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# Multiscale measures of equilibrium on finite dynamic systems

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## Abstract

This article presents a new method for the study of the evolution of dynamic systems based on the notion of quantity of information. The system is divided into elementary cells and the quantity of information is studied with respect to the cell size. We have introduced an analogy between quantity of information and entropy, and defined the intrinsic entropy as the entropy of the whole system independent of the size of the cells. It is shown that the intrinsic entropy follows a Gaussian probability density function (PDF) and thereafter, the time needed by the system to reach equilibrium is a random variable. For a finite system, statistical analyses show that this entropy converges to a state of equilibrium and an algorithmic method is proposed to quantify the time needed to reach equilibrium for a given confidence interval level. A Monte-Carlo simulation of diffusion of A\* atoms in A is then provided to illustrate the proposed simulation. It follows that the time to reach equilibrium for a constant error probability,  $t_e$ , depends on the number,  $n$ , of elementary cells as:  $t_e \propto n^{2.22 \pm 0.06}$ . For an infinite system size ( $n$  infinite), the intrinsic entropy obtained by statistical modelling is a pertinent characteristic number of the system at the equilibrium.

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## 1. Introduction

In the field of materials science, phenomena such as diffusion, fatigue crack growth, and wear for example involve dynamical models. Some states of the system are modified in time and generally tend to settle at a final value. For an isolated system, the second principle of thermodynamics involves that the most probable state leads to the maximal entropy on average. If in the ideal case of an infinite system this equilibrium state can never be obtained, equilibrium is only reached after a finite time for a finite system size. How to define equilibrium for discretised systems? In the usual case, entropy must be maximal. However, when stochastic simulations such as the Monte-Carlo method are used, entropy can not only be defined by Boltzmann definition but is related to its statistical estimation. This consists in dividing the system into a phase space. The size of the elementary cell is difficult to choose, particularly when the system is numerically simulated. We shall then (1) study the system with different decreasing divisions, (2) give a measure on each cell, (3) analyse this measure at different scales, and (4) find an unscaled measure of the state of the system. The main problem is to define a measure on this system. There is a remarkable likeness between information and entropy in physics, which allows to solve the problem of Maxwell's demon. Brillouin [1] proved that information could be considered as the negative of the system's entropy called "Negentropy". Entropy measures the lack of information and gives the total amount of information missing on the micro-states of a system. However, the tools used to quantify Negentropy remain theoretical mathematical objects rather than applied mathematical ones [2]. In the

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Information Theory, we must start by giving a precise definition of the word “Information”. The problem involves a certain number of possible answers. Information is a function of the ratio of the number of possible answers before and after a logarithmic law is retained to ensure the additivity of information. This theory first described by Shannon [3] is used in classical problems relating to information (coding, computer science, and telecommunication). There are powerful tools to quantify information in a discretised system associated with the multifractal theory [4,5], to analyse the concept of measure at different scales and to model it by some power laws. If the measure is well chosen, then it can be related to the entropy of the system via the Shannon entropy [3]. However, this theory describes the system in term of probability and then the system is seen as an infinite set. When physician observed a system, it is by nature a finite one (i.e. a sample) and then all probability measures are become statistical estimators meaning that all probabilities are estimated with uncertainly. As all multifractal measure that leads to calculate some space dimensions are based on probability calculus then, due to intrinsic fluctuation, dimensions becomes uncertain. El Naschie proved that Cantorian space-time  $\varepsilon^\infty$  possess an irreducible uncertainly [6] that amounts to a realistic resolution of the measurement problems. Consequently, all topological dimensions and Hausdorff dimensions must be described in terms of expectation [7] proving that nature is fundamentally and irreducibly statistical [8]. In a first part, we shall give a brief introduction of multifractal formalism and propose a relation between entropy and information. In a second part, we shall apply these concepts to Monte-Carlo simulation to analyse the kinetic and scaling laws of a dynamic system.

## 2. Mathematical definitions

A few mathematical definitions will now be introduced. The fractal dimension is insufficient to define the geometry and to give a quantitative description of a measure taken on a set. From the definition of the Hausdorff dimension, we can define the  $f(\alpha)$  exponent which characterises the fractal dimension of the  $E_\alpha$  subset. The  $f(\alpha)$  spectrum can be obtained from the  $D_q$  curves thanks to the Legendre transform:

$$\tau(q) = (q - 1)D_q \quad (1)$$

$$\alpha = - \frac{\partial \tau(q)}{\partial q} \quad (2)$$

$$f(\alpha) = \tau(q) - q\alpha \quad (3)$$

This Legendre transform being mainly used in thermodynamics, with the following analogy:

$$f(\alpha) \Longleftrightarrow \text{entropy} \quad \tau(q) \Longleftrightarrow \text{free energy}$$

$$\alpha \Longleftrightarrow \text{energy} \quad q \Longleftrightarrow \text{inverse temperature}$$

Indeed, the characteristic shape of the plots of  $f(\alpha)$  versus  $\alpha$  is reminiscent of the dependence on  $E$  of the entropy for a thermodynamic system [5]. In particular the Dimension of Information  $D_1$ , can be defined for  $q = 1$  in Eq. (3) and leads to:

$$D_1 = \alpha(1) = f(\alpha(1)) = \lim_{\varepsilon \rightarrow 0} \frac{S(\varepsilon)}{\log \varepsilon} \quad (4)$$

where

$$S(\varepsilon) = \sum_{i=1}^{N(\varepsilon)} \mu_i(\varepsilon) \log \mu_i(\varepsilon) \quad (5)$$

can be seen as entropy measured at the size  $\varepsilon$ . From Eqs. (4) and (5), one gets  $S(\varepsilon) = S_0 \varepsilon^{-D_1}$ . As the system is discretised, the smallest cell will be equal to unity, as defined in the Non-Standard Analysis, and does not tend to the null value. A minimal cell size lower than a critical value  $\varepsilon_c$  is really physically meaningless since  $\varepsilon < \varepsilon_c$  would lead to a more precise specification of the system than allowed by quantum theory defined by the Heisenberg' uncertainly principle. Therefore,  $S_0 = \lim_{\varepsilon \rightarrow 1} S(\varepsilon)$  is the intrinsic entropy value of the system that does not depend on the size of the cells. In conventional cases,  $\mu_i$  will be the fraction of the total set mass contained in the  $i$ th box. In the following section, we propose to study the relevance of the intrinsic entropy on a discretised system obtained by the Monte-Carlo simulation. At the outset, the system is far from equilibrium. It tends to equilibrium to maximise the statistical entropy when increases time.

### 3. Monte-Carlo simulation

The phenomenon, which is presented above is the diffusion of  $A^*$  atoms in  $A$ . This system is computed for two-dimensional systems represented by a  $n^2$  Boolean matrix ( $0 = A$ ;  $1 = A^*$  Atom) with  $n^2/2$   $A$  atoms on the right part of the matrix (Fig. 1).

The  $A$  jump elementary process occurs as follows: on average and for each iteration, each  $A^*$  atom can jump randomly in one of the four directions in order to occupy an empty neighbouring site. One crore Monte-Carlo simulations (MCS) are carried out for seven different sizes of the system ( $8^2$ ,  $16^2$ ,  $32^2$ ,  $64^2$ ,  $128^2$ ,  $256^2$ , and  $512^2$  cells). Then the Box Counting Algorithm [5] is applied onto each system at different times.  $X(t, n)$  is the system defined at time  $t$  with a system of size  $n^2$  that contains  $n^2/2$   $A^*$  particles. For each system  $X(t, n)$ , the quantity of information  $S(\varepsilon)$  is computed for different sizes  $\varepsilon$  that follow a dyadic decreasing size. By plotting  $S(\varepsilon)$  versus  $\log(\varepsilon)$ , the regression line is a straight line that allows us to calculate the slope,  $D_1$ , and the intrinsic entropy  $S_0$  by the intercept thanks to the least square method. Fig. 2 shows the  $S_0$  evolution versus simulation time for the seven different system sizes (each point is the mean of several simulations). As can easily be shown, the entropy  $S_0$  increases with time: diffusion increases the information of the physical system. Moreover, when the process reaches equilibrium, an asymptote occurs leaving unchanged the values of entropy we shall call  $S_0^{\text{Eq}}$ , the intrinsic entropy of equilibrium. To analyse more precisely this asymptote, 10,000 systems  $X(5000, 32)$  were simulated at the thermodynamical equilibrium ( $A$  and  $A^*$  atoms are uniformly distributed and then the entropy is maximal) and  $S_0^{\text{Eq}}$  are computed. Then the probability density function of  $S_0^{\text{Eq}}$  is plotted (Fig. 3) and follows a Gaussian law that is similar to the law of entropy fluctuation of a system at equilibrium [9]. Entropy variation entails information variation quantified by the intrinsic entropy. As shown by El Naschie [8], most

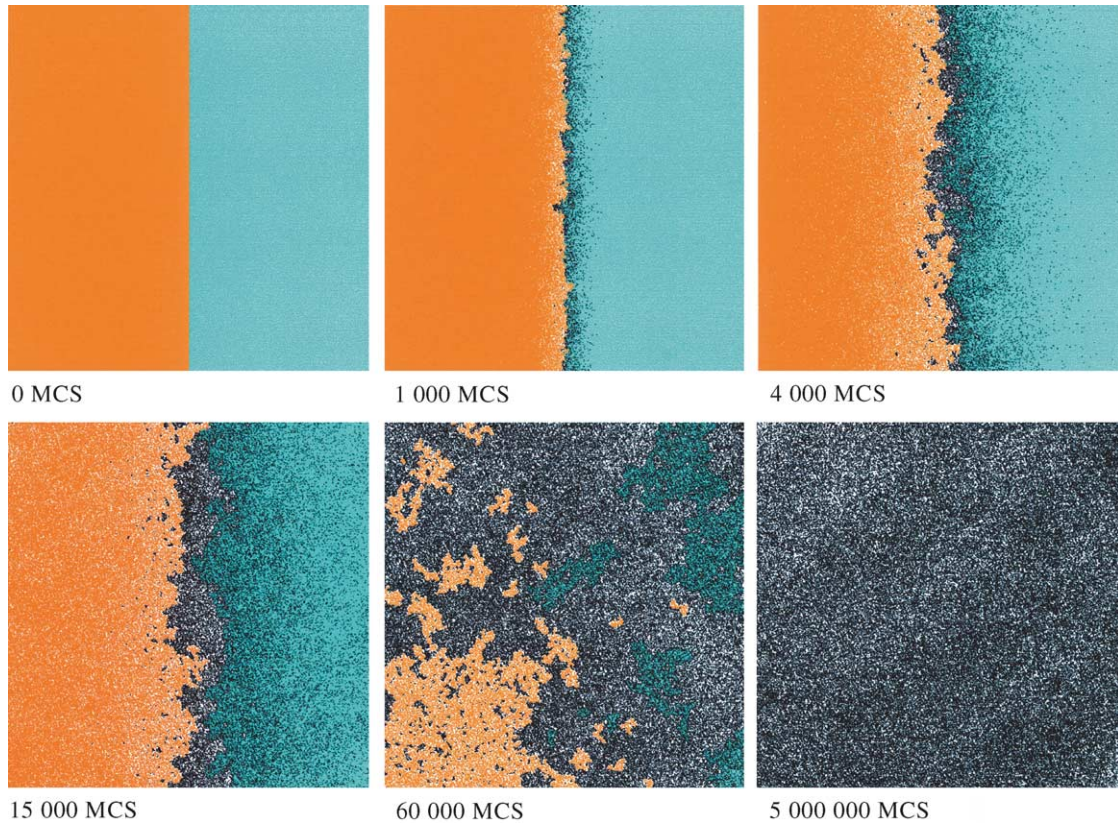


Fig. 1. Monte-Carlo simulation of the diffusion of  $A^*$  atoms (left part of the matrix) in  $A$  atoms (right part). Iterations represent the number of random jumps per atom called Monte-Carlo steps (0, 1000, 4000, 15,000, 60,000 and 5,000,000 MCS). The orange colour represents the higher sizes of site percolation clusters of  $A^*$  and respectively the blue colour the higher sizes of site percolation clusters of  $A$ . Black cells represents the  $A^*$  atoms and white ones the  $A$  atoms that both are not included in the percolation clusters. Notes that the percolation threshold at equilibrium is  $p_c = 0.5927460$  and as the number of  $A^*$  and  $A$  are identical ( $p = 0.5 < p_c$ ), no percolation is present.

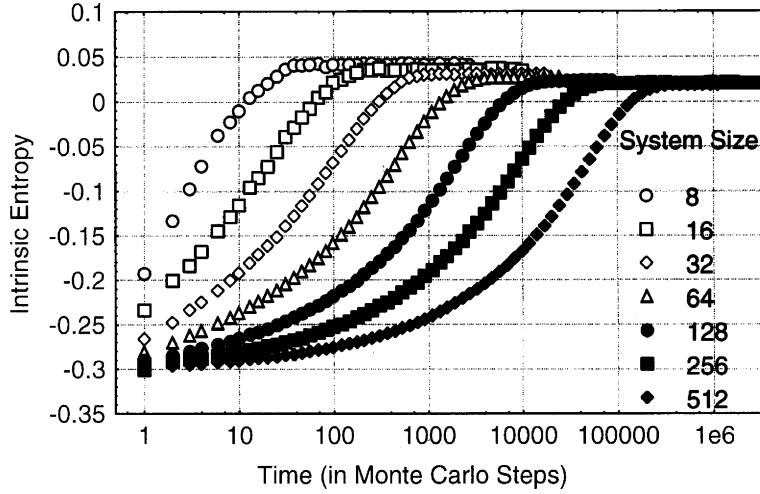


Fig. 2. Plot of the intrinsic entropy  $S_0$  evolution versus simulation time (in Monte-Carlo step) of the Monte-Carlo simulation of the diffusion of  $A^*$  atoms in  $A$  atoms for seven different system sizes ( $8^2$ ,  $16^2$ ,  $32^2$ ,  $64^2$ ,  $128^2$ ,  $256^2$  and  $512^2$  cells). All points are the mean of several simulations.

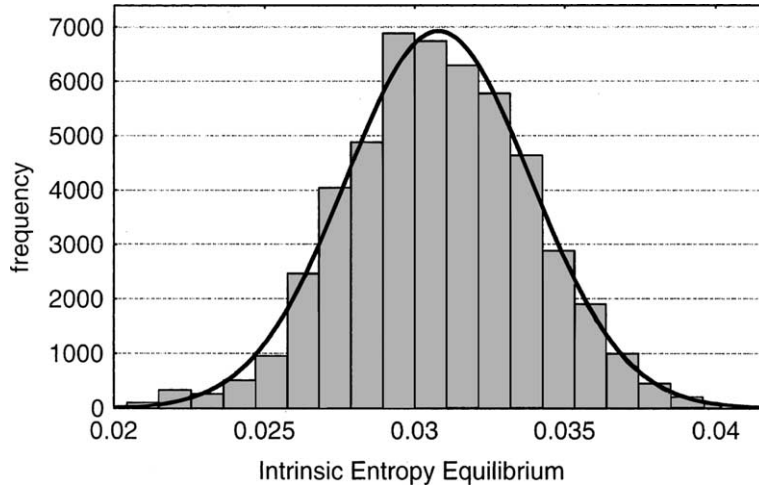


Fig. 3. Histogram of intrinsic entropy  $S_0^{\text{Eq}}$  at equilibrium for a system size of  $32^2$  cells. The histogram is obtained by 50,000 simulations of the equilibrium and the Gaussian PDF is plotted with mean  $\mu_{S_0^{\text{Eq}}} = 0.0308$  and standard deviation of  $\sigma_{S_0^{\text{Eq}}} = 0.00308$ .

statistics of fundamental processes related to basic problems are Gaussian and fundamental statistics are a subcategory of Gaussian distributions that involves some fluctuations in the information dimension.

### 3.1. Equilibrium time

Then the question is “Is equilibrium reached and how long does it take?” We shall prove that this question has no physical sense in absolute and one has to admit a probability error to the answer. We postulate that the equilibrium time will be the time  $t_e$  in which  $S_0(t_e) = S_0^{\text{Eq}}$ . However, this equality can only be true in a statistical sense with a given confidence level. Let us analyse results obtained for the  $32^2$  cells system: as  $S_0^{\text{Eq}}$  follows a Gaussian PDF with mean  $\mu_{S_0^{\text{Eq}}} = 0.0308$  and standard deviation of  $\sigma_{S_0^{\text{Eq}}} = 0.00308$ , at 95% for the confidence interval, we find  $S_0(t_e) = 0.0246$  and from Fig. 4 the value of  $t_e = 600$  MCS is obtained. “Does this mean that after 600 MCS equilibrium is reached?” In

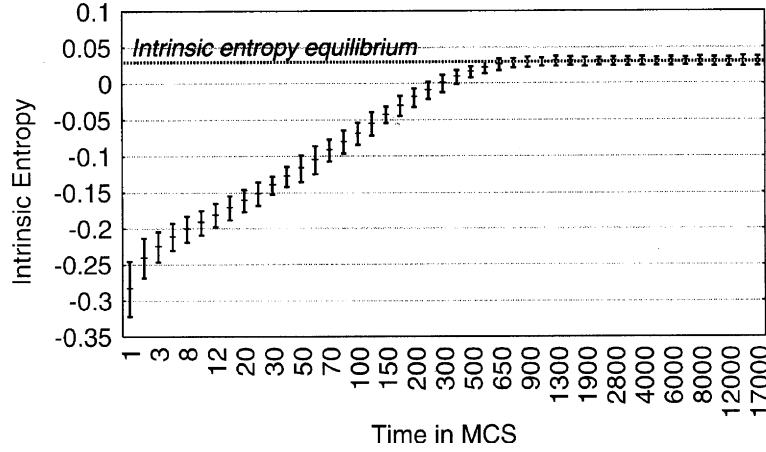


Fig. 4.  $S_0$  intrinsic entropy variation versus simulation time (in Monte-Carlo step) for the Monte-Carlo simulation of the diffusion of  $A^*$  atoms in  $A$  atoms for a system size of  $32^2$  cells. All points are the mean of several simulations. Each bar represents the mean values and the 95% confidence interval obtained by 50,000 simulations.

fact, in a philosophical sense, it is impossible to give either positive or negative answer. This theory only asserts that we cannot answer positively. In fact, we will prove that the quantity of information is not large enough to reject the state of equilibrium if the equilibrium is not reached. Suppose that instead of observing one system, we observe  $p$  systems that follow the same dynamic structure. Then the entropy can be averaged at each Monte-Carlo step, and as  $S_0(t_e)$  follows a Gaussian PDF, the standard deviation of the mean will also follow a Gaussian PDF with standard deviation equal to  $\sigma_{S_0(t_e)}/\sqrt{p}$ . Two important remarks have to be made:

Let us note  $\Delta S_{0,p,n}^{\text{Eq}} = S_0^{\text{Eq}}(t_{e,n}) - S_0^{\text{Eq}}(\hat{t}_{e,n,p})$  where  $\hat{t}_{e,n,p}$  is an estimation given by statistical analyses to determine the equilibrium time of a system of size  $n^2$  with  $p$  simulations and  $t_{e,n}$  is the real unknown time to reach equilibrium. Therefore,  $\Delta S_{0,p,n}^{\text{Eq}}$  represents the sampling error made on measuring the intrinsic entropy.

- For a given  $n$ ,  $\Delta S_{0,p,n}^{\text{Eq}}$  decreases (in mean) as  $p$  increases. Consequently,  $t_e$  will increase with the number of observation  $p$ : the more frequently a dynamic system is observed, the longer the time of equilibrium is. It becomes impossible to assert that equilibrium is reached only in an asymptotically sense that is not implicitly numerically obtained.
- For  $p$  fixed, one gets  $\lim_{n \rightarrow \infty} \Delta S_{0,p,n}^{\text{Eq}} > 0$  and as a consequence  $t_e$  will always increase with  $n$  for a fixed number of observations  $p$ . It is impossible to affirm for any system size that equilibrium is reached for a given number of observations of the system.

The main problem is now to answer the following question: “at the limit, does the system reach its equilibrium?” In other words, “Is the intrinsic entropy a pertinent measure to detect asymptotically the equilibrium state?” To answer, it is first necessary to estimate the standard deviation of  $S_0(\hat{t}_{e,n,p})$  noted  $\sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,p})}$  that depends on the size of the system and the number of observations for the mean computation. For only one observation, the value of  $\sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,1})}$  versus the system size,  $n$ , was plotted in Fig. 5 which gives by regression analysis  $\sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,1})} \propto n^{-1/5}$ . Then from  $p$  observations of the system, one gets from the Central Limit Theorem  $\sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,p})} \propto n^{-1/5} p^{1/2}$ . As consequence,  $\lim_{n \rightarrow \infty} \lim_{p \rightarrow \infty} \sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,p})} = 0$  and with a probability equal to 1, it is possible to affirm that the equilibrium state is reached at the limit, and then our intrinsic entropy is an asymptotic measure of the equilibrium state and the time to reach equilibrium in a finite discretised system.

However, for a discretised system, the size and the number of observations are finite and the affirmation that equilibrium is reached cannot be stated without any error probability. Let us now define two probability errors:

$\delta$ : error of rejecting erroneously the equilibrium state although equilibrium is reached.

$\beta$ : error to accept the equilibrium state although it is not reached.

Let  $\Delta S_{0,p,n}^{\text{R}} = (S_0^{\text{UnEq}}(t) - \overline{S_0^{\text{Eq}}(\hat{t}_{e,n,p})}) / \sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,p})}$  (with  $\overline{X}$  is the mean of  $X$ ) the reduced error on the equilibrium state: the higher  $\Delta S_{0,p,n}^{\text{R}}$  is, the lower error  $\beta$  is (for a fixed value of error  $\delta$ ). Under Gaussian assumption of the  $S_0^{\text{Eq}}(\hat{t}_{e,n,p})$  PDF, the  $\beta$  values could be modelled by:

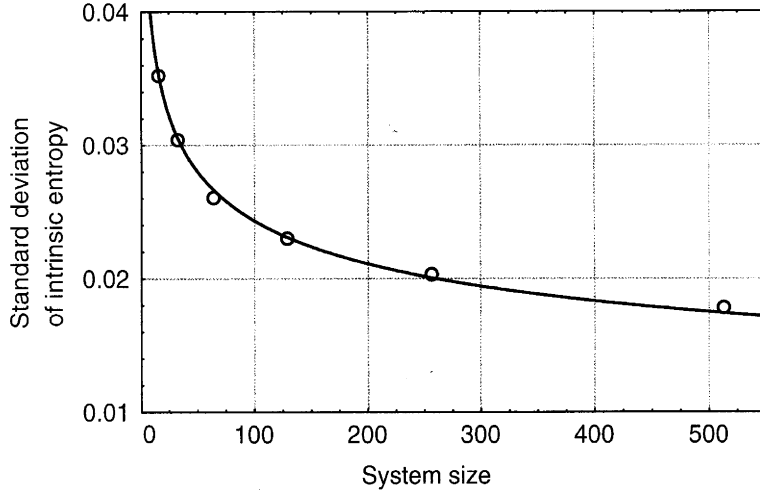


Fig. 5. Evolution of intrinsic entropy at the equilibrium  $S_0^{\text{Eq}}(\hat{t}_{e,n,p})$  versus the size of the system. The fitting line gets the following regression equation  $\sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,p})} = 0.06n^{-0.2}$  obtained by the least square method.

$$P(\Delta S_{0,p,n}^R) = 1 - \beta(\Delta S_{0,p,n}^R) = F(u_{1-\delta} - \Delta S_{0,p,n}^R \sqrt{P}) \quad (6)$$

with  $F(u) = \int_{-\infty}^u \frac{1}{\sqrt{2\pi}} \exp(-\frac{u^2}{2}) du$  and  $F(u_z) = \delta$ . For the system size  $n = 32$  we have plotted the different curves  $P(\Delta S_{0,32,5}^R), P(\Delta S_{0,32,10}^R), \dots, P(\Delta S_{0,32,35}^R)$  for a fixed risk  $\delta = 0.0001$ . Let us now illustrate these curves by an example: we choose to make an error of 1/10,000 ( $\delta = 0.0001$ ) that our simulation rejects the equilibrium although equilibrium is reached. We accept with a 10% error ( $P(\Delta S_{0,p,n}) = 0.9$ ) to accept the equilibrium state although it is not reached and will only be reached after 70 MCS ( $t = \hat{t}_{e,32,p} - 70$ ). From the histogram in Fig. 3, one gets  $\overline{S_0^{\text{Eq}}(\hat{t}_{e,n,p})} = 0.0295$ ,  $\sigma_{S_0^{\text{Eq}}(\hat{t}_{e,n,p})} = 0.00308$  and for 70 MCS (Fig. 2) one gets  $S_0^{\text{UnEq}}(t) = 0.0285$ . Then according to Fig. 6, we report the point (0.9, 0.0285) and we must process 48 simulations, or physically observe the system 48 times.

### 3.2. Equilibrium time determination

We shall now introduce an original algorithm to detect the time to reach equilibrium. As can be observed in Fig. 4,  $S_0(\hat{t}_{e,n,p})$  becomes constant at equilibrium from a statistical point of view.  $S_0(\hat{t}_{e,n,p})$  PDF approximately follows a Gaussian PDF with homogeneous variances. Let us note  $S_0(t_{i,n,p})$  the  $i$ th measure of entropy for the  $p$ th system of size  $n$  (with  $t_{i,n,p} < t_{i+1,n,p}$ ,  $i \in \{1, \dots, I\}$ ,  $p \in \{1, \dots, P\}$ ). Let us note  $i_e$  the time indicia such that  $t_{i_e,n,p}$  will be the time to reach equilibrium and then  $S_0(t_{i_e,n,p}) = S_0(t_{i_e+1,n,p}) = S_0(t_{i_e+2,n,p}) = \dots = S_0(t_{I,n,p})$  in a statistical sense.

We shall then introduce the algorithm to test this equality. The equilibrium hypothesis will lead to:

$$\mu[S_0(t_{i_e,n,p})] = \mu[S_0(t_{i_e+1,n,p})] = \dots = \mu[S_0(t_{I,n,p})] \quad (7)$$

where  $\mu[S_0(t_{k,n,p})]$  is the mean of the intrinsic entropy calculated for a system of size  $n$  with  $P$  simulations obtained at time  $t_k$  (we will note also  $\sigma^2[S_0(t_{k,n,p})]$ , the variance at the intrinsic entropy at same state).

By analysis of variance (ANOVA) we test the hypothesis  $\mu[S_0(t_{i,n,p})] = \mu[S_0(t_{i+1,n,p})] = \dots = \mu[S_0(t_{I,n,p})]$  at the significant level  $\delta$ .

At equilibrium  $\sigma^2[S_0(t_{i_e,n,p})] = \sigma^2[S_0(t_{i_e+1,n,p})] = \dots = \sigma^2[S_0(t_{I,n,p})]$  and we shall note  $\sigma^2[S_0(t_{i_e,\dots,I,n,p})]$  the estimation of these variance entropy given by ANOVA. In the same way, we shall note  $s^2[S_0(t_{i_e,\dots,I,n,p})]$  the variance of the entropy between each different time and then the random value  $F[S_0(t_{i_e,\dots,I,n,p})] = s^2[S_0(t_{i_e,\dots,I,n,p})] / \sigma^2[S_0(t_{i_e,\dots,I,n,p})]$  will follow a Snedecor probability density function  $\Phi$  at  $(I - i_e, (P - 1)(I - i_e + 1))$  degrees of freedom noted  $\phi_{I-i_e, (P-1)(I-i_e+1)}$ . Let us finally note  $\Pi[S_0(t_{i_e,\dots,I,n,p})]$  the critical probability such that:

$$\int_{F[S_0(t_{i_e,\dots,I,n,p})]}^{\infty} \phi_{I-i_e, (P-1)(I-i_e+1)} d\phi = \Pi[S_0(t_{i_e,\dots,I,n,p})] \quad (8)$$



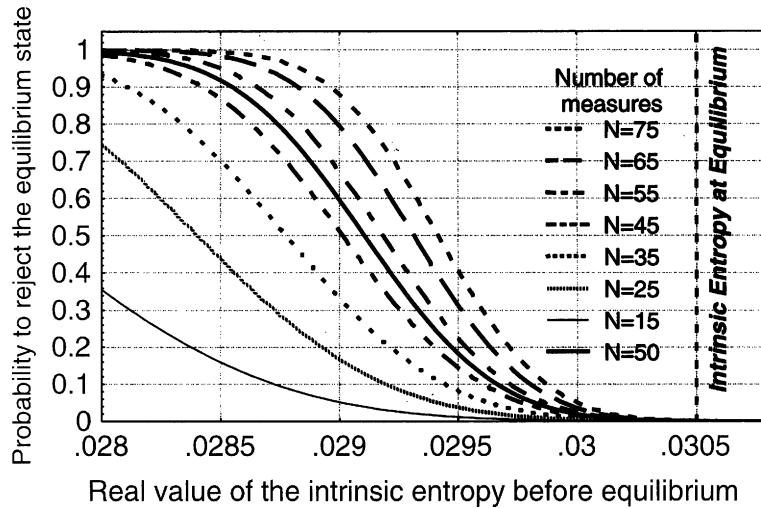


Fig. 6. Probability to reject erroneously the equilibrium state although it is not reached for different numbers of measures of the system for a fixed risk  $\delta = 0.0001$  (probability error to reject the equilibrium state although equilibrium is reached) versus the real value of the entropy before equilibrium  $S_0^{\text{UnEq}}(t)$ .

Suppose that we erroneously affirm that all the systems, at time  $t_{i_e-1,n,p}, t_{i_e,n,p}, t_{i_e+1,n,p}, \dots, t_{I,n,p}$ , are at equilibrium (this is false because we include the unequilibrated system  $S(t_{i_e-1,n,p})$ ), then the  $s^2[S_0(t_{i_e-1,n,p})]$  will increase and  $\sigma^2[S_0(t_{i_e-1,n,p})]$  will statistically stay unchanged. Therefore, the value  $F[S_0(t_{i_e-1,n,p})]$  will increase and the probability  $\Pi[S_0(t_{i_e-1,n,p})]$  to reject erroneously the equilibrium state will decrease.

The research of the equilibrium time algorithm can now be described in five steps:

- Step 0: Choice of a probability to reject erroneously the equilibrium state:  $\delta$ ,  
 Choice of the system size:  $n$ ,  
 Choice of the repetition simulation number:  $P$ ,  
 Choice of the number of MCS times:  $I$ ,  
 Computing simulations.
- Step 1: Initialisation: equilibrium subscript time  $t_e = 1$ .
- Step 2: Calculus of  $F[S_0(t_{i_e,n,p})]$ .

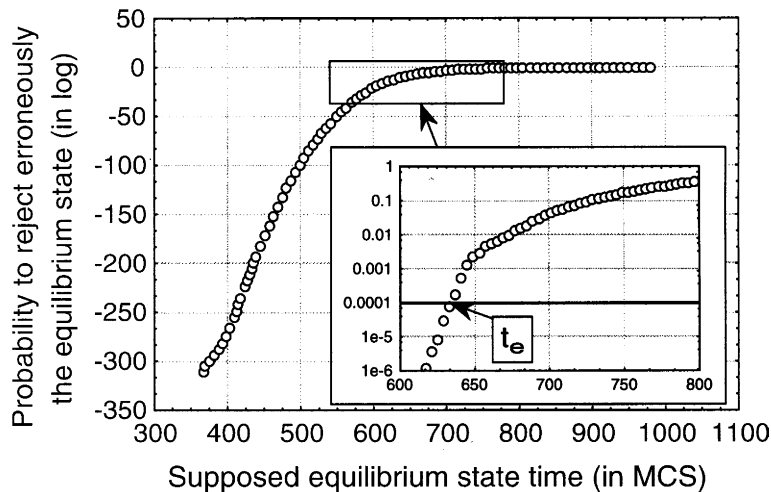


Fig. 7. Evolution of the probability to reject erroneously the equilibrium state,  $\Pi[S_0(t_{1,\dots,1000,32,100})]$ , versus the supposed equilibrium time for a system size of  $32^2$  cells. For the values of  $\delta = 0.0001$ , the equilibrium time is  $t_e = 635$ .

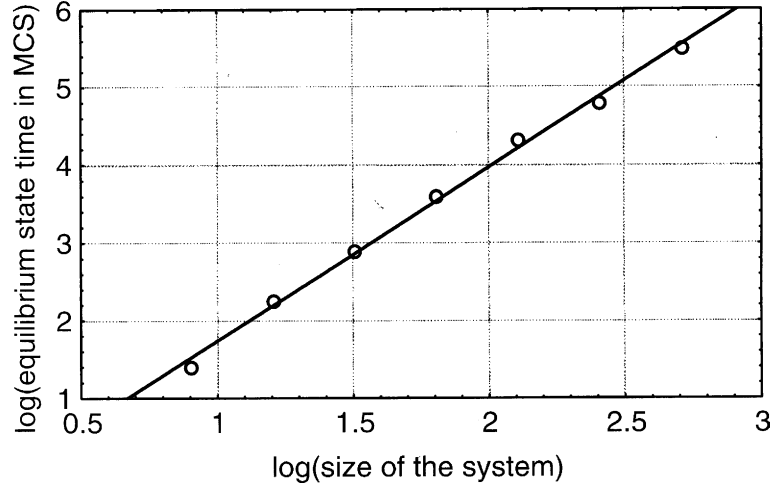


Fig. 8. Plot of the equilibrium time  $t_e$  in MCS (in log co-ordinate) versus the size of the system  $n$  (in log co-ordinate). The points obey a linear fit ( $r^2 = 0.996$ ) given by the regression equation  $\log(t_e) = -0.495 + 2.23 \log(n)$ .

Step 3: Integral evaluation of the probability:  $\Pi[S_0(t_{i_e}, \dots, I, n, P)]$  that represents the probability to reject falsely the hypothesis Eq. (9).

Step 4: If  $\Pi[S_0(t_{i_e}, \dots, I, n, P)] < \delta$  then  $i_e = i_{e+1}$  go to Step 2 or else Continue.

Step 5: Equilibrium time is  $t_e$ .

Fig. 7 represents the evolution of the integral evaluation of the probability  $\Pi[S_0(t, \dots, 1000, 32, 100)]$  versus time  $t$ . We shall choose the value of  $\delta = 0.0001$  and then get the equilibrium time  $t_e = 635$ . For each size of the system, the  $t_e$  time when equilibrium is reached is statistically calculated with the method described below. Then  $\log(t_e)$  is plotted (Fig. 8) versus the system size (in log-log co-ordinates). The points obey a linear fit ( $r^2 = 0.996$ ) with a slope of the 2.22 for the regression line meaning that  $t_e \propto n^{2.22 \pm 0.06}$ , where  $n^2$  is the number of elementary cells. The equilibrium time follows a power law with respect to the size of the system. From a different point of view,  $n$  can be seen as a characteristic length of the system and we get  $n \propto t_e^{0.45 \pm 0.01}$ . The rate exponent 0.45 is lower than the well-known exponent of the diffusion shown by Einstein that is 0.5. This fact can be explained by the border effect that inverses the flux of atoms and then decreases the diffusion rate.

#### 4. Intrinsic entropy, anti-entropy and unscaled intrinsic entropy

From Fig. 2, it can be observed that the value of the intrinsic entropy at equilibrium decreases when the size of the system increases but the decrease is lower and lower as the size of the system increases. We shall then plot the value of the equilibrium intrinsic entropy versus the system size (Fig. 9). Thanks to the non-linear regression with a very high coefficient of correlation ( $r^2 = 0.99997$ ), we get the following power law for the intrinsic entropy:

$$S(t_{i_e}, n, P) = 0.0066_{\pm 0.0005} + 0.0593_{\pm 0.0002} / n^{0.263 \pm 0.006} \quad (9)$$

The intrinsic entropy represents the amplitude factor of the scaling law of the entropy in the phases system and is equal to the minimal entropy compatible with the Heisenberg' principle. Two remarks have to be made according to the definition of anti-entropy defined Michael Conrad [10]. We have shown that the intrinsic entropy follows a Gaussian law (truncated) meaning that fluctuations still occur at all scales. As entropy is defined as the maximal probable state, fluctuations will decrease locally entropy i.e. create anti-entropy at all the scales [10]. The main interesting results is that the intrinsic entropy depends on the size of the macroscopic system that can be seen as an isolated system (universe). Intrinsic entropy at equilibrium decreases when size of macroscopic system increases (Figs. 2 and 9). Thanks to the multiscale evaluation of the information, the Intrinsic Entropy possesses the properties of the vertical approach introduced by Conrad [11]: complex system can be seen as a kind of percolation network in which information is transduced from macro- to micro-scales and amplified from micro- to macro-scale and then must consider the interplay of phenomena at all scales. These properties can be explained by an analogy between the recorelation and decorre-

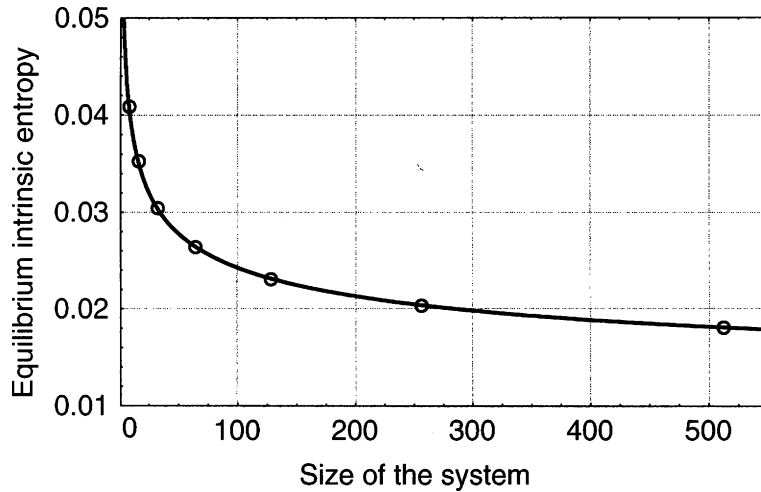


Fig. 9. Plot of the equilibrium intrinsic entropy versus the system size. Regression equation is given by  $S(t_{ic,n,p}) = 0.0066_{\pm 0.0005} + 0.0593_{\pm 0.0002}/n^{0.263_{\pm 0.006}}$ .

lation processes [12] and intrasec entropy. Decorrelation increases entropy due to the phase decorrelation of the wave function describing the system following the linear superposition principle. However, recorrelation process can be seen as a continual recorrelation of the quantum mechanic phase factor that will decrease entropy or create anti-entropy. Following this theory [13], the smaller the scale, the greater the contribution to decorrelation and the longer the scale, the greater the contribution of recorrelation. In our system description, the greater the system, the higher the probability to obtain some correlated structures that increase the order and therefore decrease the mean quantity of information at all the scale that finally decrease the intrinsic entropy. In a philosophical sense, the higher the observable universe, the higher the probability to met some organised micro-systems at all the scales and this “self-organisation” is characterised by the intrasec entropy.

A new definition of the entropy  $S_{\infty}$  can be stated by taking  $S_{\infty} = \lim_{n \rightarrow \infty} S(t_{ic,n,p})$ , the entropy obtained for an infinite system size, which we call the unscaled intrinsic entropy, we get  $S_{\infty} = 0.0066_{\pm 0.0005}$ .  $S_{\infty}$  is a characteristic number of the system at equilibrium independently of the system size. In another publication, we shall show that this entropy has the same characteristics as the mixed entropy.

## 5. Conclusion

We have shown that the multifractal analysis allows a simple description of a discrete dynamic system. Particularly, the study of the information dimension that can be related to the entropy is pertinent to analyse the rate to reach equilibrium. The main interest in the multifractal formalism is to quantify a measure at different scale and then it is possible to build independent indicia scale. With this approach, we have built an unscaled entropy to characterise the state of the system. It will then be possible to use some usual procedures of the descriptive statistics to quantify different physical characteristics such as the time used to reach equilibrium and to propose some power laws that describe the kinematics of the physical process. The unscaled entropy defined in this paper is a powerful quantity to analyse dynamical systems such as those based on simulations as for dynamical molecular simulation, Monte-Carlo simulation and of course chaotic systems. The relation between the quantity of information and the physical entropy is an analogy rather than equivalence. In a future article, we shall prove that there exists a duality, rather than an analogy, between our unscaled entropy and thermodynamic entropy thanks to the thermodynamic cost of information computation.

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## References

- [1] Brillouin L. Science and information theory. New York: Academic Press; 1956.
- [2] Zurek WH. Complexity, entropy and the physics of information. Addison-Wesley; 1990.
- [3] Shannon CE. Bell System Technical Journal 1948;27:379–423, 623–56.
- [4] Bunde A, Havlin S. Fractals and disordered systems. Springer; 1995.
- [5] Peitgen HO, Jrgens H, Saupe D. Chaos and fractals new frontiers of science. Springer-Verlag; 1992.
- [6] El Naschie MS. On the uncertainty of Cantorian geometry and the two-slit experiment. Chaos, Solitons & Fractals 1998;9(3):517–29.
- [7] El Naschie MS. Cobe satellite measurement, hyperspheres, superstrings and the dimension of space–time. Chaos, Solitons & Fractals 1998;9(8):1445–71.
- [8] El Naschie MS. Branching polymers and the fractal Cantorian space–time. Chaos, Solitons & Fractals 1998;9(1/2):131–41.
- [9] Rief F. Fundamentals of statistical and thermal physics. New York: McGrawHill; 1965.
- [10] Conrad M. Anti-entropy and the origin of initial condition. Chaos, Solitons & Fractals 1996;7(5):725–45.
- [11] Conrad M. Across-scale information processing in evolution, development and intelligence. BioSystems 1996;38:97–109.
- [12] Conrad M. Quantum gravity and life. BioSystems 1998;46:29–39.
- [13] Conrad M. Origin of life and the underlying physics of the universe. BioSystems 1998;42:177–90.