Editors:
Prof. Nikos E. Mastorakis, Technical University of Sofia, Bulgaria
Prof. Anca Croitoru, University "Al. I. Cuza" of Iasi, Romania
Prof. Valentina Emilia Balas, "Aurel Vlaicu" University of Arad, Romania
Prof. Eduard Son, Russian Academy of Sciences, Moscow, Russia
Prof. Valeri Mladenov, Technical University of Sofia, Bulgaria

RECENT ADVANCES in MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY

Proceedings of the 10th WSEAS Int. Conf.
on MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY (MCBC'09)

Prague, Czech Republic, March 23-25, 2009

Recent Advances in Biology and Biomedicine
A Series of Reference Books and Textbooks

ISBN: 978-960-474-062-8
ISSN: 1790-5125

Published by WSEAS Press
www.wseas.org

RECENT ADVANCES in MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY

RECENT ADVANCES in MATHEMATICS and COMPUTERS in BIOLOGY AND CHEMISTRY

Proceedings of the 10th WSEAS International Conference on MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY (MCBC'09)

Prague, Czech Republic
March 23-25, 2009

Recent Advances in Biology and Biomedicine
A Series of Reference Books and Textbooks

Published by WSEAS Press
www.wseas.org

ISSN: 1790-5125
ISBN: 978-960-474-062-8

RECENT ADVANCES in MATHEMATICS and COMPUTERS in BIOLOGY AND CHEMISTRY

Proceedings of the 10th WSEAS International Conference on MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY (MCBC'09)

Prague, Czech Republic
March 23-25, 2009

Recent Advances in Biology and Biomedicine
A Series of Reference Books and Textbooks

Published by WSEAS Press
www.wseas.org

All papers of the present volume were peer reviewed by two independent reviewers. Acceptance was granted when both reviewers' recommendations were positive.
See also: http://www.worldses.org/review/index.html

ISSN: 1790-5125
ISBN: 978-960-474-062-8

World Scientific and Engineering Academy and Society

RECENT ADVANCES in MATHEMATICS and COMPUTERS in BIOLOGY AND CHEMISTRY

Proceedings of the 10th WSEAS International Conference on MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY (MCBC'09)

Prague, Czech Republic
March 23-25, 2009

Preface

This year the 10th WSEAS International Conference on MATHEMATICS and COMPUTERS in BIOLOGY and CHEMISTRY (MCBC'09) was held in Prague, Czech Republic. The Conference remains faithful to its original idea of providing a platform to discuss theoretical and applicative aspects of molecular dynamics, biochemistry, biophysics, quantum chemistry, molecular biology, bioengineering, biotechnolgies, medical imaging, chemical engineering, nuclear biology and medicine, impulsive differential equations in biology etc. with participants from all over the world, both from academia and from industry.

Its success is reflected in the papers received, with participants coming from several countries, allowing a real multinational multicultural exchange of experiences and ideas.

The accepted papers of this conference are published in this Book that will be indexed by ISI. Please, check it: www.worldses.org/indexes as well as in the CD-ROM Proceedings. They will be also available in the E-Library of the WSEAS. The best papers will be also promoted in many Journals for further evaluation.

A Conference such as this can only succeed as a team effort, so the Editors want to thank the International Scientific Committee and the Reviewers for their excellent work in reviewing the papers as well as their invaluable input and advice.

The Editors

Table of Contents

Plenary Lecture 1

Particle Methods Applied in Biology and Chemistry

Professor Franck Assous
Ariel University Center & Bar-Ilan University
ISRAEL
E-mail: franckassous@netscape.net

Abstract: Particle method is a well-known approach that has been used for a long time in charged particle beams or plasma physics modeling. In recent years, particle based methods have become widespread tools for approximating solutions of ordinary/partial differential equations in a variety of fields. In these methods, a solution of a given equation is represented by a finite set of particles, located in points xi and carrying masses ωi. Equations of evolution in time are then written to describe the dynamics of the location of the particles and their weights. The aim of this lecture is to show that this method can provide a useful tool of simulation in biology and chemistry. In the first part, we recall the principles and the basic properties of the particle method. Numerical and algorithm considerations are also exposed. In the second part, examples of reformulation of problems from other fields, like chemistry and biology, which allow the use of particle based modeling, are presented.

Brief Biography of the Speaker: Professor Franck Assous received a Ph.D. degree in Applied Mathematics from the University of Paris (France). He then received the French "Habilitation a Diriger les Recherches" degree from the University of Toulouse (France). He worked more than 14 years at the Atomic French Agency (CEA) as a senior researcher. In parallel, he was teaching at the ENSTA School of Engineers (Paris) as an Assitant Professor, then at the Versailles University as an Associate Professor. He is currently working in Israel, where he is Professor of Applied Mathematics at the Ariel University Center (Israel), and at the Bar-Ilan University (Israel). His research project include numerical methods for Partial Differential Equations, with a particular interest for problems arising from models in the field of computational electromagnetism and plasma physics, originated from the need to compute precisely the motion of charged particles for plasma physics applications. He is also interested in studying the relations between different fields (cross-disciplinary research), particularly applications of mathematical and numerical methods applied to physics, chemistry and biology.

Plenary Lecture 2

Advanced Classification and Regression Algorithms

Assoc. Professor Dana Simian
Faculty of Sciences
University Lucian Blaga of Sibiu
ROMANIA
E-mail: dana.simian@ulbsibiu.ro

Abstract: The aim of this paper is to present and analyzed new classification and regression algorithms and applications of these algorithms for different kind of data. One of the practical applications of our algorithms is in the ecological characterization of different areas.
Generally, the task of classification is to find a rule, which based on external observations assigns an object to one of several classes. A classification task supposes the existence of training and testing data given in the form of data instances. Each instance in the training set contains one target value, named class label and several attributes named features. One of the approaches used for solving the problem of binary or multiclass classification is represented by SVM algorithm. SVM models are obtained by convex optimization and are able to learn and generalize in high dimensional input spaces. The goal of SVM is to produce a model which predicts target value of data instances in the testing set which are given only the attributes. A very powerful idea, which can be used not only in SVM algorithms, is the kernel method. Using an appropriate kernel, the data are projected in a space with higher dimension in which they are separable by a hyperplane. Usually simple kernels are used but the real problems require more complex kernels. The kernel substitution can be used to define many other types of learning machines distinct from SVMs.
We introduce and analyze multiple kernels based on simple kernels. Our intention was to study the possibility of obtaining nonlinear multiple kernels using simple classifiers and to analyze their performance comparing with other multiple kernels. Therefore we choose, first, for experiments the most common data sets, used in a great number of papers and taken from libsvm website. Second, we used different types of data obtained in the monitoring process of many ecological areas from Romania.
In order to take advantage of possible correlations between the outputs to improve the quality of the predictions, we also consider the Support Vector Regression method (SVR). SVR is based on the theory of Support Vector Machines and belongs to the category of reproducing kernel methods. The kernel is viewed as the covariance of a second order Gaussian process. SVR builds a model, f, of the output of a system that depends on a set of factors. One of the problems we confront with, in the ecological characterization of different areas is the quantification of the outputs of our system. In order to apply SVR method, we make a regression analysis for studying the relationships among the outputs of our system.

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 Babes-Bolyai of Cluj-Napoca, Romania and the Ph.D. from Babes-Bolyai University of Cluj- Napoca, Romania. She graduated many courses in Computer Science. She is the head of the Department of Computer Science from the Faculty of Sciences, University Lucian Blaga of Sibiu, Romania. She has a great experience in algorithms and numerical methods for modelling and optimization. She published 15 books, more than 60 articles and participated in the editorial board of 22 scientific publications (proceedings of international conferences).
She organized 5 special sessions within WSEAS conferences and 2 international workshops on topics related to algorithms and computational techniques in modeling, approximation and optimization. She was a member of many scientific committees of international conferences.. She was plenary speakers in 3 international conferences. She is reviewer of many scientific publications. She was involved as director of many research grants. She has been included in “Who is Who in the World” in 2006 and in the “IBC Foremost Engineers of the World”, 2008.

Plenary Lecture 3

Statistical Global Metabolic Control Analysis

Profesor Zelimir Kurtanjek
University of Zagreb
Faculty of Food Technology
CROATIA
E-mail: zkurt@pbf.hr

Abstract: Metabolic Control Analysis (MCA) is a mathematical theory stemming from elec-trical engineering network analysis applied to biological systems. Availability of annotated genome, metabolomics and proteomics of numerous industrial important microorganism leads fundamental research of industrial microbiology "in silico". From engineering point of view, open are possibilities for computer design of synthetic genome for development of new tech-nologies, most importantly for bioenergetics based on synthetic microorganism with inte-grated photosynthesis and fermentation metabolisms. The main obstacles toward this far reaching goal are not in chemical synthesis of genome, but rather in biological and computer analysis of intricate metabolism control on a molecular level. At present, most of MCA analy-sis is based on steady state (homeostatic constraint) analysis and study of "one factor at a time" infinitesimal effects of perturbations of each individual enzyme and metabolite concen-tration on metabolic fluxes and individual reaction rates. This work introduces the concept of global sensitivity based on simultaneous variation of a complete set of enzymes and metabo-lite concentrations (elasticities) in finite ranges of activities (concentrations). Perturbations are defined by corresponding finite ranges of concentrations and corresponding general probabil-ity density distributions. The flux sensitivities are determined as first and second order rela-tive multidimensional variances. The first order effects are reflection of variation of each in-dividual enzyme. Importantly, the second order effects imply synergic effects of the whole ensemble of enzymes which completely escapes in the traditional MCA analysis. The disper-sions of fluxes due to each enzyme are evaluated through computer simulation and Fourier Amplitude Sensitivity Test algorithm. The implications of the proposed theory are demon-strated by computer simulation of theoretical metabolism pathways and experimental analysis of E. coli central metabolism unsteady perturbation by glucose impulse.

Brief Biography of the Speaker: Zelimir Kurtanjek was born in 1946 in Zagreb, Croa-tia. He graduated in 1971 with engineering degree in physics from the Department of Sci-ences, University of Zagreb. He completed postgraduate studies in Technical Cybernetics at Faculty of Technology, University of Zagreb. In 1975 he enrolled at the postgraduate study in chemical engineering at the Department of Chemical Engineering, The University of Houston, TX, USA. In 1979 he received doctoral degree under mentorship of Prof. Dan Luss in the Laboratory for Reaction Engineering. He completed his postdoctoral studies with Prof. G. Froment at the Department of Chemical Engineering, University of Gent, Belgium. During 1991. he was a visiting professor through EU project TEMPUS at the Department of Biologi-cal Sciences, University of Ulster, Coleraine, Northern Ireland. Since 1980 he is employed at the University of Zagreb, Faculty of Food Technology and Biotechnology, University of Za-greb as a professor of chemical engineering. He is teaching reactor engineering, mathematical modeling and process control to students of biochemical, chemical and food engineering.
In his scientific work he is interested in modeling and control of reactors, modeling of bioprocesses and food processes, and application of AI methods in modeling and process con-trol. He has published over 50 papers in international and national journals. Since 1976 he is a member of American Institute of Chemical Engineers, a delegate of Croatia in European Fed-eration of Biotechnology, and also is a member of Croatian Society of Chemical Engineers, Croatian Society of Biotechnology, and Croatian Technical Academy. He is editor in chief of Chemical and Biochemical Engineering Quarterly and a member of the editorial board of Food Technology and Biotechnology journals.

Plenary Lecture 4

Introduction of an Hamiltonian Function and a Canonical Representation Aimed at a Possible Driving of the Evolution of a Cells Colony

Professor Joseph Quartieri
Department of Physics, Engineering Faculty
University of Salerno
Via Ponte don Melillo 1, I-84084 Fisciano (SA)
ITALY
E-mail: quartieri@sa.infn.it
Co-Authors:
Professor Stefano Steri
Department of Mathematics, University of Napoli
Dr. Claudio Guarnaccia
Department of Physics, Engineering Faculty
University of Salerno

Abstract: A new method to approach the problem of solving PDEs by means of Lie series expansion has been deeply investigated by the author (in cooperation with Professor S. Steri) in several papers and the application to biomathematical topics has been performed. The treatment of a cells colony and its evolution has been modelled with a non linear Cauchy problem (evolutionary PDE) and solved by Lie series. The conditions that ensure the existence and the uniqueness of the solution have been presented. Then the control of a drug has been introduced and described by a time dependent parameter.
In our recent studies we are dealing with the following problem: how to introduce the Hamiltonian function in an analytic nonlinear evolutionary process and how to gain a canonical representation of the process by a double series of equations, similarly to what is done in Physics and in finite optimal processes theory. By this way, we are conducted to introduce adjoint variables, namely generalized momenta, to be considered together with the positional variables.
In this work we present a remarkable illustration of the procedure to be followed, developing in details the task for the biological problem above described, the study of a controlled birth and death stochastic process, in which generalized momenta have a clear interpretation. In fact the meaning and the role of new adjoint functions is here suitably discussed. In the end, the possibility to perform an optimum control on the drug action is mentioned, with a particular interest to the application of a minimum principle a la Pontryagin.

Brief Biography of the Speaker: Prof. Joseph Quartieri is full professor of Physics in the Engineering Faculty of University of Salerno. He belongs to the Physics Department "E.R.Caianiello" of the same University. From 1997-98 he is the coordinator of all the Physics courses in the Engineering Faculty. From 2006 he is also in charge of Medical Physics course at Medicine and Surgery Faculty of University of Salerno.
He got graduated cum laude in Nuclear Physics at Naples University in 1974. From 1980 to 1986 he worked as researcher at National Research Centre (CNR). From 1980 he took several teaching positions as assistant professor, and in 1985 he became associated professor at Engineering Faculty of Rome University "Tor Vergata". From 1997 he moved to the Engineering Faculty of Salerno University. He got a scientific association with the National Institute for Nuclear Physics (INFN), in the Salerno's group and participated in the Physics Department "E. R. Caianiello". He is author of hundreds of papers in several relevant international journals.

Authors Index