PROGRAM OF THE

INTERNATIONAL CONFERENCE OF COMPUTATIONAL METHODS IN SCIENCES AND ENGINEERING (ICCMSE 2003)

Kastoria, Greece 12-16 September 2003

Conference center: Technological Educational Institute of Western Macedonia, Kastoria Campus Fourka area, Kastoria

Friday 12 September 2003

18:00 – 21:00 Registration

19:00 – 19:30 Opening. Dr. T.E. Simos (Invited Chair of ICCMSE 2003). Greetings from Dr. Z. Kalogiratou (Chair of the Organizing Committee).

19:30 – 21:00 Wine Reception

Saturday 13 September

Session: "Computational Physics I"

Saturday 13 September

ROOM: 10

Chair: Prof. V. Drakopoulos

9:00-9:30   V. Drakopoulos
Comparing Sequential Visualisation Methods for the Mandelbrot Set

9:30-10:00   A. Gaitanis, M. R. Freedman and N. M. Spyrou
Verification of a Simple Technique for the Removal of Motion Artefacts in Electrical Impedance Epigastrography Signals

10:00-10:30   J. L. Guisado, F. Jimenez-Morales, J. M. Guerra
Application of Shannon's Entropy to Classify Emergent Behaviors in a Simulation of Laser Dynamics

10:30-11:00   Coffee break

11:00-11:30   R. Hoppe and W. Litvinov and T. Rahman
Modelling and Computation of Axially Symmetric Flows of Electrorheological Fluids

11:30-12:00   A. Kaczanowski, K. Malarz and K. Kulakowski
Hysteresis Loop of a Nanoscopic Magnetic Array

Session: "Computational Engineering I"

Saturday 13 September

ROOM: 9

Chair: Prof. D. Karalekas

9:00-9:30   P. Abad
Components for Time Serie Receiver Clock Offset in GPS Solutions

9:30-10:00   F. A. Batzias, N. P. Nikolaou, A. S. Kakos and I. Michailides
Modelling the Natural Gas Consumption in a Changing Environment

10:00-10:30   F. A. Batzias, A. S. Kakos and N. P. Nikolaou
Computer Aided Dimensional Analysis for Knowledge Management in Chemical Engineering Processes

10:30-11:00   **Coffee break**

11:00-11:30   Y. S. Boutalis and O. I. Kosmidou
A Feedback Linearization Technique by Using Neural Networks: Application to Bioprocess control

11:30-12:00   G. Castellano, A. M. Fanelli and C. Mencar
Deriving Prediction Intervals for Neurofuzzy Networks

Session: "Computational Mathematics I"

Saturday 13 September

ROOM: 8

Chair: Dr. J. Vigo-Aguiar

9:00-9:30   H. Ramos, J. Vigo-Aguiar
     Variable Step-Size Störmer Methods

9:30-10:00   H. Ramos, J. Vigo-Aguiar
     A Note on the Selection of the Step-Size in the Variable Step-Size Störmer Method

10:30-11:00   **Coffee break**

11:00-11:30   J. Vigo-Aguiar, H. Ramos
     VS-VO Numerov Method for the Numerical Solution of the Schrödinger Equation

11:30-12:00   Dr. J. Vigo-Aguiar
     Exponential Fitting BDF formulas

12:00-12:30   M. De'Michieli Vitturi, F. Beux
     Nonlinear Pressure and Temperature Waves Propagation in Fluid Saturated Rock

Session: "Computational Methods I"

Saturday 13 September

ROOM: 3

Chair: Dr. Ch. H. Tsitouras

9:00-9:30   N. Orfanoudakis, H. Hatziapostolou, E. Mastorakos, E. Sardi, K. Krallis, N. Vlachakis, S. Mavromatis
Design, evaluation measurements and CFD Modelling of a Small Swirl Stabilised Laboratory Burner

9:30-10:00   T. Levitina and E. J. Brändas
Multitaper Techniques and Filter Diagonalisation – a Comparison

11:00-11:30   M. Lambiris, Ch. Tsitouras and K. Evmorfopoulos
Four-Step, Two-Stage, Sixth-Order, P-Stable Methods

10:30-11:00   *Coffee break*

11:00-11:30   S. Tsitmidelis, M. V. Koutras, V. Zissimopoulos
Reliability Bounds Improvement Via Cut Set or Path Set Rearrangements

11:30-12:00   N. J. Daras
Markov's Property and Generalized Padé-Type Approximants

12:00-12:30   G. Wei and N. Mousseau, P. Derreumaux
Protein Folding Simulations Using the Activation-Relaxation Technique

Session: "Computational Mathematics II"

Saturday 13 September

ROOM: 2

Chair: Dr. Z. Kalogiratou

9:00-9:30   O. Angulo, J. C. Lopez-Marcos
Numerical Integration of a Size-Structured Cell Population Model in an Environment of Changing Substrate Concentration

9:30-10:00   Z. Kalogiratou, Th. Monovasilis, T. E. Simos
Numarical Solution of the Two-Dimensional Time Independent Schrödinger Equation with Exponential-Fitting Methods

10:00-10:30 Z. Akdogan, M. Demirci and O. Sh. Mukhtarov
Sturm-Liouville Problems with Eigendependent Boundary and Transmissions Conditions

10:30-11:00 Coffee break

11:00-11:30 M. Kunik
Kinetic Solution of the Boltzmann-Peierls Equation – Part I

11:30-12:00 S. Qamar
Kinetic Solution of the Boltzmann-Peierls Equation – Part II

Keynote Lecture:

Saturday 13 September

ROOM: 9 AND 10

Chair: Dr. T. E. Simos

12:30-13:30   Professor J. C. Butcher

Some Numerical Methods for Stiff Problems

13:30   LUNCH

Keynote Lecture:

Saturday 13 September

ROOM: 9 AND 10

Chair: Prof. G. Maroulis

17:00-18:00 T. Levitina and E. J. Brändas

Numerical Quadrature Performend on the Generalized Prolate Spheroidal Functions

18:00 – 18:15   COFFEE BREAK

Session: "Computational Physics II"

Saturday 13 September

ROOM: 9

Chair: Dr. T.E. Karakasidis

18:15-18:45   **T. E. Karakasidis, A. B. Liakopoulos, N. S. Cholevas**
Parallel Molecular Dynamics Simulation of Lennard-Jones Liquids on a Small Beowulf Cluster

18:45-19:15   **P. Kolorenc, J. Horacek, K. Houfek and M. C. Zek, G. Mil'Nikov, H. Nakamura**
Calculation of Vibrational Excitation of Diatomic Molecules Below Dissociative Attachment Threshold

19:15-19:45   **M. H. X. Liang & B. Wetton, T. G. Myers**
Combined Air and Rivulet Flow and Application to Fuel Cells

19:45-20:15   *Coffee break*

20:15-20:45   **Y. Li, Shao-Ming Yu and P. Chen**
A Parallel Adaptive Finite Volume Method for Nanoscale Double Gates Mosfets Simulation

20:45-21:45   **M. S. Magdon-Maksymowicz, A. Dydejczyk, P. Gronek and A. Z. Maksymowicz**
Simulation of the Switching Curve in Antiferromagnetic Ising Model

Session: "Computational Engineering II"

Saturday 13 September

ROOM: 8

Chair: Prof. F. Grodin

18:15-18:45   C. S. Chew, K. S. Yeo and C. Shu
Simulation of Incompressible Flows Across Moving Bodies Using Meshless Finite Diffrerencing

18:45-19:15   A. Chortaras, Y. Guo, M. M. Ghanem, F. O. Bunnin
Automatic Generation of Software Components for Real Options Modelling

19:15-19:45   M. Darbandi, K. Mazaheri-Body, S. Vakilipour
A Pressure Weighted Upwinding Scheme for Calculating Flows on Unstructured Grids

19:45-20:15   *Coffee break*

20:15-20:45   E. E. Gdoutos, A. A. Giannakopoulou and D. A. Zacharopoulos
Stress Analysis and Failure Mechanisms of Compose Materials with Debonded Interfaces

20:45-21:15   F. Grondin and G. Mounajed, A. Ben Hamida and H. Dumontet
Digital Concrete: A Multi-Scale Approach for the Concrete Behavior

Session: "Computational Methods and String Manipulation Techniques for Molecular Biology"

Saturday 13 September

ROOM: 10

Chair: Prof. A. Tsakalidis and Dr. C. Makris

18:15-18:45   K. Perdikuri, C. Makris, A. Tsakalidis
Discovering Regularities in Biosequences: Challenges and Applications

18:45-19:15   R. Clifford and M. Sergot
Distributed Suffix Trees and Their Application to Large-Scale Genomic Analysis

19:15-19:45   M. Christodoulakis, C. S. Iliopoulos, Kunsoo Park, J. S. Sim
Implementing Approximate Regularities Extended Abstract

19:45-20:15   Coffee break

20:15-20:45   Y. Panagis, E. Theodoridis, K. Tsichlas
Data Structuring Application for String Problems in Biological Sequences

Session: "Computational Mathematics III"

Saturday 13 September

ROOM: 2

Chair: Dr. J. Vigo-Aguiar

18:15-18:45   E. Afjei, M. H. Arbab
Magnetostatic Field Analysis by Employing Absorbing Boundary Condition

18:45-19:15   I. Arregui, J. J. Cendan and C. Vazquez
A Duality Method for the Compressible Reynolds Equation. Application to Simulation of Read/Write Process in Magnetic Storage Devices

19:15-19:45   Coffee break

19:45-20:15   F. Balibrea, J. L. G. Guirao and F. L. Pelayo
An Environment for Computing Topological Entropy for Skew-Product Transformations

20:15-20:45   M. K. Banda
Variants of Relaxed Schemes and two-Dimensional Gas Dynamics

Sunday 14 September

Session: "Computational Chemistry I"

Sunday 14 September

ROOM: 10

Chair: Prof. S.C. Farantos

9:00-9:30   **K. Daoulas and V. G. Mavrantzas**
Atomistic Monte Carlo Simulation Studies of Polymer Melts Grafted on Solid Substrates

9:30-10:00   **G. Cerruela Garcia, I. Luque Ruiz, M. A. Gomez-Nieto**
A New Algorithm to Obtain All Maximum Common Subgraphs in Molecular Graphs Using Binary Arithmetic and Constraints Satisfaction Model

10:00-10:30 ***Coffee break***

10:30-11:00   **S. Itoh, M. Igami**
A Hybrid Molecular Dynamics Simulation Method for Solids

11:00-11:30   **H. Kaya, M. Kaplan, H. Saygin**
A Recursive Algorithm for Finding HDMR Terms for Sensitivity Analysis

11:30-12:00   **P. Becker**
Charge, momentum, and spin density: Towards a unique modelisation and a joint refinement of experimental data

12:00-13:00   **LUNCH**

Session: "Computational Physics III"

Sunday 14 September

ROOM: 8

Chair: Prof. H. Katsuragi

9:00-9:30　　T. E. Karakasidis
Vibrational Properties of $NiO(110)$ Surface by Molecular Dynamics Simulation

9:30-10:00　　Y. Li
An Iterative Method for Single and Vertically Stacked Semiconductor Quantum Dots Simulation

10:00-10:30 Coffee break

10:30-11:00　　H. Katsuragi and H. Honjo
Monotonic Scaling of the KPZ Growth with Quenched Disorder

11:00-11:30　　M. Darbandi, S. O. Torabi
The Study of Seepage Through Embankments Using a Moving Finite Volume Method

12:00-13:00　　LUNCH

Session: "Computational Engineering III"

Sunday 14 September

ROOM: 9

Chair: Prof. D. Hristopoulos

9:00-9:30   **D. T. Hristopoulos**
Simulation of Spart an Random Fields

9:30-10:00   **K. Konstantinidis and I. Andreadis**
On the Use of Color Histograms for content Based Image Retrieval in Various Color Spaces

10:00-10:30 **P. V. Kyratsis, D. A. Panagiotopoulos, D. V. Kakogiannis**
Computer Aided Engineering for Theoretical Studies of Vehicle

10:30-11:00 Coffee break

11:00-11:30 **M. Liapi, K. Alketas Ougrinis**
The Transmutation of the Architectural Synthesis. Morphing Procedures Through the Adaptation of Informational Technology

11:30-12:00 **D. G. Pavlou, N. V. Vlachakis, M. G. Pavlou, V. N. Vlachakis, M. Kouskouti, I. Statharas**
*Foundamental Solution of the Cracked Dissimilar Elastic Space*

12:00-13:00 **LUNCH**

Session: "Computational Mathematics IV"

Sunday 14 September

ROOM: 2

Chair: Prof. G. M. Amiraliyev

9:00-9:30   T. M. Alkhamis
Computational Method for Unconstrained Optimization Functions with Noise

9:30-10:00   M. Al-Refai
Convergence Analysis for an Iterative Method for Solving Nonlinear Parabolic Systems

10:00-10:30   G. M. Amiraliyev
Uniform Numerical Method for a Quasilinear System with Boundary Layer

10:30-11:00   *Coffee break*

11:00-11:30   R. Anguelov, P. Kama and JM-S Lubuma
Nonstandard Theta-Method and Related Discrete Schemes for the Reaction-Diffusion Equation

11:30-12:00   N. Moir
A New Class of Methods for Solving Ordinary Differential Equations

12:00-13:00   LUNCH
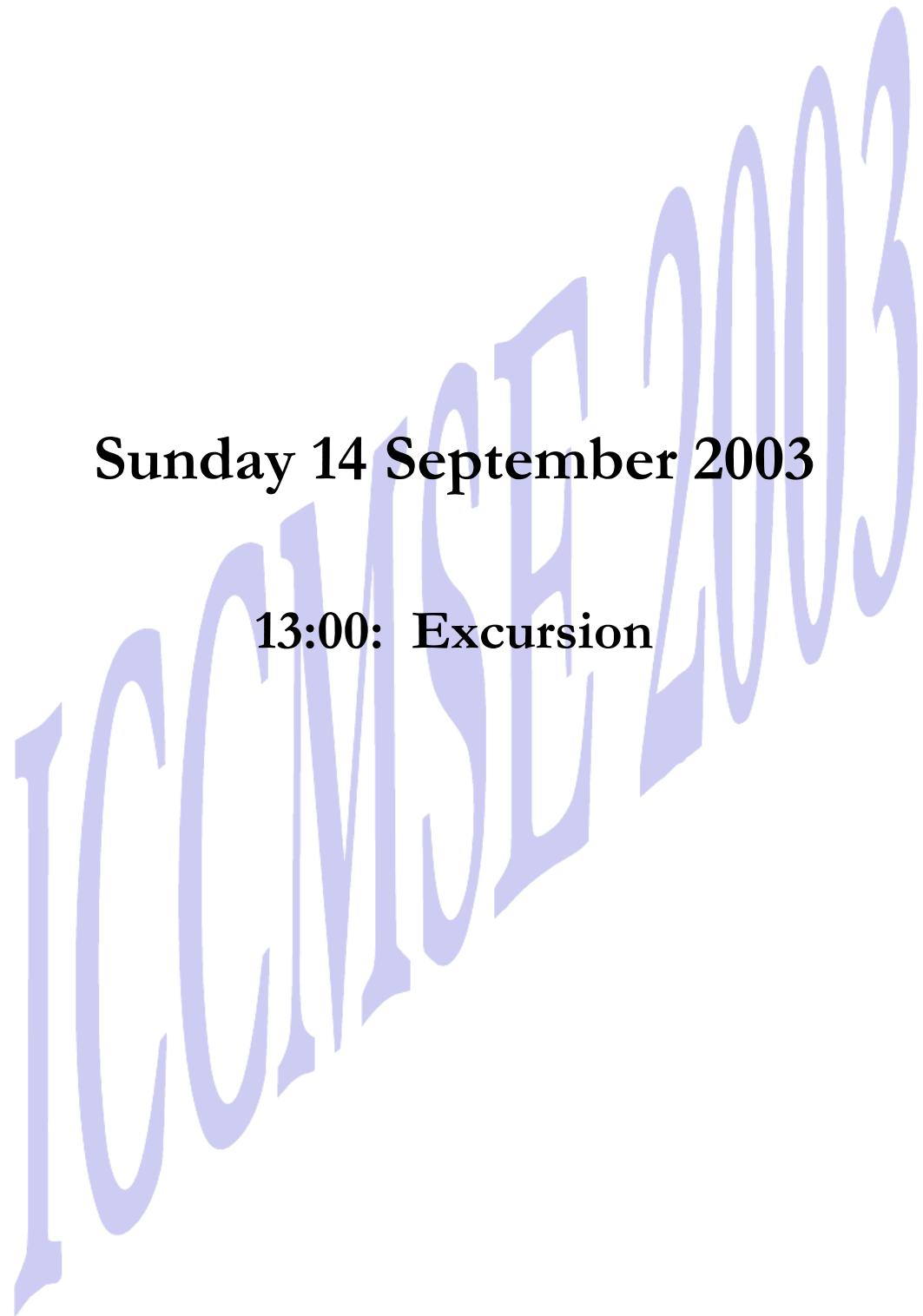
Sunday 14 September 2003

13:00: Excursion

Sunday 14 September 2003

13:00: Central Dinner

Monday 15 September

Session: "Computational Biology and Medicine"

Monday 15 September

## ROOM: 2

Chair: Prof. Dž. Belkić and Prof. K. Belkić

9:30-10:00   V. N. Christofilakis, Ch. Alexopoulos
Modeling the State and Behavior of an Enzyme Using UML – an Object Oriented Approach

10:00-10:30   G. Lappas and V. Ambrosiadou
Binary and Multicategory Classification Accuracy of the LSA Machine

10:30-11:00   *Coffee break*

11:00-11:30   J. Roca J. R., J. Roca, J. Martinez and F. J. Martinez, F. J. Gil and J. A. Alvarez-Comez
Feasibility of Closed-Loop Target Controlled Infusion of Intravenous Anaesthesia

Session: "Computational Finance"

Monday 15 September

ROOM: 1

Chair: Prof. L. J. Streckert
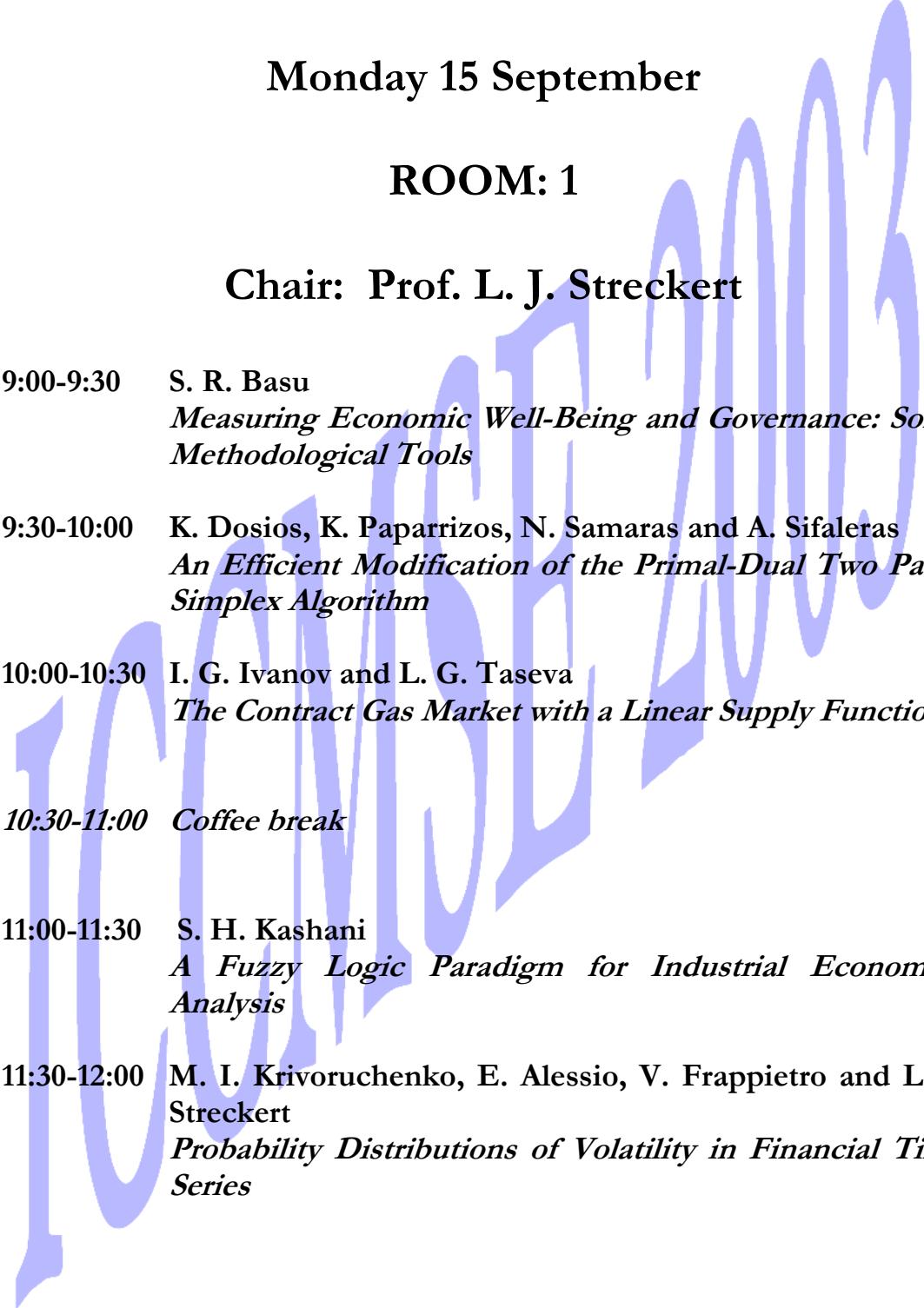
9:00-9:30   S. R. Basu
Measuring Economic Well-Being and Governance: Some Methodological Tools

9:30-10:00   K. Dosios, K. Paparrizos, N. Samaras and A. Sifaleras
An Efficient Modification of the Primal-Dual Two Paths Simplex Algorithm

10:00-10:30 I. G. Ivanov and L. G. Taseva
The Contract Gas Market with a Linear Supply Function

10:30-11:00 *Coffee break*

11:00-11:30   S. H. Kashani
A Fuzzy Logic Paradigm for Industrial Economics Analysis

11:30-12:00 M. I. Krivoruchenko, E. Alessio, V. Frappietro and L. J. Streckert
Probability Distributions of Volatility in Financial Time Series

Session: "Soft Computing and Emerging Systems"

Monday 15 September

ROOM: 3

Chair: Dr. V. Kodogiannis

9:00-9:30   I. Petrounias, A. Tseng, P. Chountas
Constraint Based Web Mining

9:30-10:00   E. Wadge, V. Kodogiannis, D. Tomtsis
Neuro-Fuzzy Ellipsoid Basis Function Multiple Classifier for Diagnostic of Urinary Tract Infections

10:00-10:30   I. Petrounias and A. Assaid
Temporal Web Log Mining Using Olap Techniques

10:30-11:00   *Coffee break*

11:00-11:30   D. Tomtsis, V. Kodogiannis, E. Wadge
Optical PH Measurement using Chromatic Modulation

11:30-12:00   K. Sivagurunathan, P. Chountas, E. El-Darzi
Representation & Modelling of Electronic Patient Records

Session: "Computational Mathematics V"

Monday 15 September

ROOM: 9

Chair: Dr. G. Papageorgiou

9:00-9:30   **P. J. Garcia-Nieto**
Numerical Simulation of Scavenging of an Urban Aerosol by Filtration Taking Into Account the Presence of Coagulation, Condensation, and Gravitational Settling

9:30-10:00   **G. Papageorgiou and Ch. Tsitouras**
Runge-Kutta Research at NTUA

10:00-10:30 Coffee break

10:30-11:00 **E. Francomano, A. Tortorici, E. Toscano, G. Ala and F. Viola**
Wavelet-Like Bases for Electromagnetic Transients in Electric Power Substations Grounding Systems

11:00-11:30 **Ming-Gong Lee**
Application of Automatic Differentiation in Numerical Solution of a Flexible Mechanism

SYMPOSIUM

<u>Title:</u> "Computational Methods for the Molecular Sciences"

PART I

Monday 15 September

ROOM: 10

Chair: Prof. G. Maroulis

9:00-9:40   **A. Rizzo**
Birefringences: A Challenge for Both Theory and Experiment

9:40-10:00   **A. Haskopoulos and G. Maroulis**
Intermolecular Interactions of $\left(H_2O\right)_2$

10:00-10:40   **U. Hohm, L. Zarkova**
Accurate Thermophysical Properties of Neat Globular Gases and their Binary Mixtures Determined by Means of an Isotropic Temperature-Dependent Potential

10:40-11:00   *Coffee break*

11:00-11:40   **G. Maroulis**
Electric Hyperpolarizability Calculations

11:40-12:00   **N. Karatsis and G. Maroulis**
Molecular Structure and Electric Polarizability in Sodium Chloride Clusters

12:00-12:30   **Z. Xiong and N. C. Bacalis**
Generalization of Laguerre Orbitals Toward an Accurate, Consise and Practical Analytic Atomic Wave Function

Keynote Lecture

Monday 15 September

ROOM: 9 AND 10

Chair: Prof. Dž. Belkić

12:30-13:30 Prof. Karen Belkić

The Need for a Paradigm Shift in Data Analysis for Biomedical Spectroscopic Imaging through Magnetic Resonance in Oncology

13:30   LUNCH

Keynote Lecture

Monday 15 September

ROOM: 9 AND 10

Chair: Prof. Karen Belkić

17:00-18:00 Prof. Dž. Belkić

Unique Virtues of the Padé Approximant for High-Resolution Signal Processing

18:00-18:15   COFFEE BREAK

Session: "Electron Densities and Density Functionals"

Monday 15 September

## ROOM: 10

Chair: Ajit J. Thakkar

18:15-18:45 N. Russo, T. Marino, E. Sicilia and M. Toscano
Past, Present and Future Challenge of Density Functional Theory Based in Molecular Sciences

18:45-19:15 J. M. Ugalde
The Electron-Pair Density and the Modeling of the Spherically Averaged Exchange-Correlation Hole

19:15-19:45 Coffee break

19:45-20:15 Ajit J. Thakkar
Density Functionals for Moments of the Electron Momentum Distribution

20:15-20:45 H. Nakatsuji
Structure of the Exact Wave Function: Progress Report

Session: "Computational Mathematics VI"

Monday 15 September

ROOM: 2

Chair: Prof. J. C. Bucher
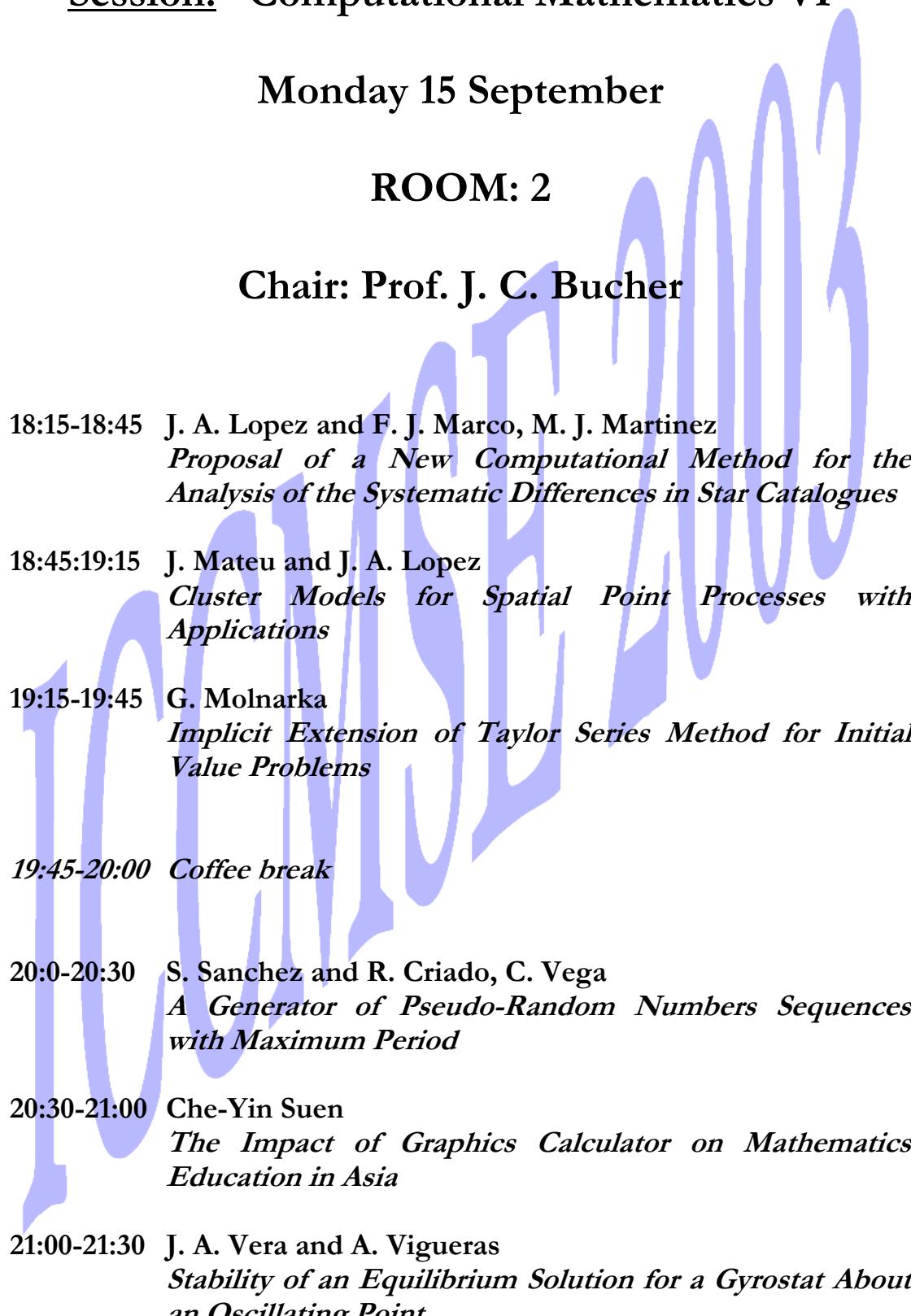
18:15-18:45   J. A. Lopez and F. J. Marco, M. J. Martinez
Proposal of a New Computational Method for the Analysis of the Systematic Differences in Star Catalogues

18:45:19:15   J. Mateu and J. A. Lopez
Cluster Models for Spatial Point Processes with Applications

19:15-19:45   G. Molnarka
Implicit Extension of Taylor Series Method for Initial Value Problems

19:45-20:00   Coffee break

20:0-20:30   S. Sanchez and R. Criado, C. Vega
A Generator of Pseudo-Random Numbers Sequences with Maximum Period

20:30-21:00   Che-Yin Suen
The Impact of Graphics Calculator on Mathematics Education in Asia

21:00-21:30   J. A. Vera and A. Vigueras
Stability of an Equilibrium Solution for a Gyrostat About an Oscillating Point

Session: "Computational Physics IV"

Monday 15 September

ROOM: 3

Chair: Dr. L.A.A. Nikolopoulos

18:15-18:45   L. A. A. Nikolopoulos
A Finite Element Approach for the Dirac Radial Equation

18:45-19:15   Y. V. Skorov, B. J. R. Davidsson, G. N. Markeleov
Consistent Kinetic Model of Innermost Cometary Atmosphere and Boundary Layers of Cometary Nucleus

19:15-19:45   Coffee break

19:45-20:15   L. A. A. Nikolopoulos
B-Splines: A Powerful and Flexible Numerical Basis for the Continuum Spectrum of the Schrodinger Equation. An Application to Hydrogenic Atomic Systems

20:15-20:45   E. Vamvakopoulos, G. A. Evangelakis, D. G. Papageorgiou
Solidification of Pb PRE-Covered Cu(111) Surface

Session: "Computational Engineering IV"

## Monday 15 September

ROOM: 9

Chair: Prof. D. Karalekas
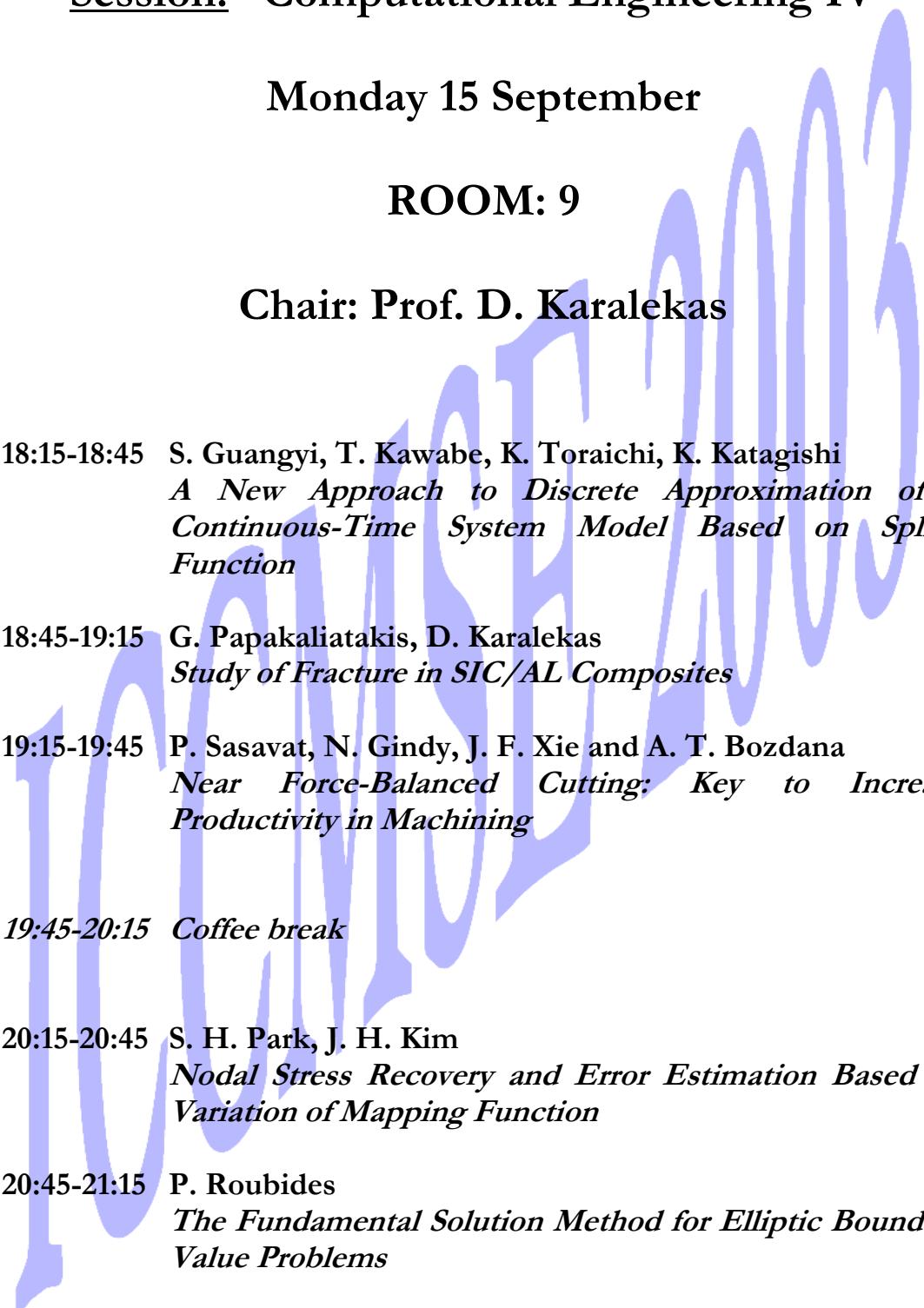
18:15-18:45   S. Guangyi, T. Kawabe, K. Toraichi, K. Katagishi
A New Approach to Discrete Approximation of a Continuous-Time System Model Based on Spline Function

18:45-19:15   G. Papakaliatakis, D. Karalekas
Study of Fracture in SIC/AL Composites

19:15-19:45   P. Sasavat, N. Gindy, J. F. Xie and A. T. Bozdana
Near Force-Balanced Cutting: Key to Increase Productivity in Machining

19:45-20:15   Coffee break

20:15-20:45   S. H. Park, J. H. Kim
Nodal Stress Recovery and Error Estimation Based on Variation of Mapping Function

20:45-21:15   P. Roubides
The Fundamental Solution Method for Elliptic Boundary Value Problems

Session: "Mathematical Chemistry"

Monday 15 September

ROOM: 8

Chair: Dr. Sonia Nikolic
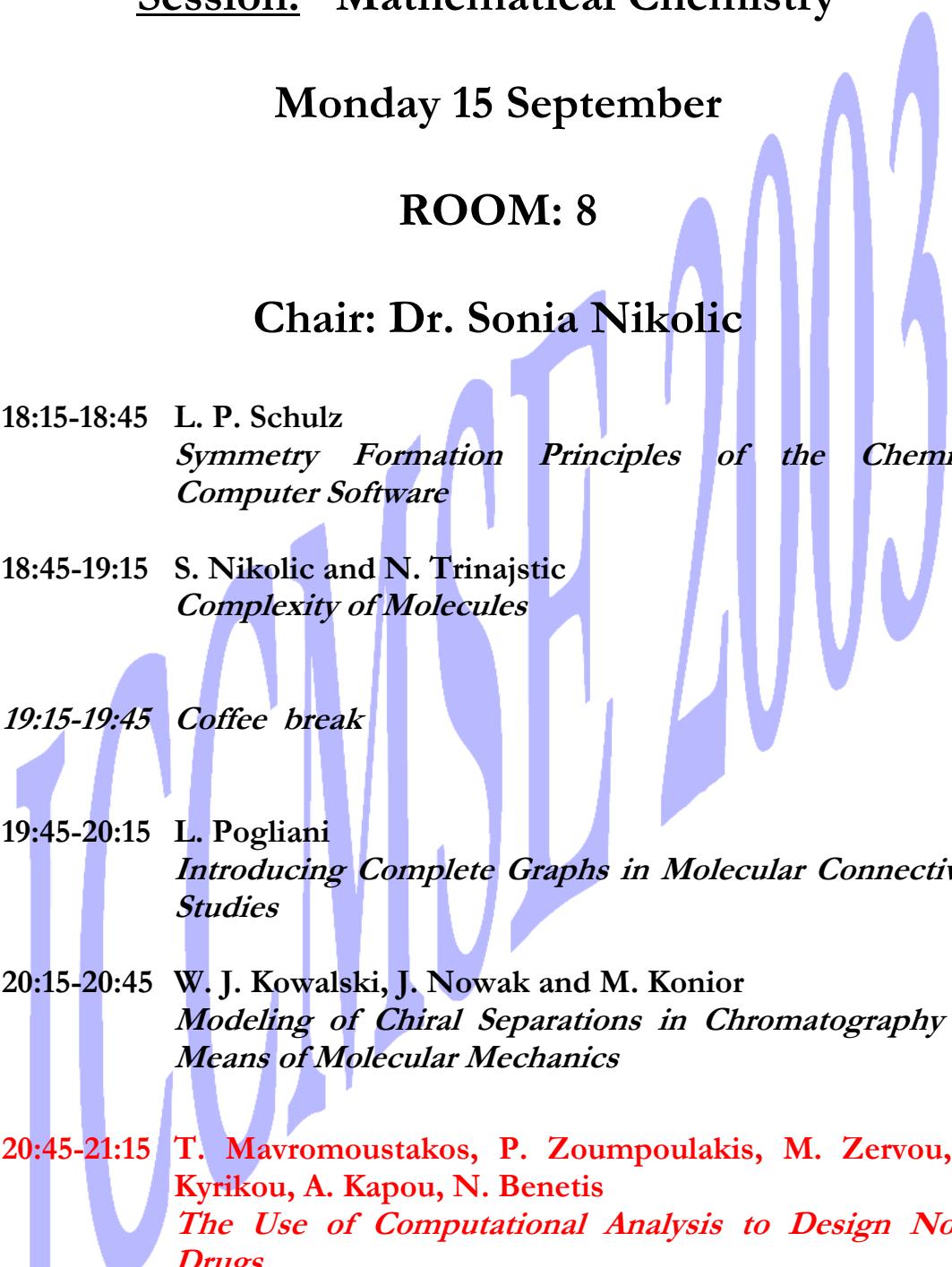
18:15-18:45   L. P. Schulz
Symmetry Formation Principles of the Chemical Computer Software

18:45-19:15   S. Nikolic and N. Trinajstic
Complexity of Molecules

19:15-19:45   Coffee break

19:45-20:15   L. Pogliani
Introducing Complete Graphs in Molecular Connectivity Studies

20:15-20:45   W. J. Kowalski, J. Nowak and M. Konior
Modeling of Chiral Separations in Chromatography by Means of Molecular Mechanics

20:45-21:15   T. Mavromoustakos, P. Zoumpoulakis, M. Zervou, I. Kyrikou, A. Kapou, N. Benetis
The Use of Computational Analysis to Design Novel Drugs

Tuesday 16 September

SYMPOSIUM

Title: "Computational Methods for the Molecular Sciences"

PART II

Tuesday 16 September

ROOM: 10

Chair: Prof. G. Maroulis

9:00-9:40   **S. C. Farantos**
Bifurcation Phenomena in Molecular Vibrational Spectroscopy

9:40-10:00   **P. Karamanis and G. Maroulis**
Electric Properties of Substituted Diacetylenes

10:00-10:40   **A. M. Kosmas**
Theoretical Structural and Relative Stability Studies of Isomeric and Conformeric Forms of XOOY Peroxides $\left(X = H, CH_3, CI, Br, I, Y = CI, Br \right)$

10:40-11:00   ***Coffee break***

11:00-11:40   **S. Wilson**
On the Systematic Construction of Molecular Basis Sets

11:40-12:20   **C. Pouchan**
Calculations of anharmonic vibrationnal spectra: From triatomics to mediumsize molecular systems

12:20-13:00   **B. F. Minaev and H. Ågren**
Enzymatic Spin Catalysis Involving O_2 (Must be Deleted)

Session: "Computational Mathematics VII"

Tuesday 16 September

ROOM: 2

Chair: Prof. M.N. Vrahatis

9:00-9:30   **L. S. Illiadis, S. H. Spartalis**
Fundamental Fuzzy Relation Concepts of a D.S.S. for the Estimation of Natural Disasters' Risk (The Case of a Trapezoidal Membership Function)

9:30-10:00   **G. Hanna and J. Roumeliotis**
Collocation and Fredholm Equations of the First Kind

10:00-10:30   **E. Camouzis, R. Devault, G. Papaschinopoulos**
Period Two Trichotomy on $X_{N+1} = \dfrac{a + \gamma X_{N-1} + \delta X_{N-2}}{X_N + X_{N-2}}$

10:30-11:00   ***Coffee break***

11:00-11:30   **E. C. Laskari, G. C. Meletiou, D. K. Tasoulis, M. N. Vrahatis**
Data Mining and Cryptology

11:00-12:00   **N. G. Pavlidis, K. E. Parsopoulos and M. N. Vrahatis**
Computing Nash Equilibria Through Particle Swarm Optimization

Session: "Computational Engineering V"

Tuesday 16 September

ROOM: 9

Chair: Prof. J. Roumeliotis

9:00-9:30   J. Roumeliotis
Axisymmetric Rigid Bodies in Creeping Flow

9:30-10:00   J. K. Sakellaris
Finite Element Analysis for Weakly Coupled Magneto –
Thermo-Mechanical Phenomena in Shell Structures

10:00-10:30 G. Papakaliatakis
Computational Study of the Crack Extension Initiation in
a Solid Propellant Plate with a Circular Hole

10:30-11:00 *Coffee break*

11:00-11:30 S. V. Shepel, S. Paolucci
Finite Element Level Set Formulations for Modelling
Multiphase Flows

11:30-12:00 J. P. Suarez and P. Abad, A. Plaza, M. A. Padron
Computational Aspects of the Refinement of 3D Complex
Meshes

12:00-12:30 E.G. Varagouli, T.E. Simos and G.S. Xeidakis
Fitting a Multiple Regression Line to Travel Demand
Forecasting: The Case of the Prefecture of Xanthi,
Northern Greece

Session: "Computational Chemistry II"

Tuesday 16 September

ROOM: 8

Chair: Dr. T.E. Simos

9:00-9:30   T. Rusu and M. Pinteala, V. Bulacovschi
Artificial Intelligence Methods Used in the Investigation of Polymers Properties

9:30-10:00   Shenghua Shi and Atsuo Kuki
A Simple Approach to a Multi-Objective Design with Constraints in Compound Selection for Drug Discovery

10:00-10:30 Coffee break

10:30-11:00   G. D. Verros
Computer Aided Estimation of Molecular Weight and Long Chain Branching Distribution in Free Radical Polymerization

Session: "Computational Methods II"

Tuesday 16 September

ROOM: 3

Chair: Dr. Ch. Tsitouras

9:00-9:30   **A. P. Grinko, M. M. Karpuk**
About One Approach to the Minimization of the Errors of the Tutoring of the Neuron Networks

9:30-10:00   **E. Miletics**
Energy Conservative Algorithm for Numerical Solution of ODES Initial Value Problems

10:00-10:30   **I. Ntzoufras, A. Katsis, D. Karlis**
A Bayesian Statistical Modeling for the Distribution of Insurance Counts

10:30-11:00   Coffee break

11:00-11:30   **E. S. Tentis, D. P. Margaris, D. G. Papanikas**
Transient Simulation of Large Scale Gas Transmission Networks Using an Adaptive Method of Lines

11:30-12:00   **M. M. Karpuk**
About the Possibility of Applying the Neuron Networks for Determining the Parameters of Uniaxial Films on the Basis of the Ellipsomentric measurements

12:00-12:30   **S. Zimeras, F. Georgiakodis**
Bayesian Models for Medical Image Biology Using Monte Carlo Markov Chains Techniques

END OF CONFERENCE

Poster Session I

Saturday 13 September

16:00 – 17:00

E. Kefalidis and T.E. Simos
P-stable Multiderivative Methods with Minimal Phase-Lag for the Numerical Solution of the Schrödinger Equation

A. Episkopakis, D. Nikolopoulos, K. Arvanitis, N. Dimitropoulos, G. Panayiotakis, D. Cavouras and I. Kandarakis
Modeling the Detective Quantum Efficiency of Scintillators Used in Medical Imagins Radiation Detectors

D. Glotsos, P. Spyridonos, P. Petalas and G. Nikiforidis, D. Cavouras, P. Ravazoula, P. Dadioti and I. Lekka
Support Vector Machines for Classification of Histopathological Images of Brain Tumour Astrocytomas

I. Kalatzis, N. Pikiouras, E. Ventouras and I. Kandarakis, C. C. Papageorgiou and A. D. Rabavilas, D. Cavouras
Probabilistic Neural Network Versus Cubic Least-Squares Minimum-Distance in Classifying EEG Signals

Kalatzis and N. Piliouras, D. Pappas, E. Ventouras and D. Cavouras
Probabilistic Neural Network Classifier Versus Multilayer Perceptron Classifier in Discriminating Brain Spect Images of Patients with Diabetes from Normal Controls

L. Bayon, J. M. Grau, M. M. Ruiz and P. Suarez
New Developments on Equivalent Thermal in Hydrothermal Optimization. An Algorithm of Approximation

Poster Session II

Monday 15 September

16:00-17:00

Z. A. Anastassi and T. E. Simos
A Family of Optimized Runge-Kutta Methods with Five Stages and Fourth Order for IVPS with Oscillating Solutions

Th. Monovasilis, Z. Kalogiratou, T. E. Simos
Exponential-Fitting Symplectic Methods for the Numerical Integration of the Schrodinger Equation

D. Nikolopoulos, P. Liaparinos, S. Tsantis, D. Cavouras and I. Kandarakis, G. Panayiotakis
Radiation Detection Efficiency Evaluation of YAP;CE Scintillator by Monte-Carlo Methods

P. Spyridonos, P. Petalas, D. Glotsos, G. Nikiforidis, D. Cavouras, P. Ravazoula
Comparative Evaluation of Support Vector Machines and Probabilistic Neural Networks in Superficial Bladder Cancer Classification

P. Theocharakis, I. Kalatzis and N. Piliouras, N. Dimitropoulos, E. Ventouras and D. Cavouras
Relationship Between Carotid Plaque Composition and Embolization Risk Assessed by Computer Processing of Ultrasound Images

P. G. Bagos, Th. D. Liakopoulos and S. J. Hamodrakas
Maximum Likelihood and Conditional Maximum Likelihood Learning Algorithms for Hidden Markov Models with Labeled Data-Application to Transmembrane Protein Topology Prediction

Poster Session III

Tuesday 16 September

12:30-13:30

A. Sharma
The Generalised Mass-Energy Equation $\Delta E = AC^2 \Delta M$; *Its Mathematical Justification and Application in General Physics and Cosmology*

S. Tsantis, I. Kalatzis, N. Piliouras, D. Cavouras, N. Dimitropoulos, G. Nikiforidis
Computer-Aided Characterization of Thyroid Nodules by Image Analysis Methods

S. Tsantis, D. Cavouras, N. Dimitropoulos, G. Nikiforidis
Denoising Sonographic Images of Thyroid Nodules Via Singularity Detection Employing the Wavelet Transform Modulus Maxima

D. Sakas and T. E. Simos
Symmetric Multistep Methods with Minimal Phase-Lag for the Approximate Solution of Orbital Problems

I. Z. Emiris and Th. Nikitopoulos
Structured Matrix Perturbations for Molecular Conformations