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Numerically robust spectral methods for crystal plasticity simulations of heterogeneous materials

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ABSTRACT

Efficient spectral methods are developed to predict the micromechanical behaviour of plastically deforming heterogeneous materials. The direct and mixed variational conditions for mechanical equilibrium and strain compatibility are formulated in a framework that couples them to a general class of non-linear solution methods. Locally evolving micromechanical fields in a sheared polycrystalline material governed by a phenomenological crystal plasticity constitutive law are used to validate the methods, and their performance at varying material heterogeneities is benchmarked. The results indicate that the solution method has a dominant influence on performance and stability at large material heterogeneities, and significant improvements over the conventional fixed-point approach are obtained when higher-order solution methods are employed. Optimal solution strategies are devised based on this and applied to an idealised dual-phase polycrystalline aggregate.

1. Introduction

Mapping the mechanical properties of microstructures in relation to its myriad configurations is a fundamental task in the design optimisation of heterogeneous materials (Kalidindi, 2012). Traditional methods to characterise microstructure–property relationships are expensive and slow as they rely heavily on experimentation. Alternatively, high-fidelity numerical predictions can be used to effectively substitute this process. In recent years, powerful numerical tools have been developed to predict rigorous bounds on the effective response of statistically defined classes of microstructural aggregates (Lebensohn et al., 2004). More accurate predictions rely extensively on the use of the finite element method (FEM) to obtain locally resolved micromechanical fields (Cailletaud et al., 2003; Mika and Dawson, 1999; Clayton and McDowell, 2003). However, the size of the representative microstructural volume element (RVE) that can be treated by FEM calculations is limited by the large computational cost involved. A promising alternative to FEM in recent years has been the spectral method.

The spectral method was originally introduced by Moulinec and Suquet (1994, 1998) to compute the micromechanical response of elastic composite materials, and has since been generalised to rigid-viscoplastic (Lebensohn, 2001) and elasto-viscoplastic (Lebensohn et al., 2012) materials, with Eisenlohr et al. (2013) developing a further extension to the case of finite strains and general (arbitrary) constitutive descriptions. The spectral method has been successfully applied to treat polycrystalline materials (Grennerat et al., 2012; Lebensohn et al., 2008; Lebensohn et al., 2009; Lebensohn et al., 2013; Lefebvre et al., 2012), and its efficiency over FEM in this context has been demonstrated (Prakash and Lebensohn, 2009; Liu et al., 2010; Eisenlohr et al., 2013).

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Applications to heterogenous materials, however, are limited by the slow convergence of the fixed-point iterative method when it is applied to materials with a large contrast in the local stiffness (Michel et al., 2001). Several approaches have been proposed to overcome this limitation. Accelerated schemes have been introduced by Eyre and Milton (1999) and Monchiet and Bonnet (2012) for materials with large property contrasts. For the case of materials with infinite property contrasts Michel et al. (2001) suggested a method based on augmented Lagrangians that is also suitable for the simulation of void growth (Lebensohn et al., 2013). Improved convergence has also been demonstrated through the use of Fourier space filtering strategies (Kaßbohm et al., 2006; Brisard and Dormieux, 2010) and efficient alternatives to the fixed-point solution method of the original approach (Zeman et al., 2010; Brisard and Dormieux, 2010).

However, these approaches are limited to the treatment of simple material models. An extension to the case of general constitutive descriptions in a finite-strain context, which is better suited to describe plastically deforming heterogeneous materials, is the aim of the present study. A direct and mixed variational approach is used to formulate accelerated spectral methods in a framework that can leverage efficient non-linear solution methods. A flexible implementation of finite-strain crystal plasticity constitutive models (Roters, 2011; Roters et al., 2012) is then interfaced with these methods for physically appropriate models of the underlying deformation mechanisms in heterogeneous materials. The proposed methods are validated for polycrystalline materials and simple representations of dual-phase microstructures are then used to illustrate their performance.

This study is organised as follows: the derivation of the direct and mixed spectral formulations are presented in Section 2 followed by an outline of their numerical implementation in Section 3. In Section 5, the proposed methods are validated and the results of simulations as outlined in Section 4 are discussed. A summary is provided in Section 6 along with perspectives for future applications.

2. Theory

2.1. Kinematics

$\mathcal{B}_0 \subset \mathbb{R}^3$ is a hexahedral microstructural domain of interest on which a macroscopic deformation gradient $\overline{\mathbf{F}}$ is imposed. The resulting deformation defines a field $\boldsymbol{\chi}(\mathbf{x}) : \mathbf{x} \in \mathcal{B}_0 \rightarrow \mathbf{y} \in \mathcal{B}$ mapping points $\mathbf{x}$ in the reference configuration $\mathcal{B}_0$ to points $\mathbf{y}$ in the deformed configuration $\mathcal{B}$. This deformation map can be decomposed as the sum of a locally fluctuating displacement field $\widetilde{\mathbf{w}}$ and the imposed macroscopic displacement field

$$\boldsymbol{\chi}(\mathbf{x}) = \overline{\mathbf{F}}\mathbf{x} + \widetilde{\mathbf{w}}(\mathbf{x}), \tag{1}$$

for which periodicity conditions are enforced in the sense that $\widetilde{\mathbf{w}}^- = \widetilde{\mathbf{w}}^+$ on corresponding surfaces $\partial\mathcal{B}^-$ and $\partial\mathcal{B}^+$.

The total deformation gradient, given by $\mathbf{F} = \partial\boldsymbol{\chi}/\partial\mathbf{x} = \boldsymbol{\chi} \otimes \nabla = \mathrm{Grad}\boldsymbol{\chi}$, can similarly be decomposed as the sum of the imposed macroscopic deformation gradient, $\overline{\mathbf{F}}$, and the locally fluctuating displacement gradient, $\widetilde{\mathbf{F}}$:

$$\mathbf{F} = \overline{\mathbf{F}} + \widetilde{\mathbf{F}} \qquad \text{with } \widetilde{\mathbf{F}} = \frac{\partial\widetilde{\mathbf{w}}}{\partial\mathbf{x}} = \widetilde{\mathbf{w}} \otimes \nabla = \mathrm{Grad}\widetilde{\mathbf{w}}. \tag{2}$$

2.2. Static equilibrium

The material response is governed by an arbitrary rate-dependent constitutive law that relates the deformation gradient to the first Piola–Kirchhoff stress, $\mathbf{P}$, at every material point in the reference configuration through a strain energy density functional, $\mathcal{W}$:

$$\mathbf{P}(\mathbf{x}) = \frac{\delta\mathcal{W}}{\delta\mathbf{F}(\mathbf{x})} = \mathbf{f}(\mathbf{x}, \mathbf{F}, \dot{\mathbf{F}}, \boldsymbol{\xi}), \tag{3}$$

where $\boldsymbol{\xi}$ is a set of evolving internal variables. $\mathbf{P}$ at $\mathbf{x}$ may be a function of its neighbourhood, as in the case of a nonlocal material point model.

2.2.1. Direct variational formulation

In the direct formulation, the equilibrium deformation field is obtained by minimising $\mathcal{W}$ over all admissible deformation fields (*i.e.* satisfying the prescribed macroscopic deformation field and local periodicity conditions in the sense of Eq. (1)). In the absence of external body forces, the stationary condition expressed in real and Fourier[1] space follows as:

$$\min_{\boldsymbol{\chi}} \mathcal{W} \Rightarrow \mathrm{Div}\ \mathbf{P}(\mathbf{x}) = \mathcal{F}^{-1}[\mathbf{P}(\mathbf{k})\, i\mathbf{k}] = \mathbf{0}, \tag{4}$$

which is equivalent to finding the root of the residual body force field

[1] Quantities in real space and Fourier space are distinguished by notation $Q(\mathbf{x})$ and $Q(\mathbf{k})$, respectively, with $\mathbf{x}$ the position in real space, $\mathbf{k}$ the frequency vector in Fourier space, and $i^2 = -1$. $\mathcal{F}^{-1}[\cdot]$ denotes inverse Fourier transform.