New model for crack growth using random walkers *

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Abstract

In close analogy to diffusion limited aggregation (DLA) and inspired by a work of Roux, a random walker algorithm is constructed to solve the problem of crack growth in an elastic medium. In contrast to conventional lattice approaches, the stress field is not calculated throughout the whole medium, but random walkers are used to detect only the hot sites on the surface of the crack. There, an analytically calculated Green’s function is used to determine the stress field. The complicated boundary condition on the crack surface is simulated by a special sticking-rule walk. Using this new method we generate crack-clusters up to sizes of 20,000 particles on simple workstations within reasonable time. We simulate several different boundary conditions, like uniaxial tensile, pure shear and isotropic tensile load. We study the influence of several parameters representing the material strength or fatigue. Furthermore we study the effect of anisotropic walks. As a result, we reproduce with this new model typical experimental crack shapes and are able to simulate the essential features of realistic cracks.

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1 Introduction

The study of non-equilibrium growth models has been extremely popular in the past few years. Especially the Laplacian growth phenomenon has been studied extensively and applications of it can be found in a large variety of fields, e. g. electrodeposition [1], fluid-fluid displacement [2] or growth of bacteria colonies [3]. One reason for its popularity is, that a numerical simulation of this process can be done extremely efficiently using diffusion-limited aggregation (DLA) [4]. Using highly optimized programs [5, 6] it is possible to grow huge DLA clusters containing up to 50 million particles [7, 8].

However, this paper is not devoted to DLA, but inspired by this efficiency and success of DLA and by a work of Roux [9] we will attack the problem of crack growth in an elastic medium [10, 11, 12]. Here, to an elastic material a certain load is applied and eventually cracks develop, which grow until the material breaks apart. Although highly developed numerical techniques, which are mainly based on lattice models, exist [13, 14], the simulation of crack growth is even on today’s supercomputers restricted to a few thousand broken bonds or even less. Thus, new techniques are urgently needed, which might allow for large crack growth simulations maybe on workstations.

As was pointed out by many researchers [15, 16], there exist some remarkable formal similarities between the vectorial elasticity problem — which is governed by the Lamé equation — and the scalar electricity problem — which is governed by the Laplace equation. It was even shown by Roux, that it is formally possible to construct a Green’s function of the Lamé equation using a certain type of vectorial random walkers in a similar way one constructs a Green’s function of the Laplace equation. The latter one can of course simply be interpreted as a density of random walkers and is thus much easier to implement than a formal, vectorial random walker, which is much more difficult to interpret. However, although Roux’s ideas are very clear, an actual numerical implementation of them and a check of their practicability is still missing.

In the current paper we will discuss his ideas and will present a new algorithm for crack growth. For this purpose we will construct a DLA-like random walker method, in which the random walkers are used to find the
“hot” (highly stressed) sites along the surface of a crack, i. e. those which are most likely to break. Here, ‘DLA-like’ is not meant in the sense of ‘probabilistic’ used in [17, 18, 19, 20] to characterize these crack growth models, but in a sense that we explicitly use random walkers to transport information from the boundaries towards a crack.

The use of random walkers will introduce disorder and noise into the simulation. But since real material are typically spatially disordered and inhomogeneous, this noise can be justified and interpreted physically as an inherit randomness. It does not have to be introduced by hand like in typical lattice models, but is an implicit feature of the model.

The outline of this paper is as follows. In section 2 we will give a short introduction into the problem of crack growth. We will briefly present and extend Roux’s ideas and we will discuss the reasons, why a direct numerical simulation of his method is not practical. In section 3 we will introduce a new model for crack growth by drawing an analogy to DLA. We will use random walkers and an analytically calculated Green’s function to transport the information about surface forces towards a crack, which is represented as a cluster of particles. We will also discuss the treatment of the boundary condition along the crack, which turns out to be the most difficult ingredient of the model. Then, in section 4 we shall present the results of this model and will study several variations of it in order to understand the influence of the numerical parameters. Here, we will compare our model to experimental and analytical results. In section 5 we will critically discuss the method and, finally, in section 6 we will summarize our results.

2 Relation between crack growth and random walks

Consider a $d$ dimensional infinite elastic medium with Poisson ratio $\nu$. In equilibrium this system can be described in terms of the stress field $\sigma$ which obeys

$$\text{Div}\sigma = 0. \quad (1)$$

Together with Hooke’s law this can be reformulated in terms of the dis-
placement field \( u \) and one obtains the Lamé equation

\[
(1 - \nu(d - 1))\nabla^2 u + \nabla(\nabla \cdot u) = 0. \tag{2}
\]

A crack in such a system can be interpreted as an additional force free surface, which thus has to obey the boundary condition

\[
\sigma \cdot n = 0. \tag{3}
\]

Here one has to point out, that unlike in DLA this boundary condition at the crack surface is not formulated in terms of the displacement field — which corresponds to the potential in the Laplace equation — but in terms of the stress field, which is related via Hooke’s law to a spatial derivative of \( u \). As we will show later, this peculiarity requires a special treatment of the crack surfaces.

Apart from those equilibrium conditions one can formulate the condition for the growth of a crack in terms of the stress component parallel to the crack surface \( \sigma_\parallel \). This has to exceed a critical value \( \sigma_c \), which is directly connected to the intermolecular cohesion forces, and then the growth velocity of the crack \( v_n \) is determined by

\[
v_n \propto (\sigma_\parallel - \sigma_c)^\eta \tag{4}
\]

where \( \eta \) is a heuristic parameter which is often simply set to one. This rule for crack growth only takes into account crack growth through cleavage and completely ignores bending terms. The equations (2, 3, 4) formulate the problem of crack growth as a nonlinear moving boundary problem.

To give a closed picture of the problem we shall now recall very briefly the main ideas of Roux \[9\] in order to be able to extend and comment them. The fundamental idea of his work is to define a Markovian random walk process that constructs a matrix, which finally leads to a Green’s function of the Lamé equation. This is done in complete analogy to the Laplacian case, which we will find as a special case of the following derivation.

Therefore, consider an elastic material with an unknown displacement field \( u \), which is a result of the boundary conditions. Our task is to obtain this field at point \( x \) in terms of the boundary displacements. Therefore
consider the following Markovian process: A random walker starts at point $x$ and makes a first, elementary jump of length $r$ into a random direction $e_1$. After averaging over all possible directions $e_1$ one defines at $x$ a new vector $(Q_r \ u)(x)$ as

$$(Q_r \ u)(x) = \left\langle Q(\ e_1) \cdot u(\ x + r \ e_1) \right\rangle_{e_1}$$

(5)

where the elementary step matrix $Q(\ e)$ is defined as

$$Q(\ e)_{ij} = (\alpha \cdot \frac{1}{2} + (1 - \alpha) \cdot d \cdot e \otimes e)_{ij} \equiv (\alpha \cdot \delta_{ij} + (1 - \alpha) \cdot d \cdot e_i e_j)$$

(6)

and $\alpha$ is a parameter that will be determined later.

As usual in Markov processes this elementary step is iterated. Consequently, after performing $N$ independent steps — each of length $r$ — one defines at $x$ the new vector

$$(Q_r^N \ u)(x) = \left\langle Q(\ e_N) \cdots Q(\ e_1) \cdot u(\ x + r \ e_1 + \cdots + r \ e_N) \right\rangle_{e_1 \ldots e_N}$$

(7)

By considering its spatial Fourier transform

$$(Q_r^N \ u)(k) = \int (Q_r^N \ u)(x) \exp(-i \ k \ x) \ dx = Q_r^N(k) \cdot u(k)$$

(8)

one can evaluate the limit of vanishing step length $r \to 0$ and diverging number of steps $N \to \infty$, while keeping $t = N r^2$ fixed. One easily obtains with the central-limit theorem

$$\lim_{N \to \infty, r \to 0} Q_r^N(k) = Q_t(k) = \exp \left( -\frac{t}{2d(d+2)} \left[ (2\alpha + d) \ k^2 + 2d(1 - \alpha) \ k \otimes k \right] \right) \equiv \exp(M).$$

(9)

After transforming this quantity back into real space, it is easily seen that the Fourier transform

$$\left( Q^t \ u \right)(x) = \int Q^t(\ r) \cdot u(\ x + r) \ dr.$$

(10)
provides a solution of the following general equation for the vector field $V(\mathbf{r}, t)$

$$\frac{\partial V}{\partial t} = \frac{(2\alpha + d)\nabla^2 V + 2d(1 - \alpha)\nabla(\nabla \cdot V)}{2d(d + 2)}$$  \hspace{1cm} (11)

The stationary limit $\partial V/\partial t = 0$ of this equation obviously provides the Lamé equation if one chooses $\alpha$ appropriately

$$\alpha = \frac{d(1 - 2\nu(d - 1))}{2(d + 1 - d\nu(d - 1))}$$  \hspace{1cm} (12)

and identifies $V(\mathbf{r}, t)$ with the displacement field $u(\mathbf{r}, t)$.

In summary, in this formulation the problem of determining a time-dependent Green’s function $Q^t(\mathbf{r})$, which is used in (10), has been formulated in terms of a random walk. Obviously eq. (11) shows the type of Markov process that one has to perform in order to solve Lamé’s equation. Anyhow, we shall show in the following that although exact, it is not practical to construct an algorithm directly from (11).

A direct and naive implementation of (11) would involve the following steps. One would launch a random walker at a boundary site $\mathbf{r}_i = x + \mathbf{r}$ at which the displacement $u$ is known. The walker would undergo an isotropic random walk until it touches a crack at point $\mathbf{r}_f = x$. During the walk one would calculate the product of the elementary step matrices $Q(e_N) \cdots Q(e_1)$ and would finally average at $x$ over the vectors $Q(e_N) \cdots Q(e_1) \cdot u(r_i)$ of all incoming random walkers. One would then have to extrapolate to the limit $r \to 0$ — which at least in this algorithm necessarily leads to $N \to \infty$ — and according to (10) this procedure should finally yield the required solution.

But although this process strongly reminds one of the process to construct the Green’s function of the Laplace equation with random walkers, there are several differences which result in important difficulties. Unlike in DLA the history of each walk is here extremely important. The product matrix is explicitly dependent on each individual step $e_i$ and therefore the path on which the walker travels from its initial to its final point is extremely important. Thus, the contribution of each individual walk to the average (11) is arbitrarily small.
On the other hand it is necessary to take the limit $N \to \infty$ and thus the number of factors to calculate the product matrix grows rapidly. But since the eigenvalues of $Q(e)$ are not equal to unity the product matrix $Q(e_N) \cdots Q(e_1)$ has an uncontrollable norm, which either diverges or vanishes exponentially fast. From this follows, that also the modulus of the resulting vector $Q(e_N) \cdots Q(e_1) \cdot u(r_i)$ is uncontrollable. Similar arguments show immediately that not only the modulus, but also the direction of the resulting vector is uncontrollable. The consequence of these considerations is, that a naive implementation of the algorithm suggested by (7) results in enormous statistical fluctuations of both the modulus and the direction of $(Q_N^N u)(x)$, which cannot be suppressed in numerical simulations.

Another important point is, that the previously described algorithm neglects the presence of a crack, which substantially changes the stress field. It is also not easily possible to include the boundary condition at the crack (3), because it is expressed in terms of the stress field, which is not included in the previous derivation. Of course one could reformulate the boundary condition in terms of the displacement field, but this requires spatial derivatives of the displacement field which are even less accessible than the displacement itself.

However, the previous considerations showed that one purpose of the random walkers is to construct the matrix $Q^t(r)$, which is the basis of (10). But in an infinite system this matrix, which is actually already the average of all product matrices of walks starting at the origin and terminating at $r$, can be calculated analytically. Thus, one could evaluate (10) directly using random walks, which would then only be used to determine the initial and final positions $x$ and $x + r$. Here, the history of each individual walk is no longer relevant and thus one does not obtain the huge fluctuations described before.

$Q^t(r)$ is obtained by a Fourier transformation of (9) into real space (see Appendix). Finally one finds

$$Q^t(r) = \frac{1}{2\pi} [f_s(r, t) + f_a(r, t)] \cdot 1 - \frac{1}{2\pi} f_a(r, t) \cdot 2 \frac{r \otimes r}{r^2}$$

(13)
\[ f_s(r, t) = \exp \left( -\frac{r^2}{4\lambda_1 t} \right) + \frac{4\lambda_1 t}{4\lambda_2 t} \exp \left( -\frac{r^2}{4\lambda_2 t} \right) \]
\[ f_a(r, t) = \left( 1 + \frac{4\lambda_1 t}{r^2} \right) \exp \left( -\frac{r^2}{4\lambda_1 t} \right) - \left( 1 + \frac{4\lambda_2 t}{r^2} \right) \exp \left( -\frac{r^2}{4\lambda_2 t} \right) \]

This result has to be commented in several respects.

It is clearly seen from the form of the two functions \( f_s \) and \( f_a \), that the underlying elementary process is a random walk. They consist of two Gaussians, which are the result of the diffusion of free particles launched at the origin of an infinite domain. The limiting case of the pure Laplacian is obtained by setting \( \nu \to -\infty \). In this case \( Q^t(r) \) simplifies to the Green’s function of the corresponding Laplace problem, which is a pure Gaussian.

Since one requires \( t = Nr^2 \) to be fixed, one has introduced a new, free time variable. But none of the recent and efficient implementations of DLA algorithms uses an explicit time definition. In DLA the time it takes for a walker to reach a cluster is not relevant. Here, \( k \) explicitly enters \( Q^t(r) \).

The previously calculated \( Q^t(r) \) is only valid in an infinite domain. In \( (7) \) one averages essentially over all possible random walks that connect the origin with the point \( r \). But in the presence of a crack, many of the walks terminate at the crack before reaching \( r \). Also those walks are taken into account in eqs. \( (7-10) \) to calculate \( Q^t(r) \). This deficiency could be altered by considering only those walks, which do not leave a restricted area, like in calculations of “first-passage-times”, but this case cannot be calculated analytically.

Equation \( (10) \) leads to the solution of the Lamé equation only in the stationary limit \( t \to \infty \). But in this limit \( Q^t(r) \) vanishes identically, which means that one only obtains the trivial solution \( u(r) \equiv 0 \).

As a result one obtains, that also a numerical simulation of \( (10) \) — although technically possible — cannot be done, since mainly the time variable \( t \) cannot be interpreted in a simulation.

The essential result of the previous considerations is, that the matrix \( Q^t(r) \) plays the role of a Green’s function of the time dependent problem \( (11) \) and the original algorithm simply provides a prescription how to construct...
it using random walks. On the other hand, one would in all cases end up with a Green’s function in an infinite domain, which in fact can be calculated directly and analytically.

3 Algorithm

From the previous sections it is clear that the use of the original random walker method always ends up in the calculation of a Green’s function for the displacement field. Both, the boundary condition at the crack surface and the breaking criterion, are usually given in terms of the stress field which is related to the spatial derivative of the displacement field using Hooke’s law. Thus it seems natural to calculate the Green’s function for the stress field analytically and use this to construct a random walker algorithm.

Therefore, consider an infinite domain in the absence of cracks which is kept fixed at infinity. At the origin one applies a point force \( F \) which generates a stress field \( \sigma^*(r) \) throughout the whole system and is governed by \( \text{Div} \sigma^* = F \cdot \delta(r) \). Using the method of Kolossov-Mushkelishvili \([21, 22]\) we can calculate the stress field in the whole system and obtain

\[
\begin{align*}
\sigma_{xx}^* &= 2 \Re \left( \frac{c}{z} \right) + \Re \left( \frac{zc}{z^2} + \chi \frac{\overline{z}}{z} \right) \\
\sigma_{yy}^* &= 2 \Re \left( \frac{c}{z} \right) - \Re \left( \frac{zc}{z^2} + \chi \frac{\overline{z}}{z} \right) \\
\sigma_{xy}^* &= -\Im \left( \frac{zc}{z^2} + \chi \frac{\overline{z}}{z} \right)
\end{align*}
\]

where we represent all 2d vectors as complex numbers

\[
\begin{align*}
z &= x + iy \\
c &= \frac{F_x + iF_y}{2\pi(1 + \chi)} \\
\chi &= 3 - 4\nu
\end{align*}
\]

and \( \Re(z) \) ( \( \Im(z) \) ) denote the real (imaginary) part of \( z \). Now one has to take into account that the probability for a random walker, that is launched from the center of a circle of radius \( r \), to reach a certain element \( d\varphi \) at the
perimeter of this circle is \( p \, d\varphi = d\varphi/2\pi r \). This term has to be divided out of (15) and therefore we define
\[
\sigma = 2\pi |z| \sigma^*.
\]
(17)

Using this Green’s function \( \sigma \), which is the basis of the following algorithm, we define a new method to determine the stress field in the medium:

1. Since (1) is linear, we can obtain the solution for a line of forces as a superposition of elementary point forces. Like in DLA, where each point which is kept at a nonzero potential is interpreted as a source of walkers, each point force acts also here as a source of random walkers. Random walkers are launched — like in DLA one at a time — with equal probabilities from each point \( r_i \) where a force \( F_i \) is applied. All forces are usually of unit strength. Each walker undergoes an ordinary random walk until it touches a particle of the cluster located at point \( r_f \). Afterwards one calculates the stress tensor \( \sigma \left( r_f - r_i, F_i \right) \) according to (17) and accumulates this stress in the counter of the appropriate surface element (see below).

2. A crack is represented as an aggregate of particles of unit diameter. Like in DLA the growth of a crack has to be initiated by locating a seed particle at some point, which then acts as a single microcrack, from which the crack grows. Since we expect strong fluctuations during the growth of the crack we use a special scheme to reduce the fluctuations and get a better estimate of the stress field. It is well known from DLA that the introduction of anisotropic noise-reduction schemes [23, 24] immediately leads to strong lattice effects. Although similar schemes have not shown such effects in lattice models of crack growth [25] we try to avoid possible problems, and therefore our scheme must not define any surface nor prefer any direction. The crack is represented by the particles as indicated in figure 1: Each particle represents two stress counters, one for each crack surface. Only the particles at the tip of a branch, i. e. those with only one parent particle but no children, have one single counter. In these counters the stresses \( \sigma \) carried by the incoming walkers are accumulated.
3. Obviously the correct boundary condition (3) is not obeyed by simply calculating stresses according to (17), but an unbalanced force

\[ \vec{F}_{\text{unbal}} = \sigma \cdot \vec{n} \neq 0 \]

remains. Therefore, we apply a virtual balancing force

\[ F_{\text{bal}} = -\sigma \cdot n \] (18)

to the appropriate surface element at \( r_f \), which exactly compensates the spurious shear component \( \tau \) and stress component perpendicular to the crack surface \( \sigma_\perp \). Thus it is in principle sufficient to accumulate at the crack only the stress component parallel to the crack surface \( \sigma_\parallel \). But on the other hand we will show later that the shear component will be essential to determine the direction into which the crack grows and thus we accumulate at \( r_f \) the shear component as well as \( \sigma_\parallel \). As was said above, a random walker is started at each point where a force is applied. Consequently, the walker has to be restarted from \( r_f \) and is reinserted into the system, this time with the new force \( F_{\text{bal}} \). This process of constantly reinserting the walker into the system is repeated until the modulus of \( F_{\text{bal}} \) drops below a certain threshold, which in our simulations is typically chosen as \( 10^{-8} \). Afterwards the walker is discarded and a new walker is started. This repeated process can be interpreted as a method to relax the stress at the surface and can best be understood in terms of a boundary integral method [26]. Physically this process is like a multiple scattering method. A similar situation occurs in DLA in simulations of viscous fingering with nonvanishing surface tension [27, 28, 29] or in simulations of electrochemical deposition with nonvanishing surface impedance [30]. Both cases are mapped to a simulation of sticking probability DLA, in which the walker stops at the cluster with a probability smaller than unity.

4. Next we have to define a growth rule. Here it has to be stressed that the growth of the crack must not be governed by the fact that the crack is touched by a walker, but only the accumulated stress tensor should determine the growth of the crack. Since the stress tensor is symmetric, it defines eigenvalues and eigenvectors, which determine the principal stresses and principal stress directions. The eigenvalues also allow to
distinguish between tensile and compressive stress, because both have a different sign. Now, we provide two material parameters: one for tension $\sigma_t$ and one for compression $\sigma_c$. They represent the material strength under the corresponding load. Especially the strength under tensile load $\sigma_t$ can be related to the intermolecular cohesion forces. If either of them is exceeded by one eigenvalue, the crack grows and a new particle is added to the crack. The direction into which to put the new particle is determined by the eigenvector of the other eigenvalue. This breaking rule is chosen such that for a pure uniaxial tension the crack grows perpendicular to the direction of the force. In this growth rule only the principal stresses, which are purely tensile or compressive, are checked against the material strength. This situation is similar to the growth rule in the central-force model [31], in which also no shear or bending modes are used to break a bond.

5. Once the crack has grown it has to release its stress. Here, we study two different situations. In the first one the stress is only released locally, i.e. only the stress counter of the particle to which a new particle is added is cleared, while all other counters keep their values. This situation can physically be compared to a material in which fatigue plays an important role since even a small load can accumulate and break a sample if it is acting long enough. In the second situation we study a global relaxation. In this scheme we not only clear the counter of the particle at which the crack has grown, we also clear all counters in the entire cluster after the crack has grown by $M$ particles. The parameter $M$ is a fatigue parameter. The first situation can be expressed in terms of this parameter as $M = \infty$.

4 Results

In the following we are going to present the results obtained by simulating the previous method. We simulated several different boundary conditions: uniaxial tension and compression, isotropic tension and pure shear (fig. ). In order to compare with experimental results we also simulated a four point shear geometry and another geometry used in experiments. We furthermore studied the influence of material strength and fatigue.
The length scale in all following simulations is the particle diameter and all applied forces have unit length, which defines the unit of the stress.

4.1 Basic results

In the following we will present the results of three different simulations with the boundary conditions uniaxial tension, isotropic tension and pure shear. The material strengths are typically chosen to be \( \sigma_t = 20 \) and \( \sigma_c = -20 \) (sc. the applied forces are of unit size). Thus, the system breaks equally well under compression and under tension. Since the stress components parallel to the crack surface of one walker are typically around \( 0.5 \), at least \( N = 40 \) walker have to touch a certain site before the cluster can grow. As the seed of all clusters we place two particles with unit diameter at the points \((0,0.5)\) and \((0,-0.5)\). This initial geometry is chosen arbitrarily, but simulations with other geometries show that the results depend neither on the number nor on the specific geometry of these seed particles. The Poisson ratio is \( \nu = 0.2 \) and the fatigue parameter is \( M = 10 \). All clusters have a size of 6,000 particles.

In figure 3 we show a typical result of a simulation of uniaxial tension. Here, forces are located along the lines \( \vec{r} = (\pm 2000, y) \), \( y \in [-2000, 2000] \) and point into the positive (negative) \( x \) direction. One obtains essentially a one-dimensional, straight crack without side branches that grows perpendicular to the direction of the force. This result is physical and can easily be observed in experimental and other numerical studies.

In figure 4 we show a typical result of a simulation of pure shear. In this simulation all forces are again located along the lines \( r = (\pm 2000, y) \). But now the forces are pointing into the positive (negative) \( y \) direction to produce a pure shear field. Although we use the same microcrack as in the previous simulation the shape of the crack is now drastically altered. The resulting cracks show a pronounced cross-like shape. This main shape is a result of the pure shear field, whose stress tensor contains only off-diagonal elements, and thus the eigenvectors always point into a \( 45^\circ \) angle from a surface. We have to remind, that this shape is not a lattice effect but a consequence of the applied forces.

The reason for the symmetry of the cross-like shape is that the material strengths for tension and compression are symmetric, \( \sigma_c = -\sigma_t \). The
case of asymmetric strength will be shown later. The cross-like shape under symmetric breaking conditions has been observed in other numerical studies \cite{18, 14} on much smaller length scales. In experiments this shape is usually not observed, because the material strength for tension is usually smaller than for compression.

One also observes small side branches which form right angles with the main branch. We have to stress, that these right angles cannot be the result of lattice effects because the whole method is formulated off-lattice. Our simulations are the first off-lattice simulations which show this behavior. The formation of right angles is completely determined by the cracking process and has a physical origin: Since there are no restoring forces acting on the crack surface, the boundary condition (3) only allows stresses parallel to the surface. Consequently side branches can only grow perpendicular to the main branches in the vicinity of the main crack.

A typical result for a crack pattern under isotropic tension is shown in figure 5. Here, the radially outward pointing forces are located along a circle of radius 2000. One obtains a ramified structure which can clearly be distinguished from DLA: The typical tip-splitting instability vanished and the side branches show again a tendency to grow perpendicular to their main branches.

4.2 Fatigue

As a first variation we want to study the influence of the fatigue parameter by setting $M = \infty$ while keeping all other parameters fixed. Physically we simulate now a material in which a small load can accumulate and can damage the material. Eventually this can lead to the formation of a large crack.

Since we use $M = \infty$ we need much less walkers to reach the material strength and can simulate much larger cracks. Here, we show cracks containing 20,000 particles.

Under uniaxial tension (fig. 6) we obtain again a narrow straight crack perpendicular to the applied load, but we observe the formation of many small side branches, which grow perpendicular to the main crack and which can themselves form perpendicular side branches. We have to stress again
that the formation of perpendicular side branches is not a result of lattice effects but quite physical. However, the formation of multiple side branches is not physical and thus we obtain, that the fatigue parameter is essential to describe the physical processes.

Under shear load (fig. 7) we observe the formation of the cross-like main branches. Like in the previous case the introduction of fatigue leads also in this case to the formation of many small side branches which again may form side branches themselves. This leads eventually to a dendritic shape of the crack.

Very interesting is the result under isotropic tension (fig. 8). Like in the previous cases we obtain a ramified main crack which is covered with many small side branches. Again we observe that these side branches grow perpendicular to the main branch. This fact is particularly interesting in this geometry since here no growth direction is favored by the boundary condition and thus the right angles can only be explained by the previously given physical arguments. Furthermore one has to notice the stability of the crack tips which do not show a tendency to split. One rather observes the appearance of side branches behind the crack tip.

### 4.3 Variation of the material strength

In this section we want to discuss the effect of the material strength on the results of the simulation. We set the strength to two extreme values: either to zero or to ±100 while keeping \( M = \infty \) fixed.

In the figures 9 – 11 the results for \( \sigma_c = \sigma_t = 0 \) are shown. Setting both values to zero means, that the crack grows as soon as it is touched by a walker.

In the uniaxial tension experiment (fig. 9) the crack remains its elongated shape but the number and shape of the side branches changed drastically. They completely lost their straight appearance and are much more ramified. Also the pronounced 90° angles vanish. Now, the crack looks very much like a DLA cluster with anisotropic sticking probability.

In the shear simulation (fig. 10) the global cross shape of the crack is still present. But here in contrast to the uniaxial case the right angles
between main and side branches and the very straight shape of all branches
are still present. Amazingly, the dendritic shape of the cracks under shear is
extremely stable and is not destroyed even in the limit of zero strength.

In the case of isotropic tension (fig. 11) almost all features emphasized
above are gone. The cluster does no longer reveal side branching and 90°
angles between branches or screening of curved cracks. The resulting crack
looks like a typical DLA cluster of the corresponding size.

As a result one obtains, that in the limit of zero strength our model
crosses over into a anisotropic DLA like behavior. This is readily explained
because in the limit of zero strength the noise generated by the random
walkers dominates over the structure imposed by the outer boundaries. But
the vectorial character of the problem is not completely gone. It introduces
an intrinsic anisotropy as is clearly seen by comparing the uniaxial and the
shear case: In the first case one still obtains one straight crack perpendicular
to the force, whereas in the latter case one obtains the cross like shear crack.
Such a peculiarity cannot be found in the scalar DLA.

In the figures 12–14 the results for $\sigma_c = \sigma_t = 100$ are shown. In the
shear simulation (fig. 12) one observes that the dendritic shape of the crack
is extremely stable. Even in the limit of high noise reduction the dendritic
shape of the four main branches does not change. Neither the number nor
the size of the main branches seems to decrease. Also in the case of uniaxial
tension (fig. 13) the overall shape of the cluster does not change. One still
observes a straight structure with many side branches and even the side
branches that grow parallel to the main branch remain. In the isotropic
geometry (fig. 14) one observes that the main and the side branches tend to
be straighter and the overall crack seems to be less ramified. Here one can
see clearly the tendency of side branches to grow perpendicular to the main
branches.

4.4 Asymmetric strength

Here we want to address the question of asymmetric strengths. In typical
real material like concrete one usually finds the behavior $|\sigma_c| > |\sigma_t|$. Thus, as
special cases we want to comment on the situation, that the material only
breaks under tension: $\sigma_c = -\infty$, $\sigma_t = 20$. We also studied the opposite case
in which the medium breaks only under compression: \( \sigma_t = \infty, \sigma_c = -20 \).

The most obvious change in the result is obtained in the shear experiments (fig. 15). As soon as one strength is chosen much larger than the other one, only one of the diagonal main branches remains. The curvature of the crack is purely a boundary effect. In fact, according to the breaking mode either one or the other diagonal is selected. This is in complete agreement with previous simulations. One also finds that the pronounced dendritic shape that was observed earlier has completely vanished and the single crack does no longer contain any side branch at all.

A similar observation can be made in the uniaxial tension simulation (fig. 16). If one only allows breaking under tension one obtains a single straight crack perpendicular to the force direction. Again, all side branches disappear. In the other case, in which only the breaking under compression is allowed, the crack perpendicular to the load direction disappears and a single crack parallel to the load direction is observed. This effect is readily understood with the Young experiment: A tensile load on an elongated bar will not only increase the length of the bar but it will also influence the width of the bar, according to the Poisson ratio. Thus, the breaking mode observed here is a result of the positive Poisson ratio.

The suppression of compressive breaking seems to have the smallest effect in the isotropic case (fig. 17). Here, there seems to be no difference between a crack generated only for tensile breaking and a crack generated under tensile and compressive cracking: One observes 90° angles between main and side branches, one observes side branching rather than tip splitting and one obtains the screening behavior described earlier.

### 4.5 Experiments

We also reproduce with our new model real experiments performed on concrete. As an example we want to show the results obtained for the “four-point-shear experiment” [32] and a mixed “tensile-shear experiment” [33].

In the four point shear experiment a concrete sample containing two notches in it to initiate the fracture process at well defined points is loaded with four shear forces as indicated in figure 18. One has to mention, that in the experiments of course finite samples are used, which imposes additional
boundaries on the simulation. In our simulation we simplify this and apply four forces to an infinite plane. But we showed with a boundary-integral calculation of the stress field that this simplification does not lead to substantial difficulties. For simplification we describe the notches by two single particles at the respective positions (fig. 18). The geometrical relations for the location and the magnitude of the forces are the same as in the experiment.

The result of our simulation is shown in figure 19, whereas the result of experiments is shown in figure 20. Both results show the same behavior: One observes curved cracks, which start with an almost 45° angle and cross over into a straight behavior: In the initial stages of growth the crack develops according to a pure shear field generated by the two forces between which the microcracks are located. This results in an roughly 45° angle. If the cracks get larger the situation changes and growth occurs according to a compressive field generated by the two forces located near the notch.

In the experiment one obtains in the end one large and one small crack, while we observe in the simulations a symmetric situation. One observes experimentally that initially two cracks start to grow, but one of them stops after one has reached the yield stress. This yield stress is not accessible in our simulations, which is the reason for the symmetric crack pattern.

In the second calculation we simulated another experiment also performed on a concrete sample which is known as load-path 2: To a concrete sample first a tensile load is applied until a crack of a certain size developed, then it is unloaded and a tensile shear load is applied. The result of our simulation (fig. 21) of this experiment is compared to the experimental results (fig. 22). One observes first a long straight tensile crack as a result of the tensile load. During the second load phase the diagonal shear cracks emerge.

4.6 Biased walks

In all simulations described above the walkers performed an isotropic random walk. This is in agreement with the calculations of Roux. In this section we want to consider the case of biased random walks, in which each walker jumps into a preferred direction.

One physical motivation of the bias is the following. The stress \( \sigma \) and the strain field \( \varepsilon \) lead inside an elastic medium to an elastic energy \( U \) which is
stored in the fields

\[ U = \frac{1}{2} \varepsilon_{ij} \sigma_{ij} \quad (19) \]

In our case of an infinite and isotropic elastic medium with a point force \( \vec{F} \) at the origin this can be calculated at point \( \vec{r} \) as

\[ U(\vec{r}) \propto 1 + 2 \frac{(2 - \nu)(1 + \nu)}{(1 - \nu)^2} \cdot \cos^2 \varphi \quad (20) \]

where \( \cos \varphi \propto \vec{F} \cdot \vec{r} \). Now, we consider the regions with high elastic energy as hot regions in which crack growth is most likely. Thus it is reasonable to let the walker preferentially diffuse into these regions by using an angular jump probability of the type

\[ p(\varphi) \propto 1 + \alpha \cdot \cos^2 \varphi \quad (21) \]

where \( \alpha \) is now a free model parameter and \( \varphi \) is the angle between jump and force direction.

Since we must not overestimate the contribution of each walker to the stress counters at the crack surface, we now have to accumulate scaled stresses

\[ \tilde{\sigma}(r_i - r_f, F) = \frac{\sigma(r_i - r_f, F)}{p(\varphi)} \quad (22) \]

where \( \cos \varphi \propto (r_i - r_f) \cdot F \). Here we take into account the anisotropic distribution of walkers.

In this formulation the walkers diffuse preferentially into the direction of the force, which is certainly a good choice for walkers that are launched at the outer boundary. But if one considers the walkers that are relaunched at the crack surface, this might lead to unphysical effects: Since all walkers diffuse until they touch the crack, the relaunched walkers might touch the crack again in an angle \( \varphi \approx \pi/2 \) which finally leads to \( \tilde{\sigma} \to \infty \). Thus, we still overestimate the contribution of individual walkers. This shows, that the bias does not only increase the density of walkers in certain regimes of space, but it also shifts the balance between the walkers launched at the outer boundary and at the crack. Therefore, we also consider a second possibility of a bias, in
which the walkers preferentially diffuse perpendicular to the force direction

\[ p(\varphi) \propto 1 + \alpha \cdot \sin^2 \varphi \]  \hfill (23)

The figures 23 and 24 show typical crack structures generated with a cosine-type and sine-type bias under isotropic tension. Each structure was generated for a bias parameter \( \alpha = 10 \), a Poisson ratio \( \nu = 0.2 \), material strength \( \sigma_{ct} = \pm 20 \) and a fatigue parameter \( M = 10 \). The structure for the cosine-bias contains 2,000 particles whereas the structure for the sine-bias contains 6,000 particles.

The cosine-type bias leads to very regular needle like cracks (fig. 23) while the sine-type bias produces a completely new structure (fig. 24).

Here, we observe very typical properties. The generated crack is very similar to the ones observed in the experiments by Lemaire and Van Damme \cite{34}. With a sine-type bias one obtains a very pronounced \( 90^\circ \) behavior: Initially all side branches grow perpendicular to their main branches. Like the cracks produced by Van Damme et al. the branches bend and side branches appear only on the outer side of the curved crack. Furthermore we observe, that again the crack tips are very stable and do not show a tip-splitting instability.

### 4.7 Quantitative analysis

All crack patterns shown above have a fractal structure which shall be analyzed in terms of the dependence of the radius of gyration \( R_g \) on the crack size \( N \). Therefore we generated five clusters for each geometry uniaxial tension, shear and isotropic tension and each parameter set case 1.: high strength \( \sigma_{ct} = \pm 100 \) and strong fatigue \( M = 10,000 \) and case 2.: low strength \( \sigma_{ct} = \pm 30 \) and weak fatigue \( M = 10 \). The results are shown in the figures 25–27. In all cases we find a fractal behavior

\[ N \propto R_g^{D_f} \]  \hfill (24)

where the fractal dimensions \( D_f \) are summarized in the following table.

The fatigue-parameter \( M \) successfully suppresses side branching so that the resulting structures are essentially one dimensional as can be seen from
the fractal dimensions in the second case: here the fractal dimensions are close to unity. In the case of strong fatigue — case 1. — the fractal dimensions for shear and isotropic tension are considerably lower than the fractal dimension of DLA, which is the result of the observed stability of the crack tips. Only the fractal dimension of the uniaxial-tension simulations is very large and indicates that the continuous side branching might lead to a compact structure.

We also measured the fractal dimensions of the simulations using biased walks. For each case sine- and cosine-type bias we generated five cracks under isotropic tensile load. The results are shown in figure 28. Again, one observes a fractal behavior with dimensions

\[
D_f = \begin{cases} 
1.03 \pm 0.05 & \text{cosine-type bias} \\
1.23 \pm 0.04 & \text{sine-type bias}
\end{cases}
\] (25)

One observes that a cosine-type bias leads to one-dimensional, needle-like structures, whereas the sine-type bias leads to ramified fractals.

5 Discussion

As has been shown above, our new random walker method for crack growth successfully reproduces well known experimental results and results of previous small scale simulations using lattice methods.

The major advantage of our method is the complete absence of any lattice whatsoever. All three ingredients, the walk, the breaking criterion and the growth direction, have been formulated completely in a continuum language. Therefore all lattice effects — like the well known anisotropy in lattice-DLA — are avoided. The observed anisotropies — like the pronounced cross-like structure under shear load — have a physical origin and are no artifacts.
This fact is particularly interesting for the observed right angles between main and side branches. We have to stress again that this off-lattice method reproduces this important physical property of real cracks. In fact, we are not aware of other simulations which reproduce this fact without using a structured lattice.

An important feature of crack growth is the structural disorder of real materials. This disorder is implicitly included in our method by the use of random walkers, which introduces annealed disorder into the simulation.

Another advantage of our method is that by using optimized algorithms all calculations are easily done on workstations. Actually, our calculations are all performed on simple SPARC2 stations. They use about 5MB main memory for a 20,000 particle cluster. The typical run time for one cluster is in the order of 10–15 hours. By altering the strength and the fatigue parameter this time can be much shorter but also much longer. The interested reader can obtain all source codes from the author.

One disadvantage of our method is that it is not easily possible to measure the displacement field \( u \) since the whole algorithm is based entirely on the stress field \( \sigma \). Therefore it is not yet possible to measure stress-strain relations or energy release curves, which are of course important physical quantities. For the same reason it is also not possible to simulate experimental situations in which not the load but rather the displacement is controlled. However, one might argue that in the present stage one is restricted to infinitely stiff materials with vanishing displacements.

The last point to be discussed is the fact that — except for the case of the biased walks — a walker undergoes an ordinary, unbiased random walk before touching the cluster. Thus, the probability that a walker reaches a certain site is implicitly governed by the Laplace equation. However, this does not impose a wrong, Laplacian screening behavior, which has two reasons. The first reason for this is, that the condition for relaunching a walker is completely determined by the Lamé equation and the boundary condition \( (3) \) and, thus, by the elasticity problem. Furthermore one has to notice that both, the Laplace and the Lamé equation share the property, that the important fields, the electric and the stress field, diverge at tips. This is just an explanation of the fact that DLA clusters — like real cracks — preferentially grow at tips. This property is the reason why we chose random walkers to sample the hot
sites of the cracks. In our simulation we can even enhance this tip growth by strongly reducing the effect of fatigue and thereby inhibiting the growth of side branches. Thus, the fact that random walks are used to determine the “hot sites” of a crack is not in conflict with our aim to simulate crack growth.

As an additional possibility we studied the case of biased walks, in which the bias is calculated from the applied forces. For this case we have generated cracks which are very similar to experimental ones observed by Lemaire and Van Damme [34]. Although we do not yet fully understand the physical meaning of the bias parameter $\alpha$ we believe that further research into this direction will lead to new and interesting results.

6 Summary

In the present work we have studied the possibilities to implement a novel way to simulate crack growth by using random walkers. Inspired by Roux we have discussed stochastic algorithms — which are suggested by his original work — to solve the Lamé equation. Although he showed an exact relation between random walkers and elasticity, a direct implementation of the method shown in his work is not practical, because it is not possible to suppress the strong fluctuations and to reach useful averages. However, his work showed that it is indeed possible to treat problems different from Laplacian ones with random walkers. Inspired by the closely related DLA algorithm — which has been very successful in solving problems of Laplacian growth — we have then constructed a different and new method to attack the crack growth in elastic media.

Here, the random walkers are no longer used to construct a Green’s function, but are rather used to detect the hot sites in a crack, which are the next ones to grow. The formulation of the walk and the growth rule is purely made in the continuum to avoid all lattice effects. We are able to reproduce with this new method older results which have been obtained using other, conventional methods on smaller systems. We are also able to simulate experiments that have been performed on concrete.

Although we restricted ourselves to the special case of Lamé’s equation in
the framework of linear elasticity, in principle our method can be extended to other growth phenomena. It may be interesting to investigate this aspect.

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A Appendix

Since the matrix $M$ in the exponent of (1) is symmetric, it can be diagonalized and thus $Q^t(k)$ can be evaluated in closed form. One obtains in two dimensions

$$Q^t(k) = \frac{1}{k^2} \begin{pmatrix} k_2^2 \exp_2 + k_2^2 \exp_1 & k_1 k_2 \{ \exp_2 - \exp_1 \} \\ k_1 k_2 \{ \exp_2 - \exp_1 \} & k_1^2 \exp_1 + k_1^2 \exp_2 \end{pmatrix}$$

(26)

where $\exp_i = \exp(-t\lambda_i k^2)$ and $\lambda_1$ and $\lambda_2$ are the eigenvalues

$$\lambda_1 = \frac{2 \alpha + d}{2d(d+2)}$$

$$\lambda_2 = \frac{3d + 2 \alpha (1-d)}{2d(d+2)}$$

(27)

of $M$. Now, the Fourier transformation into real space

$$Q^t(r) = \int Q^t(k) \exp(i k \cdot r) \frac{d^2 k}{(2\pi)^2}$$

(28)

involves the calculation of integrals of the type

$$\int \frac{k_i k_j}{k^2} \exp(-t \lambda k^2) \exp(i k \cdot r) \frac{d^2 k}{(2\pi)^2}.$$  

(29)

Using polar coordinates the evaluation of the angular integration leads to Bessel functions of the first and second kind, $J_0(x)$ and $J_2(x)$

$$\int_0^{2\pi} \cos^2 \varphi \cdot \exp(ik \cdot r \cos(\varphi - \varphi_r)) d\varphi = \pi [J_0(kr) - \cos(2\varphi_r)J_2(kr)]$$

$$\int_0^{2\pi} \sin^2 \varphi \cdot \exp(ik \cdot r \cos(\varphi - \varphi_r)) d\varphi = \pi [J_0(kr) + \cos(2\varphi_r)J_2(kr)]$$

(30)

$$\int_0^{2\pi} \sin \varphi \cos \varphi \cdot \exp(ik \cdot r \cos(\varphi - \varphi_r)) d\varphi = \pi [-\sin(2\varphi_r)J_2(kr)]$$
The remaining radial integration involves an integral of Bessel functions and Gaussians and finally one obtains

\[ Q_t(r) = \frac{1}{2\pi} [f_s(r, t) + f_a(r, t)] \cdot \frac{1}{2\pi} f_a(r, t) \cdot 2 \frac{r \otimes r}{r^2} \]  

(31)

where

\[ f_s(r, t) = \frac{\exp \left(-r^2/4\lambda_1 t\right)}{4\lambda_1 t} + \frac{\exp \left(-r^2/4\lambda_2 t\right)}{4\lambda_2 t} \]

\[ f_a(r, t) = \left(1 + \frac{4\lambda_1 t}{r^2}\right) \frac{\exp \left(-r^2/4\lambda_1 t\right)}{4\lambda_1 t} - \left(1 + \frac{4\lambda_2 t}{r^2}\right) \frac{\exp \left(-r^2/4\lambda_2 t\right)}{4\lambda_2 t} \]  

(32)

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