An Equation-free Multiscale Method: A Result of Extending the Quasicontinuum Method to Irregular Structures

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Keywords: *multiscale, quasicontinuum, scale separation, higher-order*

The quasicontinuum (QC) method was first developed to reduce the computational costs of atomistic computations [1]. It allows to preserve the full atomistic description in small regions of interest and coarse-grains the atomistic model elsewhere. As such, it combines aspects of reduced order modelling approaches and concurrent multiscale approaches. For two decades, the QC method was only applied to conservative atomistic models. Not long ago however, it was extended towards discrete dissipative models that can for instance be used to model fibre networks, foams and printed structures [2]. The extension to beam models also enlarged its application range [3].

An important drawback of the QC method is that it can only be applied to lattice models (in which each node/atom is connected to its neighbouring nodes/atoms in the same manner). Work was performed to extend the method towards irregular discrete models and resulted in a QC approach that shows similarities to FE^2 approaches. Consequently, those extensions come with similar advantages and disadvantages as computational homogenisation approaches.

In this presentation we will show a different extension of the QC method towards irregular discrete models. The extension is effectively a numerical generalisation of the QC method and has the advantage that the resulting framework remains fully nonlocal. Consequently, the approach can relatively straightforwardly be employed for higher-order interpolation schemes at the macroscale. This will be demonstrated by higher-order examples in which irregular, planar beam models with damage are considered.

We consider that the resulting approach has two main advantages. First, no macro-to-micro and micro-to-macro relations need to be defined. This means amongst others that no boundary conditions at the microstructure need to be applied. This is an advantage because for higher-order interpolation fields at the macroscale, these boundary conditions are not trivial. The second advantage is that the separation-of-scales principle does not apply to the method. Hence, the user does not have to worry if scale separation is present.

References

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