International Journal of Engineering Science 78 (2014) 124–133

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

Interpolation–free discrete modeling with gradient matrix: Case study of edge dislocation in linearly elastic crystal

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ARTICLE INFO

Article history:
Received 19 November 2013
Received in revised form 11 February 2014
Accepted 12 February 2014
Available online 5 March 2014

Keywords:
Linear elasticity
Crystals
Dislocations
Gradient matrix
Modeling

ABSTRACT

A meshless and interpolation-free (MIF) method of numerical modeling in solid mechanics has been formulated with a gradient matrix extending the gradient operation to discrete data. Nodal strains and, consequently, stresses in this method are expressed immediately in terms of nodal displacements and the stress divergence in terms of nodal stresses that makes it possible to get the stress balance equation in a truly discrete form. A trial MIF model where nodal points correspond to atom positions is employed for a rectilinear edge dislocation in a linearly elastic crystal. Both the resulting stress level at the dislocation core, close to the theoretical crystal strength, and respective core dimensions prove to be realistic physically whereas calculated long-range stresses asymptotically approach the related continuous fields known in an analytical form for the dislocation in linearly elastic isotropic continuum.

1. Introduction

Interpolations are inherent in numerical models of continuum mechanics aimed to obtain approximate continuous solutions of constitutive equations. In particular, kinematics in the widely used finite element method (FEM) is formulated with a priori shape functions expressing a velocity field inside each finite element (FE) in terms of its nodal velocities (Gallager, 1975; Zienkievicz, 1970; Zienkievicz, Taylor, & Zhu, 2005). Such interpolations associated with the meshing intrinsic in FEM result in some generic drawbacks of this method. On the one hand, the corresponding approximate fields have artificial singularities at FE nodes, edges or faces reducing the solution accuracy. On the other hand, when physically prescribed discontinuities are considered FE faces (edges in 2D) should be placed on respective interfaces whereas nodal points must be duplicated there. Even with such complications, however, the singularities of arbitrary shape functions will remain irrelevant to actual discontinuities, which arise between material structural elements of rather complex shape. For example, it would be hard to use shape functions ascribed to whole grains, which are polyhedrons with more than 20 apices. That is why, in particular, FEM models of polycrystal deformation usually subdivide each grain into a lot of more primitive elements (Kanjarla, Van Houtte, & Delannay, 2010; Roters et al., 2010) and become highly consumptive.

Apart from the above mentioned limitations, FEM models become too much awkward in application to large deformations, moving boundaries or propagating cracks, where the mesh should be repeatedly updated. In order to avoid re-meshing troubles, meshless extensions of FEM have been developed where shape functions are associated with scattered nodal points rather than certain domains between them and such points may be readily shifted, added or removed in simulation. Detailed

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http://dx.doi.org/10.1016/j.ijengsci.2014.02.015
0020-7225/

reviews of meshless models (Belyschko, Krongauz, Organ, Fleming, & Krysl, 1996; Chen, Lee, & Escandarian, 2006; Fries & Matthies, 2004; Ullah & Augarde, 2013) are available and the author in no way claims to survey an extremely rich variety of related works. However some geometric aspects of them significant for the present paper should be addressed. The moving least square (MLS) approach (Belytschko, Gu, & Lu, 1994; Nayroles, Touzot, & Villon, 1992) and the reproducing kernel particle method (RKPM) (Liu, Jun, & Zhang, 1995; Liu, Li, & Belitschko, 1997), different in their mathematical origins Lancaster and Salkauskas (1981) and Lucy (1977), respectively, and rather similar in implementation are most often employed to derive approximate displacement fields. Such fields are usually treated with appropriately smooth shape functions related to individual nodes, weight functions reflecting the local influence of these nodes, and partly overlaying supports of the latter, which may be considered as domains of their influence. Along with the principal re-meshing problem thus eliminated, other serious troubles inherent in FEM are also reduced, in particular artificial singularities between neighboring FEs. Besides, properly modified meshless methods become superior to FEM in treating physically prescribed discontinuities (Fries & Matthies, 2004). To this end nodal supports (normally disks in 2D and balls in 3D) are limited by considered physical interfaces (Belytschko, Lu, & Gu, 1994) or discontinuous enrichment functions are added to continuous approximations (Belytschko, Ventura, & Xu, 2002).

Despite the above considered advantages, meshless models still are not widely applied in the engineering routine because they are much more computationally expensive than those of FEM owing to highly complicated treatment of employed shape and weight functions (Belyschko et al., 1996; Chen et al., 2006; Fries & Matthies, 2004; Pan, Sze, & Zhang, 2004; Ullah & Augarde, 2013). Furthermore, related approximations for displacement fields usually are not interpolations in a rigorous sense because at nodal points they may differ from respective nodal variables. Such deviations become undesirable when imposing essential boundary conditions and necessitate special treatments (Fernandez-Mendez & Huerta, 2004; Ullah & Augarde, 2013). Another computational complication of meshless modeling is due to error estimation procedures (Chung & Belytschko, 1998; Lee, Chung, & Choi, 2003) in the adaptive discretization essential in this numerical method. Meanwhile, since both the latter and FEM have specific limitations, efforts have been undertaken to find a reasonable compromise between them. Thus in a coupled FE/meshless method (Ullah, Combs, & Augarde, 2013) the whole model is first treated with FEM and then some domains are converted into meshless zones if a predefined error measure is violated. In the extended FEM (XFEM) reviewed in Belytschko, Gracie, and Ventura (2009), where certain formal grounds of the meshless method are used and known properties of physical discontinuities are embodied in special enrichment functions, cracks, dislocations and boundaries considered with a fixed mesh may cross FE volumes. Smoothed FEM (SFEM), where conventional mesh-based shape functions have been smoothed within FE (Liu, Nguyen, Dai, & Lam, 2007), at their nodes (Nguyen-Thoi, Vu-Do, Rabczuk, & Nguyen-Xuan, 2010), edges (Liu, Nguyen-Thoi, & Lam, 2009) or faces (Nguyen-Thoi, Liu, Lam, & Zhang, 2009), are also cited as competitors to the meshless method, although they retain the re-meshing problem.

Computational drawbacks related to both the mesh-based and meshless shape functions could be avoided if numerical methods were *truly discrete* that is not only meshless but also interpolation-free, and the present paper is an effort in this direction. The author has limited himself to a rather brief overview of the conventional methods, mentioned above, just because of the indicated principal distinction of the proposed approach. An essential prerequisite to develop the meshless and interpolation-free (MIF) approach in solid mechanics is the increasing computational power that makes it possible to process very high densities of nodal points and, hence, to image and to consider simulation results in terms of nodal variables only. Besides, MIF models would appear to be particularly applicable to physically discrete (e.g. crystalline) structures having no stiff matter in interatomic space. Indeed, any assumption of strain distribution over this space would be completely speculative, whereas geometrically small deviations of similar structures from equilibrium states still should be linearly elastic. Therefore a mechanistic approach remains reasonable since the strain and, hence, stress tensor can be ascribed to a rather small number of adjacent atoms (not less than four in 3D or three in 2D) as if they were nodal points of a virtual continuum fragment. At the same time, although the density of discretization is rapidly increasing, the current mesh-based and meshless methods could not plainly get rid of continuous approximations because the latter are used in calculating stiffness terms and, eventually, nodal forces and stresses. Therefore a challenging question arises of how to allow for the material stiffness with no suggestion for continuous fields between scattered nodal points.

In the present paper, aimed to develop a MIF method of numerical modeling, an elastic response with the material elastic modulus is considered exclusively at nodal points, whereas an underlying local strain at each node is derived depending on displacements of neighboring nodes. The predetermined number of thus involved neighbors depends on computational and physical reasons. In order to implement such a method, one should express constitutive equations of solid mechanics in a truly discrete form that is first of all to extend the conventional gradient operator directly to nodal variables. An appropriate extension proposed by Zisman and Ermakova (2006) has been called gradient matrix and applied to the strain mapping (Zisman, Ivanov, Lomov, & Verpoest, 2006) and to the imaging of crystal curvature (Zisman, Van Boxel, Seefeldt, & Van Houtte, 2008) later on. This matrix is uniquely expressed in terms of nodal coordinates contained in whatever differentiation domain and derives from the corresponding data sampling the uniform gradient component, thus extracting only a linear part of an underlying continuous field and neglecting *unknown* residual errors. Similar residuals, like inaccuracy of arbitrary shape functions, are inherent in discrete models. In any case, the denser situated nodal points, the smaller such errors. In the present paper the gradient matrix will be employed in order to express nodal strains and hence stresses immediately in terms of nodal displacements. Furthermore, to properly extend the stress balance equation and thus to enable the discrete MIF modeling in solid mechanics, the divergence operation will also be expressed in a truly discrete form.