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To our beloved ones

Preface

Increasing computing power in the last decades has given mathematical modeling an ever greater impulse and made it a very important tool to solve problems coming from industry. The European Consortium for Mathematics in Industry (ECMI) was founded 20 years ago by mathematicians from ten European universities to foster the use of mathematics to help European industry and commerce to pose and solve their problems. The aims of ECMI are to (a) promote the use of mathematical models and mathematics in industry, (b) form applied mathematicians capable of working effectively in industry and (c) work for these goals at the European scale. Efficient problem solving often requires the use of results in different mathematical fields, yet no single applied mathematician may be able to cover the whole subject. By providing a European research network, ECMI can bring together experts from a wide geographical range.

Since 1986, ECMI has incorporated many more institutions and industries throughout Europe and it has been consolidated as a brand name for Industrial Mathematics. Twenty years later, the biannual ECMI conference was celebrated for the first time in Spain, at the Universidad Carlos III de Madrid. This is a young university created in 1989. Technological studies and departments are located at the Leganés campus where the conference was held. Moreover, University Carlos III participates in the Leganés Scientific and Technological Park, together with the Autonomous Region of Madrid and the city of Leganés. They contribute to place Madrid at the forefront of research and development in Spain.

The scientific program covered a wide variety of topics related to technological sectors (aerospace and automotive industry, materials and electronics, information and telecommunication technologies, energy and environment, biology, biotechnology, life sciences, imaging) and to finances and economics. The different origin of participants helped making the conference multidisciplinary. Active participation of industry was intended, with reasonable success. The present volume includes a part of the contributions to the conference, selected after a refereeing process. It is a pleasure to see that six plenary speakers have submitted papers for this volume. Vincenzo Capasso in his "Alan Tayler" lecture, besides presenting his scientific work on statistical geometric measure applied to medicine and materials science, recalls some of the challenges for Mathematics in Industry listed in the first ECMI brochure produced by Alan Tayler and himself in 1994, relates them to the present situation of an enlarged Europe, and tells us how these challenges remain important and pressing for us today. Antonio Barrero (Seville), Alfredo Bermúdez (Santiago), Russel Caflisch (UCLA), Luis Campos (Lisbon) and Pierre Degond (Tolouse) illustrate with their contributions the breadth of applications and variety of techniques that are embraced by ECMI. ECMI's commitment to educating students in Industrial Mathematics is reflected in the fact that many papers were given by students. The Wacker Prize, offered for a Master's Level thesis on an industrial problem was awarded to Filippo Terragni, in line with the tradition of excellent work by previous winners. Many of the minisymposia and special sessions included the activities of ECMI Special Interest Groups. Of the 35 minisymposia organized for the conference, many are gathered in this book, usually preceded by a short explanation about their contents. A number of contributed papers complete the volume. I hope that these proceedings will contribute both to show interesting and relevant mathematical problems and methods, and to strengthen cooperation between academia and industry, the absence of which is a major weakness of the European Science-Technology system.

As President of ECMI and on behalf of the ECMI Council, I wish to thank all those who have contributed to the success of the Conference. Among them the participants, the speakers, the International Scientific Committee and the National and Local Organizing Committees. Organizing this meeting has been possible thanks to the efforts of many people both at the Spanish national and local level to whom we are very grateful. In particular all the members of the Modeling, Simulation and Industrial Mathematics Group at Universidad Carlos III worked hard to run a smooth and successful conference which would not have been possible without their help. The dedication of our university congress bureau, Congrega, was also essential for the conference success. Ms. Bárbara Tapiador's help was very important to process the manuscripts that are gathered in the present book. I am grateful to my co-editors, Gloria Platero, Miguel Moscoso and José Manuel Vega for their invaluable help.

Lastly, the support of our sponsors is gratefully acknowledged: Ministerio de Educación y Ciencia (grant MTM-2005-24569-E), Comunidad de Madrid (grant S-0505/ENE/0229), Universidad Carlos III de Madrid, Universidad Politécnica de Madrid, Consejo Superior de Investigaciones Científicas (CSIC), Instituto de Tecnológico de Química y Materiales "Álvaro Alonso Barba", Ayuntamiento de Leganés and Springer.

Madrid, May 2007 *Luis L. Bonilla, President of ECMI*

Contents

Part I Plenary Lectures

On the Mean Geometric Densities of Random Closed Sets, and Their Estimation: Application to the Estimation of the Mean Density of Inhomogeneous Fibre Processes
V. Capasso and A. Micheletti 3

Synthesis of Micro and Nanoparticles from Coaxial Electrified Jets
A. Barrero and I.G. Loscertales 35

Numerical Simulation of Induction Furnaces for Silicon Purification
A. Bermúdez, D. Gómez, M.C. Muñiz, P. Salgado, and R. Vázquez 48

Growth and Pattern Formation for Thin Films
R.E. Caflisch 66

On Waves in Fluids: Some Mathematical, Physical and Engineering Aspects
L.M.B.C. Campos 73

Quantum Diffusion Models Derived from the Entropy Principle
P. Degond, S. Gallego, F. Méhats, and C. Ringhofer 106

Statistical Aspects of Size Functions for the Description of Random Shapes: Applications to Problems of Lithography in Microelectronics
A. Micheletti, F. Terragni, and M. Vasconi 123

Part II Minisymposia

Minisymposium "Flow Control in Aircrafts"
A. Abbas and J.M. Vega 137

Using Non-Normality for Passive Laminar Flow Control
C. Cossu, L. Brandt, J.H.M. Fransson, and A. Talamelli 139

On the Catalytic Effect of Resonant Interactions in Boundary Layer Transition
X. Wu, P.A. Stewart, and S.J. Cowley 146

Stabilization of Tollmien–Schlichting Waves by Mode Interaction
C. Martel, E. Valero, and J.M. Vega 157

Acoustic Streaming and Lower-than-Laminar Drag in Controlled Channel Flow
P. Luchini 169

Recent Progress in the Use of Compliant Walls for Laminar Flow Control
P.W. Carpenter 178

Minisymposium "Global Flow Instability"
V. Theofilis 188

Helical Instability and Breakdown of a Batchelor Trailing Vortex
M.S. Broadhurst and S.J. Sherwin 191

A Finite-Element Alternative for BiGlobal Linear Instability Analysis
L.M. González 196

Numerical Considerations in Spectral Multidomain Methods for BiGlobal Instability Analysis of Open Cavity Configurations
J. de Vicente, E. Valero, and V. Theofilis 201

Minisymposium "Analysis of Dynamical Problems in Turbomachinery"
C. Martel and R. Corral 207

Modal Identification of Mistuned Bladed Discs
M. Berthillier, B. Salhi, and J. Lardiès 208

Aeroelastic Instability of Low-Pressure Rotor Blades
R. Corral and J.M. Gallardo 214

Recent Advances in Numerical Analysis of Nonlinear Vibrations of Complex Structures with Friction Contact Interfaces
E.P. Petrov 220

Minisymposium "Numerical Methods for Conservation Laws"
G. Russo 225

Central Runge–Kutta Schemes for Stiff Balance Laws
G. Puppo and G. Russo 226

Flow Calculations using Shock Capturing Schemes Based on Power Limiters
S. Serna 231

A Comparison Between Relaxation and Kurganov–Tadmor Schemes
F. Cavalli, G. Naldi, G. Puppo, and M. Semplice 236

Minisymposium "Multibody Dynamics"
B. Simeon 241

The Reverse Method of Lines in Flexible Multibody Dynamics
C. Lunk and B. Simeon 242

Fast Simulation of Quasistatic Rod Deformations for VR Applications
J. Linn, T. Stephan, J. Carlsson, and R. Bohlin 247

Simulation and Optimization of Suspension Testing Systems
M. Speckert and K. Dreßler 254

Minisymposium "Some Topics in Astrodynamics and Space Geodesy"
J.M. Gambi and P. Romero 259

Optimal Station Keeping for Geostationary Satellites with Electric Propulsion Systems Under Eclipse Constraints
P. Romero, J.M. Gambi, E. Patiño, and R. Antolin 260

International Reference Systems for Astrodynamics and Space Geodesy
M. Folgueira, N. Capitaine, and J. Souchay 265

Post-Newtonian Covariant Measurement Formulations in Space Geodesy
J.M. Gambi, M.L. García del Pino, M.C. Rodriguez, M. Salas, and P. Romero 270

Minisymposium "Clean Coal Conversion Technologies"
C. Dopazo and P.L. Garcia-Ybarra 276

Mathematical Modelling of Coal Particles Combustion in Pulverised Coal Furnaces
A. Bermúdez, J.L. Ferrín, A. Liñán, and L. Saavedra 277

Transport of Particles and Vapors in Flue Gases and Deposition on Cold Surfaces
J.L. Castillo and P.L. Garcia-Ybarra 284

A Comprehensive Mathematical Model of Flue-gas Desulfurization
N. Fueyo, A. Gomez, and J.F. Gonzalez 290

Determination of the Kinetic Parameters of a Pulverized Fuel from Drop Tube Experiments
S. Jiménez and J. Ballester 296

Minisymposium "Mathematical Problems in Oil Industry"
A. Fasano 301

An Asphaltene Precipitation Model Using a Lattice Approach
S. Correra 302

Formation and Growth of Wax Deposit in the Pipelining of Crude Oils
S. Correra, D. Merino-Garcia, A. Fasano, and L. Fusi 307

Simulations of the Spurt Phenomenon for Suspensions of Rod-Like Molecules
C. Helzel 312

Minisymposium "Flow in Porous Media"
N. Svanstedt 317

Multiscale Stochastic Homogenization of Convection-Diffusion Equations
N. Svanstedt 318

Numerical Approximation of Boundary Layers for Rough Boundaries
N. Neuss 323

Upscaling in Nonlinear Thermal Diffusion Problems in Composite Materials
C. Timofte 328

Effective Two-Phase Flow Models Including Trapping Effects at the Micro Scale
C.J. van Duijn, H. Eichel, R. Helmig, and I.S. Pop 333

Minisymposium "Shallow Water and Simulation of Environmental Flows"
C. Parés 340

ADER DG and FV Schemes for Shallow Water Flows
C.E. Castro and E.F. Toro 341

Numerical Simulation of Bedload Sediment Transport Using Finite Volume Schemes
M. Castro Díaz, E.D. Fernández Nieto, and A. Ferreiro Ferreiro 346

New Trends and Applications in Oceanographic Numerical Modelling
L. Ferrer, Ad. Uriarte, and M. González 351

Study and Development of Numerical Models for the Simulation of Geophysical Flows: The DamFlow Project
M.J. Castro, A.M. Ferreiro, J.A. García, J.M. González, and C. Parés 356

On Variational Data Assimilation for 1D and 2D Fluvial Hydraulics
I. Gejadze, M. Honnorat, F.X. Le Dimet, and J. Monnier 361

Minisymposium "Multiscale Problems in Materials"
A. Carpio 366

An Asymptotic Solution of Aggregation Dynamics
Y. Farjoun and J. Neu 368

Atomistic Simulations of the Incipient Plastic Deformation Mechanisms on Metal Surfaces
O. Rodríguez de la Fuente 376

Critical Thickness for Misfit Dislocation Formation in InAs/GaAs(110) Heteroepitaxy
I. Plans, A. Carpio, L.L. Bonilla, and R.E. Caflisch 381

Discrete Dislocation Dynamics in Crystals
M.P. Ariza, A. Ramasubramaniam, and M. Ortiz 387

Interconnection of Continuum and Discrete Models of Dislocation Pile-ups
R.E. Voskoboinikov, S.J. Chapman, and J.R. Ockendon 392

Simplified P_N Models and Natural Convection–Radiation
R. Pinnau and M. Seaïd 397

Minisymposium "Nonlinear Charge and Spin Transport in Semiconductor Nanostructures"
G. Platero 402

Electronic Transport in Nanowires at Different Length Scales
A.-P. Jauho 404

SU(4) Kondo Effect in a Mesoscopic Interferometer
R. López 421

Josephson Effect and Magnetic Interactions in Double Quantum Dots
F.S. Bergeret, A. Levy Yeyati, and A. Martín-Rodero 426

Quantum Shuttle: Physics of a Numerical Challenge
A. Donarini 431

Microscopical Model for Hyperfine Interaction in Electronic Transport Through Double Quantum Dots: Spin Blockade Lifting
J. Iñarrea, G. Platero, and A.H. MacDonald 440

Rabi Dynamics in Driven Tunneling Devices
R. Sánchez and G. Platero 444

Quantum-Transmitting-Boundary Algorithm with Local Spin–Orbit Coupling
L. Serra and D. Sánchez 449

Spintronic Transport in II–VI Magnetic Semiconductor Resonant Tunneling Devices
D. Sánchez 454

Hysteretic Linear Conductance in Single Electron Transport through a Single Atom Magnet
J. Fernández-Rossier and R. Aguado 460

Minisymposium "Ferromagnetic Carbon Nanostructures"
T. Makarova and M.A.H. Vozmediano 466

Ferromagnetic Carbon Nanostructures
T.L. Makarova 467

Looking for Ferromagnetic Signals in Proton-Irradiated Graphite
M.A. Ramos, A. Asenjo, M. Jaafar, A. Climent-Font, A. Muñoz-Martín, J. Camarero, M. García-Hernandez, and M. Vázquez 477

Ferromagnetism and Disorder in Graphene
M.P. López-Sancho, M.A.H. Vozmediano, T. Stauber, and F. Guinea . . . 483

Topological Defects and Electronic Properties in Graphene
A. Cortijo and M.A.H. Vozmediano 488

Transport Through a Graphene Transistor
F. Guinea, A.H. Castro Neto, and N.M.R. Peres 494

Minisymposium "PDAE Modelling and Multiscale Simulation in Microelectronics and New Technologies"
G. Alì and R. Pulch 499

Domain Decomposition Techniques for Microelectronic Modeling
G. Alì, M. Culpo, and S. Micheletti 500

A Concept for Classification of Partial Differential Algebraic Equations in Nanoelectronics
A. Bartel and R. Pulch 506

Numerical Simulation of a Class of PDAEs with a Separation of Time Scales
B. Chachuat and P.I. Barton 512

Model Order Reduction for Nonlinear Differential Algebraic Equations in Circuit Simulation
T. Voss, A. Verhoeven, T. Bechtold, and J. ter Maten 518

Minisymposium "Numerical Methods for Semiconductor Kinetic Equations (COMSON Minisymposium)"
A. Majorana 524

Comparing Kinetic and MEP Model of Charge Transport in Semiconductors
A. Majorana and V. Romano 525

A Deterministic Solver to the Boltzmann-Poisson System Including Quantization Effects for Silicon-MOSFETs
M. Galler and F. Schürrer 531

Minisymposium of the ECMI SIG "Shape and Size in Medicine, Biotechnology and Material Sciences"
A. Micheletti 537

Size Functions Applied to the Statistical Shape Analysis and Classification of Tumor Cells
A. Micheletti and G. Landini 538

A Mathematical Morphology Approach to Cell Shape Analysis
J. Angulo 543

Reconstruction of Transducer Pressure Fields from Schlieren Data
R. Kowar 548

Plant Growth Modeling
N. Morozova, N. Bessonov, and V. Volpert 553

Minisymposium "New Trends in the Analysis of Functional Genomics Data"
J.M. Carazo and A. Pascual 559

Bayesian Classifiers with Consensus Gene Selection: A Case Study in the Systemic Lupus Erythematosus
R. Armañanzas, B. Calvo, I. Inza, P. Larrañaga, I. Bernales, A. Fullaondo, and A.M. Zubiaga 560

The Quest for Biological Significance
A. Sánchez and J.L. Mosquera 566

Functional Classification of Genes Using Non-Negative Independent Component Analysis
M. Chagoyen, H. Fernandes, J.M. Carazo, and A. Pascual-Montano . . . 571

New Trends in the Analysis of Functional Genomic Data
D. Montaner, F. Al-Shahrour, and J. Dopazo 576

Minisymposium: "Inverse Problems and Applications"
O. Dorn and M. Moscoso 581

A Robustness Analysis of the Iterative Multi-Scaling Approach Integrated with Morphological Operations
D. Franceschini, M. Donelli, R. Azaro, and A. Massa 582

Iterative Microwave Inversion Algorithm Based on the Adjoint-Field Method for Breast Cancer Application
O. Dorn, M. El-Shenawee, and M. Moscoso 587

Iterative Microwave Inversion for Breast Cancer Detection Using Level Sets
N. Irishina, M. Moscoso, and O. Dorn 592

Characterization of Reservoirs by Evolving Level Set Functions Obtained from Geostatistics
R. Villegas, O. Dorn, M. Moscoso, and M. Kindelan 597

Reconstruction of Simple Geometric Objects in 3D Optical Tomography Using an Adjoint Technique and a Boundary Element Method
A. Zacharopoulos, O. Dorn, S.R. Arridge, V. Kolehmainen, and J. Sikora 603

High Contrast Electrical Impedance Imaging
N. Polydorides 608

Minisymposium "Finance" (Oxford)
S. Howison and K. Schmitz 613

Pricing Exotic Options Using Strong Convergence Properties
K. Schmitz Abe and M. Giles 614

Credit Contagion in a Structural Framework
H. Haworth 630

The Valuation of Elementary Exotics with Strike Resets
E.C.K. Yu 637

Minisymposium "On Optimal Strategies of Multivariate Passport Options"
J. Kampen 643

Foresight Bias and Suboptimality Correction in Monte–Carlo Pricing of Options with Early Exercise
C.P. Fries 645

On the American Option Value Near its Exercise Region
E. Chevalier 650

Free Boundary Problems in Mathematical Finance
J. Chadam 655

Optimal Strategies of Passport Options
J. Kampen 666

Minisymposium "Meshfree Methods for the Solution of PDEs"
M. Kindelan 671

Solving One-Dimensional Moving-Boundary Problems with Meshless Method
L. Vrankar, E.J. Kansa, G. Turk, and F. Runovc 672

Meshless Simulation of Hele-Shaw Flow
F. Bernal and M. Kindelan 677

Minisymposium: "Mathematical Models for the Textile Industry"
T. Götz 683

Dynamics of Curved Viscous Fibers
S. Panda, N. Marheineke, and R. Wegener 685

Modeling and Simulation of Non-Woven Processes
M. Günther, R. Wegener, and F. Olawsky 691

Asymptotics of Fiber Spinning Equations
T. Götz, A. Klar, and A. Unterreiter 697

Three-Dimensional Elastica for Modelling Fibre Assemblies
R.B. Ramgulam and P. Potluri 703

Effective Properties of Nonwoven Textiles from Microstructure Simulations
A. Wiegmann 708

Minisymposium "Approximate Algebraic Techniques for Curves and Surfaces"
B. Jüttler 713

Computing the Intersection Curve Between a Plane and the Offset of a Parametric Surface
F. Carreras, L. Gonzalez–Vega, and J. Puig-Pey 714

Approximating Offsets of Surfaces by using the Support Function Representation
J. Gravesen, B. Jüttler, and Z. Šír 719

Semantic Modelling for Styling and Design
C.E. Catalano, V. Cheutet, F. Giannini, B. Falcidieno, and J.C. Leon 724

Minisymposium "Web-based Learning Environments in Applied Mathematics"
M. Heiliö 729

An Industrial Application of an Integrated Framework for Production of Interactive Documents
G.M. Grasso, C.L.R. Milazzo, and S. Runci 731

An e-Learning Platform for Applications of Mathematics to Microelectronic Industry
G. Alì, E. Bilotta, L. Gabriele, P. Pantano, and R. Servidio 736

Web Based System for Graduate Studies: Optimization, Games, and Markets
M. Heiliö and J. Mockus 741

Web-Tool on Differential Equations
P. Miidla 746

Part III Contributed Papers

Model and Method to Increase the Thermal Efficiency of Micro-Heat Exchangers for Aerospace Applications
A. Velazquez, J.R. Arias, and B. Mendez 753

Influence of Trailing Jet Instability on the Dynamics of Starting Jets
C. Marugan-Cruz, M. Vera, C. Martinez-Bazan, and G. Pawlak 758

Modelling and Computational Analysis of the Dynamic Crash Behaviour of Fabric Reinforced Composite Automotive Structures
E.V. Morozov and V.A. Thomson 763

Theoretical Modeling of Flame–Acoustic Interaction
M.L. Bondar, J.H.M. ten Thije Boonkkamp, and R.M.M. Mattheij 768

Air-Blown Rivulet Flow of a Perfectly Wetting Fluid on an Inclined Substrate
J.M. Sullivan, S.K. Wilson, and B.R. Duffy 774

The Effect of the Thermal Conductivity of the Substrate on Droplet Evaporation
G.J. Dunn, S.K. Wilson, B.R. Duffy, S. David, and K. Sefiane 779

The Effect of Particles on Linear and Weakly Nonlinear Instability of a Two-Phase Shallow Flows
A. Kolyshkin and S. Nazarovs 784

Water Quality Simulation of a Future Pit Lake
A. Bermúdez, L.M. García García, P. Quintela, and J.L. Delgado 790

Optimal Management and Design of a Wastewater Purification System
L.J. Alvarez-Vázquez, E. Balsa-Canto, and A. Martínez 795

Estimation of Fuzzy Anomalies in Water Distribution Systems
J. Izquierdo, M.M. Tung, R. Peréz, and F.J. Martínez 801

Investigation of the Evolution and Breakup of Electrically Charged Drops
S.I. Betel, M.A. Fontelos, U. Kindelán, and O. Vantzos 806

Homogeneous Nucleation of Dipole Domains and Current Self-Oscillations in Photoexcited Semiconductor Superlattices
J.I. Arana and L.L. Bonilla 812

Numerical Analysis of a Nickel-Iron Electrodeposition Process
N. Alaa, M. Iguernane, and J.R. Roche 817

A Simplified Finite Element Formulation for Spray Transfer GMA Weld Pools
M. Edstorp 822

Numerical Solution of a Non-Local Elliptic Problem Modeling a Thermistor with a Finite Element and a Finite Volume Method
C.V. Nikolopoulos and G.E. Zouraris 827

Numerical Solution of 3D Magnetostatic Problems in Terms of Scalar Potentials
A. Bermúdez, R. Rodríguez, and P. Salgado 833

Optimization Methods for a Wifi Location System
A. Martínez, L.J. Alvarez-Vázquez, F. Aguado-Agelet, and E. Balsa-Canto 838

Flow in the Canal of Schlemm and its Influence on Primary Open Angle Glaucoma
A.D. Fitt 843

A One-Phase Model for Air-Breathing DMFC Cells with Non-Tafel Kinetics
M. Vera and F.J. Sánchez-Cabo 848

Optimising Design Parameters of Enzyme-Channelling Biosensors
D. Mackey and A.J. Killard 853

Breast Nodule Ultrasound Segmentation Through Texture-Based Active Contours
M. Alemán-Flores, L. Álvarez, and V. Caselles 858

A Contrast Invariant Approach to Motion Estimation: Validation and Application to Motion Estimation Improvement
V. Caselles, L. Garrido, and L. Igual 863

A Mathematical Model for Prediction of Recurrence in Bladder Cancer Patients
C. Santamaría, M.B. García-Mora, G. Rubio, and J.L. Pontones 868

Use of the Fourier Transform in the Distributions Sense for Creation Numerical Algorithms for Cone-Beam Tomography
O.E. Trofimov 873

Shapley Value vs. Proportional Rule in Cooperative Affairs
R. Amer, F. Carreras, and A. Magaña 877

A Wide Family of Solutions Based on Marginal Contributions for Situations of Competence–Cooperation with Structure of a Priori Coalition Blocks
J.M. Giménez 882

Time-Varying Grids for Gas Dynamics
F. Coquel, Q.L. Nguyen, M. Postel, and Q.H. Tran 887

Meshless Poisson Problems in the Finite Pointset Method: Positive Stencils and Multigrid
B. Seibold 892

Basics of a Differential-Geometric Approach to Diffusion: Uniting Lagrangian and Eulerian Models on a Manifold
M.M. Tung 897

Diagnostic Modelling of Digital Systems with Binary and High-Level Decision Diagrams
R. Ubar, J. Raik, H. Kruus, H. Lensen, and T. Evartson 902

Numerical Integration in Bayesian Positioning
H. Pesonen and R. Piché 908

Singular Problems With Quadratic Gradient Term
A. Vitolo 913

Pattern Matching for Control Chart Monitoring
D. Cantone and S. Faro 918

Index Characterization in DAE Circuit Models Without Passivity Assumptions
A.J. Encinas and R. Riaza 923

Fingerprint Classification using Entropy Sensitive Tracing
P. Mihăilescu, K. Mieloch, and A. Munk 928

An Invariant Domain Preserving MUSCL Scheme
C. Berthon 933

A Stable CE–SE Numerical Method for Time-Dependent Advection–Diffusion Equation
R. Company, E. Defez, L. Jódar, and E. Ponsoda 939

A Random Euler Method for Solving Differential Equations with Uncertainties
J.C. Cortés, L. Jódar, and L. Villafuerte 944

Cubic-Matrix Splines and Second-Order Matrix Models
M.M. Tung, L. Soler, E. Defez, and A. Hervás 949

Part IV Color Plates

Color Plates 957

Part V Contributor Index

List of Contributors 985

Part I

Plenary Lectures

On the Mean Geometric Densities of Random Closed Sets, and Their Estimation: Application to the Estimation of the Mean Density of Inhomogeneous Fibre Processes

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Dedicated to Alan Tayler

Preface [VC]

It has been a great honour for me to deliver the "Alan Tayler Lecture" in this ECMI Conference, to honour one of the leading founders and Presidents of ECMI. I have collaborated with Alan for many years, especially during my term as Chairman of the Educational Committee, and later during the first ECMI-HCM Project. While he was already very ill, he found the way to participate (even though only for a couple of days) in a workshop in Milan, opening ECMI to the Italian academic and industrial community, and highly supported the birth of MIRIAM (the Milan Research Centre for Industrial and Applied Mathematics).

I had a rewarding experience around the early 1990s producing, in a strict collaboration with Alan, the first ECMI Brochure [CT94] (see the ECMI web site) in order to advertise the specific role of ECMI within academia and industry in Europe.

It was clear to me that he had a vision of how to establish in Europe a co-operative action by the most active groups in the applications of mathematics to real world problems; I wish to remind the key issues stated in the brochure, since I may claim that these are still update.

"Realising the need of interaction between universities and research groups in industry, the European Consortium for Mathematics in Industry (ECMI) was founded in 1986 by mathematicians from ten European universities.

...

Mathematics, as the language of the sciences, has always played an important role in technology, and now is applied also to a variety of problems in commerce and the environment.

European industry is increasingly becoming dependent on high technology and the need for mathematical expertise in both research and development can only grow.

. . .

These new demands on mathematics have stimulated academic interest in Industrial Mathematics and many mathematical groups world-wide are committed to interaction with industry as part of their research activities.

In 1986 ten of these groups in Europe founded ECMI with the intention of offering their collective knowledge and expertise to European Industry.

The experience of ECMI members is that similar technical problems are encountered by different companies in different countries. It is also true that the same mathematical expertise may often be used in differing industrial applications.

If European industry is to compete in world markets it should take advantage of the competitive edge which may be gained from using European mathematical expertise.

No single European country is likely to have sufficient expertise of mathematical knowledge whereas ECMI can provide a comprehensive coverage of mathematical skills and their diverse applications." [CT94]

We are now facing the challenge of a larger European Union.

Alan had anticipated this by promoting an ECMI "patronage", financially supported by the EU, of those countries usually called "Central Europe", such as Čekia, Hungary, Poland, Romania, Slovakia.

I am sure that he would have liked to participate in the process of complete integration of all the new entries in the ECMI system.

Going back to the ECMI Brochure, a major scope of ECMI was identified as follows.

"C. TO OPERATE ON A EUROPEAN SCALE

Academic resources in Mathematics for Industry are also scarce and distributed across Europe; industrial needs are widely spread. Exchange and interactive programmes are necessary in training, research and industrial collaboration if there is to be an effective transfer of knowledge and skills. The EC is encouraging ECMI to involve relevant groups in Eastern Europe as Associate members."

As part of this encouragement, the EC provided funds to ECMI for organising a series of workshops in those countries, in collaboration with recognised colleagues at the local level. Thus anticipating the enlargement of the political Europe.

In my opinion, having the EC approved a significant enlargement of Europe towards East, listing soon 27 member states, ECMI, as an enlarged Consortium, should find new ways to exploit the best of the scientific resources of the old and the new member states together, to actively participate in the building up of a common competitive Europe. As far as scientific competence is concerned, there are excellencies in all regions of Europe, some of them well identifiable also in the new member states; a genuine will to sustain competence of Europe should go through ways to exploit all of them, with the usual ECMI cooperative attitude.

Another anticipation envisaged by Alan has been the shift of meaning of the key word "Industry" in the ECMI system.

"This collaboration may also be extended to developing mathematical models for the environment, earth sciences, biology and finance." [CT94]

We have already achieved the inclusion of what we call **Economathematics**, and today we are facing a further shift of attention towards **Medicine and Biotechnology**.

All over the world leading experts of **Mathematics for/in Industry**, are participating actively in the development of **Mathematics for/in Medicine**, thus undertaking the further challenge of contributing to the development of innovative methods for diagnosis and treatment of relevant diseases, from cancer to infectious diseases.

My own presentation here is aimed to showing an example of how mathematics, originally developed for mining industry or more in general for material science and chemical industry, is now moving to deal with problems of interest in medicine.

At first this research was motivated by polymer industry in Europe, and constitutes one of the most important success stories of collaborative research within ECMI, that was supported within the first HCM Project coordinated by Alan Tayler. As a documentation of the cooperation between different research teams in Europe within the ECMI Special Interest Group on "Polymers", the volume "Mathematical Modelling for Polymer Processing. Polymerization, Crystallization, Manufacturing", edited by myself, was published as Volume 2 in the **ECMI Series on Mathematics in Industry by Springer-Verlag, Heidelberg 2002**, showing an additional success story of ECMI: the start of the **Springer Series on Mathematics in Industry**.

1 Introduction

Many processes of biomedical or material science interest may be modelled as birth-and-growth processes (germ–grain models), which are composed of two processes, birth (nucleation, branching, etc.) and subsequent growth of spatial structures (cells, vessel networks, etc.), which, in general, are both stochastic in time and space. These structures induce a random division of the relevant spatial region, known as random tessellation (see Fig. 1). A quantitative description of the spatial structure of a tessellation can be given, in terms of the mean densities of interfaces (n-facets).

In applications to material science a main industrial interest is controlling the quality of the relevant final product in terms of its mechanical properties; as shown, e.g. in [FC98], these are strictly related to the final morphology

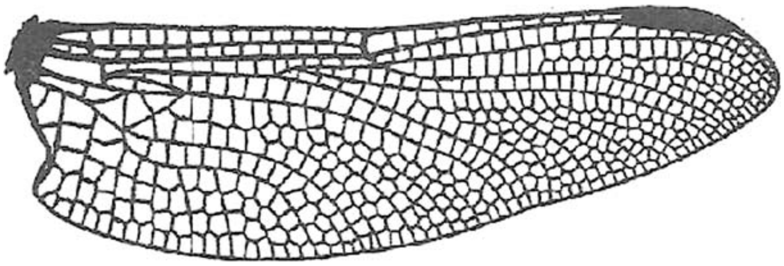

Fig. 1. The spatial tessellation generated by vessels in a dragonfly wing

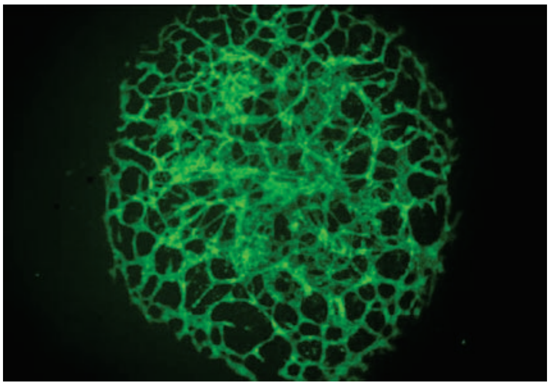

Fig. 2. Vascularization of an allantoid [Credit: Dejana et al. 2005]

of the solidified material, so that quality control in this case means optimal control of the final morphology.

In medicine, an important area of application of birth-and-growth processes and other models of stochastic geometry is tumour-induced angiogenesis. It can be modelled as a fibre process of Hausdorff dimension 1 in the relevant 2D or 3D space.

Tumour-induced angiogenesis is believed to occur when normal tissue vasculature is no longer able to support growth of an avascular tumour. At this stage the tumour cells, lacking nutrients and oxygen, become hypoxic. This is assumed to trigger cellular release of tumour angiogenic factors (TAFs) which start to diffuse into the surrounding tissue and approach endothelial cells (ECs) of nearby blood vessels. ECs subsequently respond to the TAF concentration gradients by forming sprouts, dividing, and migrating towards the tumour. A summary of these mechanisms can be found in the recent paper by Carmeliet [JK01] (see also Figs. 2–4 where examples of real or simulated vascular networks are depicted).

Initially, the sprouts arising from a parent vessel grow essentially parallel to each other. It is observed that once the finger-like capillary sprouts have

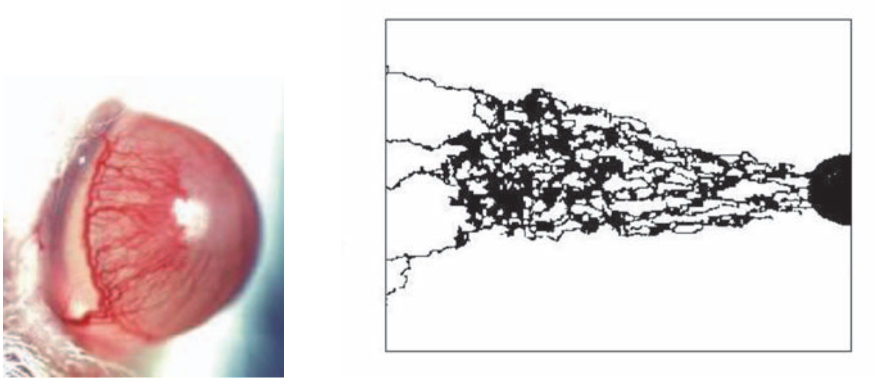

Fig. 3. *Left*: Angiogenesis on a rat cornea [Credit: Dejana et al. 2005]. The white spot is a pellet implanted in the cornea containing an angiogenetic substance, emulating the effect of a tumour. *Right*: A simulation of an angiogenesis due to a localized tumour mass (*black* region on the *right*) (from [CA99])

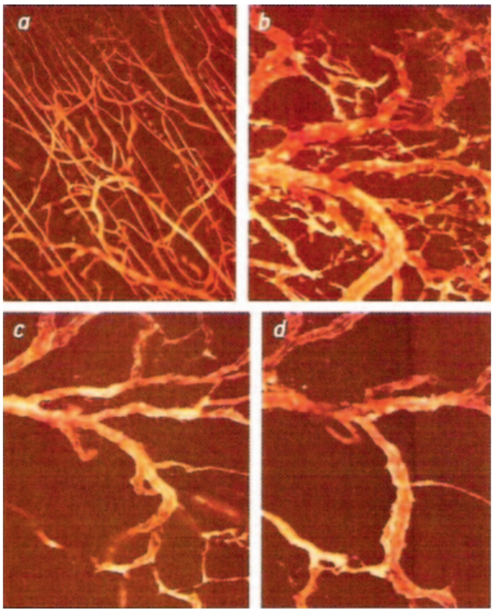

Fig. 4. Response of a vascular network to an antiangiogenic treatment (from [JK01])

reached a certain distance from the parent vessel, they tend to incline towards each other, leading to fusions called anastomoses. Such fusions lead to a network of vessels. On the other hand the sprout branching dramatically increases while approaching the tumour mass, eventually resulting in vascularization.

The coupling of the branching and growth process to the underlying chemical gradients is limited by the local density of the existing capillary network, thus leading to a mathematical strong coupling of this density and the kinetic parameters of the branching and growth process.

The study of angiogenesis has such potential for providing new therapies that it has received enthusiastic interest from the pharmaceutical and biotechnology industries. Indeed, dozens of companies are now pursuing angiogenesis-related therapies, and approximately 20 compounds that either induce or block vessel formation are being tested in humans. Although such drugs can potentially treat a broad range of disorders, many of the compounds now under investigation inhibit angiogenesis and target cancer. Intriguingly, animal tests show that inhibitors of vessel growth can boost the effectiveness of traditional cancer treatments (chemotherapy and radiation). Preliminary studies also hint that the agents might one day be delivered as a preventive measure to block malignancies from arising in the first place in people at risk for cancer.

In developing mathematical models of angiogenesis, the hope is to be able to provide a deeper insight into the underlying mechanisms which cause the process. It is therefore essential that predictive mathematical models are developed, capable of producing precise quantitative morphological features of developing blood vessels. Such models might be used for predicting the evolution of tumours (prognosis), and identifying optimal control strategies (medical treatment).

Unfortunately, a satisfactory modelling of angiogenesis requires a theory of stochastic fibre processes, evolving in time, and strongly coupled with underlying fields. In this case the theory of birth-and-growth processes (or branching-and-growth processes), developed for volume growth, cannot be applied to analyse realistic models, due to intrinsic mathematical difficulties, coming from the dependence of the kinetic parameters from the geometric spatial densities of the existing tumour, or capillary network itself [CM05,McDou06].

All these aspects induce stochastic time and space heterogeneities, thus motivating a more general analysis of the stochastic geometry of the process. The formulation of an exhaustive evolution model which relates all the relevant features of a real phenomenon dealing with different scales, and a stochastic domain decomposition at different Hausdorff dimensions, is a problem of high complexity, both analytical and computational.

Anyway statistical methods for the estimation of geometric densities may offer significant tools for diagnosis and dose/response analysis in medical treatments.

In the modelling of the above-mentioned systems it is of great importance to handle random closed sets of different (even though integer) Hausdorff dimensions. Following a standard approach in geometric measure theory, such sets may be described in terms of suitable measures. For a random closed set of lower dimension with respect to the environment space, the relevant measures induced by its realizations are singular with respect to the Lebesgue measure, and so their usual Radon–Nikodym derivatives are zero almost everywhere.

In Sect. 2 an original approach is reported, recently proposed by the research group of the authors, who have suggested to cope with these difficulties by introducing generalized densities (distributions) *á la Dirac–Schwartz*, for both the deterministic case and the stochastic case. In this last one, mean generalized densities are of interest.

These instruments may then help to formulate stochastic models (that is solving direct problems) for the over-mentioned applications; they also suggest methods for the solution of the related inverse problems, including methods of statistical analysis for the estimation of geometric densities of a stochastic fibre process that characterize the morphology of a real system. We apply such methods to real data, taken from the literature, and to simulated data, obtained by existing computational models of tumour-induced angiogenesis.

These methods can be used for validating computational models, and for monitoring the efficacy of possible medical treatment.

1.1 Nomenclature

We remind that a *random closed set (RACS)* Ξ in $\mathbb{R}^d$ is a measurable map

$$\Xi : (\Omega, \mathcal{F}, \mathbb{P}) \longrightarrow (\mathbb{F}, \sigma_{\mathbb{F}}),$$

where $\mathbb{F}$ denotes the class of the closed subsets in $\mathbb{R}^d$, and $\sigma_{\mathbb{F}}$ is the $\sigma-$algebra generated by the so-called *hit-or-miss topology* (see [Mat75]).

The theory of Choquet–Matheron shows that it is possible to assign a unique probability law associated with a *RACS* Ξ in $\mathbb{R}^d$ on the measurable space $(\mathbb{F}, \sigma_{\mathbb{F}})$ by assigning its *hitting functional* T_Ξ.

This is defined as

$$T_\Xi : K \in \mathcal{K} \longmapsto P(\Xi \cap K \neq \emptyset),$$

where $\mathcal{K}$ denotes the family of compact sets in $\mathbb{R}^d$.

Actually we may consider, equivalently, the restriction of T_Ξ to the family of closed balls $\{B_\varepsilon(x); x \in \mathbb{R}^d, \varepsilon \in \mathbb{R}_+ - \{0\}\}$.

In dependence of its regularity, a random closed set Θ_n with Hausdorff dimension n (i.e. $\dim_{\mathcal{H}} \Theta_n(\omega) = n$ for a.e. $\omega \in \Omega$), may induce a random Radon measure

$$\mu_{\Theta_n}(\cdot) := \mathcal{H}^n(\Theta_n \cap \cdot\,)$$

on $\mathbb{R}^d$ ($\mathcal{H}^n$ is the n-dimensional Hausdorff measure), and, as a consequence, an *expected measure*

$$\mathbb{E}[\mu_{\Theta_n}](\cdot) := \mathbb{E}[\mathcal{H}^n(\Theta_n \cap \cdot\,)]$$

(for a discussion about measurability of $\mathcal{H}^n(\Theta_n)$ we refer to [BM97, Z82]).

In several real applications, it is of interest to study the density (said *mean density*) of the measure $\mathbb{E}[\mu_{\Theta_n}]$ [BR04], and, in the dynamical case, its evolution in time [Mol92, Mol94]. Here we present a synthesis of a theory of random distributions as generalized densities of random measures, and mean geometric densities as expected values of random generalized densities, as proposed in [CV06c]. In particular we introduce a *Delta formalism*, á la Dirac–Schwartz, for the description of random measures associated with random closed sets of lower dimensions, such that the well known usual Dirac delta at a point follows as a particular case (see, for instance, [Jones82, KF70, Vlad79]).

In dealing with mean densities, a concept of *absolutely continuous random closed set* arises in a natural way in terms of the expected measure; indeed, an interesting property of a random set in $\mathbb{R}^d$ is whether the expected measure induced by the random set is absolutely continuous or not with respect to the d-dimensional Lebesgue measure ν^d. Thus, it is of interest to distinguish between random closed sets which induce an absolutely continuous expected measure, and random closed sets which induce a singular one. To this aim we introduce definitions of *discrete*, *continuous*, and *absolutely continuous* random closed set, coherently with the classical 0-dimensional case, in order to propose an extension of the standard definition of discrete, continuous, and absolutely continuous random variable, respectively (see also [CV06a, CV06b]).

2 Generalized Densities

In the sequel we will refer to a class of sufficiently regular random closed sets in the Euclidean space $\mathbb{R}^d$, of integer dimension n.

Definition 1 (n-regular set). *Given an integer $n \in [0, d]$, we say that a closed subset S of $\mathbb{R}^d$ is* n-regular*, if it satisfies the following conditions:*

(i) $\mathcal{H}^n(S \cap B_R(0)) < \infty$ *for any* $R > 0$

(ii) $\lim_{r \to 0} \frac{\mathcal{H}^n(S \cap B_r(x))}{b_n r^n} = 1$ *for* $\mathcal{H}^n$*-a.e.* $x \in S$

Here b_n denotes the volume of the unit ball in $\mathbb{R}^n$.

Remark 1. Note that condition (ii) is related to a characterization of the $\mathcal{H}^n$-rectifiability of the set A ([Fal85], p. 256, 267, [AFP00], p. 83).

We may observe that if A_n is an n-regular closed set in $\mathbb{R}^d$, we have

$$\lim_{r \to 0} \frac{\mathcal{H}^n(A_n \cap B_r(x))}{b_n r^n} = \begin{cases} 1 & \mathcal{H}^n\text{-a.e. } x \in A_n, \\ 0 & \forall x \notin A_n; \end{cases}$$

as a consequence (by assuming $0 \cdot \infty = 0$), for $0 \le n < d$ we have

$$\begin{aligned} \lim_{r \to 0} \frac{\mathcal{H}^n(A_n \cap B_r(x))}{b_d r^d} &= \lim_{r \to 0} \frac{\mathcal{H}^n(A_n \cap B_r(x))}{b_n r^n} \frac{b_n r^n}{b_d r^d} \\ &= \begin{cases} \infty & \mathcal{H}^n\text{-a.e. } x \in A_n, \\ 0 & \forall x \notin A_n. \end{cases} \end{aligned}$$

It is well known that every positive Radon measure μ on $\mathbb{R}^d$ can be decomposed as

$$\mu = \mu_{\ll} + \mu_{\mathbb{P}\mathrm{erp}},$$

where $\mu_{\ll}$ and $\mu_{\mathbb{P}\mathrm{erp}}$ are the absolutely continuous, and the singular parts of μ, respectively, with respect to ν^d, the usual Lebesgue measure on $\mathbb{R}^d$.

It then follows that $\mu_{\ll}$ admits a (nontrivial) Radon–Nikodym derivative with respect to ν^d, which is known as its density; while the Radon–Nikodym derivative of $\mu_{\mathbb{P}\mathrm{erp}}$, with respect to ν^d, would be zero ν^d- a.e.

Anyhow in analogy with the usual Dirac delta function $\delta_{x_0}(x)$ associated with a point $x_0 \in \mathbb{R}^d$ (a 0-regular closed set), a density can be introduced also for $\mu_{\mathbb{P}\mathrm{erp}}$, in a generalized sense, according to Definition 2 [KF70].

Definition 2 (Generalized density). *We call* $\delta_{\mu_{\mathbb{P}\mathrm{erp}}}$, *the* generalized density (*or, briefly, the* density P) *of* $\mu_{\mathbb{P}\mathrm{erp}}$, *the quantity*

$$\delta_{\mu_{\mathbb{P}\mathrm{erp}}}(x) := \lim_{r\to 0} \frac{\mu_{\mathbb{P}\mathrm{erp}}(B_r(x))}{b_d r^d},$$

finite or not.

Clearly, if A_n is an n-regular closed set in $\mathbb{R}^d$ with $n < d$, then the measure

$$\mu_{A_n}(\cdot) := \mathcal{H}^n(A_n \cap \cdot)$$

is a singular measure with respect to ν^d. Based on Definition 1, the quantity

$$\delta_{A_n}(x) := \lim_{r\to 0} \frac{\mathcal{H}^n(A_n \cap B_r(x))}{b_d r^d},$$

(finite or not), can now be introduced as the (generalized) density associated with A_n.

With an abuse of notations, we may introduce the linear functional δ_{A_n} associated with the measure μ_{A_n}, as follows:

$$(\delta_{A_n}, f) := \int_{\mathbb{R}^d} f(x)\mu_{A_n}(\mathrm{d}x),$$

for any $f \in C_{\mathrm{c}}(\mathbb{R}^d, \mathbb{R})$, having denoted by $C_{\mathrm{c}}(\mathbb{R}^d, \mathbb{R})$ the space of all continuous functions from $\mathbb{R}^d$ to $\mathbb{R}$ with compact support. In accordance with the usual representation of distributions in the theory of generalized functions, we formally write

$$\int_{\mathbb{R}^d} f(x)\delta_{A_n}(x)\,\mathrm{d}x := (\delta_{A_n}, f).$$

Define the function

$$\delta^{(r)}_{A_n}(x) := \frac{\mathcal{H}^n(A_n \cap B_r(x))}{b_d r^d},$$

and correspondingly the associated measure