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Quasicontinuum Approach Applied to Inelastic Materials

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Abstract: The quasicontinuum (QC) method was proposed by Tadmor, Ortiz and Phillips [3] in 1996. The original application of this computational technique was a simulation of large atomistic systems with regular lattices described by long-range conservative interaction potentials. Extension to non-conservative interaction was done by Beex et al. [1]. In the present work, the QC technique is applied to an irregular set of particles connected by discrete plastic links representing e.g. a fibrous material. QC models for plastic materials are constructed within the framework of the microplane theory. Accuracy, efficiency and specific properties of QC microplane models are evaluated by comparison of results with the pure particle approach.

Methodology

The key idea of QC is to reduce the computational cost by reducing degrees of freedom (DOF) of the fully atomistic approach. Instead of dealing with all atoms, a small relevant subset of atoms is selected to represent the whole system. These atoms, the so-called repatoms, are used to approximate the DOF of other atoms. atoms. In applications of the QC idea to particle models, the selected representative particles are referred to as the repnodes.

The description of the 2D material with plastic properties is based on the idea of microplanes. The relation between the stress and strain vectors is used on planes with various orientations, so-called microplanes. The macroscopic stress and strain tensors are obtained by a summation of all these vectors under the assumption of kinematic constraint. The orientation of each microplane is defined by its unit normal $\boldsymbol{n}$. The strain vector ε^n on the microplane is the projection of the strain tensor, $\varepsilon_i^n = \varepsilon_{ij} n_j$. Then the normal strain on the microplane is

$$\varepsilon_N = n_i \varepsilon_i^n = n_i \varepsilon_{ij} n_j. \tag{1}$$

The constitutive elasto-plastic law is defined on microplane level and the macroscopic stress tensor is obtained by integral formula

$$\sigma_{ij} = \frac{2}{\pi} \int_{\Omega} \sigma_N n_i n_j. \tag{2}$$

Numerical simulations have been performed using the open-source finite element code OOFEM [2]. In OOFEM implementation, nodes with interpolated DOF are realized with a special type of node called hanging node. Linear interpolation of hanging nodes is used. Links connecting particles are modeled as perfectly elasto-plastic.

Results

The proposed model has been tested in uniform tension. The geometry of the tested example is depicted in Fig. 1 (left). A significant narrow region is realized in the middle and final plastic mechanism is expected there. If this region is realized with repnodes, the QC model provides very accurate description. But if this region is realized only with microplane elements, the final plastic mechanism is not captured exactly; see Fig. 2. The QC model with repnodes is compared with the fully resolved particle model. The strain error in the last time step is depicted in Fig. 1 (right). Time saving is more than 20%.

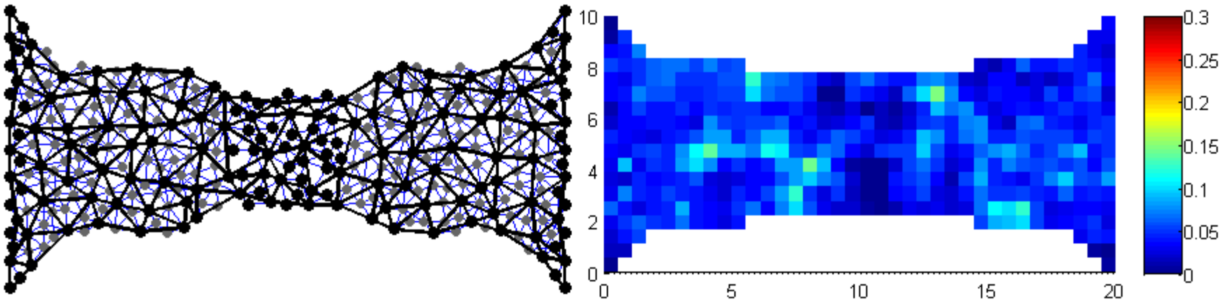

Fig. 1: Interpolation mesh with repnodes and absolute strain error divided by submitted strain.

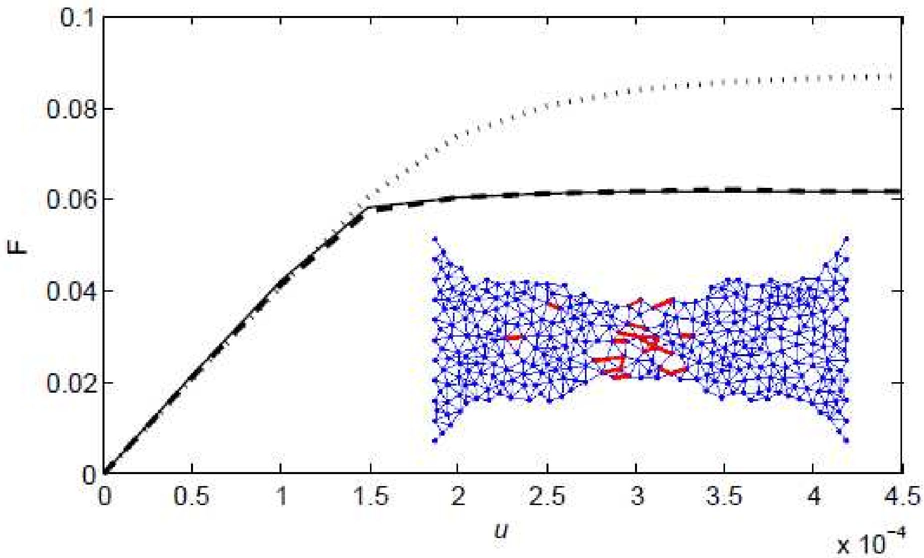

Fig. 2: Force-displacement diagram for fully resolved particle model (solid), microplane model with repnodes in the narrow region (dashed) and without extra repnodes (dotted). Deformed particles with links in plastic state (red).

Conclusions

The QC-based method leads to a substantial reduction of unknown DOF and computational demand. The error caused by this reduction can be effectively reduced by suitably setting the region of high interest. Finally, a significant simplification of the problem can be reached at the price of an acceptable error. The presented example shows that the QC microplane model provides a very good description of the particle model with plastic links if the final plastic mechanism is captured by repnodes.

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References

[1] L. Beex, R. Peerlings, M. Geers, A multiscale quasicontinuum method for dissipative lattice models and discrete networks. Journal of the Mechanics and Physics of Solids, 64 (2014) 154−169.

[2] B. Patzák, OOFEM – an object-oriented simulation tool for advanced modeling of materials and structures. Acta Polytechnica, 52 (2012) 59−66.

[3] E.B. Tadmor, M. Ortiz, R. Phillips, Quasicontinuum analysis of defects in solids. Philosophical Magazine A, 73 (1996) 1529−1563.