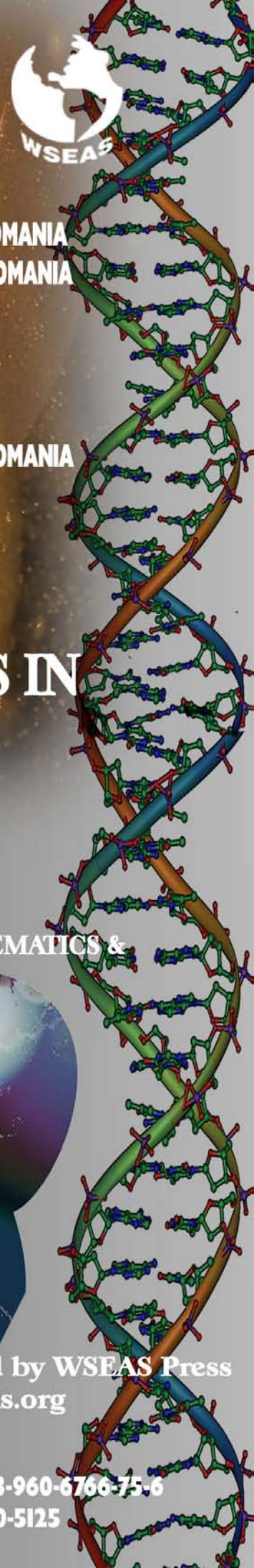


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MATHEMATICS AND COMPUTERS IN BIOLOGY AND CHEMISTRY

Bucharest, Romania, June 24-26, 2008

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COMPUTERS IN BIOLOGY & CHEMISTRY (MCBC '08)**

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Preface

This book contains the proceedings of the 9th WSEAS International Conference on MATHEMATICS & COMPUTERS IN BIOLOGY & CHEMISTRY (MCBC '08) which was held in Bucharest, Romania, June 24-26, 2008. This conference aims to disseminate the latest research and applications in Mathematical Models (Deterministic and Stochastic), Modelling and Simulation, Experiments and Computer Analysis, Statistics, Optimization, Computer Science (Data Bases, Data Structures, Software Engineering, Reliability), Computational Intelligence (NN, FL and EC), Practical Methods, Bio-Engineering, Chemical Engineering and other relevant topics and applications.

The friendliness and openness of the WSEAS conferences, adds to their ability to grow by constantly attracting young researchers. The WSEAS Conferences attract a large number of well-established and leading researchers in various areas of Science and Engineering as you can see from <http://www.wseas.org/reports>. Your feedback encourages the society to go ahead as you can see in <http://www.worldses.org/feedback.htm>

The contents of this Book are also published in the CD-ROM Proceedings of the Conference. Both will be sent to the WSEAS collaborating indices after the conference: www.worldses.org/indexes

In addition, papers of this book are permanently available to all the scientific community via the WSEAS E-Library.

Expanded and enhanced versions of papers published in this conference proceedings are also going to be considered for possible publication in one of the WSEAS journals that participate in the major International Scientific Indices (Elsevier, Scopus, EI, ACM, Compendex, INSPEC, CSA see: www.worldses.org/indexes) these papers must be of high-quality (break-through work) and a new round of a very strict review will follow. (No additional fee will be required for the publication of the extended version in a journal). WSEAS has also collaboration with several other international publishers and all these excellent papers of this volume could be further improved, could be extended and could be enhanced for possible additional evaluation in one of the editions of these international publishers.

Finally, we cordially thank all the people of WSEAS for their efforts to maintain the high scientific level of conferences, proceedings and journals.

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Plenary Lecture I

Phenomenological Universalities as a new tool for experimental and cross-disciplinary research



Professor Pier Paolo Delsanto

Chair of Structural Mechanics, Bioindustry Park of Canavese
Bioinformatics and High Performance Computing Lab
Politecnico of Torino,
ITALY

E-mail: pier.delsanto@polito.it

Abstract: Phenomenological Universalities represent a new tool for the classification and interpretation of observed or experimental data in the context of cross-disciplinary research. Also they can act as a “magnifying glass” to finetune the analysis and to quantify the difference among similarly looking datasets. In particular, the class U2 is of special relevance, since it includes, as subcases, all growth models proposed to date. In this presentation we show that it may be applied, in a simple fashion, to a variety of problems of interest in biomedicine and in the context of elastodynamics. The results suggest the application of different fitting equations from the ones which are currently adopted, and the use, in several contexts, of fractal dimensioned variables.

Brief Biography of the Speaker: Academic degrees: Laurea (MS.) in Physics, University of Torino, 1963; Ph.D. in Physics, University of Torino, 1965; "Libera Docenza" (Habilitation) in Physics, University of Roma, 1971. Positions: 1966-1969 University of Frankfurt, Germany. (Fellow of the A. von Humboldt Stiftung and Research Associate), 1969-1984 University of Puerto Rico, Mayaguez, USA. (Professor with tenure). 1982-1983 Duke University, Durham, NC, USA (Visiting Professor – In sabbatical leave from the University of Puerto Rico). 1984-1987 Naval Research Laboratory, Washington D.C. (Research Physicist). 1987 to date: Politecnico di Torino (Italy), Full Professor. Also, for the years 1994-2000: Director of the National Institute for Condensed Matter Physics (INFM)-Politecnico of Torino Research Unit. Miscellanea: Coordinator of many national and international research projects (1980-2003), e.g. BRITE EURAM, COPERNICUS (Europe), and NSF, ARO, NATO (USA). Coordinator of the European Science Foundation programme NATEMIS, 2000-2005, with seven countries involved. Consultant to the Naval Research Laboratory, 1987-1999 and 2003-2004 and to the Los Alamos National Laboratory, 2000-2002. Also, from 2004 Consultant to the NIH supported “Center for the development of a virtual tumor” (CVIT), Boston, Mass. Co-leader of the Modeling-Simulation Working Package of the EU-funded AERONEWS Project, (6th Framework Programme for European Scientific Research), see ww.kulac.ac.be/AERONEWS. Invited Speaker, Guest Editor, Chair and/or Co-Organizer in many international conferences and meetings. Editor of the books: 1) “New Perspectives on Problems in Classical and Quantum Physics”, Gordon and Breach, 1997-1998, in two volumes. 2) “The universality of Nonclassical Nonlinearity, with applications to NDE and Ultrasonics”, Springer, 2006. Editor-in-chief (one out of three) of the electronic journal “Theoretical Biology and Medical Modelling”. Professor ad Honorem at the Universities of Puerto Rico, USA and Brazov, Romania. Invited Professor (or equivalent) at several Universities, such as Melbourne (Australia) , Montreal (Canada) , Cagliari (Italy), etc. Outstanding Performance Award: Naval Research Laboratory, 1985 and 1986. A.Berman Research Publication Award for outstanding paper: Naval Research Laboratory, 1994.

Plenary Lecture II

Nucleic Acid Structural Properties Identified by Genomic Signal Analysis



Prof. Paul Dan Cristea

Corresponding Member of Romanian Academy
Director of the Romanian Bioinformatics Society
Biomedical Engineering Centre,
University "Politehnica" of Bucharest,
ROMANIA

E-mail: pcristea@dsp.pub.ro

Website: http://www.acad.ro/academia2002/acadrom/pag_ist.htm

Abstract: The conversion of nucleotide sequences into digital genomic signals allows using signal processing methods for the analysis of genomic data. This approach reveals surprising regularities in the distribution of nucleotides and pairs of nucleotides, in both prokaryotes and eukaryotes. These structural and statistical restrictions of genomic sequences would be difficult to identify by using only statistical and pattern matching methods, as in standard symbolic sequence analysis. Long range regularities make the structure of a genome be less like that of a "plain text", which simply conveys a semantics in accordance to a grammar, and more like that of a "poem", which obeys additional structural rules that give "rhythm" and "rhyme". A direct application of these regularities is predicting nucleotides in a sequence, when knowing the preceding ones, in a way similar to time series prediction. This approach attempts to model processes such as DNA replication, DNA transcription, or mRNA translation, and allows to explore the possibility of low level error correction. Moreover, genomic signal analysis (GSA) reveals the hidden ancestral structure of nucleotide sequences, before their re-structuring under the selective pressure of species separation. GSA is also efficient in the analysis of pathogen variability. This is important for the molecular level detection of mutations that induce drug resistance, providing the clinician with information needed for a fast and accurate decision, and avoiding the lengthily and expensive phenotypic clinical studies requesting pathogen culture. The talk will present result in the molecular study of variability of Human Immunodeficiency Virus, performed in cooperation with Dr. Dan Otelea from the National Institute of Infectious Diseases "Prof.Dr.Matei Bals", and of Mycobacterium tuberculosis, in cooperation with Dr. Dorina Banica from the National Institute of Pneumology "Prof. Dr. Marius Nasta", Bucharest, Romania and Dr. Karin Rodewald, Max-Planck – Institute of Biochemistry, Martinsried, Germany.

Brief Biography of the Speaker: Paul Cristea graduated the Faculty of Electronics and Telecommunications (UPB - University "Politehnica" of Bucharest, Romania, 1962), the Faculty of Physics (University of Bucharest, 1969), and has a Ph.D. in Technical Physics (UPB, 1970). Since then his research and teaching activities covered an large area of Electrical Engineering and related domains including topics like Digital Signal and Image Processing, Genomic Signals, Neural and Evolutionary Systems, Computerized Medical Equipment, Evolutionary Intelligent Agents, Intelligent e-Learning Environments. He is the author or co-author of more then 130 published papers, 11 patents and contributed to more then 20 books in these fields. He is currently affiliated with UPB, the Biomedical Engineering Center (general director) and the Vrije Universiteit Brussel, Belgium, the ETRO Department. He is a corresponding member of the Romanian Academy and director of the Romanian Bioinformatics Society.

Plenary Lecture III

Processing of Polymer Matrix Nanocomposites with Carbon Nanotubes



Professor José M. Kenny

European Centre for Nanostructured Polymers, UdR INSTM,
University of Perugia, NIPLAB - INSTM, UdR Perugia, 05100 Terni – ITALY

E-mail: jkenny@unipg.it

Website: <http://www.unipg.it/materials>

<http://www.nanofun-poly.com>

<http://www.ecnp.eu.org>

Abstract: Carbon nanotubes (CNTs) are innovative materials with enormous potential because of their outstanding mechanical and physical properties [1]. Their utilization to prepare polymer composites is very important in several fields like electromagnetic shielding, touch screens and static charge dissipation. In this regard the possibility to realize a fully integrated nanotube-reinforced epoxy system represents a promise for the preparation of composite materials with outstanding mechanical properties and multi-functional features [2,3]. However, the incorporation of nanotubes is not a trivial task mainly if a good dispersion for a chemical grafting to the polymer matrix are mandatory to maximize the advantage of nanotube reinforcement. Here we report our recent activities on the processing of polymer matrix nanocomposites with carbon nanotubes and, in particular, the chemorheological aspects that affect the interaction of nanofillers and the matrix. Specific models are applied to describe the kinetics of the different reactive processes and the changes of the polymer structure. Regarding the polymer-nanotube interaction, the plasma treatment for the functionalization of carbon nanotubes represents a novel approach easy to scale up to industrial application. More recently there were a lot of attempts to fluorinate carbon nanotube sidewalls in such manner [4-7]. In this work we report how plasma functionalized single-walled carbon nanotubes (F-CNTs) can be used as precursors for the compatibilization with polymeric matrices for preparing an integrated nanotube composite material. The results show the emergence of specific interactions of cross-linking between thermosetting matrix and amino-functionalized CNTs during the cure reaction with an improvement of the mechanical properties with respect to those prepared with un-functionalized CNTs. The possibility of using functionalized CNTs to make possible a “mix and match” approach towards classes of hybrid materials will be reported suggesting the possibility of tuning the electrical properties by combining the electric field in the assembling processing. Moreover it was demonstrated as electrophoretically deposited CNT thin films provide a simple route to obtain layered functional nanostructures by growing homogeneous films of carbon nanotubes and infiltrating polymer or monomer, followed by in situ polymerization. Some examples where electrophoretically deposited SWCNT films were infiltrated with monomer and then the monomer was polymerized are reported [8].

Brief Biography of the Speaker: Professor José M. Kenny got his PhD in Chemical Engineering from the University of South (Bahia Blanca, Argentina). He is Full Professor of Materials Science and Technology at the University of Perugia, where he also teaches Polymer Technology and Materials Nanotechnology. Moreover, Prof. Kenny is the President of the Board of the ECNP: European Centre for Nanostructured Polymers installed by the 11 core-partners of the European Network of Excellence NANOFUN-POLY. Prof. Kenny is the Director of the International PhD Program on Materials Nanotechnology and of the European Master on Polymer Nanotechnology coordinated by the University of Perugia in collaboration with several European Universities. Both programs are supported by the European Network of Excellence NANOFUN-POLY and the ECNP coordinated by Prof. Kenny. During his career Prof. Kenny has been visiting and research professor in the following universities: University of Naples (1984-1991), University of Connecticut: (1989) University of Washington (1990), Washington University of Saint Louis (1991). He has published more than 300 papers in international scientific journals and books related to the processing technologies of polymers, composites and nanocomposites. Prof. Kenny has directed

more than 100 final projects for the degree in Materials Engineering and more than 30 PhD theses on Industrial Engineering and Materials Nanotechnology. He has coordinated several Italian and international research projects and is member of several scientific societies: he is currently Past-President of the SAMPE Europe (Society for the Advancement of Material and Process Engineering) and recently has been elected member of the Board of the Italian Industrial Association of Composite Materials.

Plenary Lecture IV

Complex Procedure for Evaluating the Fatigue Wear of Tibial Inserts for Patients with Abnormal Walking



Professor Lucian Capitanu

Department of Tribology
Institute of Solid Mechanics of Romanian Academy
Constantin Mille 15, Bucharest
ROMANIA
E-mail: luciancapitanu@yahoo.com
Website: <http://www.imsar.ro>

Co-Authors:

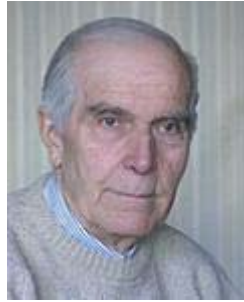
Luigi Vladareanu, Aron Iarovici, Justin Onisoru
Department of Continuum Mechanics
Institute of Solid Mechanics of Romanian Academy
Constantin Mille 15, Bucharest
ROMANIA

Abstract: In a previous paper [1] the authors established the basis for implementing control strategies for some Knee Prosthesis Simulator by intermediate of Programmable Logical Controllers in Open Architecture structure. The authors describe there a method for estimating the fatigue wear based on experimental tests and numerical simulations of tribological behavior of the Knee Prosthesis under common activities loading. But the loading cycles are standard ones from the literature, it means that could be significant differences between the loadings used in simulator and the real ones especially when abnormal walking is still maintaining after Knee Arthroplasty. It results that, due to the cumulative nature of fatigue wear, these differences will accumulate leading to inaccurate predictions on prosthesis fatigue. This work try to present a more complex procedure which allows for transferring the real loads from the patient artificial knee to the knee simulator control system, by intermediate of kinematic acquisition, evaluation of joint loadings and dynamic simulation of joint contact. Practically, the data resulting from motion analysis of the patient activities will be processed by a specialized code (AnyBody Modelling System) which will determinate the motion dynamic loadings of the joint. Based on these processed data, a detailed joint tribological model will allow for determination of contact dynamics based on Finite Element Analyses and will generate the customized evolution of each one of the controlled knee simulator degrees of freedoms. Use of the method described here will generally improve the accuracy of lifetime predictions based on experimental data obtained in a Knee Prosthesis Simulator, allowing for customizing the tests for each patient.

Brief Biography of the Speaker: Title of qualification awarded: Senior Researcher; Head of Tribology and Biotribology Department, Scientific Manager of Institute of Solid Mechanics of Romanian Academy. Principal subjects-occupational skills covered: Tribology of classic materials, fatigue wear, lubrication, contact mechanics; Tribology of plastics and composite materials; Biotribology of Knee and Hip Endoprostheses. Doctorate coordinator in Tribology and Biotribology. Main subjects and professional skills: PhD studies related to friction and wear of thermoplastics reinforced with glass fibers. Member of Academic Assosiations: Full Member of European Society of Biomechanics (ESB), Founder member of Romanian Association of Tribology. Main author of 4 books in tribology of composite materials and biotribology of orthopedic prostheses.

Plenary Lecture V

EU Objective of 120g CO₂/km Emission for New Cars a Challenge for Tribology



Professor Ivan Iliuc
Department of Tribology
Institute of Solid Mechanics of Romanian Academy
Romanian Academy,
ROMANIA
E-mail: iiliuc@yahoo.com

Abstract: Passenger cars produce about 12 % of overall EU GHG emissions (CO₂) and transport sector with about 20 % is the second biggest emitter of GHG among all sources. Since 1990, EU has reduced transport emissions by 5 % but the contribution of road transport increased by 26 %. In order to accomplish the Kyoto requirements it is clear that transport emissions should also be reduced. A new decision of EU Commission from Feb 2007 specific the average emission in EU 27 should be 120 g/km by 2012. For several decades the most cost-effective method of reducing CO₂ emissions from cars will be to improve fuel efficiency. There are many ways of further improving the fuel efficiency of conventional engines and cars, among them: ignition systems that ensure complete combustion of the fuel available, improved compression at low engine loads, engine and gear friction reduction, six-speed manual transmission, stop-go systems, cylinder deactivation and other. Tribology will help to realize the above improvement by using low friction lubricant, adequate additive and modifying the frictional surface. The paper presents the problems and solutions, which were found.

Brief Biography of the Speaker: IVAN ILIUC, born in Bucharest at 12.11.1932. Education: M. Sc. 1958 Chemical Engineering-Polytechnic University of Bucharest, Ph.D 1970 in Tribology –at Polytechnic University of Bucharest. Career/Employment: Institute of Applied Mechanics, researcher, 1960-1970; Head of Laboratory for application of radioactive tracers in wear measurements 1968-1980, Institute of Physics and Technology of Materials Senior scientific researcher, Head of Tribology Department, 1980-1990; Institute of Solid Mechanics Head of Tribology Department 1990- 2000. Romanian Academy Ph.D Adviser 1991- today; Institute of Solid Mechanics, Deputy Director 1990-1995. Domain of interest: i) Wear and friction processes of materials; ii) Protection of surfaces, lubrication; iii) Friction and anti-wear properties of thin and thick layers; iiiii Development of measurement devices involved in tribology (ex. Digital profilometer, high sensitivity wear measurement devices). Honours, Awards, Fellowships: Prize of Romanian Academy “Traian Vuia 1964, Dozent Stipendium of the Alexander von Humboldt Foundation 1970-1971; Member of the Romanian Society of Tribology; Member of the German Society of Tribology (GfT). Publications: number of papers in refereed journals:45; number of communications to scientific meetings and invited conference : 18; number of books: 2: Tribologia Straturilor Subtiri (Romanian Academy publishing house) 1974; Tribology of Thin Layer (Elsevier) 1980.

Plenary Lecture VI

New trends in multivariate approximation and optimization



Associate Professor Dana Simian
Department of Computer Science,
Faculty of Sciences,
University Lucian Blaga of Sibiu
Romania
E-mail: dana.simian@ulbsibiu.ro

Abstract: Multivariate approximation and optimization appear in modeling real systems. The aim of this lecture is to present new algorithms and computational techniques for solving practical problems of approximation and optimization and to make a comparison between them. In the first part, genetic algorithms, ant and wasp behaviour algorithms are taken into account and applied to agent-based approaches to manufacturing scheduling and control in distributed manufacturing systems and to adaptive multiagent systems. In the second part we present new results in multivariate interpolation and polyspline and their applications in image processing and classification theory. A reformulation of the problem of multivariate interpolation which allows the use of methods taken from artificial intelligence make a connection between the two parts of the presentation. As a conclusion, problems from many other fields, like chemistry, biology, medicine which can be solved using the presented algorithms and techniques are presented.

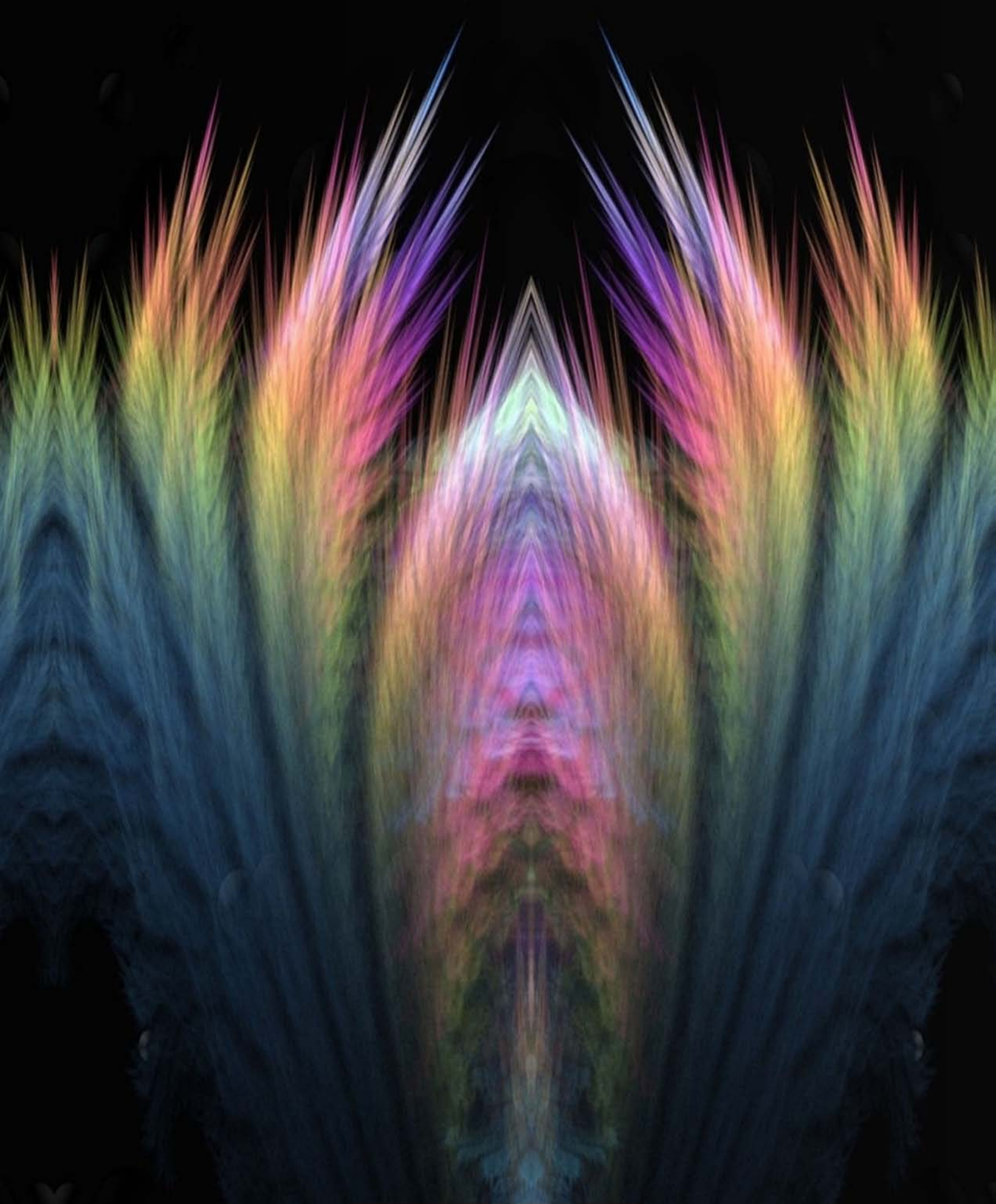
Brief Biography of the Speaker: Dana Simian received the diploma in engineering from the University of Sibiu, Romania, the diploma in Mathematics - Informatics from the University Babeş-Bolyai of Cluj-Napoca, Romania and the Ph.D. in Mathematics from Babeş-Bolyai University of Cluj-Napoca. She is Assoc. Prof. to the Department of Computer Science, Faculty of Sciences, University Lucian Blaga of Sibiu, Romania. She has a great experience in algorithms and numerical methods for modelling and optimization. She organized two special sessions within WSEAS conferences and an international workshop on topics related to modeling, approximation and optimization. She was a member of many scientific committees of international conferences. She has published more than 40 papers on a wide variety of subjects relating to multivariate interpolation, optimization, modeling, multiagent systems. She is co-editor of 4 WSEAS book series. She is author of 10 scientific books. She has been included in "Who is Who in the World" in 2006. She participated in many research grants.

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