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ADVANCED TOPICS on MATHEMATICAL BIOLOGY and ECOLOGY

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Proceedings of the 4th WSEAS INTERNATIONAL CONFERENCE on MATHEMATICAL BIOLOGY and ECOLOGY (MABE '08)

Acapulco, Mexico, January 25-27, 2008

Mathematics and Computers in Science and Engineering
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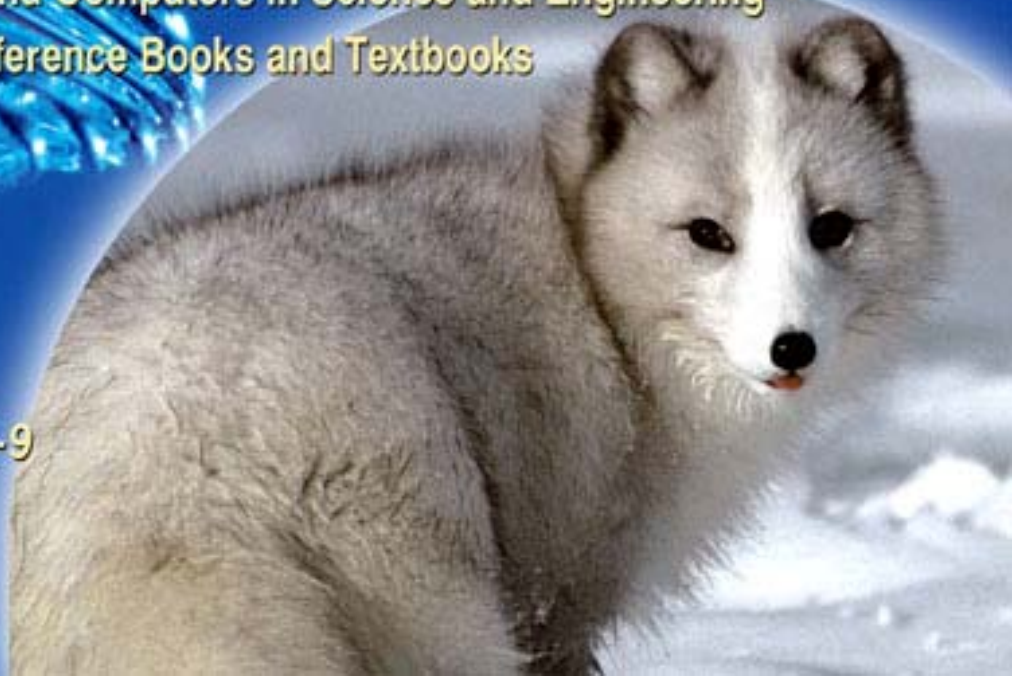

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Preface

This book contains proceedings of the 4th WSEAS International Conference on Conference on Mathematical Biology and Ecology (MABE'08) which was held in Acapulco, Mexico, January 25-27, 2008 The WSEAS Mathematical Biology and Ecology Conference was started in Udine, Italy, January 2005 and then held in Miami, Florida, USA, January 2006. It was also held in Gold Coast, Queensland, Australia, January 2007 and this year in Acapulco, Mexico. The Society (WSEAS) has also organized many other separate or joint conferences on Biology, Biochemistry, Biophysics, Bioengineering, Biotechology, Ecosystems, Ecology, Oceanology, Forest Science, Environment, Development etc... well as their impact and their interaction with other areas of Modern Engineering and Science. The relevant titles could be retrieved from the web site: www.worldses.org/history.htm

The 4th WSEAS International Conference on Mathematical Biology and Ecology (MABE'08) aims to disseminate the latest research and applications in the afore mentioned fields. 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 these 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, 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).

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

The Editors

Plenary Lecture I

Receiver Operating Characteristic (ROC) Curve: A Tool for Describing and Comparing Continuous Diagnostic Tests

Professor Ivana Horova
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Abstract: The ROC methodology has been developed in 1950's. It is derived from signal detection theory where it is used to determine if an electronic receiver is able to satisfactory distinguish between signal and noise. Recently there has been an increased use of ROC curves for assessing the effectiveness of continuous diagnostic markers in distinguishing between healthy and diseased individuals. The most common parametric methods to estimate the ROC curve are based on bi-normal or bi-logistic model. But problems can occur if the distributional assumptions are not satisfied. Non-parametric methods do not have any distributional assumptions and are an ideal alternative for ROC curve analysis. In this lecture two different approaches to nonparametric estimates via kernel methods are presented. The first method is based on kernel estimates of cumulative distribution functions and the second one uses the fact that, in statistical terms, ROC curve is the non-null distribution function of the P-value. We conduct a simulation study to compare ROC curves obtained by proposed methods to data sets one of which fulfils the assumptions for bi-normal model. In conclusion, these methods are applied to medical data.

Plenary Lecture II

Conquering the time scale problem in biophysics and materials science

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Abstract: Driven by ever more powerful computational resources, simulation methods have become increasingly important to compliment experimental investigations in many scientific disciplines. Increasingly such methods are not only used to understand biological or physical phenomena, but to predict the outcome of experiments not yet performed or to the design biological effectors or nano materials with specific properties. Unfortunately structure formation in biological systems, as well as in many other areas of the nano science, occurs on time scales that are billions of times longer than the individual time step of present-day optimistic simulation methods. Here I will discuss an alternate approach, based on the development of atomistic free-energy forcefields, which can circumvent this "time-scale gap" for many scientific applications. I will present recent results of large-scale simulations for biomolecular structure formation (protein folding and protein structure prediction), drug-design and nano-material simulations with this approach. Perspectives of this approach for world-wide distributed computing and further scientific applications will be discussed.

Brief Biography of the Speaker: Wolfgang Wenzel studied physics at the University Bochum starting in 1983. As a Fulbright fellow he moved to Ohio State University (Columbus, Ohio, USA) in 1985 where he graduated 1989 with a Ph.D. in physics. He stayed as a postdoctoral fellow in the laboratory of Prof. Ken Wilson until his return to Germany in 1992, where he joined the department of physics of Dortmund University. In 2001 he became a group leader for computational nanophysics at the newly founded Institute for Nanotechnology at the Research Center Karlsruhe, one of Germany's national laboratories. Together with his group he works on the development of predictive simulation methods to accurately describe slow processes in various scientific fields: these include the POEM (protein optimization with energy methods) for biomolecular structure simulation, including protein folding, docking and structure prediction; the FlexScreen high-throughput in-silico screening approach for drug development and efficient simulation techniques for the description of nano-materials (http://www.fzk.de/biostruct).

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