, and an alternative contour integral to define their own metric of **J**. They too did not investigate consistency with LEFM, but rather focused on developing traction-separation relations for use in cohesive zone simulations.

In this article, we present a novel methodology for calculating the **J**-integral. We construct continuum variable fields from atomic data that are consistent with the continuum Euler balances of mass, momentum and energy, then use these fields in the traditional contour/surface integral expressions to estimate the **J**-integral. Our approach to estimate continuum fields from atomic data originated with Irving and Kirkwood's work (Irving and Kirkwood, 1950) (which was later continued by Noll, 1955). They established the consistency between Dirac delta weighted atomic point data and continuum fields through a correspondence between Newton's law governing the evolution of the particles and Euler's "hydrodynamic" balance laws governing the continuum. Hardy extended the averaging technique from Dirac delta weight functions to continuous kernels (Hardy, 1982; Root et al., 2003), see also Zimmerman et al. (2004), Webb et al. (2008) for review and applications. Hardy's and others' use of coarse-grained averages of atomic data has been shown by many researchers to be superior to per-atom data alone, in particular the atomic stress based on the virial theorem, with regards to producing results consistent with continuum mechanics theory. For example, Cormier et al. (2001) showed that for the analysis of stress fields in the vicinity of an elastic inclusion, the use of coarse-graining produced fields closer in agreement with continuum estimates than did the per-atom virial stress. More recently, Admal and Tadmor (2010) conducted an in-depth analytical and numerical study of how Hardy's expression for stress and the virial stress compare with each other and with other metrics used for estimating stress from atomistics. By examining cases of both homogeneous and inhomogeneous deformation, they conclude that the Hardy stress definition possesses higher accuracy and quicker convergence with averaging domain size than the other methods studied, including the coarse-grained (i.e. volume-averaged) virial stress.

Hardy's work, based in an Eulerian description of motion, was subsequently reformulated in the Lagrangian framework natural for solids by the authors in Zimmerman et al. (2010). Given Eshelbian mechanics dependence on the material frame, it is rational to adopt the Lagrangian description. Our Lagrangian, kernel-based method, unlike that of previous work, has the benefits of preserving path independence down to a surprisingly small size. It must be emphasized that without this property any contour-based method that purports to give an estimate of **J** is questionable. In addition, the proposed method has excellent correspondence with linear elastic fracture and defect mechanics with regard to critical values and trends for idealized problems where there are analytical solutions. These properties will be demonstrated with numerical simulation of fundamental defect types in Section 5. Section 2 provides a brief summary of the continuum **J**-integral theory. Section 3 gives a concise summary of the continuum field estimators needed to calculate the **J**-integral and Section 4 discusses the various aspects of consistency, e.g. between stored energy and stress, needed to obtain accurate **J**-integral estimates from atomic data. As mentioned, in Section 5 representative simulations are given to validate the method and display its numerical properties. Lastly, the paper is concluded with a discussion of future work.

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