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Unification of local and nonlocal models within a stable integral formulation for analysis of defects

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ABSTRACT

Employing the discrete Cauchy-Born rule with the principle of virtual work done, a generalized model is formulated with the hope to unify local and nonlocal continuum frameworks. Despite the conventional mapping of the microscopic bond from the undeformed configuration, the consistent derivation requires a transformation on the Average Deviation of Lattice (ADL) vector in the region of influence. The new conversion proffers flexibility to the framework for the analysis of nonuniform distribution of particles in the field. We also found a compact mapping matrix which converts surface-based forces (stresses) to the nonlocal body-based forces. The transformation matrix allows reconstructing continuum models at a lower length scale in a discrete setting. To see the credibility of the model, fracture evolution in SCB specimen made of Polymethyl methacrylate (PMMA) is simulated, and the results are compared with experiments which admit an acceptable agreement.

1. Introduction

The recent advancements in developing new materials with a broader application made scholars revisit conventional constitutive models and frameworks. Besides, the description of empirical data challenges them to have a closer look at materials in a lower scale. Classical Continuum Theories (CCTs) allow a continuous spread of matter in the body and sets the equations of motion holding the local action solely. In additions, CCTs are based on partial differential equations (PDE). These assumptions narrow the validity of the CCT to those macro-level responses where the loading length scale is much larger than the physical length scales. But in the case of loading with a microscopic length scale, the classical prediction differs from experimental observation. Short wavelength excitations, analysis of porous media and state-of-the-art nanomaterial such as carbon nanotube are some examples that CCT failed to describe them accurately. Eringen (1976). Moreover, several experiments showed that mediums with smaller cracks have higher fracture resistance than a body with a larger one, while the CCT does not consider the effect of crack dimensions. To avoid such restrictions of the CCT, Voigt (1887) added a couple- forces to the conventional force-traction to model nonlocal interaction. Eringen verified that a nonlocal description is proficient at predicting a broad range of wavelengths Eringen (1972). The nonlocal theory was improved to be capable of predicting crack growth. Eringen pointed out that unlike the CCT, the stress distribution close to the crack tip is bounded. Eringen (1972) proposed a failure criterion by comparing cohesive stress to atomic bonds strength. Although the suggested nonlocal theory points the bounded stresses at the crack tips, the derivatives of the field variables are preserved

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in the formulation. Eringen, Speziale, and Kim (1977) improved their nonlocal theory to model Griffith crack and later, he Ari and Eringen (1980) noted that the results of nonlocal Griffith crack model are in a good agreement with Elliott's lattice model (1947). Nevertheless, the governing equations were written based on the partial differential equations which are still ill-defined on discontinuity. Generally, the nonlocality comes into the picture by adding strain derivative to the standard constitutive relation or defining strain averaging (Eringen et al., 1977). Despite other nonlocal theories which use derivative of field variable, Rogula (1982) proposed a nonlocal theory based on field variable. But the model was written for one-dimensional problems. Silling (2000) proposed a derivative-free framework capable of analyzing multi-dimensional problems. The PD framework may be considered as an intermediate route between the classical and molecular dynamics (MD) approaches. Since it characterizes spatial interaction via integration, a PD equation can solve problems with discontinuities without resorting to any special treatment Silling (2000). Based on this advantage, the PD framework finds its application not only in mechanics (Silling, 2000) but also in areas like thermo-mechanics (Kilic & Madenci, 2010), electromigration (Gerstle, Silling, Read, Tewary, & Lehoucq, 2008), heat conduction in a body involving discontinuity (Bobaru & Duangpanya, 2012) etc. However, its original bond-based (BBPD) version faces a serious limitation because of its restriction on Poisson's ratio. Besides, the BBPD does not distinguish between volumetric and distortional deformation. The reason behind such limitations in BBPD is traced back to its assumption of equal and opposite pairwise forces between two particles within a bond. As an important step forward, Silling came up with a modification of the BBPD formalism and proposed state-based peridynamics (SBPD) (more precisely ordinary SBPD) in Silling, Epton, Weckner, Xu, and Askari (2007), which could resolve many of the issues associated with the original BBPD approach. Unlike the BBPD, the forces in a bond are unequal in ordinary SBPD (Warren et al., 2009). However, the interaction forces within a bond are still considered as collinear. The SBPD framework is successfully applied in different areas of mechanics, e.g. plasticity (Silling et al., 2007), visco-elasticity (Kilic, 2008), visco-plasticity (Foster, Silling, & Chen, 2010; Taylor, 2008), dynamic brittle fracture (Ha & Bobaru, 2011), delamination in composite material (Xu, Askari, Weckner, & Silling, 2008), branching phenomena (Agwai, Guven, & Madenci, 2011) etc. But owing to its assumption of collinear forces along a bond, the ordinary SBPD is not applicable to non-linear anisotropic materials (Warren et al., 2009). Such limitation has led to further development, and non-ordinary SBPD has been proposed (Warren et al., 2009). Unfortunately, the non-ordinary SBPD is also scourged with difficulties in implementations. It may suffer from instability arising from the weak coupling of particles in the definition of deformation gradient. Responses via the non-ordinary SBPD may also show zero energy modes (Breitenfeld, Geubelle, Weckner, & Silling, 2014). Despite all the effort to improve laws and models (Chang, 2010; Ghosh & Arroyo, 2013; Maranganti & Sharma, 2007; Zhang, Jiao, Sharma, & Yakobson, 2006) a consistent connection between microscale and continuum level is not well defined. Most of the developed continuum models are not capable of capturing the evolution of microscopic defects such as crack within the framework. The existence of defects, such as imperfection and voids may affect the susceptibility of structure because of inception and growth of defects from an atomic level to the macroscopic scale. Several studies show that evolution of fracturing of brittle materials may not be presented via linear fracture mechanics (Buehler, van Duin, & Goddard III, 2006; Mattoni, Colombo, & Cleri, 2005; Mura, 1993; Remmers, de Borst, & Needleman, 2008; Yukutake, 1989). It started with bond-based peridynamics (Silling, Zimmermann, & Abeyaratne, 2003) which brought up some obstacles to have realistic modeling due to the extreme simplification of particle interactions in the domain. The concept of state in peridynamics framework was introduced to remove some of the restrictions (Silling et al., 2007; Silling & Lehoucq, 2010). However, the new concept required advanced mathematical tools to be implemented in the framework. Moreover, it has been shown that there is a huge instability in the response of the problem (Breitenfeld et al., 2014). Our recent study proposed a discrete Lagrangian-based framework to characterize the response of an elastic body at a length scale of interest (Sarkar, Nowruzpour, Reddy, & Srinivasa, 2017). A great benefit of adopting the Lagrangian description is its flexibility in characterizing coupled multibody-interaction. In this paper, we present a systematic approach to constructing new nonlocal derivative-free formulation from classical constitutive models. This study could be an effort for the unification of local and nonlocal framework to analyze problems incorporating discontinuities and defects. In Section 2, we present nonlocal deformation in a body based on Discrete Cauchy-Born Rule (DCBR). The new definition compacts the state of deformation at a point of a discrete system into a second-order tensor. In Section 3, we derive a nonlocal derivative-free energetically-conjugate pair using nonlocal rate of work done in the continuum. In Section 4, a transformation matrix is introduced to map surface-based forces (conventional stress) to body-based ones. This transformation makes the continuum particle capable of interacting with the nonlocal region. In Section 5, using peridynamics approach for calculation of strain energy release rate (G), we present a new suitable energy-based criterion for the framework to predicts failure in brittle materials. In Section 6, a numerical investigation is done to show the credibility of the new development in analyzing mixed-mode fracture toughness of the semi-circular bend specimen made of PMMA. Finally, some concluding remarks are drawn in Section 7.

2. Directionality operator

Here, we present a projection principle for upscaling microscopic information, which allows non-trivial directional information to develop a variable in a continuous or discrete system. The principal was obtained by employing a stochastic