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COMPUTATIONAL ASPECTS OF FRACTURE SIMULATIONS WITH LATTICE MODELS

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Abstract

This paper deals with some basic techniques used in numerical simulations of fracture with lattice models. The influence of the element type and mesh orientation on the fracture pattern is shown by simulating an experiment on a concrete plate subjected to shear loading. It was found that beam elements with three degrees of freedom per node, especially with a random orientation of the beams in the lattice, give the best comparison with the experiment. Yet, also the element size turned out to be important. A new fracture law is outlined which uses principal tensile stresses in each node of the lattice to determine the beam to break. For the implementation of heterogeneity in the model a method is developed which uses digital images of the real microstructure of a material. The crack patterns obtained from simulations on a lattice under a few basic loading conditions using this new method are very realistic.

1 Introduction

Heterogeneous materials have complicated fracture mechanisms, which are related to their microstructure. The use of linear elastic fracture mechanics to analytically describe these mechanisms is very hard, since the fracture patterns consist of a main crack, with various branches, secondary cracks and microcracks. To gain some more insight into the problem the use of numerical tools is a good option. Studies in theoretical physics indicated that lattice type models can be quite successful for the simulation of fracture processes in heterogeneous materials, see, for instance, Herrmann and Roux (1990). These models were adopted for specific applications such as to simulate fracture in concrete, see, for instance, Bažant et al. (1990) or Schlangen and van Mier (1992), or in ceramics, see, for instance, Curtin and Scher (1990) or Jagota and Bennison (1994). In these models a material is discretized as a lattice consisting of small spring or beam elements that can transfer forces, see Fig. 1. The simulation of fracture is realized by performing a linear elastic analysis of the lattice under loading and removing (or partially removing) an element from the mesh that exceeds a certain threshold, for example strength or energy.

The results that are obtained from simulations with lattice models, however, depend strongly on the used fracture criterion and the chosen element and/or mesh type. To obtain realistic results it is important that the relation between the implemented disorder in the model and the heterogeneity of the material that is to be simulated is as close as possible.

In this paper the elastic equations as well as the fracture procedure of the model are explained in detail. Different solving techniques for the set of linear elastic equations are discussed. In section 3 the differences in crack patterns obtained from simulations where the element type, beam length and mesh orientation are varied will be shown. Furthermore the effect of various fracture criteria on the simulated crack patterns is presented. Also a short discussion is given of various methods to implement disorder in the lattice and the relation of this disorder to the microstructure of the material.



Fig. 1. Regular triangular lattice of beams (a), external forces and deformations on a single beam element (b) and stress-strain relation for an element (c). (Reprinted from Schlangen (1993))

2 Elastic equations of lattice model

2.1 Set of equations

In this section the elastic equations of the two-dimensional lattice model with beam elements will be described. Each of the beams in the lattice can transfer, in general, normal force (F), shear force (Q) and bending moment (M) as shown in Fig. 1b. The relations between these forces and the corresponding displacements (Fig. 1b) for the endpoints (i and j) of a beam can be expressed as follows:

$$F_i = \frac{EA}{l}(u_i - u_j) \tag{1}$$

$$Q_i = \frac{12EI}{l^3}(v_i - v_j) - \frac{6EI}{l^2}(\phi_i - \phi_j)$$
⁽²⁾

$$M_{i} = \frac{6EI}{l^{2}}(v_{j} - v_{i}) + \frac{4EI}{l}(\phi_{i} - \frac{\phi_{j}}{2})$$
(3)

in which E is the Youngs modulus, l is the length, A is the cross sectional area, and I is the moment of inertia of a beam element, (u, v) are the translational displacements, and ϕ is the nodal rotation. Equations (1-3) use simple beam theory; see, for example, Herrmann and Roux (1990). For a lattice with regular geometry, like that shown in Fig. 1a, E, l, A and I are in principle equal for all elements. However these parameters could be varied, element by element or according to a superimposed microstructure, in order to implement heterogeneity.

To construct the system of equations for the complete lattice, each element matrix has to be multiplied with the appropriate rotation matrix, see Schlangen and Garboczi (1995), and positioned correctly in the system matrix. The final set of equations for the system is of the form:

$$b = \mathbf{A}x\tag{4}$$

in which b is the load vector, A is the stiffness matrix, and x is the displacement vector.

2.2 Solving the equations

When solving the set of linear elastic equations for a lattice under an applied load, the load vector and the stiffness matrix are known and the displacement vector is to be determined by solving eq. (4). One method to solve the set of equations, which is used in most of the previous simulations with the lattice model developed at the Stevin Laboratory, is to use a direct solver which finds the inverse of A, for instance by Gaussian elimination. More information about this procedure can be found in many finite element textbooks; see, for instance, Cook et al. (1989). A faster way to find a solution for the set of equations is by the conjugate gradient method, Press et al. (1988). Recently, see Schlangen and Garboczi (1995), a special version of a conjugate gradient solver, see Garboczi and Day (1995) is implemented in the lattice model. In this algorithm the displacement vector x is solved iteratively by minimizing the functional G, which has the dimensions of energy,

 $\mathbf{G} = 0.5x\mathbf{A}x - bx$

The advantage of a conjugate gradient solver becomes even larger for fracture simulations. Breaking an element and thus removing it from the lattice is a local effect. This implies that the resulting changes in the deformation vector and in G will be small. Therefore only a few iteration steps will be needed to relax the system and find the next element to remove. It should be noted that more iterations of the algorithm are necessary to converge to a solution when the difference in components of the system matrix becomes large. This will happen, for example, when simulating a multi-phase composite where one phase is much stiffer than the other phases. In that case preconditioning of the matrix can help to speed up the process, Batrouni and Hansen (1988).

When a direct solver is used the complete system usually has to be resolved every time an element is removed. However, in this case the method of structural variation could also be used, see Majid et al. (1978) and Jirásek and Bažant (1994). In this method, the inverse of the matrix A is used to update the displacement vector when an element is removed from the mesh, so that a full-scale solution is not needed every time. This does require a large amount of computer memory, since the inverse matrix must be stored. Although for a lattice of beams the stiffness matrix is sparse, the inverse of that matrix is generally not. For a general system of N nodes, the inverse of A is of size $(3N)^2$, which can be enormous. Clearly, the method of structural variation will be useful only for small systems.

2.3 Elastic moduli and fracture criterion

The 2-D elastic moduli tensor for a regular triangular lattice of beams, which is elastically isotropic, Feng et al. (1985), can easily be derived analytically by evaluating the elastic energy of a unit cell of the lattice under a uniform strain (hydrostatic or simple shear):

$$bulk \ modulus: \ \kappa = \frac{\sqrt{3}}{2} \frac{EA}{l} \tag{6}$$

shear modulus:
$$\mu = \frac{\sqrt{3}}{4} \frac{EA}{l} \left(1 + \frac{12I}{Al^2} \right)$$
 (7)

Poisson's ratio:
$$\nu = \frac{\kappa - \mu}{\kappa + \mu} = \frac{\left(1 - \frac{12I}{Al^2}\right)}{\left(3 + \frac{12I}{Al^2}\right)} - 1 < \nu < \frac{1}{3}$$
 (8)

For rectangular beam elements with unit thickness the Poisson's ratio is equal to:

$$\nu = \frac{\left(1 - \left(\frac{h}{l}\right)^2\right)}{\left(3 + \left(\frac{h}{l}\right)^2\right)} \tag{9}$$

To simulate fracture a breaking rule must be defined. Different criteria for fracture have been adopted and can be found in the literature; see,

for instance, Herrmann and Roux (1990), Schlangen (1993), Jagota and Bennison (1994), Beranek and Hobbelman (1994) and van Vliet and van Mier (1994). The main idea is that an element of the lattice will break when a predefined threshold for some quantity, for example tensile stress or elastic energy, is exceeded in that element.

In stead of removing just one element, it can be decided to remove more elements from the lattice before relaxing the system again. This can be a method to simulate dynamic in stead of static loading. Yet, in that case a relation has to be found between the number of elements that is removed in a step and the rate of loading.

In the simulations in section 3 of this paper in each step a beam is removed from the lattice when:

$$\frac{F}{A} > f_t \tag{10}$$

where F is the normal tensile force in the beam, A is the cross sectional area, and f_t is the tensile strength of the beam. Thus the local behaviour of a beam element is perfectly brittle. The stress-strain relation of such an element is plotted in Fig. 1c. After removing one beam element the system is relaxed again. Yet, an error is made when using this fracture law. This will be discussed in section 4.

3 Element and mesh dependency

3.1 Influence of element type on the crack pattern

A lattice of springs or beams is a discretization of a continuum. The number of degrees of freedom in the nodes of a lattice determines the type of continuum that is represented by the lattice. In this section a comparison is made of results of fracture simulation using regular triangular networks with different kinds of elements. The experiment shown in Fig. 2a is simulated with elements having 1, 2 or 3 degrees of freedom, respectively, in each node. In the experiment, see Nooru-Mohamed (1992), a concrete plate is loaded in shear. The crack pattern that was found in the test is plotted in Fig. 2a.

In the first simulation the elements can only transfer normal force, and thus the lattice is equivalent to a central force spring network, Meakin et al. (1989), Bažant et al. (1990) and Burt and Dougill (1977). Equation (1) corresponds to this network. This network is a discretization of a linear elastic continuum with a value of the Poisson's ratio fixed at 1/3. In the second simulation, the elements can also support a shear force, incorporating Eq. (1) and half of Eq. (2), $Q_i = \frac{12EI}{l^3}(v_i - v_j)$. These elements with normal force and shear force are isomorphic to a spring network with central force plus rotational springs, Jagota and Bennison (1994) and Curtin and Scher

(1990). This second network is a discretization of a linear elastic continuum with a general value of Poisson's ratio (but less than 1/3). In the third case elements with normal force, shear force and bending moments are used, Herrmann et al. (1989), Schlangen and van Mier (1992) and Jagota and Bennison (1994). Here all three equations, Eq. (1-3), must be included. This lattice is a discretization of a higher order continuum, a Cosserat elastic continuum, Herrmann and Roux (1990), again with a general value of Poisson's ratio less than 1/3. For a more complete overview of different lattice models the reader is referred to Herrmann and Roux (1990).



Fig. 2. Geometry and crack pattern of shear experiment on concrete plate, according to Nooru-Mohamed (1992) (a), simulated crack patterns in mesh with springs (b), spring and shear elements (c) and beam elements (d). (Reprinted from Schlangen and Garboczi (1995))

The results of the three simulations are shown in Fig. 2b-d. In the simulations no heterogeneity was implemented to separate problems of implementation of disorder and the ability of a lattice to describe a continuum. The crack patterns differ appreciably between the lattices with different elements. In the lattice with only normal force in the elements, one straight crack is obtained. When two degrees of freedom per node are used, the cracks start at the correct angle, but the cracks stay straight and do not curve. In the simulations with the beams with three forces, the crack pattern is much closer to the experimentally observed pattern. In all three cases, however, it can also be seen that the crack patterns are influenced by the principal directions of the mesh. This phenomenon is further discussed in the next section.

3.2 Influence of mesh orientation on the crack pattern

The effect of mesh orientation on crack patterns when using the beam elements, with three forces, is illustrated in the next example. In Fig. 3 crack patterns are shown of simulations of the same experiment as in the previous section, using four lattices with different beam orientations. In the first mesh beam elements in a square grid are used (Fig. 3a). The second lattice, shown in Fig. 3b, is the same as that shown in Fig. 2d. In the third simulation, shown in Fig. 3c, again a triangular lattice is used, but the mesh is rotated 90°. In the last simulation (Fig. 3d) a special random lattice is used. The cross sections and moments of inertia are chosen in such a way that the lattice represents a homogenious medium, as explained in Schlangen and Garboczi (1995). In all four simulations two overlapping curved cracks are obtained, yet there are differences in crack shape due to the different orientation of the meshes. The simulation using the homogeneous random lattice resembles the experiment most closely. It is expected, however, that a regular lattice with implemented disorder can lead to simular results.



Fig. 3. Simulated crack patterns in square (a), regular triangular (b), rotated regular triangular (c) and random triangular (d) mesh. (Reprinted from Schlangen and Garboczi (1995))

3.3 Influence of beam size in the lattice

To study the influence of the size of the beams in the lattice on the fracture behaviour, an example is shown taken from Schlangen (1995). A triangular lattice (Fig. 4b) having periodic boundary conditions in the horizontal direction is loaded in tension in the vertical direction. Two different strengths in a ratio of 1.0 to 3.0 are assigned to the respective elements. The meshes consist of 25% low strength (1.0) and 75% high strength (3.0) elements. The size of the beams has been varied. Four different analyses are performed, with meshes consisting of 8, 16, 32, and 64 elements in horizontal direction.

The crack patterns of the meshes with different element sizes are comparable, however there is a large difference in load-crack opening response, see Fig. 4a. The curves are always the average response of ten simulations with different low and high strength beams chosen randomly. The mesh with the largest elements (8) shows the most ductile response. This can be explained from the fact that the crack width is larger and thus more energy is released if an element is removed in a coarse mesh compared to a fine mesh. This results in larger deformations. The above shows that we have to be careful in varying the beam size.



Fig. 4. Load-crack opening (a) and crack patterns (b) for simulations in which the fineness of the mesh is varied. (Reprinted from Schlangen (1995))

4 Fracture law

4.1 Discussion of fracture laws

In the above simulations the stress in a beam element is calculated using eq. (10) in which the normal force in a beam is divided by the cross section. However this is not always correct. If a uniform strain is applied to a triangular lattice of beam elements, it is clear that all the elements carry only normal forces and thus stresses in all directions are equal. Yet, when a uniaxial strain is applied to a triangular lattice, the stress calculated with this fracture law depends on the direction of loading.

In order to explain this phenomenon the following analysis is performed. A triangular lattice of beams, with equal properties, having periodic boundary conditions in one direction is loaded in tension in the other direction, see Fig. 6. If the lattice is loaded in horizontal (X) direction using the old fracture law, a straight crack is obtained and also a load-crack opening response with descending branch, see Fig. 6. When the lattice is loaded in the vertical (Y) direction, however, the descending branch stays high and all the vertical beams in the lattice break. Next to this difference in crack propagation and the shape of the load-crack opening response, the maximum load depends on the direction of loading. A uniaxial strain in horizontal direction results in a 33% higher stress than a uniaxial strain in vertical direction on the same lattice.

In most of the simulations performed earlier, see Schlangen (1993), the contribution to the stress in the fracture law consisted of the normal force in a beam as well as part of the bending moment. This, however, has no positive effect on the directionality in the lattice which is discussed above.

In Beranek and Hobbelman (1994) and van Vliet and van Mier (1994) a normal force and shear force in a beam are combined as in Mohr's Circles to obtain a value for the stress in a beam. It is not checked, but the author believes that also with this fracture law no improvement concerning the directionality of the lattice is obtained.

In the remainder of this section a new fracture law is explained. The main difference with the aforementioned fracture laws is that in the new law a stress is calculated in each node in stead of each beam. All the beams connected to a node contribute to this stress. The procedure for calculating the stress is outlined in Fig. 5. In a node a cut is made like in Fig. 5a. Out of all the normal and shear forces (the bending moment is not included) in the beams at one side of the cut two resulting forces F_{node} and Q_{node} iare computed, see Fig. 5b. This is done for all angles between 0 and 2π . The angle is determined for which the normal force is maximal. The shear force for that angle is equal to zero, see Fig. 5c. The cross sections of the beams in the direction perpendicular to the cut for which the normal force is maximal are determined as shown in Fig. 5d. Then a stress σ_{node} is determined as shown in Fig. 5e. Thereafter the beam for which the tensile stress divided by the tensile strength is maximum is removed from the lattice. Note that for a lattice representing a homogeneous material (i.e. a lattice in which all the beams have an equal strength and stiffness) all the beams in a node have the same stress and thus the same breaking point.



Fig. 5. Lattice with forces in beam elements (a), resulting normal and shear forces perpendicular to a nodal cut (b), maximum normal force $F_{node,max}$ in the node (c), cross sections corresponding to angle with $F_{node,max}$ (d) and resulting stress in the node (e)

The relation between the stress found following this procedure, σ_{node} , and the real stress σ (which is the local stress in a medium as a result of a globally applied stress on the lattice) can be determined from the angles in the lattice. The real stress σ is the local stress in a node as a result of a globally applied stress on the lattice. For beam elements with rectangular cross section and unit thickness the relation is:

$$\sigma = \sqrt{3} \frac{h}{l} \sigma_{node} \tag{11}$$



Fig. 6. Load-crack opening diagram (a) and crack patterns (b) for lattice loaded in tension in X and Y direction using the old and new fracture law.

With the new fracture law the same example as discussed above, the triangular lattice with periodic boundary conditions in one direction and tensile load in the other direction, is simulated. In Fig. 6 it can be seen that the same crack pattern is obtained for the lattice loaded in X and Y direction and that the maximum loads as well as the complete load-crack opening diagrams match almost perfectly.

4.2 Compression and splitting in a homogeneous mesh

In the previous section it has been shown that the new fracture law gives good results for uniaxial tensile loading. But what about tensile splitting and compression? In this section simulations with the old and new fracture law are compared for these types of loading. A square triangular lattice of beams that have equal properties is used. One beam in the centre is removed to introduce an imperfection for the crack to start. The resulting crack patterns are plotted in Fig. 7. Fig. 7a and 7b show the crack patterns for a lattice loaded in tensile splitting in horizontal and vertical direction, using the old fracture law. In the simulations shown in Fig. 7e and 7f the new fracture law is used for the same loading case. With the old fracture law and splitting in vertical direction the same phenomenon is observed as in the tensile simulation of the previous section. Only the beams in the direction of the tensile stress fail. In the simulation of Fig. 7b a sort of splitting behaviour is found, vet the crack is not in the middle where it should be. With the new fracture law the simulated crack patterns show a much improved behaviour. It is not shown here, but also the load-crack opening response for both loading directions match with the new fracture law.

In Fig. 7c,d (old fracture law) and 7g,h (new fracture law) the crack pat-

terns are shown for a lattice loaded in compressive in both directions. There is no constraint assumed at the supports. With the old fracture law rather strange crack patterns are observed (7c,d). The lattice loaded in horizontal direction (7d) did not fracture at all, since the normal forces in all the beams were compressive. The simulations with the new fracture law show again better behaviour. However, it should be mentioned that the crack patterns for compression, also with the new fracture law, are influenced by the prefered direction in the triangular mesh, as already explained in section 3.2. As discussed a random lattice would give better results. Yet, a regular lattice with implemented heterogeneity will also do quite well as will be shown in the next section.



Fig. 7. Crack patterns for a lattice loaded in tension splitting (S) or compression
(C) in vertical (V) or horizontal (H) direction using the old (O) or new
(N) fracture law: S-V-O (a), S-H-O (b), C-V-O (c), C-H-O (d), S-V-N
(e), S-H-N (f), C-V-N (g) and C-H-N (h)

5 Back to reality: concrete fracture

In the previous sections some basic features of lattice modelling are explained. All cases are studied for the homogeneous case. Yet, the actual goal is to simulate fracture in a real material. Real materials are in general not homogeneous, and therefore fracture will be influenced by the microstructure of the material. The heterogeneity has to be implemented to simulate the fracture process correctly. The scale at which information is required should be taken into account too. Different techniques have been used in the past to implement disorder. These techniques all have their own application (scale) for which they will give good results. This will not be discussed here further; only some different options are mentioned briefly:

• Randomly assigning different properties, if desired following a certain distribution, to the elements in the lattice, see, for instance, Herrmann et al. (1989) and Schlangen (1993).

• Using a mesh with random geometry, but equal properties for the beams, see, for instance, Burt and Dougill (1977) and Schlangen (1993).

• Generate a microstructure and project this on a regular lattice of beams and assign different properties to the beams depending on their position, see, for instance, Schlangen and van Mier (1992) and Jagota and Bennison (1994).

• Use a combination of the previous two, a random geometry and a generated grain structure, see, for instance, Bažant et al. (1990).





In the simulations shown in this section a method is used in which the microstructure is implemented in a direct way. An image of a real piece of material is taken. In this case an image of a mortar, see Fig. 8a. By using image processing techniques the image is split into three phases, i.e. particles, mortar and voids, see Fig. 8b. A lattice of 19931 beam elements is projected on top of this image and different properties are assigned to the elements in the different zones, Fig. 8c. The elements in the aggregates, mortar and interface between them are given a strength and stiffness in the ratios: 10, 4 and 2 respectively. In the voids no elements are placed. The purpose of the simulations below was not to find a real match with experiments, but to show that the trend is similar to what happens in the real material.

Four simulations are performed using the mesh of Fig. 8c. The loading cases are uniaxial tension (Fig. 9a), tensile splitting (Fig. 9b) and two compression cases (Fig. 9c,d). The new fracture law explained in section 4.1 is used. In the uniaxial tension simulation (Fig. 9a) two cracks start from both sides of the specimen. This, because no rotation of the ends is allowed. Pieces of material still bridging the two crack faces can be seen, as was observed experimentally, see van Mier (1991). This causes a ductile response. In the tensile splitting case (Fig. 9b) a crack starts in the centre of the specimen and propagates to the loading points. The stress-crack opening curves for the two tension cases are plotted in Fig. 10a. Both show a softening behaviour. The stress in the splitting case is about 16% higher than the stress in the uniaxial tension case, which is comparable to what is observed experimentally.

For the compression case the boundary conditions are varied. In the simulation shown in Fig. 9c the nodes where the compressive loads are applied are free to move horizontally (zero boundary restraint). In the other case (Fig. 9d) these nodes are fixed (infinite boundary restraint). In the case of free boundaries (Fig. 9c) diagonal cracks, or shear bands, are found. Fixed boundaries (Fig. 9d) leads to hourglass type crack patterns. This behaviour is already observed in many experimental work, see, for example, van Vliet and van Mier (1995).



(a)





Fig. 9. Crack patterns for a lattice loaded in tension (a), tensile splitting (b), compression with free (c) and fixed (d) boundaries

The stress-crack opening diagrams are plotted in Fig. 10b. Compared with the real behaviour of concrete the simulated results are not so good. For the simulation with free boundaries a softening behaviour is obtained. For the fixed case no descending branch is found. Of course this is different from what is found experimentally. However there are two major differences between the simulation shown and an experiment with fixed boundaries. Firstly, in an experiment the boundaries are never completely fixed (restrained). Secondly, the three-dimensional effect due to the boundary restraint becomes very important. A two-dimensional simulation is not sufficient in that case. Further research is required to get the load-displacement response correct for compressive loading.

A comparison of the maximum stress in the uniaxial tensile case with the compression case with free boundaries shows that the stress in the compression case is about 10 times higher. This is realistic for concrete.



Fig. 10. Stress-crack opening diagrams for lattice loaded in tension and tensile splitting (a) and compression with free and fixed boundaries (b)

6 Discussion and conclusions

In this paper numerical aspects of lattice models for the simulation of fracture are discussed. It is shown that lattice models should be used with care. Sometimes results that are found are caused by the model and not by the behaviour of the material that is modelled.

For fracture, the results that are obtained strongly depend on the element type chosen. Beam elements with three degrees of freedom per node seem to give the best agreement with experimentally obtained crack patterns.

The shape or orientation of the beams in a lattice also influences the simulated crack patterns, with the cracks tending to follow the mesh lines. This disadvantage can be circumvented by using a random lattice which is made elastically homogeneous.

The results that are obtained from simulations also depend on the size of the elements in the lattice. The stress-strain behaviour becomes more ductile for increasing element size.

A new fracture law is proposed which uses the maximum tensile stress in each node to determine which element should be fractured. In contradiction to previously used fracture laws, the stress which is determined does not depend on the direction of loading applied on the lattice.

In section 5 a method is outlined to implement the heterogeneity of a material in a direct way. A digital image of the microstructure of a mortar is used to assign different properties to the elements in the lattice. A lattice in which heterogeneity is implemented following this method is subjected to a few basic loading conditions. The crack patterns obtained from these simulations look very realistic. However, the problem that still remains is how to determine the input parameters for strength and stiffness for the elements in the lattice. For concrete, especially data for the strength and stiffness of the interfacial zone between aggregates and mortar are unknown. Probably a combined experimental and numerical investigation, as proposed by Vervuurt and van Mier (1995), will lead to appropriate values.

Finally, a remark will be made about the application of lattice models. It is not realistic to state that lattice models will ever be used to analyse structural members on a material level. The use of lattice models, however, can be very helpful to study the fracture behaviour of a material and how this behaviour will change if the properties of the individual components change. Furthermore, lattice models can be a useful tool for developing stronger and better materials.

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