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A variational formulation of dissipative quasicontinuum methods

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ABSTRACT

Lattice systems and discrete networks with dissipative interactions are successfully employed as mesoscale models of heterogeneous solids. As the application scale generally is much larger than that of the discrete links, physically relevant simulations are computationally expensive. The QuasiContinuum (QC) method is a multiscale approach that reduces the computational cost of direct numerical simulations by fully resolving complex phenomena only in regions of interest while coarsening elsewhere. In previous work (Beex et al., *J. Mech. Phys. Solids* 64, 154–169, 2014), the originally conservative QC methodology was generalized to a virtual-power-based QC approach that includes local dissipative mechanisms. In this contribution, the virtual-power-based QC method is reformulated from a variational point of view, by employing the energy-based variational framework for rate-independent processes (Mielke and Roubíček, *Rate-Independent Systems: Theory and Application*, Springer-Verlag, 2015). By construction it is shown that the QC method with dissipative interactions can be expressed as a minimization problem of a properly built energy potential, providing solutions equivalent to those of the virtual-power-based QC formulation. The theoretical considerations are demonstrated on three simple examples. For them we verify energy consistency, quantify relative errors in energies, and discuss errors in internal variables obtained for different meshes and two summation rules.

1. Introduction

Conventional continuum theories discretized by Finite Element (FE) approaches become problematic at small length-scales and complex material behaviours. In these cases, the underlying microstructure or even the atomistic crystal structure comes into play. This introduces nonlocality, and requires discrete simulations such as structural lattice computations or Molecular Statics (MS) in order to capture the physics properly. Discrete conservative systems are in their full description conveniently formulated within a variational framework, in which their behaviour follows a minimization of a potential energy $\mathcal{E}$, i.e.

$$\boldsymbol{r} = \arg\min_{\widehat{\boldsymbol{r}} \in \mathscr{R}} \mathcal{E}(\widehat{\boldsymbol{r}}), \tag{1}$$

where $\widehat{\boldsymbol{r}} \in \mathscr{R}$ denotes an arbitrary admissible vector collecting the positions of all lattice atoms (or particles), $\mathscr{R}$ denotes a configuration space, and $\boldsymbol{r} \in \mathscr{R}$ a suitable minimizer, see e.g. Tadmor and Miller (2011), Section 6. For application-scale problems, the construction of $\mathcal{E}$ and the solution of (1) entails excessive computational efforts because of two facts:

F1. A large number of atoms and bonds contained in fully-resolved systems leads to considerable expenses associated with the solution of the Euler–Lagrange equations involving large-scale energy gradients and Hessians.
F2. For the assembly of energies, gradients, and Hessians,[1] all atoms or bonds have to be individually taken into account.

The QuasiContinuum (QC) methodology, originally formulated by Tadmor et al. (1996), and extended in various aspects later on, e.g. Curtin and Miller (2003) and Miller and Tadmor (2002, 2009), overcomes F1 and F2 in two steps. First, *interpolation*, based on a number of selected representative atoms, or *repatoms* for short, constrains the displacements of the remaining atoms in the lattice,

$$\boldsymbol{r} = \boldsymbol{I}(\boldsymbol{r}_{\text{rep}}), \tag{2}$$

[1] In MS, it is standard to employ quasi-Newton or completely Hessian-free minimization schemes, requiring only energies and gradients, cf. e.g. Tadmor and Miller (2011), Section 6.2. Contrary to MS, lattice systems are usually solved using a Newton-Raphson scheme that requires also Hessians.

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where $\boldsymbol{r}_{\text{rep}} \in \mathscr{R}_{\text{rep}}$ stores the positions of all the repatoms, and $\mathscr{R}_{\text{rep}}$ denotes a subspace of the original configuration space $\mathscr{R}$. Because the dimension of $\mathscr{R}_{\text{rep}}$ is usually much smaller than that of $\mathscr{R}$, deficiency F1 is mitigated. The second involves *summation*, in which the energy and governing equations of the reduced model are determined by collecting the contributions only from so-called *sampling atoms*, in analogy to numerical integration of FE method. As a result, an approximation $\widehat{\mathcal{E}}$ to $\mathcal{E}$ in (1) is minimized, which resolves F2. Section 3 of this paper presents a more detailed discussion of the two QC approximation steps. Other techniques and further details can be found e.g. in Tadmor and Miller (2011); Iyer and Gavini (2011) and Luskin and Ortner (2013).

Also at length scales larger than the nanoscale (atomistic length scale), many materials possess discrete underlying structures—regular, irregular, or random—at the micro- or meso-scale; typical representatives are fibrous materials such as paper (Kulachenko and Uesaka, 2012; Liu et al., 2010) or textile (Potluri and Manan, 2007). In such materials the bonds between the fibres (or yarns) take the role of atoms in atomistics. However, since the involved length-scales are larger, the interactions of these "atoms" (i.e. particles) often comprise dissipative processes. Hence, the original QC formulation developed for purely conservative interactions cannot be employed. Initial theoretical developments to lift this limitation have been provided by Beex et al. (2014c, d) for fibre plasticity and bond-sliding failure. For the derivation the authors have used a non-variational thermodynamically-consistent framework that employs the following virtual-power statement

$$\dot{\widehat{\boldsymbol{r}}}^{\mathrm{T}} \boldsymbol{f}_{\text{int}} = \dot{\widehat{\boldsymbol{r}}}^{\mathrm{T}} \boldsymbol{f}_{\text{ext}}, \quad \forall \dot{\widehat{\boldsymbol{r}}}. \tag{3}$$

In Eq. (3), the dot denotes the derivative with respect to time; the vectors $\boldsymbol{f}_{\text{int}}$ and $\boldsymbol{f}_{\text{ext}}$ store components of resulting internal and external forces. This means that the left- and right-hand sides can be identified as the internal and external powers; for further details see Beex et al. (2014c), Section 2.1. Let us note that in the ideal, smooth and consistent case, the formulation of Eq. (3) would be connected to the one of (1) via the relation $\boldsymbol{f}_{\text{int}} - \boldsymbol{f}_{\text{ext}} = \partial \mathcal{E}(\widehat{\boldsymbol{r}})/\partial \widehat{\boldsymbol{r}}$. Throughout this paper, the QC approach based on Eq. (3) will be referred to as the *virtual-power-based QC*. The virtual-power-based QC framework has been employed in various contexts and proven to be efficient while accurate, see e.g. Beex et al. (2014c). However, from this formulation, it is not entirely clear whether the governing equations derived from Eq. (3) are also energetically consistent; it may happen that some terms are missing, cf. e.g. Rokoš et al. (2016), Table 1, for an example in continuum gradient plasticity. Variational approaches may furthermore be considered to provide finer information about system evolution such as microstructure pattern formation or phase transition, see e.g. Ortiz and Repetto (1999), Carstensen et al. (2002), and Schröder and Hackl (2013). In the case of adaptivity, better error estimates and mesh refinement capabilities for localized phenomena (such as damage) can be explored in highly nonlinear problems, cf. e.g. Radovitzky and Ortiz (1999). From a broader perspective, the variational formulation offers a consistent framework convenient for, e.g., the rigorous treatment of evolutions that exhibit discontinuities in time, investigations of structural stability using energy landscapes arising from time-incremental minimization, or direct employment of non-linear optimization algorithms. Finally, the variational formulation allows us to extend the conservative QC methodology to an entire class of rate-independent internal mechanisms in a natural way.[2]

[2] In principle, extensions to inertial and viscous effects are possible as well. For the sake of simplicity and clarity, any rate effects are omitted throughout this contribution, and the interested reader is referred to Mielke and Roubíček (2015), Chapter 5 and references therein.

The goal of this paper is therefore to reformulate the virtual-power-based QC framework for internal dissipative processes in terms of variational principles and show that the obtained solutions *coincide* for both formulations in the case of plasticity with isotropic hardening. To that end, a suitable potential Π will be constructed such that

$$\boldsymbol{q} \in \arg\min_{\widehat{\boldsymbol{q}} \in \mathscr{Q}} \Pi(\widehat{\boldsymbol{q}}), \tag{4}$$

describing the state of the system in analogy to (1). Here, however, $\boldsymbol{q}$ denotes a general state variable that also includes internal dissipative variables. Furthermore, $\mathscr{Q}$ is an abstract state space, and the inclusion sign $\in$ indicates that the potential Π is generally nonsmooth or may have multiple minima. In analogy to standard QC, a reduced variable $\boldsymbol{q}_{\text{red}} \in \mathscr{Q}_{\text{red}}$ and an approximate energy $\widehat{\Pi}$ will be introduced in order to alleviate F1 and F2. In what follows, the approach based on Eq. (4) will be referred to as the *variational QC*. Its construction falsifies the statement presented in Beex et al. (2014c), Section 1, claiming that the solution to Eq. (3) *cannot* be obtained by direct minimization of an energy potential.

In order to construct the full energy potential Π, we employ the variational formulation of rate-independent processes as introduced in an *abstract setting* by Mielke and Roubíček (2015) that is closely related to applications in continuum mechanics. Earlier studies were provided e.g. by Francfort and Marigo (1993), Han and Reddy (1995), Francfort and Marigo (1998), Ortiz and Stainier (1999), Charlotte et al. (2000), Hackl and Fischer (2008), Conti and Ortiz (2008), and Kochmann and Hackl (2010). Section 2 of this paper first briefly introduces definitions and basic principles of the theory. Second, the approach is reformulated in the particular context of discrete lattice systems.

The governing equations associated with (4) will be addressed in Section 4, where we recall the Alternating Minimization (AM) method, see also Bourdin et al. (2000). Since the energy potential Π for plasticity is nonsmooth, we will also briefly discuss the return-mapping algorithm suitable for its minimization.

Before closing this contribution by a summary and conclusions in Section 6, we perform numerical tests on three benchmark examples presented in Section 5, two of which have been adopted from Beex et al. (2014c), Section 4, and Beex et al. (2015b), Section 4.2. We demonstrate that both approaches, represented by Eqs. (3) and (4), lead to energetically-consistent solutions for the exact and central summation rules presented in Beex et al. (2011) and Beex et al. (2014b). The third example then presents both global as well as local quantities for an indentation test. Finally, we show that despite the significant dimension reduction and time savings achieved by the QC method, the obtained errors in stored and dissipated energies due to interpolation and summation are rather low: the relative errors in energies do not exceed 4%, while the simulation time is decreased by a factor of 4–30 depending on the triangulation, loading, and geometry.

2. Rate-Independent variational plasticity

2.1. General considerations

The variational formulation for rate-independent processes comprises several steps and relies on two principles (S) and (E), which are described below (for details see Mielke, 2002; Mielke and Theil, 2004; Mielke, 2004 and Mielke and Roubíček 2015). The state of the system within a fixed time horizon $[0, T]$ is described in terms of a non-dissipative variable $\boldsymbol{r}(t) \in \mathscr{R}$, and a dissipative component $\boldsymbol{z}(t) \in \mathscr{Z}$. The latter specifies all irreversible processes at time $t \in [0, T]$, where t denotes a pseudo-time parametrizing the quasi-static evolution process. The state of the system is fully characterized by the state variable $\boldsymbol{q}(t) = (\boldsymbol{r}(t), \boldsymbol{z}(t)) \in \mathscr{Q} = \mathscr{R} \times \mathscr{Z}$.

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