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COMPARISON OF QUASICONTINUUM APPROACHES USING VARIOUS LEVELS OF SIMPLIFICATION

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Abstract: *Atomistically based simulations of materials with disordered microstructure often lead to a high number of degrees of freedom (DOFs) and extreme computational costs. The quasicontinuum method (QC) is a multiscale simulation technique which combines fast continuum and exact atomistic approaches. The key idea of QC is to reduce the computational cost by reducing degrees of freedom of the fully atomistic approach. In the present work, the QC idea is applied to particle systems with elastic-brittle links representing a specific material microstructure. Three approaches using various levels of simplification based on the idea of QC are described and implemented. Accuracy and specific properties of QC-inspired approaches are evaluated by comparing the results with the fully resolved particle model.*

Keywords: Quasicontinuum method, finite elements, discrete particle model, elasto-brittle material.

1. Introduction

The quasicontinuum method (QC) was originally proposed in (Tadmor et al., 1996). The original application of this multi-scale technique was a simplification of large atomistic lattice models described by long-range conservative interaction potentials. In this paper the idea of QC is applied to discrete disordered particle systems with short-range elastic-brittle interactions.

2. Methods

The key idea of QC is to reduce the number of DOFs and the associated computational cost without losing the exact atomistic description in regions where it is required. Therefore, two types of regions in the investigated domain are considered. In regions of high interest, the pure particle approach is required and all particles carry their own independent DOFs. By contrast, in regions of low interest, continuum assumptions are used (Miller & Tadmor, 2002). The simplification is then implemented in two steps: interpolation of DOFs and homogenization of microstructure. In this work, three approaches that differ by the level of simplification based on the QC idea are outlined, implemented in the OOFEM platform (Patzák, 2012) and compared with the pure particle model in 2D. All presented approaches have been developed and explained in more detail in (Mikeš & Jirásek 2015).

2.1. Pure particle approach (A1)

This approach does not use any simplification. Every single particle represents a node with independent DOFs. All links are taken into account explicitly and contribute directly to the stiffness matrix. Consequently, this approach provides the "exact" result, which is used as a reference solution for evaluation of accuracy and efficiency of the following simplified approaches.

2.2. Hanging nodes approach (A2)

The first model reduction technique is based on approximation of certain DOFs. In the regions of low interest, only a small subset of particles is selected to carry independent DOFs. These so-called *repnodes*

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represent the vertices of a triangular mesh which is used to interpolate the DOFs of other particles called hanging nodes because their DOFs are not independent but are "hanging" on appropriate repnodes. By contrast, in the regions of high interest, all particles are selected as repnodes to provide the exact particle representation.

2.3 Global homogenization approach (A3)

In this approach, 2D or 3D finite elements are used not only to interpolate DOFs but also to replace the stiffness that corresponds to the microstructure, so that a substantial number of links can be removed from the particle model. Material properties of 2D elements are identified by homogenization of one global effective elastic stiffness tensor, which is assembled from the contribution of all links. According to (Stránský et al., 2010), such a tensor can be evaluated as

$$\boldsymbol{D}_e = \frac{1}{V}\sum_{i=1}^{N_t} L_i E_{t_i} A_i (\boldsymbol{n}_i \otimes \boldsymbol{n}_i \otimes \boldsymbol{n}_i \otimes \boldsymbol{n}_i) \tag{1}$$

where $\boldsymbol{n}$ is the unit vector specifying the direction of the given link, E_t is the Young modulus of the link, A is its cross-section area and L is its length. The sum is taken over N_t links occupying volume V.

2.4 Local isotropic (A4) and anisotropic (A5) homogenization approach

The idea of these approaches is the same as for A3 with the difference that the evaluation of the effective material stiffness tensor is done for each element separately. The stiffness tensor of each element is obtained only from the contributions of the parts of the links that are located in this element. Then the material parameters are identified from the corresponding stiffness tensor for each element. The A4 approach identifies the stiffness of all elements as isotropic whereas A5 considers all elements as arbitrarily anisotropic with the exact anisotropic stiffness matrix.

3. Results and conclusions

The presented example is an L-shaped beam with geometry and boundary condition according to Fig. 1. The material of the links is considered as elastic-brittle, with failure occuring at the critical level of tensile strain. Before the critical value is reached, the link is considered as purely elastic. The region of high interest is located around the nonconvex corner and along the expected crack trajectory; see Fig. 1 (right). The geometry of microstructure is generated randomly. Five different realizations with the same parameters have been used. Different realizations of microstructure lead to different crack trajectories and force-displacement diagrams; see Fig. 2. The results are evaluated as an average over all five random realizations of microstructure.

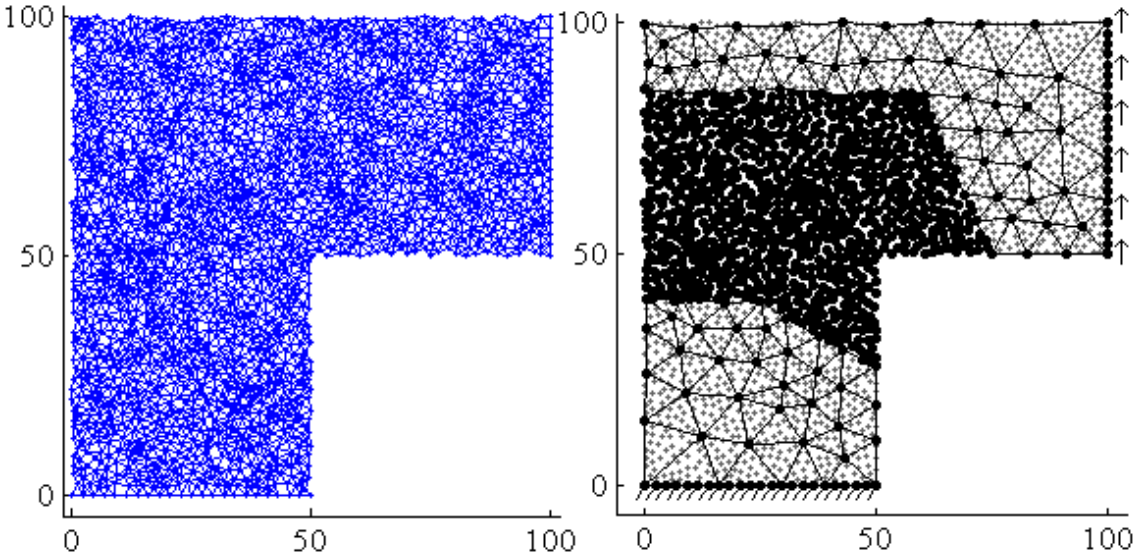

Fig. 1: Example of microstructure geometry (left). Quasicontinuum model with boundary conditions (right), regions of high interest, repnodes with interpolation elements (black), hanging nodes (grey).

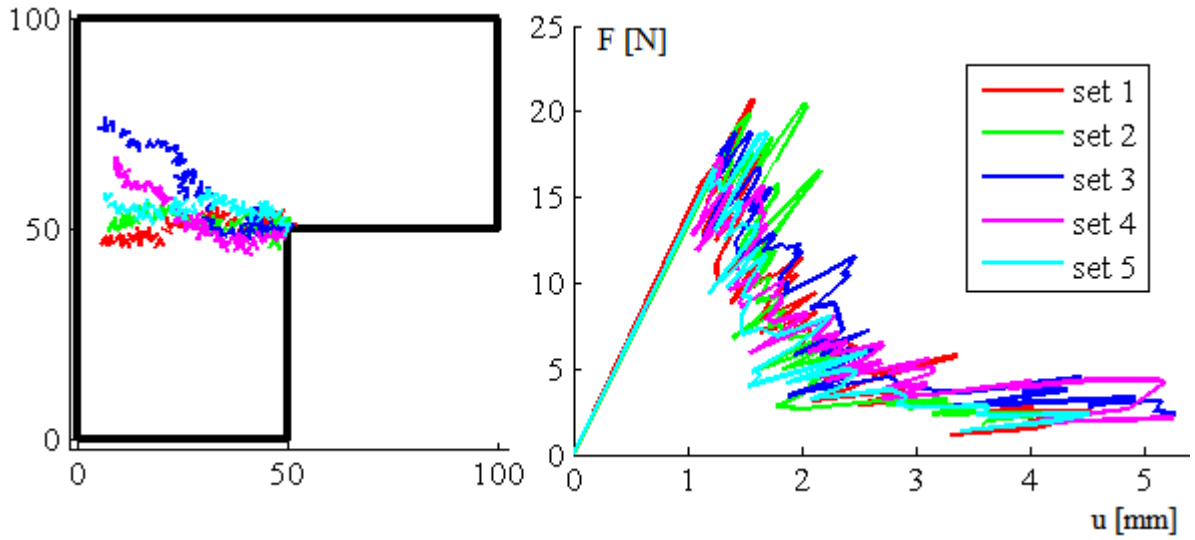

Fig. 2: Crack trajectories (left) and corresponding force-displacement diagrams (right) for five random microstructures generated with the same parameters.

The accuracy of the presented simplifying approaches A2-A5 is evaluated with respect to the exact approach A1. Relative errors in terms of displacement and force are plotted in Fig. 3. The relative error in macroscopic stiffness and the error measured in the terms of a global strain error indicator defined as

$$e^2{}_{A2} = \frac{1}{2}\sum_{i=1}^{N_t} L_i E_{t_i} A_i \left(\varepsilon_{A2_i} - \varepsilon_{A1_i}\right)^2 \tag{2}$$

are plotted in Fig. 4. Numerical values of all errors in the first step are listed in Table 1. The initial response of A3 is significantly stiffer. The error of A3 decreases as the crack propagates because the major part of deformation takes place in the region of high interest. It is surprising that A4 is less stiff (more accurate) than A5 with more sophisticated homogenization and even than A2 with the exact microstructure. It is because both the interpolation and the anisotropic homogenization make the final response stiffer. By contrast, isotropic approximation of an anisotropic stiffness tensor may

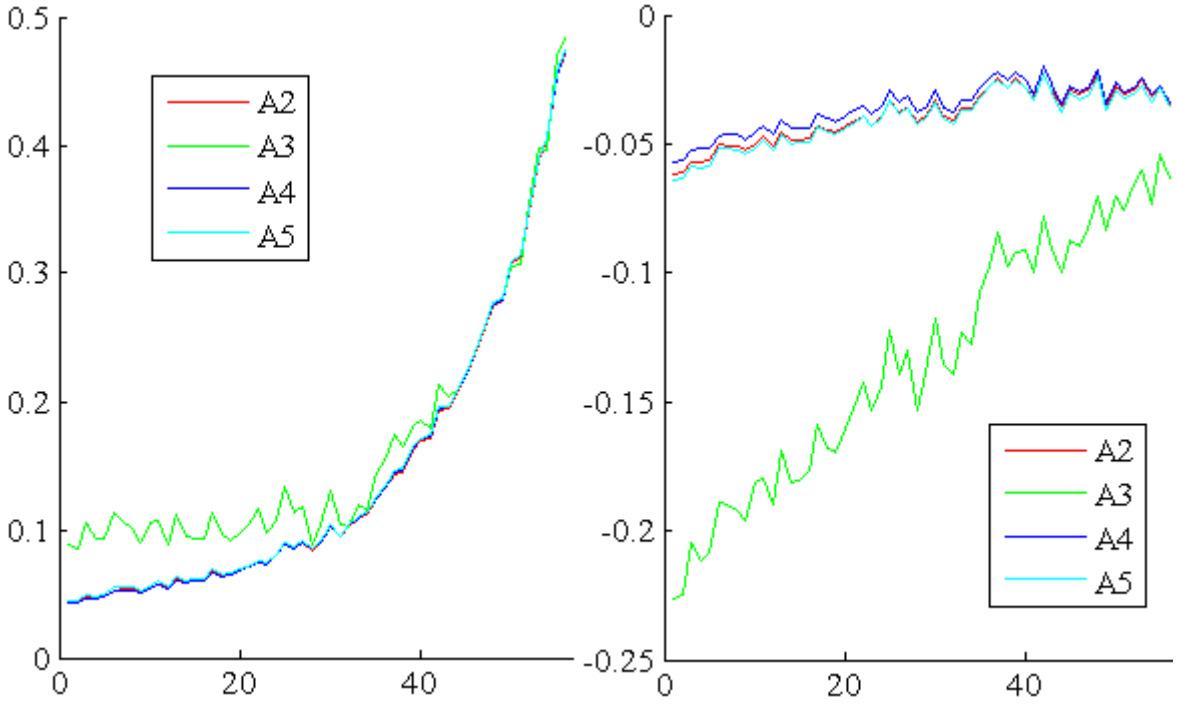

Fig. 3: Relative force error (left) and relative displacement error (right) as a function of number of cracked links.

result in a loss of stiffness in some directions. In A4 these two types of error act against each other and thus A4 appears to be the most accurate (in terms of stiffness) but its accuracy cannot be guaranteed. This can be observed if the error is measured in strain. According to the strain error indicator, the best approach is A2 with interpolation only, while A5 with the most accurate anisotropic homogenization is only slightly worse and A4 takes the 3rd place; see Table 1.

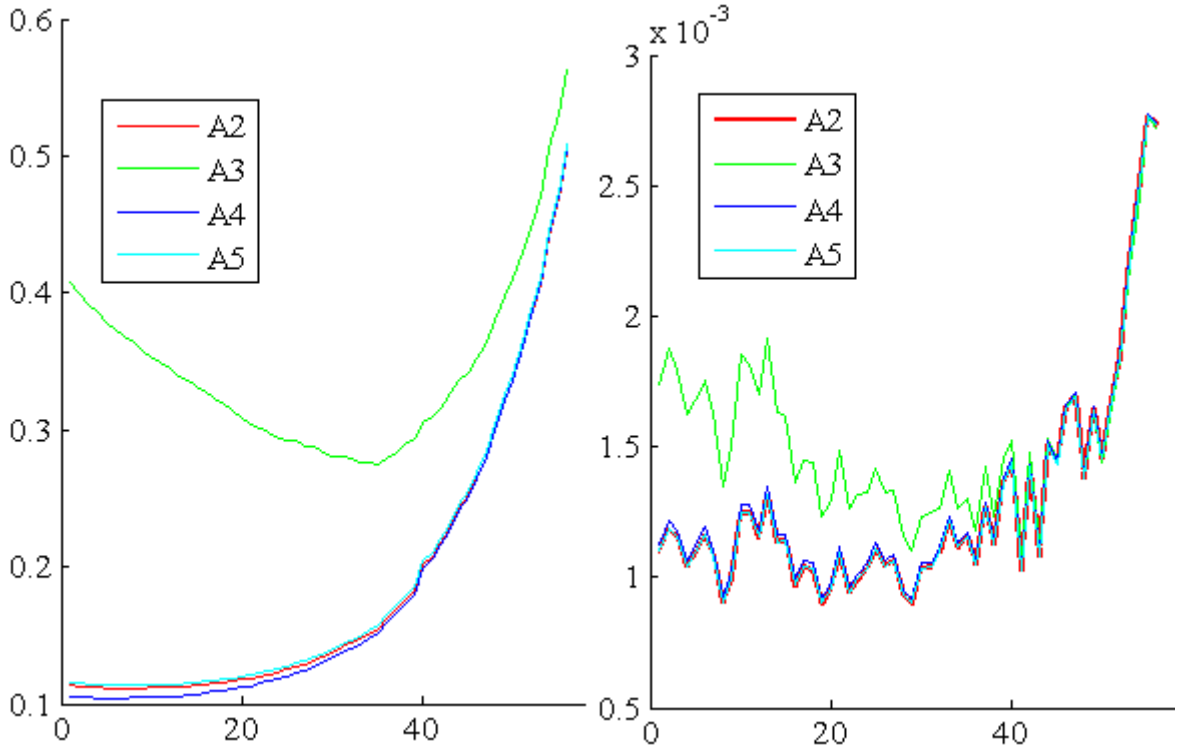

Fig. 4: Relative stiffness error (left) and global strain error indicator (right) as a function of number of cracked links.

Tab. 1: Table of accuracy of different approaches.

Method	Displacement error	Force error	Stiffness error	Global strain error indicator
A2 hanging nodes	-6.18%	4.47%	11.33%	2.258E-03
A3 global homogenization	-22.63%	8.88%	40.75%	3.622E-03
A4 local isotropic homog.	-5.73%	4.23%	10.56%	2.324E-03
A5 local anisotropic homog.	-6.38%	4.48%	11.58%	2.264E-03

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