Large Scale Simulations and Visualizations of a N-ary Fragmentation Model*

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Abstract. The numerical results of simulations of a N-ary fragmentation process are presented. Its main assumptions are: Continuous bi-dimensional material; Uniform and independent random distribution of the net forces; Every fragment fracture stops with constant probability p. Furthermore, the material has q random point flaws that interact with the maximal net forces to produce the fracture. By large-scale simulations, it was obtained a power law for the fragment size distribution for a wide range of the parameters of the model. Its visualizations simulate fragmentation in brittle materials, like glass.

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1 Introduction

Fragmentation processes are common phenomena in Nature and Technology. In refs. [11, 14, 15] is given a long enumeration of some natural fragment size distributions of high energetic instantaneous breaking of brittle objects. This experimental evidence predicts a power-law behavior for small fragment masses:

$$F_X(s) = P(X(s) \leq s) \approx \alpha s^{-\beta} \tag{1}$$

where s is the fragment's area or volume. The β exponent varies between 1.44 and 3.54, see refs. [11, 14, 15].

A mean-field type approximation to describe the fragmentation process can be formulated by means of the rate equations, see ref. [12]:

$$\frac{\partial c(x,t)}{\partial t} = -a(x)c(x,t) + \int_x^\infty c(y,t)a(y)f(x/y)dy \tag{2}$$

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where: $c(x, t)$ is the concentration of fragments of mass less than x at time t, $a(x)$ is the rate at which fragments of mass x break into smaller ones, and $f(x/y)$ is the conditional probability that a fragment of mass x was produced from a fragment of mass $y \geq x$. Using scaling and homogeneity assumptions, some exact results were obtained. Several two dimensional fragmentation models have been analytically studied by the application of the rate equations, see refs. [2, 3, 6, 13].

The collision phenomena of solid but brittle discs with similar size were studied in ref. [9]. A molecular network of faults is considered to define the fracture process. Using large-scale simulations and molecular dynamics techniques, they were obtained the velocity, size and position distributions of the generated fragments. By means of a dynamical model of granular solids, it was numerically determined a critical point between damage and fragmentation behavior of the collision of solid disks, see ref. [10]. These techniques techniques have also been applied for the study of different models for fracture and fragmentation in materials that present a previous distribution of cracks and/or flaws, see ref. [1].

The statistical properties of a recursive d-dimensional fragmentation process were studied in refs. [7, 8]. In 2 dimensions, a rectangle breaks up in 4 rectangles with fragmentation probability $0 < p < 1$ and with probability $q = (1 - p)$ it becomes "frozen". By an analytical study it was determined that the volume distribution is a sum of power-laws. For the small volume limit $(v \to 0)$ it was obtained an approximate algebraic volume distribution:

$$F_X(v) = P(X(v) \leq v) \approx \tfrac{\gamma(1-p)}{d} v^{-\gamma} \tag{3}$$

where $\gamma = 2p^{\frac{1}{d}}$. Furthermore, it was proved that this fragmentation model is non self-averaging.

A simple model for two-dimensional binary fragmentation was numerically studied in refs. [4, 5]. Its main hypothesis are: Random distribution of the values and positions of the net forces that produce the binary fracture; The fragmentation is generated by a deterministic criterion; Every fragment fracture stops at each time step with probability p; Existence of a minimal fragment size m_{fs}. By large-scale simulations, it was obtained an approximate power law behavior for the fragment size distribution for a wide range of the parameters of the model.

In this work, is numerically studied a two-dimensional N-ary fragmentation process, which generalize the model in refs. [4, 5]. In this process, the number of fragments generated is a random variable and the breaking criterion is deterministic. In addition, it is considered that the material as a random distribution of point flaws. In what follows, the model is defined and the numerical results for 4-ary fragmentation are discussed.

2 Definition of the N-ary Fragmentation Model

The material is a continuous square of linear size 1. At the initial situation, see figure 1, there are net forces of traction (or compression), denoted by f_x and f_y, acting on the material at random positions and directions. They correspond to uniform and independent distributed random numbers in $[0,1]$. In addition, there are q point flaws located at random positions that remain fixed during the fragmentation process. At each step, all the fragments will be broken in n fragments unless they satisfy the stopping condition. The sum of the area of the new fragments will be the same of the original fragment. This fact is introduced in order to fulfill the mass conservation assumption.

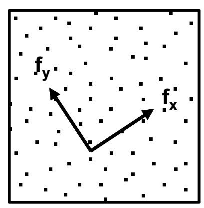

Figure 1. Fragmentation initial situation with q=80 random point flaws

The hypothesis of the model are:

(a) Point Flaws: The initial fragment is the unit square with q random point flaws, see figure 1, that remains fixed during the fragmentation process. In this work, for the simulations, the number q will be chosen constant with value $q = 100$.

(b) Fracture Forces: For each fragment there are fracture forces f_x and f_y that are applied at random positions of the fragments. The random distribution of the forces will obey a Uniform distribution in $[0,1]$. Moreover, the fragmentation process is self-similar, see for instance refs. $[2,8]$.

(c) n-ary Fragmentation: At each step all the fragments will be broken in n (even number) fragments independently, like in a cascade process, unless they satisfy the stopping condition:

- (c1) $\frac{n}{2}$ Fragments are obtained from the application of the forces, i.e. the fracture or cutting plane in this case is the plane perpendicular to the random direction of the larger net force.
- (c2) $\frac{n}{2}$ Fragments are obtained due to the existence of flaws in the material. The $\frac{n}{4}$ cutting planes are the planes with normal perpendicular to the

line defined by the point of application of the larger force and the position of one of the $\frac{n}{4}$ nearest point flaws. In this work was chosen $n = 4$. In this case, two fragments are generated by the interaction of the nearest point flaw with the position of the application of the larger net force.

An example of the initial step fracture is shown in figure 2.

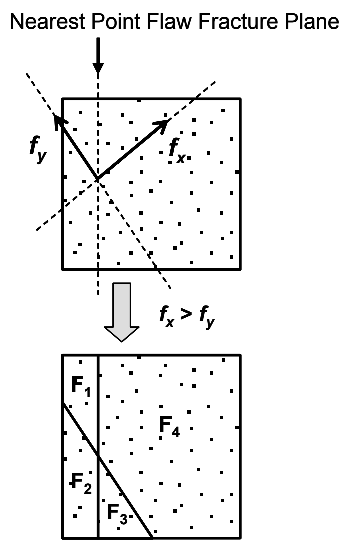

Figure 2. Example of a initial step fragmentation

The parameter n can be a constant or a random variable with Uniform or Poisson distribution, for example.

(d) Mass Conservation: The sum of the size of the new fragments generated will be the same of the original fragment. These n fragments are generated such that the sum of the area of them will be the same of the original fragment.

(e) Random Stopping: There are three situations in which the fragmentation process of a particular fragment stops:

(e1) If the area of the fragment to be broken is smaller than the minimal fragment size or cutoff: m_{fs}, see ref. [**?**].

(e2) There is a probability p that the fragmentation process stops.

(e3) Every fragment has a resistance r to the breaking process represented by the parameter $0 \leq r \leq 1$. A fragment breaks only if the maximum of the net forces acting on it is greater than r. This parameter will be chosen uniform and constant, i.e. remains fixed during the fragmentation process.

The stopping criterion applies for a fragment of area less or equal to a parameter a_c called critical area, introduced in order to represent the fact that greater fragments have more probability to be broken than the smaller ones.

The fragmentation model defined by (a) to (e) is a two-dimensional self-similar stochastic process that verify the Markov property. A theoretical study of this stochastic process is very difficult due to its complexity. For this reason in the next section, the results of the numerical study implemented by large-scale simulations are presented. The main objective of this study was to determine the fragment size distribution.

3 Numerical Results: 4-ary Fragmentation

The methodology for the simulations was the following:

1) The parameters p, r, a_c and m_{fs} are chosen within the following ranges:

$$\begin{aligned} 0.01 \leq p, r \leq 0.20 \\ 0.01 \leq a_c \leq 0.05 \\ 0.00005 \leq m_{fs} \leq 0.0005 \end{aligned} \tag{4}$$

   The value of q was fixed in 100 during the simulations.
2) The results were averaged over 1000 independent random initial conditions, characterized by the initial net forces and the random distribution point flaws.
3) It was chosen 4-ary fragmentation since it is the minimal even number to produce non-binary fragmentation.
4) The fragmentation process evolves according to the rules (a) - (e) defined in section.

The simulations were performed in a distributed way using the *spmd* model. For 1000 initial conditions were used 10 *slaves* each of one computing the fragment size distribution for 100 different initial conditions. A *master* program gathered the results from the slaves. The *speed-up* is practically equals to the numer of *slaves*.

It was determined that the fragment area distribution $f(s)$ follows approximately a power law distribution, for a wide range of the parameters of the model:

$$f(s) \cong \alpha s^{-\beta(p,r,a_c,m_{fs})} \tag{5}$$

The power-law exponent depends on the main parameters of the model: The stopping probability p, the resistance r, the critical area a_c and the minimal fragment size m_{fs}. The exponent of the power-law shows an increase with respect to [5] due to the existence of the point flaws random distribution.

In figure 3 the fragments size distribution $f(s)$ is shown for: $p = r = 0.01, 0.02, 0.03$ and $a_c = 0.01$, $m_{fs} = 0.0001$.

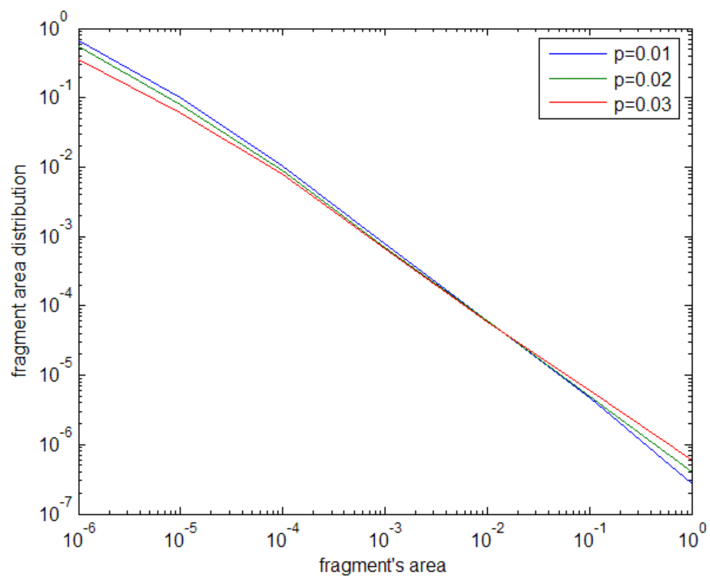

Figure 3. Fragment area distribution for $a_c = 0.01, m_{fs} = 0.0001$ and $p = r = 0.01, 0.02, 0.03$

The deviation from the power law behavior for small area of the fragments is a finite size effect. The deviation from the power law behavior for large area of the fragments is originated by the parameter a_c.

For $a_c = 0.01$ and $m_{fs} = 0.0001$, the exponent β is a power-law of $p = r$ in the interval $[0.01, 0.05]$:

$$\beta = 0.8121 p^{-0.0734} \tag{6}$$

with correlation coeficient $\rho = 0.97$. The specific values of β are shown in table 1:

p	0.01	0.02	0.03	0.04	0.05
β	1.14	1.08	1.05	1.03	1.01

Table 1. Exponent β as a function of $p = r$.

In figure 4 it is shown how the fragmentation process looks for different sets of parameters: a_c, m_{fs} change while p, r remain fixed in the same value. The visualizations the model are very complex with patterns of fracture that simulate real fragmentation processes in brittle materials like, for instance, glass.

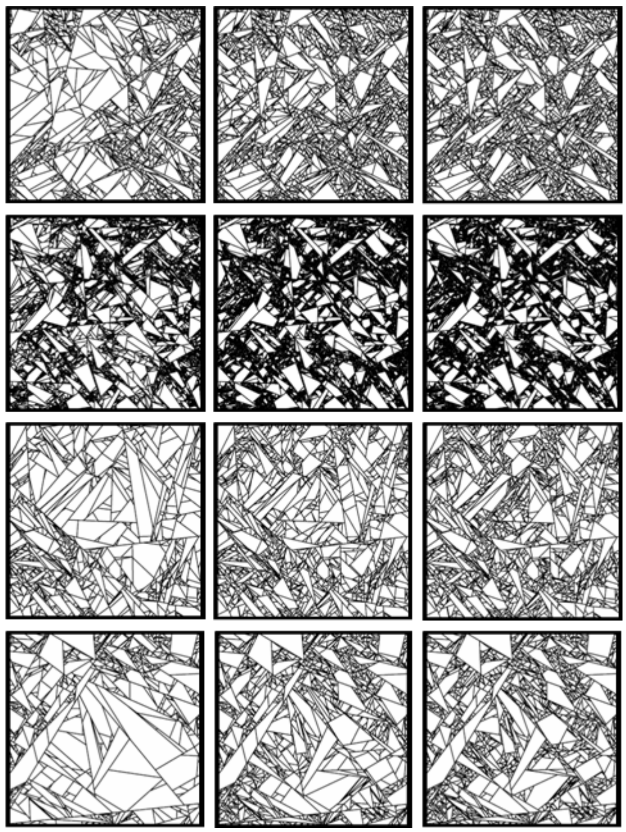

Figure 4. Visualizations of fragmentation process for different set of parameters. First row: $p = r = 0.1$, $a_c = 0.01$, $m_{fs} = 0.0005$. Second row: $p = r = 0.1$, $a_c = 0.01$, $m_{fs} = 0.00005$.Third row: $p = r = 0.15$, $a_c = 0.01$, $m_{fs} = 0.0005$. Fourth row: $p = r = 0.15$, $a_c = 0.03$, $m_{fs} = 0.0005$.

From figure 4 it can be affirmed that:

- If the parameter p is increased, the frequency of larger fragments increases.
- If the parameter a_c is increased, the size of larger fragments increase.
- If the parameter m_{fs} is decreased, the smaller fragment typical size decreases.

4 Conclussions

In this work, it was numerically studied a model for N-ary fragmentation. The main characteristic of this model are: existence of a random stopping and a fracture criterion based on the nearest point flaw and maximal net force. By large-scale simulations, it was determined an approximate power law behavior for the fragments area distribution. We affirm that these results are due to:

1) The mass conservation assumption.
2) The existence of fragments that cannot be broken further: minimal fragment size.
3) Deterministic criterion for the 4-ary fracture process based on the maximum net force and the nearest point flaw.
4) The random stopping condition

The visualizations of this model are very complex with patterns of fracture that simulate real systems.

References

1. Abraham, F., Portrait of a Crack: Fracture Mechanics Using Parallel Molecular Dynamics, IEEE Computational Science and Engineering, Vol. 4, N. 2, pp. 66-78, 1997.
2. Ben-Nai, E., P. L. Krapivsky, Multiscaling in Fragmentation, Physica D, Volume 107, Issues 2-4, pp. 156-160, 1 September 1997.
3. Ben-Nai, E., P. L. Krapivsky, Fragmentation with a Steady Source, Physics Letters A, Volume 275, Issues 1-2, pp. 48-53, 2 October 2000.
4. Hernandez, G., Discrete Model for Fragmentation with Random Stopping, Physica A, Volume 300, Issue: 1-2, pp. 13 - 24, November 2001.
5. Hernandez, G., Two-Dimensional Model for Binary Fragmentation Process with Random System of Forces, Random Stopping and Material Resistance, Physica A, Vol. 323, Iss. 1, pp. 1 - 8, March 2003.
6. Krapivsky, P. L., E. Ben-Nai, Scaling and multiscaling in models of fragmentation, Physical Review E, Vol. 50, N. 2, pp. 3502-3507, November 1994.
7. Krapivsky, P. L., E. Ben-Nai, I. Grosse, Stable Distributions in Stochastic Fragmentation, Journal of Physics A, Volume 37, Number 25, pp. 2863-2880, February 2004.
8. Krapivsky, P. L., I. Grosse and E. Ben-Nai, Scale invariance and lack of self-averaging in fragmentation, Physical Review E, Vol. 61, N. 2, pp. R993-R996, February 2000.
9. Kun, F., H. J. Herrmann, Fragmentation of Colliding Discs, Int. Journal of Modern Physics C, Vol. 7, N^o 6, pp. 837 - 855, 1996.
10. Kun, F., H. J. Herrmann, Transition from damage to fragmentation in collision of solids, Physical Review E, Volume 59, Issue 3, pp. 2623-2632, March 1999.

11. Lawn, B. R., T. R. Wilshaw, Fracture of Brittle Solids, Cambridge University Press, 1975.
12. Redner, S., in Statistical Models for the Fracture of Disordered Media, H. Herrmann and S. Roux (eds.), Random Materials and Processes Series, Elsevier Science North Holland Publishers, 1990.
13. Rodgers, G. J., M.K. Hassan, Stable distributions in fragmentation processes, Physica A, Vol. 233, Iss. 1-2, pp. 19-30, 1996.
14. Turcotte, D.L., Fractals and Fragmentation, Journal of Geophysical Research, Vol. 91, pp. 1921-1926, 1986.
15. Turcotte, D. L., Fractals and Chaos in Geology and Geophysics, Second Edition, Cambridge University Press, 1997.