Discrete models for two- and three-dimensional fragmentation

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Received 16 February 1995; revised 1 March 1995

Abstract

We study an iterative stochastic process as a model for two- and three-dimensional discrete fragmentation. The model fulfills mass conservation and is defined on two- and three-dimensional lattices of linear size \(2^n\). At each step of the process the "most stressed" piece is broken in the direction of the maximum net force, which is a random variable. Despite their simplicity, reflected in deterministic fracture criteria and simple random forces acting on the materials, our models present complex features that reproduce some of the experimental results that have been obtained. For some regimes a log-normal and a power law behavior are obtained for the fragment size histogram. For this reason we propose them as basic models that can be substantially refined to describe the fragmentation process of more realistic models.

1. Introduction

Fragmentation processes are common phenomena in nature. In Refs. [1–3] Turcotte, Lawn and Wilshaw gave a long enumeration of natural fragment size distributions (fragments from weathering, asteroids, coal heaps, rock fragments from nuclear and chemical explosions, projectile collisions, etc) for which power-laws were measured with exponents ranging from 1.9 to 2.6 concentrating around 2.4. In some way, power law behavior for small fragment masses, seems to be a common characteristic of the instantaneous breaking of brittle objects.

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There are careful experiments in one dimension, see Ref. [4], in which long thin glass rods are broken by vertically dropping them. Depending on the height from which the glass rods are dropped, the fragment size distribution varies from a log-normal shape, for smaller heights, to a power law for increasing heights. Stochastic models for one-dimensional fragmentation can be found in Ref. [5], where the fracture points are chosen randomly. Power-law, exponential and log-normal fragment size distributions can be obtained depending on the a priori fracture points distribution. By the introduction of a minimal fragment size (a piece that cannot be broken further) and a Poisson distribution for the number of fragments into which pieces are broken, a power law behavior is obtained at some stages of the fragmentation process.

In Ref. [6], a hierarchical model for the fragmentation of gas clouds via gravitational condensation is developed, under the assumptions of mass conservation and no presence of pressure. Initially, clouds split (condense) into \( q \geq 2 \) equal mass parts. The process continues in a self-similar way such that the dynamic equations can be solved analytically. Further assumptions on the model allow one to prove that the fragment mass distribution follows a power law behavior in the steady state.

A mean-field type approach to describe the fragmentation process can be formulated through the concentration \( c(x, t) \) of fragments of mass less than \( x \) at time \( t \) by the rate equations, Ref. [7]:

\[
\frac{\partial c(x, t)}{\partial t} = -a(x)c(x, t) + \int_{x}^{\infty} c(y, t)a(y)f(x/y)dy,
\]

where \( a(x) \) is the rate at which fragments of mass \( x \) break into smaller ones (this quantity is supposed not to depend on time) and \( f(x/y) \) is the conditional probability that a fragment of mass \( x \) was produced from a fragment of mass \( y \geq x \). Some exact results are obtained in Ref. [7], if some further assumptions are made about \( f(x/y) \). In general the solutions of the former equations are, however, very difficult to obtain.

Stochastic processes which are discrete in space and time have also been studied as models for fragmentation phenomena using cellular automata. In Ref. [8] two- and three-dimensional cellular automata are proposed to model the power law distribution resulting from shear experiments of a layer of uniformly sized fragments. The fracture probability of a fragment is determined by the relative size of its neighbors. A larger probability is obtained for fragments with a larger number of equal size neighbors. If two blocks have the same fracture probability then a random decision is made. The process continues until no blocks of equal size are neighbors. In all cases a power law fragment size distribution is obtained, with an exponent that depends on the parameters of the model.

In this paper we present simple models which consider the local rupture process of a compact block of material and in that sense go beyond mean-field [7] or abstract hierarchical models [6]. As compared to previously introduced stochastic automata [8] we introduce a quantitative measure for the applied stresses. In some sense our models are a generalisation of Ref. [4] to higher dimensions.
2. The model

We propose discrete stochastic processes in two and three dimensions which fulfill mass conservation. We consider two- and three-dimensional lattices of linear size $2^n$. The fracture process is defined deterministically, based on microscopic models of forces.

As initial situation (see Figs. 1(A) and 2(A)), each corner of the lattice has an uniformly distributed random number between $[0, 1]$, which represents the net "force" value applied on this corner. This is an abstraction of the externally imposed load to a set of just four points per fragment and therefore these corner forces cannot be regarded as real forces applied at the corners. The net forces acting on the lattice can be computed from these numbers for each direction. At each step the most stressed piece is broken into two equal size (volume or area) fragments. An example of Y-axis fracture in two dimensions can be seen Fig. 1(B), while a fracture example in three dimensions due to X-axis compression can be seen Fig. 2(B).

Our objective is to measure the fragment size histogram for our models, and investigate under what circumstances these simple models present power law behavior in the limit.
of small fragments. With these results we will be able to show that even these simple models of fragmentation, based on microscopic random strength considerations and deterministic fracture criteria, can give a range of interesting results that agree with some of the experimentally available data.

In what follows, we will define the mechanisms needed for each step of the stochastic fracture process. These definitions will be made for the three-dimensional case. The 2D case is a particular case that can be obtained by disregarding the net force in the Z-axis and the forces \( f_4, f_5, f_6, f_7 \). At each time step the following features must be considered:

(a) The definition and interpretation for the net forces as functions of the random numbers in the corners.

For this purpose, we will consider two classes of "forces": compression and shear forces. They will be computed from the random numbers by (see Figs. 1(A) and 2(A)):

Compression:

\[
\begin{align*}
  f_x &= |f_0 - f_3| + |f_1 - f_2| + |f_4 - f_7| + |f_5 - f_6|, \\
  f_y &= |f_0 - f_1| + |f_2 - f_5| + |f_4 - f_8| + |f_6 - f_7|, \\
  f_z &= |f_0 - f_4| + |f_1 - f_5| + |f_2 - f_6| + |f_3 - f_7|.
\end{align*}
\]  

Shear:

\[
\begin{align*}
  f_x &= |(f_0 - f_3) - (f_1 - f_2)| + |(f_4 - f_7) - (f_5 - f_6)|, \\
  f_y &= |(f_0 - f_1) - (f_2 - f_3)| + |(f_4 - f_5) - (f_6 - f_7)|, \\
  f_z &= |(f_0 - f_4) - (f_1 - f_5)| + |(f_2 - f_6) - (f_3 - f_7)|.
\end{align*}
\]  

The modulus is considered for both kinds of forces because we are interested in the total forces acting on the material. The forces are supposed to follow the one-dimensional Hooke's law. Thus they can be interpreted as deformations.

(b) A criterion to choose the piece of material to be broken.

Based on the above definitions for the net forces, the more "stressed" piece of the material is broken. The piece with maximum "stress" among the axis is selected. Precisely, a piece \( P_1 \) with net forces given by \( (f^1_x, f^1_y, f^1_z) \) is more stressed than a piece \( P_2 \) with forces \( (f^2_x, f^2_y, f^2_z) \) if:

\[
\max(f^1_x, f^1_y, f^1_z) \geq \max(f^2_x, f^2_y, f^2_z),
\]  

which defines an order relation among the pieces of the material depending on the distribution of the forces.

(c) A criterion to choose the orientation of the fracture in the selected piece.
Once the piece to be broken is selected by applying the criterion defined in (b), the fracture orientation must be defined. In this case the decision is straightforward: The fracture or cutting plane is the plane perpendicular to the direction of the larger net force. For instance, in Fig. 2(B) the cutting plane is YZ since the maximum net force is $f_x$. Two new pieces are generated, with equal volume or area corresponding to the half of the volume or area of the original piece. This insures mass conservation.

(d) A criterion to define how the breaking process continues.

The idea of our model is to continue the fragmentation process in a self-similar way. In order to do that we have to define the new scalar forces acting on the corners of the generated pieces at each stage of the process. The forces in corners that already exist are maintained for the new piece, as can be seen in Figs. 1(B) and 2(B). But 8 (4 for the 2D case) new corner forces $f'_0,f'_1,f'_2,f'_3,f'_4,f'_5,f'_6,f'_7$, must be defined. We will also impose Newton’s law of action = reaction, thus only 4 (2 for the 2D case) new forces must be defined. In Fig. 2(B), for example, we have in the YZ cutting plane:

\[
\begin{align*}
  f'_0 &= f'_3, \\
  f'_1 &= f'_2, \\
  f'_4 &= f'_7, \\
  f'_5 &= f'_6.
\end{align*}
\]

Analogous equations are obtained for the XZ and a XY cutting planes. We will consider two possible ways to choose these numbers. The first one is to choose random numbers that are given by a random convex combination between the corresponding values of the corner’s forces. In the example that we are considering (Fig. 2(B)) this definition reduces to:

\[
\begin{align*}
  f'_0 &= af_0 + (1 - a)f_3, & f'_1 &= bf_1 + (1 - b)f_2, \\
  f'_4 &= cf_4 + (1 - c)f_7, & f'_5 &= df_5 + (1 - d)f_6,
\end{align*}
\]

where $a, b, c, d$ are uniformly distributed random numbers between 0 and 1. This kind of model will be called Model A. The equations for the XZ and XY cutting planes are similar.

In the second case, the new forces are independently distributed random numbers between 0 and 1 without any dependence on the previous forces. This kind of model will be called Model B.

(e) A stopping criterion for the fragmentation process.

At this point we have to consider the discrete nature of the model. We are considering a lattice of size $2^n \times 2^n \times 2^n$. This implies that we cannot continue the breaking process forever. We have to define stopping criteria, that can also be considered as typical for the evolution of the fracture process. It seems natural to impose that it is not possible to break a piece perpendicular to the direction in which it has a length of unity.

We will consider two stopping criteria. In the first one we stop the global fragmentation process if an attempt is made to break the maximally stressed piece perpendicular to
a unit length side. We call this criterion "fast stopping". The second one will be to continue the fragmentation process in such event with the second most stressed piece and so on, until even the least stressed piece cannot be broken. In this case, all pieces of the material have at least one side of length unity when the process stops. We call this criterion "relaxed stopping".

The definitions stated before define a stochastic process discrete in time and space that satisfies the Markov property, since, at each time step the knowledge of the sizes of the pieces and its stresses, determines which piece must be broken. The choice of the piece is made in a deterministic way, but the stress configuration on each step of the model is randomly constructed. The analytical study of the model is very difficult. For this reason we will present a numerical study which involves large scale simulations of our models.

3. Results

In this section we present and discuss the numerical results obtained from the study of our models defined in the last section. We average our results over many independent random initial conditions, characterized by the initial force configuration, i.e., the eight random forces. Since the simulations are rather time consuming we consider between 1000 and 5000 initial conditions for the 2D models, while for the 3D models we could only average our results over 200 to 1000 initial conditions. The system linear size is \( N = 2^n \) where \( N \) for our simulations will be equal to 128, 256, 512, 1024, 2048 in the 2D case and it will be equal to \( N = 32, 64, 128, 256 \) for the three-dimensional case.

For each model we computed the fragment size (area or volume) histogram obtained from the fragmentation process. The maximum number of steps the stochastic process can make is \( N^2 = 2^{2n} \) for the 2D and \( N^3 = 2^{3n} \) for the 3D case, which corresponds to the situation in which there are only cubes of unit length. This gives a very large upper bound for the evolution time that was observed for the models with relaxed stopping criterion. For the fast stopping criterion in 2D, a transient time of order \( O(N) \) was observed.

3.1. 2D Results

Let us first consider the fast stopping criterion under compression (Eq. (3)) and shear (Eq. (4)) for Models A and B. We will show only the results for compression forces, because the ones for shear are similar. From Figs. 3 and 4 it is clear that both processes do not have enough time to generate a large quantity of small area fragments. In the case of Model A the frequency of big area fragments is almost zero and the fragment size concentrates around the linear size of the lattice. Thus fragments with a long x or y axis length are generated very soon, and because of the definition of the stopping criterion, no further breaking is made on medium size area fragments. The
fragment size histogram follows an approximately log-normal law, while the number of fragments generated decreases at an exponential rate. On the other hand, in Model B the frequency of big area fragments is significantly greater than for small areas and the histogram has a longer tail at large fragments than a log-normal distribution. This is because the independent choice of the stresses allows greater fracture probabilities for a piece which was just broken than in Model A. But this also produces a faster stopping.

In Figs. 4 and 5 we can compare the fragmentation processes for both types of forces. The shear forces produce a greater number of big area fragments with a long side than the compression forces.

Next we consider the relaxed stopping criterion again only for Models A and B using Eq. (3) since the results for shear forces are similar. The fragment size histograms are shown in Figs. 6(A) and (B). The computations were very time consuming (4 days on a Sparc 10) due to the quadratic time evolution for the relaxed stopping criterion. From Figs. 6(A) and (B) we find indication that both models generate a power law visible essentially in the limit of small areas. If \( F(s) \) denotes the number of fragments with area \( s \) divided by the total number of fragments generated, we suppose:

\[
F(s) \sim \alpha s^{-\beta}, \quad s \to \infty.
\]
Fig. 5. Fragmentation process example of Models A and B using Eq. (4), shear forces, and fast stopping criterion.

Fig. 6. Area of fragments histogram for 2D Models A and B using Eq. (3) and relaxed stopping criterion for \( N = 128, 256, 512, 1024 \) and averaging over 5,000 samples.

The effective exponents are different for both models and were computed from the estimated slopes for large areas. In the case of compression we obtain for Model A an exponent \( \beta = 2.1 \pm 0.4 \) while for Model B we have obtained \( \beta = 1.5 \pm 0.3 \). This last exponent being smaller that two cannot be asymptotically valid for infinite size. In nature this poses in principle no problem since the original block always gives an upper cutoff. In the case of shear forces we have obtained similar exponents. These exponents are, however, not very trustworthy since we expect corrections to scaling for small areas because the true asymptotic scaling should hold in the limit of large areas.

As we have said before, for the Model A the number of fragments generated is
significantly larger, since by definition of the stress configuration the pieces obtained from the fracture process in Model B have higher probability to be chosen again than in Model A. This fact leads to faster stopping and to smaller exponents.

The fragmentation at the end of the process can be observed for the relaxed stopping in Figs. 7(A) and (B) for compression forces. For Model A the elementary size pieces seem to be uniformly distributed all over the lattice, while for Model B, they concentrate in some regions.

3.2. 3D Results

In the 3D case, we have studied the Models A and B considering the net forces defined by Eqs. (3) (i.e. compression forces) and only with the relaxed stopping condition.

In the relaxed stopping case very long computing times are expected. As in the 2D case the number of fragments generated increases according to \( N^d \) where \( N \) is the linear size of the lattice. The maximum number of fragments is \( N^3 \); for Model A approximately \( 0.3N^3 \) fragments were generated, while for Model B their number is \( 0.2N^3 \). So, we must restrict our simulations to small sizes, more precisely \( N = 32, 64, 128, 256 \) and rather low statistics.

Taking into account the former considerations we show the numerical results in Figs. 8(A) and (B). The log-log plot of the fragment size histograms show for Models A and B a larger curvature than for the 2D case. In the limit of small volumes the curve does not depend on the size of the lattice and seems to remain as the lattice size grows. This reflects a fact that correction to scaling effects are larger in three dimensions than in two dimensions. It seems impossible to assert that it is a power-law or to make any predictions about the exponents.

4. Conclusions

In this work simple models for two- and three-dimensional discrete fragmentation were studied. They have two main features: random distribution of the forces that
generate the fragmentation and deterministic criteria for the fracture process at each step of the fragmentation. Different behaviors were obtained for the fragment size distribution which includes log-normal and power law behavior, depending on the definition of the parameters of our models, which are: the scalar net forces acting on the fragments; the selection of the piece to break; the choice of the fracture orientation; the definition of how the fragmentation process must continue and finally, the definition of a criterion to stop the fragmentation. The power law distribution is a non-trivial result which reproduces empirical results of some highly energetic fracture processes.

The fast stopping feature produces very fast convergence of the fracture process, roughly linear the size of the system, while the relaxed stopping produces transients of order $O(N^d)$ where $d$ is the dimension of the model. The two different choices for the new stresses on the fragments generated from the fracture process introduce no significant differences for all the models considered. The independent random choice increases the probability of breaking small area fragments, and also increases the probability of breaking pieces which have recently been broken.

The 2D results allow us to predict a power law behavior for both models of forces.

Fig. 8. Volume of fragment histogram for 3D Models A and B using Eq. (3) and relaxed stopping criterion and averaging over 1,000 samples.
(compression and shear) and for both Models A and B in the limit of $N \to \infty$. But this is not the case in 3D. We remark that the 2D power law was obtained for simple random forces distribution and deterministic fracture criteria. We claim that with our models, a wide range of definitions will produce the power-law behavior.

The existence of elementary pieces that cannot be broken anymore introduces an arbitrary assumption. This limitation can be avoided by considering models that are discrete in time but not in space. We are actually developing such spatially continuous models taking into account similar assumptions as in the discrete models studied here.

Acknowledgements

This work was partially supported by PG041-92 94, U. de Chile, C-10003 Fundación Andes and EEC. G. H. wishes to acknowledge financial support of the EEC through a "Marie Curie" fellowship.

References