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Young Researchers

Modelling Biological Processes

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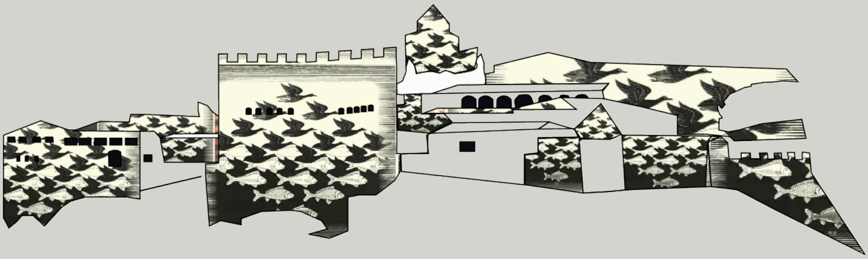
BOOK OF ABSTRACTS

BIOMAT 2012

Self-organization & collective dynamics in the Life Sciences

swarms, biofilms, traffic



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1. Binary interaction algorithms for the simulation of flocking and swarming dynamics

Microscopic models of flocking and swarming takes in account large numbers of interacting individuals. Numerical resolution of large flocks implies huge computational costs. Typically for N interacting individuals we have a cost of $O(N^2)$. We tackle the problem numerically by considering approximated binary interaction dynamics described by kinetic equations and simulating such equations by suitable stochastic methods. This approach permits to compute approximate solutions as functions of a small scaling parameter at a reduced complexity of $O(N)$ operations. Several numerical results show the efficiency of the algorithms proposed.

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2. Optimization problems in radiotherapy dosimetry planning

Selecting a suitable radiation strategy for any given patient is a key issue in radiotherapy. To achieve that aim, one has to determine the dose which achieves better tumour control probability over a selected planning target volume, as well as the manner to deliver it which minimizes damage on nearby healthy tissues and organs at risk. To do this, the clinicians involved have to select one among several (usually few) tentative dose distributions, and to make that choice they largely rely on personal experience rather than on quantitative arguments. For this reason, the development of computational tools that may help in such decision-making process is a long-standing goal in the field.

In this talk we will consider one aspect of the general problem described above. Specifically, a mathematical model will be presented to select a dose distribution which achieves efficient radiobiological effects on actual clinical situations. Our model is formulated as a variational problem where suitable constraints are included to account for clinical requirements and operational limitations [1]. Under appropriate assumptions on the radiobiological data and parameters involved, the problem thus obtained is shown to possess a unique solution. The relevance of such solution will then be discussed by means of a retrospective study involving a number of clinical cases.

[1] J.C.L. Alfonso, G. Buttazzo, B. García-Archilla, M. A. Herrero and L. Núñez, A class of optimization problems in radiotherapy dosimetry planning, *Accepted in AIMS DCDS-B* **17; 6(3)**, (2012).

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3. A new family of traveling wave solutions to a non–linear reaction diffusion system

We present the analysis of traveling wave solutions to a nonlinear flux limited PDE coupled with a Fisher–Kolmogorov– Petrovski–Piskunov type reaction term. It is found that for wave speeds high enough there exist classical traveling wave solutions, but as the wave velocity lowers we get a structural bifurcation into discontinuous traveling waves that are reminiscent of hyperbolic shock waves. These particular solutions may be relevant in biological contexts as they provide models by which the whole solution (and not just the bulk of it, as it is the case with classical traveling waves) spreads through with finite speed.

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4. A new probabilistic approach to crowd dynamics for applications in built environment

Performaces of real world pedestrian facilities, such as pedestrian loads on footbridges or walkway serviceability, are evaluated in probabilistic terms in the current engineering and architectural practice. Bearing this in mind, a new probability-based approach to the modeling of crowd flows is proposed. The position of each pedestrian in a given walking area is expressed in terms of a time-evolving probability measure, whose evolution law is deduced consistently with non-local anisotropic microscopic models of the behavior of single walkers, including mutual pedestrian interactions. This approach allows one to account for uncertainties in initial/boundary conditions of crowd flow, as well as to provide occupancy statistics, without making use of several repeated simulations based on random sampling algorithms.

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5. The hierarchical structure of throphic networks

The research in the field of ecological networks is becoming more and more relevant given the increasing pressure that ecosystems are facing, which makes the study of their topology especially interesting due to its interconnectance with the dynamical processes taking place on them.
One of the most characteristic features of the structure of food webs is the existence of trophic levels: the prey of any given species tend to occupy similar levels within this

structure. Many models have been put forward to account for this food-web topology, all of them reliant on some kind of hidden variable – ecological niche, genetic distance, etc – with the niche model, one of their main exponents, becoming a kind of a benchmark for the study of food webs.
However, we show that a hierarchical network of this sort requires two parameters to be properly described: the coherence of the hierarchy and the contiguity of the prey. We also put forward a simple self-assembling network model, in which species are added sequentially to the network and prey are selected according to their trophic level, a purely structural property. This shows that realistic food-web topologies can be generated without need for any hidden variable.

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6. Modelling radiotherapy for low–grade gliomas

Gliomas are infiltrative brain tumours. This implies a problem for clinicians: the main part of the tumour is invisible because the cell density is underside the detection threshold [1] and it is not possible to make a resection of the whole tumour without removing healthy brain tissue. Inevitably an anaplastic transformation occurs, that rapidly causes the demise of the patient.

Even if radiotherapy allows to improve the quality of life, after a certain time, the tumour restarts to grow. Radiotherapy leads to damages to the DNA strands, causing apoptosis of dividing cells in a short time (in about 1 day). One would expect to observe a sudden decrease of the radius of the tumour just after the treatment. On the contrary, the tumour decrease is quite slow and can continue during sereval months.

Apparently, the velocity change due to the post radiotherapy is a prognostic factor for low-grade gliomas and seems to be a quantitative parameter to predict long-term outcomes [2]. This agrees with an other study wich shows that the velocity is an important survival criterion [3].

In a previous work [4], we applied a diffusion-proliferation model to patients and we estimated the age of the patient at the onset of the tumour. In parallel, we analysed biopsy samples of about 10 low-grade gliomas and we showed that edema is responsible for the MRI-defined abnormalities (work in progress). In this work, we modify the model to take into account edema and we apply it to patients who received radiotherapy.

We demonstrate that our model reproduces quite well the real data. This model could be used to estimate the duration of the treatment efficacity.

[1] J. Pallud *et al*, Diffuse low-grade oligodendrogliomas extend beyond MRI-defined abnormalities, *Neurology* **74**, (2010), 1724–1731.

[2] J. Pallud *et al*, Dynamic imaging response following radiation therapy predicts long-term outcomes for diffuse low-grade gliomas, *Neuro-Oncology*, (2012), 496–505.

[3] E. Mandonnet *et al*, Continuous growth of mean tumor diameter in a subset of grade II gliomas, *Annals of Neurology* **53**, (2003), 524–528.

[4] C. Gerin *et al*, Improving the time-machine: estimating date of birth of grade II gliomas, *Cell Proliferation* **45**, (2012), 76–90.

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7. Stochastic Amplification in Neural Networks

The cerebral cortex exhibits complex patterns of oscillations even in the absence of external stimuli. Deciphering its nature, structure and function are challenging tasks. Cortical local field potentials are bistable and can fluctuate spontaneously between a quiescent (Down) and an active (Up) state, generating slow δ oscillations (also known as Up-and-Down States). Experimental evidence shows that spontaneous high oscillations (in the $\beta - \gamma$ band) emerge within Up states [1]; remarkably, similar oscillations do not appear in Down states. Moreover, this rhythm within Up states seems to be a collective phenomenon given that individual neurons do not lock to it. Our conclusion, supported by both theory and simulations, is that the collective phenomenon of "stochastic amplification of fluctuations" –previously described in other contexts such as Ecology [2] and Epidemiology– explains in an elegant manner, beyond model-dependent details, all the intriguing phenomenology of Up-and-Down states*.

[1] A. Compte, M.V. Sanchez-Vives, D.A. McCormick, X.J. Wang, *J. Neurophysiol.* **89**, (2003), 2707–2725.

[2] A.J. McKane, T.J. Newman, *Phys. Rev. Lett.* **94**, (2005), 218102–218105.

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8. The meaning of niche: Cause or consequence of food-web structure?

Food webs –networks of predators and prey– have long been known to exhibit intervality: species can be ordered along a single axis in such a way that the prey of any given predator tend to lie on unbroken intervals. Although the meaning of this niche dimension has remained a mystery, it is assumed to be the reason behind the highly non-trivial structure of food webs. For decades, therefore, most food-web modelling has been based on assigning species a niche value by hand. However, going on empirical evidence and a simple self-assembling network model, we show that realistic intervality can come about as a consequence of biologically plausible mechanisms that do not require an a priori ordering. We conclude that the niche dimension – in the sense used for modelling – is in fact an emergent property of food-web structure [1].

[1] S. Johnson, V. Domínguez-García and M.A. Muñoz, The meaning of niche: Cause or consequence of food-web structure?, *Submitted*.

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9. A new interaction potential for swarming models

We consider a self-propelled interacting particle system, which has been frequently used to model complex behavior of swarms such as fish schools or birds flocks. Typically, the model is equipped with the Morse potential. For this and other potentials patterns such as aligned flocks and rotating mills emerge in particle simulations. These stationary states can however not be computed a priori in general, except for some special cases such as one-dimensional flocks. We present a class of interaction potentials, that we call Quasi-Morse potentials, which likewise generate flocks and rotating mills. However, their stationary states can be explicitly computed as (affine) linear combinations of up to three elementary functions, only whose scalar coefficients have to be obtained numerically. No time evolution needs to be simulated. The potentials are constructed from certain solutions of linear PDEs and fulfill all desirable biological properties. We present the formulae for the mill and flock solutions, verify our results by comparing to corresponding particle simulations and illustrate parameter dependencies.

[1] J. A. Carrillo, S. Martin, V. Panferov, A new interaction potential for swarming models, *submitted* preprint: arxiv.org/abs/1204.2567

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10. Modeling biofilms formation and evolution in drinking water distribution systems using a multi-agent approach

Biofilms develop in drinking water distribution systems (DWDs) as complex communities of microorganisms bound by an extracellular polysaccharide polymer, the glycocalyx, which provides them structure, protection and helps to retain food. These communities of organisms form spontaneously in the presence of moisture and bind strongly against the initial repulsion at the inner pipe wall and modified it as capture more nutrients and new bacteria.

A developed biofilm is very strong and a problem when you need a clean and disinfected environment. Apart from the health risk that biofilms in DWDSs may be, due to them role as microbial pathogens reservoir [1] biofilms are responsible for many other DWDSs problems. For example: aesthetical deterioration of the water, proliferation of higher organisms, operational problems, biocorrosion, consumption of disinfectant, etc. Although in most countries regulated quantities of residual disinfectant are present in the DWDSs these are not enough to avoid the presence of biofilms in these systems. So nowadays, biofilms represent a paradigm in the management of water quality in all DWDS. A number of studies have been approached on the reasons and effects of the biofilms in DWDSs, both in the microbiological and in the engineering fields. The survival and regrowth of microorganisms in DWDSs can be affected by not only biological factors but also interaction of various physico-chemical and hydraulics factors. The DWDSs constitutes the major part of water treatment utilities. In these systems many biological and physicochemical reactions occur creating heterogeneous habitats in the same distribution system over time and space, making biofilms exist at different levels in these systems. Many are the factors within the DWDS that affect biofilms development.

The aim of our study is modeling biofilms formation and evolution in DWDSs using the currently available information of the DWDSs physical and hydraulic conditions that affect biofilm development. This will be done using Multi-Agent Systems (MASs) as modeling tool to achieve this purpose.

A multi-agent system consists of a population of autonomous entities (agents) situated in a shared structured framework (environment). These agents operate independently but also are able to interact with their environment, coordinating themselves with other agents. This coordination may imply cooperation if the agent society works towards common. Thus, in a cooperative community, agents have usually individual capabilities which, combined, will lead to solving the entire problem. But cooperation is not always possible and there are instances where agents are competitive, having divergent goals. In this later case, the agent also should take into account the actions of the others. However, even if the agents are able to act and achieve their goals by themselves, it may be beneficial to partially cooperate for better performance, thereby forming coalitions. Turning on to coordinating activities, either in a cooperative or a competitive environment, one basic way to solve the potential conflicts that may arise among agents is by means of negotiation. Negotiation may be seen as the process of identifying interactions based on communication and reasoning regarding the state and intentions of other agents. There are some properties which agents should satisfy [2]: reactivity, perceiving their environment; pro-activeness, being able to take initiative; and social ability, interacting with other agents. Besides, the agents are computationally efficient because concurrency of computation is exploited as long as communication is kept minimal. We dispose of agents with redundant characteristics which offer system reliability. This system is easy to maintain by the agent modularity that allows us to handle their properties locally. Agents are able to organize themselves to adapt their activity on different environments and even to solve different problems. Regarding the environment, a list of their more important characteristics is the next: it structures the multi-agent system as a whole; it manages resources and services, maintaining ongoing activities in the system and defining concrete means for the agents to communicate.

The studies about biofilm resulted in descriptive and functional knowledge of biofilms. Biofilms modeling allows to check hypothesis on their mechanisms and to predict its evolution depending on time. The agents are defined as bacterial colonies cores; due to the high biofilm density reached in these systems. Theses cores mimic the behavior of individual bacteria. Once agents have been defined and their relationships established, a schedule of combined actions on these objects defines a processes occurring, in their environment, over time. In this study the environment is represented by the inner part of a pipe where the biofilms develop. This study attempts to build a multi-agent biofilm model, based on a limited number of basic interactions between bacteria and hydraulics and physical characteristics of the pipes in DWDSs, but able to represent the spatial and temporal variation of attached biofilm quantity.

[1] M. Wooldridge, An Introduction to MultiAgent Systems - Second Edition, *John Wiley & Sons*, (2009).

[2] J. Wingender, Biofilms in drinking water and their role as reservoir for pathogens, *International Journal of Hygiene and Environmental Health* **214**, (2011), 417–423.

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11. How do social insects manage to form geodesic paths in a bounded region?

Social insects are an important example of complex collective behavior. In particular, ant colonies develop different tasks as foraging, building and allocation [1]. While they search for food they deposit a pheromone that it is considered as a crucial element in the mechanism for finding minimal paths. The experimental observations suggest that the model should include the presence of pheromone and the persistence (tendency to follow straight paths in the absence of other effects).

In our study [2], we will consider ants as random walkers where the probability to move in one or another direction is influenced by the concentration of pheromone near them (*reinforced random walks*). We are mainly interested not in an individual random walker but rather on a large number of random walkers, their collective behavior, and the possibility for them to aggregate forming geodesic paths between the nest and the boundary.

We investigate the behavior of ants in a disk of 50cm of diameter. The statistical analysis performed from the measurements in real experiments show that, in absence of chemotactic stimuli, ants follow a distribution formed by a normal distribution plus a pareto tail. Our computational and analytical results show that in order for the ants to follow shortest paths between nest and boundary, it is necessary to superimpose to the ants' random walk the chemotactic reinforcement. It is also needed a certain degree of persistence so that ants tend to move preferably without changing their direction much.

[1] B. Hölldobler and K. Wilson, *The ants, Berlin: Springer*, (1990).

[2] M. Vela-Pérez, M.A. Fontelos and J.J.L. Velázquez, Ant foraging and minimal paths in simple graphs, *Submitted for publication*.

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12. Non–planar front propagation and its properties for space–heterogeneous reaction–diffusion equation. Cylindrical type domain

We are concerned in this paper with travelling wave solutions in the cylinder of following equation

$$\begin{cases} u_t - \Delta u = f(x_1 - ct, y, u) & t > 0,\ x_1 \in \mathbb{R},\ y \in \omega \\ \partial_\nu u(t, x_1, y) = 0 & t > 0,\ x_1 \in \mathbb{R},\ y \in \partial\omega, \end{cases} \tag{1}$$

$c > 0$ is the propagation speed, ν denotes the exterior unit normal vector field to a cylindrical domain Ω, $u(t, x) : (\mathbb{R}^+, \emptyset) \to \mathbb{R}$, and $f : (\emptyset, \mathbb{R}^+) \to \mathbb{R}$.

This kind of equation was first introduced in [1] in one dimension case, and was generalized in [2] and [3] for multidimensions to study a more general model of the impact of climate change on the dynamics of biological species, that are sensitive to say the temperature range.

In the present paper, we would like to extend the results of [3] in the infinite cylinder Ω by allowing a greater generality assumption on the function f, this can be viewed as a more general class of "favourable zone". We set up the analogous results to [3] such as the necessary and sufficient conditions for existence and uniqueness of travelling front, that is the solution of the type $u(t, x_1, y) = U(x_1 - ct, y)$, characterized by the sign of the generalized principal eigenvalue $\lambda_{1,N}$. We also present in this paper some further properties of travelling front such as asymptotic behaviour and monotonicity, which were not discussed in [3].

We also consider the behaviour of solutions at large time, describing the shape of solution close to extinction point for a more general class of f. The convergence of solutions in L^1, which can be interpreted in biological view point as the persistence or extinction of the total population is also established here.

Finally, we discuss solutions of the following equation

$$\begin{cases} u_t = \Delta u + f(t, x_1 - ct, y, u) & t > 0,\, x \in \mathbb{R},\, y \in \omega \\ \partial_\nu u(t, x_1, y) = 0 & t > 0,\, x \in \mathbb{R},\, y \in \partial\omega, \end{cases} \tag{2}$$

where f is periodic in the first variable t, such equation can be viewed as representing the seasonal dependence of f. We will prove that there is exactly one travelling wave solution of the equation above with analogous conditions on f as the first part. The approach for the previous case are still useful for this kind of equation. However, we emphasize that the travelling front is no longer monotone in time in this case. Some new ideas have been introduced to deal with the difficulties arising in this problem.

[1] H. Berestycki, O. Diekmann, K. Nagelkerke, P. Zegeling, Can a Species Keep Pace with a Shifting Climate?, *Bull. Math. Biol.* **71(2)**, (2008), p. 399–429.

[2] H. Berestycki, L. Rossi, Reaction-diffusion equations for population dynamics with forced speed, I - The case of the whole space, *Discrete Contin. Dyn. Syst.*, **21(1)**, (2008), p. 41–67.

[3] H. Berestycki, L. Rossi, Reaction-diffusion equations for population dynamics with forced speed, II - Cylindrical type domains, *Discrete Contin. Dyn. Syst.*, **25(1)**, (2009), p. 19–61.

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