# Kinetic Monte Carlo algorithm for thermally induced breakdown of fiber bundles

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Fiber bundle models are one of the most fundamental modeling approaches for the investigation of the fracture of heterogeneous materials being able to capture a broad spectrum of damage mechanisms, loading conditions, and types of load sharing. In the framework of the fiber bundle model we introduce a kinetic Monte Carlo algorithm to investigate the thermally induced creep rupture of materials occurring under a constant external load. We demonstrate that the method overcomes several limitations of previous techniques and provides an efficient numerical framework at any load and temperature values. We show for both equal and localized load sharing that the computational time does not depend on the temperature; it is solely determined by the external load and the system size. In the limit of low load where the lifetime of the system diverges, the computational time saturates to a constant value. The method takes into account the secondary failures induced by subsequent load redistributions after breaking events, with the additional advantage that breaking avalanches always start from a single broken fiber.

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## I. INTRODUCTION

Under a constant external load most materials exhibit a time-dependent response and fail in a finite time. Beyond its high technological importance the understanding of such creep rupture phenomena addresses several fundamental problems for statistical physics as well. The complexity of creep rupture arises from the fact that, depending on the type of materials, it can have a wide variety of microscopic origins, from the existence of frictional interfaces, through the viscoelasticity of the constituents, to thermally activated aging processes [1,2]. Recent experimental investigations have revealed the high importance of thermally activated degradation in creep phenomena [1,3–6], from the fracture of bundles of collagen fibers in biomaterials [7] and complex fluids [8] through gels [9] and solids [1,10], with consequences reaching even to geological scales [4].

Most theoretical approaches to the fracture of heterogeneous materials are based on discrete models composed of lattices of springs [11], beams [12], or fibers. Among the modeling approaches the fiber bundle model (FBM) plays a crucial role, since it captures the main ingredients of the fracture of disordered materials but it is still simple enough to facilitate analytical calculations in the mean-field limit [13–21]. In FBMs the specimen is discretized in terms of parallel fibers which are subject to a longitudinal external load. The fibers have identical elastic properties but stochastically distributed breaking thresholds. Under a quasistatically increasing external load first the weaker fibers break in the bundle. The load of broken fibers must be overtaken by the remaining intact ones, which in turn may also exceed their respective failure threshold and fail. Hence, a single breaking event may induce an entire avalanche, which goes on until it is arrested by some strong fibers or it destroys the entire system [1,2,15,20–24].

During the past decades several extensions of FBMs have been proposed to enable their application to the problem of damage-enhanced creep in various types of materials [1,2,20–27]. In order to obtain a theoretical understanding of the effect of thermally induced damage accumulation on the process of creep rupture, recently Guarino *et al.* introduced a simple fiber bundle approach which has proven very successful [5,28–30]. In the simplest case of the model a bundle of homogeneous fibers is considered (i.e., all the fibers have the same failure strength), which is then subject to a constant sub-critical external load. The evolution of the system is driven by thermal noise: the local stress on fibers has thermally induced fluctuations which may lead to breaking. The main advantage of this simple model is that several interesting macroscopic features of the system can be derived analytically, e.g., it has been demonstrated that the lifetime of the bundle has an Arrhenius-type dependence on the load and temperature even when the fibers have disordered strength [5,29,30]. However, on the microscopic level computer simulation is an indispensable tool to obtain information about the stochastic dynamics of thermally induced fracture. The direct computer implementation of thermally induced stress fluctuations imply serious limitations on the available range of temperature and load values and on the system size.

In the present paper we propose a kinetic Monte Carlo (KMC) algorithm which provides an efficient framework to investigate the thermally induced creep rupture of fiber bundles. We demonstrate that the KMC-FBM overcomes the main limitations of previously used algorithms [21,31–33], allowing for a better understanding of thermally induced rupture processes. After presenting the algorithm we focus on its efficient implementation and performance analysis. The advantages of the KMC-FBM are illustrated by comparing the load, temperature, and system size dependence of the CPU time to those of the traditional method of direct Monte Carlo (MC) sampling.

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## II. FIBER BUNDLE WITH THERMAL NOISE

To study the time evolution of thermally activated fracture processes, recently Guarino *et al.* introduced an extension of the FBM which proved to be successful in spite of its simplicity [5,5,21,28,30]. In the following we summarize the main ingredients of the model construction and present the direct computer implementation of the dynamics of the model.

### A. Model construction

In the model we consider $N_0$ parallel fibers on a square lattice of size $L$. The fibers have a linearly elastic behavior characterized by an identical Young modulus $E$. Structural heterogeneity of the material can be captured by introducing random strength $\sigma_{\text{th}}^i$ for fibers $i = 1, \ldots, N_0$ with a probability density $p_{\text{th}}(\sigma_{\text{th}})$. The bundle is subject to a constant external load $\sigma$ parallel to the fibers' direction such that the load falls below the fracture strength $\sigma_c$ of the sample. To take into account the effect of thermal noise in the fracture process, it is assumed that the local load on fibers $\sigma_i$, $i = 1, \ldots, N_0$ has time dependent fluctuations $\xi(t)$ so that the load of fiber $i$ at time $t$ reads as

$$\sigma_i = \sigma_i^* + \xi_i(t), \tag{1}$$

where $\sigma_i^*$ denotes the deterministic part of the load arising from the external driving and from the load transferred from broken fibers. Thermally induced stress fluctuations $\xi$ are characterized by a Gaussian distribution with zero mean and a temperature dependent standard deviation

$$p(\xi, T) = (1/\sqrt{2\pi T}) \exp(-\xi^2/2T). \tag{2}$$

The system evolves in discrete time steps sampling new values of $\xi$ independently of each other. The fibers break when the local load on them exceeds their failure strength

$$\sigma_i > \sigma_{\text{th}}^i. \tag{3}$$

After such primary fiber breakings induced by thermal fluctuations, the load of broken fibers has to be redistributed over the remaining intact ones. Investigating fracture problems two limiting cases of load redistribution have a high relevance: in the case of equal load sharing (ELS) all surviving fibers overtake equal fractions of the load [5,15,16,18,19,25,28,30,34]. ELS ensures that the stress distribution remains homogeneous in the bundle until the end of time evolution, which makes it possible to obtain the most important macroscopic characteristic quantities of the system by analytical means. In the case of localized load sharing (LLS) the load of a broken fiber is equally distributed over its intact nearest neighbors in the square lattice, resulting in a high stress concentration along the perimeter of failed regions [21,32,33]. Most real cases lie between these two limits, however, comparing ELS and LLS results can reveal the effect of the inhomogeneous stress field in the breaking process. It follows from the model construction that the system has a finite lifetime $t_f$ even at zero external load, i.e., thermal fluctuations always drive the system to failure, however, $t_f$ depends strongly on the load $\sigma$ and temperature $T$: as the temperature goes to 0 at any load or the load goes to the critical load of the bundle at any finite temperature, the lifetime of the system tends to $\infty$ or 0, respectively. Other parameter sets provide lifetimes between these two limits.

In the simplest setup of the model a completely homogeneous system is considered, i.e., all the fibers have the same breaking strength $\sigma_{\text{th}} = 1$ so that the only source of disorder is the thermal noise arising due to the finite temperature $T$. Under creep loading, analytic calculations in the mean-field limit of the homogeneous model have revealed that the macroscopic lifetime of the bundle has an Arrhenius-type dependence on the external load $\sigma$ and temperature $T$ [5,28]. Later it was demonstrated that the presence of disorder in the breaking thresholds $\sigma_{\text{th}}$ increases the effective temperature of the system, but the scaling form of the lifetime remains the same [30,31,35]. For the time evolution of the system under a constant load it was proven that thermally driven creep rupture reproduces the Andrade relaxation at the beginning of the process, i.e., the strain rate $\dot{\varepsilon}$ of the bundle decreases as $\dot{\varepsilon} \sim t^{-p}$ with the exponent $p = 1$ [36]. Additionally, the time-to-failure power-law acceleration of strain close to failure has also been obtained analytically [36].

### B. Computer simulation with direct sampling

Analytical calculations are mainly feasible on the macroscopic scale of the fracture process, however, serious limitations arise when studying the microscopic dynamics of the system. Under a constant subcritical load fibers primarily break due to thermal fluctuations, which corresponds to the nucleation of microcracks in the bundle. After the load of broken fibers is redistributed there may be additional fibers, the load on which exceeds the local breaking threshold. As a consequence, the thermally induced breaking of fibers can give rise to further breaking and, finally, can even trigger an entire avalanche of secondary failure events. This bursting activity represents the intermittent nucleation and propagation of cracks, which is a crucial feature of the fracture of heterogeneous materials. Under LLS, additionally to the temporal correlation of bursting failure events, complex spatial correlations arise in the bundle: fibers breaking in a burst form a connected set in the square lattice, which can be considered as cracks. Such breaking bursts generate acoustic waves in real materials which can be recorded in the form of crackling noise being the primary source of information about the microscopic dynamics of the fracture process.

Simulation techniques of the Guarino model so far have been based on the direct MC sampling of thermally induced stress fluctuations [21,31–33]. An iteration step of the algorithm at time $t$ starts with generating random stress fluctuations $\xi_i(t)$ $[i = 1, \ldots, N(t)]$ according to the distribution, Eq. (2), for all intact fibers of number $N(t)$ independent of each other. Fibers for which the total load $\sigma_i$, Eq. (1), exceeds the local breaking threshold $\sigma_{\text{th}}^i$, Eq. (3), are immediately removed from the system and the deterministic part of their load is redistributed over the remaining intact fibers according to the ELS or LLS schemes. Note that, at the same time, more than one primary breaking can occur, especially at high temperatures and loads. After the load redistribution the breaking criterion, Eq. (3), is checked again until a stable configuration is reached where all fibers can sustain the elevated load. Time is represented by an integer $t$ which is

incremented as $t \to t+1$ after an avalanche stops. Based on the algorithm, computer simulations revealed several interesting aspects of the microscopic bursting activity and spatial structure of damage of thermally activated breakdown: both the size of avalanches and the waiting times between consecutive events proved to be power law distributed, with exponents depending on the load and temperature [21,32,33]. Studying the growth dynamics and spatial structure of cracks as an interesting analogy of thermally induced failure to phase transitions was pointed out, changing the type from first order to continuous-like transition as $T$ and $\sigma$ are varied [32]. However, the algorithm has a very serious limitation, namely, the CPU time it requires is practically proportional to the lifetime of the bundle. It has the consequence that only a relatively narrow region of the $\sigma$-$T$ parameter plane could have been explored numerically [21,31–33]. For example, for the system size $L = 256$ the ranges of temperature $T$ and load $\sigma$ available with a reasonable CPU time under LLS conditions are $0.005 \leqslant T \leqslant 0.1$ and $0.01 \leqslant \sigma/\sigma_c < 1$, respectively [21,32,33].

## III. KINETIC MONTE CARLO ALGORITHM FOR THERMALLY INDUCED CRACKING

In order to overcome the limitations of directly generating the fluctuating stress field with Gaussian distributed noise we start from the transition rate of fibers between the intact and the broken states. Subjecting the bundle to a constant external load $\sigma$ the probability $p_b$ that fiber $i$ with breaking threshold $\sigma_{\text{th}}^i$ will break under the local load $\sigma_i$ reads as

$$p_b^i = 1 - P\left(\sigma_{\text{th}}^i - \sigma_i, T\right), \tag{4}$$

where

$$P(x,T) = \int_{-\infty}^{x} (1/\sqrt{2\pi T}) \exp(-x^2/2T) \tag{5}$$

is the cumulative distribution of thermal fluctuations with the probability density function, Eq. (2). Since the thermally induced breakings of fibers are independent of each other, the primary breaking can be described as a Poissonian process with the ensemble of transition rates

$$r_i \sim p_b^i. \tag{6}$$

Here index $i$ runs over the intact fibers $i = 1, \ldots, N(t)$ that are present in the system at a given time with number $N(t)$.

The KMC algorithm works as follows.

(1) *Initialization*

Time $t$ is set to $t = 0$.

(2) *Local transition rates of intact fibers*

Calculate the transition rates $r_i$ according to Eq. (4) for all intact fibers $i = 1, \ldots, N(t)$.

(3) *Cumulative transition rates*

Update the array of cumulative transition rates,

$$R_i = \sum_{j=1}^{i} r_j, \quad i = 1, \ldots, N(t). \tag{7}$$

Note that the total breaking rate of the bundle is $R_{N(t)}$, which henceforth is denoted $R$ for brevity.

(4) *Primary fiber breaking*

Choose one fiber to break randomly with a probability proportional to its transition rate. For this purpose we generate a random number $\kappa$ uniformly distributed between 0 and 1 and find that fiber $i$ for which it holds that

$$R_{i-1} \leqslant \kappa R \leqslant R_i. \tag{8}$$

(5) *Breaking event*

Remove fiber $i$ from the list of intact fibers and update $N(t) \to N(t) - 1$.

(6) *Time increment*

We determine the time $\Delta t$ elapsed to the breaking of fiber $i$ since the last breaking event using the total breaking rate $R$. For this purpose we generate a new uniformly distributed random number $\kappa'$ between 0 and 1 and obtain $\Delta t$ as

$$\Delta t = -\frac{\ln \kappa'}{R}, \tag{9}$$

which is equivalent to assuming exponentially distributed waiting times between consecutive events of rate $R$. Then time $t$ is updated as $t \to t + \Delta t$.

(7) *Avalanche of triggered breakings*

The load of the broken fiber has to be redistributed over the intact ones according to the selected load-sharing scheme. The updated load of fibers is compared to the local breaking threshold and additional breaking is induced when $\sigma_k > \sigma_{\text{th}}^k$. The removal of these fibers is again followed by load redistribution, which in turn can trigger an entire avalanche of breaking events which leads to an updated value of the number of intact fibers $N(t)$. The avalanche stops when either all remaining intact fibers can sustain their local load or there are no more intact fibers available for breaking (catastrophic avalanche).

(8) *Stopping condition*

If there are still intact fibers in the bundle $N(t) > 0$, then return to step 2; otherwise, finish.

The disorder of breaking thresholds is quenched so that breaking rates $r_i$ of Eqs. (4) and (6) have to be updated in step 2 solely due to the changing load of single fibers. It has the consequence that the efficient implementation of the ELS and LLS schemes requires different strategies. Under ELS conditions all intact fibers keep the same load, which has two important consequences: (i) the breaking rate of all intact fibers has to be updated after each avalanche, and (ii) in a triggered avalanche fibers break in the increasing order of their failure thresholds. Hence, at the beginning of the simulation the fibers are sorted in increasing order of the breaking threshold, which has to be maintained over the course of the simulation. Under LLS conditions the stress field is inhomogeneous, since the load is locally redistributed over the intact nearest neighbors of failed fibers, and large overloads build up along the perimeter of clusters of broken fibers. However, fibers which do not have broken neighbors only keep the external load $\sigma$, which is constant. It follows that in LLS simulations only a subset of fibers has to be updated, i.e., those which received load increments during the last avalanche (and survived it). The different updating schemes imply that LLS simulations can be significantly faster than their ELS counterparts, contrary to other FBMs [17–20].

## IV. TESTS OF EFFICIENCY

In order to test the efficiency of the KMC algorithm of FBMs and verify its advantages over the usual direct sampling approach, computer simulations were carried out on Intel Xeon X5680 3.6-GHz (6-core) processors. For the failure strength of fibers two disorder distributions were considered: a uniform distribution between 0 and 1 and a Weibull distribution with the probability densities

$$p(\sigma_{\rm th}) = 1, \tag{10}$$

$$p(\sigma_{\rm th}) = m\frac{\sigma_{\rm th}^{m-1}}{\lambda^m}\exp\left[-(\sigma_{\rm th}/\lambda)^m\right], \tag{11}$$

respectively. In Eq. (11) the parameter $\lambda$ sets the scale of strength values, while the exponent $m$ controls the amount of disorder of the system. For the Weibull exponent $m$ two values, $m = 2$ and $m = 3$, were considered while $\lambda = 1$ was set. Simulations were performed at different temperatures while varying the external load $\sigma$ in a broad range, $10^{-3} \leqslant \sigma < \sigma_c$. Under ELS conditions for a Weibull-distributed fiber strength $\sigma_c$ can be obtained analytically as $\sigma_c = \lambda(me)^{-1/m}$, which yields $\sigma_c \approx 0.428$ and $\sigma_c \approx 0.496$ for $m = 2$ and $m = 3$, respectively. The uniform distribution results in a lower ELS strength value, $\sigma_c = 0.25$. For LLS calculations the fracture strength $\sigma_c$ was determined by simulations [18]. Figures 1 and 2 present a comparison of the CPU time of the KMC and traditional sampling method as a function of the load for both ELS and LLS schemes, respectively. It must be noted that in the case of direct MC sampling both the temperature $T$ and the load $\sigma$ have a strong effect on the duration of simulations: the temperature $T$ determines the amount of primary breakings, while the load $\sigma$ controls the effect of triggering of avalanches of fiber failures. It follows that increasing the temperature and the load both give rise to a faster evolution and a shorter simulation time. In the case of the KMC the number of primary breaking events is always 1, irrespective of the temperature,

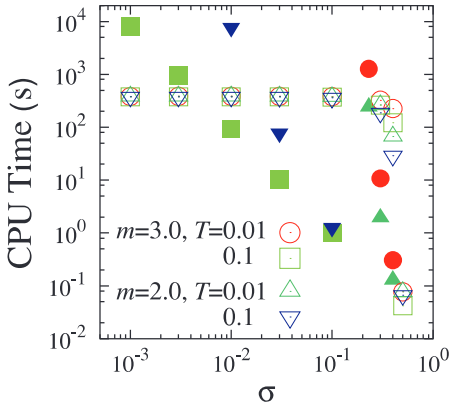


FIG. 1. (Color online) Comparison of the CPU time for simulations with the traditional approach and with the kinetic Monte Carlo (KMC). Equal load-sharing simulations were carried out with a bundle of $N_0 = 10^5$ fibers. For the quenched disorder of fiber strength Weibull distributions with $m = 2$ and 3 are considered. Results of the KMC algorithm are indicated by the open symbols, while their filled counterparts represent the results of the traditional method.

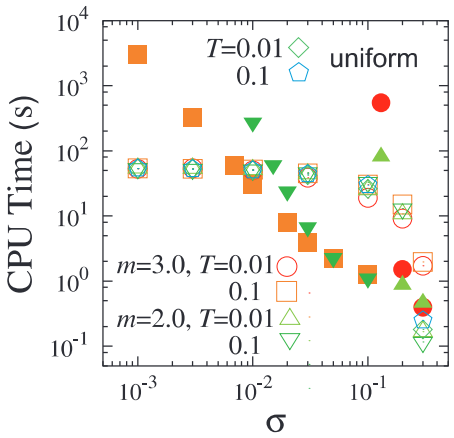


FIG. 2. (Color online) Comparison of the CPU time for simulations with the traditional approach and with the kinetic Monte Carlo (KMC). Local load-sharing simulations were carried out on a square lattice of side length $L = 256$. For the quenched disorder of fiber strength Weibull distributions with $m = 2$ and 3 and a uniform distribution between 0 and 1 are considered. Results of the KMC algorithm are indicated by the open symbols, while their filled counterparts represent the results of the traditional method.

hence, the simulation time is completely insensitive to the value of $T$. At higher loads more avalanches are triggered, which reduce the number of intact fibers of costly updates, and hence, a high load results in an acceleration of calculation. It is important to emphasize that in the limit of low load values the CPU time of the KMC converges to constant values for both ELS and LLS (see Figs. 1 and 2). The reason is that here only small avalanches are triggered and the majority of fibers break one by one in the primary phase.

Figure 3 presents the dependence of the CPU time on the number of fibers $N_0$ of the bundle for ELS and LLS simulations. Due to the global nature of the KMC algorithm the computational time increases with the square of $N_0$ for parameter values which fall in the plateau regime in Figs. 1 and 2. However, if the load is close to the fracture strength $\sigma_c$ of the bundle, a much weaker dependence is evidenced. The reason is that the most time-consuming part of the simulation

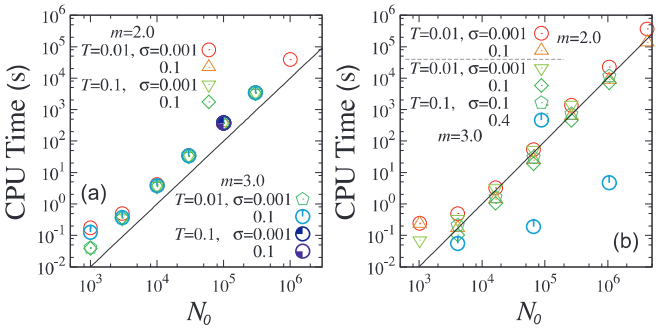


FIG. 3. (Color online) Size dependence of the CPU time of kinetic Monte Carlo simulations for ELS and LLS at several load and temperature values with two Weibull exponents. For both ELS and LLS simulations a power-law dependence on the number of fibers $N_0$ is evidenced for load values which fall in the plateau regime in Figs. 1 and 2. Straight lines represent power laws of exponent 2.

is the determination of primary breakings, i.e., the calculation of the breaking rates and finding the fiber to break due to thermal noise. However, close to failure avalanche triggering dominates, which makes a much lower contribution to the CPU time.

## V. DISCUSSION

We have presented a KMC algorithm to simulate the fracture of fiber bundles driven by thermally induced stress fluctuations under a constant external load. In the model thermal noise gives rise to Gaussian-distributed stress fluctuations which are added to the deterministic part of the local load of fibers. A fiber breaks when its total load exceeds the local failure strength. After failure events the released load is overtaken by the remaining intact fibers with either ELS or LLS, which in turn can trigger an entire avalanche of breakings. In spite of its simplicity, the model grasps the main ingredients of delayed fracture of a broad class of materials and it has proven successful in reproducing experimental observations.

Under ELS conditions and fixed breaking thresholds (no strength disorder) interesting macroscopic quantities of the system can be derived analytically, however, the microscopic dynamics of the time evolution and the microstructure of damage can only be explored by computer simulations. When the load sharing is localized or strength disorder is present in the system analytical calculations are not feasible so that theoretical investigation must rely entirely on computer simulations. The direct MC sampling of thermal fluctuations used in the literature on the model has the difficulty that the computational time is proportional to the lifetime of the system, which implies that simulations have been constrained to a narrow region of the temperature–external load parameter plane.

Our method is based on the assumption that the thermally induced primary failure of fibers is independent of each other for both load-sharing schemes. Hence, their breaking sequence can be treated as a Poissonian process and their breaking time can be obtained from the breaking rates, which depend on the load and temperature. The method ensures that at a given time only a single fiber breaks due to the driving, which then initiates an avalanche of breakings. In the present analysis we have focused on the computational aspects, implementation, and efficiency of the KMC algorithm. Tests were carried out by varying the external load and the temperature over a broad range for two types of disorder distributions of fiber strength. Simulations showed that the computational time of the model does not depend on the temperature. Increasing the external load reduces the CPU requirement because of the triggering of extended bursts which remove the numerically costly intact fibers from the system. In the limit of low loads the computational time converges to a constant determined by the system size without any dependence on the lifetime of the system. The CPU requirement grows with the square of the number of fibers except in the vicinity of the critical load, where a much weaker dependence is evidenced. Compared to the simple algorithm based on direct MC sampling of thermal fluctuations, our KMC algorithm is not limited either by the value of the temperature or by the external load; the entire $\sigma$-$T$ parameter plane is accessible by computer simulations. The only limiting factor is the system size, i.e., the number of fibers, which can be resolved by parallelization of the algorithm.

Another interesting continuous-time approach has been proposed to the time-dependent failure of fiber bundles in Refs. [25–27] based on the load-dependent lifetime of fibers. Under ELS conditions in this model a single uniformly distributed random number is sufficient to determine when a fiber breaks. In our KMC algorithm there are two sources of disorder, namely, the quenched fiber strength, which is set in the initial state, and the annealed disorder induced by thermal noise. A thermally induced primary breaking event requires two independent uniformly distributed random numbers, i.e., one of them determines which fiber breaks, while the other one is needed to obtain the time elapsed since the last breaking event. This dynamics allows us to capture also the avalanches of secondary breakings.

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