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# A Characterization of the Notion of Fluctuation

# Una caracterización de la noción de fluctuación

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### Abstract

When it is said that "something" fluctuates, what is usually meant is that it randomly increases at times and decreases at other times. The nature of that "something" undergoing those changes can be quite varied: There are fluctuations of the difference in electric potential, in pressure, in temperature, in the number of members in a population, etc. The characterization presented here of the notion of fluctuation makes possible not only the analysis of fluctuations in diverse types of systems but also an adequate comparison of the values of the fluctuations taking place in different systems. To provide some examples of the use of the notion of fluctuation introduced here, it is applied to the analysis of fluctuations occurring during diffusion processes of a gas in bicompartmental systems.

**Keywords:** notion of fluctuation, analysis of fluctuations, comparison of values of fluctuations

### Resumen

Cuando se expresa que "algo" experimenta fluctuaciones, se desea comunicar, usualmente, que ese "algo" —de manera azarosa— en algunas ocasiones aumenta y, en otras ocasiones, disminuye. La naturaleza de ese "algo" que muestra dichos cambios puede ser muy variada: hay fluctuaciones de diferencia de potencial eléctrico, de presión, de temperatura, del número de integrantes de una población, etc. Se presenta una caracterización de la noción de fluctuación que posibilita no sólo el análisis de fluctuaciones en sistemas de diversos tipos sino también una comparación adecuada de los valores de las fluctuaciones que ocurren en distintos sistemas. Para brindar algunos ejemplos del

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uso de la noción de fluctuación introducida, ésta es aplicada al análisis de fluctuaciones que tienen lugar durante procesos de difusión de un gas en sistemas bicompartimentales.

**Palabras clave:** una noción de fluctuación, análisis de fluctuaciones, comparación de los valores de fluctuaciones

**Mathematics Subject Classification:** 82C99, 82D05

# 1 Introduction

In the exact and natural sciences of interest here, when it is said that "something" fluctuates, what is usually meant is that it randomly increases at times and decreases at other times. The nature of that "something" undergoing those changes can be quite varied. There are fluctuations of the difference in electric potential (like that occurring between resistor terminals due to thermal noise), in pressure, in temperature, in the number of members in a population in diverse ecosystems, etc. ([1], [2], [3], [4] and [5]).

Quantum fluctuations will not be discussed here. The topic of this paper will be developed within a classical framework.

This article has two objectives: The first is to provide a characterization of fluctuation, a notion which may be used in systems of different types – physical, chemical and biological. The second objective is to carry out some preliminary applications of the notion addressed, using a very simplified bicompartmental system model in which gas diffusion processes take place.

This approach is rather conceptual and more oriented toward mathematical physics than toward theoretical physics. No attempt has been made to adjust the parameters of the model used, for possible predictions of experimental results. However, in section 4 mention will be made of how to proceed for this type of predictions, should one desire to use the results presented here.

The state of a system at a given instant $t$ can be represented by a vector $\vec{S}(t)$ (the vector of the state of the system depending on time) in a system of coordinates of a phase space. It will be supposed that for each event considered in which the notion of fluctuation may be used, there is a criterion such that if $\vec{S}(0)$ is known (that is, the vector of the state of the system at a certain initial instant), it is possible to determine, for any instant $t$, the most likely value of $\vec{S}(t)$; or $\vec{S}(t)$ itself can be found if the approach is deterministic. In addition, this system often displays probabilistic behavior, and the state actually assumed by the system at a given instant $t$ differs from the state mentioned above. The following notation will be used: The most probable state of the system (or that predicted by some deterministic criterion), at instant $t$, will be referred to as: $\vec{S_d}(t)$. The vector of the state corresponding to the state actually assumed by the system at instant $t$ will be known as $\vec{S_p}(t)$. The fluctuation corresponding to the system described, at instant $t$, will be defined as the product of two factors. One of these factors is the modulus of the difference $\vec{S_p}(t) - \vec{S_d}(t)$: $|\vec{S_p}(t) - \vec{S_d}(t)|$. Note that this modulus can be considered as the "distance" between the two states mentioned above: the state really assumed by the system at $t$ and the most probable state for that system at $t$ (according to a criterion to be specified), or the state predicted at $t$ by a deterministic approach. The other factor is a "normalization factor", which should make it possible to compare the value of that fluctuation with values of other fluctuations. These other fluctuations can correspond to the same system at other instants and in diverse situations (such as that of having let the system evolve from an initial state that is different from that previously considered), or to other systems of the same type, or even to those of a different type. The following normalization factor is proposed: $\frac{1}{|\vec{S_d}(t)|}$. Therefore, it is possible to express $F(t)$, the fluctuation of the system at instant $t$, as follows:

$$F(t) = \frac{|\vec{S_p}(t) - \vec{S_d}(t)|}{|\vec{S_d}(t)|} \tag{1}$$

## 2 A very simplified model of a bicompartmental system in which gas diffusion takes place

Consideration will be given to a system with two compartments, $C_1$ and $C_2$, with the same volume and the same shape. The system is kept at a constant temperature $T$. Both compartments are separated by a divider in which there is an orifice. It will be admitted that inside these compartments there can only be molecules of a particular gas, and $N_1(t)$ and $N_2(t)$ will be used to refer to the numbers of molecules of that gas contained in compartments $C_1$ and $C_2$, respectively, at instant $t$. Given the mathematical approach used, it will be accepted that $t$ can take on the values $0, 1, 2, 3, \ldots$. The lapses between two consecutive instants are intervals of time which have not been specified because they are not significant in this study. Suppose, for example, that the lapse between the consecutive instants 0 and 1 (or between instants 1 and 2, 2 and 3, etc.) is 0.1 s. In that case “3” would refer to 3 tenths of a second (0.3 s), 17 to 1.7 s, etc. Of course, the symbols $N_1(0)$ and $N_2(0)$ will be used to refer to the numbers of molecules in compartments $C_1$ and $C_2$ at an initial instant 0 s.

In order to simplify the computations required, for this paper extraordinarily small numbers of molecules will be considered as compared to, for instance, Avogadro's number ($N \simeq 6.02 \times 10^{23}$), the number of molecules contained in a mole of gas.

The bicompartmental system mentioned above is illustrated in figure 1.

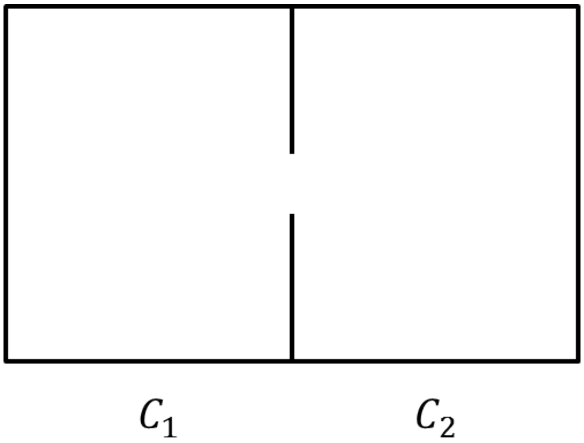


Figure 1: System of two compartments – $C_1$ and $C_2$ – in which gas diffusion processes take place.

If a deterministic diffusion process is considered, it is necessary to specify the value of the diffusion constant ($k$) and the meaning of $k$. The algorithm to be used to describe the diffusion process is the system of equations in finite differences specified below:

$$\left.\begin{aligned} N_1(t+\Delta t) &= N_1(t) - kN_1(t) + kN_2(t) \\ N_2(t+\Delta t) &= N_2(t) - kN_2(t) + kN_1(t) \end{aligned}\right\} \tag{2}$$

If $\Delta t$ is taken as the unit of time (for example, 0.15 s), the system of equations is:

$$\left.\begin{aligned} N_1(t+1) &= N_1(t) - kN_1(t) + kN_2(t) \\ N_2(t+1) &= N_2(t) - kN_2(t) + kN_1(t) \end{aligned}\right\} \tag{3}$$

The meaning of the first equation is as follows: The number of molecules of gas in $C_1$, at instant $t+1$, is equal to the number of molecules that were in $C_1$ at instant $t$, minus $kN_1(t)$ (the number of molecules of gas which during lapse $\Delta t$ – the unit of time – have left $C_1$ and entered $C_2$, due to the diffusion process), plus $kN_2(t)$ (the number of molecules of gas which during lapse $\Delta t$ have left $C_2$ and entered $C_1$). It is characteristic of diffusion processes for the number of molecules that leave $C_1$ and enter $C_2$ during $\Delta t$ to be directly proportional (with the proportionality constant equal to $k$) to the number of molecules contained in $C_1$ at instant $t$. In addition, the number of molecules leaving $C_2$ and entering $C_1$ during that $\Delta t$, due to a diffusion process, is directly proportional (with the proportionality constant equal to $k$) to the number of molecules contained in $C_2$ at instant $t$.

The second equation (3) is interpreted analogously. For a given temperature $T$, the value of $k$ depends on the geometry of the bicompartmental system and, in particular, on the size of the orifice in the divider between the two compartments. It will be admitted that the orifice is circular and that a device will make it possible to control its diameter in order to conduct experiments with different values of $k$. In section 4, consideration will be given to the relation between $k$ and $\Delta t$.

For the first example of a deterministic diffusion process, suppose that the following data are valid:

$N_1(0) = 1000$, $N_2(0) = 0$, and $k = 0.1$.

The corresponding diffusion process has been graphed in figure 2.

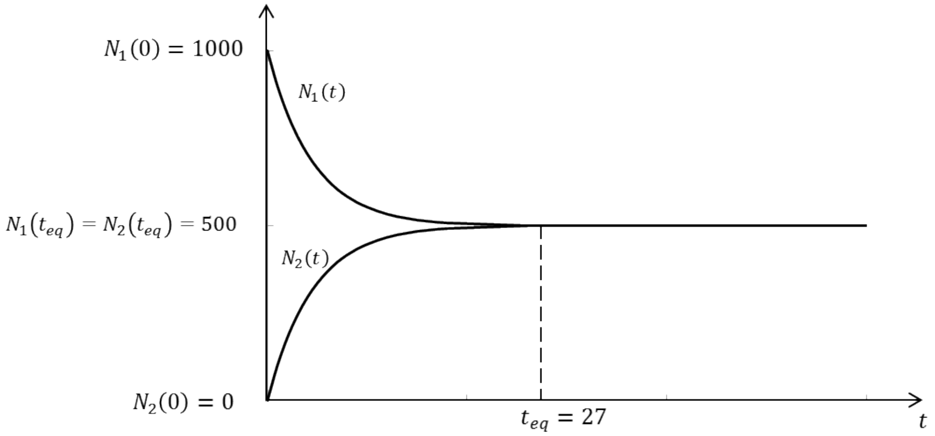


Figure 2: The diffusion process in the bicompartmental system represented in figure 1, such that $N_1(0) = 1000$, $N_2(0) = 0$, and $k = 0.1$, according to a deterministic approach.

During the diffusion process, the number $N_1(t)$ of molecules contained in $C_1$ decreases, and the number $N_2(t)$ of molecules contained in $C_2$ increases. A situation of equilibrium is reached such that the values of $N_1(t)$ and $N_2(t)$ are equal. The instant when that occurs will be called "instant of equilibrium" – $t_{eq}$. Starting at $t_{eq}$, the values of $N_1(t_{eq})$ and $N_2(t_{eq})$ remain constant, according to the deterministic approach used for the diffusion process. This does not mean that after $t_{eq}$, there is no longer any exchange of molecules of gas between $C_1$ and $C_2$; however, that exchange is such that in each $\Delta t$ the number of molecules leaving each compartment is equal to the number of molecules entering.

The diffusion process can be addressed also from a probabilistic approach. Recall that with a deterministic approach, the value of $k$ makes it possible to compute the number of molecules which, in an elemental lapse $\Delta t$, will leave the compartment and enter the other. Likewise, with a probabilistic approach, that number of molecules can also be calculated. (The result may be different from that obtained with the deterministic approach.) When using the probabilistic approach, the probability $p_d$ that any molecule of gas of those considered will go, during $\Delta t$, from one compartment to the other is made equal to $k$ (the diffusion constant used in the deterministic approach). Thus, for example, if $k = 0.1$, then the probability $p_d$ that any molecule which at any instant $t$ is in $C_1$ will be in $C_2$ at instant $t + 1$ becomes 0.1. In addition, the probability that any molecule which at any instant $t$ is in $C_2$ will be in $C_1$ at instant $t + 1$ is also 0.1. Of course, the probability that any molecule which at any instant $t$ is in either of the two compartments will remain in the same compartment at instant $t + 1$ is equal to the difference between 1 and the probability $p_d$ specified. The reason is that for any molecule, at any instant, the probability that it will be in either of these two compartments is 1.

Consider once again the bicompartmental system in conditions such that $N_1(0) = 1000$ and $N_2(0) = 0$. The evolution of the state of the system with a probabilistic approach can be specified by recurring to computational simulation. Also take any particular molecule of gas, at any instant $t$, in either of the two compartments. If one wishes to decide whether that molecule will be in the same compartment at instant $t + 1$, or whether it will have moved into the other compartment, it is useful to take into account the unit segment shown in figure 3.

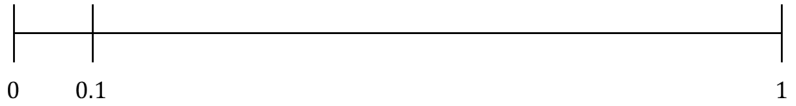


Figure 3: Segment with a length of 1, in which the value 0.1 has been indicated.

A genuine random number generator is required to obtain a number between 0 and 1. (For this purpose, the Hybrid Random Number Generator (HRNG) was used [6].) Let $R$ be the random number generated between 0 and 1, with ten decimal digits. If $R > 0.1$, it is considered that the molecule at $t + 1$ will be in the same compartment in which it is at $t$, and if $R < 0.1$, it is considered that $t + 1$ will be in the other compartment. Two pertinent questions then arise:

(a) What should be decided if $R = 0.1000000000$?

(b) What should be decided if $R = 0.0999999999$?

One acceptable way of proceeding is the following: It can be admitted in the situation described in (a) that if decimal digits continue to be obtained randomly, at some point one of those digits will be different from 0. In that case, one would have to conclude that the molecule is, at $t + 1$, in the same compartment. Likewise, in the situation described in (b), it could be admitted that if decimal digits continue to be obtained randomly, one of them will be different from 9, and one would have to conclude that the molecule is in the other compartment at $t+1$. Another acceptable way to proceed is as follows: If $R$ is equal to either of the numbers 0.1000000000 or 0.0999999999, a new value for $R$ will be generated, and the procedure will be repeated until $R$ no longer has a value equal to either of those two numbers. When this occurs, the established criterion will be applied to decide which compartment the molecule is in at $t+1$. The procedure described, based on obtaining random numbers between 0 and 1, is applied to each molecule in the system, to decide (according to the probabilistic approach) what happens to that molecule; that is, whether it remains in the compartment or goes into the other compartment, during each $\Delta t$, between the initial instant and that considered the final instant for the purposes of the study conducted.

If computer simulation is used to study the diffusion process, with the probabilistic approach, in this bicompartmental system, and with the initial conditions $N_1(0) = 1000$, $N_2(0) = 0$, and it is accepted that $p_d = k = 0.1$, the results obtained are like those shown in figure 4.

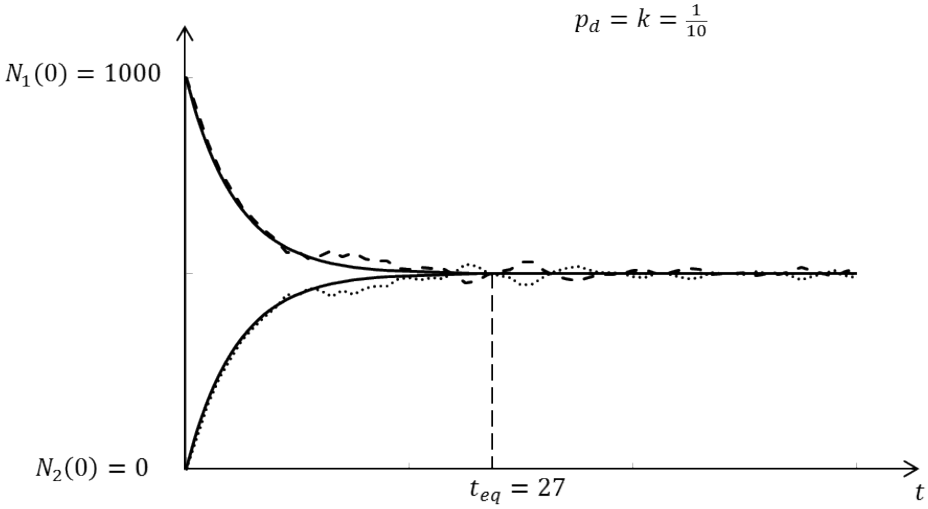


Figure 4: $N_1(t)$ (- - -) and $N_2(t)$ (··········) according to the probabilistic approach. ($N_1(t)$ and $N_2(t)$ according to the deterministic approach, previously represented in figure 2, are indicated by the solid line.)

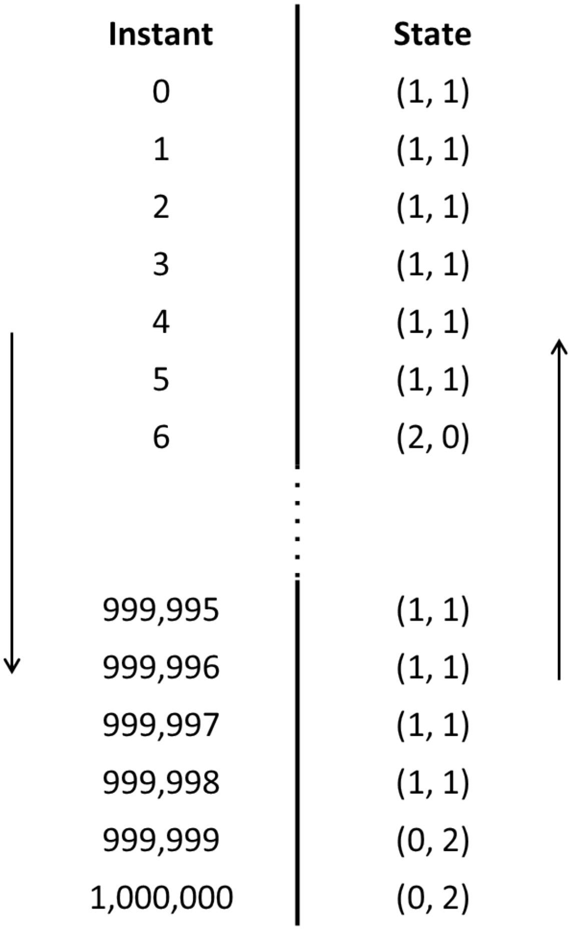
It can be observed that the diffusion process considered deterministically differs from that considered probabilistically. In the latter approach, the system that attains the state of equilibrium may leave it.

According to the second principle of thermodynamics applied to an isolated system (one which does not exchange either matter or energy with the outside), the entropy of the system is non-decreasing, and it attains its maximum value when the system reaches the state of equilibrium, where it remains indefinitely. Entropy can be interpreted as a measurement of disorder in the system. Thus, the system reaches its highest degree of disorder in the state of equilibrium and it does not become ordered spontaneously. The description of the evolution of the system from the probabilistic perspective, that of statistical mechanics, is different. According to the approach of this branch of physics, if the system reaches the state of equilibrium, it can go farther away spontaneously. In this paper, it has been supposed that the results obtained with the probabilistic approach using computer simulation correspond to those obtained in real experiments. In other words, with this approach, the entropy can decrease. When this occurs, the order of the system increases.

Consider a bicompartmental system containing only two molecules. Let $p_d = 0.1$.

One possible way of referring to the different states of the system, according to the extremely simplified model used, is as follows: an ordered pair such that the first element of that pair specifies the number of molecules in $C_1$, and the second element of that ordered pair is the number of molecules contained in $C_2$. With this notation, different states of the system may be indicated as $(0, 2)$, $(1, 1)$ and $(2, 0)$. Using computer simulation, the evolution of the system was observed according to the probabilistic approach, for 1,000,001 instants.

The first 6 states and the last 6 states, assumed by the system at the different instants considered, are shown in figure 5.



| Instant | State |
|---|---|
| 0 | (1, 1) |
| 1 | (1, 1) |
| 2 | (1, 1) |
| 3 | (1, 1) |
| 4 | (1, 1) |
| 5 | (1, 1) |
| 6 | (2, 0) |
| 999,995 | (1, 1) |
| 999,996 | (1, 1) |
| 999,997 | (1, 1) |
| 999,998 | (1, 1) |
| 999,999 | (0, 2) |
| 1,000,000 | (0, 2) |

Figure 5: States assumed by the bicompartmental system containing 2 molecules, for 1,000,001 instants. The lefthand arrow indicates the direction of the “arrow of time” and the righthand arrow indicates the direction opposite to that of the “arrow of time”.

For systems of this type, with any number of molecules, the probability that at a given randomly selected instant, the system will be in each of the possible states can be calculated, using concepts of macrostates and microstates, and techniques of combinatory calculus. (It is supposed that whoever randomly chooses an instant does not know what the initial state of the system was.) The probabilities that the system will be in states $(0,2)$, $(1,1)$ and $(2,0)$ will be known as $p(0,2)$, $p(1,1)$, $p(2,0)$, respectively.

When going along the list of states through which the system has passed (both in the direction of the arrow of time and backwards), it is also possible to compute the probabilities that the following sequences of consecutive states will be found:
$((0,2),(0,2)), ((0,2),(1,1)), ((0,2),(2,0)), ((1,1),(0,2)), ((1,1),(1,1)), ((1,1),(2,0))$, $((2,0),(0,2)), ((2,0),(1,1))$, and $((2,0),(2,0))$.

If one goes along the list in the direction of the arrow of time, the corresponding probabilities are:
$p_{t,+}((0,2),(0,2)), p_{t,+}((0,2),(1,1)), p_{t,+}((0,2),(2,0)), \ldots$, and $p_{t,+}((2,0),(2,0))$.

If one goes along the list in the direction which is reverse to the arrow of time, the corresponding probabilities are:
$p_{t,-}((0,2),(0,2))$, $p_{t,-}((0,2),(1,1))$, $p_{t,-}((0,2),(2,0))$,$\ldots$, and $p_{t,-}((2,0),(2,0))$.

It will be explained below why, from the perspective of physics, it is not only interesting but also very significant that the following equalities are valid:
$p_{t,+}((0,2),(0,2)) = p_{t,-}((0,2),(0,2))$, $p_{t,+}((0,2),(1,1)) = p_{t,-}((0,2),(1,1))$,$\ldots$, and $p_{t,+}((2,0),(2,0)) = p_{t,-}((2,0),(2,0))$.

This type of equalities are valid for systems with any number of molecules. Thus, for example, for a bicompartmental system with 1000 molecules, equalities such as the following may be established:
$p_{t,+}((540,460),(490,510)) = p_{t,-}((540,460),(490,510))$, and $p_{t,+}((400,600),(650,350)) = p_{t,-}((400,600),(650,350))$.

For comparison purposes, the values of the probabilities of finding the different possible pairs of consecutive states are provided at the end of this paragraph, for the bicompartmental system discussed containing 2 molecules. The frequencies with which these pairs appear on the list of the 1,100,001 states mentioned, when going in the direction of the arrow of time and backwards, are given as well. The nomenclature used for these frequencies, which is analogous to that used for the corresponding probabilities, is easily interpreted.

$$p_{t,+}((0,2),(0,2)) = p_{t,-}((0,2),(0,2)) = 0.2025$$
$$f_{t,+}((0,2),(0,2)) = 0.20215 \qquad f_{t,-}((0,2),(0,2)) = 0.20250$$

$$p_{t,+}((0,2),(1,1)) = p_{t,-}((0,2),(1,1)) = 0.045$$
$$f_{t,+}((0,2),(1,1)) = 0.04488 \qquad f_{t,-}((0,2),(1,1)) = 0.04483$$

$$p_{t,+}((0,2),(2,0)) = p_{t,-}((0,2),(2,0)) = 0.0025$$
$$f_{t,+}((0,2),(2,0)) = 0.00249 \qquad f_{t,-}((0,2),(2,0)) = 0.00254$$

$$p_{t,+}((1,1),(0,2)) = p_{t,-}((1,1),(0,2)) = 0.045$$
$$f_{t,+}((1,1),(0,2)) = 0.04483 \qquad f_{t,-}((1,1),(0,2)) = 0.04488$$

$$\begin{aligned}
&p_{t,+}((1,1),(1,1)) = p_{t,-}((1,1),(1,1)) = 0.41\\
&f_{t,+}((1,1),(1,1)) = 0.41016 \qquad f_{t,-}((1,1),(1,1)) = 0.41016
\end{aligned}$$

$$\begin{aligned}
&p_{t,+}((1,1),(2,0)) = p_{t,-}((1,1),(2,0)) = 0.045\\
&f_{t,+}((1,1),(2,0)) = 0.04504 \qquad f_{t,-}((1,1),(2,0)) = 0.04499
\end{aligned}$$

$$\begin{aligned}
&p_{t,+}((2,0),(0,2)) = p_{t,-}((2,0),(0,2)) = 0.00250\\
&f_{t,+}((2,0),(0,2)) = 0.00254 \qquad f_{t,-}((2,0),(0,2)) = 0.00249
\end{aligned}$$

$$\begin{aligned}
&p_{t,+}((2,0),(1,1)) = p_{t,-}((2,0),(1,1)) = 0.045\\
&f_{t,+}((2,0),(1,1)) = 0.04499 \qquad f_{t,-}((2,0),(1,1)) = 0.04504
\end{aligned}$$

$$\begin{aligned}
&p_{t,+}((2,0),(2,0)) = p_{t,-}((2,0),(2,0)) = 0.2025\\
&f_{t,+}((2,0),(2,0)) = 0.20291 \qquad f_{t,-}((2,0),(2,0)) = 0.20291
\end{aligned}$$

It can be observed that the different frequencies are reasonable approximations to the corresponding probabilities.

The larger the number of molecules contained in the bicompartmental system, the greater the effort required to compute probabilities of this type. Although the results of these calculations have not been included below, the results concerning certain pairs of frequencies of the type considered have been provided. They were computed based on two sequences of 10,001 states. The sequences were obtained by computational simulation, operating with $p_d = 0.1$. The initial state $(50, 50)$ was used for one of these sequences of states, and $(500, 500)$ for the other. The values obtained for those pairs of frequencies are:

$$\begin{array}{rr}
f_{t,+}((48,52),(45,55)) = 0.0051 & f_{t,-}((48,52),(45,55)) = 0.0051\\
f_{t,+}((47,53),(54,46)) = 0.0010 & f_{t,-}((47,53),(54,46)) = 0.0011\\
f_{t,+}((44,56),(49,51)) = 0.0027 & f_{t,-}((44,56),(49,51)) = 0.0029\\
f_{t,+}((506,494)),(505,495) = 0.0120 & f_{t,-}((506,494)),(505,495) = 0.0130\\
f_{t,+}((523,477),(521,479)) = 0.0002 & f_{t,-}((523,477),(521,479)) = 0.0003\\
f_{t,+}((521,479),533,467)) = 0.0001 & f_{t,-}((521,479),533,467)) = 0.0002
\end{array}$$

Once again, it can be observed that the frequencies computed when going along the list of sequences of 10,001 states in the direction of the arrow of time are approximately equal to those corresponding to the frequencies computed under time reversal.

For systems such as the one observed, with any number of molecules, the probabilities of the types mentioned can be computed using the concept of macrostate (coinciding with the notion of state found here) and that of microstate, along with combinatorial techniques. The corresponding calculations are not included in this article, but the following should be recalled: Given the notion of state – that is, macrostate – used, the number of microstates corresponding to that state is the number of possible distributions of the molecules of gas in $C_1$ and $C_2$, compatible with that state, under the supposition that the different molecules are distinguishable. Thus, $N_\mu(N_1(t), N_2(t))$, for $(N_1(t) + N_2(t)) = N$, will denote the number of microstates corresponding to the state $(N_1(t), N_2(t))$. This number can be computed as follows:

$$N_\mu\left(N_1(t), N_2(t)\right) = \binom{N}{N_1(t)} = \binom{N}{N_2(t)} = \frac{N!}{N_1(t)!N_2(t)!}$$

All the microstates in the system are considered to be equally probable. Consequently, the more microstates there are that correspond to that state (or macrostate, if the terminology from mechanical statistics is used), the more probable it is that a state will be assumed by the system. The state of equilibrium of a system, of those systems able to reach that state in which entropy attains its maximum value, is that corresponding to the highest number of microstates.

Equalities such as $p_{t,+}((n_i, n_j), (n_k, n_l)) = p_{t,-}((n_i, n_j), (n_k, n_l))$, for $n_i + n_j = n_k + n_l = N$ (where $N$ is the total number of molecules contained in the system considered), have – as indicated above – important implications from the perspective of physics. Suppose that the system evolves according to the probabilistic approach for an unlimited period (i.e., infinite: $t = 0, 1, 2, \dots$). Let us also admit that someone randomly selects a subsequence which is as large as desired, from the infinite sequence of states, starting at the instant $t = 0$. Anyone selecting that subsequence of states has the option of considering the states that compose it, in the order given by the direction of the arrow of time, or in the direction opposite to the arrow of time. If that person shows that subsequence to others, such as experts in mathematics, physics and computing, without specifying in which direction the results are presented, they will not be able to discern whether they correspond to the arrow of time or to the reverse.

It must be emphasized that the preceding conclusion is correct if it is admitted, as specified above, that the system evolves during an infinite time (producing an infinite sequence of states), and that the subsequence of consecutive states was randomly selected. In this situation, regardless of how low the probability is that the system will spontaneously assume any of the possible states, if that probability (as does occur) is different from 0, then that state will be assumed by the system. For example, this can occur with either of the two states in which the system is farther from equilibrium. This can occur not only once but also as many times as desired if a large enough subsequence has been used. Suppose, for instance, that the system contains $N$ molecules, $N$ being a number which is as large as desired. Thus, for the model of the system considered, there are $2^N$ possible microstates. Given that either of the microstates has the same probability of occurring, that probability equals $\frac{1}{2^N}$, but only one microstate corresponds to either of the two states that are farthest from equilibrium. Therefore, if one of the states of the subsequence considered is selected at random, the probability that the state chosen will be $(N, 0)$ is equal to $\frac{1}{2^N}$. Suppose that one takes a subsequence made up of $V$ consecutive states, such that $V = 2^N \cdot S$, where $S$ is also a natural number as large as desired. What is, then, the approximate number of times that the state $(N, 0)$ will appear in that subsequence? The answer is as follows: $\frac{1}{2^N} \cdot V = \frac{1}{2^N} \cdot 2^N \cdot S = S$.

In spite of the above, it is usually considered that the phenomenon of the diffusion of a gas containing a high number of molecules (like Avogadro's number), in a system like that analyzed here, starting from a point that is very far from equilibrium, is an irreversible process (even if a probabilistic approach is used, that of statistical mechanics). Why? The answer is closely related to the following: The hypothesis that the time required to generate the sequence of states from which one subsequence is randomly chosen is infinite is not realistic; it corresponds to an extremely idealized situation. If that system (with such a large number of molecules of gas) is observed, starting at an initial state very far from the state of equilibrium, for a reasonable time for human capabilities, it can be noted that it has, according to the predictions of the probabilistic approach, an evolution which is very similar to that predicted by the deterministic approach. This difference between the predictions is due to the presence of small fluctuations, according to the probabilistic approach. The larger the values of the fluctuations are, as considered in section 3, the lower the frequencies of the fluctuations.

# 3 Applications of the notion of fluctuation described to bicompartmental systems of the type addressed in section 2

In figure 6, the results of the states at instant $t$, corresponding to the system of the type described, have been displayed for the deterministic approach and for the probabilistic approach.

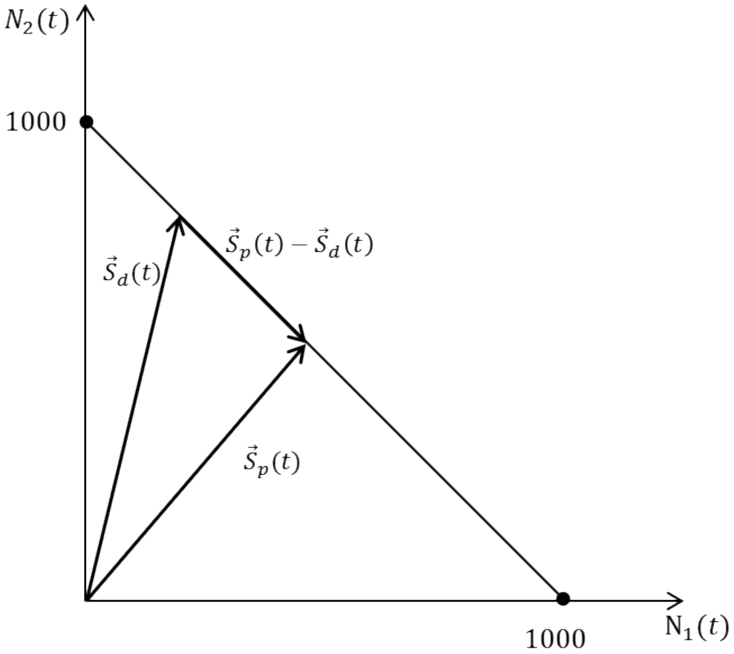


Figure 6: Representation of $\vec{S_p}(t)$, $\vec{S_d}(t)$, and $\vec{S_p}(t) - \vec{S_d}(t)$, for a bicompartmental system with $N$ molecules, where $N = N_1(t) + N_2(t) = 1000$.

In this case, equation (1) becomes:

$$F(t) = \frac{\left(\left({}^{p}N_1(t) - {}^{d}N_1(t)\right)^2 + \left({}^{p}N_2(t) - {}^{d}N_2(t)\right)^2\right)^{\frac{1}{2}}}{\left({}^{d}N_1^2(t) + {}^{d}N_2^2(t)\right)^{\frac{1}{2}}} \tag{4}$$

In (4), ${}^{d}N_1(t)$ and ${}^{d}N_2(t)$ symbolize the values of $N_1(t)$ and $N_2(t)$ computed with the deterministic approach specified in the system of equations (2); and ${}^{p}N_1(t)$ and ${}^{p}N_2(t)$ symbolize the values of of $N_1(t)$ and $N_2(t)$, obtained by computer simulation, using the probabilistic approach.

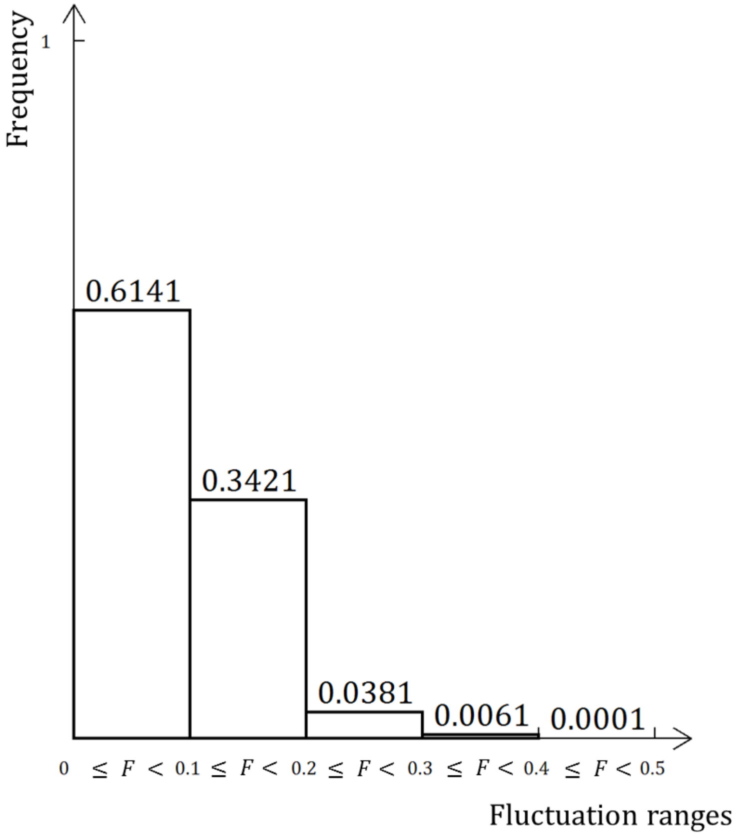
Although the fluctuation – $F(t)$ – as expressed in (4) for instant $t$, depends explicitly only on time, actually it depends also on $N_1(0)$, $N_2(0)$ and $k$. Indeed, ${}^{p}N_1(t)$ and ${}^{d}N_1(t)$ are functions of $N_1(0)$ and $N_2(0)$.

Equation (4) was used to compute fluctuations both in situations in which the system was nearing equilibrium and in others in which it was moving away from it.

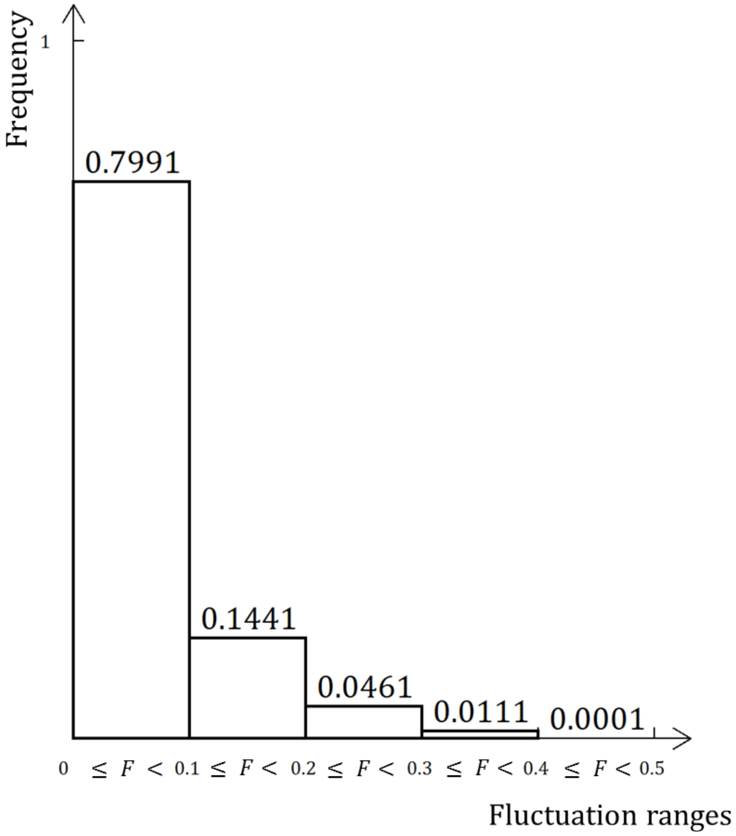
First, concerning fluctuations, the behavior of a system of the type considered in section 2 was analyzed as it evolved from the initial state – $(100, 0)$. With $k = 0.1$, it was observed that the system reached the state of equilibrium – $(50, 50)$ – at instant $t = 18$ (i.e., $t_{eq} = 18$), when using the deterministic approach. Of course, the behavior described with the deterministic approach repeats itself, with no variations, every time that the system is left to evolve from the same initial state. On the contrary, the behavior of that same system, when described with the probabilistic approach, and studied using computer simulation, can lead to different sequences of states, each time that the system is allowed to evolve from $(100, 0)$, the initial state specified.

A sequence of 1000 "experiments", was conducted by letting the system evolve according to the probabilistic approach, from the initial state $(100, 0)$, with $p_d = 0.1$, until the final instant $t_f$, equal to the instant of equilibrium which was found with the deterministic approach; hence, $t_f = 18$. The distribution of the fluctuations computed for instant $t_f = 18$, in those 1000 computer simulation "experiments" is displayed in figure 7a in the histogram, where various ranges of values of fluctuations are shown on the x-axis. For each of these ranges, the frequency with which the values of the fluctuations computed can be found within that range is indicated.

In the histogram in figure 7b, the same procedure was used except for $t_f$; the fluctuations described above were computed for $t_f = \frac{1}{2}t_{eq} = 9$.



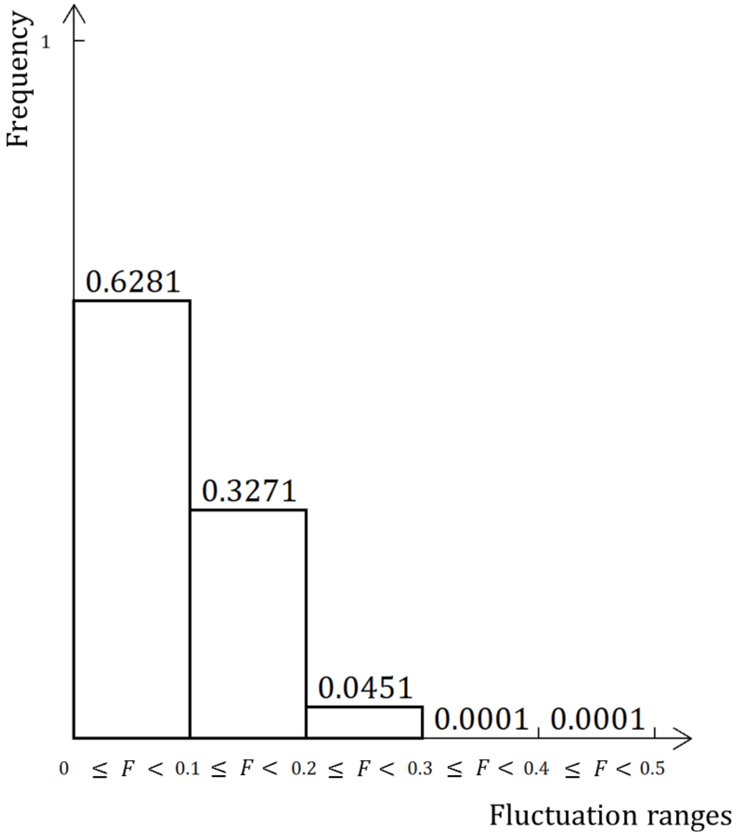
(a) Distribution of fluctuations for 1000 experiments, with initial state $(100, 0)$, $k = p_d = 0.1$, and $t_f = 1t_{eq} = 18$.



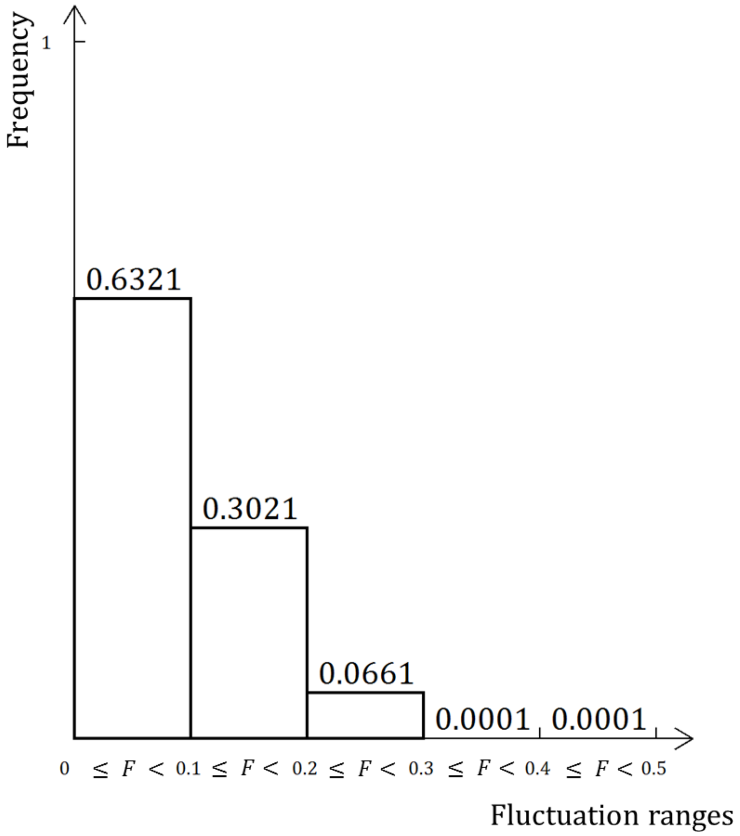
(b) Distribution of fluctuations for 1000 experiments, with initial state $(100, 0)$, $k = p_d = 0.1$, and $t_f = \frac{1}{2} t_{eq} = 9$.

Figure 7: Distributions of fluctuations for two sets of “experiments”of computational simulation in which the bicompartmental system is allowed to evolve starting at a state far from equilibrium.

In figures 8a and 8b, the same type of histogram represents the results obtained when letting the system evolve from the state of equilibrium – $(50, 50)$ – until instants $t_f = 100$ and $t_f = 50$, respectively. Note that in this case where the initial state is that of equilibrium, according to the deterministic approach the system remains in that state, and shows no variations. In contrast, just as in the previous case, the trajectories of the states may vary for each of the “experiments” of the two sets of 1000 “experiments” conducted for each set according to the probabilistic approach. For each “experiment” pertaining to one of these sets of 1000, $t_f = 100$ was used. Thus, it was possible to find the distribution of the fluctuations for $t_f = 100$. On the other hand, for each of the “experiments” of the other set of 1000 “experiments”, $t_f = 50$ was used, and the distribution of the fluctuations for $t_f = 50$ was found.



(a) Distribution of fluctuations for 1000 experiments, with initial state $(50, 50)$, $k = p_d = 0.1$, and $t_f = 100$.



(b) Distribution of fluctuations for 1000 experiments, with initial state $(50, 50)$, $k = p_d = 0.1$, and $t_f = 50$.

Figure 8: Distributions of fluctuations for two sets of "experiments" of computational simulation in which the bicompartmental system is allowed to evolve starting at a state of equilibrium.

# 4 Discussion and perspectives

Although it is not the objective of this paper to make predictions about experimental results based on the extremely simple model of the bicompartmental system presented, it should be pointed out that, in principle, it would be feasible to do so. Take, for example, the deterministic approach described in the system of equations (2). Experimentally, how could the values for $N_1(t)$, $N_2(t)$ be found at each instant $t$, for a real system of this type? It might be done, for example, by using a device which measures pressure $P_1(t)$ in compartment $C_1$ and another device of the same type to measure pressure $P_2(t)$ in compartment $C_2$. As accepted, the system would be kept at a constant temperature $T$. Under these conditions, the laws of gases for known volumes of $C_1$ and $C_2$ (which are equal) make it possible to estimate $N_1(t)$ and $N_2(t)$.

How can the value to be attributed to $\Delta t$ be determined once a certain value is established for $k$? The answer to this question enables one to note that the values $\Delta t$ and $k$ are closely related, according to the treatment for the diffusion phenomenon described here. Suppose that one begins an experiment with a certain amount of gas in $C_1$ and no gas at $C_2$. Therefore, $N_1(0)$ can be estimated, as mentioned above, based on $P_1(0)$. Suppose that in the real bicompartmental system, the starting point is a situation where $P_1(0)$ has a certain value due to the presence of a specific quantity of gas (e.g., 2 moles of gas) in $C_1$. Admit also that at instant $t = 0$, the quantity of gas in $C_2$ is zero. The system is permitted to evolve until $P_1(t) = \frac{3}{4}P_1(0)$, and it is possible to determine the instant $t$ for which the preceding equation is fulfilled. That instant will be known as $t_M$. Moreover, in the deterministic model provided by equation (2), operating with a value of $k$ fixed at 0.01, for example, it is seen that after a particular number of elemental lapses $\Delta t$ (equal to $M$), $N_1(t) = \frac{3}{4}N_1(0)$. In other words, it is verified that $N_1(t) = \frac{3}{4}N_1(0)$, when a period of time equal to $M\Delta t$ has elapsed, starting at $t = 0$. It is justified then to consider that the following equality is verified: $t_M = M\Delta t$. Therefore, $\Delta t = \frac{t_M}{M}$. Recall that $t_M$ was measured and $M$ was determined according to the evolution of the deterministic model given by (2). Thus, the value of $\Delta t$ has been found for the $k$ specified – $k = 0.01$. These, then, are the parameters necessary for the model to be able to make predictions on the real system. Suppose, for example, that one wants to predict how much time is required from $t = 0$, for a real system to reach a situation such that $P_2(t) = \frac{4}{5}P_1(t)$, having started from the same initial conditions described above. For this purpose, the deterministic model is allowed to evolve from its initial state until $N_2(t) = \frac{4}{5}N_1(t)$, and it is found for how many $\Delta t$ must the model evolve to reach that state. Suppose that the time $Q\Delta t$ has elapsed and that situation has been reached, but now the value of $\Delta t$ is known in "real time". Thus, the value of $Q\Delta t$ is known. This then will be the prediction of the deterministic model used concerning the time that should elapse so that in the real system the situation indicated above can be attained.

One possible objection regarding the deterministic model used here is that it is implemented by a system of equations based on finite differences; it is not an approach that makes use of differential equations, as do others more commonly found in current physical-mathematical methods. Nevertheless, it can be shown that by operating with a small enough value of $k$, one may come as near as desired to the results obtained using a system of differential equations. This topic will be developed elsewhere.

Another possible objection which may be more fundamental is that the characterization of the states used here could be viewed as so extremely simplified that it could lead to erroneous results. Hence, for example, if it is deemed necessary to assign values to 6 coordinates (3 of position and 3 of velocity) to specify the state at that certain instant $t$ of each of molecule in a system containing $N$ molecules, a $6N$ dimensional phase space must be used to represent, with a point in that space, the state of the system, at a particular instant. Moreover, the trajectory of this point in that phase space describes the evolution (i.e., the time-based sequence of states) of the system of $N$ molecules considered. Now then, this characterization of the system is very suitable for certain objectives, but characterizations of greater or lesser analytical depth should be used for other objectives. The characterization (of the state of the bicompartmental system) developed in this article consists of specifying – for each instant $t$ – how many molecules $N_1(t)$ are contained in $C_1$, and how many molecules $N_2(t) = N - N_1(t)$ are contained in $C_2$, with $N$ being the total number of molecules in this system. The notion of fluctuation provided can be generalized for more sophisticated specifications than that used here to characterize the state of the system.

One might question the normalization factor used and propose $\frac{1}{|\vec{S}(t_{eq})|}$ instead. However, many systems do not reach a state of equilibrium. In particular, the number of elements composing them may change with time. For these systems, that possible alternative normalization factor would be inadequate. Therefore, a normalization factor was introduced as a useful option in cases of this type as well.

In other studies, an analysis will be conducted regarding the dependence of the fluctuations on (1) the size of the systems (that is, of the number of their components), and (2) the time elapsed from the initial instant, $t = 0$, until the instant when they are computed.

Fluctuations in areas of interest to biology, such as population dynamics, enzymology and metabolic networks, will also be addressed.

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