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PREFACE

BIOLOGY, PHYSICS AND NONLINEAR SCIENCE

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This special issue of the *Journal of Nonlinear Mathematical Physics (JNMP)* is devoted to **Nonlinear Mathematical Biophysics**.

The first part of the present century and the end of the previous one have witnessed an impressive acceleration in the development of Biology, both at the experimental and at the theoretical level. This development of Biology also took with itself on the one hand a growing role of Mathematics, and on the other a greater interaction with Physics.^a

The present Special Issue does, as its title suggests, concentrate on Biological issues which are closer to the scope of *JNMP*; that is, it deals with nonlinear biological and biophysical processes and attempts to treat them according to the standards of Mathematical Physics. Even with such a specification, the number of biological subjects which should enter in such a collection is huge; this issue does actually, with a quite arbitrary choice due to the issue editor, focus mainly on two special subjects, i.e. on the one hand the *Nonlinear dynamics of biological macromolecules* (in particular, DNA), and on the other the *Mathematical aspects of the theory of Evolution*.

I hope these papers will be of interest to the readers of *JNMP*, and maybe will attract some mathematical physicists, and more generally nonlinear scientists, to this beautiful subject. Hopefully, this will also result in more Nonlinear Mathematical Biophysics papers appearing in *JNMP*.

It is probably worth adding a few words, and bibliographical indication, in guise of Introduction to the Papers collected here; needless to say, no attempt at completeness of discussion or of references is attempted (nor thinkable), and the selection of sources reflects my own preferences — and favors books and review papers.

^aThis is also witnessed by the appearance of a growing number of textbooks on the subject, see e.g. [2, 7, 23, 29, 41, 61–63, 82].

Nonlinear dynamics of macromolecules

The nonlinear dynamics of macromolecules, and in particular of DNA, has been widely studied in the last decades; different communities have followed different approaches, ranging from all-atoms numerical simulations (necessarily involving only a short part of the DNA macromolecule) to extremely simplified models, considering DNA as an elastic rod or as an assembly of identical units with one or few degrees of freedom per unit.

To give an idea of the complexity of the molecule, we just mention that DNA is made of an assembly of nucleotides, organized in two long chains, which are themselves organized into a double helix, which winds into higher order structures, up to chromosomes [13]. Each of the nucleotides is made of about 30 atoms (depending on the nitrogen base included in it, see below), and each chain includes, depending on the species, a very large number of nucleotides, e.g. $2.2 \cdot 10^8$ in the longest human chromosome [37]; all in all, we are facing a system with about 10^{10} degrees of freedom.

The nucleotides are made of two different parts: the external one is a sugar-phosphate group, connecting to the same groups of adjacent nucleotides to form the long backbone chains; the internal one (linked by a covalent bond to the sugar ring) is a nitrogen base, which can be of four types: Adenine (A), Guanine (G), Cytosine (C) and Thymine (T). The bases at corresponding sites on opposite chains must be one of the Watson–Crick pairs (A-T or G-C) [91] and link to each other via H-bonds (two for A-T, three for G-C). The genetical information is coded in the base sequence, i.e. in the inhomogeneous part of the DNA double chain. The reader is referred e.g. to [13, 34, 83, 89] for more detail on DNA.

Needless to say, such a structural complexity — which corresponds to a wealth of different biological functions — defies any attempt of detailed description in terms of Mathematical Physics modelling (and not only). Thus analytically-oriented researchers have focused on specific aspects of DNA functioning and have developed simplified models for the dynamics of DNA involved in these functions, in particular selecting relevant degrees of freedom and considering certain other ones as effectively frozen due to their large activation energy. The resulting models have just a few degrees of freedom — usually one or two — per nucleotide.

These simple *mesoscopic* nonlinear models are attractive to mathematical physicists; they can be roughly classified into two classes, depending on the kind of motions they are primarily focusing on (corresponding to different biological processes undergone by DNA), i.e. *vibrational* and *torsional*; the most widely studied models are associated, respectively, with the names of Peyrard, Bishop and Dauxois [74, 75] (see also [5, 6, 14, 15]), and to that of Yakushevich [95] (see also [40, 86, 98, 99]). The interest in these soliton-bearing models, surely due also to the success of the theory of Davydov’s soliton [19] in alpha-helices, was started by the pioneering paper by Englander *et al.* [30], and continued since then. The interested reader can consult the books by Peyrard and Dauxois [77] and by Yakushevich [96], or the review paper by Peyrard [72]; see also [17, 71, 73, 76]. Nowadays, these models face the challenge put by data obtained in single-molecule experiments [10, 11, 50, 81, 84, 85].

Several papers in this Special Issue are concerned with DNA and with this class of DNA models. I would mention first of all the paper by Ribezzi–Crivellari, Wagner and Ritort [80] dealing with the problem of determining proper parameters in DNA modelling, and focusing in particular on kinetic parameters for DNA hairpins under tension. The paper by Ogden, Saccomandi and Sgura [66] deals with a phenomenological continuum model of DNA, and in particular aims at describing DNA overstretching. The paper by

Joyeux [43] and the one by Rapti, Rasmussen and Bishop [79] both deal with the transfer-integral operator method for the study of one-dimensional models of DNA, in the first case within an approach leading to a pseudo-Schroedinger equation and in the second one within the Peyrard–Bishop–Dauxois approach. The latter is also the framework in which Theodorakopoulos [88] discusses several phenomena in genomic DNA, and how parameters can be chosen, and computation performed efficiently. The work by Zdravkovic [100], which also contains a large Bibliography, considers a version of the Peyrard–Bishop model, first considered by Dauxois [18], which takes into account the peculiar helicoidal geometry of DNA. Finally, the remaining two papers both consider inhomogeneous DNA models. The work by Yakushevich [97] looks in detail at the rotational dynamics of a pair of bases, subject to intrapair interaction as well as to stacking interactions with nearby base pairs, taking also into account the helicoidal geometry; in their work Cadoni, De Leo and Demelio [12] study numerically the inhomogeneous version of a “composite” DNA model in which the nitrogen base and the sugar-phosphate backbone are modelled by different degrees of freedom, showing how the homogeneous degree of freedom dominates and allows for long-lived solitons despite inhomogeneities.

Mathematical aspects of the theory of Evolution

The use of mathematical tools to study the evolution of a population goes back to Leonardo da Pisa, also known as Fibonacci; and the discovery by Mendel of the laws of heredity in diploid species is surely a relevant example of application of Statistics to Biology.

Leaving aside such noble ancestors, in the XXth century several scientists attempted at a quantitative analysis of Darwin’s theory of Natural Evolution, starting with the classical works by Haldane, Fisher and Wright in the twenties [31, 32, 38, 39, 94] (transmitted to a wider community by Dobzhansky [22]); it should also be recalled that the FKPP reaction-diffusion equation [33, 47, 90] was developed by Fisher and by Kolmogorov, Petrovsky and Piskunov to describe the diffusion of an advantageous gene in a population. See e.g. [16, 53, 59] for more recent discussions of Evolution by mathematically-oriented leading biologists.

As well known Evolution is based on the interplay of *Competition* (for the available — and necessarily limited — resources), and *Mutation*. It is thus not a surprise that the dynamics of populations of interest for Evolution is nonlinear^b, and that stochastic effects are relevant in it — albeit one can within certain approximations just consider average behaviors.

One should not overlook the relevance of *neutral evolution*, which is of stochastic origin. This was actually already considered by Darwin: indeed, in the very first part chapter IV of *The Origin of Species*, immediately after the very famous phrase introducing the concept of natural selection, i.e. “*This preservation of favourable variations and the rejection of injurious variations, I call Natural Selection*”, Darwin adds: “*Variations neither useful nor injurious would not be affected by natural selection, and would be left a fluctuating element,*

^bLinear behavior and hence exponential growth are obtained in the so called malthusian model (actually Malthus’ work was devoted to showing the inconsistency of such a linear model), which applies for unlimited resources; nonlinearity sets in as a consequence of limited resources and hence of competition to secure them.

as perhaps we see in the species called *polymorphic*". In modern times, neutral evolution was introduced and studied mathematically by Kimura [16, 45, 46, 67].

The basic quantitative function attached to a species in Darwin's approach is its *fitness*, i.e. the expected number of descendants per individual in the given species. This is a statistical quantity, and it will depend on the environment; in general it depends also on the details of the competition for resources, i.e. on the fraction of other species or groups present in the overall population and hence competing with the given one. Thus the fitness is a function (in general, nonlinear) of the composition of competing populations and of the genetic character of a given species.

The general public is aware of the approach via *game theory* through the popular book by Dawkins [20]; deeper treatments are provided e.g. by [3, 52, 57, 58, 60, 92]. Roughly speaking, this approach amounts (at least in its simpler form) to the assumption that the fitness of a species depends linearly on the relative abundance of other competing species in the overall population. This assumption is quite reasonable, and produces meaningful predictions, in a range of situations.

Needless to say the linearity hypothesis is not always valid, and one has to resort to different approaches; there will be a *fitness landscape* modelling the evolutionary possibilities, more and less like an energy landscape describing the possibilities for the time evolution of a thermal system (in the biological case the stochastic effects are due to random mutations, the rate of mutations being somehow an analogue of the temperature). Physicists and mathematical physicists are naturally attracted by this approach based on Statistical Mechanics (see e.g. [69] for a very readable introduction).

It was also realized that Evolution is at work not only on animals and more generally on living being, but also at the molecular level [24, 26, 44], which of course provided opportunity for experiments showing Evolution at work on short timescales. The work of Eigen [24, 26] introduces the key concept of a *quasi-species* [8, 25, 27, 48, 93].

The combination of these two concepts, fitness landscape and quasi-species, is at the basis of the modern mathematical theory of evolution [35, 36] (see also [21, 49, 65, 68, 70, 87]).^c It would make no sense to attempt even a very cursory description of this here^d, so I will just stop these few words now.

Several papers in this Special Issue are concerned with the mathematical theory of Evolution. The work by A.G.M. Neves [64] provides some rigorous results on the Eigen quasispecies model (see above) in the so called "sharp-peak landscape", analyzing the case with a periodically changing optimal genome. In their work, F. Bagnoli and P. Liò [4] discuss how the interplay of mutations and selection (i.e. of the two basic ingredients of Evolution) organizes the fitness landscape. Last but not least, in their review K. Jain and S. Seetharaman [42] discuss nonlinear deterministic equations in biological evolution; that is, they consider models of biological evolution in which the population frequency changes

^cOne should be warned that while the basic mathematical tools are simple enough when considering species which reproduces asexually, the situation becomes quite more involved in the case of sexual reproduction, i.e. of recombination of genetic material proceeding from different parents [9, 56, 78].

^dI will just mention that it is nowadays possible to study Evolution *in vitro*, thanks to experiments on evolution of very simple living beings such as viruses [28, 51, 55]; this study is confirming the vision of Darwin, and providing new hints for further developments of the theory [1, 54].

deterministically with time (considering average behaviors), this change being described by nonlinear equations.

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