A QUASICONTINUUM APPROACH TO MODELING DISCRETE MICROSTRUCTURES

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Summary The quasicontinuum method, which was developed for atomic lattices, is extended to a more general class of microstructural models in which discrete points interact via discrete interactions. Such models allow one to study the influence of small-scale features (e.g. defects) in large-scale problems in a natural fashion, but may be prohibitively expensive. The quasicontinuum method allows one to reduce the resolution of the description where appropriate, so that realistic simulations become feasible. The conventional, energy based method is reformulated in terms of a virtual power balance. The summation rules used to account for the influence of discarded lattice points are also revisited. The performance of the resulting method is illustrated by an example.

INTRODUCTION

Discrete lattice models consisting of trusses or beams are often successfully employed to model the microstructure of solid materials. These intrinsically simple models naturally capture the discreteness and associated scale effects of discrete microstructures, e.g. of fibrous materials. But also scale effects in other materials, for which a discrete representation of their microstructure is not immediately obvious, such as concrete and polymers, have been successfully modeled using discrete lattices.
A disadvantage of lattice models is their computational cost. Practically relevant models of macroscopic problems require solving large systems of equations. A remedy consists in replacing the discrete model by an effective continuum in regions of little interest. However, formulating such an equivalent continuum may not be trivial and handshaking procedures are required to couple the continuum regions to fully resolved lattice regions.
In this contribution we pursue a different approach, which is entirely computationally based and thus does not require the use of an equivalent continuum. It is based on the quasicontinuum (QC) method for atomic lattices [1,2]. The QC method uses interpolation and summation to lower the resolution of the discrete (atomic) lattice model where appropriate. On the other hand, the full lattice description is used in regions of interest. A natural transition can be made between the two regions and no equivalent continuum or handshaking procedures are required. This allows one to model defects and other local features in full detail, and nevertheless capture their macroscopic effect – including scale effects – efficiently.
Here we extend the QC method from atomic lattices to a more general class of discrete lattice models of microstructures. In particular, two modifications are made: (i) the interpolation is introduced via a virtual power statement rather than the conventional energy minimization to allow for dissipative phenomena, and (ii) a new summation rule is proposed to efficiently and accurately formulate the resulting equations. The method is finally illustrated by a two-dimensional example.

THE QUASICONTINUUM METHOD FOR DISCRETE MICROSTRUCTURES

In the QC method, two approximations are introduced to reduce the computational cost of large-scale lattice models: interpolation and summation [1,2].
Interpolation is used to reduce the number of degrees of freedom of the system. A small number of lattice points are selected to represent the displacements of the entire lattice. These lattice points are referred to as representative points or reppoints. The space between them is triangulated and within each triangle linear interpolation is used to constrain the displacements of the remaining lattice points to those of the reppoints (see Step 1 in Figure 1). Where the displacement fluctuations are small, the distance between the reppoints can be large. This leads to a coarse domain in which the lattice points move in an affine manner per triangle and a large gain is made in terms of degrees of freedom. In regions with rapid displacement fluctuations, each lattice point is taken as a reppoint, so that the exact lattice is recovered. In these so-called fully resolved regions, no computational gain is made.
Conventionally, the interpolated displacements are inserted in an expression for the potential energy of the (atomic) lattice. This energy is then minimized with respect to the displacements of the reppoints. This assumes that the interactions between the lattice points (atoms) are reversible and can be characterized by an interaction potential. This restriction may be lifted by adopting a virtual power statement as the basis for interpolation. As a result, irreversible interactions which are often encountered in microstructures may be incorporated, such as elastoplastic, viscoplastic, or damageing elements and bonds. Conservative (elastic) interactions are a special case, in which the equations obtained coincide with those of the conventional, energy based QC method.
Although interpolation reduces the number of degrees of freedom of the system, all lattice points still contribute to the power/energy of the system and all of these contributions must be accounted for. This is where the second

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approximation comes into play. A so-called summation rule is employed to estimate the contribution of all lattice points based on a limited number of lattice point evaluations (Step 2 in Figure 1). The lattice points that are used for this sampling procedure are referred to as sampling points. Their contribution is multiplied by a weight factor to account for the remaining lattice points. Several summation rules have been proposed in the literature for atomistic lattices, leading to different versions of the QC method.
For lattices of discrete truss elements, simpler and more efficient summation rules may be formulated on an element by element basis [3,4]. The simplest of these, the so-called central summation, uses only one sampling point in the interior of each triangle to represent all lattice points within the triangle. In addition, the reppoints also acts as sampling points. As a result, in the fully resolved region all lattice points are accounted for individually. In coarser regions, on the other hand, the central sampling points become more prominent and a large gain is made.

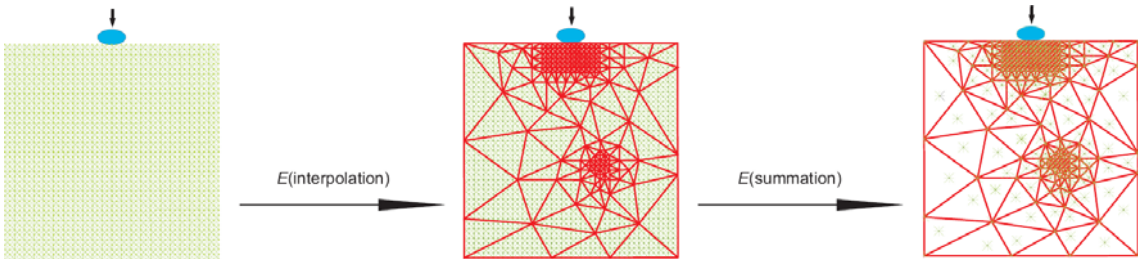

Figure 1: The two reduction steps introduced in the QC method; in both steps an error may be introduced.

EXAMPLE

To show some of the capabilities of the virtual power based QC methodology, it is applied to a two-dimensional X-braced network of elastoplastic trusses which contains a stiff inclusion at the center. The network is subjected to simple shear. A triangulation is used which is dense (fully resolved) near the inclusion and coarser towards the boundaries of the domain. The interpolated lattice has only 6% of the number of degrees of freedom of the original lattice. Furthermore, the central summation rule of [4] selects only 9% of all lattice points as sampling points; these are shown in Figure 2, in which the colors indicate the plastic strain in the individual trusses. Comparisons with direct simulations of the full lattice show that the results in the regions of interest are accurate within 10%, despite the coarse discretization used. A higher accuracy can be reached if the size of the fully resolved region is increased.

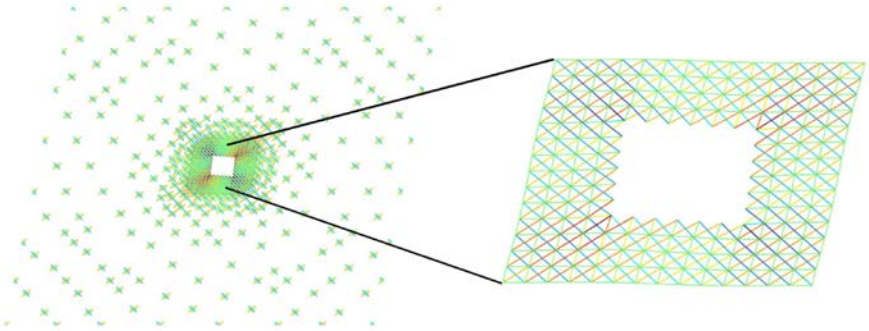

Figure 2: The plastic strains of the trusses at all sampling points (left) and of the sampling points in the fully resolved region (right) predicted by the virtual power based QC method. Red trusses are in tension, blue trusses in compression.

CONCLUSION

The QC method has been introduced as a computational multiscale method for discrete lattice models of microstructured materials. It allows one to study the influence of small-scale features in large-scale problems. No additional (continuum) modeling assumptions need to be made, as the scale bridging is entirely discrete and computational.

References

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