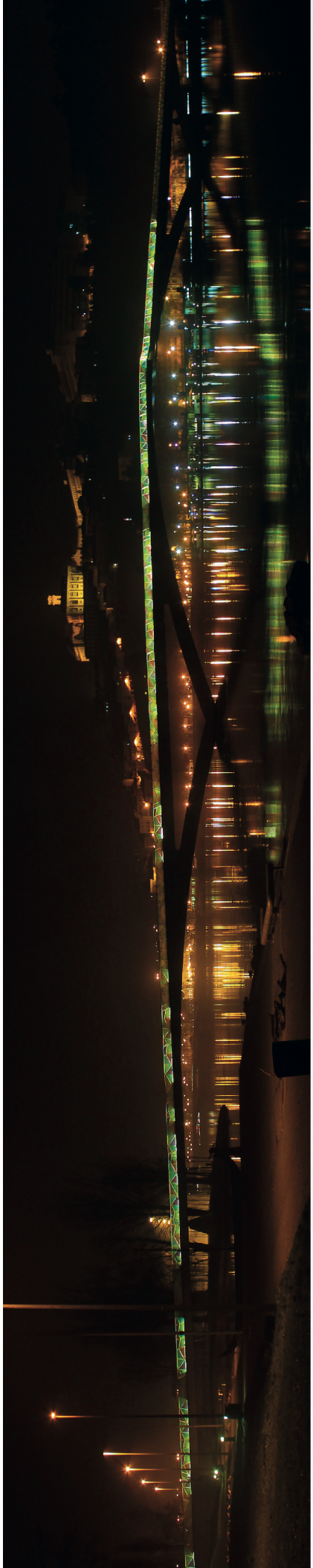

MATHEMATICS OF COMPLEX SYSTEMS

FROM PRECISION MEDICINE TO SMART CITIES

Department of Mathematics
University of Coimbra, Portugal
December 5-6, 2016

WELCOME MESSAGE

Dear colleagues,

It is an honor and a pleasure to welcome you to this workshop "Mathematics of Complex Systems: from precision medicine to smart cities" organised as an initiative of the UT Austin — Portugal CoLab Program.

The main purpose of this meeting is to enhance collaborations between scientists and researchers of different areas of the UT Austin — Portugal community who wish to be involved in the emerging field of complexity theory, in particular in the understanding of the nature and the behaviour of complex systems, such as cities or cells. This will be an opportunity to reinforce the Portuguese scientific and technological outreach, strengthening our scientific interactions and making new connections with established experts of the different topics covered in this event.

We hope that you find this forum inspiring, both for scientific interaction and informal discussions.

We would like to thank all speakers and participants for being here today. And, we also would like to express our sincere gratitude to the Centre of Mathematics of the University of Coimbra and Department of Mathematics of the Faculty of Sciences and Technology of the University of Coimbra for providing generous support and hosting the workshop at their premises.

Finally, we encourage all of you to visit the beautiful city of Coimbra. We hope you will find some time to explore the old university campus, the uptown ("Alta") and Sofia, recently classified by UNESCO as World Heritage sites.

Coimbra, December 5, 2016

Adérito Araújo

Raquel Barreira

João Gouveia

Verónica Quítalo

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RELEVANT INFORMATION

Conference venue

This workshop will take place in the Department of Mathematics of the University of Coimbra (DMUC) which is located located in the main campus of the university.

Conference rooms and registration desk

The plenary lectures will be held in Room 2.4 of the Department of Mathematics. Parallel sections will be at the same building, in Room 2.4 and Room 2.5. An information and registration desk will be near the conference rooms.

Internet access

To have internet access you may use the computers on the ground floor of DMUC, where you can use your login and password. If you are using your own laptop, you can find in your registration folder the email address and password that will grant you access to the *eduroam* wireless network.

Coffee breaks

The coffee breaks will take place on the second floor's hall.

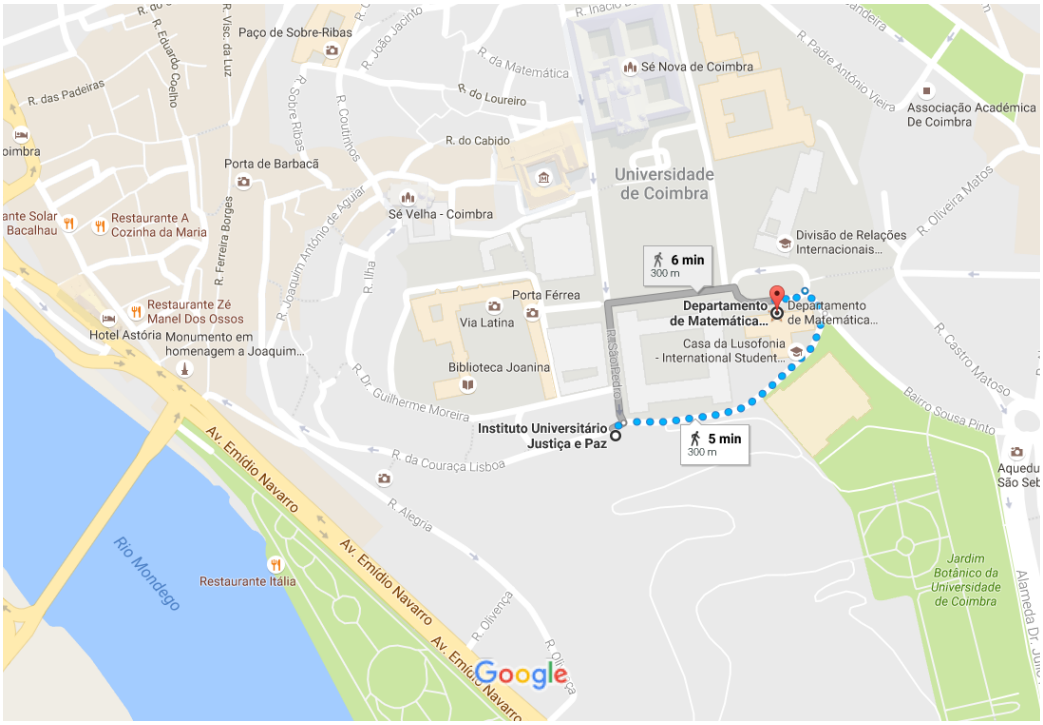
Instructions for speakers

Each lecture room is equipped with a PC, video projector and blackboard. Please be aware that each oral presentation has a 30 minutes slot (25 minutes + 5 minutes for questions).

As early as you can, and in any case before the beginning of your section, go to the assigned room to upload your presentation. PDF files are preferred. You can also use your own laptop but, in that case, please be aware that the time of your talk will be reduced due to change of computers. If you have videos or any other special feature, please test the presentation in advance of your section.

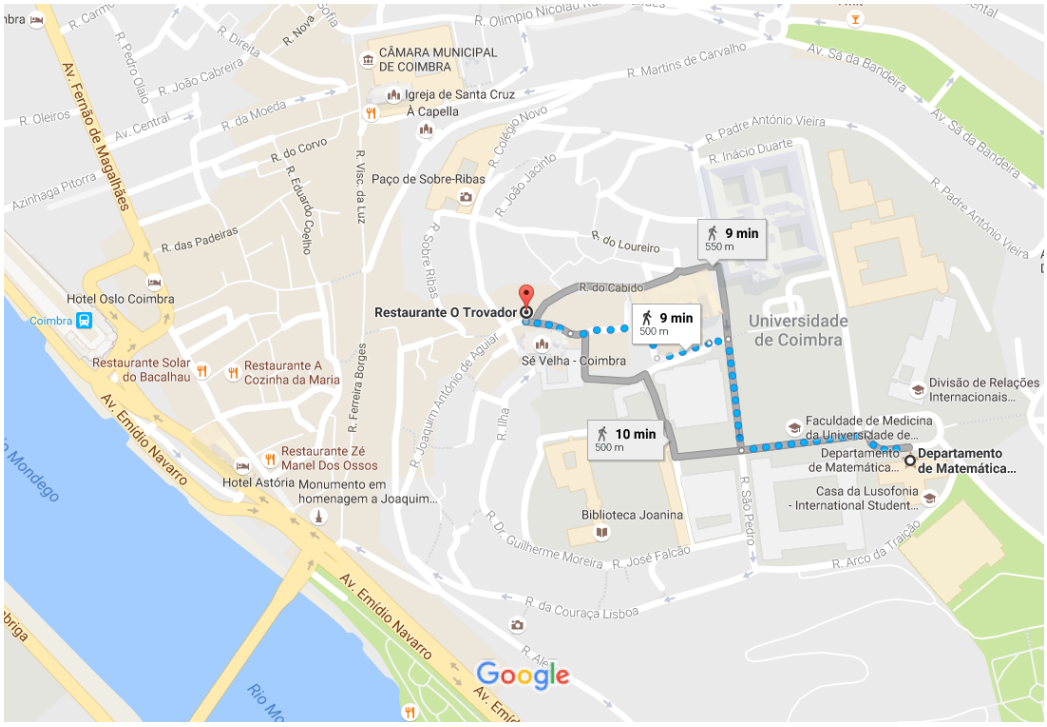
Lunches

Lunches will be served in Instituto de Justiça e Paz, IJP, from 13:00 to 14:00.



Conference dinner

The workshop dinner will take place at “Restaurante O Trovador” at 19:30. It is located on the hill, in the heart of the medieval town, next to the old cathedral and to the historical university campus.



PROGRAM

Timetable

	Monday 5 December 2016	Tuesday 6 December 2016
8:30-9:00	Reception + welcome section	
9:00-10:00	Philip K. Maini	Des Higham
10:00-11:00	Gonçalo Correia	Anotida Madzvamuse
11:00-11:30	Coffee break	Coffee break
11:30-13:00	Mini-symposia: MS1_PM; MS2_SC	Mini-symposia: MS5_PM; MS6_SC
13:00-14:30	Lunch	Lunch
14:30-15:30	Luís Rocha	Mini-symposia: MS7_PM; MS8_SC
15:30-16:00	Coffee break	Coffee break
16:00-17:30	Mini-symposia: MS3_PM; MS4_CS	Mini-symposia: MS7_PM; MS8_SC
19:30	Conference dinner Restaurant "Trovador"	

Plenary lectures

Monday, December 5

Room 2.4: 9:00-10:00
Philip K. Maini: Modelling Collective Cell Motion in Biology

Room 2.4: 10:00-11:00
Gonçalo Correia: The Role of the Car in the XXI Century: applying mathematical programming models to manage and assess the potential of car-pooling, car-sharing and car-automation

Room 2.4: 14:30-15:30
Luís Rocha: Structure and Dynamics of Complex Systems: from social media mining to control of biochemical networks

Tuesday, December 6

Room 2.4: 9:00-10:00
Des Higham: Models and Algorithms for Dynamic Networks

Room 2.4: 10:00-11:00
Anotida Madzvamuse: The Numbers for Cell Motility: novel approaches for whole cell migration

Mini-symposia

Monday, December 5

Room 2.4: 11:30-13:30
MS1_PM: Models in population dynamics
Organizer: Raquel Barreira
11:30-12:00 Jorge M. Pacheco: Population dynamics through hierarchically embedded Markov chains
12:00-12:30 Fabio Chalub: Optimal vaccination strategies and rational behaviour in seasonal epidemics
12:30-13:00 Jan Haskovec: Discrete and continuum modeling of biological network formation

Room 2.5: 11:30-13:30
MS2_SC: Complex transport system problems
Organizer: António Pais Antunes
11:30-12:00 Joana Cavadas: Optimization models for the integration of transit and parking policies
12:00-12:30 Daniela Dias: Modelling population exposure to traffic-related air pollution in complex urban systems
12:30-13:00 António Pais Antunes: Airport capacity management under IATA guidelines: modeling approach and real-world application

Room 2.4: 16:00-17:30
MS3_PM: Mathematical model of the cardiovascular system
Organizeres: Raquel Barreira and Paula Faria
16:00-16:30 Telma Santos: Data assimilation procedure applied to cardiovascular problems in 3D domains
16:30-17:00 Jorge Tiago: Boundary control problems in hemodynamics: mathematical analysis and numerical simulations
17:30-17:30 Oualid Kafi: On the mathematical modeling of atherosclerosis disease

Room 2.5: 16:00-17:30
MS4_CS: Mathematics of complex systems
Organizeres: João Gouveia and Paula Faria
16:00-16:30 Álvaro Gomes: Evolutionary algorithms for building energy efficiency and end-use energy resources management
16:30-17:00 S.X. Toh Ariel: Swarm intelligence as an evolutionary optimization for smart cities
17:00-17:30 Diogo Baptista: Using symbolic dynamics to measure the complexity of systems

Tuesday, December 6

Room 2.4: 11:30-13:30
MS5_PM: Angiogenesis and cell motility
Organizer: Rui Travasso
11:30-11:55 Elisabeth Antoine: The in vitro artery: an instrumented platform for quantitative vascular research
11:55-12:20 Maurício Moreira Soares: Angiogenic factors produced by hypoxic cells drive anastomosis in sprouting angiogenesis
12:20-12:35 João Ramos: Mechanically-driven pattern formation in cell cultures
12:35-13:00 João Carvalho: A computational model of a positive loop feedback in endothelial cells sprouting to explain the effect of fibrinogen variants

Room 2.5: 11:30-13:30
MS6_SC: CUrban analytics: open data in action
Organizer: Raquel Barreira
11:30-12:00 Fátima Neves: From open data city portals to predictive intelligence: insights from cascais open data initiative
12:00-12:30 João Tremoceiro: The Lisbon data - present and future
12:30-13:00 Miguel de Castro Neto: Urban analytics challenges

Room 2.4: 14:30-15:30 + 16:00-17:30
MS7_PM: Mathematical methods in biology
Organizeres: Sílvia Barbeiro and Rui Bernardes
14:30-15:00 Erida Gjini: Mathematics and the battle against antibiotic resistance
15:00-15:30 Marina A. Ferreira: A framework for modelling packed cell tissues

16:00-16:30 Francisco Oliveira: The role of compartmental models in the quantification of PET imaging data and computer-aided diagnosis
16:30-17:00 Pedro Serranho: 3D retinal vascular network from OCT data
17:00-17:30 Sílvia Barbeiro: Numerical solution of time-dependent Maxwell's equations for modeling light scattering in human eye's structures

Room 2.5: 14:30-15:30 + 16:00-17:30
MS8_SC: Simply talking about complexity
Organizer: Ana M. Almeida
14:30-14.40 Ana M. Almeida: Presentation
14:40-15:00 Jorge Louçã: Why do we need mathematics in Digital Humanities - the example of media opinion modelling
15:00-15:30 Rosário Laureano: Synchronization phenomenon in complex systems

16:00-16:20 Sara Eloy: Generative properties of shape grammars
16:20-16:50 Carlos Fonseca: Mathematical models of artificial genetic representations with neutrality
16:50-17:10 Sancho M. Oliveira: EvoRBC: Evolutionary Repertoire-based Control for robots with arbitrary locomotion complexity
17:10-17:30 Tiago Baptista: Step evolution - improving the performance of open-ended evolution simulations

Abstracts, plenary lectures

The Role of the Car in the XXI Century: applying mathematical programming models to manage and assess the potential of car-pooling, car-sharing and car-automation

Gonçalo Correia
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Mobility, especially on urban environments, has been changing in the last decades, leveraged by new technologies and significant societal changes. Information technologies and new vehicles are making available new mobility solutions like the Uber car or the prospect of a self-driving fleet of shared vehicles, moreover we have deep society changes such as an ageing population who is less able to drive a car and a young population, the so called millennials, who don't want to own a car anymore. Traffic and traditional public transport have been extensively researched in the past making available a set of methods that allow private companies and public authorities to manage these systems in an efficient way. With regard to the new modes and technologies there is however still a lack of knowledge on how to run them or even what type of changes they will introduce in the mobility system. In this plenary session I will be describing different uses of mathematical programming in both, disclosing the impacts, and finding management strategies for three mobility disrupters: car-pooling (several people in the same car), car-sharing (sequential usage of the same car by different people) and automated vehicles.

Models and Algorithms for Dynamic Networks

Des Higham
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In many modern applications we can record interactions that appear and disappear over time. This type of dynamic network arises, for example, in on-line human behaviour (emails between individuals), in transport (flights between cities) and in city sensors (correlations between measurements). Some of the key concepts from traditional network science must be adapted or generalized in this dynamic setting. In this talk I will focus on (a) a modelling framework that allows us to quantify and test hypotheses from the social sciences and (b) an approach to monitoring node centrality that has proved useful on very large social media networks. Results will be illustrated on real data sets.

The numbers for cell motility: Novel approaches for whole cell migration

Anotida Madzvamuse
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In this talk, I will present a novel approach for whole cell tracking based on geometric partial differential equations for the cell surface motion where the physics of the migrating cell is easily encoded. In order to fit to experimental data an optimal control framework using phase-field theory is presented. A highly efficient, adaptive and fast multigrid solver is then employed to allow for realistic 2D and 3D simulations. Numerical examples will be exhibited that show the applicability of the mathematical framework for whole cell migration.

Modelling Collective Cell Motion in Biology

Philip K. Maini
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Collective cell motion, either in the form of individual cells signalling to each other, or moving as a sheet, is very common in biology. Here, I will present a hybrid discrete cell-based model for cranial neural crest cell invasion and a model for epidermal cell movement in intestinal crypts. The models will be compared with experimental results.

Structure and Dynamics of Complex Systems: from social media mining to control of biochemical networks

Luís Rocha
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The structure of networks has provided many insights into the organization of complex systems. The success of this approach is its ability to capture the organization of multivariate interactions, and how it changes in time (network evolution) without explicit dynamical rules for node variables. As the field matures, however, there is a need to move from understanding to controlling complex systems. This is particularly true in systems biology and medicine, where increasingly accurate models of biochemical regulation have been produced. More than understanding the organization of biochemical regulation, we need to derive control strategies that allow us, for instance, to move a mutant cell to a wild-type state, or revert a mature cell to a pluripotent state. Here I present two concepts developed in our group aimed at supporting this goal. First I will present the concept distance backbone, the invariant subgraph of the distance closure of weighted graphs [Simas and Rocha, 2015]. This backbone allows us to identify redundant edges in the computation of shortest paths; we show that there is massive redundancy in many networks in different domains, including social media, Wikipedia, functional and structural brain networks, citation, air traffic, etc [Simas et al, 2016]. Since shortest-paths and diffusion distances play a role in information dynamics unfolding on brain networks [Kolchinsky et al, 2014] and knowledge networks [Ciampaglia et al, 2015], removing redundant edges can facilitate computation and discovery of important pathways in many applications. Secondly, I will present the schema redescription methodology, used to remove redundancy from automata rules to reveal their canalization properties, thus simplifying the characterization of control in large models of natural networks, such as systems biology models of biochemical regulation [Marques-Pita and Rocha, 2013]. We demonstrate that canalization (measured as effective connectivity) is an order parameter of Boolean Network (BN) dynamics, and a major factor in network controllability [Gates and Rocha, 2016; Marques-Pita, Manicka and Rocha, 2016].

Abstracts, mini-symposia

The *in vitro* artery: an instrumented platform for quantitative vascular research

Elizabeth E. Antoine[1], **Abdul I. Barakat**[1]

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Although vascular disease is a leading cause of mortality, *in vitro* tools for controlled, quantitative studies of vascular biological processes in an environment that reflects physiological complexity remain limited. Computational models provide invaluable insight regarding the dynamics of cardiovascular disease and inform stent design strategies; however, the availability of in vitro devices for validation of numerical work remains critically limited [1, 2].

We have developed a novel *in vitro* artery that allows deployment of endovascular devices including stents, quantitative real-time tracking of cellular responses, and detailed measurement of flow velocity and lumenal shear stress using particle image velocimetry [3]. The wall of the *in vitro* artery consists of an annular collagen hydrogel containing smooth muscle cells (SMCs) and whose lumenal surface is lined with a monolayer of endothelial cells (ECs). The system has *in vivo* dimensions and physiological flow conditions and allows automated high-resolution live imaging of both SMCs and ECs. To demonstrate proof-of-concept, we imaged and quantified EC wound healing, SMC motility, and altered shear stresses on the endothelium after deployment of a coronary stent. In addition, we have adapted the algorithms developed for quantification of the *in vitro* artery for use with similar but simpler 2D experimental systems.

The *in vitro* artery and accompanying post-processing tools provide a unique platform suited for a broad array of research applications. For example, quantitative data obtained from the *in vitro* artery can inform *in silico* models of cellular migration, wound healing, and cardiovascular disease progression. Wide-scale adoption of this system promises to enhance our understanding of important biological events affecting endovascular device performance and to reduce dependence on animal studies.

Keywords: endothelial wound healing; *in vitro* artery; stent; shear stress; collagen hydrogel; quantitative cellular imaging

Acknowledgments. This project was supported by a Whitaker International Program postdoctoral fellowship and by an endowment in Cardiovascular Cellular Engineering from the AXA Research Fund.

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Airport Capacity Management under IATA Guidelines: Modeling Approach and Real-world Application

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Due to the rapid growth of air traffic, demand often exceeds available capacity in the busiest airports worldwide. This may lead to significant airport congestion, creating serious problems of delays and, consequently, high costs for airports, airlines and passengers. To cope with this problem, airports may expand their capacity by building new airport facilities and/or developing new air traffic management technologies. However, these types of interventions are generally investment-intensive, very time-consuming, or sometimes even infeasible in the densest urban areas. Alternatively, airports may implement demand management mechanisms. These mechanisms aim to constrain flight demand at periods when airport capacity is expected to be exceeded by distributing flights more evenly over the day. The IATA slot allocation process is the key demand management mechanism practiced by the busiest airports outside the United States (more than 300 airports worldwide). Under this process, the airports provide a value of "declared capacity", which specifies the number of "slots" available for landings and takeoffs per hour and/or intervals of 15 minutes. For each season, the airlines submit their slot requests to a slot coordinator that must allocate the available slots in the most neutral, transparent and non-discriminatory way. The underlying slot allocation process, established in IATA's World Slot Guidelines, is very complex, with multiple criteria, rules and priorities. Recently, some optimization models have appeared in the literature aiming to support slot coordinators to better accommodate airlines' preferences at congested airports. However, these models are not yet compliant with the IATA guidelines as well as with some important airport's operational and regulatory constraints. This research develops a new modeling approach to support slot coordinators in the decisions they make during the slot allocation process, while complying with the IATA guidelines and other constraints. Results from the application of this approach are shown for a case study involving the Madeira airport (FNC).

Keywords: Airport Management; Demand Management; Slot Allocation; Optimization

Swarm Intelligence as an Evolutionary Optimization for Smart Cities.

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The digitalization age of the electric network systems in Smart Cities uptakes an interactive communication platform and energy management systems. Smart Grid Systems however behave stochastically, highlighting the complexities of maintaining an optimal dispatch of distributed generation. Therefore, a proposed optimization method is studied to develop a future solution in solving the digital grid constraints. This paper incite an assessment on the most represented optimization methods that have been studied by recent scholars [1],[2] and [3], to address the digital grid phenomenon as adverted by [4]. Among various methods, the development of swarm intelligence such as Particle Swarm Optimization Algorithms (PSO) is considered to be one of high performance solution in tackling the varied demanding task of a digital grid. Taking into account of other technology options such as cogeneration systems [5], the swarm intelligence approaches is most useful when integrated in a smart grid architecture that calls for optimization in stochastic processes.

Keywords: Optimization; Swarm Intelligence; Smart Cities; Digital Grid

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Step evolution - improving the performance of open-ended evolution simulations.

Tiago Baptista

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A common issue in Artificial Life research, and mainly in open-ended evolution simulations, is that of defining the bootstrap conditions of the simulations. One usual technique employed is the random initialization of individuals at the start of each simulation. However, by using this initialization method, we force the evolutionary process to al- ways start from scratch, and thus require more time to accomplish the objective. Artificial Life simulations, being typically, very time consum- ing, suffer particularly when applying this method. We describe a technique we call step evolution, analogous to incremental evolution techniques, that can be used to shorten the time needed to evolve complex behaviors in open-ended evolutionary simulations. We further present an extension to this technique that automates the process of stepping the simulation. We provide results from experiments done on an open-ended evolution of foraging scenario, where agents evolve, adapting to a world with a day and night cycle. The results show that the employment of this technique can improve both the overall success of simulation runs, and the time needed to evolve the observed behaviours.

Keywords: Artificial life, Multi-agent systems, Open-ended evolution, Incremental evolution.

Using symbolic dynamics to measure the complexity of systems

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The study of nonlinear dynamical systems, in particular the study of time series, is a current topic in financial systems and in control systems of chaotic systems: mechanical, climatic, electronic, robotic, decision, biological, neural, etc. Describing the behavior and measure of the complexity of time series, obtained from non-linear systems, systems involving several variables or from numerical methods, represent a great challenge. The approach presented here uses symbolic dynamics, to overcome this difficulty. The proposed method was applied in melanocytic lesions to compare and classify different type of melanocytic lesions.

Numerical solution of time-dependent Maxwell's equations for modeling light scattering in human eye's structures

Adérito Araújo, Sílvia Barbeiro, Maryam Khaksar Ghalati
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In this work we discuss the numerical discretization of the time-dependent Maxwell's equations using a leap-frog type discontinuous Galerkin method. We focus on deriving stability and convergent estimates of fully discrete schemes. We consider anisotropic permittivity tensors, which arise naturally in our application of interest. An important aspect in computational electromagnetic problems is the implementation of the boundary conditions. We present some numerical examples to illustrate the theoretical results and also in the context of modeling scattered electromagnetic wave's propagation through human eye's structures. Finally, we also briefly discuss the multi-scale nature of the problem. In a small scale, we use Maxwell's equations to compute parameters that could be used as inputs to larger scale simulations namely using Monte Carlo methods.

Keywords: Maxwell's equations, fully explicit leap-frog discontinuous Galerkin method, stability, convergence, light scattering in the retina.

Acknowledgments. This work was partially supported by the Centre for Mathematics of the University of Coimbra – UID/MAT/00324/2013, funded by the Portuguese Government through FCT/MCTES and co-funded by the European Regional Development Fund through the Partnership Agreement PT2020; by the Portuguese Government through the BD grant SFRH/BD/51860/2012.

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A computational model of a positive loop feedback in endothelial cells sprouting to explain the effect of fibrinogen variants

João Carvalho[1], **Sonja E.M. Boas**[2,3], **Roeland M.H. Merks**[2,3]
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A computational model was developed to describe the angiogenesis-like invasion of endothelial cells (sprouting) into fibrin matrices. Using an *in vitro* assay of sprouting in fibrin matrices, Weijers *et al.* [1] showed that the composition of fibrin changes the sprouting progress: there was more ingrowth on high molecular weight (HMW) than on low molecular weight (LMW) fibrin. As it is not yet clear which mechanisms regulate this process, the processes that drive the reduced ingrowth in LMW as compared to HMW fibrin were studied using a hybrid computational model, cell-based and continuum, that describes the experimental tests. From the results obtained in this simulation, it is proposed that it is present a local positive feedback mechanism between urokinase receptor (uPAR), plasmin and Transforming Growth Factor $\beta 1$ (TGF$\beta 1$). This, due to stochastic fluctuations in the different concentrations, leads to some cells in the monolayer to invade the matrix and to produce sprouts. Plasmin-mediated fibrin degradation by invading cells releases TGF$\beta 1$ from the matrix which locally stimulates cells to increase fibrin degradation, leading to a positive feedback loop. Including the experimental observation that LMW binds less TGF$\beta 1$ than HMW fibrin, the model predicts reduced sprouting in LMW as compared to HMW [2].

Keywords: biological modeling; endothelial cells sprouting
Acknowledgments. Partially supported by the research grant SFRH/BSAB/113464/2015.

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Optimization Models for the Integration of Transit and Parking Policies

Joana Cavadas[1], **Nikolas Geroliminis**[2], **Vikrant Vaze**[3], **António Pais Antunes**[1],
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Public transit systems are not only essential for urban mobility but also as a reliable system to address the current environmental and economic concerns. However, these systems are usually a source of financial problems worldwide scale, as their revenues are rarely enough to cover their expenses.

In this context, four strategic mixed integer non-linear optimization models were developed to integrate transit and parking systems by managing transit fares and parking fees so that local transportation authorities can simultaneously improve transit modal shares and decrease the operating deficits of public transit companies.

These models were applied to cities divided into zones, where trips can be made by car, bus, or not made at all if travel costs are considered too high by travelers. Logit models of the generalized costs are used to describe modal choice, considering transit fares and parking fees as decision variables. Based on the existence or not of competition among operators/companies, two different approaches were considered. On the one hand, three out of the four models assume a cooperative environment, dealing with different goals (maximizing the joint social benefits or minimizing the joint deficits) and traffic behavior assumptions (static or dynamics). On the other hand, a competitive environment was addressed with a two-stage optimization model aiming at finding the Nash equilibrium for each stage where the payoff is the net revenue achieved by each operator/company.

The integrated transit-parking planning models developed provide a better understanding of how pricing schemes affect the city mobility dynamics. They also provide insights into how an unlucrative transit system can become profitable by only managing transit fares and parking fees while ensuring reasonable levels of service. Furthermore, aspects such as congestion, parking capacity or transit system supply can also be positively affected by adjusting transit fares and parking fees.

Keywords: transit planning; parking planning; integrated transit-parking; optimization modeling.

Optimal vaccination strategies and rational behaviour in seasonal epidemics

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We consider a fixed size population divided in three different classes: **S**usceptible, **I**nfeccious and **R**ecovered. In particular, we consider a classical SIR dynamics: ($S + I \xrightarrow{\beta} 2I$, $I \xrightarrow{\gamma} R$, $R \xrightarrow{\alpha} S$) where the infecctious term $\beta(t)$ is a periodic function. We include in the model a periodic *vaccination function* $p(t)$, such that the trasition $S \xrightarrow{p} R$ is also allowed.

We show the existence of an optimal vaccination $p_{\rm opt}$, in the sense that it can be approximated by vaccination functions able to prevent outbreaks and all these other functions will necessarily imply the existence of a vaccination effort at least equal to the vaccination effort of $p_{\rm opt}$. For some examples, we are able to show explicitly $p_{\rm opt}$ as a function of β.

Finally, we introduce a population of rational individuals and we will show how the *voluntary vaccination* affects the dynamics. In particular, we consider that each individual is *rational*, i.e., each individual decides freely, according the the available information, if he or she is willing or not to be vaccinated. To this end, we will couple a system of differential equation with principles from game theory. We prove the existence of a Nash-equilibrium vaccination function $p_{\rm Nash}$ (i.e., when all individuals in the population are rational) and, for some simple examples, we show explicit formulas for $p_{\rm Nash}$.

Modelling Population Exposure to Traffic-related Air Pollution in Complex Urban Systems

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With the urgent need to reduce the high levels of air pollution observed in cities, ambitious traffic policies have been established by many European countries. However, debates still surround these measures, highlighting the need to investigate cost-effective means to assess their benefits on human health. Therefore, due to the complexity imposed by a city as an urban system, solutions to the grand challenges we face in cities must therefore be developed by a comprehensive approach, involving an understanding of complex interactions between different components of the system.

Our ongoing research aims to respond to this need seeking a decision-support tool for urban transport and air quality management, in particular to support local authorities in the promotion of "healthy transport policies". For this purpose, an integrated approach is being developed at urban scale to quantify how the changes associated with alternative traffic measures will affect population exposure to traffic-related air pollution, by combining transport-emission-dispersion-exposure models within an integrated modelling framework.

In order to achieve the defined goal, the main objectives of our current work are focused on evaluating the effectiveness of different traffic measures in terms of emission reductions and air quality improvements and their spatial distribution. The numerical system implemented is based on three modelling tools: (i) the macroscopic traffic flow model VISUM; (ii) the new road traffic emissions and energy consumption model QTraffic; and (iii) the air quality dispersion model AUSTAL2000. The modelling tools were linked and tested on the city of Coimbra.

By adopting an integrated modelling approach, the current work stresses the need to assess the overall role of road transport impacts within cities to evaluate the sustainability of urban mobility policies, focusing on the complex interactions between different aspects of the city, from the source to the receptor.

Keywords: transport planning; road traffic emissions; urban air quality; numerical modelling.

Generative properties of shape grammars

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The talk will focus on shape grammars and how they can capture design languages and are used as generative design tools to generate a large variety of design alternatives. A shape grammar is a set of rules that apply step by step to shapes to generate a language of designs. I'll start by a general introduction to shape grammars highlighting the concepts and formalism used and introduce the work of George Stiny and James Gips [1, 2] in order to present the basis of this system. Formalisms of shape grammars as algebras, weights, labels and concepts of emergence, embedding and sub-shape will be highlighted [3]. Emergence is a structural concept of shape grammars and it consists on the unanticipated or accidental outcomes of a design derivation. In design practice emergence is one of the main features that triggers creativity. Shape grammar research has shown that, within a strictly circumscribed space of designs, it is possible to be creative and generate innovative designs [4]. The difficulty in developing a computer design system that supports emergence has divided the shape grammar community into two groups. On one side there are the ones that are interested in exploring the pure power of shape grammars and don't make efforts to develop computer programmes and on the other side the ones that want to develop computer systems even if not addressing features like emergence which will also decrease the creativity aspect of the grammars. Finally, I'll end with some examples of analytical grammars and original grammars, the former more aiming at capturing existing design languages and the later aiming at developing totally new languages of design. Discussion will be done on the possibilities that both bring to shape research and to the exploration of design alternatives.

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A framework for modelling packed cell tissues

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In a packed tissue neighbouring cells exert high pressure on each other at all times. These mechanical interactions play an important role on the dynamics of the tissue and therefore cannot be neglected [1]. We propose a framework to model this type of systems based on a geometric representation of individual cells. The cells interact with each other aiming at minimizing a local potential energy, subjected to non-overlapping constraints. This gives rise to a non-linear non-convex minimization problem, for which there are unfortunately not many tools available. In this talk, I will show an algorithm we have developed for this type of problems: the damped Arrow-Hurwicz algorithm [2], as well as some examples and numerical results. This framework can be very useful in the study of packed tissues, as it helps to predict the impact of inter-cellular forces on the dynamics of the whole tissue, which can not be easily addressed through laboratory experiments.

Keywords: modelling cell tissue; mechanical interactions; non-convex optimization; sphere packing.
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Mathematical Models of Artificial Genetic Representations with Neutrality

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Kimura's neutral theory of molecular evolution [1] addresses the fact that most mutations at the genotypic level are not expressed in the phenotype, and suggests that random genetic drift is of great importance in natural evolution. Sets of genotypes connected by such neutral mutations form potentially large *neutral networks* [2] within which natural selection cannot play a direct role. However, it is understood that the accumulation of neutral mutations may potentiate the occurrence of beneficial mutations at a later stage.

Studies of neutrality in genotype-phenotype mappings have been conducted both in biology and in evolutionary computation [3]. In particular, Fonseca and Correia [4] proposed a family of uniformly redundant binary representations based on error-control codes. Such representations can exhibit various degrees of redundancy, neutrality, and other properties believed to influence the performance of evolutionary algorithms, such as connectivity, locality, and synonymity [5], and have allowed this influence to be studied experimentally to some extent [6].

In this work, a mathematical framework for the study and characterisation of Fonseca and Correia's representations is developed, leading to the definition of suitable equivalence classes and to the partitioning of the representation space with respect to neutral network structure and connectivity. The practical implications of the proposed framework are also discussed.

Keywords: Mathematical models; genetic representations; neutral networks; evolutionary computation.
Acknowledgements. This work was partially supported by a Short Term Scientific Mission (STSM) grant from COST Action CA15140 on Improving Applicability of Nature-Inspired Optimisation by Joining Theory and Practice (ImAppNIO), by national funds through the Portuguese Foundation for Science and Technology (FCT), and by the European Regional Development Fund (FEDER) through COMPETE 2020 – Operational Program for Competitiveness and Internationalisation (POCI).

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Evolutionary algorithms for building energy efficiency and end-use energy resources management

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The first step for a rational use of energy in the building sector is to incorporate building performance concerns since the early design stage. This requires evaluation and exploration of alternative solutions. However, designers are unable to manually produce more than 2 or 3 solutions. Therefore, the combined use of computer generative methods, optimization techniques, and building performance simulation tools may help overcome this issue. Generative methods produce large number of solutions allowing designers to compare and select the most promising ones. By coupling dynamic simulation tools and optimization techniques, it is possible to assess and improve the generated solutions, thus helping building practitioners in the decision making process. In this work, an evolutionary algorithm that couples an evolution strategy and local search technique is presented to generate alternative floor plan designs according to the user preferences and requirements. After generation, alternative solutions are assessed, ranked, and optimized to minimize human thermal discomfort in every building room [1].

Besides the design of more energy efficient buildings, the adequate use of energy resources and inclusion of renewable energy generation during the building lifespan is also fundamental for the promotion of a more sustainable and environmental friendly society. However, the variability and the mismatch between generation and demand raises some issues that need to be resolved. Considering the residential sector as a target to achieve a smarter use of electricity, due to the existence of a certain degree of dissociation between electricity consumption and the usage of energy services, adequate algorithms should be designed to help end-users to take the most adequate decisions regarding the optimized management of energy resources. For this purpose, a tailored evolutionary algorithm to optimize the integrated usage of multiple residential energy resources considering a large set of management strategies. Customized solution encoding and operators are developed for different groups of loads. The multiobjective model considers as objective functions the minimization of the energy cost and the minimization of end-user's dissatisfaction associated with management strategies. Results have shown that significant savings can be achieved mainly through demand response actions implemented over thermostatically [2].

Keywords: Generative building design; Building performance optimization; End-use energy resources management; Evolutionary algorithms

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Data Assimilation procedure applied to cardiovascular problems in 3D domains

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In the context of cardiovascular problems, we propose a Data Assimilation procedure to solve a non linear optimal control problem of Dirichlet type. In this procedure, real data is included in numerical blood flow simulations to obtain more realistic and accurate results. The goal is to reconstruct the blood flow profile using known data in the cost functional, available at certain parts of the 3D computational domain while assuming blood as non-Newtonian homogeneous fluid. We propose two types of control imposed at the inlet boundary: as a first step, we consider the control to be a parameter in the inlet boundary profile expression; after, we control the inlet profile assuming perpendicularity with respect to the inlet boundary. To solve this problem we propose a Discretize then Optimize (DO) approach, based on stabilized finite element methods. Some relevant work about this issue can be found for example in [4], [2], [3], [4].

Keywords: Data Assimilation; Optimal control; non-Newtonian fluids;
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Mathematics and the battle against antibiotic resistance

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The rise of antibiotic-resistant microbes poses an urgent threat to public health. Understanding the genetics, population dynamics, and control of antibiotic resistance requires integrative interdisciplinary approaches. In our research we use mathematical models to describe, simulate and study such processes, interpolating between the individual and population level. In this talk I will focus on a recent mathematical model for bacterial infection dynamics [1], which we have developed to study optimal antibiotic treatment and the role of host immunity. I will illustrate how mathematical modeling can enhance our fundamental understanding of infection ecology, provide fresh insights on resistance control and effective treatment, and pave the way to clinical applications.

Keywords: ordinary differential equations; infection dynamics; antibiotic resistance ; host immunity

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Discrete and continuum modeling of biological network formation

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Motivated by recent papers describing rules for natural network formation in discrete settings, we propose an elliptic-parabolic system of partial differential equations. The model describes the pressure field due to Darcy's type equation and the dynamics of the conductance network under pressure force effects with a diffusion rate representing randomness in the material structure. We show how the PDE system is derived from the discrete graph-based model as a mean-field-type limit. Then we present several analytical results - existence of global weak solutions and of local mild solutions and their long term behavior. Moreover, we study the structure and stability properties of steady states that play a central role to understand the pattern capacity of the system. We show that patterns (network structures) occur in the regime of small material randomness. Moreover, we present results of systematic numerical simulations of the system that provide further insights into the properties of the network-type solutions.

On the Mathematical Modeling of Atherosclerosis Disease

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This presentation is divided into two parts: (i) The inflammatory process of atherosclerosis leads to the formation of an athero- matous plaque in the intima of the blood vessel. The plaque rupture may result from the interaction between the blood and the plaque. In each cardiac cycle, blood interacts with the vessel, considered as a compliant nonlinear hyperelastic. A three dimensional idealized fluid-structure interaction model is constructed to perform the blood-plaque and blood-vessel wall interaction studies. An absorbing boundary condition is imposed directly on the outflow in order to cope with the spurious re- flexions due to the truncation of the computational domain. The difference between the Newtonian and non-Newtonian effects is highlighted. It is shown that the von Mises and wall shear stresses are significantly affected according to the rigidity of the wall. The numerical results have shown that the risk of plaque rupture is higher in the case of a moving wall, while in the case of a fixed wall the risk of progression of the atheromatous plaque is higher. (ii) Monocytes play a significant role in the atherosclerosis development. During the inflammation process, monocytes that circulate in the blood stream are activated. Upon activation, they adhere to the endothelium and extravasate through the latter to migrate into the intima. In this work we are concerned with the transmigra- tion stage. In our study, the constitutive equations for Oldroyd-B fluids are used to capture the viscoelastic behavior of monocytes. We first establish and analyze a sim- plified mathematical model describing the coupled deformation-flow of an individual monocyte in a microchannel. Then we describe the numerical implementation of the mathematical model using the level set method and show the numerical results. Further extensions of this model are also discussed.

Synchronization phenomenon in complex systems

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Whenever two ”events” seem to happen simultaneously during an extended time period, the synchrony is probably not a coincidence. The first observations related to synchronization were reported by Huygens in 1665 [1]; it was indicated by the equal periods of coupled clocks.
Until a few years ago, the study of synchrony was dispersed by very different knowledge areas, such as biology, physics or economics, through disconnected works. After a seminal paper of Fujisaka and Yamada [2], the study of synchrony has been gradually constituted as a concrete and transverse research topic. By applying the theory of dynamical systems, the complex theory or the computer science, and using the available technology, it has been possible to understand the synchrony of ”events” as coupled oscillators. In fact, groups of fireflies, pacemaker cells, lasers, pendulums or planetary orbits are all collections of (living or inanimate) oscillators. Two (or more) oscillators are said to be coupled if an appropriate communication process (physical or chemical) allows some influence between them. This influence can be bidirectional (mutual) or unidirectional. There are many different channels, both in nature and in artificial environments, which play the role of coupling between systems.
The emergent field studying the synchronization phenomena is still largely unexplored. However, it is immediately interesting for its high potential application and actually includes processes where the oscillators are replaced by chaotic systems - *chaos synchronization* - or where they are coupled in less symmetrical ways or in intricate networks.
Coupled systems are constructed from simple, low-dimensional and form new and more complex organizations, with the belief that dominant features of the underlying components will be retained. This building up approach can also be used to create a novel system which behavior is more flexible or richer than that of the components, but which analysis and control remains tractable.

Even in the so called *identical (complete) synchronization* - when the coupling is between identical chaotic systems but starting from different initial conditions - the chaos synchronization phenomenon is especially challenging. In fact, the possibility of chaotic systems oscillate in a coherent and synchronized way is not an obvious phenomenon since the *sensitive dependence on initial conditions* (that is, any infinitesimal perturbations of the initial conditions lead to the exponential divergence of nearby starting orbits) is one of the main features associated with the chaotic behavior. However, when ensembles of chaotic systems are coupled, the attractive effect of a suitable coupling can counterbalance the trend of the trajectories to separate due to chaotic dynamics.
The effectiveness of a coupling between systems with equal dimension follows of the analysis of the synchronization error. By mean of an appropriate coupling, it is possible to reach full, *asymptotical* or *practical synchronization*, depending on the coupling degree. In chaos synchronization we seek subspaces of the coupled system space - the *synchronization set* - in which a special kind of motion, which relates the coupled system, takes place.
Other synchronization regimes, in addition to the identical synchronization, are the *generalized synchronization* and the *phase synchronization*. When the systems in coupling are distinct - if they simply have different sets of parameters or even by having different dimension - the process is called generalized synchronization. It is a regime of synchronization where exists a one-to-one smooth mapping between oscillations of each system. Hence, knowing the state of one system enables us to know the state of the other system. Phase synchronization is defined as the appearance of a certain relationship between the phases of the systems in coupling while the amplitudes can remain uncorrelated.

Since the work of Pecora and Carroll [3] various coupling methods and several news concepts necessary for analyzing chaos synchronization have been developed.

In our work it was considered the synchronization phenomena of (identical or nonidentical) chaotic dynamical systems, with nonlinear unidirectional and bidirectional coupling schemes, both in continuous and discrete time [4]. In order to illustrate the coupling methods, we always use a system of two coupled chaotic systems.

In continuous time, for identical and generalized synchronization, we apply various unidirectional and bidirectional coupling schemes between Lorenz, Rössler or hyperchaotic Rössler systems with control parameters that lead to chaotic behavior. We combine several coupling schemes - diffusive linear bidirectional coupling, unidirectional coupling by control function, unidirectional coupling by dislocated negative feedback control or active-passive decomposition for several driver signals - with total or partial replacement on the nonlinear terms of the second system, a coupling version that was less explored. In some cases we only conclude about local stability of the synchronous state; the effectiveness of a coupling between chaotic systems with equal dimension follows of the analysis of the synchronization error. In other coupling schemes the sufficient conditions of global stable synchronization are guaranteed from a different approach of the Lyapunov direct method for the transversal system.

In discrete time, we study a nonlinear coupling scheme that appears in natural a family of analytic complex quadratic maps and an We are not aware about any studies of this type of coupling. It is an asymmetric coupling between two real quadratic maps. When practical synchronization is not achieved, but the difference between the dynamical variables of the systems is limited, we still can apply a chaos control technique. We obtain stable identical and generalized synchronization with some versions of the original coupling, highlighting the absence of symmetry. Two of them are generalizations promoting the use of different parameters coupling. By analyzing the difference between the dynamical variables of the systems, we obtain some results leading to stable synchronization.

Keywords: complex systems; chaos synchronization; global stability; Lyapunov direct method; Lorenz system, Rössler system; hyperchaotic Rössler system
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Why do we need mathematics in Digital Humanities – the example of media opinion modelling

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Public opinion studies became popular in the last few years, namely within the Digital Humanities research community. This gain of interest can be explained by the new dynamics of communication in a diversity of media and social networks, together with the availability of powerful computational resources allowing to gather and to process large quantities of information.

An ongoing case study will be presented regarding the news published by British newspapers during the period that conducted to Brexit. News concerning Europe are analysed, coming from three distinct political areas: far-right, right-wing and left-wing. The ongoing research aims at identifying and comparing political narratives transmitted to the population by each of these areas.

This case study will illustrate how important is the contribution of mathematics towards a multidisciplinary approach in Digital Humanities.

Urban Analytics Challenges

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Data is the fuel that powers smart cities development and today urban analytics are the main challenge we face in order to take full advantage of the potential created by the data overload resulting from the sensing capabilities, both from machines and human being, we have. In this presentation we will cover the concepts associated with smart cities, the role of open data and the arising potential of urban radiology.

From Open Data City Portals to Predictive Intelligence: Insights from Cascais Open Data Initiative

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As city efforts are been made to release large amounts of open data, the challenge is to build predictive models based on these open datasets helping to scope additional, more innovative and better governmental services and to spot emerging business and societal needs.

EvoRBC: Evolutionary Repertoire-based Control for Robots with Arbitrary Locomotion Complexity

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The use of evolutionary robotics (ER) in robots with complex means of locomotion has, so far, mainly been limited to gait evolution. Increasing the number of degrees of freedom (DOF) available to a controller significantly enlarges the search space, which in turn makes the evolution of solutions for a given task more challenging. In this paper, we present Evolutionary Repertoire-based Control (EvoRBC), an approach that enables the evolution of control for robots with arbitrary locomotion complexity. EvoRBC separates the synthesis of control into two levels: the generation of a repertoire of behavior primitives through the application of Quality Diversity techniques; and the evolution of a behavior arbitrator that uses the repertoire's primitives to solve a particular task. We evaluate EvoRBC in simulated robots with different numbers of DOF in two tasks, navigation and foraging. Our results show that while standard evolutionary approaches are highly affected by the locomotion complexity of the robot, EvoRBC is consistently able to evolve high-performing solutions. We also show that EvoRBC allows for the evolution of general controllers, that can be successfully used in robots different than those with which they were evolved.

The role of compartmental models in the quantification of PET imaging data and computer-aided diagnosis

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Positron emission tomography (PET) is a molecular imaging technique with important applications in Oncology, Cardiology and Neuroscience that uses radiolabeled molecules (radiotracers) to map molecular processes and interactions in vivo. The full potential of the technique relies on the ability to quantify the images not only in terms of the radiotracer distribution but also to obtain relevant physiological parameters that are fundamental to make intersubject and intrasubject comparisons. PET data is a 3D matrix or a sequence of 3D matrices over time (dynamic imaging) with the concentration of the radiotracer in the correspondent spatial volume (voxel). Using dynamic PET, it is possible to obtain a discrete approximation of the concentration over time. Parameters with physiological interest can then be extracted using compartmental models. Several models exist that modulate the tracer exchange between physiological compartments, which depend on the target of the radiotracer and the nature of the receptor. In this talk we summarize some of the models, notably the simplified reference tissue method [1-3], the modified reference tissue method [4-5], and two graphical methods - Patlak plot and Logan plot, for irreversible and reversible tracers respectively [6-7]. We also propose to discuss how PET imaging data has been analyzed at ICNAS for achieving reliable computer-aided diagnosis, resorting to the aforementioned techniques and our own contributions. We have focus mainly in brain function and metabolism using ^{11}C-Raclopride, ^{11}C-β-CIT, ^{18}F-FDOPA, ^{11}C-PiB, ^{11}C-PK11195, ^{11}C-Flumazenil and ^{64}Cu-ATSM. Finally, examples of their application and computer-aided diagnosis tools we have developed at ICNAS are presented [8-9].

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Population dynamics through hierarchically embedded Markov chains

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The study of dynamical phenomena in finite populations often requires the consideration of population Markov processes of significant mathematical and/or computational complexity, which rapidly becomes prohibitive with increasing population size or increasing number of individual configuration states. Ubiquitous examples are found in Darwinian evolution and social dynamics, whose state space is often sizeable. Here, I will discuss a framework that allows one to define a hierarchy of approximations to the stationary distribution of general systems amenable to be described as discrete Markov processes with time invariant transition probabilities and (possibly) a large number of states. The framework allows the efficient study of the dynamics of social and biological communities in the presence of stochastic effects — such as mutations in evolutionary dynamics and random exploration of choices in social systems — including situations when the dynamics encompasses the existence of stable polymorphic configurations, thus overcoming limitations of existing methods. The general scope of the formalism makes it relevant and widely applicable to a variety of interdisciplinary problems.

Mechanically-driven Pattern Formation in Cell Cultures

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Cell migration and adhesion are key in embryogenesis, vasculogenesis, angiogenesis and immune system response. In particular, durotaxis, the directed movement of a cell toward substrates of increasing rigidity, and its implications are yet to be fully understood. By studying the formation of patterns that emerge from cell-cell and cell-substrate interactions, it is possible to shed light on these underlying mechanisms. For that effect, the hybrid two-dimensional model of cell dynamics proposed by van Oers et al [1] was used. It couples a Finite Element Method (FEM), to calculate deformations of the extracellular matrix (ECM), and a Cellular Potts Model (CPM), to simulate cell movement and adhesion. The coupling is done by means of a cell traction force generation model, proposed by Lemmon and Romer [2], and by considering a durotaxis term in the Hamiltonian of the CPM. In order to explore this model, image analysis methods were adapted to classify and quantify the morphology of the emerging patterns of vasculogenesis. Results show that traction force needs to be tightly regulated for cells to form vessel networks. Furthermore, on the parameter region in which results the formation of a vascular network, cell-cell adhesion regulates the number and size of meshes, that is, by lowering cell-cell adhesion there is a decrease in the average size of meshes and an increase in the average number of meshes, until networks cease to emerge in the system.

Keywords: Cell migration; Durotaxis; Extracellular matrix; Cellular Potts model; Finite Element Method; Monte Carlo method; Pattern formation; Vasculogenesis.

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3D retinal vascular network from OCT data

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We will present a method to determine the 3D position of the human retinal vascular network from commercial spectral-domain (SD) optical coherence tomography (OCT) data. OCT is a noninvasive technique to collect optical properties of the human retina, therefore this method is harmless for the subject, having therefore the potential to become a screening process to diagnose alterations on the 3D location of the vessel network within the retina.

The method is divided in three steps. First one seeks the two-dimensional location of retinal vascular network on the eye fundus. this one done through support vector machines classification of properly defined fundus images from OCT data, taking advantage of the fact that on standard SD-OCT, the incident light beam is absorbed by hemoglobin, creating a shadow on the OCT signal below each perfused vessel. In a second step, the depth-wise location of the vessel is obtained as the beginning of the shadow. Finally, the classification of crossovers and bifurcations within the vascular network is also addressed.

We illustrate the feasibility of the method and show numerical reconstructions of the retinal vessel network.

Finally we will also briefly discuss some other mathematical problems that we have addressed concerning OCT, amongst which are modeling the optical properties of the human retina by proper numerical methods.

Keywords: Retina, vascular network, Optical coherence tomography

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Angiogenic Factors produced by Hypoxic Cells drive Anastomosis in Sprouting Angiogenesis

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Cancer is among the leading causes of death worldwide. Sprouting angiogenesis, the process by which new blood vessels grow from existing ones, is crucial in the growth of solid tumors, and it is also present in over seventy different pathologies [1]. In response to a chemotactic stimulus (Vascular Endothelial Growth Factor), endothelial cells of the vessel sprout can adopt either a migratory or a proliferating phenotype [2]. In this work we use a multi-scale phase field model of vessel growth [3] in 2D and in 3D coupled with blood flow hydrodynamics. We use this model to discuss the role of irrigation, endothelial cells' chemotactic response and proliferation rate as key factors in determining the morphology of vascular networks. The computation of blood flow was introduced into the model as the main quantitative element in the hypoxia regulation mechanism, allowing to determine the deactivation of VEGF production by the tissue cells as a function of tissue irrigation. Preliminary results show a significant influence in the morphology of 2D vascular networks for the case where the blood flow is taken into account in hypoxia regulation. Surprisingly in the 3D model we did not observe such influence, obtaining similar morphologies with both approaches, with and without computing the tissue irrigation. This result is unexpected and raises questions about the role of mechanical forces exerted by cells on the formation of anastomosis in 3D. Overall, these results indicate that blood flow has an important role in angiogenesis, but the active work of cells such as macrophages could be determinant in the morphology of the new capillary network.

FIGURE 1. Vessel network resulting from sprouting angiogenesis.

Keywords: angiogenesis; anastomosis; phase-field;
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Boundary control problems in hemodynamics: mathematical analysis and numerical simulations

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Flow control has been subject of extensive research during the last decades. Optimal control problems in the frame of fluid dynamics, can be applied in several real life application, from automobile to aerospace industries. Here, we present two possible frameworks for the application of control problems in hemodynamics. One related to the velocity tracking problem and another with boundary identification. We discuss theoretical aspects as well as numerical examples for which we will emphasize the computational challenges. The relevance of these techniques for the definition of a personalized tool to be used in a clinical scenario will also be emphasized.

Keywords: Optimal boundary control; Navier-Stokes equations; patient-specific simulations

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The Lisbon data - present and future

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Brief presentation of the work that Lisbon is developing in the theme of smart cities and the data that are produced.

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