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 Series 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**

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<td>9:00-9:30</td>
<td>H. Ramos, J. Vigo-Aguiar</td>
<td><em>Variable Step-Size Störmer Methods</em></td>
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<td>9:30-10:00</td>
<td>H. Ramos, J. Vigo-Aguiar</td>
<td><em>A Note on the Selection of the Step-Size in the Variable Step-Size Störmer Method</em></td>
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<td>10:30-11:00</td>
<td><strong>Coffee break</strong></td>
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<td>11:00-11:30</td>
<td>J. Vigo-Aguiar, H. Ramos</td>
<td><em>VS-VO Numerov Method for the Numerical Solution of the Schrödinger Equation</em></td>
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<td>11:30-12:00</td>
<td>Dr. J. Vigo-Aguiar</td>
<td><em>Exponential Fitting BDF formulas</em></td>
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<td>12:00-12:30</td>
<td>M. De’Michieli Vitturi, F. Beux</td>
<td><em>Nonlinear Pressure and Temperature Waves Propagation in Fluid Saturated Rock</em></td>
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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  
**Numerical 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. Liakopoulous, 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

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 Differencing

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 Composites 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*

*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 Spartan 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
Fundamental 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

Title: “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 (H₂O)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, Concise 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

   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*

*The Use of Computational Analysis to Design Novel Drugs*
Tuesday 16 September
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  
\( X = H, CH_3, Cl, Br, I, Y = Cl, Br \)

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
   \[ X_{n+1} = \frac{a + \gamma X_{n-1} + \delta X_{n-2}}{X_n + X_{n-2}} \]

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 Ellipsomeric 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

Modeling the Detective Quantum Efficiency of Scintillators Used in Medical Imagins Radiation Detectors

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