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Quasicontinuum method extended to irregular lattices

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ABSTRACT

The quasicontinuum (QC) method, originally proposed by Tadmor, Ortiz and Phillips in 1996, is a computational technique that can efficiently handle regular atomistic lattices by combining continuum and atomistic approaches. In the present work, the QC method is extended to irregular systems of particles that represent a heterogeneous material. The paper introduces five QC-inspired approaches that approximate a discrete model consisting of particles connected by elastic links with axial interactions. Accuracy is first checked on simple examples in two and three spatial dimensions. Computational efficiency is then assessed by performing three-dimensional simulations of an L-shaped specimen with elastic-brittle links. It is shown that the QC-inspired approaches substantially reduce the computational cost and lead to macroscopic crack trajectories and global load-displacement curves that are very similar to those obtained by a fully resolved particle model.

1. Introduction

Discrete particle models use a network of particles interacting via discrete links or connections that represent a discrete microstructure of the modeled material. An advantage of this approach is that discrete models can naturally capture small-scale phenomena. Therefore, a variety of sophisticated discrete material models have been developed and applied in simulations of materials such as paper [1], textile [2,3], fibrous materials [4–6], woven composite fabrics [7] or fiber composites [8]. Extensive effort has been invested into the formulation of a discrete model of concrete [9–12].

Discrete mechanical models can accurately capture complex material response, especially localized phenomena such as damage or plastic softening. However, they suffer from two main disadvantages. Firstly, a large number of particles is needed to realistically describe the response of large-scale physically relevant models. This results in huge systems of equations, which are 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.

Both of the aforementioned disadvantages of discrete particle models can be removed by using simplified continuous models based on one of the conventional homogenization procedures. However, standard continuous models cannot capture localized phenomena in an objective way and require enrichments, e.g., by nonlocal and gradient terms, which are again computationally expensive. According to Bažant [13], the most powerful approach to softening damage in the multi-scale context is a discrete (lattice-particle) simulation of the mesostructure of the entire structural region in which softening damage can occur.

Another way to reduce the computational cost of discrete particle models is a combination of a simplified continuous model with an exact discrete description in the parts where it is needed. Such a combination of two different approaches entails that some hand shaking procedure is needed at the interface between the continuous and discrete domains [14]. The quasicontinuum (QC) method is a suitable technique combining the advantages of continuous models with the exact description of discrete particle models without additional coupling procedures.

The quasicontinuum method was originally proposed by Tadmor, Ortiz and Phillips [15,16] in 1996. The original purpose of this computational technique was a simplification of large atomistic lattice models described by long-range conservative interaction potentials. Since that time, QC methods have been widely used to investigate local phenomena of atomistic models with long-range interactions [14,17]. Recently, the application of QC methods has been successfully extended to other lattices and interaction potentials. For example, an application of the QC method to structural lattice models of fibrous materials with short-range nearest-neighbor interactions has been developed by Beex et al. for conservative [18] and non-conservative [19,20] interaction potentials including dissipation and fiber sliding as well as for planar beam lattices [21], still applied to regular lattices only. An overview of applications and current directions of QC methods has been provided by Miller and Tadmor in [22,23,17] and in part IV of their book [24]. In last few years, a variational formulation of dissipative

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QC method has been done by Rokoš et al. [25], a goal-oriented adaptive version of QC algorithm has been introduced in [26] or a meshless QC method has been developed by the Kochmann research group [27]. But the application of all mentioned QC methods is still restricted only to systems with a regular geometry of particles.

In the present work, we extend the QC approach to irregular systems of particles with short-range interactions by axial forces. The main idea has been tentatively presented in a conference paper [28]. Here we proceed to a more systematic evaluation of the performance of various QC formulations applied to systems with elastic-brittle links. The proposed models are implemented in OOFEM [29–31], an open-source object-oriented simulation platform initially developed for finite element methods but extensible to other discretization methods.

The procedure that results from the QC method combines the following three ingredients:

1. Interpolation of particle displacements is used in the regions of low interest. Only a small subset of particles is selected to characterize the behavior of the entire system. These so-called *repnodes* (representative nodes) are used as nodes of an underlying triangular finite element mesh, and the displacements of other particles 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. This interpolation leads to a significant reduction of the number of degrees of freedom (DOFs) without inducing a large error in the regions of high interest.
2. A summation rule can be applied in order to eliminate the requirement of visiting all particles during assembly of the global equilibrium equations. If such a rule is not imposed, all particles need to be visited to construct the system of equations, which makes the process computationally expensive. If the summation rule is adopted, the contribution of all particles in each interpolation triangle is estimated based on sampling of the links that surround one single particle and proper scaling of their contribution. This makes the computational process faster, but some problems occur on the interface between regions of high and low interest. The piecewise linear interpolation of displacements combined with the summation rule means that the deformation is considered as constant within each interpolation element in the regions of low interest, while the deformations of individual links in the regions of high interest are evaluated exactly. Consequently, forces of nonphysical character, called the ghost forces, appear on the interface [22,32].
In our work, the summation procedure is based on homogenization of link networks contributing to the interpolation elements. Some of the links (truss elements) are selected to be processed exactly, in order to properly treat the interface between the exactly solved and interpolated domains and thus to eliminate the ghost forces.
3. Adaptivity provides suitable changes of the regions of high interest during the simulation process. A new triangulation of the interpolation mesh could be done, but this is actually not necessary because the type of region can be changed by adding repnodes before each step. A suitable change of the regions of high interest may lead to a substantial increase of accuracy and, in several specific cases, it is necessary in order to represent the correct physical behavior, e.g., in a crack propagation process. In numerical examples presented in this paper, sufficiently large fixed areas of high interest are used and additional changes during simulations do not need to be considered. For periodic lattices, efficient adaptive QC techniques have been developed in [26,32].

2. Methods

2.1. Overview

The original QC approach was developed for regularly arranged crystal lattices, in which atoms interact at a longer distance (not just with immediate neighbors) and the interaction forces can be derived from suitable potentials. In regions of low interest, displacements were interpolated in a piecewise linear fashion, using a selected set of representative atoms (repatoms). In this context, imposition of an affine displacement field on the periodic crystal lattice can be interpreted as an application of the Cauchy-Born rule.

In the present paper, we focus on discrete particle systems with short-range elastic or elastic-brittle interactions. Such systems are typically used in simulations of heterogeneous materials. Particles in these systems are distributed randomly and, in contrast to atomistic systems, do not form regular lattices, but the idea of QC can still be used.

Three approaches based on the QC idea are introduced here and are compared with the fully resolved particle model, which is considered as the reference case. Accuracy is assessed in terms of displacement and strain errors. The number and position of repnodes are adapted to achieve the optimal result.

The computational procedure consists of the following steps:

- generation of particles and of connecting links,
- selection of repnodes and generation of interpolation elements,
- application of a simplification rule,
- assembly of global equations with repnode displacements as basic unknowns,
- solution of global equations (for nonlinear models using an incremental-iterative scheme),
- post-processing of results and error evaluation.

The details of individual steps are described in the following subsections.

2.2. Generation of input geometry

In the first step, the input geometry of the particle system is generated; it is specified by the position of all particles in the system and by the information which pairs of particles are connected by links. This process depends on the type of represented material.

The second step consists of repnode selection and generation of interpolation elements. There are two possible reasons why a certain particle is selected as a repnode:

1. All particles located in a region of high interest are selected as repnodes to represent the "exact" behavior in this region.
2. In regions of low interest, a sufficient number of repnodes are needed to construct the approximation of the displacements of other particles. Such repnodes represent vertices of the interpolation elements. The basic triangulation is constructed by the T3D mesh generator [33]. Subsequently, all newly created vertices of the mesh elements are either added as new repnodes, or shifted to the position of the nearest particles, which become repnodes. The second option results in a smaller number of links that need to be solved explicitly on the interface between regions of high and low interest. Therefore, shifting the position of all mesh nodes to the nearest particles is used in all examples presented here.