Homogenization Techniques for Materials with Discrete Microstructures—a Critical Comparison

Karel Mikeš*, Ondřej Rokoš†, Franz Bormann† and Ron H.J. Peerlings†

* Department of Mechanics, Faculty of Civil Engineering
Czech Technical University in Prague
Thákurova 7, 166 29 Prague 6, Czech Republic
e-mail: Mikes.Karel@cvut.cz, web page: https://www.cvut.cz

† Department of Mechanical Engineering
Eindhoven University of Technology
P.O. Box 513, 5600 MB Eindhoven, The Netherlands
e-mail: O.Rokos@tue.nl; F.Bormann@tue.nl; R.H.J.Peerlings@tue.nl, web page: https://www.tue.nl

ABSTRACT

At sufficiently large scales, most materials can be considered as a continuum, whereas for decreasing scales, materials such as foams, textiles, concrete, or paper, reveal discrete microstructures. At the smallest scale, i.e. nano-scale, ultimately all materials become discrete, and their behaviour is dictated by the underlying atomistic lattice. When modelling of localized physical phenomena, such as dislocation or crack initiation and propagation, is of interest, the inherently non-local behaviour of the underlying discrete microstructure becomes essential, requiring accurate numerical models which capture this nonlocaly.

The most accurate option is to use discrete models directly, such as lattice or beam networks, or atomistic systems, which inherently incorporate the underlying nonlocality. Although accurate, these models suffer from prohibitive computational costs for typical engineering applications, mainly due to the large scale separation between the application length scale and the length scale of the underlying lattice spacing.

Homogenization schemes are hence required, which are capable of capturing emerging physical phenomena while being computationally tractable. In principle, two classes of approaches are available to address this problem. The first one relies on the derivation of homogenized governing equations from the underlying discrete microstructure, which are solved subsequently using standard numerical techniques for continuum problems. The most prominent physical mechanism (e.g. a dislocation or a crack) needs to be, however, included separately. Typical representatives in this class are the Peierls–Nabarro model [1], or cohesive zone model. The second option consists in considering directly an underlying discrete model, which is homogenized using suitable numerical techniques. Here the Quasicontinuum method [2] is a typical representative.

In this contribution, discussion and a critical comparison of the two classes of homogenization approaches is performed by means of two examples. The first example considers dislocation propagation and pile-up against a phase boundary in a hexagonal atomic structure, whereas the second example focuses on crack propagation in a three-point bending test of concrete specimen. In both cases, the Finite Element approach equipped with cohesive zone interfaces (using either the Peierls–Nabarro model, or an appropriate traction-separation law) is compared with the Quasicontinuum method. Accuracy and efficiency of both homogenization techniques are discussed and evaluated against full-scale simulations of the underlying discrete models.

REFERENCES

[1] Bormann, F., Mikeš, K., Rokoš, O. and Peerlings, R.H.J. The Peierls–Nabarro FE model in two-phase microstructures–a comparison with atomistics. Submitted (2019).

[2] Tadmor, E.B., Ortiz, M. and Phillips, R. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A* (1996) **73**:1529–1563.