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ON EFFICIENCY OF QUASICONTINUUM SIMULATION OF CRACK PROPAGATION IN ELASTIC-BRITTLE DISORDERED LATTICES

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Abstract: *A quasicontinuum (QC) method can effectively reduce the computational demand of atomistic simulations by combining continuum and atomistic approaches. In this paper, the QC method is applied to simulations of crack propagation in materials represented by three-dimensional disordered particle systems with elastic-brittle links. The accuracy and efficiency of different QC approaches are evaluated by comparison with the fully resolved particle model.*

Keywords: Quasicontinuum, Multiscale modeling, Lattice model, Finite elements, Elastic-brittle material.

1. Introduction

Discrete particle models can effectively capture complex material responses, especially localized phenomena such as damage or plastic softening. Such models use a network of particles interacting via discrete links or connections to represent a discrete microstructure of the modeled material. They can reproduce fine details of the microstructure and the resulting material properties if the resolution of particles is sufficiently high. On the other side, particle models have two main disadvantages: Firstly, a huge number of particles needed to describe the response of large-scale physically relevant models results in an extensive system of equations, which is expensive to solve. Secondly, the process of assembling of this system is also computationally expensive because all discrete connections must be individually taken into account.

A quasicontinuum (QC) based method can remove both of these disadvantages of high-resolution particle models. The QC method can efficiently handle regular atomistic lattices by combining continuum and atomistic approaches. Two types of subdomains are considered in a QC simulation. In the area of low interest, only a small subset of particles is selected to characterize the behavior of the entire system. These so-called *representative nodes* (in short *repnodes*) are used as nodes of an overlaid triangular finite element mesh, and the displacements of other particles (so-called *hanging nodes*) in the region of low interest are interpolated. In the regions of high interest, all particles are selected as repnodes, in order to provide the exact resolution of the particle model. Furthermore, a summation or homogenization rule can be applied in order to eliminate the requirement of visiting all particles during assembly of the global equilibrium equations.

The QC method was originally proposed in (Tadmor at al., 1996). Since that time, the QC method has been widely used and extended to applications for a variety of materials represented by regular lattices. Five QC-based approaches for simplification of irregular lattices have recently been developed by the authors (Mikeš, 2017). These approaches are based on interpolation (A2), global isotropic homogenization (A3i), global anisotropic homogenization (A3a), local isotropic homogenization (A4i) and local anisotropic homogenization (A4a).

All approaches mentioned above have been implemented into OOFEM (Patzák, 2012), an open-source object-oriented simulation platform. The accuracy and efficiency of simplified approaches is evaluated by comparison with an exact non-simplified lattice model (A1).

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2. Failure simulation

In the failure simulation of a lattice network with elastic-perfectly brittle links, the prescribed displacement is increased until the critical value of tensile strain is reached in the most stretched link. Subsequently, the link is removed and the loading is imposed again. Repeating this process results in a series of link breakages that define the macroscopic crack trajectory.

As an example, the failure of a notched beam in a three-point bending test is simulated in three dimensions. The microstructure of the beam is represented by $30 \times 60 \times 120$ randomized lattice cells, which results in 59 296 particles (with 177 823 unknown DOFs) connected by 502 172 links. The area of high interest is placed around the notch and around points with prescribed boundary conditions, see Fig. 1. Parameters of full and simplified models are listed in Tab. 1.

Tab. 1: Numbers of particles, links, elements, repnodes, hanging nodes and DOFs for various QC approaches.

	A1	**A2**	**A3, A4**
NoP	59 296	59 296	13 812
NoL	502 172	50 2172	92 138
NoE	0	4 169	4 169
NoRN	59 296	59 296	11 413
NoHN	0	47 883	2 399
NoDOFs	177 823	34 174	34 174

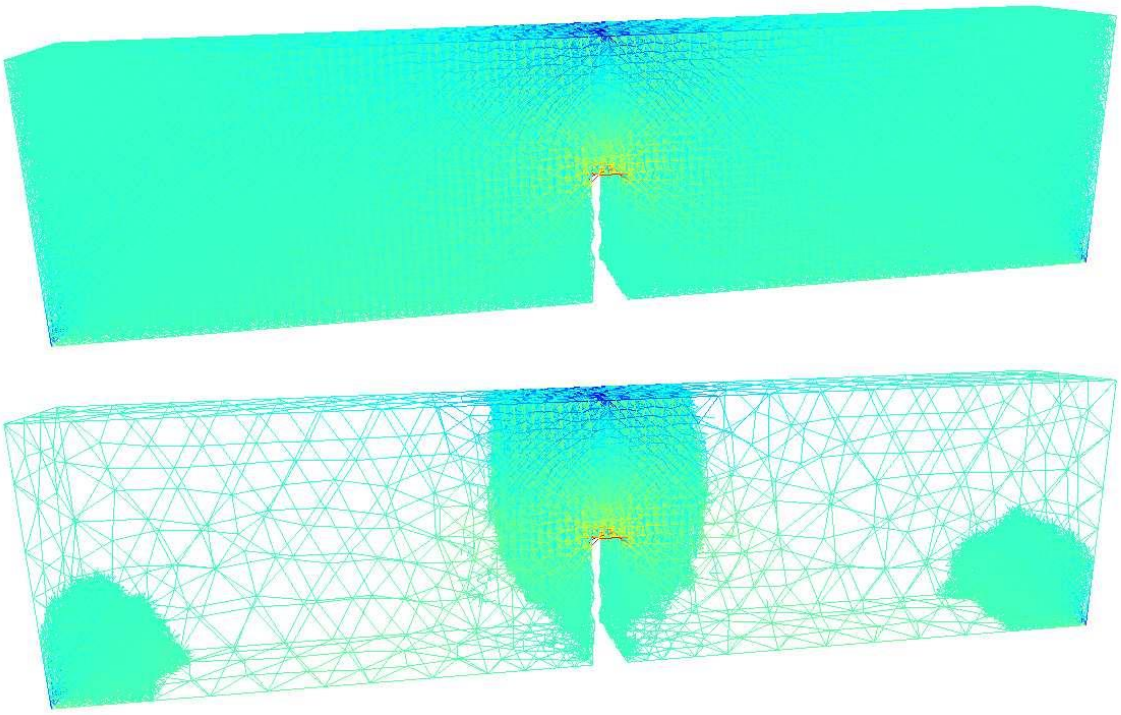

Fig. 1: Strain computed in all links for fully resolved particle model (top). Strain computed in links in area of high interest and surface edges of interpolation elements in area of low interest for simplified model (bottom).

2.1. Accuracy

For simplified approaches, the prediction of cracked links is not completely exact. The sequence of cracked links is not completely the same and some links are predicted incorrectly. However, the agreement is reasonable: Just 6 – 8 % of links cracked in the first 1500 steps computed by one of the simplified approaches are not predicted to crack in one of 2000 steps computed by exact approach, and the macroscopic shape of the crack is very similar for all approaches, see Fig. 2.

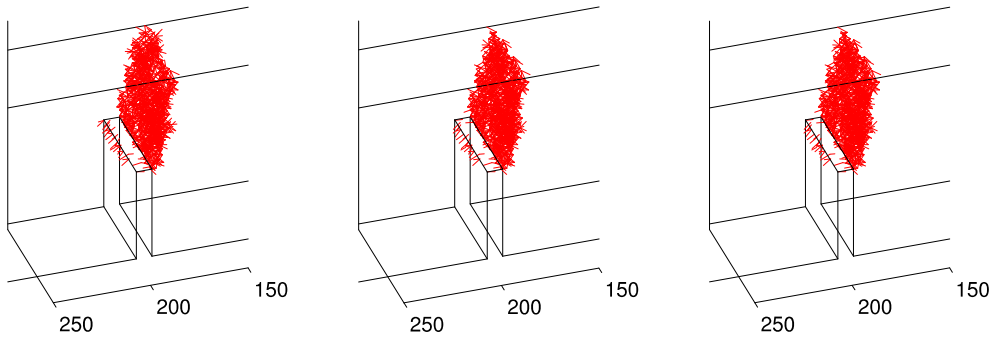

Fig. 2: Middle area of notched beam: edges of the beam (black) and cracked links (red) computed by the exact particle approach A1 (left), interpolation approach A2 (middle) and local anisotropic homogenization approach A4a (right).

The initial elastic response obtained by the simplified approaches is stiffer than the exact solution. However, the shape of the softening branch is captured by all approaches very well, see Fig. 3.

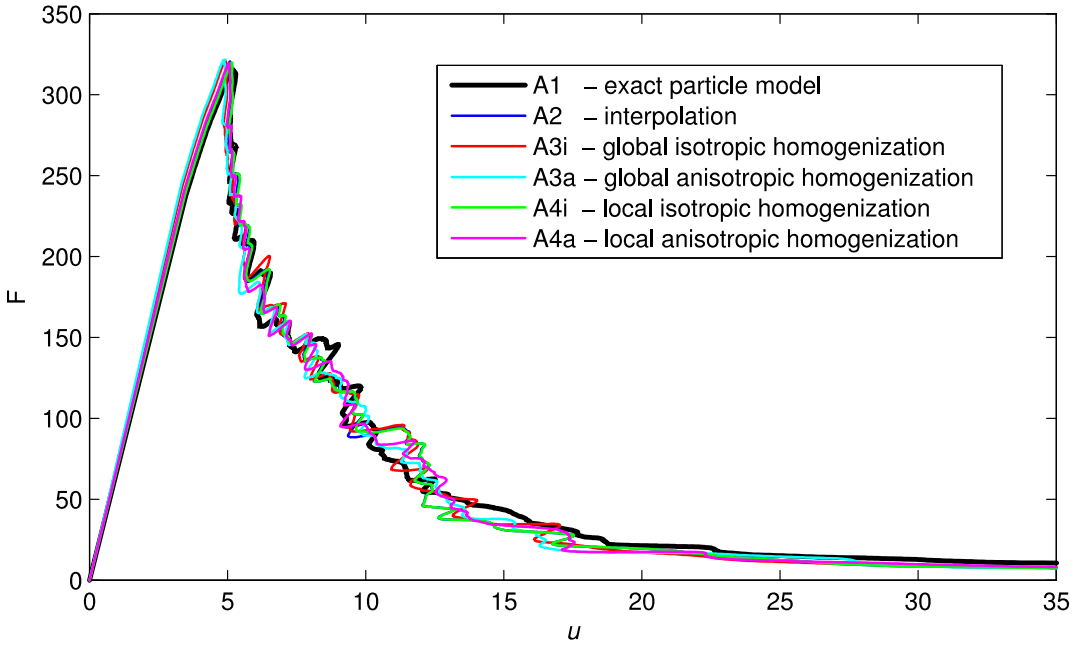

Fig. 3: Force-displacement diagrams for a microstructure with 2000 cracked links computed according to different approaches and smoothed by averaging ±25 neighboring values.

2.2. Efficiency

The QC simplification is a preparatory stage which is realized once before the actual simulation. Time consumptions of individual procedures used by a QC simplification are listed in Tab 2. A conjugate gradient solver with incomplete Cholesky preconditioning and a symmetric compressed column matrix storage scheme have been found to be the most effective combination to solve the numerical problem. The simulation times are summarized in Tab. 3. One can expect that the assembling times for systems with a huge number of hanging nodes (A2) will be significantly higher in comparison with full models (A1). An unpleasant fact is that the assembling times of A2 are even higher than the solution time of A1. The assembly of matrices with symmetric skyline storage formats is faster than the assembly in a symmetric compressed column storage format. But skyline matrices consumed more memory and, for large systems, this difference is critical. It is questionable whether the hanging nodes assembly procedure for compressed column matrix scheme can be implemented more effectively. But a more important fact is that the full assembly of the stiffness matrix or load vector needs to be done only once before the first step of simulation. Before each next step, just the influence of a cracked link connection needs to be taken into account in updating of the stiffness matrix.

Tab. 2: Time consumption of QC simplifications for various QC approaches.

Computational time [s]	**A1**	**A2**	**A3i/a**	**A4i/a**
Generate interpolation mesh	-	0.20	0.20	0.20
Transform mesh to particles	-	0.34	0.34	0.34
Find element for all particles	-	1.97	1.97	1.97
Global stiffness tensor	-	-	0.23	-
Connectivity table	-	-	-	0.13
Individual stiffness tensors	-	-	-	21.61
Total simplification time	**0 s**	**2.51 s**	**2.74 s**	**24.25 s**

In the simulation of the crack propagation process, only the time consumed by solving and updating in one step is multiplied by the number of steps. For long simulations with thousands of steps, the time of QC simplification and assembly becomes negligible and the total relative acceleration is approaching the ratio between the times needed for the solution and update by the simplified and full models. The A2 approach with interpolation without homogenization is four time faster than a full particle simulation. The approaches with homogenization (A3 and A4) achieve speed-ups by a factor of 8 – 9, see Tab. 3.

Tab. 3: Time consumption of simulation for various QC approaches.

Computational time [s]	**A1**	**A2**	**A3i/a**	**A4i/a**
QC simplification	-	2.51	2.74	24.25
Assemble stiffness matrix	2.14	12.81	0.64	0.62
Assemble load vector	1.34	5.89	0.34	0.32
Solve one step	16.06	1.85	1.77	1.73
Update one step	0.80	2.36	0.18	0.19
Simulation of 2000 steps	9 h 22 m 3 s (1.00)	2 h 20 m 41 s (0.25)	1 h 5 m 4 s (0.12)	1 h 4 m 25 s (0.11)

3. Conclusion and future work

All proposed QC approaches have been shown to be very accurate and effective in simulations of crack propagation in lattices with elastic-brittle links. Future work will deal with implementation of an adaptive algorithm which allows for changes of the area of high interest as well as of the interpolation mesh in the area of low interest.

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