Editorial:
Nonlinear Dynamics –
From Invisible Particles and Fields to the Visible Universe

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Any simple idea will be worded in the most complicated way
Malek's Law

This is the third volume in our series *Frontiers of Nonlinear Dynamics* (cp. [1,2]). It results from the 3rd European Interdisciplinary School on Nonlinear Dynamics for System and Signal Analysis EUROATTRACTOR2002 that took place in Warsaw, June 18-27, 2002, and like the previous Schools attracted researchers from very different disciplines.

It seems that *complexity* is really the key word for the whole School. But complex behavior of a system may result from simple dynamical rules – unlike it is stated in Malek's Law, simple mathematical models often work well for quite complicated systems, as for example was demonstrated for biological systems by Prof. L.Glass. *Fractal dimension* may serve as a measure of system or signal complexity (cf. [3]); however, as demonstrated in the paper by Prof. I.Procaccia and co-authors, it may be impossible to calculate "true" fractal dimension from the data since the structure of data may depend on the observer. Prof. Juliette Rouchier shows that the concept of complexity is useful also in Social Sciences. These are only some examples how EUROATTRACTOR2002 gave an excellent opportunity to young researchers to take advantage of the advanced training offered by the leading scientists and enabled cross-fertilization between different disciplines where the methods of Nonlinear Dynamics are successfully applied.

During so called Participants Presentation Sessions (PPS) young Participants could present their own ideas and scientific achievements to other Participants, Keynote Speakers and Lecturers - Members of Organizing Committee, while being subjected to a friendly peer review, with possibilities of direct exchange of the opinions concerning interests in application of Nonlinear Dynamics. At the same time the Evaluators (Keynote Speakers and Members of the Organizing Committee who were present in the lecture room) evaluated each Participant based on originality, relevance, clarity, way of presentation, and the overall impression. Three young Participants whose presentations gathered the maximum average number of points (per one Evaluator) were honoured with special OSCATTRACTOR2002 prizes – statuettes of the Egyptian God of Chaos, Nun, in Olympic colours. OSCATTRACTOR prizes have already become a tradition, honouring achievements in Nonlinear Dynamics year after year. OSCATTRACTOR2002 prizes went to: Gold – Ralph Gregor ANDRZEJAK (D); Silver – Claudia BONOMO (I); Bronze – Pawel KUKLIK (PL). Prof. Itamar PROCACCIA (Rehovot, Israel) won Special Gold OSCATTRACTOR2002 prize "for his whole-life achievements in the field of Nonlinear Dynamics, especially for his method of calculation of fractal dimension" (very widely used in scientific literature, known as *Grassberger-Procaccia method* [4]); the statuette was handled to him by Prof. Shewah Weiss, Ambassador of Israel to Poland, and by Prof. W.Klonowski, Head of the Scientific and Organizing Committees. Prof. I.Procaccia delivered also Opening Lecture *How things grow and how things break, and how Monsieur Laplace connects with all that*, explaining complexity both of fractal growth patterns and of fracture patterns in brittle media, and showing how one can develop a theory of such complex geometric objects.

In spite of our serious efforts to attract more women-scientists, and despite the fact that feminists critics of Science have argued that Chaos Theory, which is an important part of Nonlinear Dynamics, "gives a voice within Science to feminist concern" (cf. [5]) the majority of Participants and even more that of Lecturers were men.

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This volume will be of interest to scholars of very different categories, because of the interdisciplinary essence of Nonlinear Dynamics, with the "accent" on applications in Environmental and Biological Sciences.

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Lectures by Keynote Speakers

On the Fractal Dimension of the Visible Universe

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Estimates of the fractal dimension D of the set of galaxies in the universe, based on ever improving data sets, tend to settle on $D \approx 2$. This result raised a raging debate due to its glaring contradiction with astrophysical models that expect a homogeneous universe. A recent mathematical result indicates that there is no contradiction, since measurements of the dimension of the visible subset of galaxies is bounded from above by $D = 2$ even if the true dimension is anything between $D = 2$ and $D = 3$. We demonstrate this result in the context of a simple fractal model, and explain how to proceed in order to find a better estimate of the true dimension of the set of galaxies.

Key words: megafractals, correlation dimension, finite size effects

The value of the (fractal) dimension D of the galaxy distribution in the universe is an important open question in cosmology. Steadily improving observations are available giving scientists hope that enough data will allow finally to decide the highly debated issue of whether D is 3 or substantially lower (usually stated to be about 2). For example, in the recent book [1] on the "Discovery of Cosmic Fractals" it is emphatically declared that “The megafractals - the cosmic continents, archipelagos and islands - were the news brought home by the modern explorers of the cosmos, exotic, but truths nevertheless about the worlds overseas. Even if the fractal dimension and the maximum scale are still debated, megafractals cry for explanation. Their origin is the number one challenge for cosmological physics." What these authors refer to are mainly results of fractal analysis of the data sets of galaxies which indicate that the fractal dimension D of the set of galaxies is about 2 [2-4]. We build on a recent theorem of fractal mathematics [5] which indicates that these results may not be "truths nevertheless", but rather a reflection of an inherent impossibility to measure a dimension larger than 2. The true dimension may be anything between 2 and 3, and the upper number is not excluded, in agreement with standard astrophysical theories of a homogeneous universe [6]. In this way “the number one challenge" may have been resolved in an unexpected and somewhat disappointing

way, namely: when $D > 2$ *one cannot measure D* by observing the visible galaxies. In addition to explaining this result we present a partial remedy by exploring certain aspects of the data analysis that may indicate the existence of a dimension larger than 2.
In essence, the fractal analysis of any given atlas of galaxies is a simple matter, once one takes carefully into account the side issues described in [3], which deal with questions like limited angles, faint luminosities, and other observational issues. After taking in the account all these details one ends up with a set of points, or coordinates, each of which stands for a galaxy, with redshift data used to determine its distance from us (the observers). Given such a set of points $\{X_i\}_{i=1}^N$ in R^3, we define the correlation integral $C(r)$ as the number of pairs of points of this set whose distance is smaller than or equal to r,

$$C(r) = \frac{2}{N(N-1)} \sum_{i<j} \theta\left(r - \left|X_i - X_j\right|\right), \tag{1}$$

where $\theta(y)$ is the step function, unity for $y > 0$ and zero otherwise. For a fractal set of dimension D plotting $\log(C(r))$ versus $\log r$ results in a curve whose slope is the correlation dimension D_2, of the Grassberger-Procaccia algorithm [7] (see also [8, 9]). In general $D_2 \leq D$; for sets whose clustering is not singular one can expect that $D_2 = D$ [8]. For reasons related to angular restrictions and the like, in [2-4] the authors consider a quantity $\Gamma^*(r)$, which for a general fractal coincides with $C(r)/r^3$. Thus their plots should have slopes $D_2 - 3$. They find consistently $D_2 \approx 2$.
The question is then whether this is really an indication that the set of all galaxies is of dimension $D \approx 2$. We argue first that this may not be the case. In a recent paper [5] the following theorem was established: let F be a fractal set in R^3 with dimension $D > 2$. The *visible part* of the set F from a point P is the subset F_V of those points lit by a spotlight at P. *Then the part F_V that is visible to an observer can in general not have a dimension more than 2*[1].
We stress that this result is not about the projection of the set onto the celestial sphere, but about those observations in which the *distance* of each point (galaxy) is given along with its celestial coordinates (such data sets are called 3-dimensional catalogs). The meaning of the theorem is that it is in fact impossible to determine the dimension of the set of galaxies from measurements of the visible subset if the dimension of the full set is larger than 2. The basic reason for this impossibility is that galaxies “hide” behind each other when the dimension is above 2. This issue will not go away with improving the catalogs. Rather, it will become more and more important as better and better catalogs become available.
We now illustrate some aspects of this problem, and in particular show that there might be some lower bound on the true dimension when taking into account finite size effects

[1]In fact, there are really two possibilities of which the second is even more dramatic for any measurement than the first: Either the part F_V that is visible to an observer at P can in general not have a dimension greater than 2 or it may happen that the dimension of F_V depends in an essential way on the observation point P. All the known examples belong to the first class.

(which are absent in mathematical treatments of fractals, but are an evident necessity of any real-life experiment).

We first note that the catalogs provide measurement of the positions of galaxies away from us. In other words, we should consider a relatively small sphere around P and look with radial rays issuing from the sphere. In [5] it is shown that looking from a plane defines an equivalent problem, and we prefer that formulation. To further simplify the discussion in our examples we will consider a fractal embedded in 2 rather than 3 dimensions, illuminated by rays perpendicular to a randomly given baseline. In Fig. 1 we present a simple model of a fractal universe which is constructed hierarchically. At the nth level of the construction we see 4^n balls of size λ^n which are supposed to contain galaxies. At the $(n + 1)$th level each ball is further subdivided into 4 balls of size λ^{n+i}. To avoid non-generic effects we rotate the new group of balls with a random angle at each step of construction. Fig. 1 shows the set of balls at the 4th level with $\lambda = 0.4$. The fractal dimension of this example is $D = -\log(4)/\log(\lambda) = 1.5129$. The figure represents the visible set F_V (from a random line) as the lighted balls, whereas the invisible set (the complement of F_V) is shown as black balls. One can understand the theorem of [5] in the following intuitive sense. The projection (the footprint of the gray zone of Fig. 1) of the fractal on the line has dimension 1 when $D > 1$ [10, 11]. On the other hand, for the hierarchical construction up to level k, the balls have size λ^k, and thus the projection of the visible part has dimension 1 as soon as there are at least $1/\lambda^k$ visible balls (assuming they hide all others). The boundary between the gray zone and the white zone in Fig. 1 forms a graph of a function connecting the visible balls. In the kth level we call this function $f_k(x)$. Since the fractal set is constructed hierarchically, we expect a scaling relation $f_{k+1}(x) = \lambda^{-1} f_k (\lambda^{-1}x)$. This scaling relation guarantees that the graph cannot become too rough and will remain of dimension 1. To see this clearly think about the Weierstrass function $g(x)=\sum_{k=0}^{\infty} a^k \sin (b^k x)$. It is well known that the graph of this function is rough when $ab > 1$ and $a < 1$. Indeed, (cf. [12]) the Weierstrass function almost scales in the sense that

$$g(x)=a^{-1}g(bx)-a^{-1}\sin x. \tag{2}$$

The last term is smooth and its contribution to the dimension is negligible. Covering the graph with balls leads to the well known result $D = 2 — |\log a| / |\log b|$. But, in our analogous case, $a = \lambda$, $b = 1/\lambda$, leading to a 1-dimensional graph. Loosely speaking the stretching is not very strong in the y-direction, and the dimension of the graph (and hence of the visible set) remains 1. In fact, the same argument explains why in dimension $D < 1$ the visible part of a fractal has the same dimension as the fractal itself.

To illustrate these issues we consider first a fractal of dimension smaller than 2 (cf. Fig. 2). Here the visible and full sets will have the same dimension, as is demonstrated in Fig. 3, where we plot $\log C(r)$ vs. $\log r$ for both F and F_V (upper panel). Evidently the slope is the same for these sets. To demonstrate this fact further we present in the lower panel of Fig. 3 a plot of $\log C(r)$ for F vs. $\log C(r)$ for F_V. The slope of this line is unity, stressing the fact that the bulk of F is revealed in the visible subset F_V.

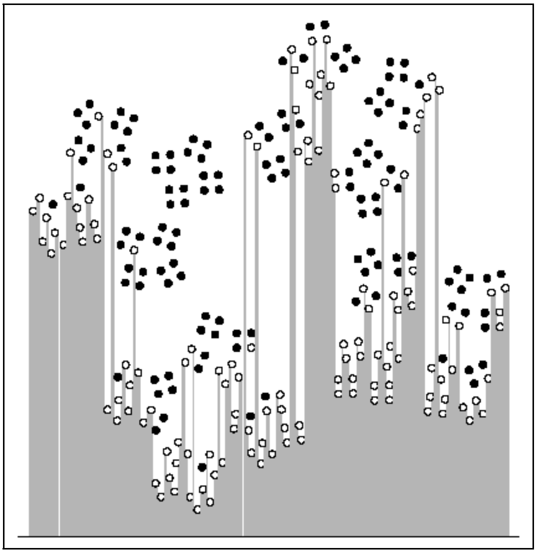

Fig. 1: A simple illustrative model for a fractal universe, drawn by a hierarchical construction at level 4, with the visible part in white, the invisible points in black. A disk is deemed visible as soon as any part of it is visible. Since the construction involves division by 4 and scale changes by $\lambda = 0.4$ the dimension is $D = -\log 4/\log \lambda \approx 1.51$.

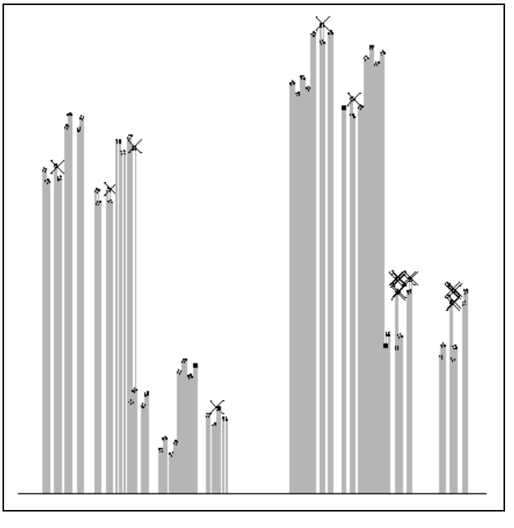

Fig. 2: A second model, as in Fig. 1, but now with dimension $D = 0.85$. Although $D < 1$, there are still hidden disks, and to make them appear more clearly, we marked them with an $\times$.

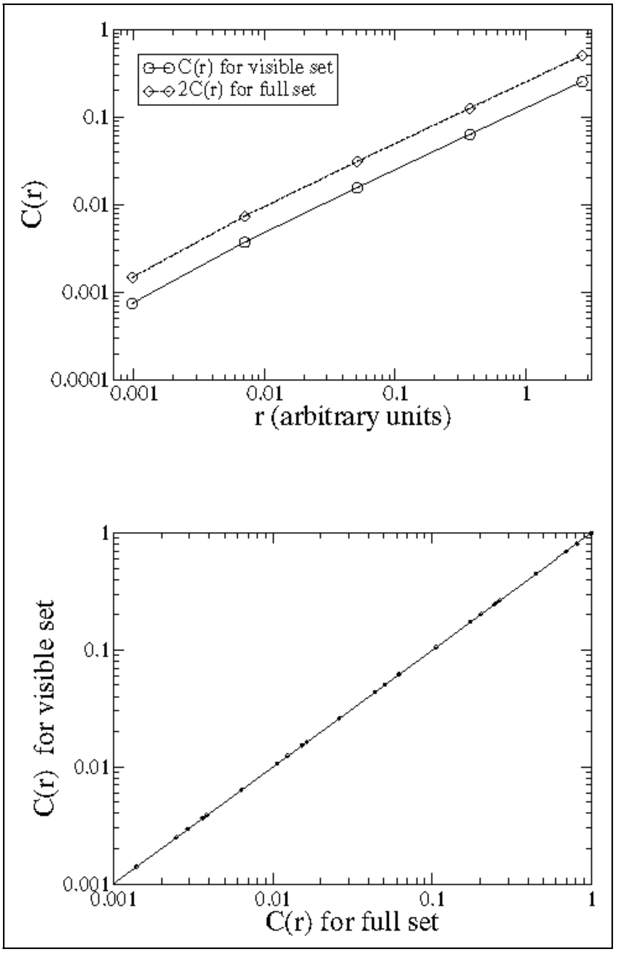

Fig. 3: Upper panel: The graphs of C(r) for the visible part and the full fractal of dimension D = 0.7, at level 6. The top curve is the binned number of pairs of points whose pairwise distance falls in the bin (in equal bins on the logarithmic scale) for the full set (multiplied by 2 to shift the curve up). The lower curve is the same for the visible part. The least square fits for the measured dimensions are D = 0.7095 ± 0.0036 and D = 0.71023 ± 0.0038. Lower panel: C(r) for the full fractal versus C(r) for the visible part at level 6. A least square fit gives a slope of 1.0002. Note that this does not at all mean that all disks are visible!

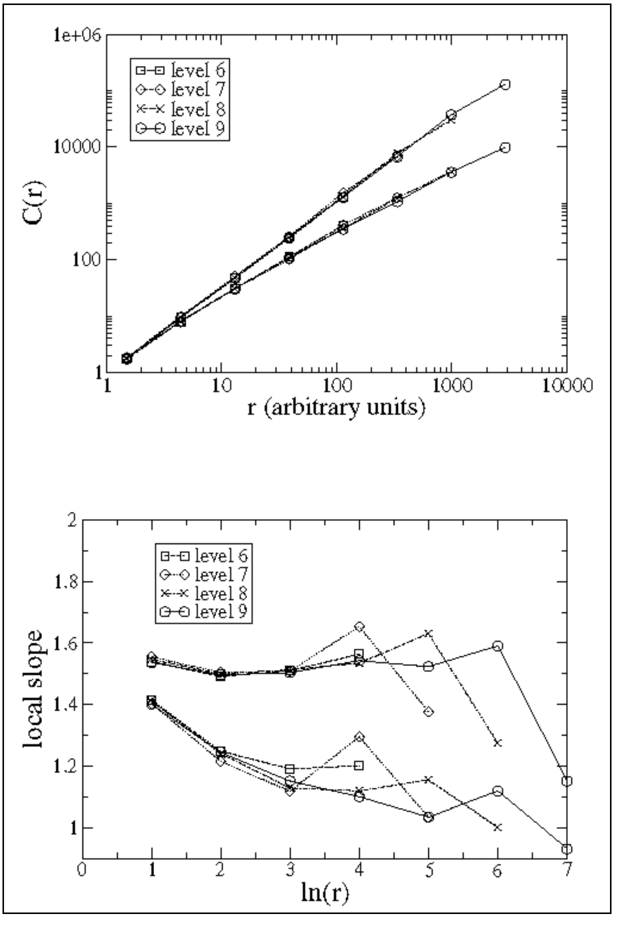

Fig. 4: Upper panel: Double logarithmic plot of C(r) vs. r for the visible and full sets of dimension D = 1.5. Shown are measurements for 4 consecutive levels of hierarchical construction (sets with 4^6 to 4^9 points). The data are normalized to collapse at the lowest available scale. Lower panel: The pointwise slopes (dimensions) of the curves in the upper panel. Note that the full set is seen to have dimension D = 1.5, while the visible part tends asymptotically to dimension 1 as the length scale increases.

The results change qualitatively when the dimension of the set is higher than 2. In the upper panel of Fig. 4 we present the double logarithmic plot of the correlation integral vs distance for F and F_V of the set of dimension 1.5 of Fig. 1. Clearly they do not scale in the same way, with the visible set settling on dimension 1 when larger and larger r are taken into account. This is underlined again by the results shown in the lower panel where the pointwise slopes of the curves in the upper panel are shown. Obviously the correlation integral for F settles nicely on dimension $D \approx 1.5$, whereas the local slope of the correlation integral for F_V tends to $D \approx 1$ as r increases. We stress that subdividing the set further in the hierarchic construction will not cure the problem. Quite on the contrary, it will make the visible set F_V a relatively smaller subset of the full set F. Unfortunately going deeper in the hierarchic construction is analogous to studying larger and deeper catalogs, so we cannot expect that newer and better data on the galaxy distributions may automatically cure the problem. We thus conclude that the results of the fractal analysis presented so far do not exclude a homogeneous universe with the fractal dimension of the full set of galaxies being as high as 3.

Lastly, we should investigate whether all is lost, or whether there is a way to probe the true dimension of the full set F from the knowledge of the visible set F_V. A modest way out is offered by the observation that the slopes of the curves in the upper panel of Fig. 4 *are very close at small* distances. This observation is underlined by the pointwise slopes of the curve in Fig. 4 at small distances. This is clearly a finite size effect which can be understood by looking again at Fig. 1. Due to the finite size of the smallest balls at this level of construction, many of the visible balls appear in groups of 4. This is due to the balls that were visible for the previous level of construction (4th in this case), mainly near the edge, but not only, which remain visible also after one step of refinement. With less degree of conviction one can also observe groups of 16 balls, or almost 16 balls, that are visible mainly near the visible edge. This finite size phenomenon will go away at the present small length scales when we subdivide many steps further, but will remain observable at the smallest available scales forever. This observation rationalizes why we get the "correct" dimension of the full set F from the smaller scales of the correlation integral.

These observations indicate that despite the mathematical impossibility of measuring the true dimension, its value may be gleaned from the behavior of the correlation integral at small scales. We stress that this possibility is not only due to close points (or galaxies) near the visible edge – also points that are far away from the observation line (or point P) contribute. Balls that are lighted at level n have high probability to give rise to a full set of lighted balls also in the next level, but not so for many subdivisions. Thus lighted balls will count the "right" dimension only with regard to small pairwise distances close to where they are. Once we try to count larger pairwise distances we unavoidable run to the problems explained above. Indeed, interestingly enough, it appears that the data analysis presented in [2-4] indicates a slight *increase* in the apparent dimension for smaller scales. We suggest that this increase may very well point to the true answer, namely, that the dimension of the set of galaxies is considerably larger than 2, and maybe even 3-dimensional in agreement with the expectations expressed in [6].

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Aspects of Fluctuations in Non-linear Biological Systems – Motion in Bistable Potentials and Selection Equations

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Two rather different topics are discussed with one common factor: they are driven by irregular influences. The first part considers the stochastic transition between potential minima over a maximum (barrier), and is treated as a Brownian motion description of reaction rates. We also discuss the related problem of "stochastic resonance", in which a small oscillating force synchronises transitions. In both these cases, the emphasis is on the formalism, and the relations between the two problems are stressed.
The other type of problem considers growth and competition equations of macromolecules, relevant for early molecular evolution on the path to the first life. Selection rules are simple and straightforward as long as competition essentially concerns limited resources. The situation gets more complex, when molecules are considered co-operative, e.g. they can catalyse growth processes. This corresponds to the hypercycle concept of Eigen, and is also a scenario for a RNA world. Components that use the support from other components may thrive, but can lead to the extermination of an entire system as the supporters may decline in the competition. As in the first part, the emphasis is on the formalism. We also take up probability aspects and problems that appear together with small probabilities and possibilities of exponential growth. Finally, the possibility of saving the co-operativity by spatial structures are discussed.

Key words: brownian motion, reaction rates, stochastic resonance, noise vs chaos, selection equations, error effects, hypercycles, RNA-world, parasites, spatial organisation

1. Introduction

At a first glimpse, the most important property of the world is that it is ordered. The order, the regularities, is what provides a meaningful existence. We look for regular laws that govern the events we see and relate them to an ordered description.

But, when we think closer, all is not order. There is always some disorder. And this is also needed to make the world meaningful. A completely ordered world, where everything was completely determined, going on as a clockwork, would be too stiff. Everything would be expected, and that also means that there could not be any development, no interesting activity.

The world needs both order and disorder. Complete order is the case at temperature zero, a frozen, regular world with no development and no time direction. Still, the world needs some order, some regularity, some structure. The disorder must not be dominating, the regular features must not be destroyed.

At the bottom, a source to disorder is the seemingly irregular motion of atoms, and also the statistical mechanical interpretation of the entropy concept which is a kind of driving force in nature, leading to the direction of time. In general, any system with a large number of more or less independent events (degrees of freedom) easily lead to uncontrolled action, what we may attribute as ”irregular behaviour”, sometimes ”noise”. An archetypal phenomenon is ”Brownian motion”, the irregular and observable motion of relatively large particles, governed by the action of small molecules. For a general survey of stochastic problems and appropriate formalism, see [1], and [2] for an overview of biological applications. Most motion inside cells as well as of the cells themselves may be described as Brownian motion.

Another source of apparent irregularity is what is referred to as ”deterministic chaos” [3]. I will here use the term (deterministic) chaos for an apparently irregular and unpredictable behaviour which at its bottom is based on a relatively simple and easily describable mechanism. In other words, disorder created by a systematic, simply described mechanism. Noise, on the other hand is disorder because of many degrees of freedom that leads to an uncontrolled behaviour. A difference between what we call noise and chaos may be a qualitative one, which depends on the number of degrees of freedom involved and the complexity of underlying events.

The theme of this article will be about the interplay between order and disorder for some quite different types of phenomena, all relevant to physical aspects of living systems.

At the lowest level, the thermal irregular atomic motion governs basic processes in an irregular manner [4, 5]. These lead to fluxes of energy, momentum and mass in all kinds of matter. The thermal fluctuations also drive structure changes and then reactions of macromolecules . Such processes can be regarded as comprised of a number of steps where a molecular system shall pass from a state with relatively low energy, over an energy barrier to a new low energy state. The energy needed for this can be provided by surrounding molecules as a Brownian motion procedure. The description of Brownian motion over a potential well and the formulation by a Fokker-Planck type of equation started with Kramers, [6], and was further developed in the 1980-s. A general survey of this formalism is found in [7].

There are also energy-consuming processes, where some energy source is used to accomplish an excitation which then leads to a passage over a barrier. Often, a process is basically of Brownian motion type, which may be accompanied by an energetic process that prevents a back flow and thus provides a unidirectional behaviour. Many muscle

processes, ion channel processes as well as cell motion mechanisms involve such steps, which again are of a basically stochastic type [8, 9].
In the brain, the basic generation of neural signals rely on the opening of ion channels [9], again governed by thermal, stochastic influences. This with necessity leads to the fact that brain signals are quite noisy[10], see also the general presentations in [11, 12]. To get a more ordered action, the brain makes use of large redundancies. Can the brain system even make benefits of noise [13]?
At a higher level, disorder enters the replication procedures that form the basis of individual reproduction and also evolution. As everywhere else, replication is not perfect and is governed by stochastic rules. There are always possibilities to introduce errors [14]. Again, this has two sides. It provides the bases of genetic variation: offsprings are never exact copies of the parents, which is the prerequisite for evolution. On the other hand, replication must also be quite accurate, most replicated molecules should be almost the same in order to get functioning individuals. As in other cases, there is a delicate balance between the necessity to have some errors and a risk that order is completely destroyed or that errors in the reproduction, the genetic variation, leads to individuals that may be destructive for a population. For the first stages of life, how could this problem have been put under control? General ideas about this were first discussed by Eigen [15].
This is a vast subject, and there is of course no chance to cover it in a single chapter as this one. The purpose here is rather to show some of the methodology used for this kind of problems, and how certain basic results can be derived. We will take up two quite different types of problems, not directly related, although there may be some common features. The first type of problem concerns transitions caused by random influences between two wells described by a potential with two minima. It is a problem of wide applications, and, as already said, treated as a problem of Brownian motion in a potential long ago by Kramers [6], and has been taken up in recent decades [7, 16 -18], also together with a related problem, that of stochastic resonance [19]: the fact that the random transitions can be synchronised by a relatively small periodic force. In connection to this, we will discuss some general aspects of random influences, i.e. noise in non-linear systems, also together with a systematic source to disorder: chaotic processes.
In the later parts of this article, we shall take up certain basic models that are thought to describe competition and evolution in primitive systems, on their way to Life.

2. Brownian Motion Description of the Passage over a Potential Barrier

Consider first the problem of a Brownian particle that moves in a potential of two wells with a barrier in between. We assume that the particle at the onset is confined to one of the wells. Because of the random force, it is possible for the particle to cross the potential barrier and go over to the other well. Our first problem is to calculate the probability rate by which this occurs.

We can write down an equation of motion, of a Langevin type [1], for this situation

$$m \frac{d^2x}{dt^2} = -\beta \frac{dx}{dt} - \phi'(x) + \xi(t) \tag{1}$$

The first term on the right hand side is due to friction damping, and β is a friction strength. $\phi(x)$ is the potential. ξ represents the random force, of white noise type with a δ-function correlation relation: $<\xi(t)\xi(t')> = 2\beta kT\ \delta(t-t')$. Note that the coefficient of this term and the damping are related. In most of the discussion, we shall use the more convenient parameter $\gamma = \beta/m$ of dimension 1/time.
The equation of motion with a linear force can be treated by analytic, exact methods. For general potentials, however, one has to use simulation methods, which are rather cumbersome and non-systematic. We will not use such an approach here, but mention that one in such cases has to be cautious about the singular function representing the random force when applying numerical methods. In particular, the velocity has no time-derivative in any point, while the existence of derivatives is usually assumed and used in integration algorithms.
We shall rather, use an equivalent description where the Brownian motion is described by a probability function $P(v,x)$ of velocity v and position x. For this, we have the Fokker-Planck equation, first considered for this problem by Kramers [6]:

$$\frac{\partial P}{\partial t} + v \cdot \frac{\partial P}{\partial x} - \frac{\phi'(x)}{m} \cdot \frac{\partial P}{\partial v} = \gamma \left[\frac{\partial (vP)}{\partial v} + \frac{kT}{m} \cdot \frac{\partial^2 P}{\partial v^2} \right] \tag{2}$$

First, consider a situation of a strong damping, in which case the velocity is almost Maxwell-distributed. We get a transition rate from the probability change with time and there is a term that represents a flow. We introduce an approximate probability:

$$P(v,x,t) \approx P_0(x,t) e^{-mv^2/2kT} + P_1(x,t) v\, e^{-mv^2/2kT} \tag{3}$$

When this is introduced in the Fokker-Planck equation, we distinguish terms of two kinds: The first type consist of those that are even in velocity:

$$\left[\frac{\partial P_0}{\partial t} + v^2 \frac{\partial P_1}{\partial x} \right] e^{-mv^2/2kT}$$

and the second type of those that are odd in v:

$$v \left[\frac{\partial P_1}{\partial t} + \gamma P_1 + \frac{\partial P_0}{\partial x} + \frac{\phi'}{kT} P_0 \right] e^{-mv^2/2kT}$$

If we integrate the Fokker-Planck equation over the velocity, the contribution that is odd in v is zero. v^2 gives a factor kT/m, so we get the relation:

$$\frac{\partial P_0}{\partial t} + \frac{kT}{m}\frac{\partial P_1}{\partial x} = 0 \tag{4}$$

To get the contribution from the odd terms, multiply the equation by the velocity and integrate. The result is:

$$\frac{\partial P_1}{\partial t} + \gamma P_1 + \frac{\partial P_0}{\partial x} + \frac{\phi'}{kT} P_0 = 0 \tag{5}$$

The process we are interested in, the passage of the barrier is slow with a time scale much larger than 1/γ. For this reason, we can neglect the time derivative in (5). Thus, (4) + (5) without time derivative make the main set of equations for our problem. There are several ways to get a result from these equations, but we will here use a scheme that is related to that of Kramers [6]. Neglecting the time derivative, (5) can be written as:

$$P_1 e^{\phi/kT} = -\frac{1}{\gamma}\frac{\partial}{\partial x}\left[e^{\phi/kT} P_0\right] \tag{5a}$$

First, we consider the general appearance of the functions P_0 and P_1. P_0 is close to a Boltzmann-distribution exp($-\phi\ /kT$) in the well. P_1 is roughly the integral over this, starting from zero at the far side of the potential maximum, increasing around the potential minimum, and then essentially constant close to the potential maximum, where it represents the flux between wells.
Now integrate (4) over the potential well, where the particle is at the onset. The integral of $\partial P_0 / \partial t$ is the time change of the total probability, W, that the particle is in that well. The corresponding integral for the P_1 -term provides the value of P_1 at the potential top. Thus:

$\partial W / \partial t = -\ (kT/m)\ P_1$ (top)

The right hand side corresponds to the rate we look for. Now, integrate our rewritten expression (5a) over the position x from the potential bottom to the top. The right hand side gives the difference between the values at the top and the bottom. We then assume a situation where the probability distribution is essentially confined to one well. Inside this well, the probability is close to the Boltzmann-type distribution exp($-\phi(x)/kT$), but at the top, P_0 which is flowing over to the other well goes down and can be put to zero. If the wells are symmetric, this is strictly so for symmetry reasons. As P_1 increases and goes to a maximum at the top, the integral at the left hand side of (5a) gets its largest values from points close to the potential top. We may there neglect the variation of P_0. Thus, the integral over the left hand side is that of the exponential function which has a maximum at the top. One gets:

$$P_1(top) \approx \frac{1}{\gamma}\frac{P_{0b}\,e^{-\Delta/kT}}{\int e^{\phi/kT}}$$

The index '*b*' refers to the potential bottom. P_{0b} is essentially the normalisation factor for the distribution. It can be assumed that the potential close to the bottom can be written as a harmonic potential: $\phi_b(x) = c_1(x-x_b)^2/2$, where x_b is the position of the potential minimum. This part will dominate the distribution, and P_{0b} is essentially the inverse of the integral of $\exp(-\phi_b(x)/kT)$, equal to $(c_1/2\pi kT)^{½}$.
The integral of $\exp(\phi(x)/kT)$ is dominated by he appearance at the top, which can be written as: $\phi_T(x) = \Delta - c_2(x-x_T)^2$. Δ is the energy height of the barrier and x_T is the position of the potential maximum.) If this is used for the integral, one gets

$$\int \exp(\varphi(x)/kT)\,dx = e^{\frac{\Delta}{kT}} \int^{x_t} e^{-c_2(x-x_t)^2/2kT}\,dx = e^{\frac{\Delta}{kT}}\sqrt{\frac{\pi kT}{2c_2}}$$

This provides the following (Kramers') result for the flow over the barrier.

$$\frac{kT}{m}P_1(\text{top}) = \frac{\sqrt{c_1 c_2}}{\gamma\pi m}\cdot e^{-\Delta/kT} \tag{6}$$

The exponential factor will always enter this kind of rate, but the factor in front is less clear. In the case of large friction it is inversely proportional to the friction coefficient γ.
There are other possibilities to derive a result like this and the precise definition of the rate may vary. The main factors remain the same. Another method is to treat this as an eigenvalue problem, and define the rate as the lowest non-zero eigenvalue, see [7], [16, 18].
The formula is valid at large damping where the most relevant time constant is given by the damping. The expression can be generalised by introducing a time constant of motion close to the top, which determines the time scale of the barrier passage. This is given by the (noise-free) differential equation at the top:

$$\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} - \frac{c_2}{m}(x - x_{top}) = 0$$

The positive time constant of an exponentially increasing x is:

$$-\frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} + \frac{c_2}{m}}$$