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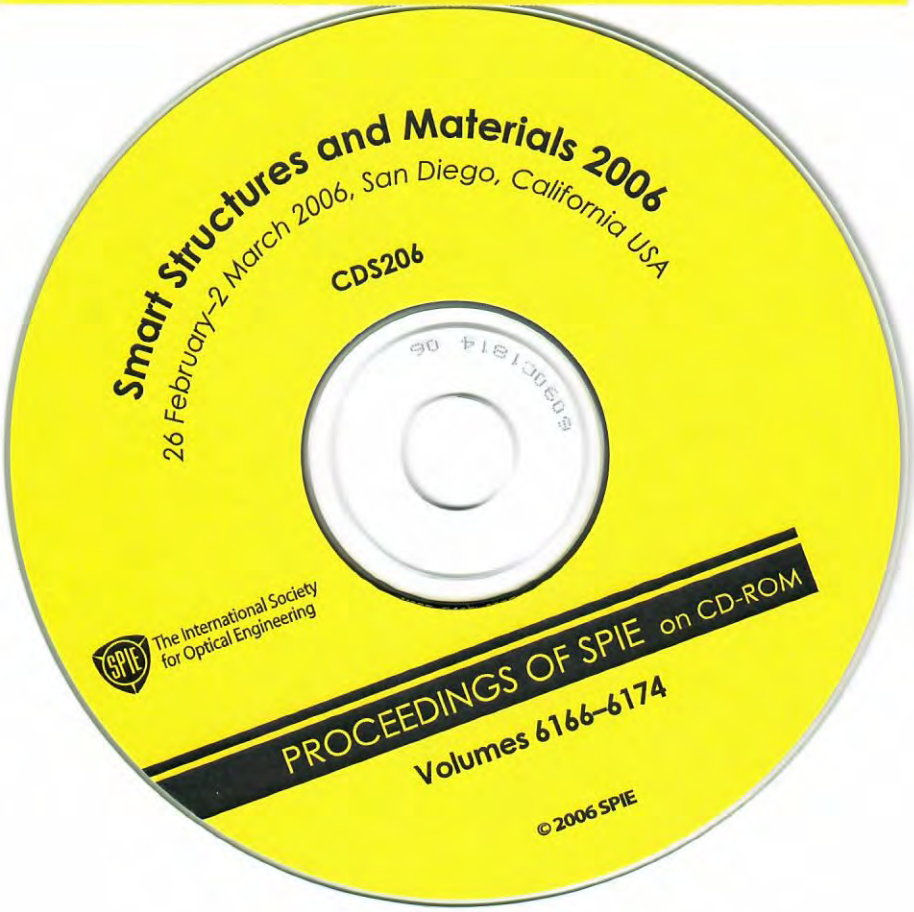

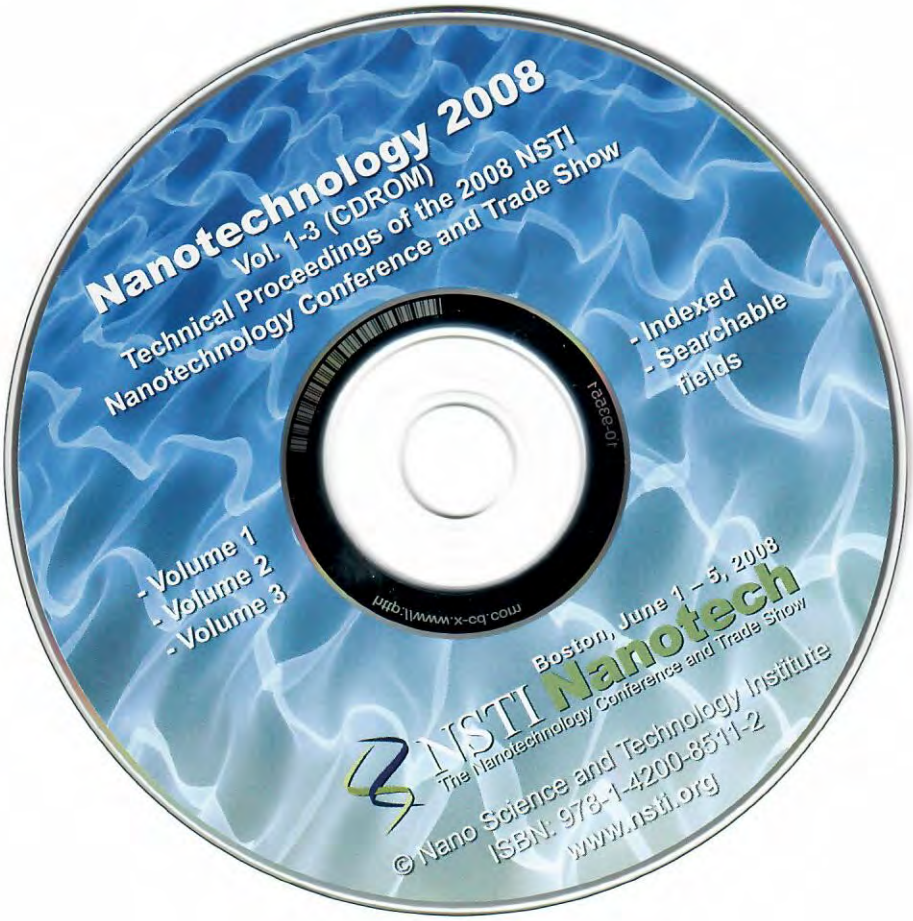
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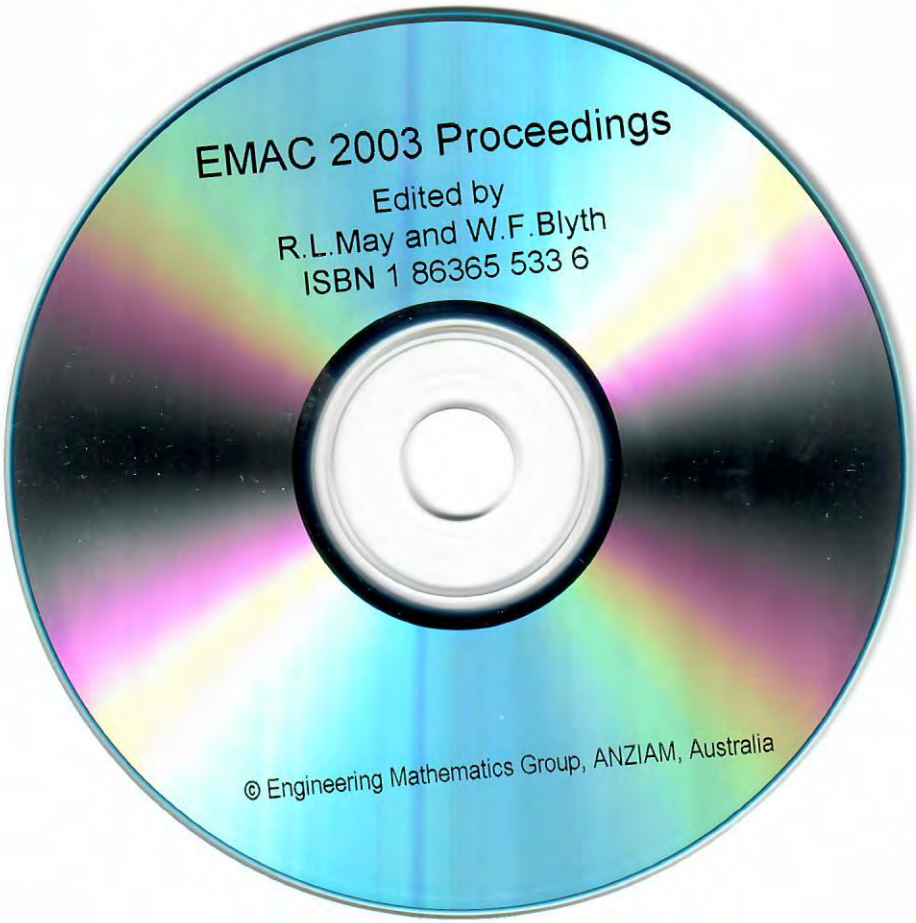
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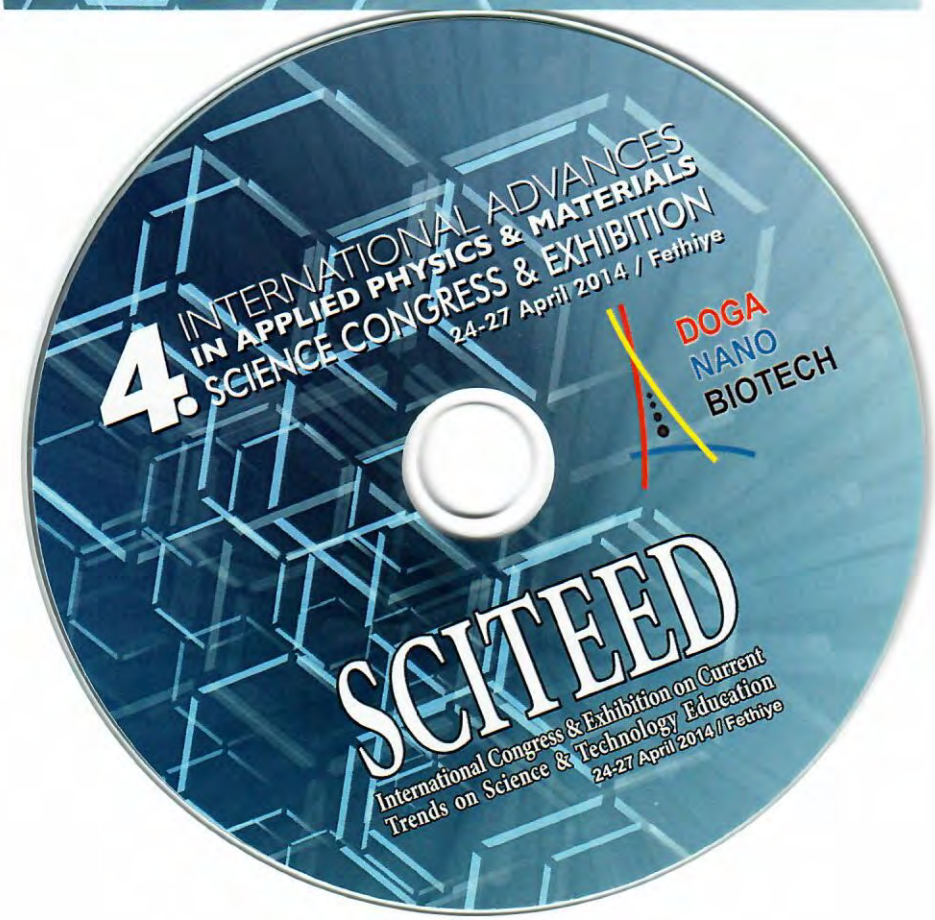
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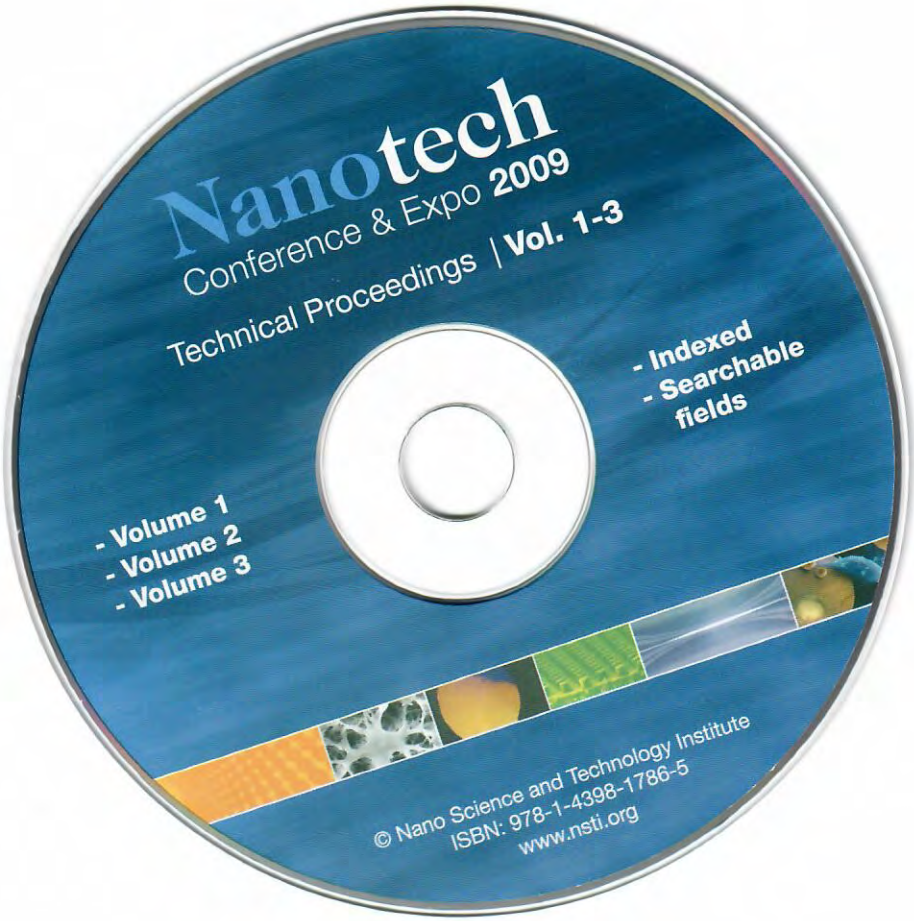
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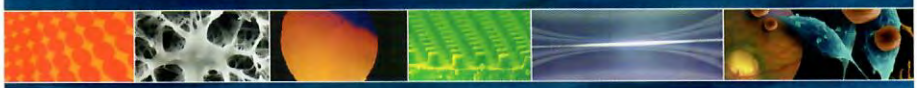

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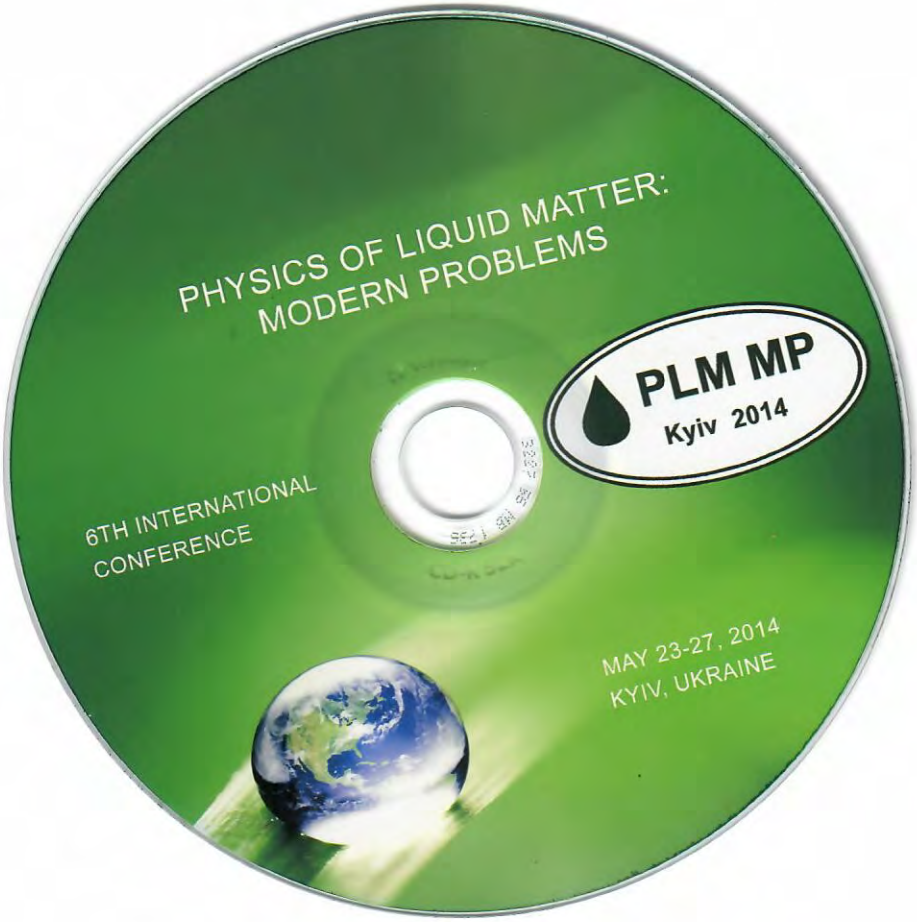
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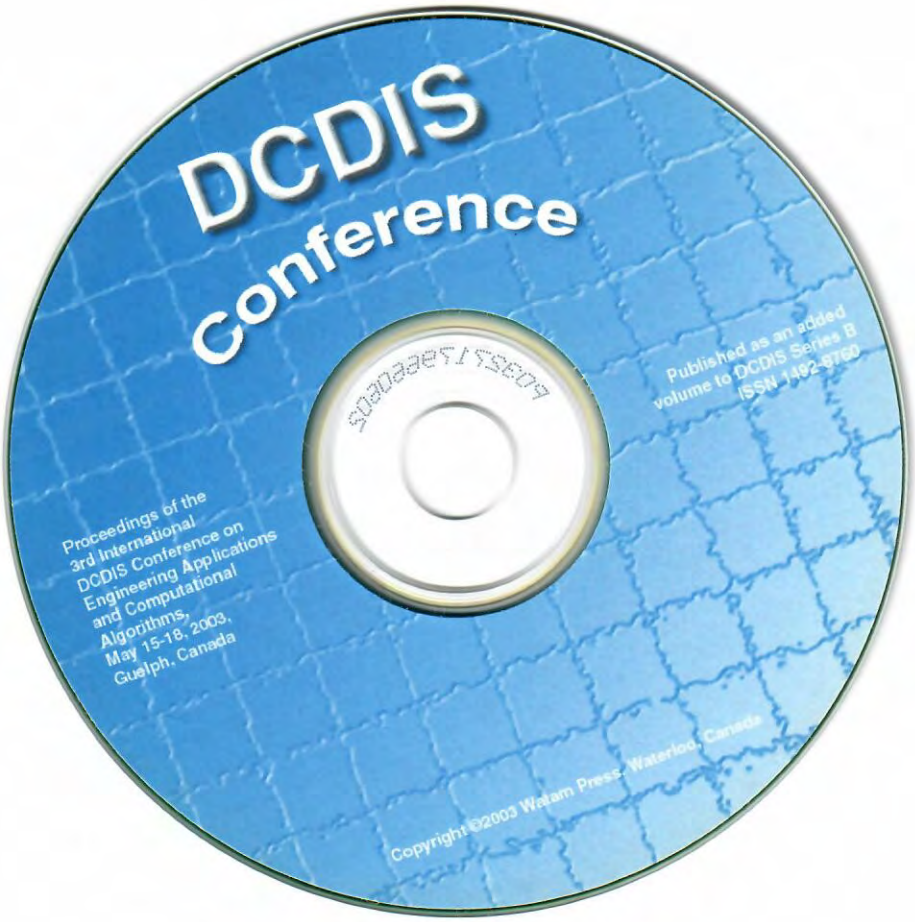
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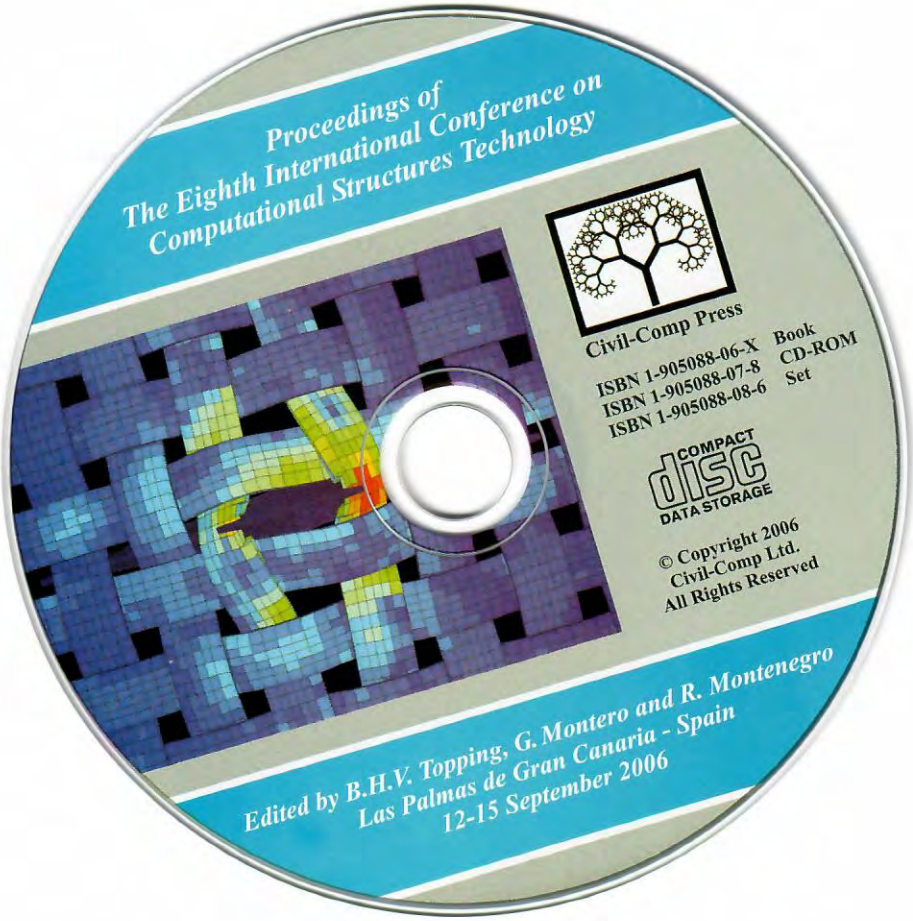
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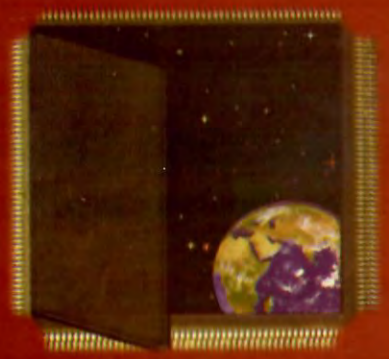

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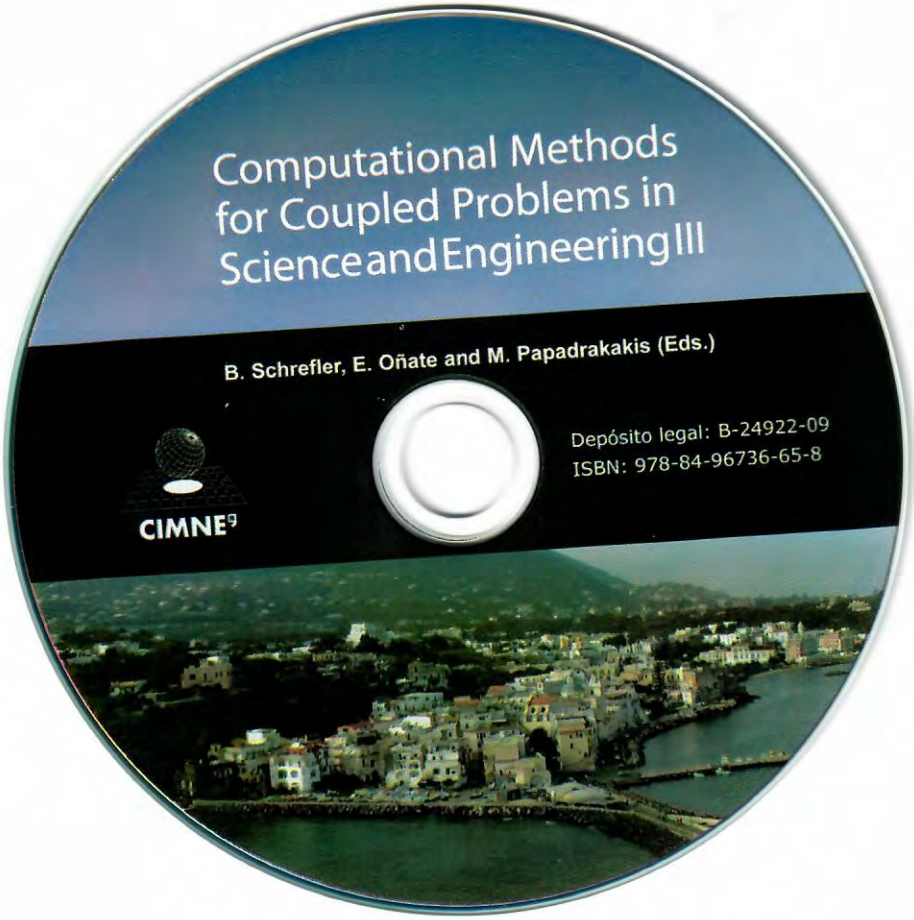
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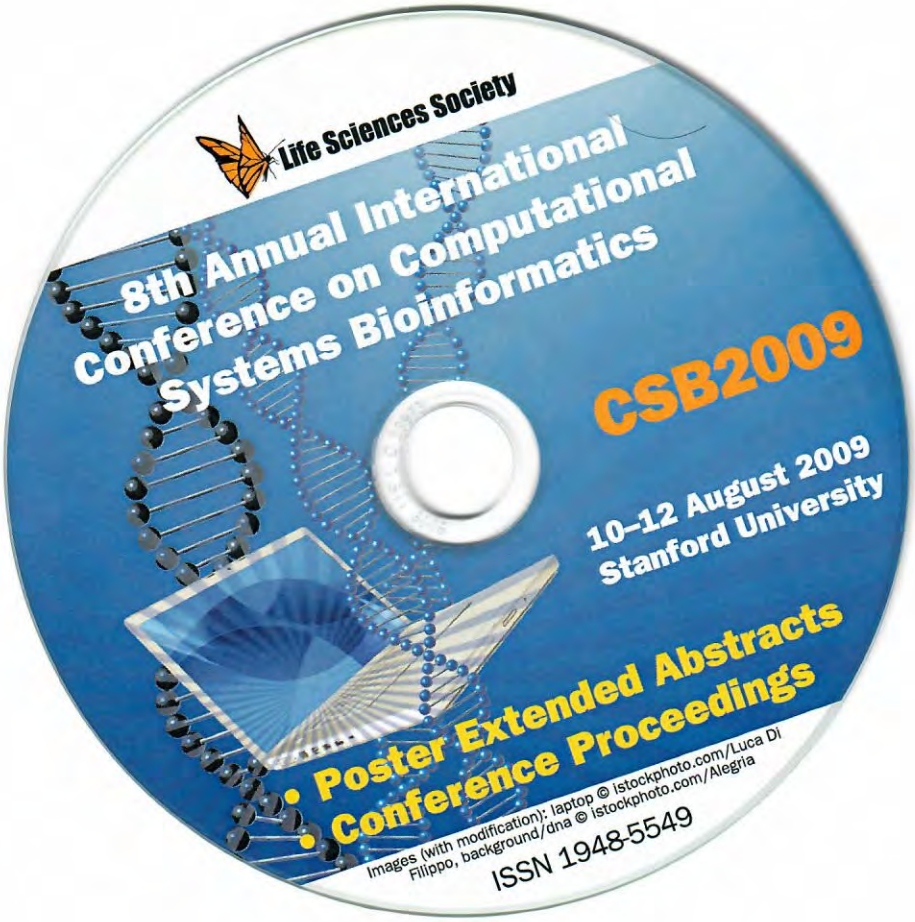
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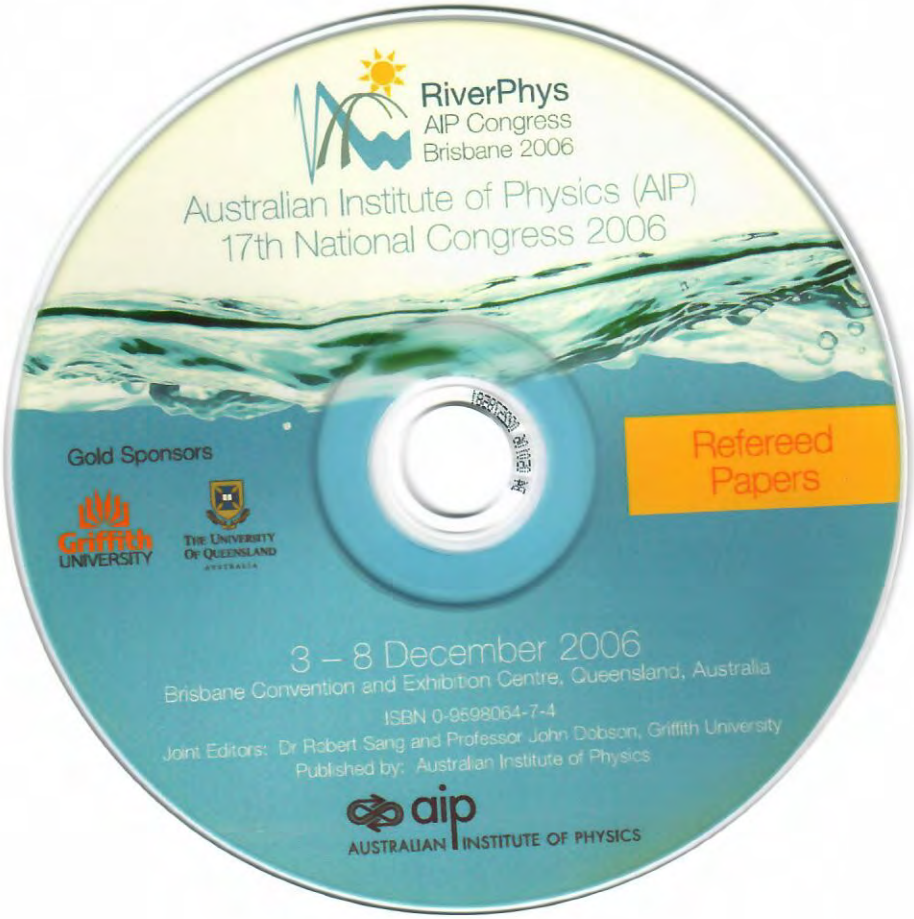
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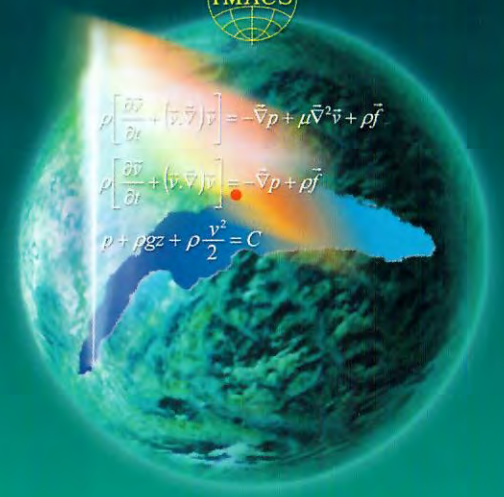

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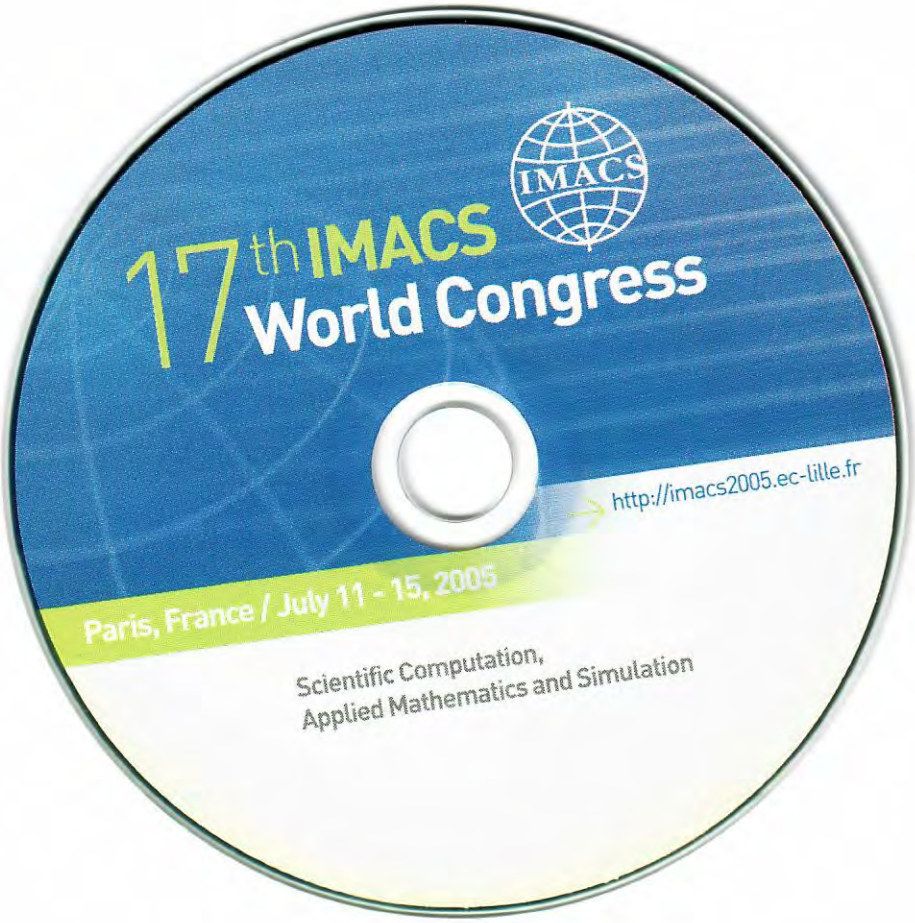
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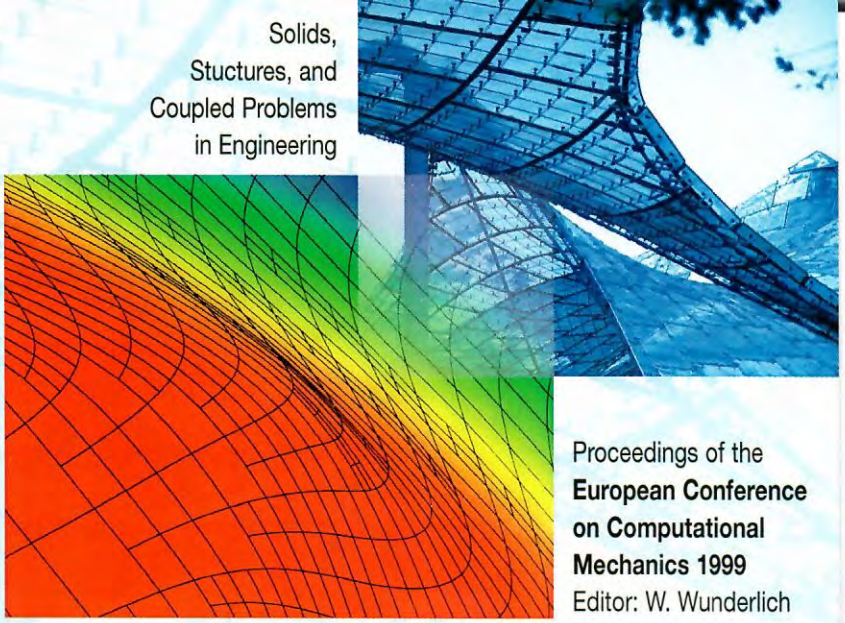

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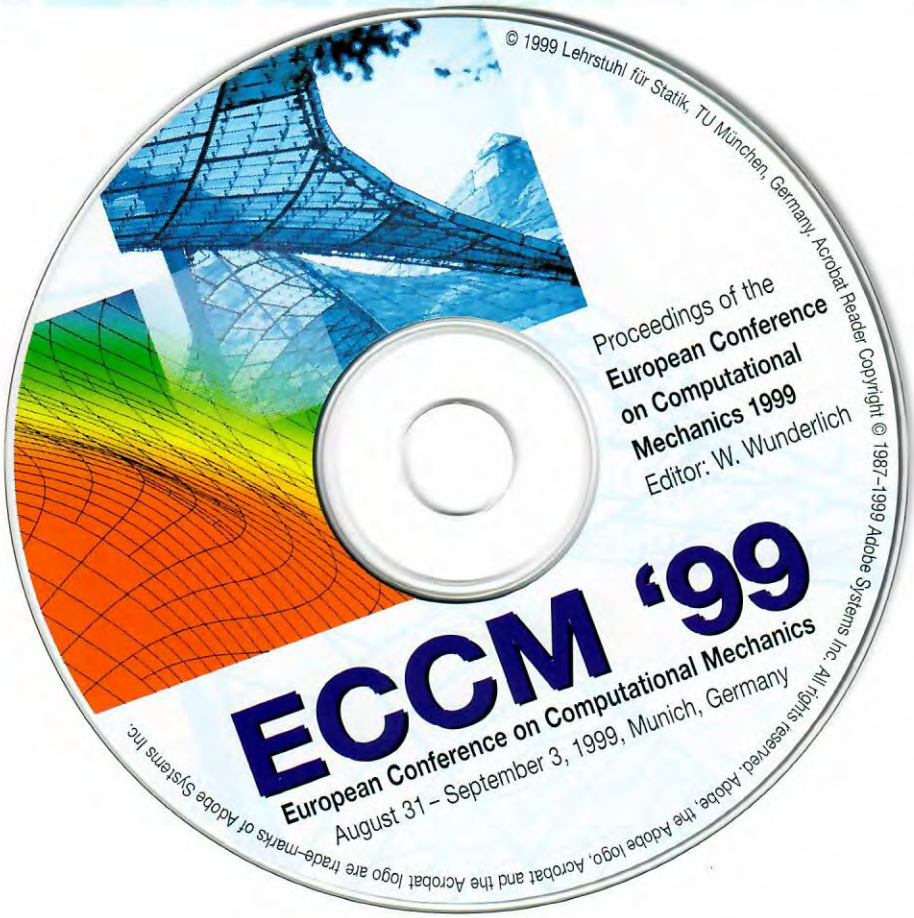

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Contents

	Preface	iii
1.	Logic	1
2.	Algebra	5
3.	Number theory	30
4.	Geometry	42
5.	Topology	57
6.	Algebraic geometry	69
7.	Lie groups and representations	77
8.	Real and complex analysis	84
9.	Operator algebras and functional analysis	116
10.	Probability and statistics	143
11.	Partial differential equations	163
12.	Ordinary differential equations and dynamical systems	187
13.	Mathematical physics	211
14.	Combinatorics	227
15.	Mathematical aspects of computer science	234
16.	Numerical analysis and scientific computing	236
17.	Applications of mathematics in the sciences	251
18.	Teaching and popularization of mathematics	263
19.	History of mathematics	268
	Late abstracts	271
	Index	275

MELNIK, p. 243

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MELNIK: Numerical Analysis of Difference Solutions in Coupled Nonstationary Electroelastic Fields Modelling

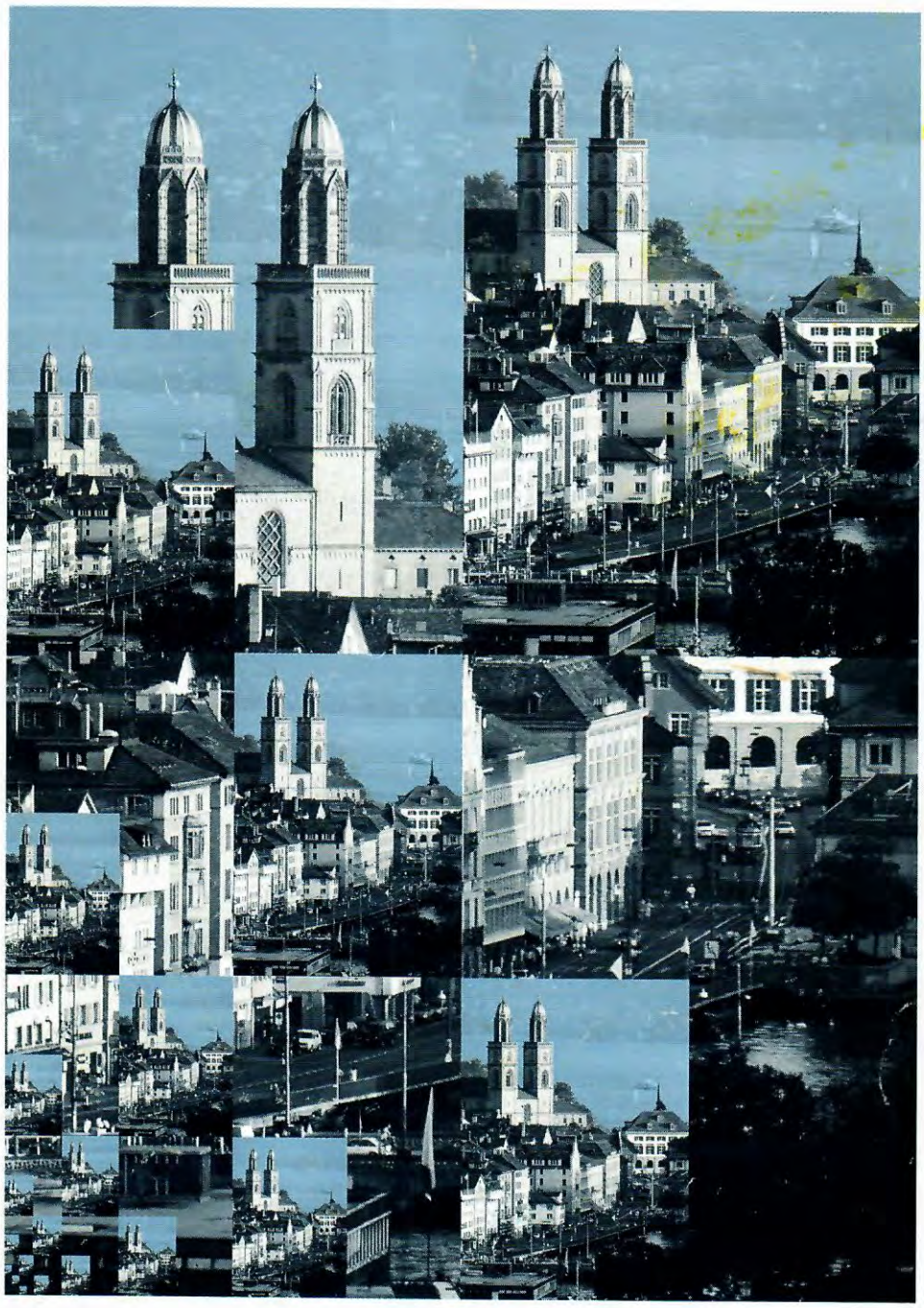
This paper deals with an efficient numerical method for the solution of coupled problems in dynamical electroelasticity. A suitable mathematical model for such types of problems is a system of second-order partial derivatives differential equations (PDDE), which does not belong to any classical kind of PDDE's, because the system contains both hyperbolic and elliptic-type equations.

Using the Faedo-Galerkin method we have been developing existence and uniqueness theory for such problems in one- and two-dimensional cases. The definitions of the generalized solution of problems are given and the existence and uniqueness theorems of the solution in Sobolev spaces are proved. The efficient difference schemes for the numerical solution of the problems are proposed. The construction of the difference schemes is based on the variational approach.

Our main results include the following: 1) the existence theorems of the unique generalised solution of the above-mentioned PDDE system have been proved; 2) computationally efficient difference schemes for coupled nonstationary electroelastic fields modelling have been proposed and convergence of the constructed difference schemes solutions have been proved; 3) the error estimates have been established (in particular, the second-order accuracy in the energy norm have been established for the above-mentioned problem); 4) constructed and theoretically grounded difference schemes have been applied to the problem on nonstationary coupled electroelastic oscillations of hollow piezoceramic cylinders and numerical results are discussed.

ICM 94
International Congress of Mathematicians
Zürich 3–11 August 1994

zürich m94



IACM

WCCM III

THE THIRD WORLD CONGRESS ON COMPUTATIONAL MECHANICS

Overseas Vocational Training Center (OVTA Center)
and
Nippon Convention Center (Makuhari Messe)
Chiba/Japan

August 1 (Monday) – 5 (Friday), 1994

Organized by
Japan Chapter of the International Association for Computational Mechanics (IACM)
Foundation for Advancement of International Science (FAIS)

P4 Numerical Methods & Computing - 4

Date & Time: Tuesday, August 2 11:00 - 13:00 Room: P

P4 - 1 A Comparison of Integral Equations for Conformal Mapping
K.Amano

P4 - 2 Variable Coefficient Explicit Runge-Kutta Methods for Stiff Equations
M.Nakashima

P4 - 3 On the Use of Exponential, Optimization Parameters When Dealing with Eigenvalue and Field Problems
P.A.A.Laura, V.H.Cortinez

P4 - 4 Asymptotic Decompositions Over Groups in Problems of Nonlinear Mechanics
I.Y.Ageyeva

P4 - 5 High Precision Programs for Solving Matrix Riccati Equations
N.Dakev, A.Cheremensky

P4 - 6 Computationally Efficient Difference Schemes for Coupled Nonstationary Electroelastic Fields Modelling
V.N.Melnik

P4 - 7 Two Improvements in the Implementation of the Gauss-Seidel Iterative Solution of Large Sparce Linear Systems
J. L.Almara

A5 Structural Dynamics - 5

Date & Time: Tuesday, August 2 15:00 - 16:30 Room: A

A5 - 1* Soil-Structure Interaction Analysis of Large Scaled Forced Vibration Test
T.Udaka, S.Kakimoto, T.Kurakake, S.Yamamoto, O.Yoshida

A5 - 2 Seismic Response Analysis of Grouped Pile Embedded Foundation by Substructure Procedure
S.Takano, Y.Yasui

A5 - 3 A Study on Effects of Grid-shaped Improved Ground against Liquefaction Failures
M.Kibayashi, T.Kawano, K.Fukuyama, S.Onimaru, M.Hatanaka, Y.Suzuki

A5 - 4 Analysis of Dynamical Characteristics and Earthquake Response for Complex Space Structure under Mutual Actun of Upstructure, Group Piles and Ground Soil
X.Shen, J.Dun, X.Shen, Y.Fan

A5 - 5 Dynamic Boundary Element Method(DBEM) Analysis of Soil - Structure System under Seismic Wave
X.Zhou, H.Feng

B5 Recent Advances in CFD - 5 Turbulent Flows II

Date & Time: Tuesday, August 2 15:00 - 16:30 Room: B

B5 - 1* LES and DNS of Turbulent Flow in an Annular Tube
H.Kawamura, S.Nakamura, S.Satake, T.Kunugi

B5 - 2 Numerical Analysis of Separated Flow in 2D 90° Bend Duct
X.Cheng, R.W.Guo

B5 - 3 Direct Numerical Simulation of Isotropic Turbulence
K.Yamamoto , I.Hosokawa, S.Oide

B5 - 4 Large Eddy Simulation of Flow Downstream of a Three-Dimensional Surface-Mounted Body
K.Nozawa, T.Tamura

B5 - 5 Finite Element Analysis of Turbulent Flow Through Expanding Axisymmetric Pipes
K.Bhatia, M.Rahman

**Keynote Lecture *Invited Lecture

P5 Numerical Methods & Computing - 5

Date & Time: Tuesday, August 2 15:00 - 16:30 Room: P

P5 - 1 Numerical Solution of The Quasihydrodynamic Device Model Based on The Half-Implict Scheme and Flux Correction Method
V.Melnik

P5 - 2 Numerical Analysis of Acoustic Gas Oscillations in Three-dimensional Regions Using Method of Geometrical Immersion
I.N.Shardakov, L.A.Golotina

P5 - 3 A Fast Computation Method of Gas Pipelines and Comparison with Experimental Data
T.Kiuchi

P5 - 4 Numerical Solving of Three-Dimensional Elastic and Acoustic Wave Problems by the Potential Methods
N.E.Ershov, S.I.Smagin

P5 - 5 Numerical Simulation of the Electrofusion Joining Process of Polyethylene Gas Pipes
M.Fukumura, M.Fujikake, K.Kitao

A6 Structural Dynamics - 6

Date & Time: Tuesday, August 2 17:00 - 19:00 Room: A

A6 - 1* Transient Dynamics and Free Vibration Formulations of Varying Cross Section Beams and Structure Elements Using Dual Reciprocity Method
F.Kasza

A6 - 2 Viscous Boundary for Wave Propagation Problem by Discrete Element Method
T.Suzuki, M.Hakuno

A6 - 3 3D Wave Propagation Analysis of 2D Irregularly Layered Media Using Hyperelement for Moving Loads
M.Nagano, M.Motosaka, M.Kamata

A6 - 4 Wave Propagation Properties of Lattice Structures -a Research of Structural Damping-
A.Nishida, Y.Hangai

A6 - 5 Computational and Analytical Methods in the Theory of Elastic Surface Waves in Bodies with Initial Stresses (Cases of Planar and Curvilinear Surfaces)
A.N.Guz

A6 - 6 A Numerical Study on One-Dimensional Thermal Waves in a Rigid Isotropic Solid
J.B.Haddow, L.Jiang

B6 Recent Advances in CFD - 6 Compressible Flows II

Date & Time: Tuesday, August 2 17:00 - 19:00 Room: B

B6 - 1** High Resolution Schemes for the Compressible Navier-Stokes Equations
H.Daiguji

B6 - 2* A TVD Solver for Two-Dimensional Viscous Flows on Unstructured Triangular Meshes
V.Magi, G.Vacca

B6 - 3 Lift and Drag Forces of an Aerofoil by the Stabilized Finite Difference Method
T.Aratani

B6 - 4 Two Dimensional Compressible Viscous Flow Analysis for Turbomachinery Blades
D.Biswas, M.Ishizuka

B6 - 5 Block Iterative Solution Strategies for Large 3D Flow Applications
S.Kharchenko, A.Yeremin, M.A.Heroux, Q.Sheikh

**Keynote Lecture *Invited Lecture

Fifth International Colloquium on Differential Equations

PLOVDIV, BULGARIA
18-23 August, 1994

First Announcement and Invitation for Participation

ORGANIZING COMMITTEE

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Address of Organizing Committee:
Stoyan Zlatev
Mathematical Faculty of the Plovdiv University
Tsar Assen Str. 24, Plovdiv 4000, Bulgaria

The Fifth International Colloquium on Differential Equations will be organized by Mathematical Society of Japan and UNESCO, with the cooperation of Association Suisse d'Informatique, Canadian Mathematical Society, Hamburg University, Kyushu University, London Mathematical Society, Plovdiv University "Paisii Hilendarski", Technical University - Berlin, Technical University - Plovdiv, Union of Bulgarian Mathematicians - Plovdiv Section, and University of Texas - Pan American.

The 32nd Australasian Applied Mathematics Conference

Masterton, New Zealand

4-8 February 1996

ANZIAM'96

Australian Mathematical Society
ANZIAM

(formerly the Division of Applied Mathematics)

The 32nd Australasian Applied Mathematics Conference

Solway Park Travelodge, Masterton, New Zealand

4-8 February, 1996

ANZIAM'96

ISBN 7259 0869 6

AMC/ANZIAM Locations

1966	Kangaroo Island
1966	Coorong
1967	Adelaide
1968	Hall's Gap
1969	Victor Harbor
1970	Lorne
1971	Smiggin's Hole
1972	Wollongong
1973	Surfers Paradise
1974	Lorne
1975	Tanunda
1976	Jindabyne
1977	Terrigal
1978	Broadbeach
1979	Leura
1980	Cowes
1981	Victor Harbor
1982	Bundanoon
1983	Perth
1984	Merimbula
1985	Launceston
1986	Wirrina
1987	Wairakei, NZ
1988	Leura
1989	Ballarat
1990	Coolangatta
1991	Hanmer Springs, NZ
1992	Bateman's Bay
1993	Hahndorf
1994	Pokolbin
1995	Busselton
1996	Masterton, NZ

Generalized Solutions of Hamilton-Jacobi-Bellman Equation from Sobolev's Classes

V. N. Melnik
School of Mathematics, University of South Australia
The Levels Campus, S.A. 5095, Australia

The connection between the maximum principle of Pontryagin (1) and Bellman's dynamic programming approach (2) is well-known when sufficient requirements on the smoothness of the Hamilton-Jacobi-Bellman-Equation (HJBE) solution are assumed. However in many cases such assumptions are excessive which makes it necessary to use the concept of generalized solutions of HJBE. A generalization of classical results is usually made in the framework of viscosity solution or in the concept of Clarke's generalized gradients. Though inclusion-type connection between (1) and (2) is established, procedures for obtaining either a solution of HJBE or an adjoint function of the optimal process are still lacking in the general case. A construction of such procedures is often precluded by the steep gradients of the solution which are typical for many applications.

In this case we propose consideration of generalized solutions of HJBE from Sobolev's classes. In fact we use Steklov's operators technique to obtain *a local optimality principle* (OP) from which we derive *generalized equations of OP* in "deterministically non-smooth" and stochastic cases. For these equations we prove the theorems on the existence and uniqueness of the solution from Sobolev's classes $W_1^{k,k}$, $k = 1, 2$. We investigate properties of the Hamiltonian of the dynamical systems described by such equations when the solution is from L_1. Our special attention is devoted to the case when the Hamiltonian produces a non-conservation law equation. The latter is the main troublemaker in many areas of mathematical modelling including drift-diffusion problems in reactive flow simulation, models of hydrodynamic type in semiconductor devices modelling, and problems in the optimal control theory. We propose an algorithm for the solution of such an equation based on the Markov-Chain-Approximation method deriving stability conditions in the explicit form.

Gerrard Liddell

ISBN 7259 0869 6

The 40th Australian Mathematical Society Conference 1996

Adelaide, South Australia

7 July – 12 July 1996

Programme and abstracts

It turns out that for groups of the form $G = \Pi_{i\in\mathbb{N}} G_i$, a countable product of locally compact groups, equipped with the group operations of pointwise multiplication and the product topology, one can prove obtain the exact same conclusion as the Glimm theorem. While it is known that Kechris' theorem fails badly for this class of groups, it turns out that one can prove a natural analogue by appealing to Sym($\mathbb{N}$), the infinite permutation group.

Dr George Willis
Department of Mathematics
The University of Newcastle
`george@frey.newcastle.edu.au`

Representations of Metrisable, Abelian Groups

Abstract: The set of measurable subsets of $[0,1]$ forms a complete metric group when equipped with the symmetric difference as the group operation and metric $d(x,y) = m(x\Delta y)$, where m is the Lebesgue measure. Every element in this group has order 2 and the group can in fact be thought of as a normed linear space over the field of order 2.

The ring of continuous endomorphisms of this group (or linear space) plays an important role in the study of continuous unitary representations of those abelian, metric groups in which every element has order 2. Insights into the structure of this ring can be obtained by thinking of endomorphisms as being infinite matrices with entries in the field of order 2. Some of these insights and their significance for representation theory will be outlined in the talk.

Dr Peter Stacey
La Trobe University

Some automorphisms of rotation algebras

The rotation algebra A_θ is the universal C^*-algebra generated by two unitaries U, V with $VU = e^{2\pi i\theta}UV$, where $\theta \in \mathbb{R}$. An automorphism of A_θ gives rise to an element of $GL(2,\ \mathbb{Z})$ and, conversely, there is a natural way of producing an automorphism of A_θ from an element of $SL(2,\mathbb{Z})$.

When θ is irrational the algebra A_θ is simple. In this case a remarkable result of Elliott and Evans shows that A_θ is an inductive limit of algebras each of which is a direct sum of two algebras of matrix valued functions on S^1.

The talk will give a brief outline of the general theory described above before describing some specific examples of automorphisms of A_θ associated with matrices of determinant -1.

John Graham
University of Sydney

Decomposition numbers for planar algebras

Jones has recently described an annular analogue $A_n(\delta)$ of the Temperley Lieb algebra $TL_n(\delta)$ which was motivated by his study of factors in the sense of von Neuman algebras. For most values of the parameter δ, these algebras (defined over the complex numbers) are semisimple and there is a simple construction for their irreducible modules. However this construction produces a family of "cell modules" for all values of the parameter. Using a "hook product" formula of Stanley which counts the linear extensions of a "forest", we obtain an explicit filtration of these modules such that the quotients are irreducible. This information determines the blocks, a formula for the dimension of the irreducible modules, the Cartan matrices, and provides a simple criterion for semisimplicity.

Dr V. Nick Melnik
(UNISA, Adelaide)

Nonlinear dynamical systems: coupling information and energy in mathematical models

Abstract: In the areas of mathematics related to modelling dynamical processes, systems and phenomena major theoretical achievements are originated from a high degree of isolation of these systems from the observer. Since the laws of science intend to represent properties of the system which remain the same under the flow of certain events this mathematical assumption seems to be a quite resonable one. Over centuries mathematicians have labeled this flow using the concept of deterministic time which in its very essence is external to the system under investigation. As a result they often attempt to represent information about the system (extractable from mathematical models at least in principle) in a homogeneous time form. In many mathematical applications ranging from gravitational astronomy to

atomic physics this simplified approach gives models which are sufficiently adequate to our experience and observations.

However, for nonlinear dynamical systems the loss of homogeneity in time is typical, and the associated time series gain coupling and non-homogeneous properties. In both existing approaches to modelling nonlinear dynamical systems (deterministic and probabilistic) neither Hamiltonian (Lagrangean) nor initial/boundary conditions for *an isolated nonlinear system* can be given with infinite precision.

First, we consider initial-boundary value mathematical models and explain why they can describe only an *a priori* dissipative system. We argue that the construction of such mathematical models for dynamical systems is always a competition between mathematical formalisation of boundary conditions (with respect to system's internal time) and of the energy conservation law (in modeler's time). We explain that the systems described by such models are not isolated being coupled with their environment. Such mathematical models provide a sound basis of human endeavours from climatology to semiconductor device theory.

No doubt, a remaining question of *an associated with such models* loss of information about the system is a very challenging problem where a wide range of new mathematical ideas have been generated in the second part of this century due to the development of optimal control theory.

In this paper we scrutinize hypothesizes on which some modern mathematical theories related to initial value mathematical models (for which the competition between boundary conditions and conservation laws is fuzzified by the Gibbs conjecture) are based. We discuss an associated question whether the human element can be eliminated in the human-system interaction from *the chain of computations/observations* (except of two points in external to the system time). We argue that if this chain is an algorithm then it is equivalent to *the normal Markov algorithm*, and we can understand, predict and model nonlinear dynamics by *the information processing of an antagonistic game type* (between a decision maker/modeler and nature). However, due to incompleteness of the available information classical results of the game theory are not applicable.

In general, a nonlinear dynamical system can expose to us both deterministic and probabilistic features subject to a spacetime scale we consider. Whatever mathematical model we use (deterministic or probabilistic) it is always the task of the decision maker/modeler to define how the coupling energy and information should be approximated in the mathematical/computational model, or to put it differently at what extent information about the system is available *a priori* and how sequential growth of information (which is not obligatory correct with the probability 1) should be processed.

NM
'96 MISKOLC
CM

SCHEDULE

Conference on

Numerical Methods and Computational Mechanics in Science and Engineering

July 15–19, 1996
University of Miskolc
Miskolc, Hungary

MISKOLCI EGYETEM 1735

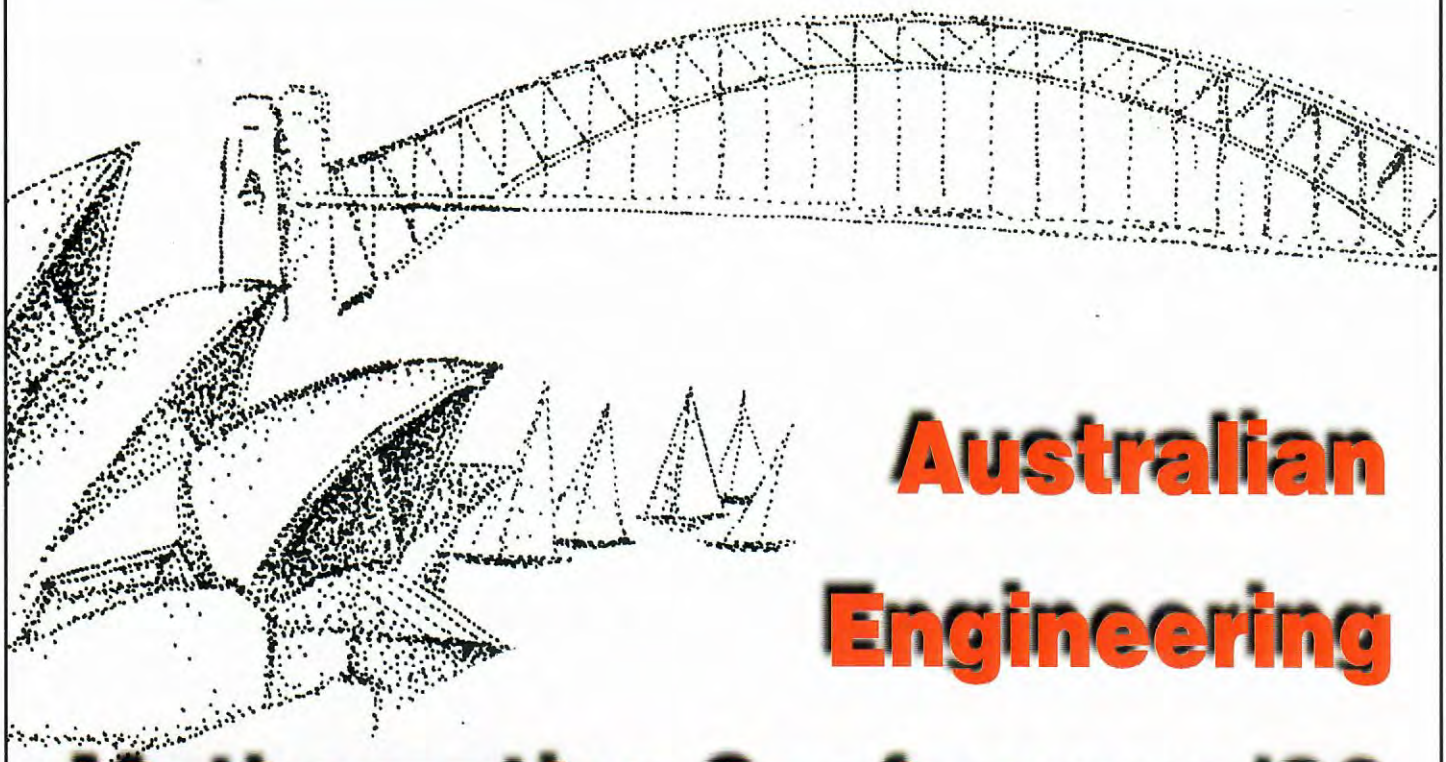
Organized by
János Bolyai Mathematical Society
University of Miskolc
Hungarian Academy of Sciences
Miskolc Committee of the Hungarian Academy of Sciences
Central European Association for Computational Mechanics

Thursday (July 18, 1996)

Session Finite Element Method II and Boundary Element Method : Lecture room II	
Chairman	I. Páczelt
8.30-8.45	G. Szeidl and I. Iván Fundamental solutions and boundary integral equations for the first plane problem of micropolar elastostatics in dual system
8.50-9.05	R. Vodicka BEM coupled formulations for contact problems
9.10-9.25	V.N. Melnik Computational models in solid state electronics: boundary element method as a Markov decision process
9.30-9.45	Y. Volpert, T. Szabó, I. Páczelt and B. Szabó Solution of mechanical contact problem using space enrichment method
10.00-10.15	H. Van der Veen A mathematical analysis of non-associated plasticity
10.20-10.35	H. Verhoeven A finite plate element for the deep drawing process
10.40-10.55	C.K. Mészényi NFEARS and its data structure
11.00-11.15	J. Rakowski Locking-free simple curved beam finite element

Session Heat Conduction : Seminar room1	
Chairman	H.-G. Roos
8.30-8.45	I. Faragó and R. Horváth On the connection between the order of the approximation and qualitative properties in the numerical solution of the heat conduction equation
8.50-9.05	M. Honneré Heat waves simulation
9.10-9.25	H.-G. Roos Finite element methods on special meshes for convection-diffusion problems
9.30-9.45	L.A. Krukier Iterative solution of steady convection diffusion equation

Session Mechanics of Structures : Lecture room IV	
Chairman	Z. Gáspár
8.30-8.45	M. Heinloo and T. Lepikult On radial deflections in circular cylindrical shells under local loading
8.50-9.05	B. Czibere-Verhoeven Application of the finite difference energy method for the geometrically nonlinear director theory of plates
9.10-9.25	I. Morachkovskaya and L.V. Kurpa A new computational analysis of thin shallow shells problems on the base of structural method of r-functions
9.30-9.45	L.V. Kurpa The computer approach to the r-functions method in problem of bending of flexible shallow shells of arbitrary shape
10.00-10.15	S. Briccoli–Bati, M. Paradiso and G. Tempesta A numerical model for the analysis of structures with unilateral constraints
10.20-10.35	M. Kowalczyk Predictor-corrector method based on homogeneous linearized system
10.40-10.55	S. Holzer Advanced finite element methods in civil engineering practice



Australian Engineering Mathematics Conference '96

Conference Programme

15-17 July 1996

The University of Sydney

An international conference presented by:

The Institution of Engineers, Australia

The Warren Centre for Advanced Engineering

The Engineering Mathematics Group
(a specialist group of ANZIAM)

Supported by: State & Regional Development, New South Wales
The Australian Technology Park Sydney Ltd
D.I.S.T International Conference Support Scheme

AEMC '96

WEDNESDAY, July 17

0900-0950 PLENARY KEYNOTE SESSION K7 — *Room:* *Main Plenary Level 4*

Session Chair: *Andrew Currie*

Presenters Name: *Professor G. Steven*
University of Sydney

Keynote Paper: The Mathematics of the Finite Element Method

0950-1050 SESSIONS 8A, 8B & 8C

Session 8A	Session 8B	Session 8C
AI & Electrical Applications IV	Engineering Mathematical Analyses & Techniques II	Mathematical Modelling V - Environmental
Room: Main Plenary	Room: Level 5	Room: Level 5
Session Chair: *David Butler*	*Session Chair:* *Alan Easton*	*Session Chair:* *Neville Fowkes*
Solving Fuzzy Non-Linear Simultaneous Equations and Its Applications in Electrical Engineering *A.T.P. So and W.L. Chan, City University of Hong Kong, Hong Kong*	Numerical Solution of Hammerstein Integral Equations Using Walsh Functions *V. Uljanov and W.F. Blyth, Royal Melbourne Institute of Technology*	Boundary Effects in Oil Spill Models *D.F. Zhang, A.K. Easton and J.M. Steiner, Swinburne University of Technology*
Robust and Simpler Ways in which Fuzzy Logic Controller is Developed *C.C. Tan and C.A. Sammons, First Robotics Industrial Science (M) Sdn. Bhd., Malaysia*	Nonconservation Law Equation in Mathematical Modelling: Aspects of Approximation *V.N. Melnik, University of South Australia*	Dimensional Analysis in Mathematical Modelling: A Case Study Using Geothermal Reservoirs *I. Pestov, Victoria University of Wellington, New Zealand*
	Solution of Boundary Integral Equations Using Wavelet Bases *J.S. Kot, D.G. Geers and N. Nikolic, CSIRO Division of Radiophysics*	Time to Ponding During Non-Constant Irrigation *P. Broadbridge and J.M. Stewart, University of Wollongong*

1050-1120 MORNING TEA
Terrace Buffet Foyer, Level 4

CTAC97

The Eighth Biennial

COMPUTATIONAL TECHNIQUES AND APPLICATIONS CONFERENCE

The University of Adelaide

Adelaide

29 September – 1 October 1997

ABSTRACTS

ANSETTAUSTRALIA

On Computational Aspects of Certain Optimal Digital Signal Processing Algorithms

Kate Melnik
Dept. of Computer Science, Flinders University of South Australia
& Roderick Melnik*
Dept. of Mathematics & Computing, University of Southern Queensland

Growing complexity of practical problems requires further development of effective numerical techniques in many areas of computational mathematics. This paper addresses the optimisation of the accuracy of the numerical evaluation of certain oscillatory integrals. Such integrals often occur as an important part of the modelling of optical systems and automatic control systems. They also occur in digital filtering, image recognition, statistical analysis of experimental data and many other problems.

We believe that the importance of the design and implementation of optimal algorithms (and algorithms close to optimal with respect to their computational characteristics) is often comparable with the importance of the design and implementation of new computer hardware. In this paper algorithms, based on the methods of quasi-solutions and residual minimisation, are constructed in order to solve a series of practical problems in digital signal processing and image recognition. These algorithms, that have been designed for the case of inaccurate data, provide automatic estimates of accuracy for problem solutions. We provide a theoretical justification of the constructed algorithms and derive their properties. A practical implementation of these algorithms is also discussed. One of the important features of the proposed algorithms is a flexible choice of options depending on practical aspects of the problems, which is a vital factor in many applications.

Modelling of Nonlocal Physical Effects in Semiconductor Plasma Using Quasi-Hydrodynamic Models

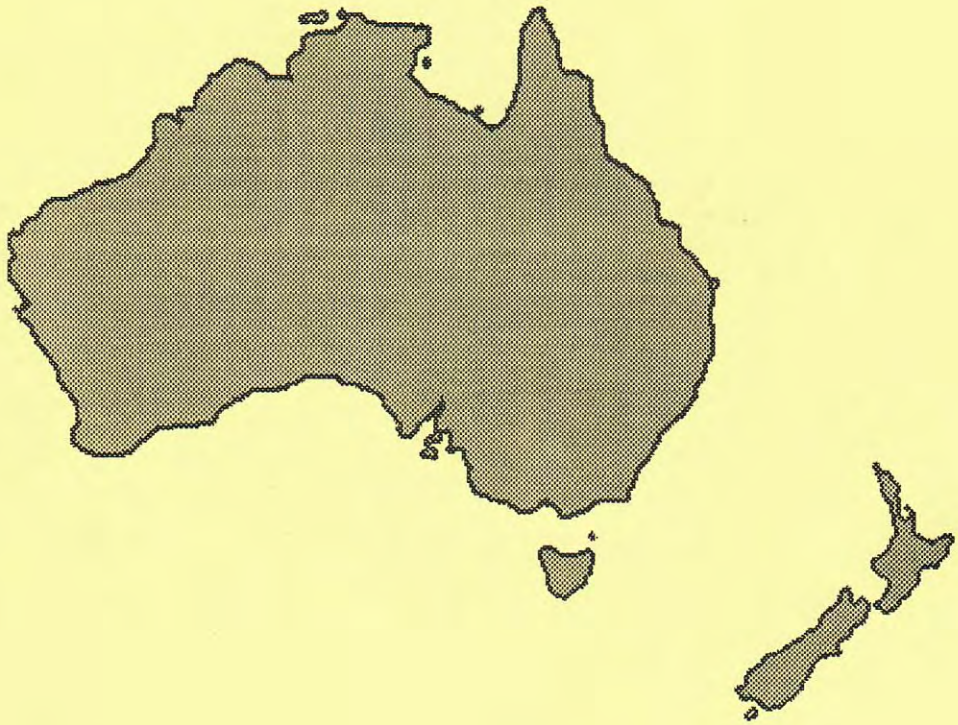
Roderick Melnik*
Dept. of Mathematics & Computing, University of Southern Queensland
& Kate Melnik
Dept. of Computer Science, Flinders University of South Australia

During recent years many problems in microelectronics have become the subject of investigation in applied mathematics providing a wide range of challenging mathematical and computational problems. In this paper we consider one class of such problems arising in computational microelectronics, namely semiconductor device modelling. We present new results obtained on the basis of non-local mathematical models. For such models mobilities of carriers become a function of carrier energy rather than the local value of electric field strength as in the classical drift-diffusion model. Our main results include the construction of effective semi-implicit difference schemes for quasi-hydrodynamic models. Such schemes belong to a wider class of exponential difference schemes that are monotone but not necessarily conservative. We present effective algorithmic realisations of these schemes and investigate their stability. Finally, we present results of computational experiments performed for realistic semiconductor devices such as silicon $p^+ - \nu - n^+$ diode structures. Such devices are widely used as microwave switches in many industrial applications. Our computational results give a quantitative picture of the physical effect of carrier velocity "splash" in the neighborhood of $p - n$ junctions. This effect, that cannot be observed using standard mathematical models of drift-diffusion type, demonstrates the non-local coupling between electric field and effective temperature of carriers. Future development of the presented work is outlined.

The 33rd Australian Applied Mathematics Conference

Lorne, Victoria

2–6 February 1997



ANZIAM'97

Pulse Evolution for Marangoni-Bénard Convection

Tim Marchant
Department of Mathematics
Wollongong University

Marangoni-Bénard convection is the process by which oscillatory waves are generated on an interface due to a change in surface tension. This process, which can be mass or temperature driven, is described by a perturbed Korteweg-de Vries (KdV) equation. For a certain parameter range, this perturbed KdV equation has a solitary wave solution with an unique steady-state amplitude for which the excitation and friction terms in the perturbed KdV equation are in balance. The evolution of an initial $sech^2$ pulse to the steady-state solitary wave governed by Marangoni-Bénard convection is examined. Approximate equations, derived from mass conservation and momentum evolution for the perturbed KdV equation, are used to describe the evolution of the initial pulse into steady-state solitary wave(s) plus dispersive radiation. Initial conditions which form one or two solitary waves are considered. A case where a steady-state solitary wave is never reached, with the wave amplitude increasing without bound, is also considered. The results from the approximate conservation equations are found to be in good agreement with full numerical solutions of the perturbed KdV equation governing Marangoni-Bénard convection.

Numerical Algorithms for First Order PDEs and Markov Chain Approximations

V. Nick Melnik
School of Mathematics
University of South Australia

There exists an intrinsic interconnection between solutions of non-smooth optimal control problems and generalized solutions of partial differential equations which contain a hyperbolic mode. In this paper we deal with generalized solutions of the first order PDE $(1 + v_\epsilon)[\partial\mu_n/\partial x + (\partial\mu_n/\partial t + f_0)/v_\epsilon] = 0$, where v_ϵ is a perturbed velocity of a dynamic system, μ_n is a decision maker function, and f_0 is a goal-dependent mapping $\mathcal{Q} \to \mathcal{B}$. By specifying Cauchy-type initial conditions and assuming that $\mu_n \in L^1(\mathcal{Q})$, this model provides an alternative description for a wide class of non-smooth optimal control problems. We are concerned with the two main questions:

- How a numerical algorithm for the definition of the function μ_n is influenced by the approximate nature of the function v_ϵ in the model itself?
- Can the well-posedness of the model be guaranteed when $n \to \infty$ and $\epsilon \to 0^+$ simultaneously?

It appears that in answering these questions the Markov Chain approximation method plays a decisive role. We argue that in an approximate description of thermodynamic systems, mathematical models occupy an intermediate place between the physical model and the computational model from which numerical algorithms can be derived. In some cases it is important to have a modelling strategy that allows a direct passage from a physical model to an algorithm for which a standard formalization can be readily provided by normal Markov algorithms.

Advance Program

ICPADM'97

5th International Conference on Properties and Applications of Dielectric Materials

May 25-30, 1997

Sheraton Walker Hill Convention Center, Seoul, Korea

SEOUL, KOREA

Organized by

The Korean Institute of Electrical and Electronic Material Engineers

Sponsored by

IEEE Dielectrics and Electrical Insulation Society

11P18 **Characteristics of Ultrafine $(CeO_2)_{0.9}(Gd_2O_3)_{0.1}$ Powders Prepared by the Glycine-Nitrate Process**
Jong-Sun Hwang, Sun-Jae Kim, Hee-Gyun Lee, Yong-Bum Lee, Ho-Yoon Nam (KOREA)

11P19 **AB Initio Simulation Approach for Computing the Effective Dielectric Constant of Random Composite Materials**
B. Sareni, L. Krahenbuhl, A. Beroual, C. Brosseau (FRANCE)

11P20 **Alkali Ion Sensitivity of K, Al implanted Silicon Dioxide**
P. K. Shin, J.T. Kim, Mikolajick, H. Ryssel (KOREA)

11P21 **The Dielectric and Mechanical Characteristics of SiO_2 Filled Epoxy Composites**
K.H. Kim, I.H. Son, M.H Kim, S.K Sin, J. H. Kim (KOREA)

11P22 **Study on the Dielectric Properties of $(Sr.Ca)TiO_3$-based Ceramics for the Capacitor Materials**
Woon-Sik Choi, Jin-Sa Kim, Chung-Hyeok Kim, Joon-Ung Lee (KOREA)

11P23 **Anomalous Properties of a Metal-Unsulator Composite in a Magnetic Field**
A.M. Satanin, V.V. Scuzovatkin (RUSSIA)

11P24 **Nonlinear Behaviour in a Composite with a Periodic Microstructure**
A.M. Satanin, V.V. Scuzovatkin, S.V. Khor'kov (RUSSIA)

13P01 **Intelligent Structures and Coupling in Mathematical Models : Examples from Dynamic Electroelasticity**
Nick Melnik (AUSTRALIA)

13P02 **Dielectric and Electrical Conductivity Studies of Flux Grown $KTiOPO_4$ and $KRbTiPO_4$ Single Crystals**
S. Selvasekarapandian, K. Vivekanandan, P. Kolandaivel (INDIA)

13P03 **Electrooptical Modulation Characteristics of Charge-Addressed Ferroelectric Crystal Spatial Light Modulator**
Liang Zhenxian (CHINA)

13P04 **Study of Dielectric Properties of Strontium Tartrate Tetrahydrate Crystals**
K. Vivekanandan, S. Selvasekarapandian, P. Kolandaivel (INDIA)

13P05 **Dielectric Properties of stabilized Barium Titanate Films**
Sang-Jin Kim, Ki-Joon Kim, Nak-Jin Seong, Joon-Ung Lee, N. Korobova, S. Park (KOREA)

15th IMACS World Congress

on Scientific Computation, Modelling and Applied Mathematics

August 24 – 29, 1997

Hotel Berlin HILTON (Germany)

IMACS
The International Association
for Mathematics and
Computers in Simulation

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Gesellschaft für Informatik e.V.

V. Belogurov (Ukraine)
Methodology of Synthesis of Systems for Water Quality Control and Monitoring

V. Bulitko, G. Bulitko, E. Nikipelova (Ukraine)
About Oscillations of Production Quality in Liquid Deposit Exploitation

D. Prochnow, C. Engelhardt, H. Bungartz (Germany)
Transport and Distribution of the Mean Settling Velocity of Particulate Matter in Rivers

S. Sheshenin (Russia)
Numerical Simulation of Water Filtration in Porous Rock/Soil Media and Related Topics

R.V.N. Melnik (Australia)
Error Dynamics and Coupling Procedures in Mathematical Climate System Models

Title of session: Computer Science
Date: Wednesday, August 27 **Time:** Evening session
Track: XVI

F. de Oliveira-Pinto (Portugal)
Certification of Large Multi-disciplinary Models

M. Korolkov, V. Bykov (Russia)
On Transfer of Fields between Numeric Models in the Course of Multidisciplinary Analysis

A. Anoprienko (Ukraine)
Tetralogic and Tetracodes : An Effective Method for Information Coding

V.V. Emelyanov, S.I. Iassinovski (Russia),
T. Stautmeister (Germany)
The Intelligent Simulation of Complex Discrete Systems

V.N. Kasyanov (Russia)
Formal Methods for Program Reusability

Title of session: Fuzzy Logic - Applications
Date: Thursday, August 28 **Time:** Morning session
Track: I

F.M. El-Khouly, E.E. El-Kholy (Egypt)
Fuzzy Implementation of Indirect Field Oriented Control of Induction Motor Drives

L. Koehl, X. Zeng, C. Vasseur (France)
A Fuzzy Logic based Fractal Dimension Estimators for Profiles

L. Mikhailov (Bulgaria), A. Nabout (Germany), A. Lekova (Bulgaria), F. Fischer (Germany)
Traffic Light Control using Fuzzy Reasoning

A. Nabout, F. Fischer, H.A. Nour Eldin (Germany)
Automated Generation of Fuzzy Rule Base for Complex System Modelling with Experimental Verification for

V. Peneva (Bulgaria)
Modelling of Uncertainities in Decision Making Systems

P. Stanev, E. Enchev, O. Manolov, J. Zaprianov (Bulgaria)
Fuzzy Navigation of an Autonomous Vehicle in Unknown Environment

Title of session: Population Dynamics
Date: Thursday, August 28 **Time:** Morning session
Track: II

K. Addi, A. Gonzalez (France)
Modelling of Vegetation Dynamics Spread

O. Bernard, J.-L. Gouz (Belgium)
Global Qualitative Validation of Biological Models: Application to the Modelling of Phytoplankton Growth

V. Davidov (Ukraine)
Stability Investigation of Biological Models with Delay

E. Endo, Y. Tamura (Japan)
Technological Progress Model of Crystalline Silicon Solar Cells by using Bi-logistic Curve

V.V. Gusarov, I.Yu. Popov (Russia)
On the Stability of Moving Solid/Fluid Interface in "Almost Quasistationary" Approximation

D. Khusainov, N. Nikiforova (Ukraine)
About One Model of Population Dynamics

M. Postan (Ukraine)
Logistic Curve of N-th Order and Compound Growth Modelling

Title of session: Petri Nets I
Date: Thursday, August 28 **Time:** Morning session
Track: III

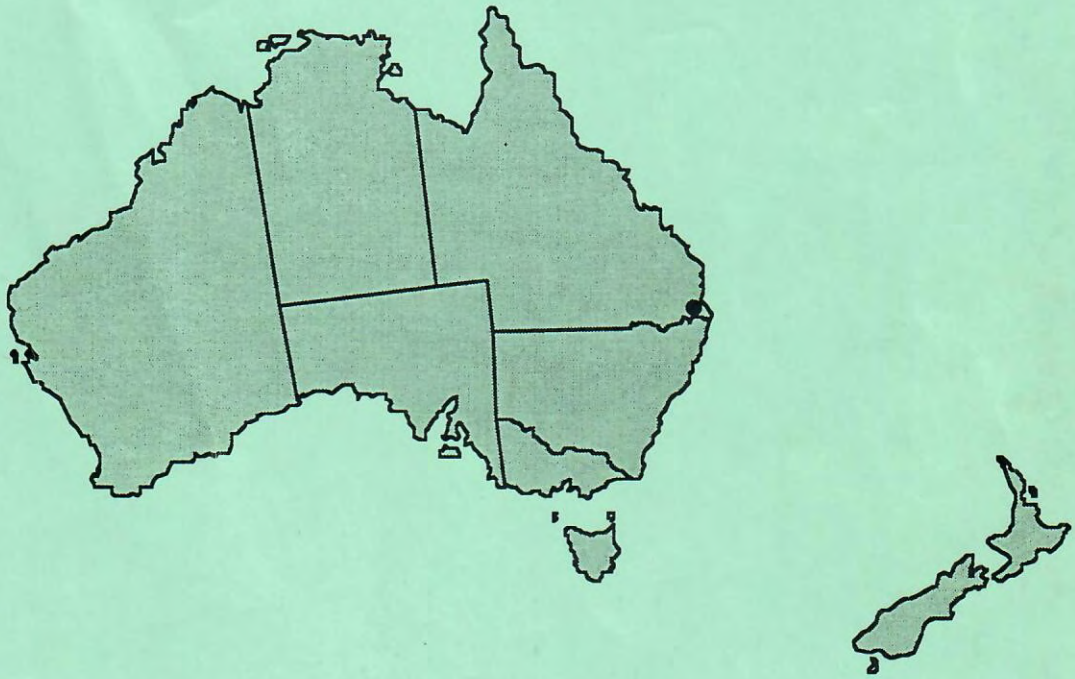
J. Desel, T. Freytag, A. Oberweis, T. Zimmer (Germany)
A Partial-order-based Simulation and Validation Approach for High-level Petri Nets

H. Li, H. Chen, G. Sun (China)
Control Synthesis for Controlled Time Petri Nets with Hard Real-time Deadlines

V.A. Nepomniaschy (Russia)
Distributed System Verification using Net and Program Models

H. Westphal (Germany)
Applying Petri Net based Supervisory Control to Stochastic DEDS

ANZIAM'98
The 34th Applied Mathematics Conference



Coolangatta, Queensland
7–11 February 1998

Australian Mathematical Society
ANZIAM
(formerly the Division of Applied Mathematics)

The 34th Applied Mathematics Conference
Coolangatta, Queensland
7–11 February 1998

ANZIAM'98

ISBN 7259 0869 6

An Arnoldi-Newton Method for Large-Scale Eigenvalue Computations

David Harrar II & Michael Osborne
Centre for Mathematics and its Applications
School of Mathematical Sciences
Australian National University

A composite Arnoldi-Newton method for general eigenvalue problems is discussed. Newton-based procedures for eigenvalue problems are capable of achieving, and even exceeding, the second-order convergence rate so characteristic of Newton's method. However, the methods require good initial data in order to insure not only a satisfactory convergence rate, but to insure convergence at all. In the context of large-scale eigenvalue problems it is often the case that this data is not available.

We propose the use of an Arnoldi method (with restarting, deflation, and shift-invert transformation) to acquire initial eigendata for use in conjunction with the powerful Newton-based procedures. Although the Newton routines are coded using complex arithmetic, we have found that it is generally satisfactory to use an Arnoldi routine which uses only real arithmetic. The computational savings are significant, and the composite method works well. Results are given for applications.

Simulation of Transient Behaviour of Semiconductor Devices with Quasi-Hydrodynamic Models

Hao He & Roderick V. Nicholas Melnik
Department of Mathematics and Computing
University of Southern Queensland

In the last four decades since van Roosbroeck's paper mathematical tools for semiconductor device simulation have been primarily based on the local equilibrium hypothesis and the drift-diffusion model or its modifications. Although *mathematical* investigation of these models has achieved some maturity the models cannot predict important *physical* phenomena such as carrier heating or velocity overshoot. Moving to the next generation of mathematical models in this field means accounting for *non-equilibrium* and *non-local* behaviour of semiconductor plasma. Indeed, in many practically important cases the assumption of thermal equilibrium becomes inappropriate and the difference between carrier temperatures and the lattice temperature has to be incorporated in the dynamics.

The challenge of semiconductor simulation using quasi-hydrodynamic models is two-fold. Firstly, for many devices such as reverse-biased diodes the problem belongs to the class of *singular singularly perturbed problems* which are known to be mathematically difficult. Secondly, challenging computational difficulties arise in software development for such problems. Both these aspects will be addressed in our talk.

Fourth World Congress on Computational Mechanics

Buenos Aires, Argentina
29 June - 2 July, 1998

ABSTRACTS

VOLUME I

International Association for Computational Mechanics

Constructive Approximations of the Convection-Diffusion-Absorption Equation based on the Cayley Transform Technique

Ivan Gavrilyuk
Dept. of Mathematics & Informatics, University of Leipzig, D04109, Germany
& Roderick Melnik*
Dept. of Mathematics & Computing, University of Southern Queensland, QLD 4350, Australia, E-mail: melnik@usq.edu.au

Convection-diffusion-reaction models arise in a wide range of applications and require quite sophisticated mathematical tools for their rigorous study. Indeed, to describe a reactive flow one has to take into account both, atomic and molecular level processes (such as diffusion transfer and chemical reactions), as well as collective phenomena (such as convection and wave processes). It is coupling between macro- and micro-levels of description that brings a major challenge to the investigation of convection-diffusion-reaction models.

In this paper we study one such model described by the nonstationary convection-diffusion-absorption equations. A quite natural approach to the solution of such problems is to use the domain decomposition method (DDM). When applied to nonstationary problems such a technique is often used in conjunction with an implicit-in-time discrete differentiation. Unfortunately, this leads to a gradual deterioration of accuracy due to the necessity of inverting certain operators associated with the problem at each time step. The same can be said about spectral and pseudospectral techniques when finite differences are used for temporal discretisation. As an alternative, during recent years attempts have been made to construct DDMs with no iterations for nonstationary problems. Such methods employ the idea of a dynamic adaptation of the computed solution to the smoothness of initial data. This idea is developed further in this paper. Recently, the first author with his collaborators established a one-to-one correspondence between the continuous initial value problem for some classes of differential equations and certain discrete initial value problems. Such a correspondence, that is essentially based on the Cayley transform technique, allows us to develop an effective numerical procedure for the solution of unsteady convection-diffusion-absorption problems. Error estimates and the results of numerical experiments will be presented.

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Printed in Santa Fe, Argentina, on March 1998 by
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CTAC99

Computational Techniques and Applications Conference and Workshops

20–24 September 1999
Australian National University
Canberra ACT 0200 Australia

Numerical Modelling of Thermoelastic Processes Using Nonlinear Theories With Thermal Relaxation Time

R.V.N. Melnik*
CSIRO Mathematical and Information Sciences, North Ryde
Roderick.Melnik@cmis.csiro.au
D.V. Strunin and A.J. Roberts
University of Southern Queensland

Abstract

A nonlinear model of thermoelasticity is solved for a ring-shaped body with special attention given to the effect of relaxation time on the body dynamics. A spectral Galerkin method is used to accurately resolve spatial structures of temperature and displacement. A sequence of solutions is obtained for gradually increasing initial amplitude of the thermoelastic wave, showing a transition from a steady harmonic wave to singular solutions. Larger values of the relaxation time are shown to result in smoother temperature profiles. The dynamics generated by a localized heat release from an external source is studied. A regime is observed in which the source excites a standing wave of the displacement while the temperature monotonically decays.

ANZIAM'99
The 35th Applied Mathematics Conference

Mollymook, NSW
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The 35th Applied Mathematics Conference
Mollymook, NSW
7–11 February 1999

ANZIAM'99

ISBN 7259 0869 6

Pollen: where does it go, where is it from?

Robert McKibbin
Institute of Fundamental Sciences, Massey University
Private Bag 11-222, Palmerston North, New Zealand

The destination of particulate material which is moved by a fluid often generates concern for environmental reasons. While the motion of solid particles such as dust and smoke components generated in industrial environments and sand from marine dredging operations are considered to be polluting because they are human-generated, there is no less concern about ash from volcanic eruptions and forest fires, and dust- and sand-storm fall-out. But some wind-borne particles are both natural and life-continuing rather than life-threatening; pollen from trees is one example. Although today's pollen may cause inconvenience to hay-fever sufferers, yesterday's can provide information on historical plant distribution through fossil deposits.

In this talk I describe some mathematical (advection-dispersion) models that can be used to describe wind-dispersed pollen and seed deposition patterns, and discuss some analytical and numerical solutions for pollen sources with simple geometry. The inverse problem of deducing source distribution from deposit patterns is briefly considered. The methods are also applicable to other wind-distributed particles.

Modelling Shape-Memory-Alloy Phase Transitions

Roderick V. N. Melnik, Anthony J. Roberts & Kerryn A. Thomas
Department of Mathematics and Computing,
University of Southern Queensland, QLD 4350

After being permanently deformed some metallic alloys can recover their original shapes upon the change of thermal conditions. During recent years this property, known as the shape memory effect, has been a subject of active research in the mathematical and engineering communities.

One of the major challenges in this field is to adequately describe structural phase transitions between different equilibrium configurations (austenite and martensite) of the metallic lattice of shape memory alloys (SMA). Since we have to deal with qualitatively different stress-strain relations in different temperature ranges, it is important to take account of the coupling between the mechanical and thermal fields in the mathematical description of the SMA dynamics (see Melnik & Roberts, *Approximate Models of Dynamic Thermoviscoelasticity Describing Shape-Memory-Alloy Phase Transitions*, in New Methods in Applied and Computational Mathematics, 1998). In this talk we present results of computational experiments on mechanical and thermal controls of phase transformations in a Cu-based shape-memory-alloy core.

ICIAM 99

the Fourth
International Congress
on Industrial and
Applied Mathematics

Final Programme

Edinburgh
SCOTLAND

5-9 July 1999

16.00 – 18.00 Contributed Presentations: Lectures

C-8 Adam Ferguson Building, Room 13

Partial Differential Equations II

Chair(s): CONSTANTIN; GRANDGIRARD

16.00–16.15 MELNIK, Roderick V N (University of Southern Queensland, Australia) *Mathematical and numerical analysis of hyperbolic models for shape-memory alloys* (p. 287)
16.15–16.30 MICHIELSEN, Bas L (ONERA, France) *A boundary integral equation for high frequency electromagnetic scattering problems* (p. 287)
16.30–16.45 CONSTANTIN, Adrian (University of Zurich, Switzerland) *Wave breaking in shallow water* (p. 249)
16.45–17.00 PASQUALI, Aldo (University of Florence, Italy) *Numerical simulations for ring spinning process* (p. 297)
17.00–17.15 LAI, Choi-Hong (University of Greenwich, UK) *An acoustic expansion method for the retrieval of noise signals in unsteady flow* (p. 283)
17.15–17.30 WANG, Hwai-Chiuan (Department of Mathematics, National Tsing Hua University, Hsinchu, Taiwan) *Semilinear elliptic problems in interior and exterior flask domains* (p. 325)
17.30–17.45 GRANDGIRARD, Virginie (Association Euratom-CEA, France) *Free boundary Tokamak plasma equilibrium computation in an infinite domain* (p. 264)
17.45–18.00 LUDWIG, Bruno (AEROSPATIALE Centre Commun de Recherches, France) *Boundary integral equations for the problem of acoustic scattering by an absorbing obstacle* (p. 285)

C-9 Adam Ferguson Building, Room 14

Dynamical Systems I

Chair(s): HABERMAN; FISCHER

16.00–16.15 BOOKER, Stuart M (Department of Mathematics, University of Dundee, UK) *Effective disruption of nonlinear electronic sub-systems* (p. 242)
16.15–16.30 STAEMPFLE, Martin (University of Glasgow, UK) *Computing the flow of dynamical systems with adaptive triangulation methods* (p. 313)
16.30–16.45 HABERMAN, Richard (Southern Methodist University, USA) *Slow passage through a saddle-center bifurcation* (p. 267)
16.45–17.00 VARLAMOV, Vladimir V (Departamento de Matematicas, Escuela Colombiana de Ingenieria, Bogota, Colombia) *Long-time asymptotic expansion for the Kuramoto-Sivashinsky equation in a disk* (p. 322)
17.00–17.15 SLEPYAN, Leonid I (Tel Aviv University and Institute for Industrial Mathematics, Israel) *Dynamic factor in impact, phase transition and fracture* (p. 311)
17.15–17.30 FENG, Bao-Feng (Kyoto University, Japan) *Numerical computation for stationary travelling-wave solutions of the Kuramoto-Sivashinsky equation: A rational spectral approach* (p. 259)
17.30–17.45 FISCHER, Oliver (Bilfinger + Berger Bauaktiengesellschaft, Germany) *Non-linear dynamic behaviour of inclined suspended cables* (p. 259)
17.45–18.00 AKHMETOV, Marat (West Kazakhstan Economical and Financial Institution, Kazakhstan) *The comparison method for vibroimpact mechanisms* (p. 234)

C-10 Adam Ferguson Building, Room 17

Optimization I

Chair(s): MULHOLLAND; FREDENHAGEN

16.00–16.15 SADOVSKI, Alexey L (Texas A&M University-Corpus Christi, USA) *A game approach to the solution of nonsmooth problems of mathematical programming* (p. 306)
16.15–16.30 BAUMANN, Helge (University of Hamburg, Germany) *Aeroassisted orbit transfer with finite thrust* (p. 241)
16.30–16.45 MULHOLLAND, Anthony J (Department of Mathematics, Glasgow Caledonian University, Glasgow, UK) *Fractal simulated annealing* (p. 290)
16.45–17.00 SØRENSEN, Allan (The Maersk Mc-Kinney Moller Institute for Production Technology, Odense University, Denmark) *A dynamical approach to global optimization* (p. 312)
17.00–17.15 GUHL, Florent (Cemagref, France) *Continuity constraint in optimization of water supply* (p. 265)
17.15–17.30 CONSTANS, Sophie (Cemagref de Bordeaux, France) *Linear formulation for optimizing disinfectant concentrations in water distribution networks* (p. 249)
17.30–17.45 FREDENHAGEN, Sigrid (Institute for Applied Mathematics, University of Hamburg, Germany) *Constrained nonlinear spline-interpolation* (p. 260)
17.45–18.00 VILAIN, Claire (INRIA, France and DIM, Chile) *Optimal power flow problem with parallelization of the security's constraints* (p. 323)

ICIAM 99

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Book of Abstracts

Edinburgh
SCOTLAND

5-9 July 1999

MCKINLEY, Iain S (University of Strathclyde, Glasgow, UK)

Stability of a ridge subject to a jet of air

In this paper we consider the linear stability of a thin ridge of fluid on a planar substrate subject to a jet of air acting normally to the substrate. We investigate two cases: one in which the jet acts at the centre of the ridge and one in which the jet is off-centre. The results of our numerical calculations are described and the conclusions of our previous quasi-static analysis of this problem are reviewed in the light of these new results. This is a joint work with Dr S K Wilson and Dr B R Duffy, University of Strathclyde, Glasgow, UK.

MEHRI, Bahman (Department of Mathematical Sciences, Sharif University Of Technology, Tehran, Iran)

Numerical solution of Neumann problem for a nonlinear Poissons equation

The following boundary value problem is considered $\nabla u = u^{\alpha}$, $0 < \alpha < 1$, in D and $\frac{\partial u}{\partial n} = g$ on ∂D we shall use finite element and boundary element methods to solve the above problem for the cases where D is a circular or an elliptical region.

MELNIK, Roderick V N (University of Southern Queensland, Australia)

Mathematical and numerical analysis of hyperbolic models for shape-memory alloys

Using the Leray-Schauder principle we analyse the well-posedness of a general nonlinear model of hyperbolic thermoviscoelasticity describing the dynamics of shape-memory alloys. The model, based on a coupled system of nonlinear partial differential equations, accounts for finite speeds of thermal disturbances by a constitutive relationship implicitly determined from the Cattaneo-Vernotte equation. By a reduction of the model to a system of differential-algebraic equations, we develop an efficient numerical algorithm for the solution of the problem. Computational results on the analysis of thermally and mechanically induced phase transitions in a shape-memory-alloy rod are presented This is a joint work with A J Roberts and K A Thomas.

MELROSE, Gordon (Old Dominion University, Norfolk, USA)

The bending problem for a simply supported strip with internal supports

The problem considered is to determine the stress distribution when a finite width rectangular plate, simply supported along its long edges, and with a pair of collinear internal supports perpendicular to these edges, is subjected to an applied load. Through standard techniques and superposition, the problem is reduced to a mixed boundary value problem, which in turn can be reformulated in terms of a hypersingular integral equation. The integral equation is solved numerically by expanding in terms of Gegenbauer polynomials.Numerical results showing the stress concentration at the ends of the internal supports are given.

MICHELETTI, Stefano (Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milan, Italy)

Mixed finite volumes for advanced transport models in semiconductors

In this communication we deal with the two-dimensional numerical simulation of semiconductor devices using advanced transport models. We propose efficient and accurate solvers based on the use of cell-centred Mixed Finite Volume methods derived from the Raviart-Thomas finite elements of lowest degree. This ensures strong conservation of electric field, current and energy fluxes, while nonnegativity of the concentrations and temperatures of the carriers is achieved through a suitable extension of the Scharfetter-Gummel method. Numerical results to validate the newly proposed stabilized method are provided. In particular, a complete electric characterization is carried out for a realistic state-of-the-art n-MOS transistor. This is a joint work with Riccardo Sacco, Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milan, Italy.

MICHIELSEN, Bas L (ONERA, France)

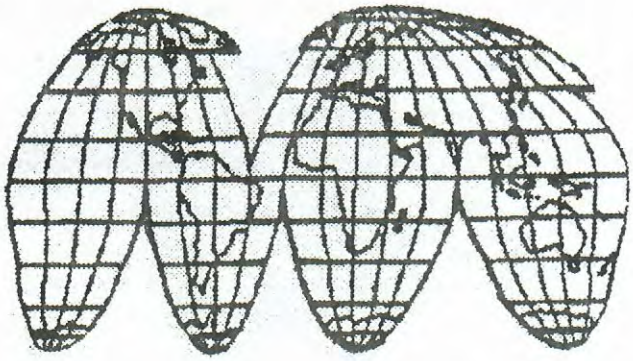
A boundary integral equation for high frequency electromagnetic scattering problems

We show uniqueness and existence for a boundary integral equation for electromagnetic scattering problems. The equation is a kind of generalised combined field integral equation based on a parametrix having the same principal symbol as the Dirichlet-to-Neumann operator of the boundary. We benefit from the high frequency localisation of the latter operator to obtain sparse systems upon discretisation. A modified version of the equation is shown to have asymptotically vanishing interactions between "hidden faces," which makes the coefficient matrices even sparser.

ABSTRACTS

of Invited Lectures and Short Communications
Delivered at

THE TENTH INTERNATIONAL COLLOQUIUM ON DIFFERENTIAL EQUATIONS



Plovdiv, Bulgaria, August 18-23, 1999

Mathematical and Numerical Analysis of Falk-Konopka-Type Models for Shape-Memory-Alloys

Roderick V. N. **Melnik**, Anthony J. Roberts & Kerryn A. Thomas

Mathematical Modelling & Numerical Analysis Group,
Department of Mathematics and Computing,
University of Southern Queensland, QLD 4350
E-mail: melnik@usq.edu.au

Keywords: dynamic thermoviscoelasticity, coupled systems, hyperbolic approximations, shape-memory alloys.

AMS Subject Classification: 35M10, 35L70, 65P05, 73F15.

This paper contributes to the development of mathematical theory of thermomechanical phase transitions in solids, in particular in shape-memory alloys. After being permanently deformed these materials can recover their original shapes upon the change of thermal conditions. This property, known as the shape-memory effect, has a wide range of applications such as solid-state heat engines, actuators, work production devices, shape-memory implants, automotive and aerospace applications.

One of the major challenges in this field is to adequately describe structural phase transitions between different equilibrium configurations of the metallic lattice of shape memory alloys. Mathematically the problem can be formulated as a strongly nonlinear system of partial differential equations that couples mechanical and thermal fields. We analyse two such models. The first model is a one-dimensional hyperbolic approximation of shape-memory-alloy dynamics, derived in our earlier paper (in New Methods in Applied and Computational Mathematics, 1999). The second model is a low-dimensional model obtained from the 3D Falk-Konopka model using centre manifold techniques. The results of the theoretical analysis are supported by computational experiments which we shall discuss.

European Control Conference ECC'99

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European Control Conference ECC'99

31. August - 3. September 1999
Karlsruhe, Germany

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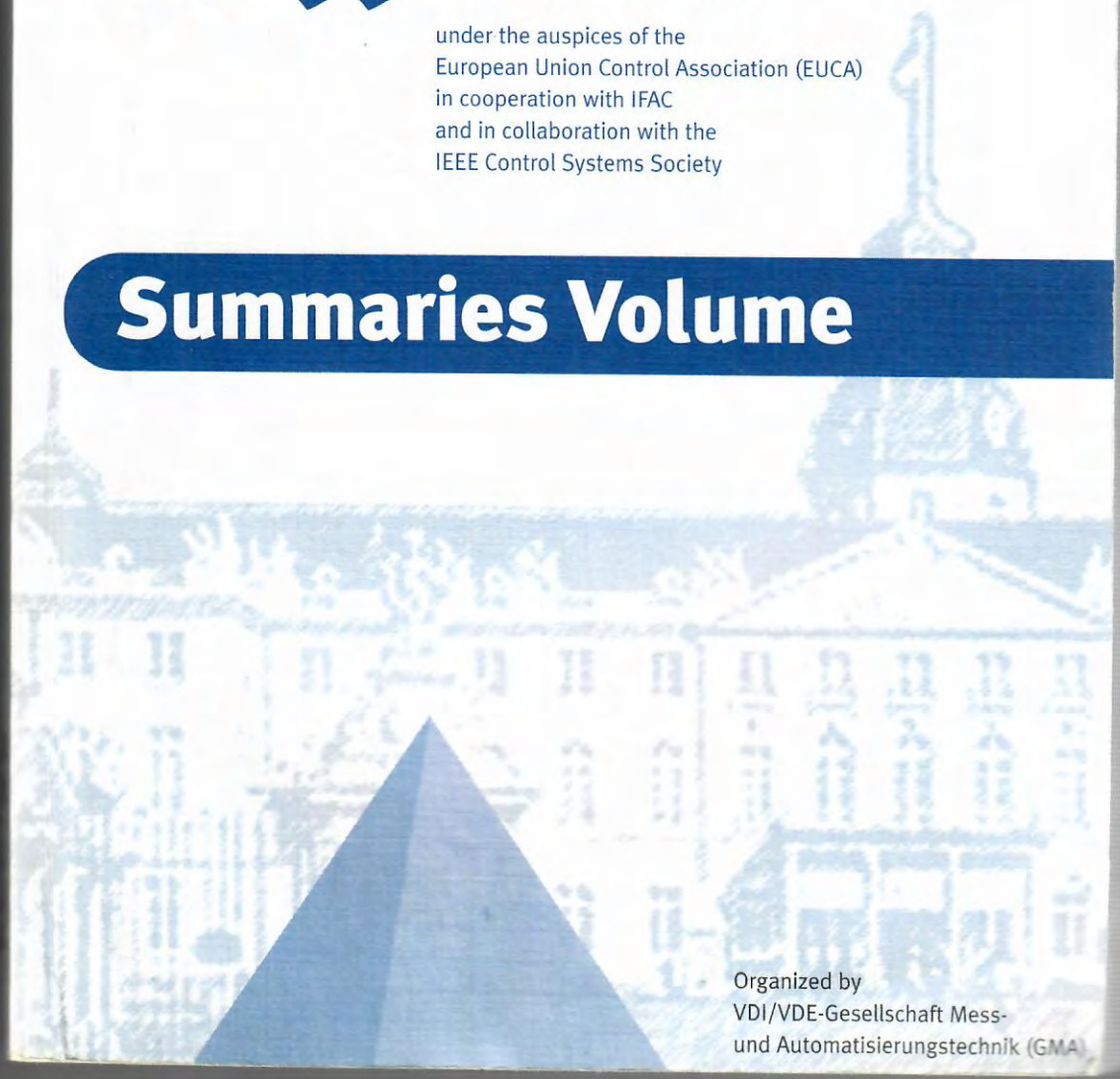
Summaries Volume



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European Control Conference 1999

31. August - 3. September 1999
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Sessions AM: Tuesday, A

Session AM-1:
H-Infinity Control .....

Session AM-2:
Stability I .....

Session AM-3:
Identification I .....

Session AM-4:
Nonlinear Controller Design Method

Session AM-5:
Model-Based Fault Diagnosis: New
(Invited Session) .....

Session AM-6:
Hybrid Systems I: Modelling .....

Session AM-7:
On-Line Process Supervision and Fa

Session AM-8:
Nonlinear Observer Design .....

Session AM-9:
Linear Systems I .....

Session AM-10:
Modelling and Control of Wastewa

Session AM-11:
Nonlinear Systems: Filtering, Robus

Session AM-12:
Target Tracking (Invited Session) .....

Session AM-13:
Variable Structure and Sliding Mod

Session AM-15:
Analysis of Nonlinear Systems .....

APPROXIMATE MODELS FOR NONLINEAR CONTROL AND HAMILTON-JACOBI-BELLMAN EQUATIONS IN NON-REFLEXIVE BANACH SPACES

R.V.N. Melnik

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Non-smooth dynamic systems appear in many applications of control and games theory. By constructing mathematical models in these fields we often have to deal with evolutionary partial differential equations (PDE), solutions of which are not smooth enough to satisfy these equations in the classical sense. A classical example is provided by Hamilton-Jacobi-Bellman (HJB) equations that approximately describe dynamics of value/cost functions which may not be differentiable everywhere. These equations can be formally derived by applying Bellman's dynamic programming approach in a heuristic manner, and much research in control theory has been devoted to the clarification of the connection between this approach and the Pontryagin maximum principle in the non-smooth and stochastic cases. This paper is devoted to the analysis of this connection under relaxed smoothness requirements in non-reflexive Banach spaces and to the approximation of HJB equations in these spaces.

The author proposes a unified treatment of non-smooth and stochastic control problems using mathematical models of HJB-type obtained with Steklov's operator technique. Until recently, the analysis of such models has been predominantly conducted in reflexive Banach spaces. The situation has changed since the introduction of the L^1 control theory. Due to new and emerging applications of control systems in engineering, non-reflexive Banach spaces play an increasingly important role in the control theory context. Non-reflexive Banach spaces become the most reasonable functional classes for perturbations in such problems where control systems have to work in a dynamic and uncertain environment. This paper contributes to the construction and the analysis of approximate PDE models for the description of control systems in such situations.

ADAPTIVE COORDINAT
MANIPULATORS FOR
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Summary

The paper presents solution of two mutually
mathematical model of multiple rigid robot
dynamic object of which the motion is constrai
synthesis of an adaptive control of multiple
papers published up to now the assumption tha
object and the environment has been widely
surfaces, and since most real contact surfaces d

The model of multiple rigid robot manipulator
of which the motion is constrained by a dynam
motion. The manipulator dynamics, the objec
account. The coordinated robots have to simu
along a predetermined known trajectory on th
force on the environment, (iii) keep the valu
maximum. The main idea used in the mod
connections with the multiple manipulators a
system of elasstically connected rigid bodies,
gravitational, damping and elasticity forces
mathematical model the adaptive control of m
synthesized. The proposed adaptive control la
model is known, but when there is uncertainty
about their nominal values. The proposed a
structure and is composed of two parts: (i) an
the multiple robots and/or object parameters, a
which is a function of the parameters identifi
theory, a theorem which proves the parameter
when the proposed adaptive control law is imp

Simulation results which verify the proposed a
in the constrained motion tasks are performed.

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eXtensible Multi-Dimensional Simulator

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As computational power increases so does the use of numerical algorithms for solving complex problems. The disciplines of physics and engineering provide many such problems requiring solutions to non-integrable nonlinear differential equations. Of common interest is the propagation of Parabolic differential equations of the form shown in Equation 1:

$$\partial_t \mathbf{A}(t, \mathbf{x}) = \mathcal{L}_{\mathbf{x}}[\mathbf{A}] + \mathbf{U}[\mathbf{A}] \,, \tag{1}$$

where $\mathbf{A}$ is a real or complex vector field which is a function of transverse coordinates $\mathbf{x}$ and propagation coordinate t, $\mathcal{L}_{\mathbf{x}}$ is a linear differential operator in $\mathbf{x}$, and $\mathbf{U}$ is some functional (possibly nonlocal in t and/or $\mathbf{x}$) of $\mathbf{A}$.

The range of problems that can be modeled by equations of this form is not small, and often the resulting numerical algorithms are computationally intensive. Computational efficiency becomes paramount, and compiled low level code (e.g. 'f77' or 'C') dedicated to the problem is in some cases an order of magnitude faster in execution than a more high level script (e.g. Matlab). But not every scientist or mathematician can be expected to be an expert low level code writer, and even then constantly rewriting or modifying code to jump from problem to problem is error prone and generally not an efficient use of their time.

XMDS is the acronym for the software package 'eXtensible Multi-Dimension Simulator' which was created to solve this problem: *XMDS transforms a high level problem description into efficient low level source code in instances where the problem is expressible in the form of Equation 1.* XMDS reads an input script file describing the problem to be modeled and then writes low level source code ('C') specifically dedicated to solving this problem. A 'C' compiler is then called to build the executable. At the heart of XMDS is the split step central difference propagation method developed by Drummond [1].

XMDS is also equipped to handle problems involving multiplicative Gaussian noises, and can implement multiple trajectories to yield mean evolution and variances. Further, XMDS is designed to be web friendly, with the input script written in XML [2] (and designed to be human readable/writable), and input/output field data written in XSIL [3], which itself is a from of XML. Utility programs can then convert XSIL formats to other formats for plotting purposes.

A prototype XMDS package has been developed and already proves to be versatile and computationally efficient, and a full initial release of this software is anticipated by the end of the year.

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Computational Analysis of Coupled Physical Fields in Piezothermoelastic Media

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Many new challenging problems in science, engineering and industry cannot be solved efficiently without invoking a *unification* of two or more physical theories that have been traditionally considered separately [1]. A classical example of such a situation is dynamic thermoelasticity where on the basis of thermodynamic theory of irreversible processes two physical theories, the elasticity theory and theory of heat conduction, are treated as a unified whole [2]. In response to a huge potential of electromechanical systems in aerospace, automotive, medical, and consumer-goods manufacturing industries, and due to an increasing interest in applications of smart materials and structures in a variety of fields, the development and applications of *physical models* that account for the coupling between thermal, mechanical, and electric fields become essential prerequisites for further technological success in these important areas.

In this paper the main focus is on computational aspects of a *dynamic model* of thermopiezoelasticity. Although the development of models capable of describing unsteady behaviour of "smart" materials (i.e. piezoceramics) has fundamental importance in many areas of applications, most studies performed in this field hitherto have dealt with stationary problems only [3]. The model under consideration in this paper is an extension of a coupled dynamic system for piezoelectrics [4] and includes the equation of motion, the Maxwell equation for electric field, and the energy balance equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \sigma_{ji,i} + F_i, \quad D_{i,i} = f_2, \quad T\frac{\partial S}{\partial t} = -q_{i,i} + Q, \quad i, j = 1, 2, 3,$$

where u_i are components of the mechanical displacement vector, ρ is the density of the material, σ_{ij} is the stress tensor, D_i are electric displacements, θ is the difference between the current, T, and the reference temperature, T_0 (i.e. $T = T_0(1 + \theta/T_0)$), F_i are components of the vector of mass forces, f_2 is the electric charge density, S is the system entropy, $\mathbf{q} = (q_1, q_2, q_3)$ is the heat influx through the system surface, and Q is the energy due to heat generation inside of the body. In contrast to [4], the full thermo-electromechanical (rather then electromechanical only) coupling is considered by employing a general form of the state equations.

Using an efficient computational algorithm developed for the solution of this problem, the effects of dynamic coupling and thermally-induced non-linearities are demonstrated for *finite piezoelectric elements* of cylindrical shape with hexagonal 6mm symmetry.

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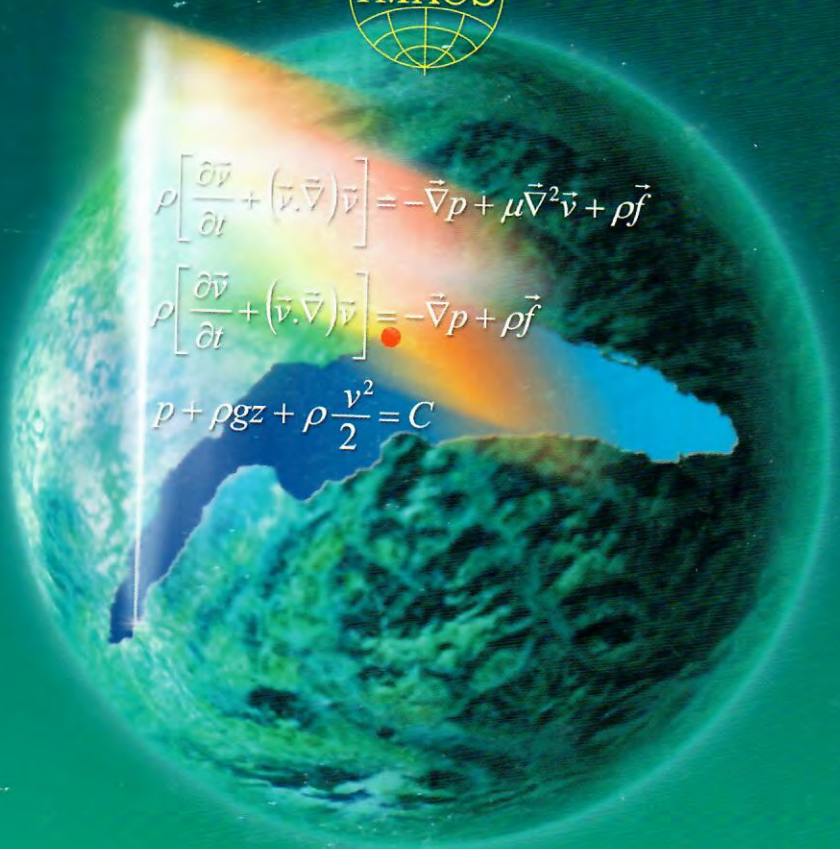

Session code:	**141**
Title:	**Nonlinear Wave Equations**
First organizer:	*Thiab R. Taha*
Institution:	*University of Georgia - USA*
Second organizer:	*Athanasios Bratsos*
Institution:	*Technological Educational Institution (T.E.I) of Athens - Greece*

Day	Time	Author(s)	Title
Wednesday	10:00	R. Melnik D.V. Strunin A.J. Roberts	**Numerical Analysis of the Behaviour of Rubber-Like Polymers with Hyperbolic Models of Nonlinear Thermoelasticity**
Wednesday	10:30	D. Fotiadis C.V. Massalas	**Wave Propagation in a Long Human Bone of Arbitrary Cross Section with a Cavity Filled with an Incompressible Viscous Fluid**
Wednesday	11:00	A.G. Bratsos Thiab R. Taha	**A Parametric Linearized Finite-Difference Method for the Solution of the Nonlinear Cubic Schrödinger Equation**
Wednesday	11:30	Otis Wright M. G. Forest K. T.-R. McLaughlin	**Some Riemann-Green Functions for the Geometric Optics Approximation of the Defocusing Nonlinear Schrödinger Equation**
Wednesday	12:00	D.A. Karpeev Constance M. Schober	**Generating Functions and Symplectic Integrators for Nonlinear Schrödinger systems**
Wednesday	12:30	M. S. Ismail Thiab R. Taha	**Finite Element Method for the Coupled Nonlinear Schrödinger Equation**
Wednesday	16:00	Drumi D. Bainov Dimitar A. Kolev	**Conditions Stimulating Blowing-up Behaviour of the Solution to an Impulsive Reaction-Diffusion Model**

C.P. Code:	**799**
Track:	**Special session**
Topic:	**Modelling and Algorithms**
Chairman	
Name:	*Michel Deville*
Institution:	*EPFL - DGM - Switzerland*
Name:	*M. Grote*
Institution:	*ETH Zürich - Switzerland*

Day	Time	Author(s)	Title
Thursday	12:00	R.V.N. Melnik A. Uhlherr J.H. Hodgkin F. de Hoog	**Applications of Distance Geometry Algorithms to Atomistic Simulation of Polymer Systems**
Thursday	12:30	Y. N. Radayev	**On the Principal Line Theory of Strain-Damage Coupled Equations and its Application to Near Crack Tip Localization Analysis**
Thursday	16:00	Constance M. Schober	**Spatiotemporal Chaos in Near-integrable PDE's**
Thursday	16:30	Sergei F. Yashkov	**Modelling Processor Sharing Queue**
Thursday	17:00	D. A. Beard	**Macroscopic Model of a Protein-DNA Complex: The Chromatin Fiber**
Thursday	17:30	Alexandre Kovalev	**On the Stability of Some Nonlinear Difference Equations of Lotka-Volterra Type**
Friday	11:00	L.E. Garey R.E. Shaw	**Solving Volterra Two-point Boundary Value Problems with Natural Auxiliary Conditions**

BOOK OF ABSTRACTS

Lausanne - Switzerland

August 21-25, 2000

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Edited by
Michel Deville
Robert Owens

EPFL
ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

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Michel Deville
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In cooperation with:
Mario Romanò
Liam Dawson
Anna Berg

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Preface

The 16th IMACS World Congress on Scientific Computation, Modelling and Applied Mathematics held in Lausanne, Switzerland, from August 21 to August 25, 2000 is sponsored by IMACS (The International Association for Mathematics and Computers in Simulation), the Swiss National Science Foundation, the Latsis Foundation, the Swiss Federal Institute of Technology Lausanne (EPFL). Industrial sponsors are Compaq, Swissair and UBS Lausanne. The city of Lausanne is also acknowledged for its generous support.

The Congress is hosted by CAPA: the Center for Advanced Parallel Applications, involving twenty-three research units within nine departments of the EPFL. Co-sponsors of the Congress are CAIMS-SCMAI (Canadian Applied and Industrial Mathematics Society), CASS (The Chinese Association for System Simulation), ESF (European Science Foundation), GAMM (German society for Applied Mathematics and Mechanics), GAMNI (Groupe pour l'Avancement des Méthodes Numériques de l'Ingénieur), GI (Gesellschaft Informatik), GMD (German National Research Center for Information Technology), HMS (Greek Mathematical Society), IFORS (International Federation of Operations Research Societies), IMA (The Institute of Mathematics and its Applications), ISGG (International Society of Grid Generation), JSST (Japan Society of Simulation Technology), MSSANZ (Modelling and Simulation Society of Australia and New Zealand), SIMAI (Società Italiana di Matematica Applicata ed Industriale), SMAI (Société de Mathématiques Appliquées et Industrielles), SMS (Swiss Mathematical Society), VKI (von Karman Institute for Fluid Dynamics), WNW (Werkgemeenschap Numerieke Wiskunde (Dutch-Flemish Numerical Analysis Community).

Over the last four decades, it has become an established tradition for a broad international community of experts from different fields to gather at IMACS world congresses. This Congress follows this IMACS tradition. About eight hundred scientists from all over the world will present and discuss new results in theory, methodology, software and applications related to basic research and industrial applications. As multi-physics simulation develops and broadens the range of possible applications, the multi-disciplinary aspects of the present trends in research are highlighted. The Congress is also a forum for informal discussion and for interactive exchange.

The proceedings on CD-Rom include keynote speakers, papers collected by session organisers who brought together scientists they knew in their own field, and finally the accepted contributed papers. The papers are presented under the various sections indicated in the table of contents. The general topics cover: 1. *Computational mathematics* 2. *Numerical mathematics* 3. *Computational physics, chemistry and biology* 4. *Artificial intelligence and computer science* 5. *Systems engineering* 6. *Application in modelling and simulation.*
Many thanks are due to many people. I would like to begin by mentioning the members of the International Program

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In the organising process and in the reviewing of the many papers we received, the help of the Local Committee has been greatly appreciated:
Alain Clappier
Giovanni Coray
Dimitris Kiritsis
Thomas Liebling
John Maddocks
Robert Owens
Leopold Pflug
Alfio Quarteroni
Michel Rappaz
Laurent Villard.

A very special thank to Rob Owens who worked a lot for the session organisation and the call for contributed papers. His skills in science and in communication were of prime help.
A special thank goes to Professor Robert Vichnevetsky, President of IMACS, who is acting as Honorary Chair of the Congress. His involvement and cooperation at each step of the Congress preparation were much appreciated.
Special thanks go also to the many session organizers. Through them and with them, we were able to set up a very nice scientific Congress programme which includes top level papers and presentations.

The Tourism Office of the City of Lausanne was a major partner in the accomodation organization dealing with smiling effiency to meet all participants requirements for hotel booking, travel arrangements, information, etc. For all that background work which is important for the success of a large conference, we thank the Tourism Office.

The daily organisational work has been carried out at EPFL by three key persons. Mario Romanò designed the Web site of the Congress. This was a première for an IMACS Congress. The decision to go on with Internet technologies made the Congress visible on the global scale and launched IMACS Congresses on the Web. The Lausanne Congress will be remembered for that innovation. Liam Dawson has been the Secretary of the Congress since the very beginning. Anna Berg joined the team later when it was recognised that with only two staff-members, we would not make it. The tireless zeal of everyone, the long hours spent in front of terminals, PC's and on the phone made possible the accomplishment of this conference. The personal involvement of everyone gave the impetus all along the (rocky) road. For that, I thank you heartily.

During the conference, a special day will be held to inaugurate the Swiss-T1 computer which is based on commodity technology and on an interconnect technology, the T-Net made by the Swiss company, Super Computing Systems. This day will celebrate an achievement of a technological research project aimed at parallel hardware for numerical simulation and associated large scale applications. It will also show the feasibility of such machines.

As a scientific congress is always a catalysing event, involving culture, sciences and culinary sensations, we will relish the banquet during a boat ride on the Geneva Lake, and delight in a concert with the "Orchestre Symphonique du Mont-Blanc", performing classical music in the Métropole Hall, sponsored by Compaq. I hope that each attendant will enjoy these unique moments, realising that such a combination of events renders the life of researchers and scientists very rewarding.

Michel Deville,
General Chair of the Congress.

Code session: 141
Nonlinear Wave Equations

A.G. Bratsos, Thiab R. Taha
A Parametric Linearized Finite-Difference Method for the Solution of the Nonlinear Cubic Schrödinger Equation 176

R. Melnik, D.V. Strunin, A.J. Roberts
Numerical Analysis of the Behaviour of Rubber-Like Polymers with Hyperbolic Models of Nonlinear Thermoelasticity 177

Otis Wright, M.G. Forest, K.T.-R. McLaughlin
Some Riemann-Green Functions for the Geometric Optics Approximation of the Defocusing Nonlinear Schrödinger Equation 176

D.A. Karpeev, Constance M. Schober
Generating Functions and Symplectic Integrators for Nonlinear Schrödinger Systems 180

M. S. Ismail, Thiab R. Taha
Finite Element Method for the Coupled Nonlinear Schrödinger Equation 180

Drumi D. Bainov, Dimitar A. Kolev
Conditions Stimulating Blowing-up Behaviour of the Solution to an Impulsive Reaction-Diffusion Model 180

D. Fotiadis, C.V. Massalas
Wave Propagation in a Long Human Bone of Arbitrary Cross Section with a Cavity Filled with an Incompressible Viscous Fluid 178

Code session: 150
Tools, Programming Environments and Algorithmics for Parallel Processing

J. Abella, S. A. Ali Touati, A. Anderson, C. Ciuraneta, J. M. Codina, Min Dai, C. Eisenbeis, G. Fursin, A. González, J. Llosa, M. O'Boyle, A. Randrianatoavina, J. Sánchez, O. Temam, X. Vera, G. Watts
MHAOTEU Tools for Memory Hierarchy Management 181

Yosr SLAMA, Mohamed JEMNI
Improving Code Generation in the Polytope Model 182

G. Folino, G. Spezzano
A Problem Solving Environment for Interactive Simulation of Bioremediation Models on Parallel Computers 182

E.M. Daoudi, A. Meziane, Y.O. Mohamed, El Hadj
Parallel TLHMM Model for Automatic Speech Recognition 183

E.M. Daoudi, E.M. Jaâra, H. Nait Cherif
Parallel Image Compression by Neural Network Techniques 184

I.V. Abalakin, S.N. Boldyrev, B.N. Chetverushkin, M.V. Iakobovski, A.V. Zhokhova
Parallel Algorithm for Solving Flow Problems on Unstructured Meshes 184

J. Kaska
A Contribution to the Analysis of the Reproduction of the Basic Machine Fonds 523

Zhongtuo Wang
Population-dynamic Approach to the Modelling of Developing New Series of Products in Enterprise 524

Eiichi Endo, Y. Tamura
Optimal Resource Allocation Model for Planning R&D on Solar Cells 524

A. Kulakowski, S. Gad, A. Yastriebow
Classical and Intelligent Models Applied to Diagnosis and Identification of Electrical Equipment of Cars 525

V.A. Vittikh, P.O. Skobelev
Developing of Multi-agent System for the Modelling of Decision Making Process for Companies with Networking Organization 526

E.M. Bronstein, S.I. Spivak
Some Problems of the Forming of an Optimal Investment Portfolio 527

C.P. code: 799
Special session - Modelling and Algorithms

Y.N. Radayev
On the Principal Line Theory of Strain-Damage Coupled Equations and its Application to Near Crack Tip Localization Analysis 529

R.V.N. Melnik, A. Uhlherr , J.H. Hodgkin, F. de Hoog
Applications of Distance Geometry Algorithms to Atomistic Simulation of Polymer Systems 530

Constance M Schober
Spatiotemporal Chaos in Near-integrable PDE's 531

Alexandre Kovalev
On the Stability of Some Nonlinear Difference Equations of Lotka-Volterra Type 531

D. A. Beard
Macroscopic Model of a Protein-DNA Complex: The Chromatin Fiber 532

Sergei F. Yashkov
Modelling Processor Sharing Queue 532

L.E. Garey , R.E. Shaw
Solving Volterra Two-point Boundary Value Problems with Natural Auxiliary Conditions 533

Numerical Analysis of the Behaviour of Rubber-Like Polymers with Hyperbolic Models of Nonlinear Thermoelasticity

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In many industrial applications we have to deal with materials that exhibit typically nonlinear thermomechanical behaviour. Rubber-like polymers are one of the most cited examples of such materials. It is not a surprising fact, inasmuch as desirable thermomechanical properties of rubber-like polymers at an economical cost made these materials relatively cheap alternative tomore traditional metallic materials in many consumer products, as well as in automotive and aircraft industries. The existing applications of polymers and the design of polymers with improved thermomechanical characteristics require the development of adequate mathematical tools to describe the coupled thermomechanical dynamics of these materials.

Although rubber-like polymers provide a classical example where nonlinear effects are essential in the adequate description of material dynamics, only few recent papers discuss numerical results obtained for these materials with general nonlinear models of coupled thermoelasticity. In dealing with the nonlinear behaviour of such materials we must give a proper weight to the fact that nonlinearities in the dynamics of rubber-like materials are closely interwoven with the effect of thermal relaxation time. Mathematical models of hyperbolic thermoelasticity, known as models with relaxation times, are based on hyperbolic-type equations for temperature. Such models deserve more attention than has been accorded them in the past. Despite an increasing attention that has been given in recent years to the numerical analysis of nonlinear effects in classical thermoelasticity, the results on the influence of the combined effects of nonlinearity and the thermal relaxation on thermomechanical properties of materials are virtually absent in the literature. However, in many cases these effects become key factors in the adequate description of the dynamical behaviour of thermoelastic systems. In particular, it is well-known that nonlinear terms in the equation of motion and the energy balance equation may lead to the formation of discontinuous profiles of displacement and temperature (shock profiles).

In the regions of such discontinuities the combined effects of nonlinearity and the thermal relaxation become signifycant. From a practical point of view, these effects are especially important in such areas as manufacturing of electronic components and process engineering to name just few.

In this paper we deal with rubber-like solid polymers that, in contrast to many other solid materials such as metals or ceramics, are energy elastic, and since they have relatively large thermal relaxation times, they demonstrate hyperbolic effects in a more pronounced fashion compared to "hard" solids.

We study numerically a combined effect of hyperbolicity and nonlinearity on the dynamics of such materials. Modelling the thermomechanical behaviour of a ring-shaped body with the Lord-Shulman-type model, we demonstrate an intrinsic connection between nonlinear effects and hyperbolicity of the dynamics. In particular, we show that the vanishing relaxation time can lead to the suppression of nonlinearities.

Applications of Distance Geometry Algorithms to Atomistic Simulation of Polymer Systems

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Polymeric materials and polymer-based composites became an intrinsic part of many new industrial materials technologies where structural engineering and material engineering research go hand in hand. This research relies heavily on the fact that the material from which the end-use structure is made can be "designed" in principle and adapted to suit specific engineering purposes. A core component in this research, both from the technological and theoretical point of view, is to be able to extract the information about the macroscopic (thermomechanical, structural) properties of polymers from their microscopic (atomistic) constitution.

Since microscopic, atomistically detailed models of materials provide a key to a better understanding of their behaviour at the macroscopic level, the development of such models and algorithms for their implementation become an important activity in industrial materials research, in particular in polymer and composite sciences. The computer-aided molecular design of structures using effective algorithms leads to the situation where compounds and composites worthy of actual synthesis can be effectively identified.

In solving molecular conformation problems, stochastic methods based on Molecular Dynamics (MD) and Monte-Carlo (MC) simulations have become quite popular amongst the researchers.

However, the computer time required for full conformational search by the MD and MC algorithms and many other stochastic search methods (genetic algorithms, e.g.) is often hardly feasible for real polymeric systems and composites. The situation is not better for

the majority of deterministic methods that, due to their exhaustive search of the conformational space, are becoming less feasible computationally when designing complex new material structures. Despite recent progress, all these methods are still computationally very demanding and, most importantly, the success of their applications to realistic polymer systems relies heavily on the choice of initial conformation. Therefore, a real challenge for these types of algorithms is to build plausible initial configurations which can then be relaxed effectively.

Although for complex polymeric systems and composites this has often proved to be a difficult task, it has to be tackled in order to provide the real opportunity to design, characterise and optimise these materials before undertaking expensive experimental work. In this talk we argue that moving towards atomistic simulations of complex polymer systems and composites, another group of stochastic search methods, known under its generic name as distance geometry (DG), will play an increasingly important role. Formulating the general distance geometry problem in atomistic simulation of materials as an optimisation problem, we apply two distance geometry algorithms to its solution and analyse their performance for bulk decane molecules. The comparative analysis of the described algorithms in applications to cross-linked polymeric structures is a natural extension of the presented work.

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Lausanne - August 21-25, 2000

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CTC 02 A-08: CTAC Numerical Analysis 8

Probabilistic and Statistical Methods in Computer Science.
Rene' Schott, *'Henri Poincare'- Nancy1*

Analysis of Complex Systems for the Condition Monitoring of a Rolling Mill.
Craig Moodie, *University of Wollongong*

Behaviour of the Laminated Circular Glass Plates.
Mehmet Zulfu Asik, *dept. of engineering sciences, metu*

A Matched Solution Method for the Lateral Variation of Longitudinal Strain in Flat Rolling.
Andrew E. Dixon, *Steel Research Laboratories*

CTC 02 A-12: CTAC Numerical Analysis 12

Interpreting Three Dimensional Information from Two Dimensional Information — a Classical Problem in Mineral Processing.
Stephen L. Gay, *The University of Queensland*

Fitting a Distribution over Random Graphs to Data.
Nicoleen Cloete, *University of Auckland, Auckland, New Zealand*

An Early Political Election Problem.
Dharma Lesmono, *University of Queensland*

Monotone Schemes for Time-Dependent Energy Balance Models.
Roderick Melnik, *University of Southern Denmark*

CTC 06 A-01: CTAC Optimisation and Design

Numerical Methods for Design of Robust Optimal Experiments.
Ekaterina Kostina, *University of Heidelberg, Germany*

Use of l_p Norms in Fitting Curves and Surfaces to Data.
Alistair Watson, *University of Dundee, UK*

V-Invariant Methods for Generalised Least Squares Problems.
Michael R. Osborne, *Australian National University*

Data Mining and Multigrid.
Linda Stals, *Australian National University*

CTC 10 A-01: CTAC Computational Fluids 1

A Comparison of Eulerian and Lagrangian Schemes for the Simulation of an Incompressible Planar Jet.
Patrick L. Morgan, *University of Sydney, Australia*

Skirting Subsets of the Plane, with Application to Marginal Stability Curves.
Geordie McBain, *University of Sydney*

Direct Simulation of Fountains with Intermediate Froude Number and Reynolds Number.
Wenxian Lin, *Engineering*

Natural Convection Flow of Air in an Inclined Open Cavity.
Morteza Nateghi, *Engineering*

CTM 02 A-01: Advances in Sinc Methods #1

Organiser: Masaaki Sugihara, *Nagoya University*

'Sinc methods' is a general name for numerical methods that are based on the use of the so-called Cardinal series of the function. During the last three decades Sinc methods have been developed and are currently being developed. Sinc methods are now recognized as the most efficient numerical methods for problems whose solutions may have singularities, or infinite domains, or boundary layers. This minisymposium presents recent advances in the Sinc methods; specifically, Sinc-Galerkin methods for ODEs and PDEs and their applications, linear solvers for Sinc-systems, Sinc-software, and theoretical foundations of the Sinc methods.

Double Exponential Transformations in Sinc Methods.
Masaaki Sugihara, *Nagoya University*

On the Ultimate Accuracy of Sinc Methods for ODEs.
Sven-Åke Gustafson, *Stavanger University*

Sinc-Galerkin Method for Solving non-Linear Boundary-Value Problems.
Ahmed Zayed, *DePaul University*

contributed talks

ICC 02_6A-06: Numerics of Fluids

Analyses of Characteristic and Up-wind Finite-Element Methods.
Masahisa Tabata, *Kyushu University*

Discontinuous Galerkin Method for the Compressible Flow Simulation.
Vit Dolejsi, *Charles University Prague*

Recovery Based Adaptation Techniques for Finite Volume Methods.
Jiøí Felcman, *Charles University*

Thermal Convection in a 3D Spherical Shell with Temperature Dependent Viscosity: a Finite Volume Approach with Advanced Pressure Correction Scheme.
Kai Stemmer *University of Münster*
Helmut Harder *University of Münster*
Ulrich Hansen *University of Münster*

ICC 03_4A-02: Oscillator Systems

Statistics of the Duffing-Holmes Oscillator under Random Excitations.
Jon Lee, *AF Research Lab, USA*

Positive Solutions of Three-Point Nonlinear Second Order Boundary Value Problem.
Youssef N. Raffoul, *University of Dayton*

Two-Step Control of Wall Mode and the Monodromy Matrix.
Henri Tasso *Max-Planck-Institut fuer Plasmaphysik*
George Throumoulopoulos *University of Ioannina*

The Dynamical Basis in the Decomposition of Forced Responses.
Julio R. Claeyssen
Teresa Tsukazan *Universidade Federal do Rio Grande do Sul*
Ines Ferreira *Universidade Federal de Santa Maria*

ICC 03_8A-07: Global Structure and Hyperbolicity

Detecting and Locating Near-Optimal Almost-Invariant Sets and Cycles.
Gary Froyland, *BHP Billiton Innovations*

EMC 02_6A-01: Computational and Theoretical Fluid Dynamics

Temperature Analysis of Journal Bearing with Axial Grooves using Computational Fluid Dynamics Technique.
Prabuono B. Kosasih, *University of Wollongong*

CFD Modelling of Thin Lubrication Film Flow.
Prabuono B. Kosasih, *University of Wollongong*

Bergan's Energy-Orthogonal Highly Non-Conforming Plate Element Approximation to the Contact Problem of Plate.
Nong Zhang, *University of Technology, Sydney*

Convergence Analysis of Non-Conforming 5-Parameter Rectangular Element.
D Shi, *Zhengzhou University, China*

EMC 11_1J-01: Applications in Engineering — from Nano to Astro

Modelling Pyramidal Quantum Dot Nanostructures.
Roderick Melnik, *University of Southern Denmark*

A Comparison between Two Types of 3D Photonic Crystals.
Geoff H. Smith, *University of Technology, Sydne*

Prediction of Extreme Forces and Moments for an Offshore Structure.
Andrew V. Metcalfe, *University of Adelaide*

Scaling and Correlation Analysis of the Northern Spiral Galaxy M51.
Jules I. Harnett, *University of technology, Sydney*

EMC 15_0G-01: Applications in Engineering — from Solar Cells to Bioreactors

Improving the Productivity of Bioreactors using Natural Oscillations.
Mark Nelson, *University of New South Wales*

A Mathematical Model of the Semiconductor-Electrolyte Interface in Dye-Sensitised Solar Cells.
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On the Existence of Solutions to Boundary Value Problems for Functional Difference Equations.
Christopher C. Tisdell, *The University of New South Wales*

Asymmetric Boundary Kernel Regression.
Mark R. Mackenzie, *University of Wollongong*

FMI 08_1P-02: NSFM Session 2

A Critique of the Risky Asset Models.
Christopher C. Heyde, *Australian National University and Columbia University*

A Model Limit Order Market.
Hugh C. Luckock, *University of Sydney, Australia*

Estimating and Predicting Volatility by Using Implied Volatilities.
Fima Klebaner, *Monash University, Australia*

Barrier Crossing Times for CIR and CEV Processes.
David B. Colwell, *The University of New South Wales*

ORC 06_7A-22: ASOR Scheduling

Two Machine Group Scheduling Problem with Sequence-Dependent Setup Times.
Rasaratnam Logendran *Oregon State University*
Nasser Salmasi *Oregon State University*
Chelliah Sriskandarajah *University of Texas at Dallas*

Computational Complexity of Scheduling with Dynamic Release Times.
Yakov Zinder *University of Technology, Sydney*
Van Ha Do *University of Technology, Sydney*

Lifted D_k^- and D_k^+ Inequalities for the Asymmetric Travelling Salesman Problem with Precedence Constraints and Related Problems.
Vicky H. Mak *The University of Melbourne*
Andreas T. Ernst *CSIRO Mathematical and Information Sciences*

Tackling the General Problem of Scheduling Parallel Machines with a Single Server.
Amir Abdekhodaee *Mathematical and Information Sciences*
Andrew Wirth *The University of Melbourne*

ORC 06_9R-13: ASOR Defence — Models 1

An Approach to Modelling the Effects of Network Centricity in Maritime Warfare.
Matthew Fewell *Defence Science and Technology Organisation*
Ian Grivell *Defence Science and Technology Organisation*

Modelling of Cloud and Foliage Obscuration using Queueing Theory Methods.
John Considine, *DSTO ISRD*

Modelling the Organisational Behaviour of Military Headquarters: a Social Scientist's Perspective.
Justin Fidock, *DSTO C2D*

Scalability and Complexity in Air Operations Analysis.
Dino Appla *DSTO AOD*
Simon Goss *DSTO AOD*
Clint Heinze *AOD, DSTO*
Mauro Iob *AOD, DSTO*
Torgny Josefsson *AOD, DSTO*
Ian Lloyd *AOD, DSTO*
David McIlroy *AOD, DSTO*
Graeme Murray *DSTO AOD*

ORC 06_9R-19: ASOR Defence — Decision support 2

Wargame Support Tools: Optimisation of Ground Combat.
Michael Haythorpe *DSTO*
Justin D. Beck *Defence Science and Technology Organisation*
Coen Van Antwerpen *Defence, Science and Technology Organisation*
Andrew W. Gill *Defence Systems Analysis Division, Defence Science and Technology Organisation*

Robustness of Communications Networks in Complex Environments — a Simulation using Agent-Based Modeling.
Adam J. Forsyth *Land Operation Division, Defence Science and Technology Organisation*
Ashley Fry *Land Warfare Development Centre, Australian Army*

Maximum Utility from Limited Vaccine Stocks: a Case Study using Agent-Based Modelling.
Adam J. Forsyth *Land Operation Division, Defence Science and Technology Organisation*
Ashley Fry *Land Warfare Development Centre, Australian Army*

Session Details

Monday (11:00-13:00)

CTC 02 A-01: CTAC Numerical Analysis 1

Complexity Issues and Singularity Detection for a Two-Dimensional First-Kind Integral Equation.
John A. Belward, *University of Queensland*

Quadratic Pencil Pole Assignment by Affine Sums.
Sylvan Elhay, *University of Adelaide*

Uncrossing the Contours — Detecting the Crossings.
Timothy Schaerf, *University of Sydney*

An H^1 Galerkin Method with Quadrature for Elliptic and Parabolic Problems.
Kassim Mustapha, *University of New South Wales*

CTC 02 A-08: CTAC Numerical Analysis 8

Probabilistic and Statistical Methods in Computer Science.
Rene' Schott, *'Henri Poincare'- Nancy1*

Analysis of Complex Systems for the Condition Monitoring of a Rolling Mill.
Craig Moodie, *University of Wollongong*

Behaviour of the Laminated Circular Glass Plates.
Mehmet Zulfu Asik, *dept. of engineering sciences, metu*

A Matched Solution Method for the Lateral Variation of Longitudinal Strain in Flat Rolling.
Andrew E. Dixon, *Steel Research Laboratories*

CTC 02 A-12: CTAC Numerical Analysis 12

Interpreting Three Dimensional Information from Two Dimensional Information — a Classical Problem in Mineral Processing.
Stephen L. Gay, *The University of Queensland*

Fitting a Distribution over Random Graphs to Data.
Nicoleen Cloete, *University of Auckland, Auckland, New Zealand*

An Early Political Election Problem.
Dharma Lesmono, *University of Queensland*

Monotone Schemes for Time-Dependent Energy Balance Models.
Roderick Melnik, *University of Southern Denmark*

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Ahmed Zayed, *DePaul University*

Monday (15:30-17:30)

CTC 02 A-09: CTAC Numerical Analysis 9

Numerical Validation of Microwave Heated Fluidised Bed Calcination of Waste Containing Ceramic Powders.
Viktor Vegh, *Queensland University of Technology*

Numerical Analysis of Lateral Movement of a Metal Strip under the Asymmetric Rolling Conditions.
Tanya Tarnopolskaya, *CSIRO Mathematical and Information Sciences*

Boundary Element Methods in the Prediction of the Acoustic Damping of Ship Whipping Vibrations.
Damien S. Holloway, *University of Tasmania*

Time Evolution of Localised Relativistic Electron States.
Jamin A. Flohr, *University of Queensland*

CTC 06 A-02: CTAC Numerical Analysis and Optimisation

Session Details

Wednesday (15:30-17:30)

EMC 02_6A-01: Computational and Theoretical Fluid Dynamics

Temperature Analysis of Journal Bearing with Axial Grooves using Computational Fluid Dynamics Technique.
Prabuono B. Kosasih, *University of Wollongong*

CFD Modelling of Thin Lubrication Film Flow.
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UC 131

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Christopher C. Tisdell, *The University of New South Wales*

Asymmetric Boundary Kernel Regression.
Mark R. Mackenzie, *University of Wollongong*

Thursday (11:00-13:00)

EMC 02_4A-02: Finite Elements and Applications

Geometric Form of the Stiffness Matrix for a Linear Triangular Mesh.
Alan K. Easton, *University of Papua New Guinea*

Anisotropic Mixed Finite Element Method for Stokes' Equations.
D Shi, *Zhengzhou University, China*

Shakedown Analysis using P-FEM and Mathematical Programming.
Son Ngo, *University of New South Wales*

Finite Element Approximation for Eigenvalue of Structural-Acoustic Coupled Problems.
X. H. Ling, *UTS*

EMC 08_7R-01: Applications in Engineering — Data Mining

Generalised Correlation Algorithms for Attribute Selection.
Alexandra Burden, *University of Wollongong*

Protecting Privacy in Genetic Databases.
Helen P. Giggins, *the University of Newcastle*

Hermite Correlation and Application.
Mark R. Mackenzie, *University of Wollongong*

Noise Addition for Protecting Privacy in Data Mining.
Md. Zahidul Islam, *The University of Newcastle*

Analysing and Interpreting Information from Questionnaires using Data Mining and Logistic Regression.
Peter Petocz, *University of Technology, Sydney*

EMC 10_3A-01: Fluids — Thin Flow and Stability

Waiting-Time and Short-Time Solutions for Thin-Film Flow.
Ebrahim Momoniat, *University of the Witwatersrand, South Africa*

The Gas-Lubricated Rayleigh Step Slider Bearing of Narrow Geometry.
Irene Penesis, *Australian Maritime College*

Some Exact Solutions of the Two Dimensional Nonlinear Shallow Water Wave Equations.
Joe J. Sampson, *Swinburne University of Technology*

Stability and Instability of Fluid Interfaces under Stress.
Stanley J. Miklavcic, *Linkoping University*

Thursday (15:30-17:30)

EMC 09_1H-01: Manufacturing — Steel 1

Improved Roll Surface Deflection Model for Strip Edge Profile Prediction.
Charlie H. McInnes, *Industrial Automation Services Pty. Ltd.*

A Finite-Difference Method Simulation of Temperature in Cold Rolling of Strip.
Hongbin Ren, *University of Wollongong*

5th International Congress on Industrial and Applied Mathematics

SYDNEY AUSTRALIA • 7-11 JULY 2003

BOOK OF ABSTRACTS

ICIAM 2003

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Book of Abstracts

ICIAM 2003

Edited by

Ross R. Moore

the particles are sectioned. However the distribution of minerals in the exposed particle sections is not the same as that for particles. For example, a particle may be composite but a section through the particle may consist of only one mineral. Particles (or particles sections) that consist of only one mineral are called liberated. Because the proportion of liberated particle sections is more than the number of liberated particles, the overall variance of the mineral distribution in particle sections is more than that for particles. In order to correct for this discrepancy an algorithm needs to be applied which performs a correction or adjustment. Stereology is the branch of mathematics that considers interpreting three dimensional information from lower-dimensional information, and hence the correction is often called a stereological correction. A number of algorithms have been developed using geometric probability equations as well as the principle of maximum entropy, and these will be reviewed. It will also be explained how it can be extended from considering particles as binary to considering them as multimineral.

CTL 08_5A-074: Fitting a Distribution over Random Graphs to Data.

Nicoleen Cloete, *University of Auckland, Auckland, New Zealand.*

The genealogy of a random sample of a population of organisms can be represented as a rooted binary tree. Population dynamics determine a distribution over sample genealogies. For large populations of constant size, and in the absence of selection effects, the coalescent process of Kingman determines a suitable distribution. Recently Neuhauser and Krone gave a stochastic model generalising the Kingman coalescent in a natural way to include the effects of selection. The Kingman coalescent is a special case of the Neuhauser Krone model obtained by setting the selection parameter to zero. The new model determines a distribution over a class of graphs of randomly variable vertex number. Because vertices have associated real scalar ages, realisations of the Neuhauser Krone process have randomly variable dimension. Our aim is to fit the model of Neuhauser and Krone to sequence data. We use Markov chain Monte Carlo methods to simulate the posterior distribution for population parameters of interest. The state of the Markov chain Monte Carlo is a random graph, with random dimension, and equilibrium distribution equal the posterior distribution. We report initial results obtained from fitting the model to simple synthetic datasets.

CTL 06_0V-092: An Early Political Election Problem.

Dharma Lesmono, *University of Queensland.*

Under the democratic systems of government instilled in many sovereign states, the party in government maintains a constitutional right to call an early election. While the constitution states that there is a maximum period between elections, early elections are frequently called. This right to call an early election gives the government a control to maximize its remaining period in power. We find the optimal control for the government by locating an exercise boundary, which indicates whether or not a premature election should be called. This problem draws upon the body of literature on optimal stopping problems and stochastic control.

CTL 13_0J-030: Monotone Schemes for Time-Dependent Energy Balance Models.

Roderick Melnik, *University of Southern Denmark.*

In the analysis of new semiconductor structures for optoelectronics quasi-hydrodynamic models play an increasingly important role. Such models are also effective in dealing with non-local, non-equilibrium effects in semiconductors[1]. In this paper we apply the generalised flow approach to construct a new difference scheme for the solution of the quasi-hydrodynamic model for semiconductor device modelling.

Although effective numerical methodologies for the solution of drift-diffusion models have been developed in the 1980s[2], the task of generalising them to quasi-hydrodynamic models is far from trivial. The major difficulty consists of changeability of the sign of $-J_n \partial_x \varphi$ in the energy balance equation which often leads to breaking-up monotonicity conditions for traditional numerical techniques. Our main result in this paper is a new difference scheme which does not violate these conditions. The analysis of this scheme and its convergence properties are investigated with numerical examples aiming at calculating dynamic characteristics of optically sensitive semiconductors, in particular of GaAs vertical field-effect phototransistor structures.

[1] Melnik RVN and He H; J. of Engineering Mathematics, **38**, (2000), pp.233-263.
[2] Polsky BS and Rimshans J; Solid State Electronics, **29**, (1986), pp.321-328.

CTC 02 A-13-3: CTAC Numerical Analysis 13

Phuoc Huynh: *Influence of Location, Number and Shape of Corrugations in Slider Bearings.* CTL 09_0H-036
Daniel May: *Validity of Modelling Urban Stormwater Quality using Neural Networks.* CTL 09_0C-014
Paul L. Brown: *Sulfidox — a Tool for Modelling the Temporal and Spatial Behaviour of Heaps containing Sulfidic Materials.* CTL 09_2F-080
Robert A. Pearson: *Strategies for Predicting Chaos.* CTL 01_0A-030

CTL 09_0H-036: Influence of Location, Number and Shape of Corrugations in Slider Bearings.

Phuoc Huynh, *University of Technology, Sydney.*

Effects of corrugation's location, number and shape on the performance of fixed-inclined slider bearings is investigated numerically, using a finite element method. It is found that the further downstream a corrugation is located, the stronger is its enhancement of the bearing's load supporting capability, relative to the smooth wall case. Load supporting capacity of the bearings is also enhanced by higher number of corrugations, but the enhancement reaches saturation rather quickly. Influence of corrugation's shape has also been considered; rectangular slots and sine waves have been used. When the corrugations are of similar size, it is seen that their shapes make little difference in the bearing capacity.

CTL 09_0C-014: Validity of Modelling Urban Stormwater Quality using Neural Networks.

Daniel May, *University of Wollongong.*

Urban stormwater quality is a significant problem requiring accurate prediction to design control measures. The development of deterministic models is hindered by the

Some examples for wave propagation in several typical media (i)-(iii) are calculated, analysed, and compared with some other theoretical and experimental data. The process of the wave reflection and diffraction is discussed.

ICL 11_6A-038: Asymptotic Study of the Edge Bending Mode of a Thin Plate.

- Dmitry D. Zakharov, *FEST, South Bank University — London*
- Julius D. Kaplunov, *Department of Mathematics*

This work is devoted to the analysis of the Rayleigh type waves of bending nature. We suggest a modified approach, started for long waves and valid for shorter wavelength. The dispersion properties of edge bending waves in isotropic plate are investigated using the averaged dynamic theory of the 2nd order (SO) asymptotic accuracy. Final boundary conditions at the edge differ from the familiar Kirchhoff theory. Results are obtained for the different Poisson ratios, the limit cases of small and large wave number are studied with deriving the analytical SO formulas for wave speed. Starting with the SO plate operator the general formulas for next iterations are deduced and used in the analysis. The wave speeds measured experimentally and those predicted by the usual Kirchhoff theory, refined theory and using the iterated operators, are compared. As shown, SO results for refined theory with iterated main differential operator lead to the better agreement with experiment even with unperturbed boundary conditions.

ICL 11_6E-017: Boundary-Value Problems of Plane Elasticity with Incomplete Boundary Conditions.

Alexander N. Galybin, *The University of Western Australia.*

This study concerns elastic boundary value problems of two types that are ill-posed due to non-uniqueness or instability of solutions. 1. Problems overdetermined on a part of the contour and undetermined on the rest of it. For instance, in contact mechanics, unknown contact stresses can be determined by measuring displacements on stress-free boundary; in fracture mechanics, monitoring crack opening displacements can reveal stresses in the process zone ahead of the crack tip. Four scalar conditions, outside the contact zone and on the crack, are known in these examples instead of two that would be necessary for well-posed problems. This leads to instability of solutions and therefore the use of regularisation methods is required. It is shown that regularisation based on the singular value decomposition method is capable to produce stable results. 2. Problems originated from investigations of tectonic stresses in the lithosphere. Data often provides stress orientations while stress magnitudes are unavailable. This leads to the problem in terms of stress orientations only, which results in the loss of uniqueness or solvability. This study reveals the number of linearly independent solutions found by analysing the orientations of boundary stresses.

EMC 11_1J-01: Applications in Engineering — from Nano to Astro

Roderick Melnik: *Modelling Pyramidal Quantum Dot Nanostructures.* EML 11_2J-029
Geoff H. Smith: *A Comparison between Two Types of 3D Photonic Crystals.* EML 13_1J-021
Andrew V. Metcalfe: *Prediction of Extreme Forces and Moments for an Offshore Structure.* EML 08_3H-020
Jules I. Harnett: *Scaling and Correlation Analysis of the Northern Spiral Galaxy M51.* EML 05_4D-044

EML 11_2J-029: Modelling Pyramidal Quantum Dot Nanostructures.

Roderick Melnik, *University of Southern Denmark.*

The formation of self-assembled quantum dots have been demonstrated in several different materials, and these low dimensional structures are expected to play a pivotal role in many micro- and nano-optoelectronic applications. It is known that the variation in the dot size and shape can produce significant energy fluctuations in the strong confinement region. In this paper, we are interested in the analysis of truncated pyramidal quantum dots which are grown from strained material systems. We base our consideration on InAs/GaAs structures. From a mathematical point of view, the problem can be seen as an eigenvalue PDE problem with discontinuous coefficients (due to different material properties of the barrier and the quantum dot). Numerical results, presented for quantum dots of different sizes, demonstrate clearly a coupling between eigenstates of the "pure" quantum dot (without wetting layer) and the quantum-well wetting layer.

EML 13_1J-021: A Comparison between Two Types of 3D Photonic Crystals.

Geoff H. Smith, *University of Technology, Sydne.*

The woodpile photonic crystal has received much attention in the literature. This is a structure consisting of layers of cylindrical rods with a stacking sequence that repeats itself every four layers. Within each layer, the rods are parallel and separated by a distance D. The distance between successive layer centers is h and the rod axes in adjacent layers are orthogonal. From a basis of two such crossed layers, we can form a vertical stack to obtain structures of various periodicities in the vertical direction. To obtain a periodicity of four layers in the stacking direction (as in the standard woodpile), rods separated by one intermediate layer are offset by a distance of $\frac{1}{2}D$ in the direction perpendicular to the rod axes.

An alternative structure having a periodicity of two layers in the stacking direction is obtained if all pairs of crossed gratings are directly above one another. Both of these structures exhibit photonic bandgaps and it is generally assumed that the 4-layer structure has larger gaps than the 2-layer one. However, we have shown that at least in metallic woodpiles, surface effects and polarization of the incident field are important, so that is conceivable that for metals the differences in the lattice structure of the two cases may not have a large effect. In this paper we make quantitative comparisons between the two structures for both the conducting and the dielectric case.

EML 08_3H-020: Prediction of Extreme Forces and Moments for an Offshore Structure.

Andrew V. Metcalfe, *University of Adelaide.*

Maximum base shears and overturning moments on a computer model of an offshore structure, during four day periods in random waves with constant sea spectrum, are obtained through time domain simulation. Estimates of probabilities of structural failure, based on these data, using a bivariate extreme value distribution are compared with estimates made from a Gibbs sampler. The effects of non-linearity in the conditional distributions of the Gibbs sampler are investigated. Methods for combining esti-

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EML 05_4D-044: Scaling and Correlation Analysis of the Northern Spiral Galaxy M51.

Jules I. Harnett, *University of technology, Sydney.*

Astronomical data analysis increasingly requires the use of sophisticated mathematical techniques, such as the structure function, autocorrelation function, Fourier series and wavelet spectra. We have found that the optimal tool is wavelet spectrum with suitable choice of the analysing wavelet. The wavelet cross-correlation function enables us to analyse the correlation between images as a function of scale as the cross-correlation coefficient depends strongly on this parameter. The wavelet spectra allow us to separate structures on different scales, in particular, features like spiral arms and diffuse extended emission.

In this paper, we present an analysis of the radio images, scaling and cross-correlation characteristics of the nearby face-on spiral galaxy M15. The cross-correlations between the images at different wavelengths show strong similarities between the total radio emission at $\lambda = 6$cm, red light and mid-infrared dust emmission on all scales. The best correlation is found between total radio emission and dust emission. Thermal radio continuum and Halpha emission are best correlated on a scale of about 1' 1.6kpc, the typical width of a spiral arm. On a similar scale, the images of polarised radio and H-alpha emission are anticorrelated, which remains undetected with classical correlation analysis.

EMC 11_1H-02: Manufacturing — Steel 2

Andrew E. Dixon: *Modelling the Attenuation of Flatness Defects at the Interstand during Hot Rolling.* EML 11_1H-022
Cheng Lu: *Thermal Effect on the Mixed Film Lubrication in Strip Cold Rolling.* EML 13_0H-013
Jianning Tang: *A Surface Roughness Model for Hot Strip Rolling.* EML 09_1V-070
Chen Lu: *Study on Snaking in the Hot Rolling of Steel Strip.* EML 06_0H-042

EML 11_1H-022: Modelling the Attenuation of Flatness Defects at the Interstand during Hot Rolling.

Andrew E. Dixon, *Steel Research Laboratories.*

In flat rolling the lateral variation of the longitudinal strains, and resulting stresses, must be small in order to minimise a defect commonly known as poor shape. This refers to the strip's inability to remain flat when external forces have been released. At the finishing mill of a hot rolling process, where the strip is rolled by a tandem train of rolling stands, it is possible for the lateral variation of plastic strains and tension to be attenuated in between stands due to plastic creep. This occurs as regions with smaller-than-average longitudinal plastic strain, being also regions of high tension from the increased elastic strain (as the strip is pulled flat), undergoes extra plastic elongation in between the rolling stands. A model is developed to describe this process and incorporates the influence of the tension control system, which maintains the total strip tension constant. This predicts the expected final variation in tension and longitudinal strain distribution under different rolling and inter-stand conditions, as well as any resulting change in strip thickness and width. This would include allowing for changes to local compressive stress conditions from strip buckling.

Engineering Applications and Computational Algorithms

Edited by Xinzhi Liu

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with structured uncertainties Using monotonization methods .....(76)
Takeshi Kawamura, Masasuke Shima

15. **Numerical Computation of Bifurcation in a Simple Baroclinic Flow** .....(82)
Gregory M. Lewis, Wayne Nagata

16. **On the Existence of Periodic Solutions of a Forced Duffing Equation** .....(88)
Chunqing Lu

17. **Solutions of a Pair of Conservation Laws with Nonconvex Flux Function** .....(92)
Sadao Shimoji

18. **A Novel Sensor-based Motion Planning Algorithm for Mobile Robots in Unknown Environments** .....(96)
Ming Lin, Jihong Zhu, Zengqi Sun

19. **Numerical Analysis of Fast Charge Transport in Optically Sensitive Semiconduntors** .....(102)
Roderick V.N. Melnik, Janis Rimshans

20. **Real Solution Structure Analysis of the Direct Kinematics for a Parallel Manipulator** .....(108)
Qizhi Wang, Zhuying Wang

21. **Numerical Approximation of the Solution for the Reaction-Diffusion System Modeling the Interaction of Two Predators and One Prey** .....(112)
Luis Fernando Hernández Moguel, Eric J. Avila Vales,
A. Estrella González, M. Escalante Torres

22. **A Piecewise-linear Map for Finding Edges in Images** .....(117)
W. Yao, R.E. Ellis

23. **Computation of the Normal Form for 1:1 Resonant Double Hopf Bifurcation** .....(121)
Pei Yu

24. **The Simplest Normal Form of Generalized Hopf Bifurcation with Perturbation Parameters** .....(127)
Pei Yu, Yuan Yuan

25. **An Approach to Adaptive Multimodal Biometric Fusion** .....(133)
Qinghan Xiao

26. **Classification Using Feature Interval Selection** .....(137)
David K.Y. Chiu, Bogdan J. Buczynski

27. **Practical Tuning of Two-Input Two-Output Takagi-Sugeno Fuzzy Controllers with Simplified Rule Consequent** .....(142)
A. Alwadie, H. Ying, and H. Shah

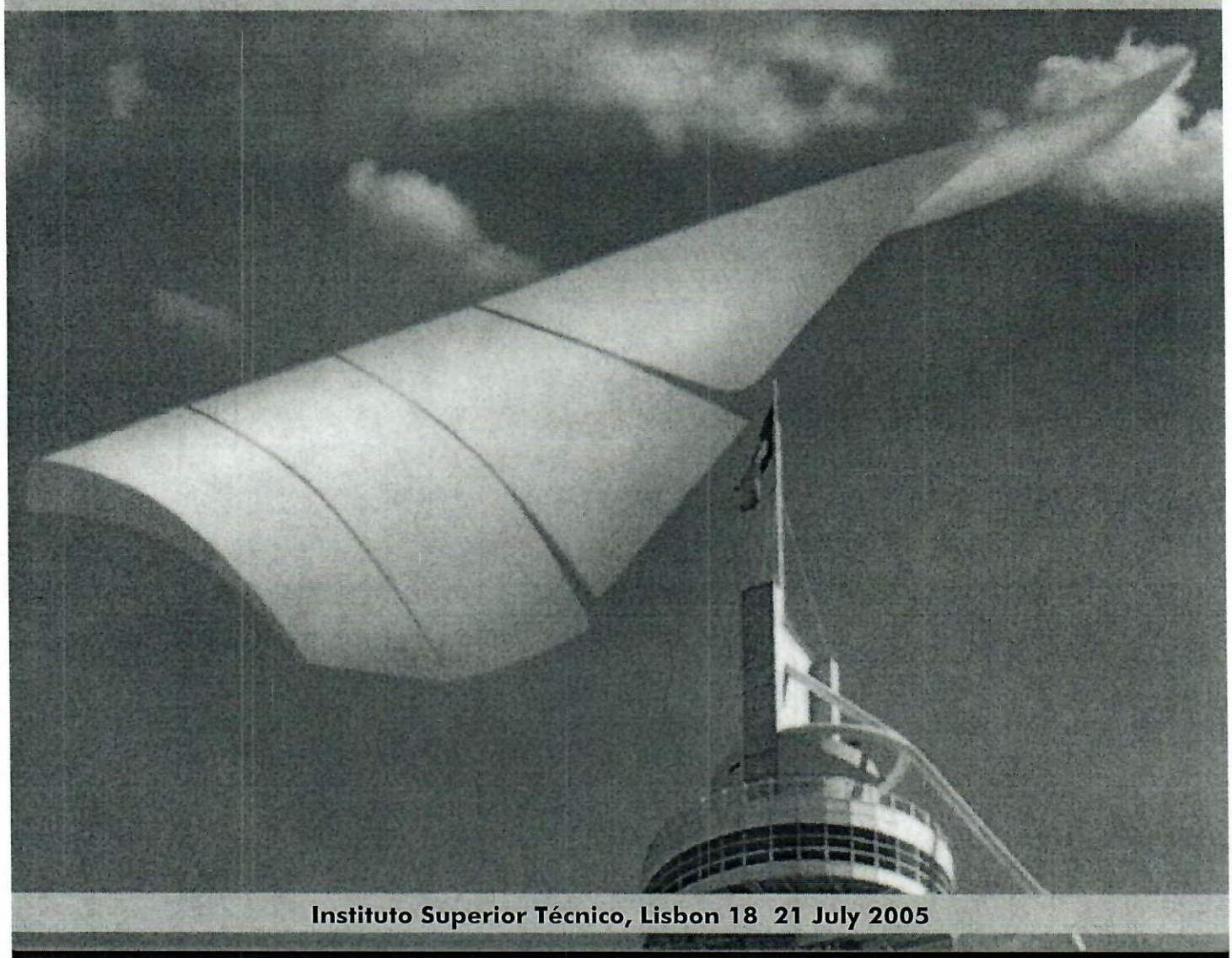
28. **A Prony Approach to Modeling of Time-Varying Fuzzy Systems** .....(147)
Trung T. Pham, Guanrong Chen

29. **Global Dynamic Optimization of Linear Time Varying Hybrid Systems** .....(153)

ECCOMAS

II ECCOMAS Thematic Conference on Smart Structures and Materials

Book of Abstracts



Instituto Superior Técnico, Lisbon 18 21 July 2005

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II ECCOMAS
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Cristóvão M. Mota Soares, Technical University of Lisbon, Portugal

Instituto Superior Técnico, Lisbon 18 – 21 July 2005

COMPUTATION OF PHASE TRANSFORMATION DYNAMICS IN SHAPE MEMORY ALLOYS BASED ON A LANDAU-GINZBURG FREE ENERGY MODEL

D. Roy Mahapatra and Roderick V.N. Melnik

Mathematical Modelling and Computational Sciences, Wilfrid Laurier University, Canada

Landau theory has been successfully applied to the solution of dynamic problems of martensitic phase transformations in alloys. On the other hand, precise mathematical description of the microstructures is known within the framework of Cauchy-Born hypothesis, although the discrete version of this description is not well elucidated for multivariant transformations in three-dimensional samples because of various computational difficulties while handling a quasi-convex minimization problem. In this paper, we develop a new Landau-Ginzburg free energy model for such a problem and demonstrate its link with the continuum description of phase transformations. This leads us to a possiblity of using the precise description of compatible microstructures in the phase-field model that allows us to improve computational effectiveness of the finite element model. The proposed formulation is general and can be applied to different types of phase transforming alloys under different thermo-mechanical loadings. Numerical results for cubic to tetragonal transformations are reported.

ANALYSIS OF INTERFACE PROPAGATION IN NIAL SLABS WITH MODELS BASED ON CONSISTENT MICROSCOPIC ENERGY REPRESENTATION

*Roderick V.N. Melnik and D. Roy Mahapatra**

** Mathematical Modelling and Computational Sciences, Canada*

In order to perform the timeresolved analysis of real shapememory alloy (SMA) devices that have truly threedimensional geometry, it is essential to develop efficient largescale computational schemes. Results on such efficent computational schemes in lowdimensional cases are known in the literature. In this paper, we develop a new 3D finite element model based on a consistent representation of microscopic Gibbs free energy by coupling the nonlinear thermoelasticity with the firstorder phase kinetics. The model is applied to study the dynamics of cubic to tetragonal transformation in a NiAl slab. We consider multivariant martensitic phases, noting that the energy representation poses the property of crystallographic group symmetry with minimum number of material constants required from either experiments or molecular dynamic simulation. The tradeoff for this minimum number is that the inversion symmetry is not preserved any longer. We analyse the propagation of the transformation interfaces in a threedimensional NiAl slab. Our major focus in this contribution is on the effect of initial texture, thermal radiation from the surface, transformation induced softening, the effects of loading rate on the transformation barrier, and on the propagation speed of the interfaces.

6ème Conférence Internationale AIMS "Systèmes Dynamiques, Equations Différentielles et Applications"

Université de Poitiers, France
25, 28 juin 2006

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- University of North Carolina Wilmington, USA

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Angiogenesis is the biological process by which networks of blood vessels are initiated and proliferate towards a mature vasculature. At the early development and growth, angiogenesis is necessary to go from the embryonic vasculogenesis into a complete and mature blood system. It is also an important factor of wound healing and tissue repairing. Unfortunately, angiogenesis is also a fundamental step in the growth of cancer tumours and in the tumoral metastasis. Recently, oncologists have suggested that the use of inhibitors of angiogenesis, an approach generically termed anti-angiogenesis, could prove effective in cancer treatment. In the present work, we consider anti-angiogenesis as a mathematical game between two players : activators of angiogenesis, willing to develop an efficient feeding network of blood vessels, and inhibitors, with a specific action on the tumour vasculature. We use a porous media model and criteria like as the pressure drop as approximation to the complex angiogenesis phenomenon. The strategies are angiogenic factors and inhibitor densities, so that we are in a topology design context. We define a static Nash game, for which we address the question of existence of an equilibrium. Numerical results illustrate how -theoretical- tumors develop multiple channels as an optimal response to optimal distribution of inhibitors.

⟶ ∞◇∞ ⟵

Blow-up estimates for some chemotaxis model

Pierre-Emmanuel Jabin
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It is well known that, for a large enough initial data, the solution to usual chemotaxis models blow up in finite time. This talk presents a way to estimate the rate of blow-up, using energy and energy dissipation. This is important in order to get stability estimates up to the blow-up time.

⟶ ∞◇∞ ⟵

Effect of Internal Viscosity on Brownian Dynamics of DNA Molecules in Shear Flow

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Xiao-Dong Yang

The results of Brownian dynamics simulations of a single DNA molecule in shear flow are presented taking into account the effect of internal viscosity. The DNA molecule is modeled as a bead-spring chain and the springs between two adjacent beads are assumed finitely extensible nonlinear elastic (FENE). A force balance on the chain leads to a stochastic differential equation governing the movement of each bead. The Euler method is applied to the solution of the model and the results for some differently disposed internal viscosities are discussed. The extensions for different values of strains are analyzed and comparison with the available experimental results is made to estimate the contribution of the effect.

⟶ ∞◇∞ ⟵

Dynamic and control of cell population : age structured model

Philippe Michel
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J. Clairambault

We address the following question: Can one sustain, on the basis of mathematical models, that for cancer cells, the loss of control by circadian rhythm favours a faster population growth? This question, which comes from the observation that tumour growth in mice is enhanced by experimental disruption of the circadian rhythm, may be tackled by mathematical modelling of the cell cycle. For this purpose we consider an age-structured population model with control of death (apoptosis) rates and phase transitions, and two eigenvalues: one for periodic control coefficients (via a variant of Floquet theory in infinite dimension) and one for constant coefficients (taken as the time average of the periodic case).

⟶ ∞◇∞ ⟵

A simplified model of TCA cycle

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Margit Heiske, Jean-Pierre Mazat and Kevin Thurley

Mitochondria play an important role in energetic metabolism in producing a large part of cellular ATP. A central role in this metabolism is played by TCA cycle (also called Krebs cycle). TCA cycle has been extensively modelized since the pioneer work of Garfinkel. Contrary to previous works our aim is to derive a simple set of differential equations able to reasonably simulate the main features of this metabolic pathway in different

and concentration scales, the dynamics of chemical kinetic systems are governed by different stochastic dynamical systems driven by Poisson noise, Brownian noise, or both. The standard Stochastic Simulation Algorithm (SSA) for chemical kinetic systems is usually limited by the multiscale nature of the genetic networks. We finally discuss the recent advances on overcoming the numerical stiffness induced by disparate reaction rates and metastability of the stochastic systems. The methods are illustrated through numerical examples.

⟶ ∞◇∞ ⟵

Mesoscopic dynamics of copolymer thin films with dispersed nanoparticles

Roderick Melnik
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Roy Mahapatra

We present a mesoscopic model for the analysis of the electroactive and flow-related properties of P(VDF-TrFE) copolymer thin films with dispersed nanoparticles for electromechanical tunability. Very large recoverable strain with tunable semiconductive and electrostrictive properties in such flexible and large-area thin films are of practical importance in micro-electronics, mechanical and bio-medical industries. Since in such a tunable copolymer film the coupled nonlinear deformation and the electrical mechanisms act over nano to macrosopic length scales, we develop a mesoscopic modeling approach. First, we derive a homogenized constitutive model that takes into account the local transport of cations in polymer, electrostriction and anhysteretic polarization. Then, based on the developed model of coupled partial differential equations, we provide a finite strain description accounting for the mesoscopic dispersion of copolymer chains. This and other key characteristics (electrical field distribution and conductivity properties) are obtained by the finite element methodology under different electromechanical loading conditions. Finally, changes in the deformation pattern of the film as a function of the copolymer volume fraction are analyzed.

⟶ ∞◇∞ ⟵

A variational approach to the moving contact line hydrodynamics

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Xiao-Ping Wang and Ping Sheng

In immiscible two-phase flows, contact line denotes the intersection of the fluid-fluid interface with the solid wall. When one fluid displaces the other, the contact line moves along the wall. A classical problem in continuum hydrodynamics is the incompatibility between the moving contact line and the no-slip boundary condition, as the latter leads to a non-integrable singularity. The recently discovered generalized Navier boundary condition (GNBC) offers an alternative to the no-slip boundary condition which can resolve the moving contact line conundrum. We present a variational derivation of the GNBC through the principle of minimum energy dissipation (entropy production), as formulated by Onsager for small perturbations away from the equilibrium. Through numerical implementation of a continuum hydrodynamic model, it is demonstrated that the GNBC can quantitatively reproduce the moving contact line slip velocity profiles obtained from molecular dynamics simulations. In particular, the transition from complete slip at the moving contact line to near-zero slip far away is shown to be governed by a power-law partial slip regime, extending to mesoscopic length scales.

⟶ ∞◇∞ ⟵

Dynamic theory and applications in smectic A liquid crystals

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A novel dynamic continuum theory is presented for smectic A liquid crystals in which the usual director **n** and unit layer normal **a** do not always necessarily coincide. Most previous dynamic continuum theories equate **n** with **a**; the theory developed here allows **n** and **a** to differ in non-equilibrium situations, work that has been motivated by the recent investigations by Auernhammer *et al.*, Soddemann *et al.* and Weinan E. The usual Oseen constraint for smectics is not imposed upon the unit normal **a**. Permeation effects are also included. After a summary of the complete dynamic equations, an application is given which shows that planar aligned layers of smectic A subjected to an arbitrary periodic disturbance are linearly stable. Boundary layer effects will also be discussed.

⟶ ∞◇∞ ⟵

Dislocation dynamics in thin films using the level set method

Yang Xiang

solutions.

⟶ ∞◇∞ ⟵

Bifurcation and Synchronization of A Synaptically Coupled FHN Neurons Model with Time Delay

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Qingyun Wang and Haixia Wang

This paper is focused on the dynamics of a coupled non-identical FHN neurons model with synaptic connection both analytically and numerically. It is shown that rich bifurcation behavior is exhibited with the variation of the coupling strength. However, a transition from the original chaotic motions to periodic ones accompanied with complex bifurcation scenario can be observed. At the same time, the frequency synchronization of the coupled neurons is studied in terms of their mean frequencies. It is also shown that a small time delay can induce new period windows with the coupling strength increasing. Moreover, it is found that the synchronization of the coupled neurons can be achieved in some parameter ranges related to bifurcation transitions. The parameter regions of different dynamic behavior are clarified.

Keywords: FHN neuron, time delay coupling, bifurcation, synchronization

⟶ ∞◇∞ ⟵

Modelling dynamics of nonlinear thermomechanical phase transformations in multidimensional shape memory alloy samples

Roderick Melnik
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D. Roy Mahapatra and L. Wang

In this contribution, we construct a new mathematical model to simulate martensitic phase combinations in shape memory alloy samples. Governing equations are obtained on the basis of the momentum balance law and a modified Landau-Ginzburg free energy functional, a generalization of the 1D Falk non-convex free-energy function. These equations are then supplemented with a kinetics model allowing us to describe the dynamics of multivariant phase transformations in three-dimensional samples. Finally, by using the Ginzburg-Landau modeling framework, we provide a methodology for linking the developed microscopic model with the atomistic reodering process that gives rise to self-accommodating microstructures. Results of numerical simulations, based on the finite-element implementation of the developed methodology, are presented.

⟶ ∞◇∞ ⟵

A Minimax Result with Applications to Adhesive Contact Problems

Dumitru Motreanu
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We show that the description in terms of unilateral Mechanics of a general model with adhesive contact naturally leads to an associated variational–hemivariational inequality. In turn, this formulation can be expressed as a critical point problem for the general class of nonsmooth functionals $I : X \to R \cup \{+\infty\}$ on a real Banach space X satisfying the structure hypothesis $I = \Phi + \Psi$, where $\Phi : X \to R$ is locally Lipschitz and $\Psi : X \to R \cup \{+\infty\}$ is convex, proper, lower semicontinuous. Here an element $u \in X$ is said to be a critical point if $\Phi^0(u; x-u) + \Psi(x) - \Psi(u) \geq 0$ for all $x \in X$. The notation $\Phi^0(u; v)$ designates the generalized directional derivative in the sense of Clarke. We focus on a recent result representing the nonsmooth version of the minimax theorem due to Brezis and Nirenberg with local linking and under presence of the splitting for the space X. This nonsmooth version was recently obtained in the paper:

R. Livrea, S. Marano and D. Motreanu, Critical points for nondifferentiable functions in presence of splitting, *J. Differential Equations*, to appear.

⟶ ∞◇∞ ⟵

DEA Analysis of Reverse Logistics of Supply Chain Integration Project Choice

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Zhi-ping Du

Abstract: logistics has a good relationship with the economic utility of supply chain and the sustainable development of environment. It has been the considerable link of supply chain research. This paper analyzes and appraises the e??ectivity of di??erent supply chain integration projects and whether considers reverse logistics or not, by establishing DEA model of supply chain integration project that is on the basis of order and synthetically considered forward and reverse logistics, .provides the

limits in the form of stochastic nonlinear Schrödinger equations.

Previous studies directed at the SNLS approximations have indicated that the self-focusing of wave energy to highly localized states can be inhibited by phase noise (modeling thermal effects) and can be restored by phase damping (modeling heat radiation).

Here it is shown that the continuum limit is probably ill-posed in the presence of spatially uncorrelated noise, at least with little or no damping, so that discrete models need to be addressed directly. Also, as has been noted by other authors, omission of damping produces highly unphysical results.

Numerical results are presented here for the first time for the discrete models including the highly nonlinear damping term, and new numerical methods are introduced for this purpose.

Previous conjectures are in general confirmed, and the damping is shown to strongly stabilize the highly localized states of the discrete models. It appears that the previously noted inhibition of nonlinear wave phenomena by noise is an artifact of modeling that includes the effects of heat, but not of heat loss.

⟶ ∞◇∞ ⟵

Closed form expressions of the probability density function for passive scalar advection by random winds and shears

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Jared Bronski, Roberto Camassa and Richard McLaughlin

We explore the evolution of the Probability Density Functions (PDF) for the random Green's functions for a diffusing passive scalar, which is also advected by a velocity field with stochastic components. These stochastic components are rapidly varying in time and they can be spatially dependent such as shears. Different analytical methods are presented to compute closed-form expressions for these PDF's or their asymptotic limits. Although computed for simple flows, these exact solutions retain mechanisms which are physically relevant. Moreover, these solutions can be effectively used as tests for more general situations where one has to resort to numerical studies of the PDF dynamics because only moment information is available.

⟶ ∞◇∞ ⟵

Spinning Rods and Passive Tracers, from Nanoscale to Table-Top scale: coherent fluctuations in the presence of thermal noise

Richard M. Mclaughlin
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Roberto Camassa, Jing Hao, Terry Jo Leiterman, Richard Superfine, Leandra Vicci and Jonathan Toledo

We present experimental measurements and mathematical predictions concerning the hydrodynamics induced by spinning rods in viscous fluids. Recent advances in nano-technology have enabled controlled manipulation of nanoscale objects immersed in fluids. Such advances allow for new biological measurements (such as physical properties of cell membranes) on length scales smaller than the wavelength of visible light, and direct observations are challenging. Moreover, on such scales, the hydrodynamics are thermally fluctuating, and observational tracers experience strong Brownian signals on top of coherent motion induced by nanoscale manipulation. As such, predictive mathematical theories are essential to interpret the observations. We discuss the hydrodynamic solutions we have developed for rods sweeping upright cones in viscous fluids. These quasi steady, three dimensional, exact and asymptotic solutions of the Stokes equations are used to study the motion of passive tracers. These predictions are shown to quantitatively match low Reynolds number experiments performed on a scaled up, table top version of the nanoscale measurements performed. In turn, the predictions on the nano-scale are considered where agreement is good, but not as good as on the macro scale. The uncertainty of the nanoscale measurements as regards missing observational information and stochastic dynamics will be discussed.

⟶ ∞◇∞ ⟵

Evaluating First Passage Times in Stochastic Evolution Equations with Jump-Diffusions and Applications in Finance

Roderick Melnik
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Di Zhang

The first passage time problem has important applications ranging from modelling in biology, physics, and chemistry to the financial market analysis. In this contribution, we focus on the first passage time problem for jump-diffusion processes described by an evolutionary stochastic differential equation with constant drift and volatility and a Poisson-like discontinuous part. It is known that a standard Monte-Carlo run for the solution

of this problem requires many thousands of time steps for each process path, while the evaluation of the density function itself would typically require many thousands of generated paths carried out by Monte-Carlo runs. In this talk we analyze a faster procedure, provide several test examples, and apply the developed methodology to pricing barrier options.

⟶ ∞◇∞ ⟵

Stochastic Dynamics of Integrable, Nonlinear Partial Differential Wave Equations

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M. Onorato and M. Serio

I discuss the stochastic dynamics of the Korteweg-deVries (KdV) and Kadomtsev-Petviashvili (KP) equations. Essentially the problems are cast with periodic/quasi-periodic boundary conditions and Riemann theta functions provide the spectral decomposition of these nonlinear PDEs. The stochastic nature of the equations is elicited by a technique common for linear PDEs in which the ordinary linear Fourier phases are taken to be uniformly distributed random numbers. In the nonlinear case the phases of the Riemann theta functions are taken to be random in the same way. Each set of random numbers thus provides a stochastic realization of a wave train which is characterized by a particular Riemann matrix. Each component in the Riemann spectrum is a "cnoidal wave" and therefore includes solitons, Stokes waves and sine waves in the formulation. A generalization of the correlation function is developed in terms of theta functions and the exact solution of the KdV and KP equations are evoked in terms of the time evolution of the power spectrum (derived analytically for the theta function solution of KdV) evolving from a particular Cauchy initial condition. The evolution of the power spectrum is carried out to infinite order, in contrast to the usual approach in which (gaussian) closure arguments are used to derive a kinetic equation which is then solved numerically to get the power spectrum evolution. I give numerical examples contrasting the finite closure kinetic equation solutions with the exact, infinite-order evolution for the KdV and KP equations. The finite closure arguments are found to destroy solitons, primarily because the individual soliton phase information is thrown away in the finite closure schemes. Instead, the infinite-order closure based on Riemann theta functions preserves the solitons perfectly. I discuss how the approach can also be applied to the study of "asymptotically integrable" evolution equations.

⟶ ∞◇∞ ⟵

Special Session 47: Applications of Dynamical Systems: Celestial Mechanics and Beyond

Marian Gidea, Northeastern Illinois University, USA
Josep Masdemont, Universitat Politecnica de Catalunya, Spain

This special session is devoted mainly to applications of dynamical systems to celestial mechanics, dynamical astronomy, space mission design, etc. The session will also discuss theoretical aspects that are relevant to these topics, such as invariant manifolds, homoclinic and heteroclinic connections, chaotic dynamics, transport, etc. Applications of dynamical systems to other areas, that share similar methods to those involved in the above topics, will also be considered.

⟶ ∞◇∞ ⟵

The dynamics around the collinear point L_3 of the RTBP

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J. M. Mondelo and M. Ollé

This talk aims towards the global description of the dynamics around the L_3 equilibrium point of the RTBP. The objects in its center manifold, including its normal behaviour, are computed by purely numerical procedures, in order to avoid the convergence restrictions of semi–analitical ones. Homoclinic phenomena is investigated. Small values of the mass parameter will be considered, in order to detect horseshoe–like motion.

⟶ ∞◇∞ ⟵

Low Energy Transfers In Space Using Chaos: Applications to Astrodynamics and Astronomy

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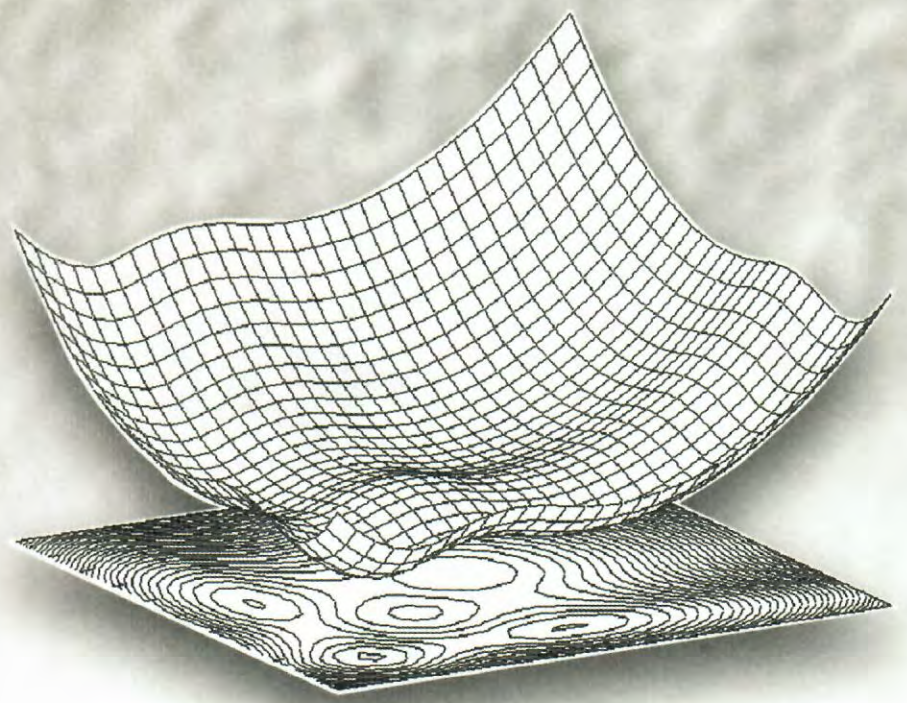
SECOND INTERNATIONAL CONFERENCE ON NONSMOOTH / NONCONVEX MECHANICS

WITH APPLICATIONS IN ENGINEERING

BOOK OF ABSTRACTS



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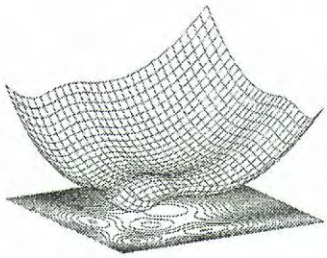

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7 & 8 July, 2006

PHASE KINETICS IN MODELLING SHAPE MEMORY ALLOYS

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SUMMARY

In this paper we propose a Ginzburg-Landau free energy model of multivariant phase transformation in shape memory alloy and its linkage with the atomistic reordering process which nally gives rise to self-accommodating microstructure. We analyze how the kinetics in uences the computation of stress-temperature induced dynamics of phase transformation in microscopic and larger length scales without attempting to solve a molecular dynamic problem in a coupled manner. Based on the variational formulation of the problem, we simulate phase transformations in a Ni-Al thin lm. The results capture well a qualitative picture of the onset of microstructure formation.

WCCM•VII

7th World Congress on Computational Mechanics

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Thursday, July 20

Session TH2: 14:20 — 16:10

	14:20	14:42	15:04	15:26	15:48
MATHEMATICAL AND COMPUTATIONAL ASPECTS OF MULTI-SCALE AND MULTI-PHYSICS — Chair: J. S. Chen, Co-Chair: Nasr Ghoniem					
Santa Monica Room	LOCALITY WITHIN A STRONGLY COUPLED TWO-SCALE MODEL FOR COMPOSITES * Ramm, E.; Hund, A.; Hettich, T.	GENERATION OF COARSE-SCALE CONTINUUM FLOW MODELS FROM DETAILED FRACTURE NETWORK CHARACTERIZATIONS * Durlofsky, L.; Karimi-Fard, M.; Gong, B.	MULTISCALE COMPUTATIONAL MODELING OF ALLOY SOLIDIFICATION Zabaras, N.; * Tan, L.	INVERSE HOMOGENIZATION: FROM EFFECTIVE PROPERTIES OF COMPOSITE TO ITS MICROSTRUCTURE Cherkaev, E.; * Bonifasi-Lista, C.; Zhang, D.	ADAPTIVE DAMAGE SIMULATION OF CONCRETE USING HETEROGENEOUS MULTISCALE MODELS * Eckardt, S.; Könke, C.
TRANSPORT AND COUPLED PROCESSES IN MICRO- AND NANOTECHNOLOGY — Chair: Melnik, Co-Chair: Povitsky					
Los Angeles Room	**KEYNOTE:** COMPUTATIONAL NANOTECHNOLOGY OF NANOMECHANICS AND THERMAL TRANSPORT IN NANOTUBES AND NANOWIRES * Srivastava, D.		MOLECULAR DYNAMIC SIMULATION ON ENHANCEMENT OF Chieng, C.	A COUPLED QUANTUM-HYDRODYNAMIC MODEL OF FIELD-EMISSION FROM CARBON NANOTUBE THIN FILMS Roy Mahapatra, D.; Sinha, N.; Yeow, J.; * Melnik, R.; Jaffray, D.	BOUNDARY SINGULARITY METHOD FOR LOW-RE SLIP FLOW Povitsky, A.; * Zhao, S.
ENRICHED FINITE ELEMENT METHODS FOR EVOLVING DISCONTINUITIES AND INTERFACES (SANCTIONED BY THE IUTAM THROUGH THE COOPERATIVE AGREEMENT BETWEEN IACM AND IUTAM) — Chair: C.A. DUARTE, Co-Chair: N.MOES					
Beverly Hills Room	SIMULATION OF CRACK BRANCHING IN DYNAMIC FRACTURE * Remmers, J.; Borst, de, R.; Needleman, A.	CONTINUOUS-DISCONTINUOUS MODELING OF DYNAMIC CRACK PROPAGATION * Pedersen, R.; Simone, A.; Sluys, B.	EXPLICIT DYNAMICS WITH X-FEM TO HANDLE COMPLEX GEOMETRIES * Nicolas, M.; Patrick, R.; Béchet, E.	XFEM-BASED CRACK DETECTION SCHEME USING A GENETIC ALGORITHM * Givoli, D.; Rabinovich, D.	
ADVANCES IN MULTISCALE METHODS — Chair: Hashmi Ben Dhia, Co-Chair: Christian Rey					
Constellation Ballroom I	DOMAIN DECOMPOSITION METHODS WITH NONLINEAR LOCALIZATION FOR POST-BUCKLING COMPUTATION OF SLENDER STRUCTURES * Rey, C.; Cresta, P.; Allix, O.; Guinard, S.	SPACE-TIME VARIATIONAL MULTISCALE MODELING FOR COMPLEX FLOWS * Munts, E.; Hulshoff, S.; de Borst, R.	LINEAR AND NONLINEAR ANALYSIS FOR SANDWICH STRUCTURES BY USING ARLEQUIN METHOD * Hu, H.; Belouettar, S.; Daya, E.; Potier-Ferry, M.	SIMULATION OF INELASTIC MATERIAL BEHAVIOR USING MDFEM * Rothert, H.; Ernst, G.; Nasdala, L.; Rolfes, R.	

	16:40	17:02	17:24	17:46	18:08
MATHEMATICAL AND COMPUTATIONAL ASPECTS OF MULTI-SCALE AND MULTI-PHYSICS — Chair: Nasr Ghoniem, Co-Chair: Hirohisa Noguchi					
Santa Monica Room	MAXIMUM ENTROPY APPROACH FOR STATISTICAL MODELING OF THREE-DIMENSIONAL POLYCRYSTAL MICROSTRUCTURES Zabaras, N.; * Sankaran, S.	MULTISCALE ENRICHMENT BASED ON PARTITION OF UNITY FOR NONLINEAR PROBLEMS Fish, J.; * Yuan, Z.	MULTIPHYSICS MODELING OF PLASMA CLEANING TECHNIQUES FOR IN SITU CONDITIONING OF VACUUM SURFACES Johnson, M.; * Hussain, M.; Truszkowska, K.; Cipollo, M.	DISLOCATION THREADING ACROSS NI-CU INTERFACE: A HYBRID ATOMISTIC-CONTINUUM APPROACH Shehadeh, M.; Lu, G.; Kioussis, N.; Banerjee, S.; Ghoniem, N.	MULTI-SCALE STRESS ASSESSMENT IN RANDOM MEDIA * Lipton, R.
TRANSPORT AND COUPLED PROCESSES IN MICRO- AND NANOTECHNOLOGY — Chair: Povitsky, Co-Chair: Melnik					
Los Angeles Room	NUMERICAL PROTOTYPE AND OPTIMIZATION OF MICROFLUIDIC MIXER * Ma, Y.; Ho, C.	MAGNESIUM PHTHALOCYANINE (MGPC) THIN FILMS AS NANOMATERIALS Puri, M.	MOLECULAR DYNAMICS SIMULATION OF POISEUILLE FLOW IN MICROCHANNELS WITH COMPLEX CROSS SECTIONAL SHAPE * Song, X.; Chen, J.	DESIGN OF NANOPARTICLE FOCUSING LENSES FOR IN-SITU NANOPARTICLE MEASUREMENT AT LOW PRESSURE CONDITION Choi, J.; * Cho, D.; Na, J.; Kim, Y.; Kim, T.	NUMERICAL SCHEMES FOR THREE DIMENSIONAL IRREGULAR SHAPE QUANTUM DOTS * Hwang, T.; Wang, W.
ENRICHED FINITE ELEMENT METHODS FOR EVOLVING DISCONTINUITIES AND INTERFACES (SANCTIONED BY THE IUTAM THROUGH THE COOPERATIVE AGREEMENT BETWEEN IACM AND IUTAM) — Chair: N. MOES, Co-Chair: J.DOLBOW					
Beverly Hills Room	EVALUATION OF J-INTEGRAL FOR SURFACE CRACKS USING X-FEM * Nagashima, T.; Miura, N.	COMBINED HYBRID CRACK ELEMENT AND XFEM FOR FRACTURE OF BRITTLE MATERIALS Karihaloo, B.; * Xiao, Q.	X-FEM SIMULATION OF PLASTIC FATIGUE CRACK GROWTH Gravouil, A.; * Elguedj, T.; Combescure, A.	ULTIMATE LOAD COMPUTATION : EFFECT OF SURFACIC DEFECTS AND ADAPTIVE TECHNIQUES Brancherie, D.; Dambrine, M.; Vial, G.; Villon, P.	SINGULARITY ENRICHMENT FOR COMPLETE CONTACT SLIDING PROBLEMS USING X-FEM * Giner, E.; Sukumar, N.; Fuenmayor, F.; Tarancon, J.
MODEL UPDATING AND EXTRAPOLATION UNDER UNCERTAINTY — Chair: Vicente Romero, Co-Chair: Francois Hemez					
Constellation Ballroom I	A METHOD FOR COMPUTATIONAL PREDICTION INVOLVING EXTRAPOLATION WHEN THE COMPUTATIONAL MODEL IS NOT COMPLETELY ACCURATE * Rutherford, B.	DEFLECTION PREDICTION FOR PRESTRESSED CONCRETE GIRDERS USING A BAYESIAN UPDATING METHOD * Chen, X.; Sheng, C.; Jacobs, L.	A METHOD FOR FEM-EMA CORRELATION AND APPLICATIONS FOR AUTOMOTIVE DOOR ASSEMBLY. * Choi, J.; Jun, I.; Cho, m.	PARAMETER ESTIMATION AND UNCERTAINTY QUANTIFICATION WITH A BAYESIAN INFERENCE APPROACH FOR SHOCK-WAVE SIMULATIONS * Kao, C.; Williams, B.	POWER/EFFICIENCY OPTIMIZATION OF A METAL HYDRIDE SORPTION COOLER UNDER QUANTIFIED DESIGN UNCERTAINTY * Lloyd, G.

Friday, July 21

Session F2: 10:50 — 12:40

	10:50	11:12	11:34	11:56	12:18
MATHEMATICAL AND COMPUTATIONAL ASPECTS OF MULTI-SCALE AND MULTI-PHYSICS — Chair: Wolfgang Wall, Co-Chair: Ekkehard Ramm					
Santa Monica Room	APPROXIMATING FLOW AND TRANSPORT EQUATIONS BY A FIRST ORDER CORRECTOR FORMULATION * Sviercoski, R.; Travis, B.				
TRANSPORT AND COUPLED PROCESSES IN MICRO- AND NANOTECHNOLOGY — Chair: Povitsky, Co-Chair: Melnik					
Los Angeles Room	NUMERICAL ALGORITHMS FOR MHD OF FLOWS OF ABLATED MATERIALS * Samulyak, R.; Du, J.; Lu, T.	KINETIC THEORY ANALYSIS OF LASER ABLATION IN SYNTHESIS OF CARBON NANOTUBES * Shusser, M.	VORTICITY DEPOSITION IN LASER-ABLATED PLUME AND EFFECT ON PLUME SHIELDING * Povitsky, A.; Zinovik, I.	MOLECULAR DYNAMICS INVESTIGATION OF HYDROGEN TRANSPORT AND STORAGE INSIDE CARBON NANOTUBES IN PRESENCE OF ELECTROSTATIC FIELD * Banerjee, S.; Murad, S.; Puri, I.	MATHEMATICAL MODELING AND NUMERICAL SIMULATION OF CHARGE TRANSPORT IN IONIC CHANNELS Sacco, R.; Chini, B.
NUMERICAL AND COMPUTATIONAL ASPECTS OF INTERFACE PROBLEMS AND APPLICATIONS — Chair: Frederic Gibou, Co-Chair: Christian Ratsch					
Beverly Hills Room	**KEYNOTE:** STRAIN IN THIN FILMS: ACCELERATED COMPUTATION AND PATTERN FORMATION * Caflisch, R.		EFFICIENT COMPUTATION OF EPITAXIAL GROWTH BY KINETIC MONTE CARLO * Smereka, P.; Devita, J.; Sander, L.; Russo, G.	AB INITIO STEP FLOW MODELS - A MULTISCALE APPROACH TO EPITXIAL GROWTH * Voigt, A.; Balykov, L.; Hausser, F.	A SECOND ORDER ACCURATE PROJECTION METHOD FOR THE INCOMPRESSIBLE FLOWS ON FULLY ADAPTIVE GRIDS * Min, C.
PARTITION OF UNITY AND EXTENDED FINITE ELEMENT METHODS: ADVANCED TECHNIQUES AND APPLICATIONS — Chair: Giulio Ventura, Co-Chair: None					
Constellation Ballroom I	HP PARTITION OF UNITY FOR SOLVING SCHRÖDINGER EQUATION IN QUANTUM MECHANICS * Chen, J.; Hu, W.	XFEM-FSI Belytschko, T.; * Wang, H.; Chessa, J.	A STUDY ON EMBEDDED DISCONTINUITIES FINITE ELEMENT TECHNIQUE * Qing, Z.; Xiaozhou, X.	COMPUTATIONAL DESIGN OF CERAMIC COMPOSITE MATERIALS WITH ENRICHED FINITE ELEMENT METHODS * Chessa, J.; Gonzalez, M.; Petla, H.	NEW METHODS TO REPRESENT PROPAGATING CRACKS WITH LEVEL SETS * Duflot, M.

polarization anizotropy in [001] plane
Phys. Rev B 71, 2005 (Buster, Zunger)

Friday, July 21

Session F3: 14:20 — 16:10

	14:20	14:42	15:04	15:26	15:48
COMPUTATIONAL NANOTECHNOLOGY WITH THE ENHANCEMENT OF HIGH-PERFORMANCE COMPUTING — Chair: Michael Leamy, Co-Chair: Shaoping Xiao					
Santa Monica Room	**KEYNOTE:** COMPUTING ISSUES IN COMPUTATIONAL NANO- MECHANICS AND MATERIALS SCIENCE DOMAIN AND ONE POSSIBLE SOLUTION 6.1 mln atoms — 1000 mln atoms Wang, S.; * Xiao, S.; Ni, J. the matrix of order 400 mln		A GENERALIZED CELL-LISTING REDUCTION FOR MOLECULAR DYNAMICS SIMULATION * Wang, D.; Hsiao, F.	NON-LOCAL QUASICONTINUUM METHOD FOR DEFORMATIONS OF CARBON NANOTUBES * Park, J.; Kim, S.; Cho, Y.; Im, S.	NON-EQUILIBRIUM MOLECULAR DYNAMICS SIMULATION OF NANOJET INJECTION: ITS DEVIATION FROM THE CONTINUUM APPROACH * Shin, H.; Yoon, W. Gomez Navarro Nature 20nm
TRANSPORT AND COUPLED PROCESSES IN MICRO- AND NANOTECHNOLOGY — Chair: Srivastava, Co-Chair: Povitsky					
Los Angeles Room	QUANTUM SIMULATIONS OF ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES IN CONVENTIONAL AND NOVEL NANOSCALE DEVICES * Ahmed, S.; Anantram, M.; Neophytou, N.; Korkusinski, M.; Klimeck, G.	NUMERICAL SIMULATION OF DIFFERENT-SIZED QUANTUM DOT ARRAY * Wang, W.; Hwang, T. 300 mln	TUNNELING THROUGH MODULATED NANOWIRES USING MODIFIED WANNIER STATES * Lassen, B.; Pedersen, J.; Willatzen, M.; Wacker, A.	MULTIPHYSICS MODELING OF HETEROJUNCTION QUANTUM DOTS * Melnik, R.; Lew Yan Voon, L.; Mahapatra, R.; Eying, K.; Pitz, J.	FLOW IN NANOTUBES BY STOCHASTIC ROTATION DYNAMICS ALGORITHM * Madadi, M.; Mehrabi, M.
NUMERICAL AND COMPUTATIONAL ASPECTS OF INTERFACE PROBLEMS AND APPLICATIONS — Chair: Christian Ratsch, Co-Chair: Frederic Gibou					
Beverly Hills Room	A HYDRODYNAMIC MODEL FOR THE GROWTH AND DYNAMICS OF BACTERIAL COLONIES * Lega, J.; Passot, T.	A MULTISCALE MATHEMATICAL MODEL OF CANCER GROWTH. * Colin, T.; Bresch, D.; Grenier, E.; Ribba, B.	LEVEL SET METHOD FOR BIFLUID FLOWS IN MICROCHANNELS * Galusinski, C.; Khadra, K.; Vigneaux, P.	MOMENT-OF-FLUID INTERFACE RECONSTRUCTION * Dyadechko, V.; Shashkov, M.	DISCRETIZATION OF DIRAC DELTA FUNCTIONS IN LEVEL SET METHODS Tsai, R.
PARTITION OF UNITY AND EXTENDED FINITE ELEMENT METHODS: ADVANCED TECHNIQUES AND APPLICATIONS — Chair: Jack Chessa, Co-Chair: None					
Constellation Ballroom I	MESHFREE MULTIGRID METHODS WITH DISTANCE FIELDS Tsukanov, I.; * Shapiro, V.	DYNAMIC CRACK PROPAGATION IN THIN SHELLS WITH THE PHANTOM NODE METHOD Belytschko, T.; * Song, J.	P-ADAPTIVE CK GENERALIZED FINTE ELEMENT METHOD FOR ARBITRARY POLIGONAL CLOUDS * Barros, F.; Barcellos, C.; Duarte, C.	APPLICATION OF THE EXTENDED FINITE ELEMENT METHOD FOR THE SIMULATION OF CONCRETE * Unger, J.; Könke, C.	X-FEM COUPLED WITH X-RAY MICROTOMOGRAPHY FOR 3D FATIGUE CRACK GROWTH SIMULATION Buffiere, J.; * Gravouil, A.; Ferrie, E.; Ludwig, W.

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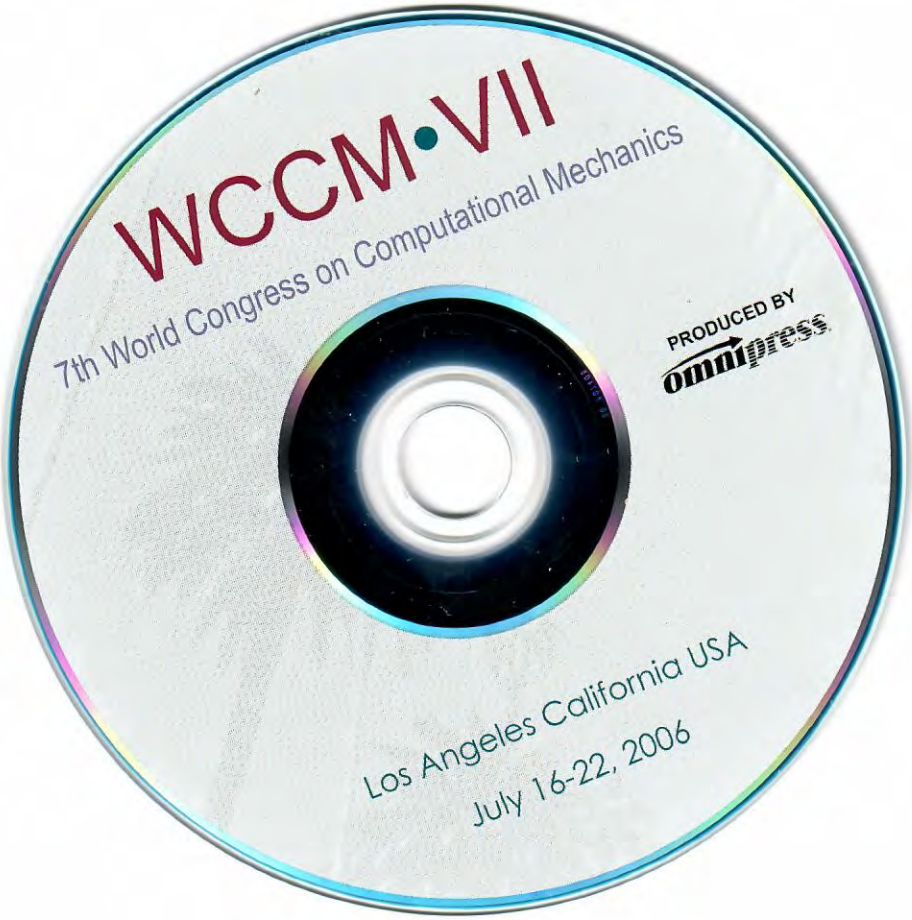
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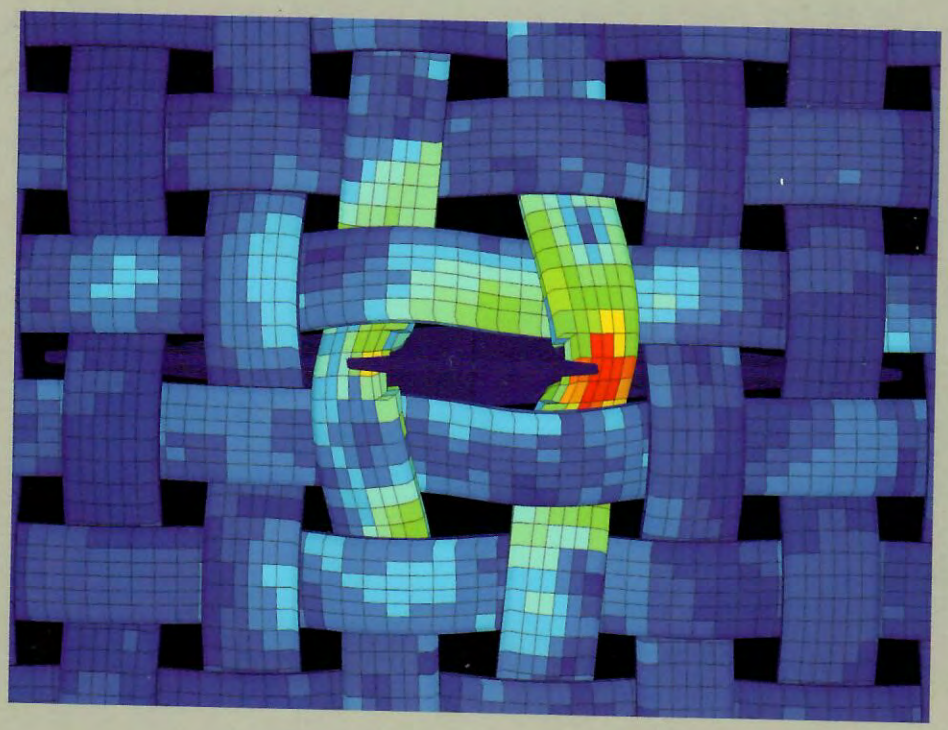

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Cover Image: Yarn failure and element stress distributions during simulation of knife penetration into a woven fabric. This image is used with the permission of W.M. Gao. For more details, see Paper 90.

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Contents

Preface

I **Computation**
Service-Lives
Session organ

1 Life Predictio
I. Mura

2 Damage Simu
Y.S. Petryna,

3 Damage Toler
C. Könke

4 A Finite Elem
Retrofitted wi
W.B. Almajed

5 Stochastic Sim
Concrete Sho
J. Li and Y. C

6 Inelastic Anal
CFRP
W.A. Thanoon

7 Nonlinear Dam
Wall Specimen
J. Li and Y. C

8 Simulations o
Polymer Bridg
W.I. Alnahhal

9 Seismic Resis
C. Butenweg

10 Multi-Objectiv
Damage Resis
M. Corvino, L

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on Computational Structures Technology,
B.H.V. Topping, G. Montero and
R. Montenegro, (Editors),
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Paper 99

Modelling Frequency Adjustment Effects Using Shape Memory Alloy Oscillators

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Keywords: vibration tuning, frequency adjustment, shape memory alloys, hysteresis.

Mechanical vibrations constitute a common phenomenon in applications of many engineering structures and systems. The result of such vibrations is usually desired to be tuned according to a specific application. In many application developments, a supplementary oscillator with a suitable frequency is attached to the primary system, by which the primary vibration can be tuned. For the cases where the primary vibration frequency is uncertain, it is always beneficial to make a supplementary vibration frequency continuously variable in a rather wide range. For construction of adaptive vibration absorbers, one kind of promising candidate material is shape memory alloys (SMA), because its stiffness can be varied by changing its temperature, due to its thermo-mechanical coupling properties [1–3].

In the present paper, we model the performance of a shape memory alloy oscillator used as a vibration absorber, which consists of a shape memory alloy rod and an end-mass. The vibration characteristic of the oscillator is continuously adjustable by changing its temperature, due to the thermo-mechanical coupling property of the shape memory alloy rod.

In order to capture the thermo-mechanical coupling property in the material, as well as hysteresis induced by phase transformations at low temperature, the mechanical behaviour of the SMA rod is first modelled using the modified Ginzburg-Landau theory by the following partial differential equation:

$$\rho\ddot{u} = \frac{\partial}{\partial x}\left(k_1(\theta-\theta_1)\varepsilon + k_2\varepsilon^3 + k_3\varepsilon^5\right) + \nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2} - k_g\frac{\partial^4 u}{\partial x^4}, \tag{99.1}$$

where u is the displacement of the rod, θ is its temperature, and $\varepsilon = \frac{\partial u}{\partial x}$ strain; ρ, k_1, k_2, k_3, ν and k_g are all material specific constants. The above model is shown be able to capture the thermo-mechanical coupling property and hysteresis induced by phase transformations, but its numerical analysis is not trivial [4].

For the convenience of the analysis, the above model is simplified. By taking into account the nature of the absorber, it can be approximated by the following model. representing a force-deformation relation for a nonlinear spring:

$$F_s = K_1\Delta\theta(x_p - x_a) + K_2(x_p - x_a)^3 + K_3(x_p - x_a)^5, \tag{99.2}$$

where K_1, K_2 and K_3 are physical constants of the SMA rod, x_p and x_a are displacements of the two ends of the SMA rod which give the measure of the rod deformation when its length is fixed. Using the above model, the governing equations of the entire system, including the primary system and the attached absorber, can be formulated as follows:

$$\begin{aligned} m_p\ddot{x}_p &+ c_p\dot{x}_p + k_p x_p - K_1\Delta\theta(x_p - x_a) + K_2(x_p - x_a)^3 + K_3(x_p - x_a)^5 = F(t), \\ m_a\ddot{x}_a &= K_1\Delta\theta(x_p - x_a) + K_2(x_p - x_a)^3 + K_3(x_p - x_a)^5, \end{aligned} \tag{99.3}$$

where m_p, k_p, and c_p are the mass, spring stiffness, and friction coefficient in the primary system, respectively; m_a is the mass in the absorber, and $F(t)$ is the excitation.

The performance of the SMA oscillator used as a vibration absorber is then simulated numerically using the developed model. It is demonstrated that the SMA oscillator can be adjusted to match various vibration frequencies by changing its temperature. It is shown that at high temperature, the SMA oscillator has a similar behaviour with linear vibration absorbers and the vibration of the primary system can be suppressed to a rather small value. The frequency response of the SMA oscillator also indicates a certain similarity between the (nonlinear) SMA absorber and linear ones. It is also demonstrated that at low temperature, the SMA absorber can be used as a general vibration damper, because it is able to dissipate energy due to the hysteresis. However, the frequency response of the absorber exhibits in this case a much more complicated behavior compared to its linear counterpart.

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Paper 274

Modelling and Analysis of PVDF Copolymer-Ceramic Composite Thin Films

D.R. Mahapatra and R.V.N. Melnik

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Keywords: piezoelectric, polymer, ceramic, free energy, poling, finite element modelling.

Polymer semiconductors and their composite variants with significant piezoelectric effect are considered as promising candidates to compete with the silicon based technology. Piezoelectric copolymer composite films, such as ultra-thin Langmuir-Boldgett films of PVDF and its copolymer with trifluoroethylene (P(VDF-TrFE)), ionic polymer, and electrostrictive elastomers have several potential applications, especially in photonics, biomedical devices, macromolecular assembly and smart structures. The category of polymer composites we are interested in this paper is the one in which the piezoelectricity, the electrical charge and the polymer dispersion interplay to produce a desired functionality. In the solid state, the dynamics of the piezoelectric copolymer (thin film) is governed by the deformation of the polymer chains which also undergo electrical polarization and transport of charge. Due to this coupled dynamics, the charge transport with dynamical changes in the conduction band of the polymeric network is of importance in photonics related applications. On the other hand, electrostriction induced mechanical motion and flexibility of the piezoelectric copolymer film is of importance for smart structural applications. Molecular level modelling of the dynamics and related observations have been reported in the literature. The macroscopic effect of linear piezoelectricity and electrostriction in piezoelectric composite structures have been studied widely. However, in polymer composites, the study of the effects which are important for small scale applications (e.g. flexible thin film device) has not been well reported in literature.

In this paper, a mesoscopic model and its finite element implementation are developed to study the dynamic visco-piezoelastic behaviour of a composite thin film made of PVDF copolymer and PZT ceramic particulate. Piezoelectric copolymers and blends we are interested in, such as PVDF-PTrFE with appropriate doping for controlled mechanical and electrical properties, are of substantial interest in microelectronics and other engineering applications. Ferroelectric ceramic particles, which can be used for doping a copolymer or a blend, have high dielectric, piezo and pyroelectric coefficients and high electromechanical coupling. However, they have poor mechanical strength, low reliability and high acoustic impedance. On the other hand, the PVDF based copolymers and reported blends have high relative compliance and flexibility and low density compared

to the piezoelectric ceramics. Therefore, an appropriate compositional structure of the above two can be useful in various applications. For processing a device-grade material, most often in the form of thin film, it is essential to polarize the polymer composite under strain. Here, the effect of the compositional variation on the effective properties are difficult to clearly identify from experiments alone. The reported studies in literature are either focused on the molecular dynamic aspect of the small-scale dynamics, as mentioned above, [1], or they are based on the linear model of piezoelasticity [2]. In addition, there are several other factors, such as the interfacial stress due to the film substrate, the free-surface energy and the dipole orientation and size dependent inhomogeneity, which can play important role in the overall structure and functions.

In order to develop a mathematical model including the above effects, first the free energy is constructed as a function of the strain, the effective polarization, and the assumed distribution functions of the polymer chains and ceramic particles in a cell. These distribution functions generally can vary over time and they are governed by the Smoluchowski equation for dispersed system [3]. Corresponding driving force includes the spatial derivative of the potential energy density. The potential energy density is expressed in terms of the bonded and nonbonded energy of molecular interaction in the cell, whereas their spatial gradient is transformed into the homogenized strain energy of the cell in the present model. Conservation laws are derived for the composite, which results in the thermomechanical equilibrium equation and the Maxwell equation of electrostatics. A coupled finite element model is developed with an element containing a number of cells. The continuum displacement, the temperature and the electric potential are determined by considering the quasi-three dimensional geometry of the thin film along with the substrate. A case of poling under controlled thermomechanical distribution over a randomly dispersed film is considered for numerical analysis. Various parametric effects of the resulting piezoelectric properties of the film under a number of poling cycles are analyzed and computational aspects of the developed code are discussed.

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ECF16

Failure Analysis of Nano and Engineering Materials and Structures

Program

Dimokritos 2, Thraki Palace Hotel

Morning Session

1. Fracture and Fatigue at the Micro and Nano scales

Chairs: I.M. Daniel (USA), A. Corigliano (Italy)

10:20

10:40 [190] **NANOINDENTATION OF CNT REINFORCED EPOXY NANOCOMPOSITES**
D. C. Lagoudas, P. R. Thakre and A. A. Benzerga

11:00 [246] **MICRO-SCALE SIMULATION OF IMPACT RUPTURE IN POLYSILICON MEMS**
A. Corigliano, F. Cacchione, A. Frangi and B. De Masi

11:20 [737] **DIFFUSION KINETICS AND MULTIVARIANT PHASE TRANSFORMATION IN SHAPE MEMORY ALLOYS**
D. Roy Mahapatra and R.V.N. Melnik

11:40 [745] **SIZE EFFECTS IN LEAD FREE SOLDER JOINTS**
A. Betzwar-Kotas, G Khatibi, A. Ziering, P. Zimprich, V. Groeger, B. Weiss and H. Ipser

Early Afternoon Session

34. Cracks in Micro- and Nanoelectronics

Chairs: B. Michel (Germany), J. Keller (Germany)

12:20 [332] **LOCAL STRAIN FIELD ANALYSIS**
B. Michel, D. Vogel, N. Sabate and D. Lieske

12:40 [295] **SIMULATION OF INTERFACE CRACKS IN MICROELECTRONIC PACKAGING**
J. Auersperg, B. Seiler, E. Cadalen, R. Dudek and B. Michel

13:00 [518] **AFM BASED FRACTURE ANALYSIS IN MICRO- AND NANOMATERIALS**
J. Keller, A. Gollhardt, D. Vogel and B. Michel

13:20 [461] **SIMULATION OF DEFORMATION AND FRACTURE BEHAVIOUR IN MICROELECTRONIC PACKAGING**
O. Wittler, H. Walter, J. Keller, R. Dudek, D. Vogel and B. Michel

13:40 [454] **EXPERIMENTAL INVESTIGATIONS FOR FRACTURE ANALYSIS OF SOLDER JOINTS IN MICROELECTRONIC**
H. Walter, C. Bombach, R. Dudek, W. Faust and B.Michel

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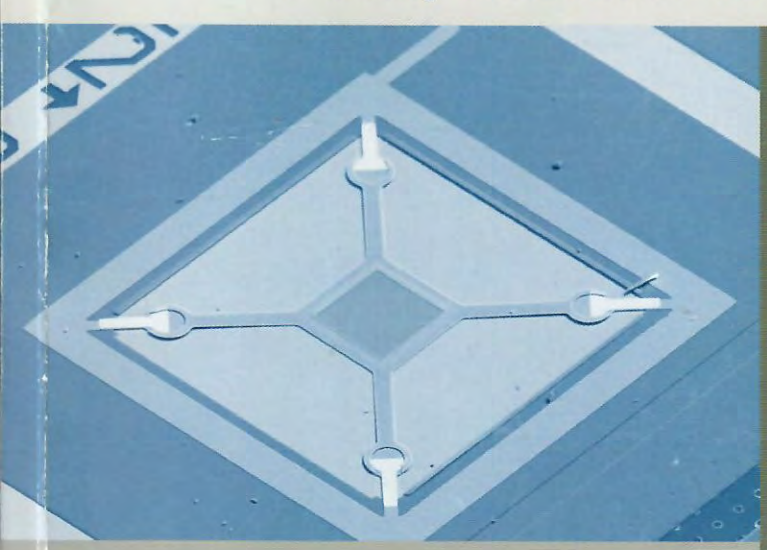

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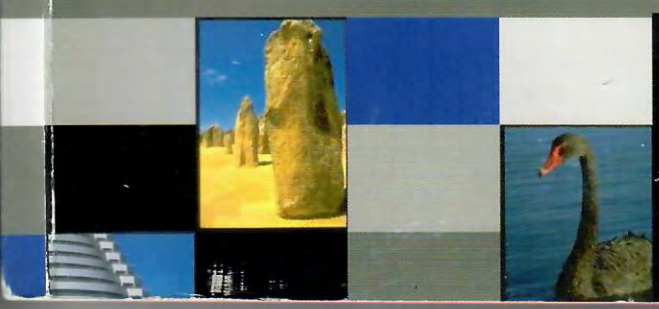

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17
665

Coupled Effects AlN/GaN Heterojunctions

Roderick V.N. Melnik[a*], D. Roy Mahapatra[a], M. Willatzen[b], B. Lassen[b],
L.C. Lew Yan Voon[c]

[a] *Wilfrid Laurier University, Waterloo, ON N2L3C5, Canada, Corresponding/presenting author:*
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[b] *Mads Clausen Institute, University of Southern Denmark, Denmark*
[c] *Department of Physics, Wright State University, USA*

Abstract

Wide bandgap wurtzite heterostructures such as AlN/GaN and ZnO/MgO are promising candidates for a number of optoelectronic device applications, where an accurate analysis of the optoelectronic properties is required. An illustrative study has been reported recently by us in [1] in the context of lattice misfit induced strain and piezoelectric effect on the resonant frequency. In many optoelectronics applications additional effects such as the charge density effect on the quantum-mechanical states may become important. Although it is well known (e.g., [2]) that the amount of net charges in the heterojunction determines the Fermi level energy of a device, what is much less understood is how strongly the strain and piezoelectricity influence the Fermi level and the evolved quantum-mechanical states. This aspect will become even more important as devices become smaller in size and more complex in shape. In this paper, we propose a self-consistent iterative scheme to analyze the coupled Poisson-Schrödinger model as an accurate representation of the mechanics of the heterojunction. The nonlinear integral for electron density $n(z)$, which acts as the coupling term, is evolved through iteration until equilibrium is reached. We restrict our attention to a three-layer system with a GaN well confined by AlN barriers (see Fig. 1). Based on the proposed self-consistent iterative scheme, we report the numerical results, which indicate significant deviation in the band structure compared to the usual one-step (not self-consistent) calculations. All the key effects, including lattice misfit, piezoelectricity and spontaneous polarization have been included in the calculations here. As seen from Fig. 2, the magnitude of strain changes drastically due to change in the mechanical boundary condition without any significant change in the electric potential. The results, that will be discussed, demonstrate also significant influence of charge density and piezoelectricity on the quasi-Fermi energy level (deviation > 100 meV when compared to one-step, non-consistent, calculations) and also concurrently on the electronic states. The proposed scheme is general enough to be employed for the analysis of complex device performance under various optoelectronic excitations.

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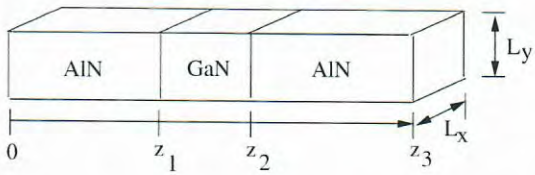


Figure 1: Three layer system with the GaN well in the AlN barriers.

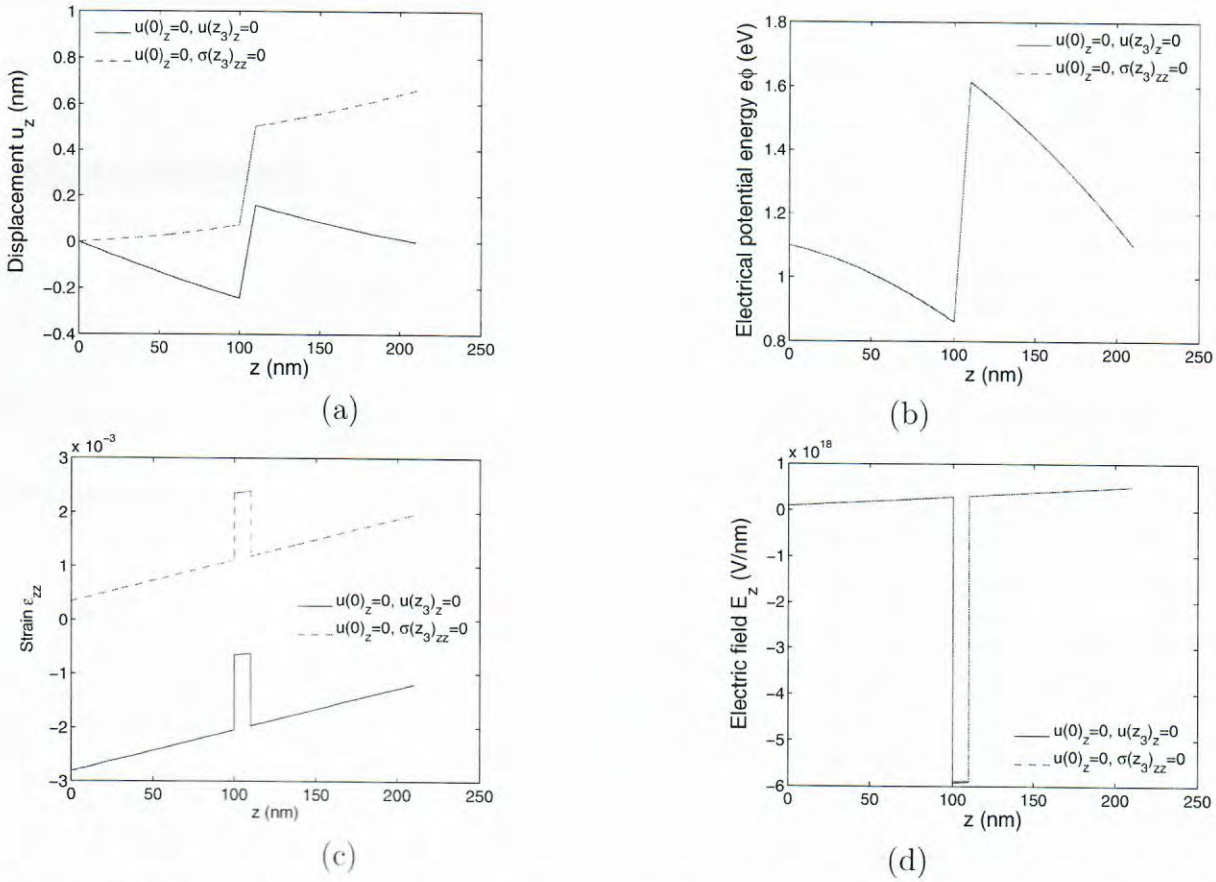
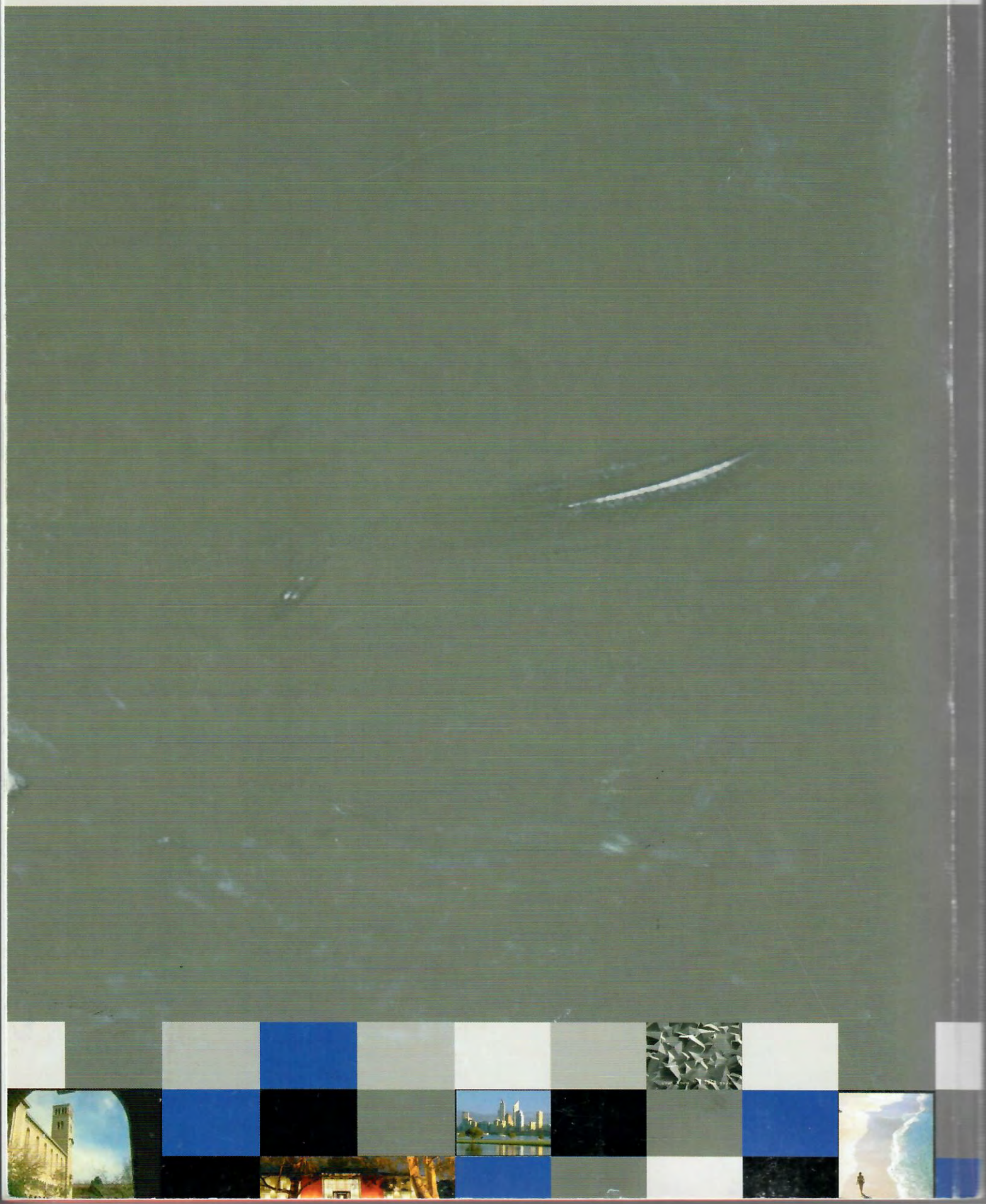


Figure 2: (a) Displacement u_z (b) electrical potential energy $e\phi$ (c) strain ε_{zz} and (d) electric field E_z under fixed-fixed and fixed-free boundary conditions applied at the two outer edges of the AlN barrier. Electric potential applied at the boundaries: $\phi(z=0) = \phi(z_3 = L_z) = 1.1/e$ V.



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Book of Abstracts

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when using chloroform matrix. Prepared layers can be used as an element of safety gas detection systems as well as low-cost analytical tool for different gas concentration during industrial chemical production. Sensor responses to hydrogen, nitrogen dioxide and alcohol vapours in air were also measured. The obtained results of dc sensitivity (S — i.e. ratio of resistance in "pure" air and that in analysed gas mixture): $S \sim 11$ to 10,000 ppm of hydrogen, $S \sim 1.5$ to 1 ppm of nitrogen dioxide, $S \sim 4$ to 40 ppm of methanol, $S \sim 5$ to 20 ppm of ethanol and $S \sim 6$ to 2 ppm of propanol.

Design and Optimisation of a MEMS-Based Tunable Fabry-Pérot Infrared Filter

Byron A. Walmsley, J.M. Dell, Yinong Liu, Xiao Zhi Hu, Mark B. Bush, L. Faraone; University of Western Australia, Australia

This study presents the theoretical design and analysis of a new surface micro-machined tuneable Fabry-Pérot (FP) infrared filter for adaptive infrared photon detectors. The proposed structure uses broad spectral range, high reflectivity distributed Bragg reflector (DBR) mirrors based on amorphous Si/air layers, resulting in very high finesse filters. The device utilises three sacrificial layers to define the air-gap in the DBR mirrors, the resonant cavity spacer, and the separation of the top mirror from the supporting flexures. The flexures are fabricated from low-temperature plasma-enhanced chemical vapour deposited (PECVD) silicon nitride (SiN_x) and Au thin films. Separation of the top mirror from the supporting flexures allows for improved fill-factors (up to 79%), as well as increased tuning range. Optical and finite element modelling of the device has shown large wavelength tuning ranges are achievable (1.5-2.5μm) at low actuation voltages (<15 V), whilst still maintaining high cavity finesse.

Temperature and Gravity Dependent *I-V* Characteristics of Organic Semiconductor Diode

S.A. Moiz[1], Kh.S. Karimov[2], M. Mehmood[1]; [1]PIEAS, Pakistan; [2]GIKI, Pakistan

In this study thin films of Poly-N Epoxipropylcarbazole (PEPC) doped by anthracene (An) were deposited over the surface of nickel substrate at different gravity conditions as 1g, 123g, 277g and 1107 g (where g = 9.81 m/sec). The Current-Voltage (*I-V*) characteristics of the devices (Ga/PEPC/Ni) were determined at different ambient temperature environment ranging from 30 °C to 60 °C with different gravity specifications. From the conductivity versus temperature response of the samples at different gravity conditions, derived from their *I-V* characteristics, it is observed that devices follow three dimension variable range hopping phenomena for their charge transport mechanism. By applying variable range hopping model, hopping conduction parameters of organic semiconductor material are estimated. From the results of these estimations, the dependence of electrical properties of the devices as a function of gravity as well as temperature is evaluated and discussed. It is also observed that device fabricated at 277g shows good electrical response as compared to the device fabricated at other gravity conditions.

Poisson-Schrödinger Model in the Analysis of Coupled Effects in Quantum Well Nanostructures

Roy D. Mahapatra[1], Roderick V.N. Melnik[1], Morten Willatzen[2], Benny Lassen[2], Lok Lew Yan Voon[3]; [1]Wilfrid Laurier University, Canada; [2]University of Southern Denmark, Denmark; [3]Wright State University, USA

In this contribution, we implement a self-consistent procedure for the solution of the Poisson-Schrödinger model applied here for the analysis of coupled effects in wide bandgap wurtzite heterostructures. Such effects are demonstrated on examples for three-layer systems, in particular AlN/GaN quantum well heterojunctions, which are promising components in a number of optoelectronic device applications. A major emphasis is given to the effects of boundary conditions, piezoelectricity and spontaneous polarization.

Numerical Modelling Study of the Sensitivity of SOS MOSFET Characteristics to Silicon Film Thickness and Back Surface Trapped Charge Variation

Karl Bertling, Aleksandar D. Rakić, Yew-Tong Yeow; University of Queensland, Australia

In this paper we present a numerical study of the sensitivity of silicon-on-sapphire MOSFET characteristics to silicon film thickness and back surface trapped charge. We demonstrate that the thickness of the film and the back surface trapped charge have a significant effect on the operation of the device and in particular the reduction of the threshold voltage.

Damage Mechanics and Experiments of Lead-Free Solder Alloy

Jun Zhou, WeiNa Hao, GuoZhong Chai; Zhejiang University of Technology, China

Based on DSCM (Digital Speckle Correlation Method), a novel video control experimental technique was developed for assessing mechanical behavior of SnAgCu solder alloy. A series of experimental tests in tension on a SnAgCu solder alloy have been conducted under various constant strain rates ranging from 10E-5/s to 10E-3/s and at 298K to 423K. The experimental results have revealed the presence of both the nucleation and growth deformation mechanisms of voids. A viscoplastic constitutive model with void damage, including strain softening and strain hardening, was developed for analyzing the effect of voids on reliability of lead-free solders. Based on the Gurson-Tvergaard plastic potential equation and orthogonal rules, the void volume fraction was used as damage variable and was introduced into the material constitutive law to simulate the macroscopic mechanical response of SnAgCu solder alloy under different temperature and strain rates. The simulation results compared with the experimental measurements. The predictions have shown the ability of the viscoplastic model coupled with void damage to correctly describe the experimental observations: nonlinearity, strain rate sensitivity and void damage evolution are well captured.

Investigation of Aging Effects in Porous Silicon

T.D. James, A. Steer, C.A. Musca, Giacinta Parish, A.J. Keating, L. Faraone; University of Western Australia, Australia

Porous silicon has many properties useful for optics applications, which include an ability to produce thin films with a wide range of refractive indices and the ability to easily fabricate multilayer structures. However porous silicon does have some non-optimal properties due to the very nature of its porous structure, namely its large surface area. The porous silicon surface is quite reactive making properties of porous silicon thin films, such as refractive index, unstable in an ambient environment. The purpose of this work is to investigate the aging of porous silicon and the effects of aging on the optical and physical properties of the thin films. Reflectance and FTIR spectroscopy are used to investigate the porous silicon layers by observing shifts in optical thickness and changes in chemical structure of the thin films. The aging process was simulated by annealing samples at temperatures such that only reactions that occur at room temperature were promoted.

Dark Current Modelling of Midwave Infrared HgCdTe Gated Photodiodes

R.J. Westerhout, C.A. Musca, J. Antoszewski, J.M. Dell, L. Faraone; University of Western Australia, Australia

HgCdTe midwave-infrared gated photodiodes were studied both experimentally and theoretically to determine the dark current mechanisms present under different surface conditions. By modifying HgCdTe photodiode equations to account for surface band-bending we are able obtain a first-order approximation to the behaviour of these gated photodiodes. A good fit to the data has been obtained for band-to-band tunnelling and surface generation-recombination current, but not for trap-assisted-tunnelling (TAT) current. This is attributed to the exclusion of interface states in the model, the complicated TAT behaviour, as well as two-dimensional effects.

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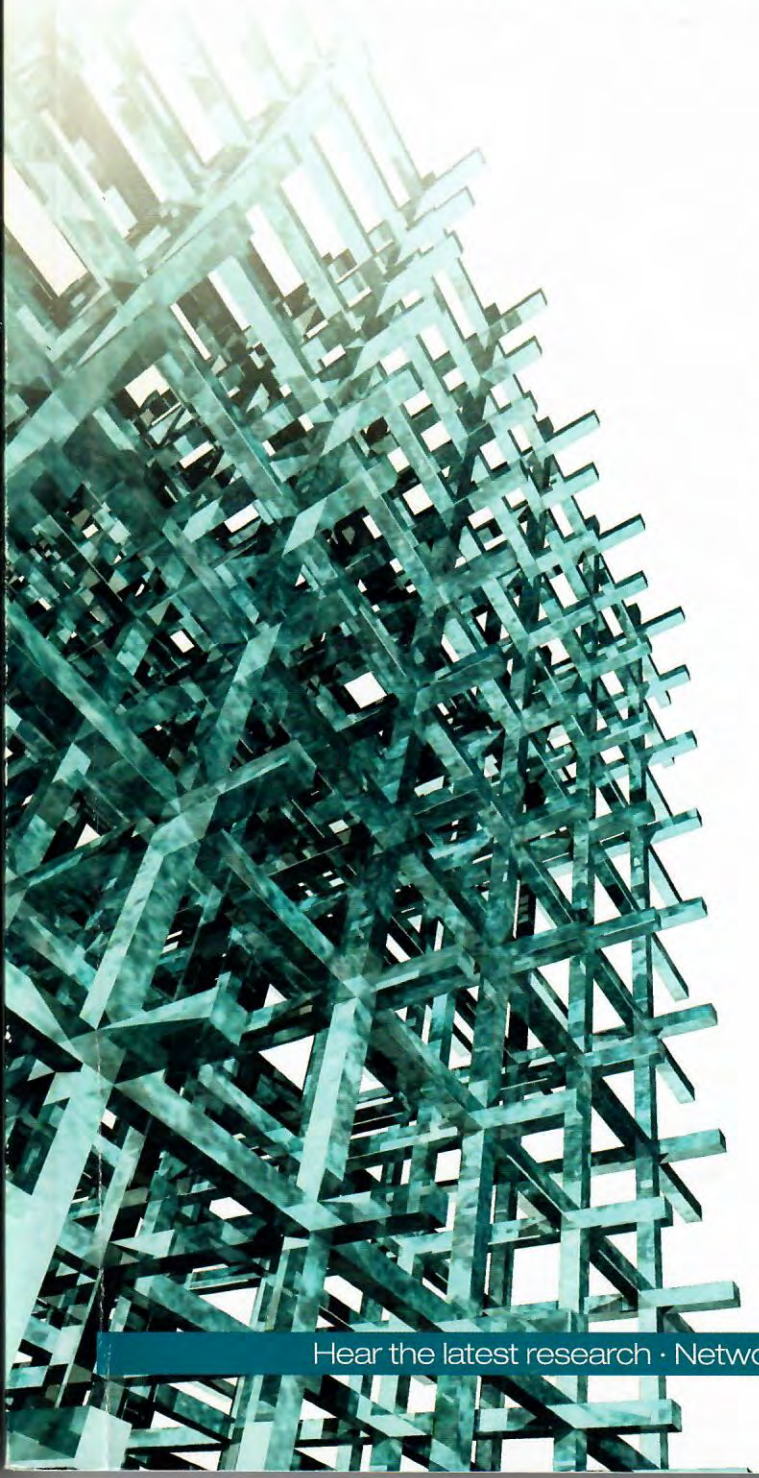

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closed position. When closed the fluid in the cell is displaced by the actuator and forced into the next sequential cell that is open. The unique pulse activated cell array format provides the ability to pump in a programmable x & y axis format.

6168-83, Poster Session

Mesoscopic dynamics of piezoelectric copolymer thin films

D. Roy Mahapatra, R. V. Melnik, Wilfrid Laurier Univ. (Canada)

Polymer semiconductors and their composite variants with significant piezoelectric effect are considered as promising candidates to compete with the silicon based technologies, especially for applications in bio-medical industry, micro/nano-scale molecular assembly, and self-sensing-actuating electronic systems. Up to date, several constitutive models have been proposed in literature for polymer chains in solvent as they are solidified. When the dynamics is studied, substantial efforts have been devoted to the analysis of the equilibrium conformations of the polymer chains and their brownian interactions in a non-Newtonian fluid. At the same time, it is known that in the solid state, the dynamics of the resulting active polymer (most often used as thin-film) are governed by the

deformation of the polymer chains that produces electric (or magnetic) polarization and surface charge. Hence, the resulting charge transport coupled with dynamical changes in the conduction band of the polymeric network is of vital importance from the device engineering viewpoint. If the charge transport (generally defined in terms of transport of the positive charges) in a polymer dominates over the molecular polarization such polymers are termed as ionic polymers. Our major focus in this studies is on another category of polymers where the piezoelectricity dominates the dynamics. Electroactive polymeric blends and copolymers based on PVDF provide typical examples of these materials where a large electrostriction (~5%) at ultra high frequencies (~1MHz) may be observed. In this context, a number of applications have already been reported where interaction of laser and UV radiation with piezoelectric polymer thin film is of significant interest. In this contribution, we develop a mesoscopic model of the coupled dynamics involving the time-dependent electromagnetics arising from the interaction of the excitation source term, nonlinear elasticity arising due to deformation of polymer chains, and charge transport. In the numerical studies, we consider electron-irradiated [P(VDF-TrFE)] copolymer, where the Gibbs free energy density is characterized by an ensemble average of conformational energies of the PVDF chains and interaction energies due to random numbers of Tr and FE doping in the blend. Since there exist multiple conformational states, the free energy density is homogenized over a mesoscopic scale. Based on this homogenized free energy density, we derive a new conservation-laws-based model. Numerical simulations aimed at identification of electrostriction patterns under different electric fields are also reported.

6168-84, Poster Session

A solid state actuator based on PEDOT/NBR system: effect of anion size of imidazolium ionic liquid

M. Cho, H. Seo, J. Nam, J. Koo, H. R. Choi, Y. Lee, Sungkyunkwan Univ. (South Korea)

The fabrication of dry type conducting polymer actuator was presented. In the preparation of actuator system, nitrile rubber (NBR) was used as a base material of the solid polymer electrolyte. Thin films of NBR (150 ~ 200 μm) were prepared by compression molding process. The conducting polymer, poly(3,4-ethylenedioxythiophene)(PEDOT) was synthesized on the surface of NBR by chemical oxidation polymerization technique, and the room temperature ionic liquids based on imidazolium salts, 1-butyl-3- methyl imidazolium X [where X= BF4-, PF6-, (CF3SO2)2N-], were introduced into the composite film. The effects of the anion size of ionic liquids on the actuator-displacement were investigated. The displacement increased with increasing anion-size of ionic liquids. The cyclic voltammetric responses and the redox switching dynamics of the actuators in different ionic liquids were studied.

6168-86, Poster Session

Deformation pattern of EAPap bending actuators with frequency and humidity

Y. Kang, W. Jung, Inha Univ. (South Korea); Y. Park, W. J. Craft, North Carolina A&T State Univ.; J. Kim, Inha Univ. (South Korea)

Electro-Active Paper (EAPap) made with cellulose is attractive as smart materials due to its merits in terms of lightweight, dry condition, large displacement output, low actuation voltage, low power consumption and biodegradability. We have observed a large bending deformation from EAPap actuators in controlled environment condition when an electric field was applied on the surface electrodes. So far, based on the cellulose structure and processing of cellulose-based EAPap, the bending deformation of the actuator is caused by the combination tion and the shear deformation of the EAPap material.

To investigate these actuation mechanisms, the deformation pattern of studied under the various parameters. The EAPap material has large region with disordered cellulose chains as well as the ordered crystal re water molecules including others can be easily detached to hydroxyl cellulose chains in the disordered regions. When an external electric fi plied, ions and water molecules can be mobile, and migrated to electr results in pure bending deformation of EAPap material due to the exp anode or cathode electrode. On the other hand, biopolymers including exhibit shear piezoelectricity due to the internal rotation of polar atom associated with asymmetric carbon atoms. Interestingly, the shear pie effect is related with the bending deformation on EAPap actuator. We ass this bending deformation caused by shear piezoelectricity in monomorpl cellulose material may not be pure bending shape. We expect that by in ing the bending deformation pattern, the migration and piezoelectric ef be determined. Experimental deformation pattern is studied with differe ity and frequency when the alternating current is applied to the EAPap and theoretical calculation will be followed.

6168-87, Poster Session

Effect of bending stiffness of the electroactive polyme element on the performance of a hybrid actuator syst (HYBAS)

T. Xu, National Institute of Aerospace; J. Su, NASA Langley Research C Jiang, P. W. Rehrig, TRS Technologies, Inc.; S. Zhang, T. R. Shout, Q. M The Pennsylvania State Univ.

An electroactive polymer (EAP)-ceramic hybrid actuation system (HYB developed recently at NASA Langley Research Center. This paper focus effect of the bending stiffness of the EAP component on the performa HYBAS and on theoretical prediction of that performance. For a consta modulus of the EAP component, the effects of length, thickness, and wi EAP component on the bending stiffness were studied. A theory based beam behavior was found to apply above a critical bending stiffness for irradiated P(VDF-TrFE) copolymer. For example, experimental data and cal modeling agree for a HYBAS with an EAP length to thickness rati However, the beam based theoretical modeling becomes invalid; i.e., the the HYBAS movement does not follow the prediction of theoretical modeli the bending stiffness is lower than a critical value. In this case, the EAP becomes an initially deformed beam. A shell based theoretical model nee developed for this situation.

6168-88, Poster Session

Polypyrrole actuators for micropump applications

J. Travas-Sejdic, P. A. Kilmartin, S. Valiavalappil, J. Hegewald, K. Li, C. S G. A. Bowmaker, R. P. Cooney, Univ. of Auckland (New Zealand)

Fluid handling devices are commonplace and traditional engineering app have enabled pumps to meet many needs. However, nearly all pumps 'moving parts' that generate wear from frictional losses. The problems ass with pumping small volumes and/or high pressures are also difficult to s from traditional engineering approaches. The aim of this programme is to a polymer-based pump which can be fabricated to move micro-/nano-lite tities of fluids with precision. Apart from nanotechnology applications, lab-on-chip designs, one possible application of such a pump is withir plantable device which could deliver very small quantities of a highly trated drug or hormone at a controlled rate.

Conducting polymer materials are attractive for such applications due to t voltage operation and the design freedom of the polymeric matrix. Here present our initial results on development of both macro- and micro-scale ing elements based on polypyrrole and substituted polypyrroles, including polypyrrole single-layer design and out-of-plane micro actuating element dard electrochemical methods, Raman spectroscopy, electron microsco mechanical-actuating testing techniques are used to evaluate the actuat ments properties. Preliminary experiments on hybrid conducting polym mer gel actuators will also be presented.

6168-89, Poster Session

New design concept for dielectric elastomer actuators

G. Kofod, Univ. Potsdam (Philippines); S. Bauer, VTT Processes (Finland) Johannes Kepler Univ. Linz (Austria); M. Paajanen, VTT Processes (Finlan

In this contribution we present a thermomechanically coupled material model for SMA based on the concept of Helm & Haupt [7] which includes the effect of pseudoelasticity as well as the shape memory effect and the external two way effect.

Experiments show that SMA materials exhibit deformations up to 20% strain if one takes into account the plastification phase which follows the austenite-martensite transformation.

For this reason we extend the latter model [7] within the scope of large strains.

Subsequently, the model is implemented into a FE code by using an innovative implicit time integration scheme.

The final aim of the research work is to investigate whether FE simulations of SMA applications, e.g. NiTI-stents and medical foot staples, should be based on large strain formulations.

If this was not the case the computational cost of such numerical investigations could be reduced significantly.

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6170-35, Session 6

Modeling the essential atomistic influence in the phase transformation dynamics of shape memory materials

D. Roy Mahapatra, R. V. N. Melnik, Wilfrid Laurier Univ. (Canada)

A physics based modeling framework to analyze the dynamics of multivariant phase transformation in three-dimensional samples of shape memory materials have been developed recently by these authors. The present paper is focused on linking the previously developed microscopic model with the atomistic reordering process that gives rise to self-accommodating microstructure. The microscopic model is based on a systematic representation of the Gibbs free energy in stress, temperature and n-dimensional order parameter space. Here n indicates the number of martensitic variants (M). Landau theory has earlier been successfully applied to solve the problem of phase-field evolution in phase transforming solids. In the context of diffusionless transformation in solids described by the Landau theory of first-order kinetics, the order parameters are the scaled ensemble averages of the atomic order variables. The diffusion kinetics model based on the time-dependent Ginzburg-Landau equation is thus the homogenized form of the spatio-temporal fluctuation due to atomic reordering. Our main objective in this paper is to study how this first-order kinetics influences the stress-temperature induced dynamics of phase transformation in microscopic and larger length-scales without attempting to solve a molecular dynamic problem in a coupled manner. This idea leads us to a thermodynamic conservation law whose characteristics are controlled by the phase kinetics. Numerical results show how this model captures the sharp interfaces and hysteretic cycles. However, while employing such microscopic model in predicting the response over large time-scales, one requires appropriate dislocation mechanisms to be accounted for. For this we turn back our attention to the dynamics of atomic ensamble by considering small clusters across grain boundaries. Depending on the

microscopic state in stress-temperature space, we introduce random dislocatio in the lattice structure and then employ a Density Functional Theory (DFT) to coup the dynamics of the clusters with the macroscopic model. This coupling is impl mented over discrete spatio-temporal scales in order to update the microscop model. Numerical simulations are reported for small samples with prescribed grai boundaries. Comparison between thermo-mechanical shake-down of Ni-Al, Ni- and Ni-Cu-Al alloys are reported.

6170-36, Session 6

Experimental test for numerical simulation of SMA characteristics and its simulation

M. Cho, S. Kim, H. Choi, Seoul National Univ. (South Korea)

Shape memory alloys(SMA) are metal alloys, which exhibit unique properties, th is, pseudo-elasticity, one-way shape memory effect(SME) and two-way shap memory effect(TWSME). SMA can exhibit interesting features such as diverse r sponses according to the induced temperature and stress. SMA changes its pro erties and material behavior progressively under cyclic loading conditions ar finally reaches stable path(state) after a certain number of stress/temperature loa ing-unloading cycles, so called 'training' completion. The presence of permane deformation, due to plastic strains or residual martensite variants during the m terial training, shifts the material characteristic curves of SMA wire.

Through the training and two-way experiments, SMA wire accumulates drast permanent (irreversible) deformation until experiencing about 50~100 cycles. A ter 300 training cycles, SMA wire is to be in a stable state. In this study, we mea sured its stress-strain curve in stable state. In addition, we observe other impo tant effects such as effect of stress induced during training, time rate of therm cycle, etc. until now, time rate of thermal cycle is not considered significantly ar only extremely slow time rate is considered in most SMA experiments and used SMA behavior simulations. Therefore to make the actuators using an SMA wi which has the fast response or short-time thermal cycle, these effects should b properly considered.

From the result of two-way experiment at each (short or long time) cycle in ph nomenological aspect, stress-strain-temperature relations and hysteresis charac teristics become changed. In short-time cycle, strain-temperature curve moves counterclockwise and the size of hysteresis envelop is large. As the time rate the thermal cycle increases, the size of the hysteresis envelop is getting small and strain-temperature curve moves along the clockwise direction above a ce tain cycle time. Above that thermal cycle time, hysteresis is fixed in the stab state. These new effects of SMA are investigated and the effect would be ex plained qualitatively.

The present work presents the experimental test using 1-D SMA wire throug two-way shape memory effect after training by thermal cycling. Through thes tests, we measured the characteristics of SMA. With the estimated SMA prope ties and effects, we compare the experimental results with the simulation result based on the SMA constitutive equation which is advanced ones including th training, thermal rate effect, etc.

6170-37, Session 6

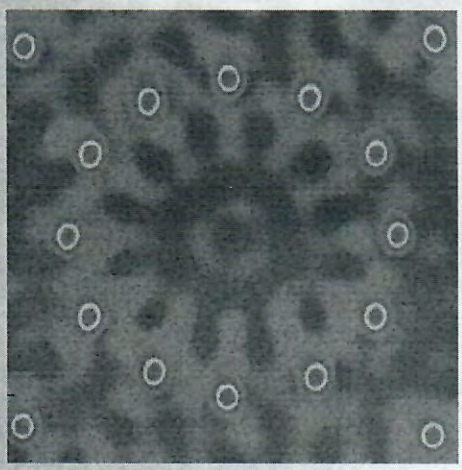
Properties of a high-temperature NiTiPd shape memory alloy in tension and compression

O. Rios, Univ. of Florida; G. Bigelow, R. D. Noebe, B. Lerch, NASA Glenn Research Ctr.; H. J. Seifert, Univ. of Florida

The numbers of specific designs and potential applications involving high-tem perature shape memory alloys have been growing in recent years, yet availabl materials for actual implementation in such plans are limited. Even in those case where promising new high-temperature shape memory alloys have been identi fied, the knowledge base for such alloys contains gaps crucial to the develop ment and implementation of these materials in actuation and other applications

We begin to address these issues by characterizing the mechanical and shap memory behavior of a Ni-30Pd-50.5Ti high-temperature shape memory alloy i both uniaxial tension and compression. Isothermal tensile and compression test were performed on the NiPdTi alloy in the martensitic and austenitic states. Whil superelastic behavior was not observed, a stress induced martensite was pro duced when the alloy was tested just above the austenite finish temperature. Thi stress induced martensite was not reversible upon unloading but could be recov

Abstract
Summaries



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- Getting Started
- Table of Contents
- Copyright
- Search

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Conference 6645: Nanoengineering: Fabrication, Properties, Optics, and Devices IV

6645-30, Session 6

Nanocoating stationary phase of MEMS-based preconcentrators and gas chromatography columns fabricated by layer-by-layer assembly of gold nanoparticles for high-speed chemical detection analysis

V. Jain, Virginia Polytechnic Institute and State Univ.; H. M. Yochum, Sweet Briar College; R. Montazami, J. R. Heflin, B. Alfeeli, S. A. Ali, M. Agah, L. T. Taylor, M. Ashraf-Khorassani, Virginia Polytechnic Institute and State Univ.

The layer-by-layer (LBL) assembly technique for adsorption of nanoscale layers has been used to form the stationary phase on the embedded walls of MEMS-based preconcentrators and multi-capillary columns for micro gas chromatography (GC). 20 and 30 nm gold nanoparticles (GNP) and 1,9-nonaedithiol have been used to deposit the LBL film stationary phase. High thermal stability for rapid heating and an easily modified active surface for gas trapping and desorption makes GNPs an ideal candidate for GC system. The thickness of the nanocoatings ranges from 10-500 nm, and it can be easily controlled in the range of 0.8 to \>50 nm per bilayer by varying the size of the gold nanoparticles. We have found that smaller nanoparticles (<30 nm) provide higher GC separation efficiency. In addition, the GNP coating on the embedded walls of a MEMS preconcentrator provides a large surface area for interaction with and trapping of gas molecules with projected detection limits in the low part-per-billion concentration range. The reduction in the overall mass of the structure allows rapid thermal desorption to generate narrow bands for injection into GC columns. The preconcentrator is fabricated using a silicon-on-glass process and has on-chip thermal control through integrated heaters and temperature sensors on the backside of the silicon wafer. This aids in reducing the separation speed by 3-4 times; making the separation of both n-alkanes from C5-C16 and polyaromatic hydrocarbons possible in less than 60 s. The ultimate goal is the development of a low-power, portable microscale fast gas chromatographic system for micrototal analysis systems (μTAS) to allow rapid, portable analysis of vapors in sample mixtures and for comparative analyses of mixture composites 'electronic nose' configurations.

6645-31, Session 6

In situ Raman scattering in nanomaterial flame synthesis

X. Liu, Rutgers Univ.

Non-intrusive, in-situ spatially and temporally precise Raman spectroscopy techniques were employed to diagnose the gas-phase synthesis of nanostructured materials. We demonstrated spontaneous Raman scattering measurements with high precision during the transition of gas-phase molecules to structured nanomaterials in strategically-chosen flame-based flow fields. Vibrational Stokes Q-branch Raman signals of major and minor species in the gas phase reaction were detected from a volume as small as 10E-12 m3. Temperature profile was determined by least-squares fitting the measured spectrum for N2 to a theoretical spectra library at different temperatures. The measurements were confirmed and combined with computational reaction fluid simulations to discover the complex mechanism behind the chemical and physical transitions. We also developed in situ laser characterization of the nano material growth by monitoring the Raman signature spectrum of interested solid particles. We finally showed the potentials of Raman scattering to combine with other techniques as a powerful tool to study the complicated two-phase related flame synthesis process.

6645-32, Session 7

Optics of thin-film silicon solar cells with efficient periodic light trapping texture

C. S. Haase, H. Stiebig, Forschungszentrum Jülich GmbH (Germany)

The interaction principle of light waves incident on a surface with a subwavelength nanostructure is a key question in the development of solar cells. Efficient thin-film solar cells based on microcrystalline silicon (μc-Si:H) or amorphous silicon (a-Si:H) with an absorber layer in the micrometer range require effective light trapping and an optimal in-coupling of the entire sun spectrum. The established approach to achieve this is the application of randomly textured transparent conductive oxides (TCO). The working principle of the nano-textured substrate is neither fully understood nor is it optimized yet. Previous investigations of light trapping in thin-film devices have been conducted with often misleading far field measurements. Optical simulations based on the Finite Integration Technique (CST Microwave Studios * (r)) are a valuable approach to analyze the light propagation in thin-film devices and study the subwavelength optics of nano-textured interfaces by solving the Maxwell equations rigorously in 3D. It allows investigating the near-field optics of a light trapping texture with a period size of ~ 1μm and considering the near-field phenomena, like optically confined modes. However, the question regarding the optimized lateral feature size, vertical height, resulting interface angle and shape of the texture is still unsolved but essential to reach high energy conversion efficiencies. Various texture designs are studied by numerical modelling using the optical constants of μc-Si:H determined at our institute.

We present a 3D simulation analysis of thin-film silicon solar cell nano-optics that gives clear design criteria for an efficient light incoupling and light trapping texture.

6645-33, Session 7

Tailored circular Bragg phenomena in TiO2 sculptured thin films through post-deposition processing

S. M. Pursel, M. W. Horn, A. Lakhtakia, The Pennsylvania State Univ.

Sculptured thin film (STF) technology is progressing from proof-of-concept experiments towards application-based devices. However, robustness and precise tuning may be needed to interface STF devices with other optical components and systems.

As deposited, PVD oxide thin films are often amorphous or nanocrystalline and may not be environmentally stable. Post-deposition annealing can be used to transform the material to a more stable crystalline state. In the circularly polarized transmittance spectrum of a TiO2 spectral hole filter before and after annealing, the location of the spectral hole (8 nm full width half max) is blue-shifted 16 nm upon annealing and x-ray diffraction verifies the transformation into a stable anatase structure. The retention and improvement of the circular Bragg phenomena as well as prediction of the associated shift may prove invaluable in making a commercial device.

Another post-deposition process that can be used to permanently shift the location of the circular Bragg regime is liquid chemical modification. This technique employs an acidic etchant to remove a small amount of material from the columns. The reduction in column diameter or change in relative index of the columns results in a well-controlled blue shift of the circular Bragg regime. After multiple immersions in HCl acid, the circularly polarized transmittance spectrum of an as-deposited "amorphous" TiO2 STF spectral-hole filter is blue-shifted 15 nm. In this paper, we will demonstrate the ability to tailor the Bragg phenomena through annealing and chemical modification.

6645-34, Session 7

Optoelectronic properties of ZnO/ZnMgO quantum well lasers with coupled self-consistent models

R. V. N. Melnik, Wilfrid Laurier Univ. (Canada); M. Willatzen, Syddansk Univ. (Denmark); D. R. Mahapatra, Indian Institute of Science (India); L. C. Lew Yan Voon, Wright State Univ.

Zinc oxide low dimensional semiconductors are materials with wide band gap and an increasing range of optoelectronics applications. Experimental evidence suggests that ZnO quantum-well (QW) lasers could, in a number of ways, outperform their GaN counterparts. Previous attempts to analyze lasing properties of ZnO/ZnMgO QW nanostructures belong to the Park's group (e.g., S.-H. Park, K.J. Kim, S.N. Yi, D. Ahn and S.J. Lee,

J. Korean Physical Soc., 47(3), 448-453, 2005).

While they did a multiband k.p theory of the gain spectrum, we note that they have not accounted for the coupling between elastic and

electric fields in a self-consistent manner, although piezoelectric and strain effect contributions influence the calculation of gain spectra.

In this contribution, we analyze the impact of both Schrodinger-Poisson and

piezoelectric couplings on the linear gain spectrum. Given the uncertainty in the band-structure parameters, we restrict our calculations to a simplified effective-mass band-structure model. In order to clarify the influence of self-consistency, many-body effects are left out. The results are reported for a QW laser nanostructure on a substrate consisting of the three main parts: two barriers of ZnMgO, each 100nm-thick, and one 10nm-thick well of ZnO.

6645-35, Session 7

Fabrication and characterization of silicon/silicon dioxide super lattices for silicon-based light-emitting devices

T. Creazzo, E. Marchena, B. Redding, T. R. Hodson, D. W. Prather, Univ. of Delaware

Silicon based light emitting materials are of particular interest for integrating electric and photonic devices into an all-silicon platform. The progress of nano-scale fabrication has led to the ability to realize silicon emitters based on quantum confinement mechanisms. Quantum confinement in nano-structured silicon overcomes the indirect bandgap present in bulk silicon allowing for radiative emissions. Two common structures that utilize the quantum mechanisms leading to light emission in silicon are nanocrystals embedded in silicon dioxide and silicon/silicon dioxide super lattices. Nanocrystals employ quantum confinement in three dimensions while the super lattice structure induces two-dimensional confinement. Strong photoluminescence (PL) has been demonstrated in both structures, confirming the presence of quantum confinement effects. Our super lattice structures are grown using plasma enhanced chemical vapor deposition (PECVD) with alternating layers of silicon and silicon dioxide. Sub-10 nanometer periods are confirmed via TEM and XRD studies. The PL dependence on layer thickness and annealing in super lattice structures is extensively investigated. While EL has been achieved in nanocrystals, it can be difficult to inject carriers due to the insulating characteristic of the oxide host. Super lattice structures hope to overcome this challenge by generating EL via lateral pumping where continuous a-Si layers circumvent the need for current to flow through oxide. This leads to the ability to design and fabricate a novel electrically pumped light emitting device on a silicon platform.

6645-36, Session 7

Function of bubble pit during readout process in PtOx type super-RENS disk

Q. Liu, The National Ctr. for Nanoscience and Technology of China (China); T. Fukaya, National Institute of Advanced Industrial Science and Technology (Japan)

In this study, the power threshold that can form recored bubbles for different cover thickness (40, 80, and 140nm)for PtOx super-RENS disk is investigated; transmittance and reflectance varying with CW-laser-irradiation time is recorded; the size and shape of the bubble before and after CW laser irradiation are measured by AFM. The optical response feature corresponding to the changes in size and shape of the bubble is also cleared. In addition, the relationship between readout times and bubble changes in size and shape of the bubble is discussed.

6645-37, Session 7

Narrowband, linear-polarization rejection filter based on columnar thin film superlattice

F. Chiadini, Univ. degli Studi di Salerno (Italy); V. Fiumara, Univ. degli Studi della Basilicata (Italy); A. Scaglione, Univ. degli Studi di Salerno (Italy); A. Lakhtakia, The Pennsylvania State Univ.

A composite structure obtained by depositing a TiO2 Columnar Thin Film (CTF) on a transparent glass substrate with a periodic array of rectangular grooves of infinite length is proposed as a narrowband, linear-polarization rejection filter.

The planewave response of the structure has been analyzed assuming the morphologically significant plane to coincide with plane of incidence.

Reflectance and transmittance spectra in the [800,900] nm wavelength range have been calculated with the assistance of the Floquet-Bloch theorem by solving the relate boundary-value problem using the Rigorous Coupled-Wave Approach.

The optical response has been systematically examined in relation to the polarization state of the incident plane wave, the radiation incidence angle, and the vapor flux angle used to fabricate the CTF.

Our results show that the proposed device rejects orthogonal linear-polarization states in different narrowband wavelength regimes. In particular, linear-polarization high-quality filters with extremely narrow bandwidths can be designed with the vapor flux angle for deposition of the CTF as the controlling parameter. The filter response can be further tuned by varying the angle of incidence.

6645-38, Session 8

Rational design of molecular self-assemblies for controlled surface patterning and molecular diffusion

D. Bléger, D. Kréher, F. Mathevet, A. Attias, Univ. Pierre et Marie Curie (France); G. Schull, L. Douillard, C. Fiorini-Debuisschert, F. Charra, Commissariat à l'Energie Atomique (France)

In order to create surface patterns, planar molecules with extended p-conjugated systems have found particularly wide use because they tend to bond in a flat-lying geometry, which allows functional groups at the molecule periphery to approach each other easily and to engage into non-covalent interactions, predominantly hydrogen bonds [1]. In this work, we developed an original approach, based on a new molecular unit designed both in order to act as a functional group used as a 'clip' between neighbouring molecules, and to pattern 2D supra-molecular architectures into specific arrangements. The opportunity to reach multiple and tunable topologies is evidenced by using scanning tunneling microscopy (STM).

More precisely, we present here first the design and the synthesis of the 'clip' based on a distyrylbenzene conjugated core and decyloxy peripheral chains. This functional group is specifically designed to ensure the recognition, mediated by the surface, of two 'functions'. In a second stage, different molecules incorporating one, two, and three 'clips' are synthesized. By using these compounds as mono- di- and trifunctional derivatives we obtained tunable dimeric organizations, polymeric-like topologies such as cyclic oligomers, linear chains as well as networks leading to controlled 2D molecular sieves [2]. We will focus on the size and shape selectivity of these sieves, and we will show that it is possible to confer a dynamics to such systems [3]. Various PAH systems differing either in shape or size were chosen as the guests. The comparison of their temperature-dependent hopping dynamics, either pure or co-adsorbed, reveals the physical mechanisms of the involved processes [4]. This allows to establish molecular-engineering rules for tuning cavity or channel selectivity, opening interesting perspectives for applications in various domains, from catalysis to biotechnologies.

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6645-39, Session 8

Fabrication of sub-diffraction-limit molecular structures by scanning near-field photolithography

G. J. Leggett, The Univ. of Sheffield (United Kingdom)

The integration of top-down (lithographic) with bottom-up (synthetic) methods remains one of the most important challenges in molecular

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679

Imaging techniques for supersonic combustion ramjet flows

Timothy J McIntyre, The University of Queensland, Australia
Kim M Hajek, The University of Queensland, Australia
Anne L Kovachevich, The University of Queensland, Australia
Halina Rubinsztein-Dunlop, The University of Queensland, Australia

Research in the Centre for Hypersonics at the University of Queensland has recently focussed on the study of flow through a supersonic combustion ramjet (or scramjet), a proposed hypersonic propulsion engine. The application of imaging techniques provides important data to complement the surface based probes that are normally implemented in ground based testing. Holographic interferometry and planar laser induced fluorescence (PLIF) techniques have both been applied to measure scramjet flows of models tested in the T4 shock tunnel facility.

Holographic interferometry offers the opportunity to make quantitative measurements of density in the flow with the restriction that it is a line of sight measurement technique. A system using a pulsed Nd:YAG laser was developed and measurements completed which visualised the flow including showing the position of shock waves due to the model and the presence of the fuel. The interferograms were analysed to provide density information about the flow.

In contrast, PLIF can be used to image more complex flows as only the gas in a laser sheet is imaged. Here, a tunable dye laser was used to excite the NO molecule and the resulting fluorescence was captured using an intensified CCD camera. This allowed the visualisation of the turbulent nature of the injected fuel but it is more difficult to obtain quantitative measurements.

The results showed that both techniques have their place in imaging these types of flows. Holographic interferometry was able to yield quantitative data averaged across the width of the flow. PLIF provided superior imaging capabilities but could not be implemented for quantitative measurements without the availability of further equipment.

680

Coupled Modeling Of Strained AlN/GaN Heterojunctions

Roderick Melnik, Wilfrid Laurier University, Waterloo, Canada
Roy Mahapatra, Wilfrid Laurier University, Waterloo, Canada
Morten Willatzen, University of Southern Denmark, Denmark
Lok Lew Yan Voon, Wright State University, United States
Benny Lassen, University of Southern Denmark, Denmark

A general three-dimensional model for the analysis of physical properties of AlN/GaN heterojunctions is presented. The model couples a multiband Schrodinger model with the Poisson equation for the electric field. The piezoelectric effect is taken into account by coupling the electric displacement to the mechanical strain in the structure via electromechanical constitutive relationships. We present results on the influence of mechanical strain and boundary conditions on the bandstructure calculation. In this context, we analyze in detail conduction and valance band energies as functions of strain and electric potential in the structure. This provides a further insight into optical properties of the structure, subject to changing electromechanical conditions. Finally, we discuss a possible extension of the presented model to account for dynamic effects.

681

Localization of polychromatic light in nonlinear photonic lattices

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Andrey A Sukhorukov, Nonlinear Physics Centre, RSPhysSE, ANU, Australia
Yuri S Kivshar, Nonlinear Physics Centre, RSPhysSE, ANU, Australia

The propagation of light in nonlinear photonic lattices has recently become a subject of intensive research. In addition to nonlinearity and the lattice depth, the light propagation is governed by two other factors: the light's wavelength and the lattice periodicity. In our work, we consider the effects that arise when changing both these factors.

We study the propagation of polychromatic light through a nonlinear photonic lattice and show that the spectrum of the light beam is greatly modified by the photonic lattice, as the blue part of the spectrum can localize into a spatial soliton, whereas the red part tends to diffract. This effect, which is, to a certain extent, present in homogenous nonlinear media as well, is drastically increased by the presence of the periodic structure.

Interfaces between two periodic lattices with different periodicity constants can be even more sensitive to changes in the light wavelength. In the linear case, light can be localized at an interface between the lattices of different periods creating the so-called surface states. If the two lattices have overlapping spectral gaps, nonlinear localization of light becomes possible even when the linear surface states are absent. If the periodicity constants are chosen adequately, it is possible to obtain a situation where the band gaps overlap for the blue, but not for the red part of the spectrum. Thus the blue part can develop into a soliton, whereas any localization of the red part is impossible. We present numerically calculated soliton solutions at the interface between nonlinear photonic lattices and show how the spectra of light beams propagating along the interface change.

682

Numerical simulation of spectral purity and dynamics in an injection-seeded pulsed optical parametric oscillator

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Pulsed optical parametric oscillators (OPOs) are useful coherent light sources for applications that require broad wavelength tunability and/or for access to wavelength regions in which there are no suitable lasers. However, OPOs have not reached their commercial potential to replace lasers in many such applications. This low acceptance may be attributed to several factors, particularly the requirement for high-quality pump lasers, the potential for optical damage to the nonlinear-optical (NLO) medium, and the complex and often unwanted behaviour that is associated with the NLO interaction.

Recently, there has been renewed fundamental interest in the performance of nanosecond-pulsed OPOs [1,2]. Effects such as frequency chirp, the breakdown of seeding during the output pulse, and reduction in backconversion have been observed under various operating conditions. Such effects offer fresh insight into the internal mechanisms at work in an injection-seeded pulsed OPO, thereby enabling us to improve the design and performance of such injection-seeded OPOs. The outcome is a low-chirp OPO system based on a periodically-poled KTiOPO4 crystal in a bow-tie cavity locked to the frequency of a narrowband cw laser that injection-seeds the NLO process; when pumped at 532 nm by a single-longitudinal-mode pulsed laser, the OPO generates pulses of narrowband signal and idler output radiation with nearly Fourier-transform-limited optical bandwidth.

Here we present new computer simulations of our high-performance OPO and compare the results with experimental data. These simulations confirm and help to explain various forms of dynamical behaviour (e.g., the transition from single-mode to multi-mode operation) that are observed in this OPO.

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[2] A. V. Smith, J. Opt. Soc. Am. B, 22, 1953 (2005)

683

Quantifying Orbital Angular Momentum Transfer in Optical Tweezers

Simon J W Parkin, The University of Queensland, Australia
Gregor Knöner, University of Queensland, Australia
Timo A Nieminen, The University of Queensland, Australia
Norman R Heckenberg, The University of Queensland, Australia
Halina Rubinsztein-Dunlop, The University of Queensland, Australia

Optical tweezers allow microscopic particles to be manipulated via the transfer of linear momentum from the trapping laser beam to the trapped particle. Advances in force measurement technology with optical tweezers enabled precision experiments in the microbiology field, for example resolution of single motor protein steps along microtubules. Optical tweezers can apply and measure forces due to linear momentum transfer, and this phenomenon has been greatly exploited. However, that they can also apply and measure torques due to angular momentum transfer has been much less exploited. In fact the total angular momentum transfer in optical tweezers has not yet been demonstrated. This demonstration is the subject of this presentation.

Light can carry angular momentum (AM) in two forms: spin (associated with circular polarisation) and orbital (associated with a helical wavefront). Spin AM can be easily transferred to optically asymmetric particles and can easily be measured through polarisation measurements. Orbital AM can also be transferred to the same particles and is particularly useful when the particle choice is limited to particles without a

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already spawned several micro devices for use in optical applications, including lenses, mirrors, waveguides, and gratings. A dispersive element has the functionality of separating input DWDM signal into its component wavelengths. To achieve this goal, an array of deformable grating light modulators is proposed. Arrays of grating light modulators are currently being developed for display applications 3,4. On the other hand, their use in DWDM applications has the potential of bringing high speed operation, low power consumption and good alignment sensitivity. We thus propose to develop a novel dispersive system for the purpose of realising the ubiquitous wavelength-selective switch. The possibility and limitation of integrating the grating light modulator array into wavelength-selective subsystem will also be examined. Numerical simulations are also being carried out to support experimental results.

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6415-66

Optical and micro-structural investigations in nanostructured doped PT and PZT piezoceramics

E. E. Dimitriu, REGO COM SRL (Romania); M. Sima, V. Ghiordanescu, National Institute for Materials Physics (Romania); R. Ramer, Univ. of New South Wales (Australia); G. V. Aldica, National Institute of Materials Physics (Romania)

An optical method for qualitative information concerning the electronic transitions in non-transparent piezoceramic materials is presented. The method is applied for investigation the electronic transition of poled lead titanate and lead titanate zirconate ceramics doped with rare earth and transitional elements, prepared by the oxide technique. The reflection spectra recorded in visible region have evidenced the presence of titanium, manganese and nickel ions in various oxidation states. Similarly, modifications of oxidation state of the additives in rare earth doped PT ceramics are confirmed by energy dispersive X-ray measurements. Inhomogeneities in the distribution of the elements concentration on the surface of piezoceramic samples, have also been reported. The electrical resistivity of a PZT relaxor material, investigated in the temperature range 20 - 500K, has revealed a metallic nonlinear dependence of resistivity as a function of temperature.

6415-67

Analysis of AlN/GaN quantum dots: coupled effects

R. V. N. Melnik, D. R. Mahapatra, Wilfrid Laurier Univ. (Canada)

We consider a general three-dimensional model for the analysis of physical properties of AlN/GaN heterojunctions. The model couples in a consistent manner a multiband Schrodinger model with the Poisson equation for the electric field, and the piezoelectric effect is taken into account by coupling the electric displacement to the mechanical strain in the structure via electromechanical constitutive relationships. We present results on the influence of mechanical strain and boundary conditions on the bandstructure calculation, including nonlinear situations. Further, for quantum dot structures, we analyze in detail conduction and valance band energies as functions of strain and electric potential.

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8.00-8.40 am	**Plenary lecture** **Nano-mechanics and multiscale problems** *Ken P. Chong* ***Chairmen: G.C. Sih, R. Ahuja***	Room A

8.45 –9.15 am	**Session IX :** **Films, layer and interface:** ***Chairmen:*** *Y.L. Bai, L. Nobile*	Room A	**Session X:** **Fatigue and crack growth** ***Chairmen:*** *T. Vu Khanh, L. Guerra Rosa*	Room B
9.15- 9.45 am	**Nanolayered MAX Phases from ab initio Calculations (96)** *R. Ahuja*		**Fatigue crack growth rate under constant amplitude loading and under tensile overloads in sheet and plate 2024 aluminum alloy (71)** *Al. Th. Kermanidis, V. K. Spiliadis, Sp. G. Pantelakis*	
9.45-10.05 am	**Two Dimensional kinetic growth on metallic and semi-conducting vicimal Surfaces = KMC simulations and rate equation approachs** *F. Dumont, C. Ramseyer, C. Girardet*		**A comparison of the fatigue behaviour of FSW and MIG weldments of two aluminum alloys (85)** *P. M. Moreira, M. A. V. de Figueiredo, F. M. F. de Oliveira, P. M. S. T. de Castro*	
10.05-10.25	**DFT Study of Interactions of Water on Kaolinite and Goethite Surfaces (97)** *D.Tunega*		**Micro-macro fatigue crack growth rate behavior of metal and polymer (10)** *G.C. Sih, H.F.Ren*	
10.25-10.45	**Modeling the adsorption of a herbicide on a carbon surface (98)** *P.Winkler R. Tscheliessnig, D. Tunega Martin H. Gerzabek*		**Application of ultrasound to accelerate fatigue (44)** *E. Statnikov, V. Ya. Korostel*	

10.45-11.05 am	Coffee break

11.05 –12.35 am	**Session XI :** **Films, layer and interface** ***Chairmen:*** *R. Ahuja, D. Tunega*	Room A	**Session XII:** **Crack models and solutions** ***Chairmen:*** *Y. Nadot, E. El Magd*	Room B
11.05 -11.35	**Plastic deformation and fracture of thin metallic films on annealing in terms of the multilevel model of a deformed solid (38)** *A.V. Panin, A.R. Shugurov*		**Fracture initiation at re-entrant corners: experiments and finite fracture mechanics predictions (45)** *A. Carpinteri, P. Cornetti, N. Pugno, A. Sapora, D. Taylor*	
11.35-11.55	**Elastic and plastic creep mechanism in thin metal films using FEM method (20)** *Ting-ting Dai, Li-Sha Niu*		**Buckling Analysis of Cracked Columns Subjected to Lateral Loads (48)** *L. Nobile*	
11.55-12.15	**Mesoscopic model for electroactive Composite Films and its applications (68)** *D. Roy Mahapatra, R.V.N. Melnik*		**Oscillating contact of isotropic elastic half-spaces (9)** *H. Y. Yu*	
12.15-12.35	**Micro-strain in copper sheets measured by X-rays diffraction (64)** *N. Hfaiedh, M. François, K. Saanouni*		**J-integral and CMOD for cracked cylinders (35)** *Miodrag Kiric*	

12.35-2.00 pm	Lunch
2.00-6.00 pm	Social program (see last page)
7.00- 8.00 pm	**Poster session**
8.00 pm	Banquet

MESO 2007 mechanics

May 13-17,

VVF les Badines, Presqu'Ile de Giens, 83408 HYERES LES PALMIERS, France

ABSTRACTS

SESSION XI

Plastic Deformation and Fracture of Thin Metallic Films on Annealing in terms of the Multilevel Model of a Deformed Solid

A.V. Panin* — A.R. Shugurov*

**Institute of Strength Physics and Materials Science SB RAS*
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ABSTRACT: The processes of plastic deformation of thin metal films subjected to thermal annealing, uniaxial tension and alternating bending are studied. The evolution of the film surface topography is examined with an atomic force microscope. The plastic flow in thin metal films under both thermal and mechanical loading is found to develop under conditions of the "chess-board" distribution of tensile and compressive normal stresses at the film-substrate interface and have a similar nature. It is shown that quasi-periodic folded structures revealing the regions, where compressive stresses reach their maximum values, are formed on the film surface in the course of loading.

KEY WORDS: Thin metal films; AFM; Annealing; Tension; Alternating bending; Plastic deformation.

Elastic and Plastic Creep Mechanism in Thin Metal Films using FEM Method

Ya-Xiong Zheng* — Li-Sha Niu* — Ting-Ting Dai* — Hui-Ji Shi*

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ABSTRACT: A whole process of the creep deformation in super-thin metal films is set up based on the study of the 2-D finite element simulation of the diffusional accommodated deformation mechanism. The simulation results present the diffusion of the point defects in grain interior. Complete creep curves are gotten by using the method above. A size dependence of the overall stress-strain response is then analyzed by altering one parameter like film thickness, grain size, loading condition, etc.

KEY WORDS: Films; FEM; Diffusion; Dislocation; Creep.

Mesoscopic Model for Electroactive Composite Films and Its Applications

D. Roy Mahapatra[a] and R.V.N. Melnik[b]

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ABSTRACT: A mesoscopic model to analyze various effects of electroactive and flow related properties of piezoelectric copolymer-ceramic composite thin film is reported in this paper. A three-phase composite with piezoelectric particulate phase, electroactive polymer phase and graft polymer-matrix phase is considered. The proposed homogenized constitutive model takes into account the local transport of cations in polymer, electrostriction and anhysteretic polarization. A finite strain description is given, which includes the mesoscopic dispersion of the copolymer chains. Finite element simulation is carried out by considering a P(VDF-TrFE)-PZT-Araldite thin film. Numerical simulations reveal diagonal shear band like patterns with small scale flow-induced regions.

KEY WORDS: Piezoelectric, polymer, mesoscopic, finite strain, thin film.

Micro-strains in copper sheets measured by X-rays diffraction

Neïla HFAIEDH* — Manuel FRANÇOIS* — Andrzej BACZMANSKI — Khémais SAANOUNI* — Krzysztof WIERZBANOWSKI****

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Authors wishing to contribute to the conference are invited to submit a two-page abstract to the conference chairman before 15 October 2006 The abstracts should be written in A4 paper (portrait orientation) with 2.5 cm margins. Times New Roman 12-point fonts should be used with single-line spacing. Abstracts will be evaluated by members of the conference scientific committee, and authors will receive notification of acceptance of their proposed contribution by 15 November 2006.

Full length papers should be received by the chairman of the organizing committee by 15 January 2007 so that there is enough time for the preparation of the volume of full papers, to be distributed to all participants.
Confirmation of participation will be required after the paper is accepted.

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Scope of the conference

Organic or inorganic substances form the basis of materials and structures that undergo a hierarchy of thresholds at the different scale although not all of them could be readily identified. The assessment depends on the size of region under consideration and the resolution of the microscopic or telescopic. Failure by cracking or by collapsing are common for materials and structures. Similar events are also known for the birth and death of distance stars and galaxies. For smaller bodies or devices, these thresholds may be less obvious. Recent interest in multiscaling has been centered on relating the behavior of the very small in contrast to the very large. In technical terms, reference can be made to bodies with large or small volume to surface ratios such that their mechanical and electrical behavior can be described by the bulk properties as an average or by the local properties of discrete particles recognizing that physical laws are not size scale invariant. Moreover,
there prevails a mesoscopic region where the particle and the bulk interplay. They lend to new behavior that were overlooked previously.
Such a dualism is not uncommon in many physical problems. The mesoscopic behavior may be loosely regarded as the transition from particle to continuum or vice versa. This transition is no doubt size and time scale size sensitive.
It can occur in solid and fluid. Topics associated with threshold phenomena are welcome for presentation in Meso 2007. They can include the following :

- Flow through capillary tubes in contrast to pipes
- Laminar and turbulent flow transition
- Heat convection of thin wire in contrast to cylinder
- Electrical conductance of macro- and nano-circuits
- Rubbery and glassy polymers
- Single- and poly-crystal behavior
- Strength of wires and round cylindrical bars
- Uni-axial and multi-axial material: linear and non-linear response
- Thin and thick plate behavior
- Brittle and ductile fracture
- Small and large crack growth behavior
- Low and high temperature effects
- Local and global material property characteristics
- Small and large bodies: size and time effects
- Specimen and structure

Related topics and those associated with life science are also welcome.
Aging of materials and animal or human cells may share a common threshold that divides longevity and early termination. Recent research on the "Klotho" gene speculates that it may be the blue print for a hormone to tell the body whether to "store" or "burn" energy. The parallel in material science would be the "available" or "dissipated" volume energy density that have been known to govern the failure behavior for a large class of materials ranging from linear to non-linear under general loading conditions and environment. Mechanics suggests that perhaps the time rate of the stored or burnt energy can be more decisive. Cell life may also be associated with a fatigue threshold as in metals. It may be linked to telomeres, the DNA at the end of chromosomes that becomes shorter whenever a cell splits in two. The establishment of a common ground for life and material science will no doubt also be confronted with the mesoscopic region. It is the lack of a precise knowledge of this transition that necessitates the notion of thresholds.

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ON PARABOLIC BOUNDARY VALUE PROBLEMS WITH SINGULARITIES ON DINI SPACE

MYKHAJLO MATIJCHUK

(CHERNIVTSY, UKRAINE)

In the cylindrical domain $Q = (0,T) \times \Omega \times E_1^+, \Omega \subset E_{n-1}$, $\partial\Omega = S$, the following linear and quasilinear boundary value problems are considered:

$$\frac{\partial u}{\partial t} = \sum_{|k|+2j=2b} A_{kj}(t,x) D_{x'}^k B_{x_n}^j u + f(t,x,u,u_x^{'},...,u_x^{(2b-1)}), \tag{1}$$

$$u|_{t=0} = \varphi(x), D_{x_n} u|_{x_n=0} = 0, B_{x_n} = D_{x_n}^2 + (2\nu+1)/x_n D_{x_n}, x_n \geq 0, \tag{2}$$

$$\sum_{|k|+2j=r_i<2b} b_{kj}^{(i)}(t,x) D_{x'}^k B_{x_n}^i u|_\Gamma = g_i(t,x,u,D_x^{r_i-1}u) \tag{3}$$

$$(i = \overline{1,bN}, \Gamma = (0,T) \times S, \nu \geq -\frac{1}{2}.$$

The Green quasifunction is constructed and an estimate of the solution is obtained for the linear problem under conditions that the coefficients of equations, boundary operators and S-surface belong to the corresponding Dini classes.

The system of solvable integral equations is associated with the quasilinear boundary problem by means of the Green quasifunction. The theorem on correctness of the problem is proved.

The problems with power singularities in coefficients associated with lower-order derivatives of equations and in boundary conditions are considered along with singularity of the coefficients of the problem on hyperplane $x_n = 0$.

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COUPLED SYSTEMS OF PDEs WITH APPLICATION TO DYNAMIC MODELING MATERIALS WITH SHAPE MEMORY EFFECTS

RODERICK MELNIK[1], LINXIANG WANG[2]

([1]WATERLOO, CANADA; [2]SYDDANSK, DENMARK)

Coupled dynamic systems of partial differential equations (PDEs) provide a foundation for many application areas in science and engineering [1,2]. Mathematical studies of such systems lead to very challenging problems, in particular when we have to deal with system nonlinearities in time-dependent situations. For a large class of nonlinear elliptic-parabolic

systems, such problems were analyzed by Professor I.V. Skrypnik and his collaborators [3].

In this contribution, we analyze another class of coupled nonlinear systems of PDEs arising in studying materials with shape memory effects [4-6]. Mathematically, the resulting models can be formulated as free boundary problems due to interfacial conditions between different phases of the material. Within the Landau framework of phase transitions based on non-monotone free energy functions, the systems of interest here are reducible to parabolic-hyperbolic equations and we discuss their mathematical treatments from both analytical and numerical perspectives.

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HOMOGENIZATION OF BOUNDARY VALUE PROBLEMS WITH NONLINEAR BOUNDARY CONDITIONS IN THICK JUNCTIONS OF TYPE 2:2:1

T. A. MEL'NYK

(KIEV, UKRAINE)

Multiscale modeling and computation is a rapidly evolving area of research that will have a fundamental impact on computational science and applied mathematics. This is connected with the prospect of development of more efficient methods that should be symbiosis of a new class of numerical and analytical modeling techniques. One class of multiscale problems is boundary-value problems in perturbed domains. There are many kinds of the domain perturbations and we need different asymptotic methods to study boundary-value problems in perturbed domains.

In recent years the interest in investigation of boundary-value problems in domains with rapidly oscillating boundaries has quickened in connection with the development of

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SOCIAL PROGRAMME

The Conference Social Programme includes a Reception Cocktail, a Dinner and a Farewell Cocktail (the Social Programme is not included in the reduced student fee).

Welcome Reception

The **Welcome Reception**, on Monday May 21st. evening, will take place in the premises of the *Archaeological Museum of Eivissa* (Museu Arqueològic d'Eivissa y Formentera)

Banquet Dinner

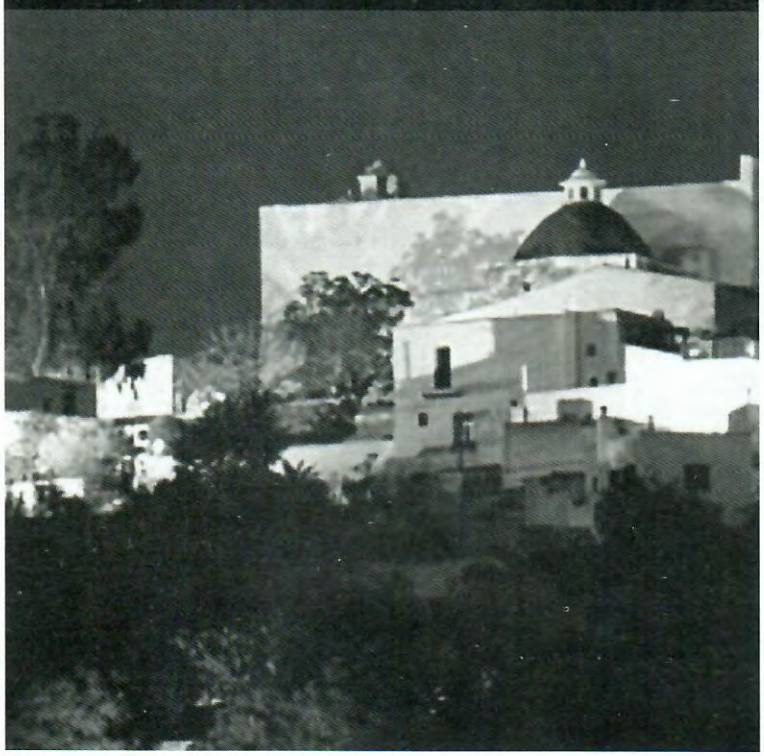
The **Conference Banquet Dinner**, on Tuesday May 22nd evening, will take place at *Can Part d'Atzaró,* a century old family finca.

Farewell Cocktail

Farewell Cocktail on Wednesday 23rd. afternoon at the Conference Venue.

Computational Methods for Coupled Problems in Science and Engineering II

Santa Eulalia, Ibiza, Spain, May 21-23 2007



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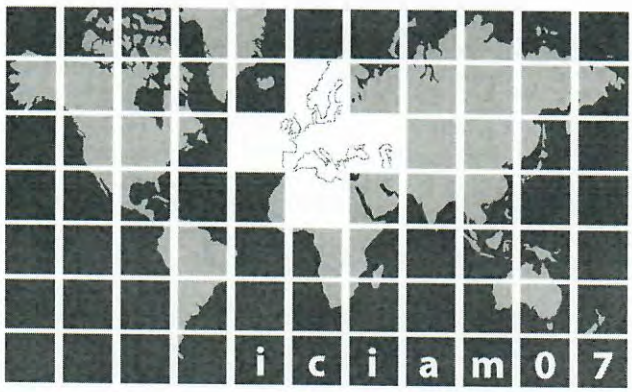

[ ] *Developments in algebraic multigrid methods for real-world applications.* **Luke Olson, Scott MacLachlan** CHN C 14 IC/MP131/020

[ ] *Nonlinear eigenvalue problems. #1* **Heinrich Voss, Elias Jarlebring** CAB G 51 IC/MP199/020

[ ] *Sparse grids for high-dimensional approximation. #1* **Michael Griebel, Markus Hegland, Christoph Schwab** KOH B 10 IC/MP1067/021

[ ] *Taylor-model methods and interval methods: applications. #1* **Markus Neher** HG E 3 IC/MP3861/024

[ ] *High-order methods for wave propagation and flow problems in complex geometries.* **Michael Dumbser, Eleuterio Toro, Claus-Dieter Munz** CAB G 61 IC/MP840/025

[ ] *Recent advances in front propagation modelling and applications. #2* **Maurizio Falcone, Regis Monneau** ETF E 1 IC/MP107/025

[ ] *Computational advances in evolving interfaces. #1* **Karol Mikula, James Sethian, Peter Frolkovič** KO2 F 150 IC/MP310/025

[ ] *Challenges for the accurate solution of Laplace eigenvalue and scattering problems.* **Timo Betcke, Lehel Banjai** KOL F 121 IC/MP196/026

[ ] *FETI, balancing, and related hybrid domain-decomposition methods. #2* **Axel Klawonn, Ulrich Langer, Barbara Wohlmuth** HG F 7 IC/MP205/026

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[ ] *Complexity of high-dimensional problems. #1* **Josef Dick, Frances Kuo** HG G 5 IC/MP102/015

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[ ] *Geometry, dynamics, and control. #2* **Dmitry Zenkov, Anthony Bloch** KOL H 312 IC/MP279/034

[ ] *Euler and space exploration. #1* **Martin Lo** KOL E 21 IC/MP40/036

[ ] *Mathematical models and computational methods for nano- and bio-technologies. #1* **Roderick Melnik, Jack Tuszynski** ML D 28 IC/MP344/036

[ ] *Recent advances in the analysis of nonlinear parabolic equations and their singular limits. #1* **Cyrill Muratov, Peter Gordon** KOL F 101 IC/MP264/040

[ ] *Quantum kinetic theory for Bose–Einstein condensation. #1* **Weizhu Bao, Hailiang Li** KOL G 217 IC/MP2055/042

[ ] *Navier–Stokes equations and related topics.* **Alex Mahalov, Yoshikazu Giga** KO2 F 174 IC/MP141/042

[ ] *Control problems for fluidodynamic models. #2* **Fabio Ancona, Benedetto Piccoli** KOL F 117 IC/MP317/046

[ ] *Boundary-value problems and integral equations. #1* **Pavel Krutitskii** KOL F 118 IC/MP417/015

[ ] *Bregman distances in optimization, inverse problems and financial mathematics.* **Elena Resmerita, Hansjoerg Albrecher** CHN F 46 IC/MP342/015

[ ] *Wavelet methods for real-world problems. #1* **Abul Hasan Siddiqi** KOL G 209 IC/MP73/054

[ ] *Approximation and analysis on the sphere. #1* **Ian Sloan, Douglas Hardin** HG G 60 IC/MP568/015

[ ] *Applied mathematics in Latin America: part 2.* **Domingo Tarzia, Julio Claeyssen** KOL G 221 IC/MP262/015

[ ] *Multigrid/multilevel approaches to the optimization of systems governed by partial differential equations.* **Robert Lewis, Stephen Nash** LFW C 4 IC/MP259/061

[ ] *Preconditioned iterative methods for PDE constrained optimization. #1* **Marcus Sarkis, Xiao-Chuan Cai** LFW B 1 IC/MP1050/043

[ ] *Control of deterministic systems under state constraints. #1* **Hélène Frankowska, Piermarco Cannarsa** KO2 F 175 IC/MP321/062

[ ] *Interior-point methods for model predictive control. #1* **Moritz Diehl, Steve Wright** HG F 30 IC/MP244/063

[ ] *Optimal control and stability analysis in dynamical systems, involving parameters.* **Mihai-Emilian Popescu** ML H 37.1 IC/MP704/063

[ ] *Shape and size in medicine, biotechnology and material Science. #1* **Vincenzo Capasso, Alessandra Micheletti** KOL F 104 IC/MP299/010

[ ] *Backward stochastic differential equations: simulations and applications.* **Emmanuel Gobet** LFW E 11 IC/MP586/013

[ ] *Probabilities meet scientific computing.* **Laurent Demanet, Lexing Ying** HG E 5 IC/MP163/015

[ ] *Geometric and stochastic aspects of the mechanics of complex bodies. #1* **Paolo Maria Mariano, Thomas Pence, Eric Vanden-Eijnden** KO2 F 152 IC/MP697/092

[ ] *Modeling, analysis and simulation of crystal defects: dislocation and surface step dynamics across the scales. #1* **Yang Xiang, Dionisios Margetis** HG E 7 IC/MP56/092

[ ] *Fast solvers for saddle-point problems with applications in fluid dynamics. #1* **Guido Kanschat, Maxim Olshanskii** HG D 5.2 IC/MP426/001

[ ] *Computational methods and investigations in cardiac modeling.* **Jacques Beaumont** CHN E 42 IC/MP243/012

ler discovered some three centuries ago, what we now call the L1, L2, and L3 *Lagrange Points*. Several of our speakers first introduced this approach to space mission design and will describe their latest work on the subject.

Although the dynamics of Euler's solutions play a fundamental role in the design of these trajectories, the use of advanced propulsion technology created many new and challenging problems. In particular the optimization of trajectories using low thrust ion engines is highly complex and interesting. Several of our speakers will address this problem.

Another interesting problem is the use of of satellites flying in formation around L2. They are typically used for astronomy missions that require long baseline interferrometers. Some of our speakers will describe the precision control of these formations in this highly nonlinear regime.

Euler would be delighted and amazed to find how his collinear orbits have made such a huge impact on space exploration and our understanding of the chaotic dynamics of the Solar System.

5218 *Space-craft insertion in unstable environments: application to formation flight near the libration points.* **Benjamin Villac** (UC Irvine, USA) IC/MT(MP40)4493/036

5219 *Invariant manifolds and the interplanetary super-highway.* **Martin Lo** (Jet Propulsion Laboratory, USA) IC/MT(MP40)4494/036

5220 *Leaving and reaching the moon from a libration-point orbit.* **Gómez-Muntané Gerard** (Universitat de Barcelona, Spain), Masdemont Josep (Universitat Politècnica de Catalunya, Spain), Elisa Maria Alessi (Universitat de Barcelona, Spain) IC/MT(MP40)4499/036

IC/MP344/036: Mathematical models and computational methods for nano- and bio-technologies. #1 ML D 28

Organiser: Roderick Melnik (Wilfred Laurier University, Canada)
Co-organiser: Jack Tuszynski (Cross Cancer Institute, Edmonton, Canada)

Most cutting edge developments that are taking place in nano and bio-technologies rely heavily on advances in mathematical modeling and computational methodologies. Examples include, but not limited to, new technologies based on low-dimensional semiconductor nanostructures such as quantum dots, nanotubes, sensors and actuators, drug discovery methodologies, protein- and macrotubule-based devices, techniques, and processes in designing biomolecular motors.

Development and integration of mathematical modeling techniques into these nano- and bio- technologies is an essential pre-requisite for further progress in this increasingly inter-disciplinary field. At the same time, problems that are arising from the development of new nano- and bio- technologies present challenges to applied mathematicians, stimulating advances in differential, difference, and integral equations, numerical analysis and computational mathematics among other fields.

This minisymposium has two aims. The first is to demonstrate some of the key mathematical and computational challenges associated with the state-of-the-art developments in new nano- and bio-technologies, focusing on several representative examples. The second is to expose the more technologically oriented part of the community to most advanced mathematical and computational techniques that are currently being developed in the field, and thus to encourage inter-disciplinary collaborations.

5221 *Multiscale simulations of complex materials for engineering and biological applications.* **Simone Melchionna** (Università degli Studi di Roma "La Sapienza", Italy), Efthimios Kaxiras (Harvard University, USA) IC/MT(MP344)2355/03

5222 *The role of nonlinearities in the biophysical properties of cytoskeletal components.* **Jack Tuszynski** (Cross Cancer Institute, Edmonton, Canada) IC/MT(MP344)2982/03

5223 *The walking molecules* kinesin *and* myosin. **Hannes Bolterauer** (Universität Gießen, Germany) IC/MT(MP344)3739/03

IC/MP264/040: Recent advances in the analysis of nonlinear parabolic equations and their singular limits. #1 KOL F 101

Organiser: Cyrill Muratov (New Jersey Institute of Technology, USA)
Co-organiser: Peter Gordon (New Jersey Institute of Technology, USA)

This minisymposium is devoted to recent advances in the analysis of reaction-diffusion and related problems which naturally arise in numerous applications such as combustion, phase transitions, and biological modeling. The focus of the talks will be on recent rigorous results on formation and global in time evolution of coherent structures. The first half of the talks will address problems of front propagation and failure in homogeneous and inhomogeneous media in the presence of advection. The second half will discuss a number of singular limits leading to the formation and non-trivial dynamics of topological defects, such as point defects, filaments and sharp reaction fronts. The analysis relies heavily on the tools of functional analysis, calculus of variations, maximum principle, and degree theory.

5224 *A variational approach to front propagation in infinite cylinders.* **Cyrill Muratov** (New Jersey Institute of Technology, USA) IC/MT(MP264)1071/04

5225 *Boundary layers and KPP fronts in a cellular flow.* **Alexei Novikov** (Penn State University, USA) IC/MT(MP264)1074/04

5226 *Traveling waves in a 2D cylinder with undulating boundary and their homogenization limit.* **Ken-Ichi Nakamura** (University of Electro-Communications, Japan) IC/MT(MP264)2062/04

5227 *Vortex and filament dynamics in Ginzburg-Landau theories.* **Giandomenico Orlandi** (Università degli Studi di Verona, Italy) IC/MT(MP264)1122/04

IC/MP2055/042: Quantum kinetic theory for Bose-Einstein condensation. #1 KOL G 217

Organiser: Weizhu Bao (National University of Singapore)
Co-organiser: Hailiang Li (Capital Normal University, PR China)

5546 *Automatic coarse-grid approximation for elliptic systems.* **Irad Yavneh** (Technion - Israel Institute of Technology) IC/MT(MP166)2521/027

5547 *Coarse-grid selection for systems of PDEs based on compatible relaxation.* **Robert Falgout** (Lawrence Livermore National Laboratory, USA) IC/MT(MP166)2581/027

IC/MP102/015: Complexity of high-dimensional problems. #2 HG G 5

Organiser: Josef Dick (UNSW Asia, Singapore)
Co-organiser: Frances Kuo (University of New South Wales, Australia)

(For abstract, see session #1 on page 329.)

5548 *Randomized algorithms and complexity for elliptic PDE.* **Stefan Heinrich** (TU Kaiserslautern, Germany) IC/MT(MP102)1256/015

5549 *A new quadrature using integration lattices.* **Xiaoyan Zeng** (Illinios Institute of Technology, USA) IC/MT(MP102)1345/015

5550 *Efficient randomized algorithm for L_∞ approximation over reproducing-kernel Hilbert spaces.* **Grzegorz Wasilkowski** (University of Kentucky, USA) IC/MT(MP102)1070/015

5551 *Algorithms for L_∞ approximation in the worst case setting.* **Frances Kuo** (University of New South Wales, Australia) IC/MT(MP98)940/021

IC/MP270/015: Computational topology and dynamics. #2 KOL F 109

Organiser: William Kalies (Florida Atlantic University, USA)
Co-organiser: Thomas Wanner (George Mason University, USA)

(For abstract, see session #1 on page 329.)

5552 *Homology algorithms and applications.* **Marian Mrozek** (Jagiellonian University, Poland) IC/MT(MP270)1193/015

5553 *Uncertainty quantification for homology computations.* **Thomas Wanner** (George Mason University, USA) IC/MT(MP270)4963/015

5554 *Rigorous continuation of equilibria of PDEs defined on rectangular spatial domains.* **Jean-Philippe Lessard** (Georgia Institute of Technology, USA), Sarah Day (College of William and Mary, USA), Marcio Gameiro (Rutgers University, USA), Konstantin Mischaikow (Rutgers University, USA) IC/MT(MP270)1628/015

5555 *Hyperbolicity, stability and monodromy of dynamical systems.* **Zin Arai** (Kyoto University, Japan) IC/MT(MP270)2608/015

IC/MP40/036: Euler and space exploration. #2 KOL E 21

Organiser: Martin Lo (Jet Propulsion Laboratory, USA)

(For abstract, see session #1 on page 329.)

5556 *BepiColombo gravitational capture and the elliptic restricted three-body problem.* **Stefano Campagnola** (University of Southern California, USA), Martin Lo (Jet Propulsion Laboratory, USA) IC/MT(MP40)4544/036

5557 *Challenges of NASA prospective libration missions.* **David Folta** (NASA Goddard Space Flight Center, USA) IC/MT(MP40)4548/036

5558 *Design strategies for libration-point missions: theory to application.* **Kathleen Howell** (Purdue University, USA) IC/MT(MP40)4549/036

IC/MP344/036: Mathematical models and computational methods for nano- and bio-technologies. #2 ML D 28

Organiser: Roderick Melnik (Wilfred Laurier University, Canada)
Co-organiser: Jack Tuszynski (Cross Cancer Institute, Edmonton, Canada)

(For abstract, see session #1 on page 330.)

5559 *On the interconvesion integral equation for relaxation and creep.* **Robert Anderssen** (CSIRO, Australia), Frank de Hoog (CSIRO, Australia) IC/MT(MP344)1401/036

5560 *Coupled nonlinear effects in nano-structures and their applications.* **Roderick Melnik** (Wilfred Laurier University, Canada) IC/MT(MP344)3238/036

5561 *Computational models for the numerical simulation of voltage-operated channels in nano-bio-electronics.* **Riccardo Sacco** (Politecnico di Milano, Italy), Bice Chini (Consiglio Nazionale delle Ricerche, Italy), Joseph Jerome (Northwestern University, USA), Massimo Longaretti (Politecnico di Milano, Italy), Giovambattista Marino (Politecnico di Milano, Italy) IC/MT(MP344)1388/036

5562 *Can we predict DNA biological activity by modelling its fluctuations?.* **Michel Peyrard** (École Normale Supérieure de Lyon, France), Santiago Cuesta Lopez (École Normale Supérieure de Lyon, France), Dimitar Angelov (École Normale Supérieure de Lyon, France), Titus Van Erp (Katholieke Universiteit Leuven, Belgium), Johannes-Geert Hagmann (École Normale Supérieure de Lyon, France) IC/MT(MP344)1563/036

IC/MP264/040: Recent advances in the analysis of nonlinear parabolic equations and their singular limits. #2 KOL F 101

Organiser: Cyrill Muratov (New Jersey Institute of Technology, USA)
Co-organiser: Peter Gordon (New Jersey Institute of Technology, USA)

Abstracts for ICIAM 07

incorporating:

GAMM Annual Meeting 2007
Embedded Meetings
Industry Days

(For abstract, see session #1 above.)

BepiColombo gravitational capture and the elliptic restricted three-body problem. **Stefano Campagnola** (University of Southern California, USA), Martin Lo (Jet Propulsion Laboratory, USA) IC/MT(MP40)4544/036

BepiColombo is the cornerstone ESA-approved mission to Mercury. It will reach its destination in 2019, after a nearly 5-year long transfer using multiple gravity assists and low-thrust propulsion. To avoid a single point failure of a classical chemical orbit insertion burn, an arrival scenario was implemented where the gravity of the Sun is exploited to weakly capture the spacecraft in a Mercury orbit. This technique can be better understood in the frame of the elliptic three-body problem model. In particular, Gravitational Capture conditions are investigated, together with the allowed region of motions for the spacecraft.

Challenges of NASA prospective libration missions. **David Folta** (NASA Goddard Space Flight Center, USA) IC/MT(MP40)4548/036

As the future unfolds for NASA in its pursuit of the Vision for Space Exploration, libration orbits play a prominent role. Both Sun-Earth and Earth-Moon regions will be exploited requiring mathematical advancements and comprehensive demonstrations. With several successful single missions, new challenges of formation flying, intra-transfer orbits, and unique station-keeping strategies take center stage. Mathematical applications to improve and otherwise optimize mission parameters are necessary to permit communication and exploration architectures of the exploration vision. Recent advancements, which apply EulerŠs grid technique, is one example. The paper focuses on potential missions and how recent advancements based on EulerŠs imaginings make these missions possible.

Design strategies for libration-point missions: theory to application. **Kathleen Howell** (Purdue University, USA) IC/MT(MP40)4549/036

Spacecraft missions to the libration points in sun–planet and planet–moon systems are of increasing interest. A number of such missions have already been launched. As the theoretical understanding of the dynamical structure in these regions of space expands, however, trajectory design to support actual mission requirements is more complex. Baseline trajectories for some recent mission scenarios are presented. Example approaches for transition of the designs to higher fidelity models is discussed.

IC/MP344/036: Mathematical models and computational methods for nano- and bio-technologies.

Organiser: Roderick Melnik (Wilfred Laurier University, Canada)
Co-organiser: Jack Tuszynski (Cross Cancer Institute, Edmonton, Canada)

Most cutting edge developments that are taking place in nano and bio-technologies rely heavily on advances in mathematical modeling and computational methodologies. Examples include, but not limited to, new technologies based on low-dimensional semiconductor nanostructures such as quantum dots, nanotubes, sensors and actuators, drug discovery methodologies, protein- and macrotubule-based devices, techniques, and processes in designing biomolecular motors.

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On the interconvesion integral equation for relaxation and creep. **Robert Anderssen** (CSIRO, Australia), Frank de Hoog (CSIRO, Australia) IC/MT(MP344)1401/036

Because of the particularization of genetic activity that they perform, rheological phenotypes are playing an increasingly important role in biotechnology research including quantitative trait loci (QTL) analysis. For the determination of such phenotypes, the viscoelastic nature of biomaterials must be taken into account. The rheological characteristics of viscoelasticity are normally modelled, as a function of the time t, in terms of the relaxation $G(t)$ and the creep (retardation) $J(t)$ functions. Different instruments are available for performing the associated relaxation and creep experiments, which generate the stress-strain relaxation and creep data from which estimates $G_{est}(t)$ and $J_{est}(t)$ of $G(t)$ and $J(t)$ are recovered. In many situations, only a single instrument is available which can only perform on of these experiments. Consequently, there is considerable interest in computational techniques which allow $J_{est}(t)$ or $G_{est}(t)$ to be determined from the other using the interconversion relationships

$$\int_0^t G(t-s)J(s)ds = \int_0^t J(t-s)G(s)ds = t.$$

Though this matter has been examined numerically in the rheological literature, a formal mathematical comparison of the two possibilities has never been undertaken. This talk will report on the results from recent mathematical investigations.

Coupled nonlinear effects in nano-structures and their applications. **Roderick Melnik** (Wilfred Laurier University, Canada) IC/MT(MP344)3238/036

We demonstrate that the conventional application of linear mathematical models to the analysis of optoelectronic properties of nanostructures in bandstructure engineering may be inadequate for new emerging applications. Examples are given for several types of low-dimensional semiconductor nanostructures, where we account consistently for nonlinear strain and piezoelectric effects in calculating their properties, and for carbon nanotube based devices such as field emitting diodes. A major focus in this talk is given to the analysis of quantum dots, where it is essential to account for coupled effects.

This is a joint work with R. Mahapatra, N. Sinha, J.T.W. Yeow, D.A. Jaffray, M. Willatzen, B. Lassen, and L. Lew Yan Voon

Computational models for the numerical simulation of voltage-operated channels in nano-bio-electronics. **Riccardo Sacco** (Politecnico di Milano, Italy), Bice Chini (Consiglio Nazionale delle Ricerche, Italy), Joseph Jerome (Northwestern University, USA), Massimo Longaretti (Politecnico di Milano, Italy), Giovambattista Marino (Politecnico di Milano, Italy) IC/MT(MP344)1388/036

A new object in cosymmetrical systems is a family of steady states with variable spectra. This case is the opposite of the symmetry situation when all the states have identical spectrum. It is very interesting to consider the effects produced by the appearance of such a continuous family. Now the nontrivial bifurcations were found in cosymmetrical problems: the delay with limit cycle branching off, new scenario of tori birth etc. The investigation of all these problems has required the development of new numerical methods and the study of approaches in the bifurcation theory of dynamical systems. The proposed talks will present recent results on the cosymmetry theme. Partially, we plan to consider: Evolution of steady states family in 2d and 3d convection in a porous medium, cosymmetrical effects in some population kinetics problems, numerical approaches to computation of steady states family, special cosymmetrical bifurcations, computer experiment on the selection of steady states from the continuous family.

The co-symmetric bifurcations in the planar filtrational convection problem: numerical results. **Vasily Govorukhin** (Rostov State University, Russian Federation) IC/MT(MP245)870/033

Theory of cosymmetry was introduced by Yudovich [1] to explain a phenomenon of existence of one-parameter family of stationary flows in the planar filtrational convection problem. It was shown that the branching of cycle of equilibria (CE) is a typical bifurcation in cosymmetric dynamical system [1]. In [2] and in many other works of these authors the theory of cosymmetric bifurcations was developed.

We investigate the planar filtrational convection problem in rectangular container numerically by Galerkin method. We consider Galerkin systems of various dimensions (up to 1000) and we study numerically the bifurcations connected mainly with CE existence.

The bifurcations of CE was found out: birth of a new family from already existing, intersection and join of CE, origin of a CE Šfrom an airŠ etc [3-4]. The bifurcations of families are connected with different CE both with stable and with unstable. The periodic, quasiperiodic and chaotic regimes were founded for different values of parameters [4]. The steady periodic regimes can occur by two ways: as a result of cosymmetric Hopf or Euler bifurcations. For some values of parameter transition from stationary movement at once to chaotic ones is possible. The bifurcation of tori branching from CE was found.

The qualitative repetition of bifurcation and consistency of bifurcation parameter values was established by different dimensions Galerkin's models investigation. We found practically all types of bifurcations studied theoretically in [2].

[1] Yudovich V.I. Matem. Zametki 49, 1991; Chaos 5 (2), 1995.

[2] Kurakin L.G. and Yudovich V.I. Chaos 10 (2), 2000; Chaos 11 (4), 2001.

[3] Govorukhin V.N. Fluid Dynamics, V. 34, No. 5, 1999.

[4] Govorukhin V.N., Shevchenko I.V., Fluid Dynamics, V. 38, No. 5, 2003; V. 41, No. 6, 2006.

Co-symmetric families of steady states in 3D convection of the incompressible fluid in a porous medium. **Vyacheslav Tsybulin** (Rostov State University, Russian Federation) IC/MT(MP245)884/033

Three-dimensional convection of the incompressible fluid in a porous medium is considered. Mimetic finite-difference schemes for the primitive variables equation are developed. The connection of a derived staggered discretization with a finite-difference approach based on the stream function (planar problem) is established. Continuous cosymmetric families of steady states are computed and stability analysis is presented.

Selection of steady states in planar Darcy convection. **Bülent Karaözen** (Middle East Technical University, Turkey), Vyacheslav Tsybulin (Rostov State University, Russian Federation) IC/MT(MP245)1732/033

Selection of steady states in the planar convection problem for the incompressible fluid in a porous medium is studied. The perturbation of initial data by adding of the harmonic deviation of boundary temperature is analyzed. Computer experiments on the selection of equilibria show that, for initial distribution (disturbance) with large amplitude, the neighborhood of a single preferable steady state is established. The question is why some patterns of fluid are more preferred than others. This problem is may be treated as a some variant of the description of separation processes. Important future problem here is a possibility to control the pattern organization.

Dynamics and family of equilibria in a population kinetics model with cosymmetry. **Katya Kovaleva** (Rostov State University, Russian Federation), Kurt Frischmuth (Universität Rostock, Germany) IC/MT(MP245)2658/033

This work continues the study have started in [1] with a system of nonlinear parabolic equations with cosymmetry. We assume three populations sharing a common space and suppose a dominant role of the unique spatial coordinate. Looking for best opportunities for their respective trades, each population may move in dependence on the current concentrations of their own kind and the other one. However, the first population (thrives on relocation of the others, while the second and third suffer from motion of the first. We use a finite-difference scheme preserving the cosymmetry property for a given problem. Two cases of boundary conditions are considered. Different scenarios of instability for the state of rest are observed. Numerical results on computation of continuous families of steady states and periodic regimes are presented and stability of the zero equilibrium are studied.

1. K. Frischmuth, V. Tsybulin, Families of equilibria and dynamics in a population kinetics model with cosymmetry, Physics Letters **A 338** (2005), 51–59.

IC/MP79/034: Pattern formation in coupled-cell systems.

Organiser: William Langford (University of Guelph, Canada)

Systems of coupled oscillators (or *cells*) occur in very diverse applications, ranging from animal gaits and neural networks to heat exchanger arrays. Earlier work focussed on systems with a high degree of symmetry, leading naturally to complex spatio-temporal patterns via equivariant Hopf bifurcation theory. Recent work includes more general architectures represented by directed graphs, and reveals new behaviors such as nilpotent bifurcations occurring in codimension one.

Synchrony in coupled systems and the vestibular system. **Martin Golubitsky** (University of Houston, USA) IC/MT(MP79)3884/034

Synchrony and phase synchrony were first studied in coupled systems using network symmetry. More generally, robust synchrony in a network of identical subsystems (cells) follows from a combinatorial condition (balanced coloring) and robust phase synchrony corresponds to symmetry in quotient networks. We review this earlier work and discuss phase shift synchrony in the context of that part of the vestibular system which connects inner ear canal nerves with neck muscle motoneurons. This later work is joint with Ian Stewart and LieJune Shiau.

Coupled cell networks: minimality and quotients. **Manuela Aguiar** (Universidade do Porto, Portugal), Ana Dias (Universidade do Porto, Portugal), Martin Golubitsky (University of Houston, USA), Maria Leite (University of Purdue, USA), Ian Stewart (University of Warwick, UK) IC/MT(MP79)3902/034

Non-isomorphic coupled cell networks can correspond to coupled-cell systems with equivalent dynamics and are called ODE-equivalent. Coupled cell systems restricted to flow-invariant subspaces defined by equality of certain cell coordinates correspond to quotient networks. In this talk we discuss some recent results related with ODE-equivalence of coupled cell networks, minimality of ODE-classes and quotients networks.

Stability computations for nilpotent Hopf bifurcations. **Maciej Krupa** (New Mexico State University, USA), Martin Golubitsky (University of Houston, USA) IC/MT(MP79)3948/034

Nilpotent Hopf bifurcations can occur in codimension one in coupled cell systems. Elmhirst and Golubitsky studied such bifurcations and obtained rather unusual branching patterns. In this work we use normal form theory to obtain stability results for some of the branches found by Elmhirst and Golubitsky. On the way to obtaining our results we determine how some of the synchrony subspaces of the network influence the structure of the normal form.

Spatio-temporal patterns in heat-exchanger arrays. **William Langford** (University of Guelph, Canada) IC/MT(MP79)3930/034

Flow-induced vibrations of the tubes in a large heat exchanger array can cause metal fatigue and failure, leading to costly repairs. A simple mathematical model is presented for the case of a rectangular array, so that the problem becomes a study of the spatio-temporal patterns in a two dimensional coupled cell system with $\mathbb{Z}_M \times \mathbb{Z}_N$ symmetry. The results presented here include all the generic equivariant Hopf bifurcations in this setting, with their onset, stability and spatio-temporal patterns, for cases with the spatial periodicities that are likely to occur, both with and without an internal $\mathbb{Z}_2$ symmetry. The predictions of this analysis are in good qualitative agreement with experiments on flow-induced vibrations in arrays of circular cylinders performed at Atomic Energy Canada Limited. This is joint work with R. Akila, Garyounis University, Benghazi, Libya.

IC/MP326/034: Symmetry aspects in biological dynamical systems.

Organiser: LieJune Shiau (University of Houston, USA)
Co-organiser: Marc Timme (Max-Planck-Institut Göttingen, Germany)

This minisymposium features novel results on models of various biological dynamics, with a focus on underlying symmetries and on breaking these symmetries. Topics range from mechanisms of muscle movements to pattern formation and non-standard dynamics in biological neural networks.

In particular, one study is about the principles of neck muscle movements in most vertebrates (including humans), based on the semicircular canal input from the ears in the vestibular (balancing) system. Two studies investigate heteroclinic networks and unstable attractors, arising naturally in networks of neural oscillators. These features lead to the phenomenon of switching between neural *encoding* states, with potential implications, among others, for odor recognition and processing in insects. Another one shows that the number density of singular points, called pinwheels, in cortical pattern forming systems follows a universal statistics, with its mean normalized density close to the mathematical constant π. A theoretical model of pattern formation in the cortex explains this result. Also, a new dynamical phenomenon is found and analyzed in the study of globally coupled neural networks. Here the dynamics shows the irregular and chaotic appearing in transients, although it is governed by negative Lyapunov exponents. A relation to *stable chaos* is also discussed.

All speakers will present the basics and symmetries of the biological systems studied, and discuss their results.

Heteroclinic networks and clustering in simple models of neural activity. **Gábor Orosz** (University of Exeter, UK), Peter Ashwin (University of Exeter, UK) IC/MT(MP326)1991/034

The dynamics of neural systems has to balance seemingly contradictory requirements of robustness to noise and sensitivity to inputs. Networks of coupled systems can however deliver this in cases where they have attractors that are heteroclinic networks giving so-called 'winnerless competition' between unstable states. We consider some specific examples motivated by work on the insect antennal lobe that convert spatially dependent inputs into spatio-temporal codes, where one can verify robustness with high sensitivity to inputs.

Stability properties of the asynchronous regime in a network of identical neurons. **Antonio Politi** (Consiglio Nazionale delle Ricerche, Italy) IC/MT(MP326)991/034

The stability of globally coupled neurons is usually carried out by following a mean field approach. With reference to a system of leaky-integrate-and-fire neurons, we develop a microscopic approach that allows for an exact stability analysis. As a result we find that the mean field approach does not always provide the correct answer. This is issue is connected to the noncommutativity of two limits: infinitely many neurons and delta-like pulses. We also discuss the occurrence of some bifurcations that break the time-invariance of the asynchronous regime and the effect of a small dilution (cutting some links) which may give rise to a linearly stable but irregular regime.

Symmetry and bifurcation in vestibular system. **LieJune Shiau** (University of Houston, USA), Martin Golubitsky (University of Houston, USA) IC/MT(MP326)1485/034

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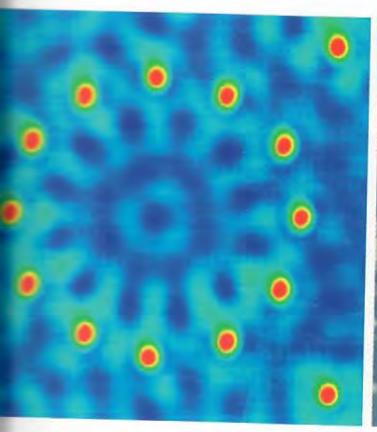

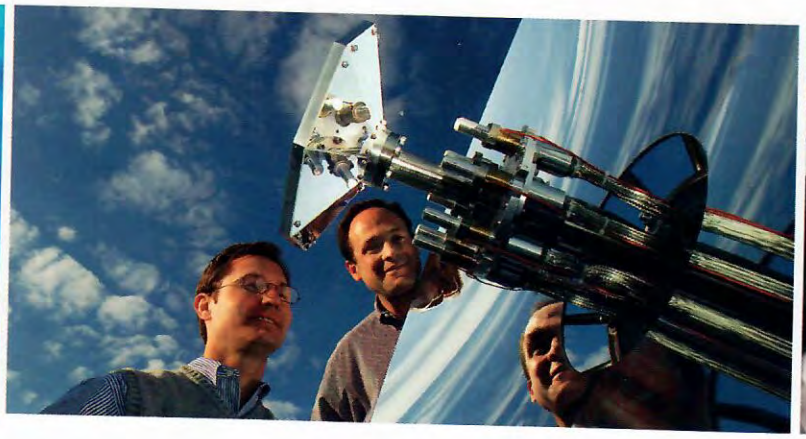

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Wednesday 29 August

SESSION 7

Conv. Ctr. 24A . . . . . Wed. 8:10 to 10:10 am

Thin Film Nanostructure Optics

Chair: **Gregory J. Exarhos**, Pacific Northwest National Lab.

8:10 am: **Optics of thin-film silicon solar cells with efficient periodic light trapping texture,** C. S. Haase, H. Stiebig, Forschungszentrum Jülich GmbH (Germany) . . . . . [6645-32]

8:30 am: **Tailored circular Bragg phenomena in TiO_2 sculptured thin films through post-deposition processing,** S. M. Pursel, M. W. Horn, A. Lakhtakia, The Pennsylvania State Univ. . . . . [6645-33]

8:50 am: **Optoelectronic properties of ZnO/ZnMgO quantum well lasers with coupled self-consistent models,** R. V. N. Melnik, Wilfrid Laurier Univ. (Canada); M. Willatzen, Syddansk Univ. (Denmark); D. R. Mahapatra, Indian Institute of Science (India); L. C. Lew Yan Voon, Wright State Univ. . [6645-34]

9:10 am: **Fabrication and characterization of silicon/silicon dioxide super lattices for silicon-based light-emitting devices,** T. Creazzo, E. Marchena, B. Redding, T. R. Hodson, D. W. Prather, Univ. of Delaware . . . . . [6645-35]

9:30 am: **Function of bubble pit during readout process in PtOx type super-RENS disk,** Q. Liu, The National Ctr. for Nanoscience and Technology of China (China); T. Fukaya, National Institute of Advanced Industrial Science and Technology (Japan) . . . . . [6645-36]

9:50 am: **Narrowband, linear-polarization rejection filter based on columnar thin film superlattice,** F. Chiadini, Univ. degli Studi di Salerno (Italy); V. Fiumara, Univ. degli Studi della Basilicata (Italy); A. Scaglione, Univ. degli Studi di Salerno (Italy); A. Lakhtakia, The Pennsylvania State Univ. . . . . [6645-37]

Coffee Break . . . . . 10:10 to 10:30 am

SESSION 8

Conv. Ctr. 24A . . . . . Wed. 10:30 am to 12:00 pm

Organic Nanostructures

Chair: **Louay A. Eldada**, DuPont Photonics Technologies

10:30 am: **Rational design of molecular self-assemblies for controlled surface patterning and molecular diffusion *(Invited Paper)*,** D. Bléger, D. Kreher, F. Mathevet, A. Attias, Univ. Pierre et Marie Curie (France); G. Schull, L. Douillard, C. Fiorini-Debuisschert, F. Charra, Commissariat à l'Energie Atomique (France) . . . . . [6645-38]

11:00 am: **Fabrication of sub-diffraction-limit molecular structures by scanning near-field photolithography,** G. J. Leggett, The Univ. of Sheffield (United Kingdom) . . . . . [6645-39]

11:20 am: **Elasticity of two-photon-fabricated nano-wires,** S. Nakanishi, Osaka Univ. (Japan); H. Sun, Jinlin Univ. (China) and Osaka University (Japan); S. Kawata, Osaka Univ. (Japan) . . . . . [6645-40]

11:40 am: **Current modulation of polymer/nanoparticle memory devices through nanoparticle engineering,** J. Ouyang, National Univ. of Singapore (Singapore) . . . . . [6645-41]

Lunch/Exhibition Break . . . . . 12:00 to 1:10 pm

SESSION 9

Conv. Ctr. 24A . . . . . Wed. 1:10 to 3:10 pm

Nanotubes

Chair: **Elizabeth A. Dobisz**, Hitachi Global Storage Technologies

1:10 pm: **Optical polarizer made of mechanically aligned carbon nanotubes,** S. Shoji, H. Suzuki, S. Kawata, Osaka Univ. (Japan) . . . [6645-42]

1:30 pm: **Optoelectronic transport studies of photosensitive ruthenium complexes with single walled carbon nanotubes,** H. Chaturvedi, J. C. Poler, The Univ. of North Carolina at Charlotte . . . . . [6645-43]

1:50 pm: **Ambient formation of highly aligned carbon nanotube networks,** M. D. Lay, P. Vichchulada, The Univ. of Georgia . . . . . [6645-44]

2:10 pm: **Analytical modeling of the current transport in carbon nanotube field effect transistors (CNT-FETs),** J. M. Marulanda, Florida International Univ.; A. Srivastava, Louisiana State Univ. . . . . [6645-45]

2:30 pm: **Nano materials for efficiently lowering the freezing point of anti-freeze coolants,** H. Hong, South Dakota School of Mines and Technology [6645-46]

2:50 pm: **Light source with carbon nanotubes field emission cathode and rare-earth doped nanocrystalline phosphors,** P. Psuja, W. Strek, Polska Akademia Nauk (Poland) . . . . . [6645-47]

Coffee Break . . . . . 3:10 to 3:30 pm

SESSION 10

Conv. Ctr. 24A . . . . . Wed. 3:30 to 4:10 pm

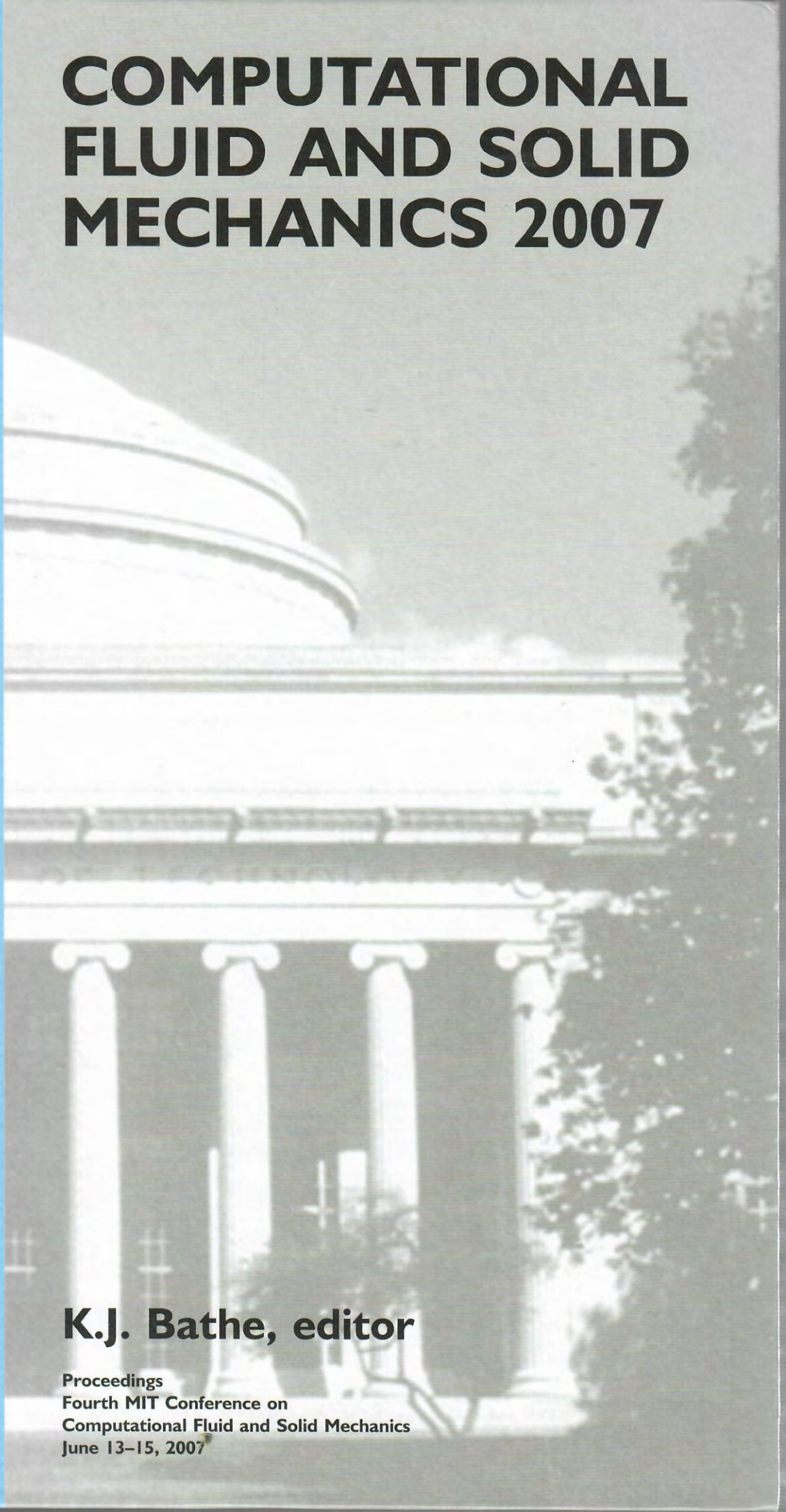
Nanowires, Nanofibers, and Nanorods

Chair: **David Bléger**, Univ. Pierre et Marie Curie (France)

3:30 pm: **Ultrahigh sensitivity nanowire photodetectors,** C. Soci, A. Zhang, B. Xiang, S. A. Dayeh, D. P. R. Aplin, X. Bao, Y. Lo, D. Wang, Univ. of California/San Diego . . . . . [6645-48]

3:50 pm: **Self-sensing of CNF and Ni nanowire/PVDF and cellulose composites using electro-micromechanical test,** J. Park, Gyeongsang National Univ. (South Korea) and The Univ. of Utah; P. Kim, J. Jang, Gyeongsang National Univ. (South Korea); D. Yoon, Korea Research Institute of Standards and Science (South Korea); G. Hansen, Metal Matrix Composites Co.; L. K. DeVries, The Univ. of Utah . . . . . [6645-50]

COMPUTATIONAL FLUID AND SOLID MECHANICS 2007



K.J. Bathe, editor

Proceedings
Fourth MIT Conference on
Computational Fluid and Solid Mechanics
June 13–15, 2007

SPECIAL ISSUE

Computational Fluid and Solid Mechanics 2007

K. J. **Bathe**	627	Preface
K. J. **Bathe** and **G. A. Ledezma**	628	Benchmark problems for incompressible fluid flows with structural interactions
K. N. **Karagiozis, M. P. Païdoussis** and M. **Amabili**	645	Effect of geometry on the stability of cylindrical clamped shells subjected to internal fluid flow
J. E. **Guilkey, T. B. Harman** and **B. Banerjee**	660	An Eulerian–Lagrangian approach for simulating explosions of energetic devices
L. **Salvatori** and **C. Borri**	675	Frequency- and time-domain methods for the numerical modeling of full-bridge aeroelasticity
C. J. K. **Lee, H. Noguchi** and **S. Koshizuka**	688	Fluid–shell structure interaction analysis by coupled particle and finite element method
R. **Melnik** and **R. Mahapatra**	698	Coupled effects in quantum dot nanostructures with nonlinear strain and bridging modelling scales
G. **Morgenthal** and **J. H. Walther**	712	An immersed interface method for the Vortex-In-Cell algorithm
A. **Liu, S. Rugonyi, J. O. Pentecost** and K. L. **Thornburg**	727	Finite element modeling of blood flow-induced mechanical forces in the outflow tract of chick embryonic hearts
X. **S. Wang**	739	An iterative matrix-free method in implicit immersed boundary/continuum methods
C. H. **Tai, K. M. Liew** and **Y. Zhao**	749	Numerical simulation of 3D fluid–structure interaction flow using an immersed object method with overlapping grids
S. M. **Mitran**	763	Metachronal wave formation in a model of pulmonary cilia
D. **Boffi, L. Gastaldi** and **L. Heltai**	775	On the CFL condition for the finite element immersed boundary method
A. **de Boer, M. S. van der Schoot** and **H. Bijl**	784	Mesh deformation based on radial basis function interpolation
R. **Unger, M. C. Haupt** and **P. Horst**	796	Application of Lagrange multipliers for coupled problems in fluid and structural interactions
A. **Frangi, A. Frezzotti** and **S. Lorenzani**	810	On the application of the BGK kinetic model to the analysis of gas-structure interactions in MEMS

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Preface

This special issue of Computers & Structures gives the papers written for the Fourth MIT Conference on Computational Fluid and Solid Mechanics. The special focus of this Conference is on *Fluid-Structure Interactions*.

The objective of the bi-annual MIT Conferences on Computational Fluid and Solid Mechanics is to bring together leading researchers and practitioners, and young researchers, in order to focus on the eight challenges in computational mechanics described in the Prefaces of the earlier MIT Conference Proceedings.[1]

The eight challenges are the development of more effective procedures for – the automatic selection and solution of mathematical models, the solution of fluid flows, the use of mesh-free methods, the solution of multi-physics and multi-scale problems, modeling uncertainties, the analysis of complete life cycles of systems, and education. Each of these challenges calls for most exciting research and developments.

While the earlier three MIT Conferences addressed all these challenges in a broad manner, the Fourth Conference focuses on the multi-physics and multi-scale challenges to analyze problems of fluid-structure interactions. The analysis of such problems has already reached great importance in many fields of engineering and the sciences; but as computational capabilities will grow, the requirements for the analysis of such problems will undoubtedly increase. Nature does not distinguish between fluids and solids, and to simulate nature more accurately, it is necessary to represent the multi-physics and multi-scale behavior of the various media encountered in one simulation model.

The papers presented at the Conference and published in this book represent in many regards the current state of the art in simulating fluid-structure interactions. As for the three earlier MIT Conferences, in addition to the presentations based on the papers published in this book, valuable presentations based on short one-page Abstracts will also be given. We are grateful for the efforts of all authors and look forward to our continued cooperation in the field of computational mechanics.

K.J. Bathe
MIT

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[1] For a description of these challenges, see Preface of *Computational Fluid and Solid Mechanics 2005*, K.J. Bathe (editor), Elsevier 2005.

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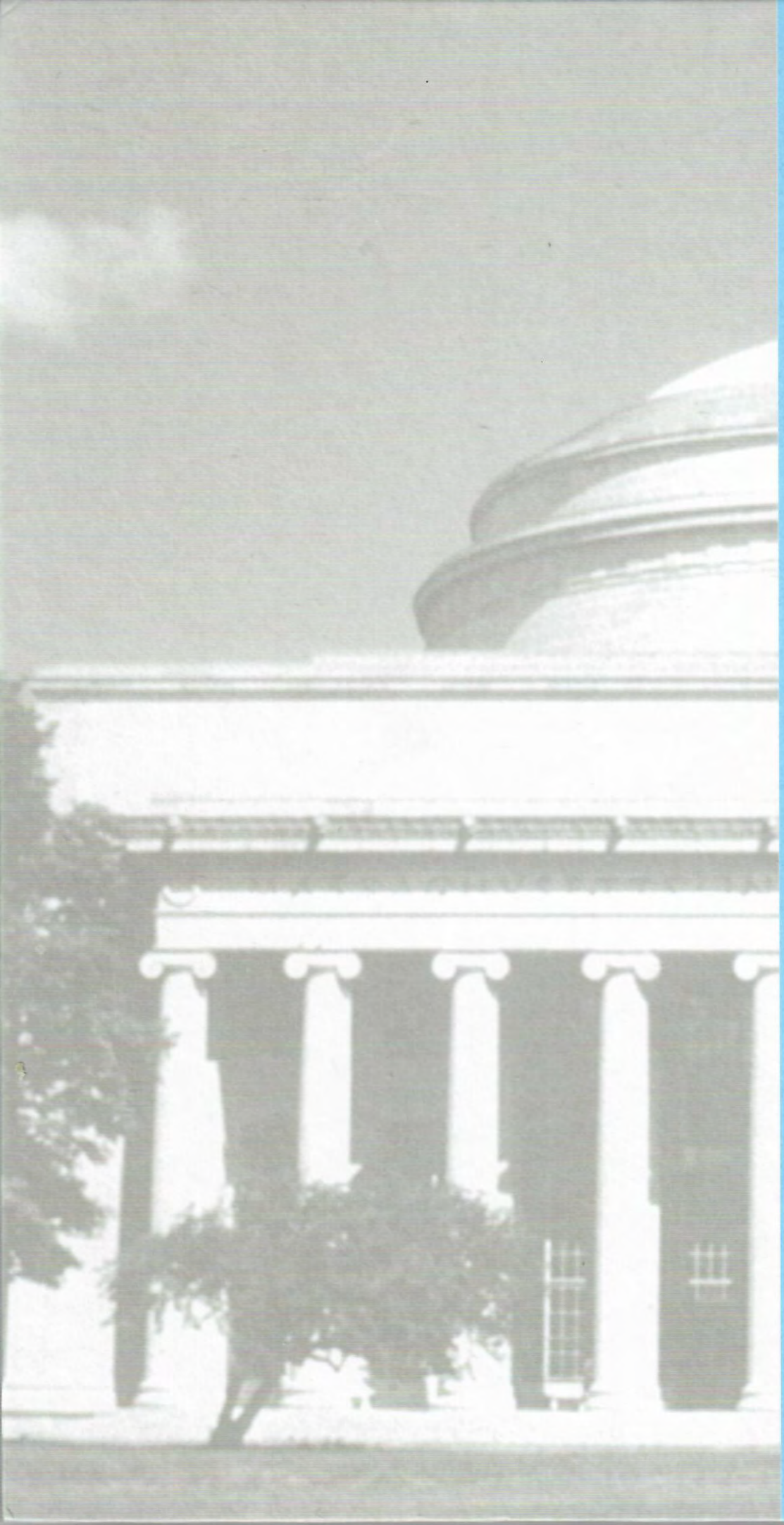

Abstracts of the Invited and Contribution Papers of CCP2008

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The 2008 Conference on Computational Physics (CCP2008) from August 5-9, 2008, in Ouro Preto, Brazil, covers several fields of computational physics.

The purpose is to continue the series of meetings that started in 1989, in which computational scientists gathered to present their latest results and interact with their peers from around the world.

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Analysis of Phase Stability of CdS Quantum Dots with First Principle MD Calculations

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Cadmium sulfide (CdS) is one of the most important wide-gap semiconductors due to its stability properties and high luminescence [1]. It has been known for a long time that the bulk CdS is highly stable and it exists in the hexagonal wurtzite phase in a wide range of temperatures, from room temperature to its melting point. Recently it has been shown that due to the large surface to volume ratio and reconstruction of surface crystal structure, the thermodynamic properties of the CdS nanostructure can differ significantly from bulk CdS [2]. For example, under appropriate conditions some wurtzite structure semiconductor materials can transform into a graphitic structure when they are in the form of thin nanoplates [3]. Since the internal pressure deduced from surface stress is very large for nanostructures, at ambient conditions, the stability phase in nanosize structures is always a high pressure stability phase structure in bulk [4]. Nevertheless, the temperature-dependent phase stability of the CdS quantum dots remains poorly understood to date. In particular, systematic calculations and comprehensive comparisons of their thermodynamic stability, as well as mechanical, electronic, and optical properties under different temperature conditions are still lacking. To fill this gap, in this work we carry out first-principle molecular dynamic (MD) calculations for CdS quantum dots of various phase structures and study temperature-dependent phase stability of these nanostructures. Based on our calculations, we analyze the relative stability of different CdS phases under different temperature conditions. Our results indicated that at the temperature range studied in this work, the phase stability sequence for the $Cd_{48}S_{48}$ nanostructure is rocksalt, wurtzite and graphitic phase, which is the same as that of bulk CdS crystal under high pressure. Although the temperature can affect the total energy of the CdS nanostructure, it can not change the phase stability sequence of CdS nanostructures in the temperature range studied in this work.

[1] K. Barnham *et al*, Applied Physics Letters, **76**, 1197 (2000).
[2]A. S. Barnard and H. Xu, Journal of Physics Chemistry C, **111**, 118112 (2007).
[3] C. L. Freeman *et al*, Physical Review Letters, **96**, 066102 (2006)
[4] C. C. Yang and S. Li, Journal of Physical Chemistry C, **112**, 1423 (2008).

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050 – MAGNETO-PHOTOLUMINESCENCE STUDIES OF CdTe/CdSe/ZnS NANOPARTICLES
Yuan-Huei Chang, C. C. Huang, L. W. Chang, C. H. Hsu, Chih-Wei Lai, Chien-Liang Liu, Pi-Tai Chou (National Taiwan University), **D. C. Lin** (National Chiao Tung University), **Y. T. Sung** (National Nano Device Laboratories), **L. C. Li** (National Chiao Tung University), **Y. W. Suen** (National Chung Hsing University), **K. W. Sun, C. P. Lee** (National Chiao Tung University)

051 – THE EFFECT OF STRAIN IN CdTe/ZnTe QUANTUM WIRES
Sunil Patil, Roderick Melnik (M2NeT Lab, Wilfrid Laurier University)

052 – EXCITATION DYNAMICS OF CdTe/ZnTe QUANTUM DOTS STUDIED IN PICOSECOND TIMESCALE
Tomasz Kazimierczuk, Mateusz Goryca, Maciej Koperski, Stanislaw Nowak (Institute of Experimental Physics, Warsaw University, Poland), **Piotr Wojnar** (Institute of Physics, Polish Academy of Sciences, Warsaw, Poland), **Jan A. Gaj, Andrzej Golnik, Piotr Kossacki** (Institute of Experimental Physics, Warsaw University, Poland)

053 – STUDY OF THE RADIATIVE RECOMBINATION PROCESSES IN TETRAPOD-SHAPED CdTe NANOCRYSTALS
Giovanni Morello, Davide Tarì, Luigi Carbone, Liberato Manna, Roberto Cingolani, Milena De Giorgi (National Nanotechnology Laboratory (NNL) of CNR-INFM, Università del Salento, Lecce, Italy)

054 – INTERFACE-INDUCED QUANTUM CONFINED STARK EFFECT: PbTe NANODOTS IN CdTe MATRIX
Roman Leitsmann, Frank Ortmann, Friedhelm Bechstedt (Friedrich-Schiller-Universität, Jena, Germany)

055 – EXCITON QUANTUM CONFINEMENT EFFECT IN NANO-STRUCTURES FORMED BY LASER RADIATION ON THE SURFACE OF CdZnTe TERNARY COMPOUND
Arturs Medvids (Riga Technical University, Latvia, Institute of Semiconductor Physics NAS of Ukraine, Ukraine), **Alexanrds Mychko** (Riga Technical University, Latvia), **Natalia Litovchenko** (Institute of Semiconductor Physics NAS of Ukraine, Ukraine), **Oksana Strilchuk, Pavels Onufrijevs, Arturs Pludons** (Riga Technical University, Latvia), **Juryi Naseka** (Institute of Semiconductor Physics NAS of Ukraine, Ukraine)

056 – EFFICIENT SINGLE-PHOTON SOURCE WITH CdSe QUANTUM DOT IN ZnSe NANOWIRE: PHOTON ANTIBUNCHING AT TEMPERATURES UP TO 220K
Adrien Tribu (CEA-Grenoble/INAC/Nanophysique et Semiconducteurs, France), **Gregory Sallen** (Institut Néel CNRS/Nanophysique et Semiconducteurs, France), **Thomas Aichele** (CEA-Grenoble/INAC/Nanophysique et Semiconducteurs, France), **Catherine Bougerol, Régis André, Jean-Philippe Poizat, Serge Tatarenko** (Institut Néel CNRS/Nanophysique et Semiconducteurs, France), **Kuntheak Kheng** (CEA-Grenoble/INAC/Nanophysique et Semiconducteurs, France)

105 – STABILITY AND ELECTRONIC PROPERTIES OF ANTISITES, VACANCIES, AND SUBSTITUTIONAL Si AND C IN GaN NANOTUBES
Márcio Luiz Colussi, **Rogério José Baierle** (Universidade Federal de Santa Maria, Chile), **Roberto Hiroki Miwa** (Universidade Federal de Uberlândia, Brazil)

106 – ACCOUNTING FOR NONLINEAR ELECTROSTRICTIVE EFFECTS IN MODELING NITRIDE NANOWIRES AND QUANTUM DOTS
Mehrdad Bahrami-Samani, **Roderick Melnik** (M2NeT Lab, Wilfrid Laurier University)

107 – OPTICAL PROPERTIES OF CATALYST FREE GROWN NANOWIRES
Detlev Grützmacher, **Hilde Hardtdegen**, **Raffaella Calarco** (Forschungszentrum Jülich, Germany)

108 – IMAGING THE ELECTRON WAVEFUNCTION IN A NANOWIRE QUANTUM DOT*
Erin E. Boyd, **Halvar J. Trodahl** (Department of Physics, Harvard University, USA), **Parisa Fallahi†** (Department of Physics, Harvard University, USA; currently at ETH, Zürich, Switzerland), **R. M. Westervelt** (Department of Physics and School of Engineering & Applied Sciences, Harvard University, USA), **Linus E. Fröberg**, **Kristian Nilsson**, **Lars Samuelson** (Department of Solid State Physics, Lund University, Sweden)

109 – ANOMALOUS LINEARLY POLARIZED EMISSION FROM FREE-STANDING NANOWIRES
Everton G. Gadret, **C. R. Biazoli**, **F. Iikawa**, **M. J. S. P. Brasil**, **T. Chiaramonte**, **M. A. Cotta** (Instituto de Física Gleb Wataghin, Unicamp, Brazil), **Mauricio M. Lima Jr.**, **Andrés Cantarero** (Instituto de Ciência de los Materiales, Universidade de Valencia, Spain)

110 – SPECTRALLY AND SPATIALLY RESOLVED PHOTOLUMINESCENCE STUDY ON SINGLE HETEROSTRUCTURED NANOWIRES
Junichi Motohisa, **Masayasu Fukui**, **Yasunori Kobayashi**, **Takashi Fukui** (Hokkaido University, Japan)

111 – THE ROLE PLAYED BY OXYGEN ON THE SURFACE PASSIVATION OF InP NANOWIRES
Marcos Dionizio Moreira, **Pedro Venezuela** (Universidade Federal Fluminense, Brazil), **Tome Schmidt** (Universidade Federal de Uberlândia, Brazil)

112 – WEAK LOCALIZATION AND QUANTUM INTERFERENCE IN Sn DOPED In_2O_3 NANOWIRES
Olivia Maria Berengue, **Adenilson José Chiquito**, **Livia Pasolini Pozzi** (DF, UFSCar, Brazil), **Alexandre José de Castro Lanfredi** (Universidade Federal do ABC, UFABC, Brazil), **Edson Roberto Leite** (DQ, LIEC/UFSCar, Brazil)

113 – ELECTRONIC PROPERTIES OF FUNCTIONALIZED ZnO NANOWIRES AND NANOTUBES
Andreia Luisa da Rosa, **Thomas Frauenheim** (Bremen University, Germany)

114 – THEORETICAL INVESTIGATION OF DEFECTIVE BC_2N NANOTUBES AS A HYDROGEN STORAGE MATERIAL
Jussane Rossato, **Rogerio Baierle** (Universidade Federal de Santa Maria, Chile), **Walter Orellana** (Universidad Andres Bello)

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Abstracts

the ZnTe barrier. The measurements are performed at 10 K. As a reverse bias is applied, the PL intensity of the QD ensemble decreases due to the tunneling of carriers out of the dots. Small dots are emptied first, which is manifested by a redshift of the inhomogenously broadened PL band. Single QD emission lines are broadened as a result of a decrease of carrier lifetime. The lifetime shortens as a consequence of the tunneling enhancement with the electric field. The broadening is more pronounced for small dots, where effective barrier heights are smaller. It is accompanied by quenching of the total PL intensity. We argue that carriers, which tunnel out faster are the holes, although characterized by a larger effective mass. Indeed, the potential confining holes in the dots is relatively shallow, as the CdTe/ZnTe valence band offset vanishes. All the confinement is therefore due to strain. We model both the broadening of a single QD emission line and the decrease of its total intensity in a semiclassical model based on WKB approximation. We obtain a common set of parameters to reproduce the experimental data. The parameters are the width of the confining potential, the ionization energy (i.e. the barrier height), and a term linear in electric field. We find that the ionization energy values are in agreement with strain induced potential wells in the valence band. The width of the confining potential significantly exceeds the QD height. This result is strongly supported by transmission electron micrographs, which show that the range of the strain field along the growth axis is about 10 nm. We suggest that the linear term is due to electric field modification of the fine structure splitting.

[Th-PB1-050]

Magneto-photoluminescence studies of CdTe/CdSe/ZnS nanoparticles

Yuan-Huei Chang *(National Taiwan University)*, C. C. Huang *(National Taiwan University)*, L. W. Chang *(National Taiwan University)*, C. H. Hsu *(National Taiwan University)*, Chih-Wei Lai *(National Taiwan University)*, Chien-Liang Liu *(National Taiwan University)*, Pi-Tai Chou *(National Taiwan University)*, D. C. Lin *(National Chiao Tung University)*, Y. T. Sung *(National Nano Device Laboratories)*, L.C. Li *(National Chiao Tung University)*, Y. W. Suen *(National Chung Hsing University)*, K. W. Sun *(National Chiao Tung University)*, C. P. Lee *(National Chiao Tung University)*

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Recently, the effect of the magnetic flux on the excitonic energy has received much attention. Optical Aharonov-Bohm effect was observed on negatively charged exciton in InGaAs/GaAs quantum ring as well as neutral exciton in type-II InP-GaAs heterostrcture. In this paper we'll present our magneto-photoluminescence studies on the optical properties of CdTe/CdSe/ZnS core-shell-shell nanoparticles. Transmission electron microscope reveals that the colloidal nanoparticles that were grown by chemical method have size of about 6 nm, with the CdTe core has diameter of 4.8 nm and the thickness of the CdSe shell and ZnS shell are 0.7nm and 0.4 nm, respectively. The band alignment between the core (CdTe) and the shell (CdSe) is a type--II band alignment and the addition of ZnS layer is to passivate the surface of CdSe and to enhance the light emitting efficiency. Magneto-photoluminescence experiment was performed at T=1.4 K with a 14 T superconducting magnet in conjunction with a green diode laser and a monochromator. PL emission centered at around 1.28 eV was observed and is due to the recombination of electrosn in CdSe and holes in CdTe. The peak could be fitted with two Guassian curves centered at 1.31 eV and 1.26 eV, respectively. As the magnetic field increase, both peak energies increase with small oscillatory structure imposed in it. In addition small oscillatory variation in the integrated PL emission intensity was also observed as the magnetic field increases. These behaviors are similar to what are reported for the Aharonov-Bohm effect on the PL emission from semiconductor with ring-like structure.

[Th-PB1-051]

The Effect of Strain in CdTe/ZnTe Quantum Wires

Sunil Patil *(M2NeT Lab, Wilfrid Laurier University)*, Roderick Melnik *(M2NeT Lab, Wilfrid Laurier University)*

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The wide band-gap semiconductors have attracted much attention due to their potential applications for short wavelength optoelectronic devices. III-V GaN-based materials are among leading materials for the fabrication of blue-green light-emitting devices [1]. However, GaN-based nanostructures are found to have higher carrier densities in generating optical gain, compared to several other alternative materials systems, as a result of a large internal

field due to the strain-induced piezoelectric and spontaneous polarizations [2]. Such alternative material systems are provided by the II-VI ZnSe-based and CdTe-based nanostructures. As recent experimental advances have opened the door to growing high-quality II-VI semiconductor heterostructures [3, 4], their theoretical studies are becoming increasingly important. Due to their potential applications in devices operating in the green region of the spectrum, CdTe/ZnTe nanostructures are of particular interest [5, 6]. CdTe/ZnTe quantum wires (QWR) are in the main focus of our present study. CdTe QWRs hosted by ZnTe are highly strained nanostructures (misfit ~ 6.0% [5, 6]). These systems provide an ideal opportunity to analyze strain effects on optoelectronic properties of QWRs, but no systematic studies of these effects have been performed so far for such CdTe/ZnTe nanostructures. In this contribution, as a first step we apply the Eshelby inclusion formulation to obtain strain fields in CdTe/ZnTe nanowires of such shapes as triangular and square, as well as of more complicated shapes such as crescent and half-ellipsoidal CdTe/ZnTe QWRs. Our main focus here is on the hydrostatic strain component, which leads to rigid shifts in band extremum, i.e. shift in optical transition energy. Our main set-up for the analysis is a QWR structure with a ZnTe buffer layer used as the substrate for the growth of QWRs. The CdTe QWR is under a compressive strain and a ZnTe barrier is lattice-matched to the substrate. We observe that the strain distributions for triangular, square, crescent and half-ellipsoidal CdTe/ZnTe QWRs are similar qualitatively to strain distributions reported earlier by O'Reilly and co-workers in the context of different material systems (e.g., [7]). We also observe that CdTe/ZnTe QWRs are greatly relaxed despite of higher initial misfit. The curved QWR boundaries lead to significant variations of strain values. We conclude that the strain effects in these nanostructures are not to be neglected. Next, we review the assumption of the strain field homogeneity and linearity of the strain-displacement relationship [8], concluding with several examples for CdTe/ZnTe QWRs, where we show that in order to explain the geometry dependence of optical transition energies, inhomogeneity and nonlinear effects may become important. Higher values of hydrostatic strain and other individual strain components lead to a situation where the band edge shift becomes larger and a modification in valence band states is observed. [1] S. Nakamura and G. Fasol, The Blue Green Diode, Springer, Berlin, 1997. [2] F. Bernardini, V. Fiorentini, and D. Vanderbilt,Phys. Rev. B 56, 10024 (1997). [3] M. V. Maksimov, I. L. Krestnikov, S. V. Ivanov, N. N. Ledentsov, and S. V. Sorokin, Semiconductors 31, 800 (1997). [4] C. Onodera, T. Shoji, Y. Hiratate, and T. Taguchi, Jpn. J. Appl. Phys. 46, 248 (2007). [5] T. W. Kim, E. H. Lee, K. H. Lee, J. S. Kim, and H. L. Park, Appl. Phys. Lett. 83,4235 (2003). [6] J. T. Woo, S. H. Song, I. Lee, T. W. Kim, K. H. Yoo, H. S. Lee, and H. L. Park, J. Appl. Phys. 102, 033521 (2007). [7] J. R. Downes, D. A. Faux, and E. P. O'Reilly, J. Appl. Phys. 82 (1997) 3754. [8] R. V. N Melnik and R. D. Mahapatra, Computers and Structures, 85(11-14), 698--711 (2007).

[Th-PB1-052]

Excitation Dynamics of CdTe/ZnTe Quantum Dots Studied in Picosecond Timescale

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Photoluminescence excited by pairs of laser pulses separated by a controlled delay has been shown to be a powerful tool to investigate transient processes in semiconductors, especially excitonic recombination [1]. It has advantage of outstanding temporal resolution limited only by the properties of light pulses. We use a version of this technique to study population dynamics in single CdTe/ZnTe quantum dots [2]. In particular we study dynamics of carrier trapping by QD after non-resonant pulsed excitation. The measurements were performed on a sample immersed in superfluid helium (at 1.8K). A special microscope, immersed together with the sample, assured a resolution better than 0.5um. A frequency-doubled femtosecond laser was used for excitation. Laser pulses were split in pairs in a Michelson interferometer setup. Time-integrated photoluminescence spectra were recorded by a CCD camera as a function of temporal separation between the two pulses in the pair. Individual lines of neutral exciton (X), biexciton (XX), and charged

[Th-PB1-104]

Possible bandgap opening in graphene due to deposited Au nanoparticles: First-principles calculations

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We perform first-principles calculations to investigate electronic and structural properties of graphene with a layer of deposited Au nanoparticles. We consider Au38 nanoparticles that can be either covered with methylthiol molecules, or not. We also consider that the nanoparticles are arranged in a hexagonal lattice, and we focus on the effect of net charge, applied electric fields, and molecular coverage on the electronic structure of the graphene + nanoparticles system. We find that covered nanoparticles interact weakly with graphene, and that the main effect of the nanoparticles on the electronic structure of graphene is a doping effect that can be modified with the application of an electric field perpendicular to the graphene plane. The system is always metallic, without the opening of a bandgap, even if the nanoparticles are charged: neither the Coulomb potential nor the weak nanoparticle-graphene interaction is able to break the graphene sublattice symmetry. In contrast, in the case of deposited bare (non-covered) Au nanoparticles, there is a relatively strong interaction between low-coordinated Au atoms and graphene carbon atoms beneath. This leads to a symmetry breaking of the graphene sublattices and to the opening of a small bandgap of a few tens of meV.

[Th-PB1-105]

Stability and electronic properties of antisites, vacancies, and substitutional Si and C in GaN nanotubes

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Spin-polarized density functional theory is used to investigate the electronic and structural properties of vacancies, antisites and substitutional Si and C in the (10,0) zigzag and (6,6) armchair GaN nanotubes. The energetic stability of those defective systems has been examined by the calculation of the formation energy (for several electronic charge states) as a function of the chemical potentials of the involved atomic species. The calculated formation energies for all defects in the nanotube system are lower than the counterparts in the bulk system. Antisites present higher formation energies as compared with substitutional Si and C impurities, introducing localized electronic levels within the nanotube band gap. For vacancies systems, in the neutral charge state, the defective levels present a spin splitting giving rise to a net magnetic moment of one Bohr magneton. Substitutional Si and C in the Ga site have the lowest formation energy and can exhibit donor properties, suggesting the formation of defect-induced n-type GaN nanotubes. Further total energy analysis of the formation energy as a function of the electronic chemical potential indicates the presence (or the absence) of those defect for a specific charge state.

[Th-PB1-106]

Accounting for Nonlinear Electrostrictive Effects in Modeling Nitride Nanowires and Quantum Dots

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Low dimensional nitride semiconductor nanostructures are promising candidates for a wide range of optoelectronic devices, including quantum dot photodectors, nanowire devices for nanophotonics and high mobility nanoelectronics, quantum dot devices for biophotonics applications, and many others [1]. Optimum opto-electromechanical characteristics of such nanostructures are dependent on their geometry, on operating conditions, and notwithstanding, on strain, piezoelectrictric, and higher order electromechanical effects which may contribute significantly to the overall properties of these structures. In [2] we demonstrated that conventional linear models could be inadequate for the analysis of optoelectronic properties of low dimensional semiconductor nanostructures, focusing our attention on nonlinear strain effects. The authors of [3] showed that nonlinear piezoelectric (elastostrictive) effects could be of significant importance for nanostructure properties (the results were exemplified with zinc-blende materials). In this contribution we focus our attention on the influence of electrostrictive effects. The quadratic electrostictive effect is an important component of electromechanical coupling in wurtzite GaN nanostructures.

Nevertheless, the analysis of this effect in the context of properties of wurtzite nanostructures is practically absent in the literature. No systematic analysis of nonlinear electrostrictive effects with multi-dimensional models has been carried out up to date. Results available in the literature are limited to the one-dimensional case (e.g., [4]) and are not applicable to the situations where a 2D/3D analysis is required. Such situations are in the main focus of this work and they include finite length nanowires and quantum dots. We start our analysis in this contribution with GaN cylindrical nanowires of 5-30nm in diameter and varying length. Our model for the analysis of nonlinear electromechanical effects is based on a general system of elasticity coupled with Maxwell's equation for the electric field. We account for the lattice mismatch via corresponding strain tensor components [2] and for nonlinear electromechanical effects via constitutive relationships where we take into account second order tensor coefficients responsible for electrostriction. It was already been known for some time (e.g., [5]) that nonlinear effects in low dimensional nitride nanostructures, such as quantum wells, can be substantial under hydrostatic pressure. We show here that in finite length nitride nanowires nonlinear electrostrictive effects can be significant even without this condition. This conclusion is also confirmed with the analysis of properties of conical (truncated pyramidal) GaN/AlN quantum dots with geometries similar to those considered in [6]. References: [1] J. Piprek, Nitride semiconductor devices: principles and simulation, Wiley-VCH, Weinheim, 2007. [2] RVN Melnik and RD Mahapatra, Coupled effects in quantum dot nanostructures with nonlinear strain and bridging modelling scales, Computers and Structures, 85(11-14), 698–711, 2007. [3] G. Bester, X. Wu, D. Vanderbilt, and A. Zunger, Importance of second-order piezoelectric effects in zinc-blende semiconductors, Physical Review Letters, 96(18), 187602, 2006. [4] M Willatzen and Lew Yan Voon, L, Static and dynamic effects due to electrostriction in GaN/AlN, J. Phys.: Condens. Matter, 19, 506202, 2007. [5] G. Vaschenko et al, Nonlinear polarization in nitrides revealed with hydrostatic pressure, phys.stat. sol. (b), 235(2), 238-247, 2003. [6] R V N Melnik and K.N. Zotsenko, Finite element analysis of coupled electronic states in quantum dot nanostructures, Modelling Simul. Mater. Sci. Eng. 12, 465-477, 2004.

[Th-PB1-107]

Optical Properties of Catalyst Free Grown Nanowires

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Semiconductor nanowires are promising candidates for a variety of nanodevices, i.e. bio- and chemical sensors /1/, nanoelectronics transistors /2/, spintronics /3/ and single photon emitter. Typically nanowires are deposited utilizing the vapour-liquid-solid (VLS) growth method using Au nanodroplets as catalyst. However, the method leads to Au contaminations. Au impurities act in many semiconductors as deep traps, disturbing the electrical and optical properties of the nanowires. Here we studied the catalyst free formation of semiconductor nanowires, namely GaN based wires on Si grown by MBE as well as the selective growth of GaAs wires on GaAs by MOVPE. GaN and InN wires have been deposited on Si (111) substrates by MBE using the substrate temperature and the III/V ratio as parameters controlling the wire growth. Transmission electron microscopy (TEM) examinations reveal a 2nm thick amorphous layer between the wires and the substrate, which is assumed to be SiNx. However, the wires are crystallographically oriented perpendicular to the surface, i.e. to the z-axis of GaN /4/. The latter still holds even when the wires are deposited on Si substrates coated with a thick SiO2. Hence the formation and orientation along the z-axis of the wires is independent of the crystallographic information of the substrate. The catalyst free growth permits the fabrication of GaN/AlN quantum structures with abrupt interfaces /4/. Photoconductivity studies show that the GaN wires exhibit a surface depletion layer, thus wide GaN wires show a pronounced Franz-Keldish effect, which diminishes with decreasing wire diameter /5/. Due to the surface enrichment of electrons in InN nanowires, the transport characteristics are sensitive to surface contaminations, in particular for quantum devices involving only a few electrons. Here, core shell structures are required defining a clean barrier towards the wire surface. First experiments have been performed growing InN/GaN core shell structures. The photoluminescence intensity of InN/GaN core shell structures is increased compared to bare InN wires, indicating a successful passivation of the surface states of the InN. The selective growth of GaAs nanowires by metalorganic vapour phase epitaxy (MOVPE) was investigated using GaAs (111) substrates patterned with a SiO2 mask. The SiO2 was patterned using e-beam lithography. SiO2 coated GaAs substrates with windows in the SiO2 film of 50-100 nm in diameter were prepared. Growth occurred only in the windows and several micron long wires with a hexagonal diameter were obtained. The smooth sidewalls are defined by the [110] facets. The selective growth into SiO2 windows allows the fabrication of regular arrays of GaAs nanowires with accurate

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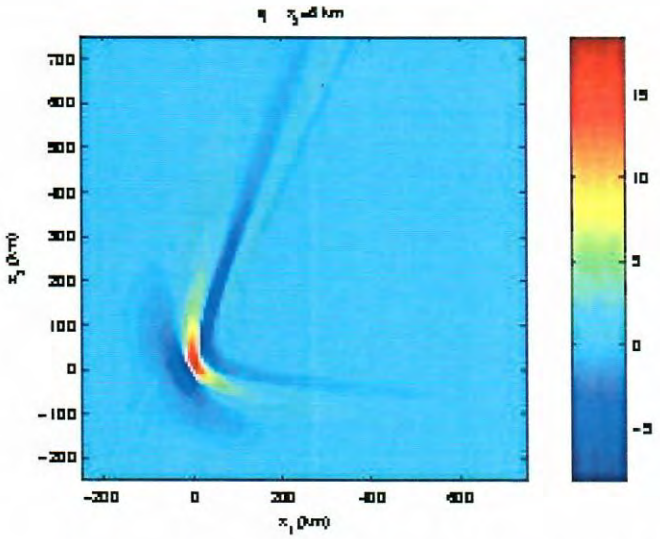

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Paper 139

Phase Transformations in Finite Length Nanowires: Analysis with Mesoscopic Models

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Keywords: phase transformations, nanowires, nonlocal models, nanostructures.

In this work we propose a simplified mesoscopic model for the analysis of nanowires of finite length. Our interest has been motivated by the fact that such nanowires can exhibit shape memory effects. This has been confirmed for a wide range of these structures, including ZnO, Cu, Ni, Al, Ag, and Au nanowires.

Here we focus on a two-dimensional analogue of what in the general three-dimensional case would correspond to cubic to tertragonal or tetragonal to orthorhombic transformations. Such a two-dimensional case deals with square to rectangle transformations which are easier to treat due to the fact that the energy as a function of lattice spacing exhibits two distinct minima corresponding to two different phases of the nanostructure.

Most results obtained up to date, both theoretical and computational, are concerned with infinitely long nanowires or infinitely large nanoplates for that matter. In this contribution, we develop a relatively simple and computationally inexpensive model to study phase transformations in finite nanostructures with our major focus given to nanowires of finite length. We note the models describing shape memory effects at the mesoscopic level such as those developed in [1] can be reduced to a two-dimensional case (and in the case of nanowires of infinite length, to the one-dimensional case). Our considerations are based on a modification of a coupled system of PDEs for the evolution of displacements and temperature [2,3]. One of the applications of the nanowires discussed in this paper stems from their integration in biomolecular technologies and we highlight the importance of the contributions of entropic elasticity in such cases.

Recently, we developed and demonstrated the application of several efficient methodologies to solve two-dimensional models describing square-to-rectangle phase transformations in materials with memory, in particular the finite volume methodology [3] and a numerical reduction procedure based on the proper orthogonal decomposition (POD) [2]. The methodology proposed in this contribution is different and is based on a combination of the Chebyshev pseudo-spectral technique combined with the domain decomposition method and second order backward differentiation. Based on this methodology, we analysed different types of nanowires and examplified our results here with Cu nanowires for different diameter-length ratio. Our results indicate that the initial pattern formation propagates towards the longitudinal boundaries of the structure when the nanowire width decreases. Based on our computational results, we provided an explanation of this phenomenon, confirming that in all cases studied here surface energy suppresses the pattern formation.

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Paper 140

Temperature-Dependent Phase Stability of CdS Quantum Dots from First-Principle Molecular Dynamic Calculations

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Keywords: quantum dots, temperature-dependent phase stability, CdS, first-principle molecular dynamic calculations.

Due to their unique optoelectronic properties and a wide range of current and potential applications, nano-sized semiconductors have attracted much attention in recent years. Among these semiconductors, cadmium sulfide (CdS), being one of the most important wide-gap semiconductors, is stable and exhibits high luminescence [1]. CdS nanostructures have found many applications in photovoltaic cells, photonic switches and optoelectronic devices. In recent years, CdS quantum dots have also been used in biolabeling, bioimaging, drug delivery and other biotechnological areas. It is due to these optoelectronic and bio-related applications, the analysis of thermal stability of CdS quantum dots becomes one of the most important avenues of research in this field. Additionally, CdS quantum dots represent an intermediate state of matter between molecular species and bulk materials. Therefore, a better understanding of their temperature dependent phase stability and phase transformations will ultimately enable us to taylor their electrical and optical properties from molecular level to bulk crystals.

It has been known for a long time that the bulk CdS is highly stable and it exists in the hexagonal wurtzite phase in a wide range of temperatures, from room temperature to its melting point 1750 °C. Recently it has been shown that due to the large surface to volume ratio and reconstruction of surface crystal structure, the thermodynamic properties of the CdS nanostructure can differ significantly from bulk CdS [2]. For example, under appropriate conditions some wurtzite structure semiconductor materials can transform into a graphitic structure when they are in the form of thin nanoplates [3]. Since the internal pressure deduced from surface stress is very large for nanostructures, at ambient conditions, the stability phase in nanosize structures is always a high pressure stability phase struture in bulk [4]. Nevertheless, the temperature-dependent phase stability of the CdS quantum dots remains poorly understood to date. In particular, systematic calculations and comprehensive comparisons of their thermodynamic stability, as well as mechanical, electronic, and optical properties under different temperature conditions are still lacking. To fill this gap, in this work we carry out first-principle molecular dynamic (MD) calculations for CdS quantum dots of various phase structures and study temperature-dependent phase stability of these nanostructures. Based on our calculations, we analyze the relative stability of different CdS phases under different temperature conditions. Our results indicated that at the temperature range studied in this work, the phase stability sequence for the $Cd_{48}S_{48}$ nanostructure is rocksalt, wurtzite and graphitic phase, which is the same as that of bulk CdS crystal under high pressure. Although the temperature can affect the total energy of the CdS nanostructure, it cannot change the phase stability sequence of CdS nanostructures in the temperature range studied in this work.

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Paper 143

Modelling Nonlinear Electro-Mechanical Effects in Nano-Heterostructures Using Domain-Decomposition Methods

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Keywords: heterostructures, lattice mismatch, electrostriction, piezoelectric, spectral methods.

In this work we analyze numerically the contributions of nonlinear electromechanical effects in nano-heterostructures, focusing on the effect of electrostriction. The main novelty of the present paper lies with the fact that the latter effect has not been analyzed in nano-heterostructures before with multidimensional models.

We start our analysis with a continuum three-dimensional axisymmetric model, accounting for complete self-consistency of electromechanical fields. Although the techniques developed here, can be applied to other material heterostructures, all our examples in this paper are given for GaN/AlN nano-heterostructures. One of the reasons for that is an increasing range of current and potential applications of these nanostructures in optoelectronic devices. We consider in our examples a cylindrical GaN/AlN nano-heterostructure which allows us to reduce the original problem to a two-dimensional model. This reduction goes with a remark that albeit the wurtzite symmetry is not axisymmetric, Navier's equations do reflect axisymmetry [1].

We note also that recently the analysis of such nanostructures have been carried out in [2]. The analysis was selfconsistent in lattice mismatches, spontaneous polarization, piezoelectric effect, and strain and has been performed by employing a linear (static and dynamic) and nonlinear (static with electrostriction) electromechanical model framework developed there. However, it was restricted to the one-dimensional situation.

In spite of the belief that a combination of dimensional effects and electrostriction could lead to interesting new physics, the problem was lacking attention partly due to a sparse experimental information on electrostrictive tensor components in the nitrides. Here, due to the availability of experimental information on the electrostriction coefficient connecting the electric field along the z-direction with the strain component, our attention was drawn to only this component of electrostriction.

In order to deal with the inherent discontinuity of the physical parameters involved and the problem of lattice mismatch, the domain decomposition methodology has been employed for our numerical (nonlinear) analysis. Chebyshev pseudospectral methods have been used for discretization in each sub-domain. Our results demonstrate clear jumps in the electric field and strain distributions across the interface between the two materials, while the mechanical field and electric displacements exhibit a continuous pattern. The effect of electrostriction has been analyzed by comparison of the results with a linear model (without electrostriction). Finally, we demonstrate a significant difference in several key parameters of nanostructures, such as the electric field and strains, while analyzing them with our multidimensional model and previous one-dimensional models.

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(which is a priori different from the temperature θ), and a phase parameter χ describing the state of the adhesion on the contact surface. The resulting equations, written both in the body and on the contact surface, are highly nonlinear, mainly for the presence of nonlinear operators (possibly degenerating) accounting for the physical constraints (as the impenetrability condition, the positivity of the absolute temperatures, consistency of the phase parameter). We prove a global in time existence result for the complete system and we investigate the asymptotic behaviour of solutions (characterizing the ω-limit set). In the isothermal case, if the damage process for adhesive bonds is reversible, we also prove uniqueness of the solution and continuous dependence on the data.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Phase Field Equations: The Next Generation

Gunduz Caginalp
University of Pittsburgh, USA
caginalp@pitt.edu

After a review of phase field equations and the distinguished sharp interface limits, this talk will focus on new results (obtained in collaboration with Xinfu Chen and Christof Eck). A new derivation from asymptotic analysis leads to a phase field model that is proven to differ by only the square of the interface thickness from the corresponding sharp interface problem. Numerical computations demonstrate the proximity of the diffuse and sharp interface problems using various sets of material parameters including those of succinonitrile experiments on the space shuttle.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Time-dependent Obstacle problems in thermohydraulics

Takesi Fukao
Gifu National College of Technology, Japan
fukao@gifu-nct.ac.jp
Masahiro Kubo

Obstacle problems, which are mathematical models of nonlinear phenomena accompanying the free boundary, have been studied. The existence and uniqueness for some systems with the Navier-Stokes equations is considered.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Phase-field systems with dynamic boundary conditions

Maurizio Grasselli
Politecnico di Milano - ITALY, Italy
maurizio.grasselli@polimi.it
Ciprian G. Gal and Alain Miranville

This talk is devoted to the mathematical analyis of a Caginalp type system subject to dynamic boundary conditions which account for possible interactions of the material with the walls enclosing it. We intend to present and discuss a number of recent results about well-posedness, global asymptotic behavior (i.e., attractors) and convergence to single equilibria.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Phase Transformations in Nanostructures: Models and Applications

Roderick Melnik
WLU/Waterloo, Canada
rmelnik@wlu.ca
Linxiang Wang, Bin Wen and Jean Zu

While a phenomenon of phase transformations in infinite nanowires and nanoplates have already been known for some time, the same cannot be said about finite low dimensional nanostructures. Only recently, evidence has been mounting that the phenomenon of phase transformations is important for finite nanostructures too, in particular when predicting opto-electromechanical properties of such structures. Based on our experience with the development of dynamic models for phase transformations at the mesoscopic level [e.g., Comput. Materials Science, 18(3-4), 141-148, 2000; Appl. Numer. Math., 57(5-7), 510-520, 2007], we report here our first attempts to describe phase transformations in finite nano-objects, focusing on the analysis of microstructure evolution. Mathematically, our model is based on a coupled time-dependent system of PDEs and is similar to the model we analyzed in [Heat and Mass Transfer, 43(6), 535-546, 2007]. Several simulation results with this model will be discussed in the context of nanostructures.

Finally, we present several computational results obtained by us with ab initio methodology. We report phase transformations in ZnO and CdS low dimensional nanostructures, including quantum dots, and analyze temperature-dependent phase stability of these objects in the context of their bio-

response of nonlinear dynamical systems undergoing periodic or quasi-periodic oscillations, whether self-excited or due to external harmonic excitation. Many decades after the first complete presentation of the method, it has been reformulated and further developed by incorporating various extensions and enhancements. The dynamic systems considered range from a simple one degree-of-freedom oscillator such as Duffing's oscillator to complex high dimensional systems with non-analytical nonlinearities in models of fluid-structural interactions. An overview will be presented of the formulation of the basic method and a brief description of the variants. For each version of the method, significant studies will be highlighted with the emphasis on insights into the accuracy of the proposed methods versus complexity and computational requirements. Subjects will include the variants of the harmonic balance method, the advantages and disadvantages of the several variants, the implementation of the variants in various applications, and possible future developments for incorporating complex nonlinearities in very high dimensional systems.

⟶ ∞ ◇ ∞ ⟵

Spatiotemporal patterns and chaotic burst synchronization in a small-world neuronal network

Qishao Lu
Beijing University of Aero. & Astro., Peoples Rep of China
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Yanhong Zheng

he spatiotemporal patterns and chaotic burst synchronization of a small-world neuronal network are studied in this paper. Synchronization parameter, similarity parameter and order parameter are introduced to investigate the dynamics behaviour of the neurons. Chaotic burst synchronization and nearly complete synchronization can be observed as the link probability and the coupling strength are large enough. It is found that with increasing the link probability and the coupling strength chaotic bursts become appreciably synchronous in space and coherent in time, and the maximal spatiotemporal order appears at some particular values of the probability and the coupling strength, respectively. The larger the size of the network, the smaller the probability and the coupling strength are needed for the network to achieve burst synchronization. Moreover, the bursting activity and the spatiotemporal patterns are robust to small noise.

⟶ ∞ ◇ ∞ ⟵

Coupled Electromechanical Effects in Nanostructures: Electrostriction in the Multidimensional Case

Roderick Melnik
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rmelnik@wlu.ca
Mehrdad Bahrami-Samani and Jean Zu

In this contribution, we analyze higher order electromechanical effects in low dimensional semiconductor nanostructures, focusing on quantum dots. While the mathematical theory of linear electromechanical interactions was put on a rigorous foundation earlier and efficient numerical procedures were developed [e.g., Appl. Math. Comp., 107, 2000, 27-55], many questions remain, already at the level of model development, in the nonlinear case. Formally, the model is based on a system of PDEs consisting of elasticity equations coupled with the Maxwell equation. In the context of nanostructures, experimental evidence suggests that a number of higher order effects may become important in predicting their properties. Nevertheless, there are no currently models that account for such effects in a consistent manner. Elastostrictive effects have recently been discussed in [PRL, 96, 2006, 187602]. However, no attempts have been made to estimate the significance of electrostrictive effects, in particular when it comes to the modeling of quantum dots where mathematical models should go beyond one-dimensional descriptions, sufficient only for quantum wells and idealized quantum wires. Nonlinear constitutive relationships, coupling mechanical and electric fields in a non-trivial manner, bring major challenges in dealing with this problem. In this contribution, we provide a systematic characterization of nonlinear electromechanical effects in low dimensional semiconductor nanostructures and report several computational results for wurtzite GaN and zinc-blende GaAs quantum dots obtained with the developed models.

⟶ ∞ ◇ ∞ ⟵

Nonlinear Semigroups and the Question of Boundary Conditions for the Tricomi Equation

John Neuberger
University of North Texas, USA

7th AIMS International Conference on Dynamical Systems, Differential Equations and Applications

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direction. Moreover, on the broad Coulomb oscillation peaks, small oscillation is appeared. The small oscillation peaks are corresponding to quantum levels *i.e.* resonant tunneling levels in the SWNT. Finally, at fully large applied gate voltage around several tens volts, the Coulomb oscillation characteristic is almost disappeared and small oscillation characteristic becomes clear. The transition of the electrical property from the Coulomb oscillation characteristic to the resonant tunneling characteristics is attributed to changing the thickness of the tunneling barriers which are Schottky barriers at the contact between SWNT and electrode metals. When small voltage is applied to the gate electrode, the thicknesses of the Schottky barriers are thick and the tunneling resistance of Schottky barriers is larger enough than quantum resistance. Therefore, carrier is fully confined in the SWNT and the Coulomb charging effects are appeared. While, when fully large voltage is applied to the gate electrode, the thicknesses of Schottky barrier are thin and the tunneling resistance of Schottky barriers is too small to confine the carrier in the SWNT. Therefore, Coulomb charging effects are lifted and the resonant tunneling characteristic remains. We also observed contour plot of second order differential conductance as a function of the gate voltage and the drain voltage. The plot shows clearly gate voltage and drain voltage dependence of the quantum levels. Thus, we succeeded in controlling electrical property of SWNT QD by applied gate voltage which transit from single-hole transistor property to resonant tunneling property.

9:00 AM

EE3, Aligned Carbon Nanotube Membranes: Transport Enhancement and Electrostatic Activity: *Bruce Hinds*[1]; [1]University of Kentucky

Carbon nanotubes have three key attributes that make them of great interest for novel membrane applications 1) atomically flat graphite surface allows for ideal fluid slip boundary conditions 2) the cutting process to open CNTs inherently places functional chemistry at CNT core entrance and 3) CNT are electrically conductive allowing for electrochemical reactions and application of electric fields gradients at CNT tips. Towards this goal, a composite membrane structure containing vertically aligned carbon nanotubes passing across a polystyrene matrix film have been fabricated. Fabrication steps, material characterization and ionic diffusion transport properties are described. Plasma oxidation during the fabrication process introduces carboxylic acid groups on the CNT tips that are modified using carbodiimide mediated coupling between carboxylic acid on the CNTs and accessible amine groups of the functional molecule. To explore the hypothesis of 'Gatekeeper' selectivity, the entrances to CNT's cores were functionalized with aliphatic amines of different lengths, charged dye molecule and an aliphatic amine elongated by spacers containing poly-peptides. The simultaneous permeation of two differently sized but equally charged molecules (ruthenium bi-pyridine [Ru-(bipy)3+2] and methyl viologen [MV+2]) was studied and relative selectivity of was seen to vary from 1.9 to 3.6 as a function of tip-functionalization chemistry. Anionic charged functional groups are seen to sharply increase flux of cationic permeates. This effect is reduced at higher solution ionic strength consistent with shorter Debye screening length screening attractive charge at the CNT core entrance. Using a hindered diffusion to model observed selectivities was consistent only with a geometry of only CNT tip functionalization, not along the length of CNT core. Bio-chemical gating of CNTs is also seen by tethering desthiobiotin to CNT tips with the reversible binding to streptavidin. The complete ATP cycle (phosphylation/ dephosphylation) can be performed on CNT tips with corresponding modulation of flux across CNT membrane. Strong electrostatic effects of binding protein are seen with enhanced cationic flux seen for the relativel open anioic protein binding at CNT tip entrance. The functional density of tethered charge molecules can be substantially increased by the use of electrochemical grafting of diazonium salts. Functionality can be forced to occur at the CNT tip entrances by fast fluid flow of an inert solvent through the core during electrochemical functionalization. The selectivity between Ru(bi-pyridine)32+ and methyl viologen 2+ flux is found to be as high as 23 with -130mV bias applied to the membrane with tethered anionic dye molecule. Changes in the flux and selectivity support a model where charged tethered molecules at the tips are drawn into the CNT core at positive bias hindering/gating flux across the membrane. Applications towards controlled transdermal drug delivery are discussed.

9:20 AM Student

EE4, Trapping Individual Carbon Nanotubes: *Anupama Arun*[1]; Paul Salet[1]; Adrian Ionescu[1]; [1]École Polytechnique Fédérale de Lausanne

A technique to deterministically manipulate individual Carbon Nanotubes (CNT) has been the brick-wall for the boom of CNT based devices. Here we demonstrate dielectrophoresis as an efficient technique to trap individual Single Walled Carbon Nanotubes (SWCNT) and Multi Walled Carbon Nanotubes (MWCNT). A coarse control on the number of nanotubes deposited was achieved by controlling the applied voltage and duration of deposition; additionally, a circuit that cuts off the electric field necessary for further CNT deposition after one single CNT deposition has been used. By using an external series resistance during dielectrophoresis, higher than the contact resistance of the carbon nanotube obtained after dielectrophoresis, we are able to limit the deposition to individual nanotubes. The contact resistance of a single SWCNT obtained by the coarse technique was found to be 80 MO. Hence we chose a limiting series resistance of 1 GO. P-type silicon substrate with resistivity of 0.1-0.5 Ocm with thermal oxide of 200 nm was used as substrate. Cr/Pt (5nm/50nm) electrodes were patterned by conventional photolithography and lift-off process. SWCNT's and MWCNT's produced by CVD process were dispersed in DI water with 1wt% surfactant SDS. The solution was sonicated and centrifuged to remove impurities. An ac signal of 5 MHz with and without series resistance was used to perform dielectrophoresis. Around 20 µl of the solution was deposited and deposition time of 120 seconds and 300 seconds were used for SWCNT's and MWCNT's respectively. The yield is better in the case of SWCNT's because they form better electrical contact with the electrodes than the MWCNT's after dielectrophoresis. The proposed fabrication is based on materials compatible with CMOS process. This opens doors to easily study individual nanotubes and to integrate CNT based devices in CMOS technology.

9:40 AM

EE5, Field Emission Enhancement in a Patterned CNT Array Cathode: D. Roy Mahapatra[1]; N. Sinha[2]; *R. Melnik*[3]; [1]Indian Institute of Science; [2]University of Waterloo; [3]Wilfrid Laurier University

Field emission (FE) from carbon nanotubes (CNTs) is difficult to characterize using simple formulae or data fitting, which is due to (1) electron-phonon interaction, (2) electromechanical force field leading to stretching of CNTs, and (3) ballistic transport induced thermal spikes, coupled with high dynamic stress, leading to degradation of emission performance at the device scale. Degradation of emission performance and occurrence of thermal spikes is undesirable for applications such as biomedical x-ray devices, where it is of great importance to have precision control of the electron beams over multiple spatio-temporal scales. Detailed physics-based models of CNTs considering the aspects (1) and (2) as mentioned above have already been developed by us (see Ref. [1-3] for details). This paper aims at analyzing a new design concept, wherein (a) the electrodynamic force field leading to strong electron-phonon interaction during ballistic transport and also (b) the usually observed reorientation of the CNT tips and instability due to coulomb repulsions can be harnessed optimally. Two additional gates on the edges of the cathode substrate are introduced in the proposed new design and magnetic field is applied from them. An array of stacked CNTs is considered on the cathode substrate. The height of the CNTs is such that a symmetric force field is maintained in each pixel with respect to the central axis parallel to vertical axis. As a result, it is expected that a maximum current density as well as well-shaped beam can be produced under DC voltage across the cathode-anode structure. In the present design, the anode is assumed to be a flat uniform conducting metal plate. The present design objective is to estimate the field emission current as function of (i) the applied magnetic field, (ii) the side-wise gate height dc with respect to the CNT height h, and (iii) the slope of stacking of the CNT tips. Simulations reveal transverse electric field distribution in the pixel, which directly influences the field emission current. Details of a coupled model involving ballistic transport of electrons, electron-phonon interaction and nonlinear deformation of CNTs due to electrodynamics forces will be discussed, followed by optimization studies involving the parameters dc/h and Vg/VDC, where Vg denotes the side-wise gate voltage and VDC denotes the DC voltage across the anode-cathode structure. Also, it will be shown how the model can be extended to a real 3D system. [1]N. Sinha, D. Roy Mahapatra, J.T.W. Yeow, R.V.N. Melnik and D.A. Jaffray, J. Compu. Theor. Nanosci., 4, 535-549, 2007. [2]N. Sinha, D. Roy Mahapatra, J.T.W. Yeow and

R.V.N. Melnik, Proc. IEEE Nano 2007, Hong Kong, Aug 2-5, 961-964, 2007. [3]N. Sinha, D. Roy Mahapatra, Y. Sun, J.T.W. Yeow, R. Melnik and D.A. Jaffray, Nanotechnology, 19, 25710, 2008.

10:00 AM

EE6, Synthesis and Characterization of Carbon Nanopearls Derived from Ni and Acetylene Using CVD Process: *Shanee Houston*[1]; Gail Brown[1]; Steve Fairchild[1]; Terry Murray[2]; [1]U.S. Air Force Research Laboratory; [2]University of Dayton

Carbon Nanopearls (CNP) are a new form of carbon nano-materials different from the well known carbon nanotubes (CNT) or buckyballs. The CNPs consists of graphitic flakes formed in a sphere structure. The term nanopearl comes from this spherical layered growth as well as the fact that the spheres are often linked together similar to a pearl necklace. The CNP radius of curvature is very small, and there is no chirality. This enables CNP to be great candidates for field emission. Carbon nanopearls (CNP) have been found to form when synthesized at 700°C using chemical vapor deposition (CVD). By using a nickel catalyst 100nm in size, CNP can be formed. Reports have shown some CNP with a size of 150nm. In this paper we report CNP with sizes ranging from 500-800nm. Raman analysis has been done to prove that sp2 carbon is formed as a result of this growth process. These results also show a narrow D and G band, which indicates a very pure sp2 carbon structure. The dip in between the two bands also indicates fewer defects in the CNP sample than what has been reported on this material so far. Additional experimental results will also be reported. It is expected that future field emission and electronic testing on these CNP will show favorable results.

Session FF: Dilute Nitride Semiconductors

Friday AM
June 27, 2008

Room: Flying A
Location: University of California, Santa Barbara

Session Chairs: Seth Bank, University of Texas at Austin

10:20 AM Student

FF1, MBE Grown Dilute Nitride Alloys of GaAsSbN Lattice-Matched to GaAs and GaSbN Quantum Wells: *Sudhakar Bharatan*[1]; Shanthi Iyer[1]; Jia Li[1]; Liangjin Wu[1]; Kevin Matney[2]; Jason Reppert[3]; Apparao Rao[3]; [1]North Carolina Agricultural and Technical State University; [2]Bede Scientific Inc.; [3]Clemson University

Dilute nitrides are an exciting new class of semiconductors based on combining GaN with III-V. Amongst the different III-V-dilute nitride material systems, N incorporation in the antimonide and mixed arsenide-antimonide systems are the most challenging due to the larger atomic size and electronegativity differences between N and Sb in comparison to N and As. In this paper we will present a comprehensive growth and characterization study of and thick GaAsSbN layers lattice matched to GaAs and GaSbN/GaSb single quantum well (SQW) heterostructures. The characterization studies include detailed structural, vibrational and optical characteristics of the structures. The effects of in-situ annealing in As ambient and ex-situ annealing in N ambient on the low temperature photoluminescence (PL) characteristics will also be presented. Both of the above alloys exhibit high crystalline quality attested by the presence of well resolved Pendellosung fringes on a triple axis (004) x-ray scan and dynamical truncation rods observed on the corresponding reciprocal space map. 8 K PL peak energy of 1 eV with a full width at half-maximum (FWHM) of 18 meV (26 meV) on ex-situ (in-situ) annealed thick GaAsSbN layers lattice-matched to GaAs have been achieved for N = 2.6%. Raman spectral analysis, the temperature dependence of the PL peak energy, and SIMS profiles indicate that the outdiffusions of N and As are suppressed and Ga-N bonding is improved in the in-situ annealed samples under As ambient, leading to higher PL intensities. In addition, indirect evidence of atomic scale ordering has been observed. These alloys exhibit pronounced s-shaped curve in the temperature dependence of the PL peak energy at low temperatures, a signature of exciton localization. The depths of these are found to be a function of annealing conditions. However, for N incorporation in GaSb with concentrations of up to 1.5%, led to highly localized N pairs/cluster states, as evidenced from the sharp and discrete features below the GaSb band edge in the low temperature PL spectra. These clearly indicate N incorporation in GaSb is a challenge. In addition, the effect of In incorporation to GaSbN SQW will also be discussed. This work is supported by Army Research Office (Contract Nos. W911NF-07-1-0577 and W911NF-07-1-0161).

10:40 AM Student

FF2, Vast Improvement of 1.55μm GaInNAsSb QW Quality by a Combination of Low Group-V Flux Growth, and Long Low-Temperature Annealing: *Hopil Bae*[1]; Tomas Sarmiento[1]; James Harris[1]; [1]Stanford University

Dilute nitride materials have been actively researched for their potential to enable low-cost high-density GaAs-based optoelectronic devices for optical communications and interconnects in the 1.2-1.6μm wavelength range. Although the growth of these materials was quite challenging, many improvements and optimizations in the growth of the material eventually enabled low-threshold (373A/cm^2 CW, 318A/cm^2 pulsed) and high power operation (250mW CW, >650mW pulsed) of 1.55μm GaInNAsSb/GaNAs lasers, as well as 1.53μm VCSELS, epitaxially grown on GaAs substrates. Our new study shows that this past state-of-the-art result was still not yet optimum, and significant additional improvement is possible, by combining two changes to the growth and annealing conditions. The quality is measured by the photoluminescence intensity of the QW samples. The first change is lowering the As and Sb fluxes, while keeping the ratio between them fixed. Roughly two times higher PL intensity is obtained by using a lower V/III flux ratio (x9, measured in beam equivalent pressure), when the growth temperature was 440°C. Lower growth temperatures resulted in lower optimum V/III flux ratio. The second improvement is annealing for longer durations at lower temperatures, compared to the 1-minute rapid-thermal anneals used in the past. This change of annealing condition resulted in another factor of two improvement in PL intensity, totaling to a factor of 4 improvement, compared to the past growth and annealing methods, which had enabled the best previously reported 1.55μm GaInNAsSb lasers. We also grew and tested "laser-like" PL samples, with doped AlGaAs cladding layers surrounding the QW, in order to determine whether the above improvements are useful for actual devices. It has been a concern that a few hours of upper-cladding or upper-DBR growth on top of QWs may over-anneal the QWs and degrade their quality. We measured the PL intensity of the samples after subjecting them to the same thermal load as from typical upper-structure growths. Our study shows that the feared degradation does not happen during upper-structure growths. In conclusion, we found a significant improvement in GaInNAsSb material quality by growing at lower group-V fluxes and annealing longer at lower temperatures than we had before. In addition, the samples grown and annealed by the new method are found to be resilient to several hours of thermal stress from the growth of upper-structures in actual optoelectronic devices. Considering that we were able to fabricate record performance lasers in the past with sub-optimum growth and annealing conditions, we expect to achieve even better laser performance to be reported at the meeting.

11:00 AM Student

FF3, Effects of N Composition on the Electronic Properties of (In)GaAsN Alloys: *Tassilo Dannecker*[1]; Matthew Reason[2]; Yu Jin[3]; John Buckeridge[1]; Stephen Fahy[1]; Cagliyan Kurdak[3]; Rachel S. Goldman[2]; [1]Tyndall National Institute; [2]University of Michigan, Department of Materials Science and Engineering; [3]University of Michigan, Physics Department

Dilute nitride semiconductor alloys are promising for long-wavelength light emitters and detectors, high performance electronic devices, and high efficiency solar cells. Typically, the electron mobility of (In)GaAs(N) alloys decreases with N incorporation, resulting in substantially lower electron mobilities than in (In)GaAs. Attempts to enhance the mobility of (In)GaAsN-based alloys have included digital alloy superlattices (SL) and modulation doped heterostructures. However, these structures are typically grown in ultra high vacuum systems where the N flux is "controlled" by a shutter. In those cases, the interface abruptness and electron mobilities are limited, since residual N is incorporated into all layers, even with the shutter closed. In this work, we have investigated the electronic properties of (IN)GaAs$_{(1-x)}$N$_x$ alloy films and (In)GaAsN/(In)GaAs

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Tuesday, July 1st 16:30 - 18:30

Minisymposium on "Mathematical Modeling and Numerical Simulation of Coupled Multiphysics Systems in Nano- and Biotechnologies" I **Room: CAS2.2 MS116A**

Minisymposium organized by Roderick Melnik and Riccardo Sacco

16:30 Modeling DNA Sequencing at the Nanoscale (Keynote Lecture)
Massimiliano Di Ventra

17:00 Multiscale - Multiphysics Simulation of Nanostructured Devices: The TIBERCARD Project (Keynote Lecture)
Aldo Di Carlo, M. Auf der Maur, M. Povolotskyi, F. Sacconi, Giovanni Romano, G. Penazzi and A. Pecchia

17:30 Modeling of Semiconductor/Electrolyte Nanostructures with Nextnano³
Stefan Birner

17:50 Three-Dimensional Strain Distributions due to Anisotropic Effects in InGaAs Semiconductor Quantum Dots
Daniele Barettin, Benny Lassen, M. Willatzen, R.V.N. Melnik and Lok Lew Yan Voon

Wednesday, July 2nd 10:30 - 12:30

Minisymposium on "Mathematical Modeling and Numerical Simulation of Coupled Multiphysics Systems in Nano- and Biotechnologies" II **Room: CAS2.2 MS116B**

Minisymposium organized by Roderick Melnik and Riccardo Sacco

10:30 Multi-Scale Simulations of DNA and Colloidal Systems with a Combined Lattice Boltzmann/Molecular Dynamics Approach
Simona Melchionna, Maria Fyta, Efthimios Kaxiras, Massimo Bernaschi and Sauro Succi

10:50 Simple Models for Extracting Compressive Rigidity of Molecules from Atomic Force Microscopy Data
Igor Sokolov and Ravi Gaikwad

11:10 Size Selective Capturing of Biomolecules and Nanoparticles by Combined Dielectrophoresis and Surface Tension
Yaling Liu, Jae-Hyun Chung and Kyong-Hoon Lee

11:30 Thermodynamic and Mechanical Properties of Simple RNA Nanostructures
Maxim Paliy and Roderick Melnik

11:50 Tissue Engineering through Simulation and Experiments
Manuela Teresa Raimondi, Federica Boschetti, Margherita Cioffi, Fabio Galbusera, Katia Laganà, Matteo Moretti and Gabriele Dubini

Wednesday, July 2nd 14:00 - 16:00

Minisymposium on "Mathematical Modeling and Numerical Simulation of Coupled Multiphysics Systems in Nano- and Biotechnologies" III **Room: CAS2.2 MS116C**

Minisymposium organized by Roderick Melnik and Riccardo Sacco

14:00 A Three-Dimensional Model of Cellular Electrical Activiy
Yoichiro Mori, Charles S. Peskin and Joseph W. Jerome

14:20 Mathematical Models of Axon Guidance: Towards the Understanding of a Key Process in Development
Giacomo Aletti, Paola Causin and Giovanni Naldi

14:40 Multiscale/Multiphysics Computational Models for Lab-On-Chip Technology Applications
Bice Chini, Joseph W. Jerome, Massimo Longaretti and Riccardo Sacco

International Center for Numerical Methods in Engineering. Barcelona, Spain.
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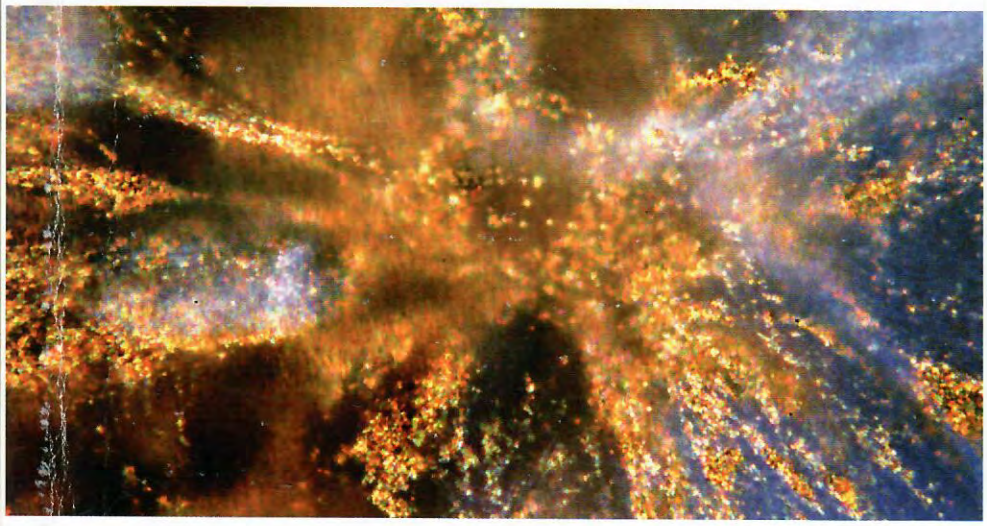

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JUNE 14 - 20, 2009 LVIV, UKRAINE

STOCHASTIC ANALYSIS AND RANDOM DYNAMICS

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ABSTRACTS

JUNE 14 - 20, 2009 LVIV, UKRAINE

APPLICATIONS OF STOCHASTIC PDEs TO MODELING THE COMPLEX SYSTEMS

Roderick V.N. MELNIK (*Canada*)

Stochastic partial differential equations (PDEs) arise frequently in the context of modeling the complex systems under random perturbations, including random dynamical systems [1]. Some such systems need to be controlled, and the resulting stochastic dynamic problems that are usually reducible to partial differential equations by using Bellman's approach lead to a number of challenges in modeling the complex systems [2, 3]. Earlier, we analyzed in detail the regularity assumptions on an adjoint process of such stochastic dynamics for nonsmooth control problems, where the control was allowed to be a discontinuous function [4]. Indeed, in situations like this (e.g., when we have to deal with the interactive dynamics between macroscopic and microscopic scales of a dynamic process), the homogenization technique, widely used for parabolic equations [5], cannot be applied, and the Hamiltonian of the problem should be approximated accounting for the consistent regularities of control and value functions [4]. In [2]. it was shown how the original stochastic dynamics can be sequentially approximated by PDEs, the general form of which was derived by applying the Steklov–Poincare operator technique.

In this contribution, we discuss the application of stochastic PDEs to modelling complex systems by exploring a connection between the training of artificial neural networks (via the dynamics of Markov chains) and the approximation of conservation law equations. The link between microscopic and macroscopic models for evolution of such systems is established via the concept of perturbed generalized dynamic systems. The discussion will be exemplified with a number of illustrative examples of network-based computational models treated here as Markov chain approximations.

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[1] W. Wang, J.Q. Duan (2007) *A dynamical approximation for stochastic partial differential equations*, J. of Math. Physics, **48** (**10**), Art. No. 102701.

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Conference Details

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B. Schrefler, E. Oñate and M. Papadrakakis (Eds.)

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Tuesday, June 9th

14:30 - 16:30 **TECHNICAL SESSIONS**

IS - Application of BEM, Meshless and Other Mesh Reduction Methods to Coupled Problems II — TuA101 Room: 1
Invited Session organized by Alain Kassab and Eduardo Divo

Turbulent Compressible Flow Analysis with Meshless Methods
K. Erhart, S. Gerace, E. Divo and A. Kassab

Generalized Finite Difference Meshless Method in Computational Mechanics and Thermofluids
S. Gerace, K. Erhart, E. Divo and A. Kassab

Multiscale Modelling of Solidification: a Meshless Approach
B. Sarler, G. Kosec, A. Lorbiecka and R. Vertnik

Model Reduction for Complex High-Tech Systems
A. Lutowska and W. Schilders

On the Meshless Simulation of Impact and Forming Models
L. Illoul, P. Lorong and F. Chinesta

Applications in Science and Engineering I — TuA102 Room: 2

Aerothermal Analysis of a Cooled Industrial Turbine Blade
F. Thirifay, J-F. Thomas and P. Geuzaine

Application and Simulation of Hydromechanical Transformers as a Vibration Isolator
A. Brysin and A. Nkiforov

Interaction and Contact of Mesoscopic Structures within Shear-Thinning Flow for Modelling the Production Process of Novel Spider Silk Materials
U.M. Mayer and W.A. Wall

Nonlocal Effects in Electromechanical Nano-Beams Via the Timoshenko Model
M. Toropova, R. Melnik and J. Zu

Simulation of the Compaction of Moulding Sand and Determination of Density Distribution using Industrial Computer Tomography (ICT) for Real Examples
A. Kadauw, J. Bast, D. Fiedler and H.C. Saewert

Coupled HM-Field System Identification - Application to Water Reservoirs
T. Lahmer, C. Könke and T. Schanz

Optimum Design in Multi-Disciplinary Problems — TuA103 Room: 3

Fuzzy and Fuzzy Random Analysis of Uncertainties of Standards Leading to Failure of Structures
L. Puklický, A. Omishore and Z. Kala

Efficient Shape Reconstruction of a Bi-Naca Aerofoil using Advanced Evolutionary Algorithms Coupled to Game Strategies
D.S. Lee, L.F. Gonzalez, J. Pèriaux and E. Oñate

Maximizing Opto-Elastic Interaction Using Topology Optimization
A.R. Gersborg and O. Sigmund

Dynamic Workflows for Multiphysics Design
T. Nguyen and J. Désidéri

Numerical Analysis for Design Optimization of an Electrostatic Micropump
E. Bertarelli, R. Ardito, M. Cioffi, K. Laganà, F. Procopio, L. Baldo, A. Corigliano, R. Contro and G. Dubini

Experimental Identification of Stochastic Loads Using a Nonlinear dynamical System Coupled with an Uncertain Linear System
A. Batou and C. Soize

Tuesday, June 9th

14:30 - 16:30 TECHNICAL SESSIONS (Cont.)

Numerical Methods for Coupled Problems II

TuA104
Room: 4

Arbitrary Langrangian Eulerian Formulation for Grids with Variable Topology
D. Isola, A. Guardone and G. Quaranta

Failure of Geometric Conservation Law for Non-Uniform Flow Simulations on Dynamic Meshes
A. Guardone and G. Quaranta

Numerical Modeling of Non-Linear Magneto-Elasticity
F. Vogel and P. Steinmann

Influence of Material Properties on Distortion and Residual Stresses During Metal Quenching Processes
A. Kumar Nallathambi, Y. Kaymak, E. Specht and A. Bertram

Mathematical Modelling of a Two-Phase Flow Trough Ejector of the CO_2 Heat Pump Unit
J. Smolka, Z. Bulinski, K. Banasiak and A.J. Nowak

Fluid-Structure Interactions II

TuA105
Room: 5

Taxonomy of Strong Coupling Fluid-Structure Interaction Schemes
U. Küttler and W.A. Wall

A Comparison of Alternative Fluid-Structure Interaction Treatments
C.A. Felippa, K.C. Park and M.R. Ross

Software Architecture and Algorithms for Coupled Fluid-Structure Simulations
J. Rang, J. Schöön and H.G. Matthies

Fluid-Structure Interaction with Multiscale Domain Decomposition Methods
E. Vergnault, O. Allix and S. Maison-Le-Poëc

Coupling The Navier-Stokes And Biot Systems For Fluid-Poroelastic Structure Interaction
S. Badia, A. Quaini and A. Quarteroni

Fluid-Structure Interaction Based on Lattice Boltzmann and *p*-FEM: Verification and Validation
St. Kollmannsberger, S. Geller, A. Duester, J. Tölke, M. Krafczyk and E. Rank

Multiscale Problems

TuA106
Room: 6

Developing Mesoscopic Models Describing Phase Transformations in Finite Nanowires and Nanoplates
R. Melnik and L. Wang

Computational Homogenization for Quasistatic Poromechanics Problems
F. Su, F. Larsson and K. Runesson

An Homogenization Model for Coupled Behavior: Application to Three Phase Electro-Magneto-Elastic Composites
R. Corcolle, L. Daniel and F. Bouillault

Computational Modeling of Inelastic Polycrystals with Internal Lengthscales
S. Bargmann, B. Svendsen, M. Ekh and K. Runesson

Two-Scale Homogenization for Periodic Mechanical Structures using the Generalized Finite Element Method
A. Hauck and M. Kaltenbacher

Modeling of Microstructure Evolution in Process with Severe Plastic Deformation
D.S. Svyetlichnyy and J. Majta

16:30 - 17:00 Coffee break

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Computational Methods for Coupled Problems in Science and Engineering III
B. Schrefler, E. Oñate and M. Papadrakakis (Eds.)

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	16:20	16:40	17:00	17:20	17:40	
Thermal Stresses I • *Professor Liviu Librescu Memorial Symposium* • Chairs: H. Hilton and C.K. Chao						
Room 407	Thermoelastic interaction between a point heat source and a coated elliptic hole; C.K. Chao, C.K. Chen, F.M. Chen	Thermal stress-focusing effect following dynamically transforming strains in a cylindrical zirconia inclusion; T. Hata	Thermal stress of strip in preheating furnace of continuous annealing line (CAL); T.C. Chen, C.H. Ho, J.C. Lin, L.W. Wu	Thermal stresses in a finite elastic cylinder; V. Meleshko, Y. Tokovyy	Thermal stresses in a rectangle under sliding built-in support of opposite sides; Y. Tokovyy, C.C. Ma	
	16:20	**16:40**	**17:00**	**17:20**	**17:40**	
Thermomechanics, Nanoeffects • Chairs: S. Chirita and B.E. Seguin						
Room 406	Frame-free continuum thermomechanics; B.E. Seguin	Effect of the thermal stresses on electronic properties of GaN/AIN nanowire superlattices; S.R. Patil, R.V.N. Melnik	On the linear thermoelasticity without energy dissipation; S. Chirita, M. Ciarletta	Measurement of the thermal conductivity of ultrathin polymers using time-domain thermoreflectance (TDTR); M.G. Ghossoub, J.H. Lee, O.T. Baris, D.G. Cahill, S. Sinha	Effect of inclusions on the reliability of film-substrate systems; K. Zhou, L.M. Keer, J.Q. Wang, X. Ai, K. Sawamiphakdi, P. Glaws	
	16:20	**16:40**	**17:00**	**17:20**		
Piezo-thermoelasticity • Chairs: O.P. Agrawal and M. Taya						
Room 405	Analytical modeling of piezo-SMA composite for thermal energy harvesting; M. Taya, O. Cem Namli	Exact solution piezothermoelastic transversely isotropic cylindrical shell under axisymmetric loading; X.W. Tangpong, O.P. Agrawal	Electro-thermo-mechanical elasticity of laminated piezoelectric finite length cylinders; T. Kant, P. Desai	Refection of piezothermoelastic waves from stress-free electroded boundary of a half-space; J.N. Sharma, V. Walia		

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Plenary Lecture 5

Low Dimensional Nonlinear Thermomechanical Models Describing Phase Transformations and their Applications

Professor Roderick Melnik
Tier I Canada Research Chair
WLU, Waterloo, ON, Canada
E-mail: rmelnik@wlu.ca

Abstract: In this plenary talk we focus on the development of low dimensional approximations to coupled nonlinear systems of partial differential equations (PDE) describing phase transformations. The methodology is explained on the example of nonlinear ferroelastic/thermoelastic dynamics. We start from the general three-dimensional Falk-Konopka model and with the center manifold reduction obtain a Ginzburg-Landau-Devonshire one-dimensional model. The Chebyshev collocation method is applied for the numerical analysis of this latter model, followed by the application of an extended proper orthogonal decomposition. Finally, we present several numerical results where we demonstrate performance of the developed methodology in reproducing hysteresis effects occurring during phase transformations and provide a survey of related methodologies and applied mathematical problems arising in this context.
Current project is a joint work with O. Tsviliuk and L. Wang.

Brief Biography of the Speaker:
Roderick Melnik is a Full Professor at the Wilfrid Laurier University in Waterloo, Canada. He is a Tier I Canada Research Chair in Mathematical Modelling. Before moving to Canada, Professor Melnik held senior professorial and research positions in the USA, Europe, and Australia. He was also a visiting fellow at the Isaac Newton Institute of the University of Cambridge , at the Institute for Mathematics and its Applications of the University of Minnesota and other research institutions in Europe, North America, and Australia. Professor Melnik's major results are in the development, analysis and applications of mathematical models based on partial differential equations and computational mathematics, focusing on coupled dynamic phenomena, systems, and processes. The areas of his research contributions include computational physics, applied numerical analysis, chemistry, and biology, non-smooth control, and stochastic differential equations. Over the past years, some of his main contributions have been to the development and applications of mathematical models in the area nano- and bionano- sciences with particular emphasis on the analysis of coupled multiscale phenomena, processes, and systems. This includes his contributions to the analysis of coupled effects in low-dimensional nanostructures, such as quantum dots, in bio-inspired and in biological systems.

Low Dimensional Nonlinear Thermomechanical Models Describing Phase Transformations and their Applications 83
Roderick Melnik, Olena Tsviliuk, Linxiang Wang

Imperfection Sensitivity and Insensitivity of Building Structures 89
Libor Puklicky

Stochastic Parametric Resonance of a Fractional Oscillator 93
Astrid Rekker, Romi Mankin

A Beam Search Method to Solve the Problem of Assignment Cells to Switches in a Cellular Mobile Network 99
Cassilda Maria Ribeiro, Anibal Tavares Azevedo

Feedback Control of Parallel-Flow Heat Exchanger Equations Using a Forwardstepping Method 106
Hideki Sano, Shin-Ichi Nakagiri

Backstepping Boundary Control of First-order Coupled Hyperbolic Partial Integro-differential Equations 112
Hideki Sano, Shin-Ichi Nakagiri

An Optimization Approach for the Job Shop Scheduling Problem 120
Jorge Magalhaes-Mendes

Fitting the Sigmoid Function Concerning a Bingham Fluid 126
Adam Marlewski, Marek Sozanski

Circular Saw Mandelbrot Set 131
Mamta Rani, Manish Kumar

Image Hiding Based on Circular Geometric Moiré 137
Minvydas Ragulskis, Algiment Aleksa, Jurate Ragulskiene

Quintic B-Spline Curve Generation and Modification based on Specified Radius of Curvature 143
Tetsuzo Kuragano

Abelian Subalgebras in Low-Dimensional Solvable Lie Algebras 151
Manuel Ceballos, Juan Nunez, Angel F. Tenorio

Computations on Transonic Inviscid Flows Past Thin Airfoils 157
Rui M. S. Pereira, Jitesh S. B. Gajjar

Using e-learning to Self Regulate the Learning Process of Mathematics for Engineering Students 165
Irene Brito, Jorge Figueiredo, Maria Flores, Ana Jesus, Gaspar Machado, Teresa Malheiro, Paulo Pereira, Rui M. S. Pereira, Estelita Vaz

Existence and Uniqueness of Positive Solutions for Degenerate Logistic Neumann Problems in a Half Space 170
Runhua Zhao, Nianpeng Wang, Wei Dong

Existence of Three Positive Periodic Solutions of Differential Equations of Second Order 174
Nianpeng Wang, Runhua Zhao, Wei Dong

RECENT ADVANCES in APPLIED MATHEMATICS

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Table of Contents

Preface 1

Committees 3

Referees 5

Invited Talk

Simulating the Molecular Basis for Alzheimer's Disease: Application of Novel Simulation and Datamining Ttechniques, Combined with Petascale Distributed Domputing 9
Vijay Pande

Genomics and Genetics

MSOAR 2.0: Incorporating Tandem Duplications into Ortholog Assignment Based on Genome Rearrangement 13
Guanqun Shi, Liqing Zhang and Tao Jiang

Characteristic Restriction Endonuclease Cut Order for Classification and Identification of Fungal Sequences 25
Rajib Sengupta, Dhundy Bastola and Hesham Ali

Ranking Genes by Relevance to a Disease 37
Shivani Agarwal and Shiladitya Sengupta

A General Graphical Framework for Detecting Copy Number Variations 47
Xiao-Lin Yin and Jing Li

Combinatorial Reconstruction of Half-Sibling Groups 59
Saad I. Sheikh, Tanya Y. Berger-Wolf, Ashfaq A. Khokhar, Isabel C. Caballero, Mary V. Ashley, Wanpracha Chaovalitwongse and Bhaskar DasGupta

Structural Bioinformatics

A Mesoscopic Model for Molecular Dynamics Studies of RNA Nanostructures 71
Max Paliy, Roderick Melnik, and Bruce Shapiro

A Set-cover-based Approach for Inexact Graph Matching 81
Misael Mongiovì, Raffaele Di Natale, Rosalba Giugno, Alfredo Pulvirenti, Alfredo Ferro and Roded Sharan

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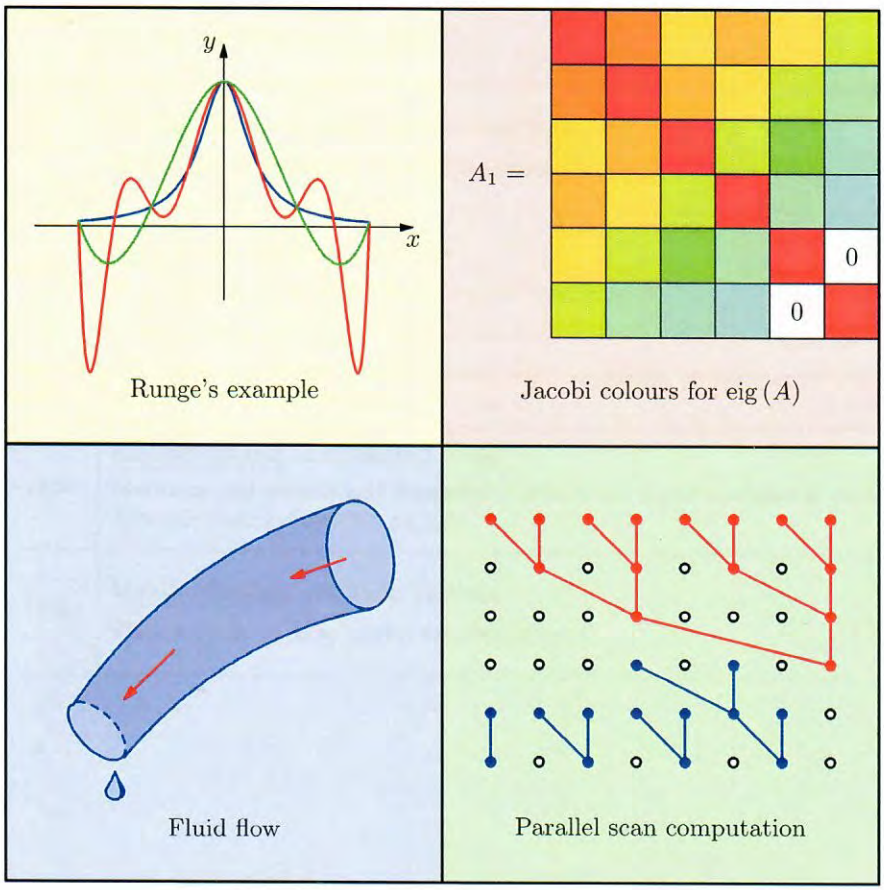

SCIENTIFIC PROGRAM

MONDAY, 11:40–12:05

Mathematical models and numerical methods for coupled nonlinear problems of dynamic thermoelasticity

Roderick Melnik and Linxiang Wang

Abstract. Initiated by the mathematical analysis of thermal stresses due to a thermal shock at the boundary in early 1950s, coupled dynamic thermoelasticity has been an important area of applied mathematics driven by challenges in the development of mathematical methods for coupled problems as well as by applications. While initially such application-driven problems relied mainly on linear models, over recent decades the class of nonlinear coupled dynamic problems of thermoelasticity has grown substantially.

In this contribution, we start from the general 3D model of dynamic nonlinear thermoelasticity, based on a coupled system of partial differential equations, which we apply for the description of shape memory alloys (SMA) dynamics and associated phase transformations. First, we apply center-manifold-based reduction procedures allowing to construct systematically new simplified models preserving essential features of the SMA dynamics. For some special cases, the reduction procedure can be carried out with the Proper Orthogonal Decomposition (POD) methodology and we demonstrate this on an example.

Then, our focus is on a mathematical model and its numerical discretization which we construct to analyze the wave propagation in shape memory alloy rods. The first order martensitic transformations and the associated effects of thermomechanical coupling are accounted for by employing the modified Ginzburg-Landau-Devonshire theory. The Landau-type free energy function characterizes different phases, while a Ginzburg term is introduced to account for the domain wall energy during phase transformations. From a mathematical point of view, the result is a system of coupled nonlinear time-dependent partial differential equations. The effect of internal friction on wave propagation patterns is analyzed under shock loadings implemented via stress boundary conditions. For practical numerical simulations of SMA samples, the constructed model of coupled nonlinear system of PDEs is reduced to a system of differential-algebraic equations, where the Chebyshev collocation method is employed for the spatial discretization, while the backward differentiation is used for the integration in time. A series of numerical experiments are carried out on copper-based SMA samples. Propagation of stress waves induced by shock loadings is analyzed for different initial temperature. It is demonstrated

that the patterns of wave propagation is complicated at low temperatures by phase transformations, while more regular patterns are observed for high temperature distributions. These observations are in agreement with experiments. Finally, the influence of viscosity effects(due to internal friction) on the overall thermo-mechanical behavior of rods is analyzed numerically.

In the reminder of this contribution, our main focus is on the development of a new model based on the Landau theory and on exploring its coupling with microstructural compatibility under the macroscopic continuum deformation framework. Computational methodologies based on finite volume and finite element implementations of the developed models will be discussed with examples.

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e–mail: lwang236@gmail.com

MONDAY, 10:55–11:20

Numerical analysis of a free piston problem

Boris Muha and Zvonimir Tutek

Abstract. The problem considered is the Stokes flow through a system of two pipes in gravity field; inside vertical pipe there is a free heavy piston. The theoretical analysis, existence and non-uniqueness of solution, has been completed recently by the authors. Here we present numerical analysis of the stationary state with respect to the angle between two pipes, diameters of the pipes and search for bifurcation points.

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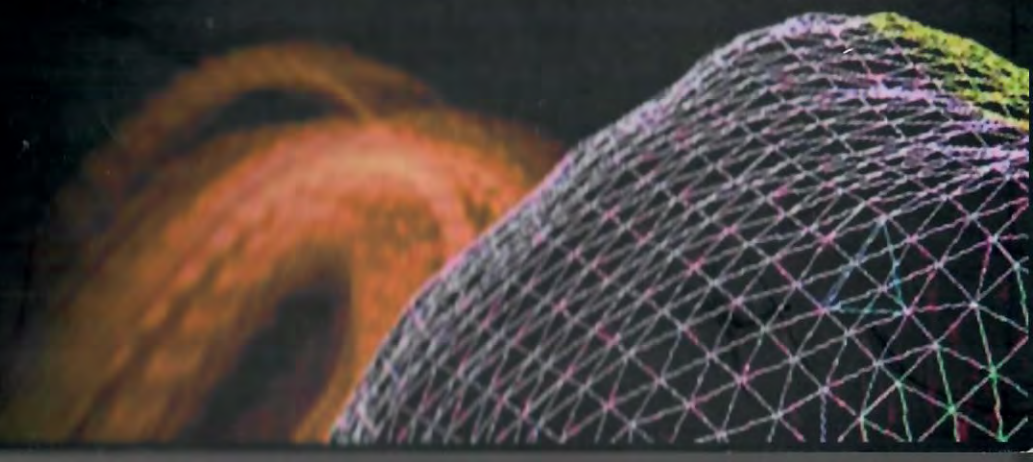

Thursday 10 December 2009

09:00-10:30 Session 2.1 *Micromechanics*

Chair: H Iyama, Yatsushiro National College, Japan

Nonlinear Multiphysics Problems of Phase Transformations in Shape Memory Alloys and Finite Length Nanostructures

R.V.N. Melnik, M2NeT Lab, Wilfrid Laurier University, Canada
O.I. Tsviliuk, JSC RB, Ukraine
L.X. Wang, Hangzhou Dianzi University, P.R. China

Experimental and numerical study on penetration of micro/nano diamond particle into metal by underwater shock wave

Shigeru Tanaka: Faculty of engineering, Kumamoto University, Japan
Kazuyuki Hokamoto, Kumamoto University, Japan
Shigeru Itoh, Kumamoto University, Japan

Application of Response Surface Method to model static and dynamic properties of MEMS structure

Adam Martowicz, Andrzej Klepka, Tadeusz Uhl
AGH University of Science and Technology, Poland

Modeling of Coupled Surface and Drag Forces for the Transport and Capture

1.Farzam Javadpour, 2.Vahid Shabro, 3.Ayodeji Jeje, and 4.Carlos Torres-Verdin4
1,2 Jackson School of Geosciences, The University of Texas at Austin, USA
2,4 The University of Texas at Austin, USA
3 University of Calgary, Canada

Coupled Multiphysics Effects in Low Dimensional Nanostructures

R.V.N. Melnik, Wilfrid Laurier University, Canada
S.R. Sunil, Wilfrid Laurier University, Canada
O.I. Tsviliuk, JSC RB, Ukraine

10:30-11:00 Coffee Break

Nonlinear Multiphysics Problems of Phase Transformations in Shape Memory Alloys and Finite Length Nanostructures

Corresponding author
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rmelnik@wlu.ca

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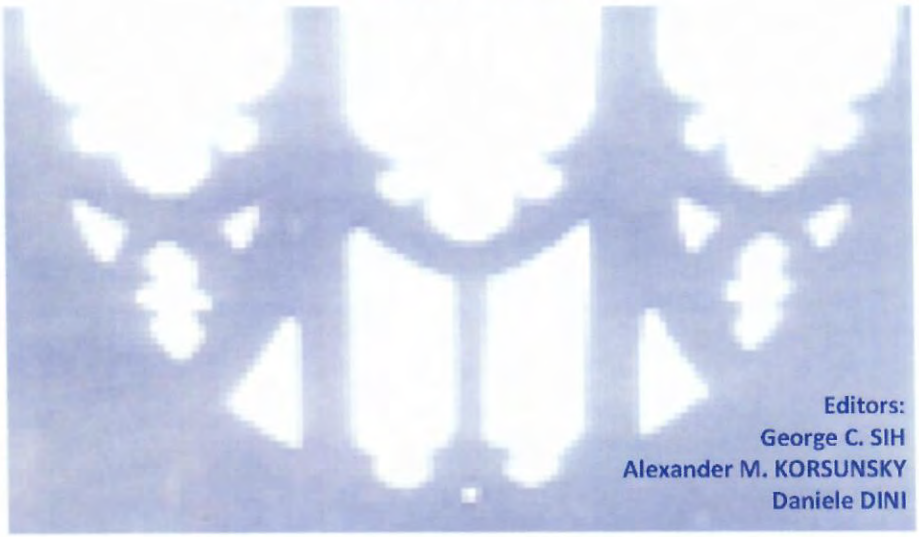
R.V.N. Melnik (M2NeT Lab, Wilfrid Laurier University, 75 University Ave W, Waterloo, ON, Canada N2L 3C5, Email: rmelnik@wlu.ca)
O.I. Tsviliuk (JSC RB, 1-3 Pivnychno-Syretska St, Kyiv 04136, Ukraine)
L.X. Wang (Faculty of Mechanical Engineering, Hangzhou Dianzi University, Xiasha, Hangzhou, 310018, P.R. China)

Some of the most intriguing examples of multiphysics problems are brought about by smart materials and structures technologies where materials with shape memory effect found numerous applications at different spatial scales. In this contribution, we start from the general 3D model of dynamic nonlinear thermoelasticity, based on a coupled system of partial differential equations, which we first apply for the description of shape memory alloys (SMA) dynamics and associated phase transformations. First, we apply center-manifold-based reduction procedures allowing to construct systematically new simplified models preserving essential features of the SMA dynamics. For some special cases, the reduction procedure can be carried out with the Proper Orthogonal Decomposition (POD) methodology and we demonstrate this on an example. Then, our focus is on a mathematical model and its numerical discretization which we construct to analyze the wave propagation in shape memory alloy rods. From a mathematical point of view, the result is a system of coupled nonlinear time-dependent partial differential equations, known as the Ginzburg-Landau-Devonshire system. The effect of internal friction on wave propagation patterns is analyzed under shock loadings implemented via stress boundary conditions. For practical numerical simulations of SMA samples, the constructed model of coupled nonlinear system of PDEs is reduced to a system of differential-algebraic equations, where the Chebyshev collocation method is employed for the spatial discretization, while the backward differentiation is used for the integration in time.

Mesomechanics 2009

Dissipation and Damage across Multiple Scales in Physical and Mechanical Systems

24-26 June 2009, Oxford, United Kingdom



Editors:
George C. SIH
Alexander M. KORSUNSKY
Daniele DINI

Mesomechanics 2009

Dissipation and Damage across Multiple Scales in Physical and Mechanical Systems

24-26 June 2009, Oxford, United Kingdom

Editors:
George C. SIH
Alexander M. KORSUNSKY
Daniele DINI

This booklet for participants contains the presentations contributed to the proceedings of the 11th International Conference on Mesomechanics 2009, held on 24-26 June in Oxford, United Kingdom.

Influence of technological imperfections on residual stress fields in riveted joints #118
E. Szymczyk, J. Jachimowicz, G. Sławinski, and A. Derewońko

Energy-based assessment of ductile tearing in a thin sheet #119
V.P. Naumenko, and I.V. Limansky

Increasing wear resistance of UHMWPE by mechanical activation and chemical modification combined with addition of nanofibers #120
S. Wannasri, S. V. Panin, L. R. Ivanova, L. A. Kornienko, and S. Piriyayon

Study of localized strain at micro-, meso- and macrolevels in AA2024 alloy by data of acoustic emission, surface strain mapping and strain gauging #121
A. V. Byakov, S. V.Panin S.V., V.V. Grenke, I.V. Shakirov, and S.A. Yussif

A virtual crystal plasticity simulation tool for micro-forming #123
S. Wang, W. Zhuang, D. Balint, and J. Lin

Numerical analysis of morphing corrugated plates #124
C. Gentilini, L. Nobile, and K. A. Seffen

Probabilistic analysis of cracked frame structures taking into account the crack trajectory #125
L. Nobile, and C. Gentilini

Enforcement of multiscaling in energy dissipation based on local pico-/nano-/micro-structure properties #127
INVITED TALK
G. C. Sih

Multi-Scale Analysis of Hydrogen-Induced Buckling in Pd Films #128
J. Cizek, I. Prochazka, M. Vlach, N. Zaludova, P. Dobron, F. Chmelik, G. Brauer, W. Anwand, A. Mücklich, E. Nikitin, R. Gemma, A. Pundt, and R. Kirchheim

Defects-enhanced flexoelectricity in nanostructures #129
S. R. Patil, and R. Melnik

Transverse crack density evolution in a single orthotropic lamina under multi-axial stresses using analytical method #130
H. Hosseini-Toudeshky, A. Farrokhabadi, and B. Mohammadi

Nonequilibrium thermodynamics approach to the mesomechanics of a deformed solid as a multiscale system #131
V.E. Panin, and V.E. Egorushkin

An extended multiscale principle of virtual velocities approach for evolving microstructure #132
D. J. Luscher, and D. L. McDowell

Statistical analyses on multi-scale features of monitoring data from health monitoring system in long cable supported bridges #133
Z. X. Li, B. J. Wu, and Y. Wang

Hydroelastic Natural Vibrations of Perforated Plates with Cracks #134
T. Liu, K. Wang, Q. W. Dong, and M. S. Liu

Power law singularity of catastrophic rupture in heterogeneous media #139
S. W. Hao, M. F. Lu, F. J. Ke, M. F. Xia, and Y.L. Bai

Mechanics and mechanisms of puncture by medical needles #140
C. T. Nguyen, and T. Vu-Khanh

Revisiting the Dang Van criterion #141
INVITED TALK
E. Charkaluk, A. Constantinescu, H. Maïtournam, and K. Dang Van

Simulation study on damage localiz
Q. Fei, A. Li, and X. Han

Eigenstrain analysis of non-uniform
T.-S. Jun, A. M. Venter, C. P. La C
A. Evans, and A. M. Korsunsky

The volume-based Strain Energy D
assessments of notched and welde
F. Berto, and P. Lazzarin

Investigation of changes in crystalli
reinforced semi-crystalline polymer
K. Schneider, A. Schöne, T.-S. Ju

Fracture and Mechanical Propertie
K. Masuda-Jindo, Vu Van Hung,

Interfaces in crystalline materials
K. E. Aifantis

Failure modeling of multiphase ste
microstructures
V. Uthaisangsuk, U. Prahl, and W

Consistent tangent stiffness for loc
J. P. Belnoue, G. D. Nguyen, and

On the accurate prediction of interf
dislocations and quadratic program
S. Reina, D. Dini, and D. A. Hills

Feasibility study of neutron strain t
B. Abbey, S. Y. Zhang, W. J. J. V

Analysis of residual stresses aroun
X. Song, I. Kyriakoglou, and A. M

Probing intra-granular deformation
F. Hofmann, X. Song, I. Dolbnya,

Digital image correlation and finite
S. Dave, X. Song, F. Hofmann, K

A combined BEM/Contact Asympto
assessment of fretting damage in b
A. Zografos, and D. Dini

Evaluation of Composite Delamina
T. Niezgoda, and A. Derewońko

Multiscale Composite FEM Modeli
T. Niezgoda, and A. Derewońko

Inverse eigenstrain analysis of resi
H.T. Luckhoo, T.-S. Jun, and A.

Micromechanical modelling of the
inhomogeneous interphase
S. Boutaleb, F. Zaïri, A. Mesbah,
J. M. Lefebvre

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Mesomechanics 2009

Defects-enhanced flexoelectricity in nanostructures

Sunil R. Patil and Roderick Melnik*

M²NeT Laboratory, Wilfrid Laurier University, 75 University Ave W, Waterloo, ON, Canada N2L 3C5

Received 1 March 2009; revised 1 May 2009; accepted 4 May 2009

Abstract

Recent studies show that low dimensional nanostructures may exhibit nonlocal electromechanical effects such as flexoelectricity. Despite the recent progress in nanostructure growth techniques imperfections such as defects are practically unavoidable. These imperfections may enhance flexoelectric effects. Therefore, the main goal of this paper is to analyze the effects of these imperfections on linear electromechanical properties and on flexoelectricity. The constitutive relations for the adiabatically insulated reversible system are derived from the total differential of the general thermodynamic Gibbs potential. The mechanical and electrical balance equations coupled through the constitutive equations are then solved with finite element method for the defective nanostructures. We focus in our study on GaN-based nanostructures which are important in electronic and optoelectronic applications. They exhibit higher magnitudes of electric field compared to other semiconductors in similar contexts. Our results are presented for GaN quantum dots embedded in an AlN matrix.

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Kyewords: Flexoelectrocity, defects, nanostructures

1. Introduction

In studying electronic and optoelectronic properties of low dimensional nanostructures for current and future applications, the linear electromechanical effects become increasingly important [1, 2, 3]. However, recent studies [1, 2, 4] show that these nanostructures also exhibit nonlinear electromechanical effects such as electrostriction [1] and nonlocal effects such as flexoelectricity [2]. Despite the universality of these phenomena in dielectrics, including centrosymmetric crystals, very little attention has been given to these effects in the context of nanostructures [2].

Lattice mismatch induced linear electromechanical effects in nano-heterostructures are now better understood [3]. At the same time, the interest to the nonlinear electromechanical effects has been growing continuously over recent years due to their importance in hetero-epitaxy grown nanostructures and other applications [5]. The recent progress in nanostructure growth techniques allows us to fabricate excellent nanostructures. Nevertheless, some imperfections such as defects are practically unavoidable. It is these imperfections that may lead to significant nonlocal electromechanical effects (in addition to lattice mismatch) such as flexoelectricity. Lattice mismatched nanostructures, such as GaN-based quantum dots (QDs) operating in high internal electric fields, of the order of 10^8

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E-mail address: rmelnik@wlu.ca

V/m, may exhibit significant inf
properties [1, 3, 4]. This fact pr
effects in GaN-based nanostru
electrostriction, in this contribut

Nomenclature

σ_{ij}	stress tensor
f_i	body mechanical force
ε_{kl}	strain tensor
G_{ijkl}	flexoelectric coefficien

2. Theory

We consider cylindrical QDs w
Governing equations for wurtzit
as well. The material constants
three-dimensional problem can
along z-axis. The electromechan

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma}{r}$$

These equations are invariant w
into a (r, z) part and a θ part,
following form for WZ nanostru

$$\sigma_{rr} = C_{11}\varepsilon_{rr} +$$
$$\sigma_{zz} = C_{13}\varepsilon_{rr} +$$
$$D_z = e_{31}\varepsilon_{rr} + e$$

Note that based on the total d
differentials of electromechanic
To take into account the lattice

$$\varepsilon_{rr} = \frac{\partial u_r}{\partial r} - \varepsilon_a, \quad \varepsilon_{zz} =$$

with $\varepsilon_a=(a_m-a_{QD})/a_{QD}$ and $\varepsilon_c=(c$
the matrix and the QD, respecti

3. Results and Discussion

We discus here our results for
are given in Fig. 1. First, we
flexoelectricity. Next, we ana
cylindrical QD and then we stu
the growth process. More preci
often the case while growing Q
clusters in the GaN QD. For c

AUTHOR INDEX

Abbey, B., 153, 155
Abdi, F., 113, 114, 117
Abdul-Latif, A., 105
Aifantis, K. E., 148
Anwand, W., 128
Bai, Y.L., 139
Balint, D., 123
Bassim, M. N., 165
Belnoue, J. P., 143, 151
Berto, F., 144
Bleck, W., 150
Boukharouba, T., 161
Boutaleb, S., 161
Brauer, G., 128
Breard, J., 170
Byakov, A. V., 121
Chamis, C. C., 112, 113, 114
Chao, C. K., 102
Charkaluk, E., 141
Charlet, K., 170
Chen, E.-P., 167
Chern, M. J., 102
Chmelik, F., 128
Choi, B.-I., 103
Cizek, J., 128
Constantinescu, A., 141
Cvijović, Z., 110
Cvijović-Alagić, I., 110
Dang Van, K., 141
Dave, S., 156
Derewońko, A., 118, 158, 159
Dini, D., 101, 152, 157
Dobron, P., 128
Dolbnya, I., 155
Dong, Q. W., 134
Dragnevski, K., 156
Egorushkin, V.E., 131
Eichlseder, W., 109
Evans, A., 143
Eve, S., 170, 171
Farrokhabadi, A., 130
Fei, Q., 142
François, M., 166
Gemma, R., 128
Gentilini, C., 124, 125
Gloaguen, J. M., 161
Gomina, M., 170
Grenke, V.V., 121
Gu, S.-T., 108
Han, X., 142
Hao, S. W., 139
He, Q.-C., 108
Hfaiedh, N., 166
Hills, D. A., 152
Hofmann, F., 143, 155, 156
Hosseini-Toudeshky, H., 111, 130
Huang, D., 113, 114
Hung, V. V., 147
Ivanova, L. R., 120
Jachimowicz, J., 118
Jalalvand, M., 111
Jernot, J.P., 170
Jun, T.-S., 143, 146, 160
Masuda-Jindo, K., 147
Ke, F. J., 139,
Kim, W.-D., 103,
Kirchheim, R., 128
Kornienko, L. A., 120,
Korsunsky, A. M., 101, 143, 146, 151, 153-156, 160, 164
Kunc, V., 117
Kyriakoglou, I., 154
La Grange, C. P., 143
Lazzarin, P., 144
Lee, S.-H., 103
Lee, M., 117
Lefebvre, J. M., 161
Li, Z. X., 133
Li, A., 142
Limansky, I.V., 119
Lin, T. H., 102
Lin, J., 123
Liu, T., 134
Liu, M. S., 134
Lu, M. F., 139
Luckhoo, H. T., 160
Luscher, D. J., 132
Maïtournam, H., 141
McDowell, D. L., 132
Melnik, R., 129
Menon, M., 147
Mesbah, A., 161
Minnetyan, L., 113, 114
Mohammadi, B., 111, 130
Mohr, J., 171
Mücklich, A., 128
Naït-Abdelaziz, M., 161
Naumenko, V.P., 119
Nguyen, C. T., 140
Nguyen, G. D., 151
Niezgoda, T., 158, 159
Nikbin, K., 117
Nikitin, E., 128
Nobile, L., 124, 125
Odeshi, A.G., 165
Panin, A., 107
Panin, S. V., 120, 121
Panin, V.E., 131
Park, H.-S., 103
Patil, S. R., 129
Piriyayon, S., 120
Prahl, U., 150
Prochazka, I., 128
Pundt, A., 128
Radi, M., 105
Reina, S., 152
Rognin, F., 117
Roos, A., 166
Rotundo, F., 164
Saanouni, K., 166
Scheider, I., 106
Schneider, K., 146
Schöne, A., 146
Seffen, K. A., 124
Shakirov, I.V., 121
Shao, J.-F., 108
Shugurov, A., 107
Sih, G. C., 101, 127
Sławinski, G., 118
Song, X., 154, 155, 156
Stockinger, M., 109
Stoschka, M., 109
Szymczyk, E., 118
Tan, W., 109
Uthaisangsuk, V., 150
van Heerden, P. R., 143
Venter, A. M., 143
Vlach, M., 128
Vorster, W. J. J., 153
Vratnica, M., 110
Vu-Khanh, T., 140
Wang, S., 123
Wang, Y., 133
Wang, K., 134
Wannasri, S., 120
Woo, C.-S., 103
Wu, B. J., 133
Xia, M. F., 139
Yazdani, F., 165
Yussif, S.A., 121
Zaïri, F., 161
Zaludova, N., 128
Zhang, S. Y., 153
Zhuang, W., 123
Zografos, A., 157

Biennial Congress of the
U.S. Association for Computational Mechanics

10TH U.S. NATIONAL CONGRESS ON COMPUTATIONAL MECHANICS

CONGRESS PROGRAM

Chair: Somnath Ghosh

July 15-19, 2009
Greater Columbus Convention Center
Columbus, Ohio, USA

USNCCM-X

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July 15-19, 2009

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The Ohio State University, College of Engineering

Thursday Technical Session 2

Room	2:20 p.m.	2:40 p.m.	3:00 p.m.	3:20 p.m.	3:40 p.m.
26 Mechanics of biological tissues					
C120	Mesoscale effective elasticity of cortical bone estimated based on high-resolution acoustic imaging (#157379)	Modeling of bone at nanostructural level (#158064)	Molecular and mesoscale disease mechanisms of Osteogenesis Imperfecta (#158490)	Cartilage impactor shape alters pore pressure: A finite element analysis (#153305)	
	Q. Grimal*, K. Raum, A. Gerisch, P. Laugier	E. Hamed*, I. Jasiuk	M. Buehler, S. Uzel*, A. Gautieri, S. Vesentini, A. Redaelli	S. Fening*, A. Goktug, M. Jones, A. Miniaci,	
52 Computational methods for fluid-structure interaction					
C121	Multigrid fictitious boundary method for vortex-induced motions of multi-cylinders in viscous flows (#158877)	A fixed mesh approach using level set function for fluid domains divided by large-deformable thin elastic structure (#157671)	Assessment of a mesh updating scheme for fluid structure interaction under ALE-FEM approach (#159692)	Multi-objective design of motion of flapping wing for micro air vehicle (#158109)	2D FSI model applied to bridge aero-elastic problems (#157865)
	D. Wan*	G. Hashimoto*, K. Ono	J. Alves*, C. Silva, N.Guevara	I. Inuzuka*, S. Yoshimura	H. Gomes*, P. Pimenta
22 Computational nanoscience and coupled multi-physics modeling of low dimensional materials					
C122	Size-dependent and strain rate effects in quantum dot nanostructures with molecular dynamics simulations (#160494)	Shape properties of quantum-confined semiconductor structures (#154417)	Modeling of GaN HEMTs (#157456)	Computational models for the simulation of third generation photovoltaic devices (#159630)	
	S. Patil, D. Mahapatra, V. Sutrakar, R. Melnik*	M. Willatzen*, J. Gravesen	Dragica Vasileska*	C. Falco, R. Sacco*, M. Verri	
05 Multimodel and multiscale approaches in solid mechanics: algorithms and applications advances					
C123	Propagation of local alterations using X-Fem within the Arlequin framework (#158559)		A light formulation for coupling discrete and finite element models (#157366)	An hamiltonian discrete element method for linear elasticity in large deformation (#159014)	Multiscale analysis by a GP method with applications to nanoscale ceramics coating (#159821)
	H. Ben Dhia*, O. Jamond		S. Gavoille, C. Rey*, A. Delaplace, C. Mariotti	L. Monasse*, C. Mariotti	J. Fan*

Thursday Technical Session 3

Room	4:15 p.m.	4:35 p.m.	4:55 p.m	5:15 p.m.	5:35 p.m.
26 Mechanics of biological tissues					
C120	Multi-Scale finite element analysis of head injury by employing micro blood vessel and nerve cell tissue models (#155707)		Microstructures in 3D affect cardiac myocyte shortening (#158156)	Stress analysis in porous media due to convection enhanced delivery (#160565)	
	E. Nakamachi*, Y. Morita, H. Kuramae		M. Curtis*, E. Budyn, T. Desai, B. Russell	O. Ivanchenko, B. Sweetman, N. Sindhwani*	
52 Computational methods for fluid-structure interaction					
C121	Numerical approaches for the quadratic eigenvalue problem on large structural acoustic systems (#157528)		An implementation of efficient FSI algorithms to parallel environments REVOCAP_coupler (#158548)	A variational multiscale based stabilized formulation of the incompressible Navier-Stokes equations for moving domain problems (#158165)	Finite-elements analysis of liquid sloshing in low gravity environment (#157718)
	G. Reese*, T. Walsh, C. Baker		S. Minami*, S. Yoshimura	A. Masud, R. Calderer*	M. El-Kamali*, J.-S. Schotté, R. Ohayon
22 Computational nanoscience and coupled multi-physics modeling of low dimensional materials					
C122	Combined boundary singularity method and molecular method for nano-fluids (#159628)	Optical properties of metal-molecular hybrid nanostructures: Insight from atomic-level first principles to continuum modeling (#158582)	Molecular simulations of liquid argon confined down to nanometer Distance (#157690)	Inverse problems for multiband modeling and design of low dimensional nanostructures (#160401)	
	S. Zhao, A. Povitsky*	R. Pachter*, P. Day, J. Duan, G. Hong	Y. Lei*, Y. Leng	R. Melnik, D. Sytnyk*	
05 Multimodel and multiscale approaches in solid mechanics: algorithms and applications advances					
C123	A partitioning algorithm to couple diffusion and elasticity for the simulation of hygromechanical wood structures of cultural heritage (#158556)	Multi-scale topology optimization of composite structures (#159949)	Implementation of higher order basis bunctions in the multiscale finite element method (#157940)	A generation algorithm of a concrete unit cell (#157382)	
	D. Dureisseix*, B. Marcon	A. Tovar*, K. Khandelwal	S. Soghrati*, I. Stanciulescu	E. Gal*, A. Ganz, L. Hadad, R. Kryvoruk	

The US National Congress of Computational Mechanics is the biennial congress of the U.S. Association for Computational Mechanics (USACM).

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Conference programme

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(with the exhibition of sensor developments and industrial samples)

Ukraine, Odessa, June 28 – July 2, 2010

PROGRAM

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28.06—02.07 2010
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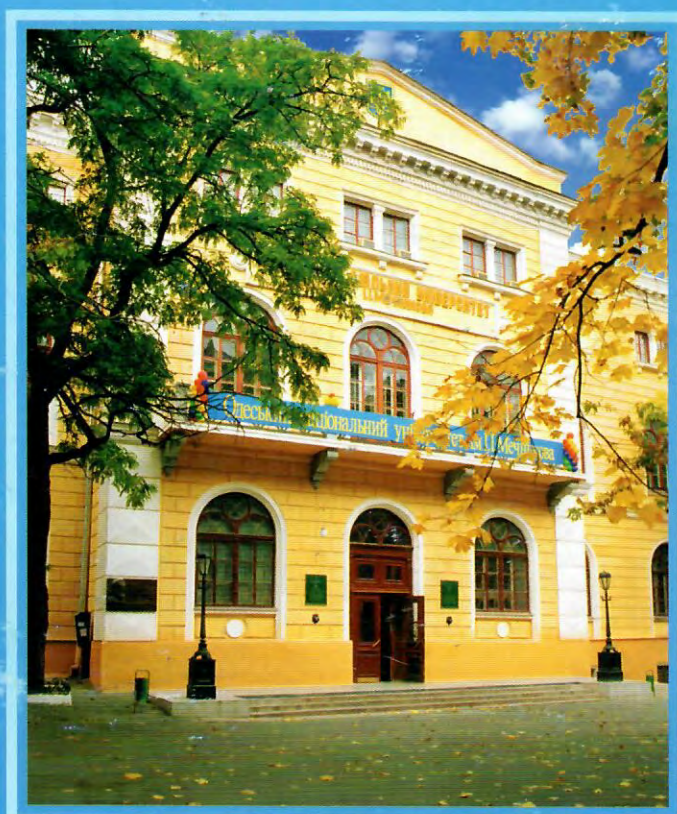
"СЕНСОРНА ЕЛЕКТРОНІКА ТА МІКРОСИСТЕМНІ ТЕХНОЛОГІЇ"
(СЕМСТ-4)

4th International Scientific and Technical Conference

"SENSORS ELECTRONICS AND MICROSYSTEMS TECHNOLOGY"
(SEMST-4)

ТЕЗИ ДОПОВІДЕЙ
BOOK OF ABSTRACTS



Україна, Одеса, 28 червня – 2 липня 2010 р.

Ukraine, Odessa, June 28 – July 2, 2010

MATHEMATICAL MODELING AND PHYSICAL PROPERTIES OF CARBON NANOTUBE SENSORS WITH STONE-WALES DEFECTS

N. Sinha[1], S. Patil[2], and R.V.N. Melnik[2]

[1] *Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge 02139, USA*

[2] *M²NeT Lab, Wilfrid Laurier University, Waterloo, Canada N2L 3C5*

The synthesis of defect-free carbon nanotubes (CNTs) continues to be a challenge, despite substantial progress and achievements in the field. Moreover, many physical properties of CNTs show significant variability which makes the study of such properties a very difficult task. For example, one of the key characteristics in such important areas of applications of CNTs as sensing, nanobiomedical X-ray devices, and various imaging probes is fluctuation of field emission current from CNTs. Indeed, experimental studies on the collective field emission from carbon nanotubes (CNTs) on metallic cathode substrate confirm wide variability of this characteristic. In a series of our recent works, we have investigated several related effects, such as the relationship between the electron-phonon transport and the mechanical deformation in the CNTs [1-4]. A systematically coupled model of randomly oriented CNTs in a thin film has been developed and a range of numerical simulations have been reported, which were able to reproduce several experimentally observed phenomena, such as a fluctuating field emission current, deflected CNT tips and the heating process.

The major premises of the present contribution lie with the fact that defects may adversely affect the performance of many CNT-based devices. However, we point out that the distinct properties of CNTs with defects can also be utilized for many applications such as sensors. Our main idea proposed here stems from the fact that by introducing Stone-Wales (SW) defects, the band gap of CNT changes and this can be related to the change in its conductivity. According to the dislocation theory [5], upon successive generation and dislocation of new SW defects an (n,n) CNT abandons its symmetry which eventually leads to the zigzag symmetry (n,0). This also results in a stepwise reduction of the diameter of the inner segment, and in a change in the electronic structure of the emerging domains. In order to use this property for sensor applications, the change in conductivity due to band gap change can be calculated using four-probe expression where the conductivity is measured by taking the reciprocal of resistivity. Among other things, we analyze the deformation parameter which changes with the applied pressure, signifying the potential of CNTs for pressure sensing applications. The results presented in this contribution indicate that by introducing SW defects in CNTs, we have a new avenue for a range of sensor applications.

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Ellipticity conditions in multiband Hamiltonian problems for the analysis of low dimensional nanostructures

Roderick Melnik and Dmytro Sytnyk

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In this contribution, we analyze multiband mathematical models for low dimensional nanostructures such as quantum dots [1, 2]. In this context we have to deal with partial differential operators (PDO) associated with certain quadratic forms. We recall that for any m–dimensional matrix PDO $H = \{h_{ij}\}_{i,j=1}^{m}$, where

$$h_{ij}^{kl} \frac{\partial^2}{\partial x_k \partial x_l}, \tag{1}$$

the associated quadratic form is defined by

$$G(\xi_1, ..., \xi_{nm}) = vMv^T, \quad v = (\xi_1, \ldots, \xi_{nm}), \tag{2}$$

where M is an $mn \times mn$ matrix composed from the elements h_{ij}^{kl}.

Then the PDO H is said to be elliptic with the increasing sequence of eigenvalues if the eigenvalues of associated M (2) satisfy

$$\lambda_i < 0, \quad \forall\, i = 0, 1, \ldots, nm. \tag{3}$$

First, we consider Hamiltonians for nanostructures with zinc-blende (ZB) crystal lattice structures. In particular, the Luttinger–Kohn (LK) 6×6 Hamiltonian for ZB has the form:

$$H^{LK} = \begin{pmatrix} \frac{1}{2}P & L & M & 0 & i\frac{1}{\sqrt{2}}L & -i\sqrt{2}M \\ L^\star & \frac{1}{6}P + \frac{2}{3}Q & 0 & M & -\frac{i}{3\sqrt{2}}(P-2Q) & i\sqrt{\frac{3}{2}}L \\ M^\star & 0 & \frac{1}{6}P + \frac{2}{3}Q & -L & -i\sqrt{\frac{3}{2}}L^\star & -\frac{i}{3\sqrt{2}}(P-2Q) \\ 0 & M^\star & -L^\star & \frac{1}{2}P & -i\sqrt{2}M^\star & -\frac{i}{\sqrt{2}}L^\star \\ -\frac{i}{\sqrt{2}}L^\star & \frac{i}{3\sqrt{2}}(P-2Q) & i\sqrt{\frac{3}{2}}L & i\sqrt{2}M & \frac{1}{3}(P+Q) & 0 \\ i\sqrt{2}M^\star & -i\sqrt{\frac{3}{2}}L^\star & \frac{i}{3\sqrt{2}}(P-2Q) & \frac{i}{\sqrt{2}}L & 0 & \frac{1}{3}(P+Q) \end{pmatrix},$$

with corresponding P, Q, M, L defined via PDOs (see [1, 2] and references therein).

Similarly, we also consider Hamiltonians for wurtzite crystal lattice structures, where we focus on the Bir–Pikus (BP) Hamiltonian in the form:

$$H^{BP} = \begin{pmatrix} F & 0 & -H^\star & 0 & K^\star & 0 \\ 0 & G & 0 & -H^\star & 0 & K^\star \\ -H & 0 & \lambda & 0 & L^\star & 0 \\ 0 & -H & 0 & \lambda & 0 & L^\star \\ K & 0 & L & 0 & G & 0 \\ 0 & K & 0 & L & 0 & F \end{pmatrix},$$

with corresponding F, H, I, K defined via PDOs (see [1, 2] and references therein).

We show that both classical LK and BP Hamiltonians lead to mathematical models that need to be augmented due to ellipticity requirements. Indeed, for many applied problems the actual physical parameters for typical materials result in problems which are not elliptic, but rather essentially hyperbolic. The solutions to such problems are not from the domain $D(H_0)$ and the eigenvalues E_i are not bounded from the below. In both cases of LK and BP Hamiltonians we demonstrate how such Hamiltonians should be augmented to satisfy the ellipticity requirements.

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НАЦІОНАЛЬНА АКАДЕМІЯ НАУК УКРАЇНИ
ІНСТИТУТ ПРОБЛЕМ МОДЕЛЮВАННЯ В ЕНЕРГЕТИЦІ
ім. Г.Є. Пухова НАН України

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Целью конференции является укрепление и развитие научно-технического сотрудничества специалистов в области математического и компьютерного моделирования в различных направлениях науки, техники и народного хозяйства. Задачи конференции: обмен новыми идеями теоретических и прикладных исследований и опытом практических разработок в области математического и компьютерного моделирования; обсуждение научных достижений в области математического и компьютерного моделирования и их реализации с использованием современных компьютерных систем; укрепление связей между наукой и производством; привлечение молодых исследователей к научному творчеству.

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ЗМІСТ

M. Resch Modern high performance computer architectues 10
А.І. Петренко Моделювання грід-систем і в грід-системах 11
С.Е. Саух Новый метод построения предобусловливателей для итерационного решения больших систем уравнений 22
M. Sosonkina Efficient calculation of vibration modes in structural mechanics .. 32
В.Ф. Евдокимов, А.А. Кучаев, Е.И. Петрушенко, В.А. Кучаев Трехмерная интегральная модель магнитного поля 32
F. Belgassem Contour compression using wavelet and piecewise 40
N. Currle-Linde, M. Resch Strategy for the development of tools for large-scale and real-time simulation 46
Y. Dorozhko, Y. Yudin, T. Krasikova, N. Currle-Linde, M. Resch An abstract language and environment for the creation and execution of experiments over distributed computers 48
Y. Kovalenko, U. Küster Performance analyzers overview 55
U Küster A language for automatic source to source transformations of fortran code for optimization and instrumentation 59
R V.N. Melnik Modelling low dimensional nanostructures, their thermo-electromechanical properties and applications in engineering, physical and 60
M Ahe, B. Lie, T. A. Hauge, Xstrata Nikkelverk Dynamic modeling and verification of a CU/NI fluidized-bed roaster 72
А.Ф. Верлань, Р.А. Абдикаримов Математическое моделирование нелинейных задач динамики вязкоупругих систем с переменной жесткостью 80
Ю.С. Авагимова., Ю.Я. Любарский Разработка экспертной системы для годового планирования ремонтов электросетевого оборудования 84
Т.В. Авдеенко, Ю.А. Мезенцев Задачи синтеза оптимальных расписаний нанотехнологических производств 88
Т.А. Аверина Статистическое моделирование пуассоновских ансамблей 96

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M. PALIY[1], R. V. N. MELNIK[1], B. A. SHAPIRO[2]

RNA Nanostructures and Their Properties: A Modelling Perspective

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Ribonucleic acid (RNA) has been proposed as a promising alternative to DNA and proteins for the design of the artificial self-assembled materials at nanoscale (see [1] and references therein). As compared to DNA and some other bio-molecules, RNA offers not only a much greater variety of interactions but also great conformational flexibility of RNA structures, making RNA a very promising functional nano-material for the design of the man-made molecular devices and systems. We first present a model based on all-atom Molecular Dynamics, demonstrating the stability and conformational dynamics of several simple RNA nanostructures. We explain the effect of the counterions and solvent, that are both known to modify strongly the stability and dynamics of RNA nanostructures, on the behaviour of the "kissing loops". This effect is very important due to the fact that the "kissing loop" motif can be used as a basic constructional element to join the simplest building blocks into a symmetric structures with their spatial dimensions lying in the range of 10-20 nm. Then, we present several promising multiscale methodologies for simulation of biomolecular systems such as RNA nanostructures, focusing on our recent efforts in the development of a hierarchy of simplified coarse-grained mesoscopic models suitable for the description of these complex systems [2].

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Photocatalytic Performance of Pyrochlore-Type Structure Compounds, Bi2MTaO7 (M = Al, Ga, Fe or In), On Alizarin Red S Degradation 73
Leticia M. Torres-Martinez, Isaias Juarez-Ramirez, Juan S. Ramos-Garza, Francisco Vazquez-Acosta, Soo Wohn Lee

Imaginary Relativity 79
Mehran Rezaei

Combined Spectral and Finite Difference Methods for a Stationary Neutron Transport Equation 91
Nikos Mastorakis, Olga Martin

An Ultrasensitive Vibrating Channel Mass Sensor based on Tunnelling Current Detection 97
Maurizio Migliore, Zakaria Moktadir, Hiroshi Mizuta

Instability of Ion-Acoustic Oscillations and Anomalous Thermal Conductivity in the Transition Region of Stellar Atmosphere 103
P. A. Bespalov, O. N. Savina

A Perpetual Evolution of Electrochemically Deposited Nano-Structured Cu Thin Films Driven by Acoustic Cavitation 108
A. Mallik, B. C. Ray

Effect of Organoclay and SEBS-g-MA Contents on Constituting Balance between Stiffness vs. Toughness in PP/SEBS-g-MA/Organoclay Nanocomposites 113
M. Ranjbar, A. Arefazar, Gh. Bakhshandeh

Numerical Analysis of the Heating Effects of an Atmospheric Air Barrier Dielectric Discharge 119
Antonis P. Papadakis, Andrew C. Metaxas

Phase-field Approach to Studying Shape Memory Effects and Thermomechanical Properties of Low Dimensional Nanostructures 125
Roderick Melnik, Linxiang Wang

Modelisation of Accumulation Barrier of Nanostructure AlGaAs/GaAs 131
I. Bouneb, M. Marir-Benabbas

Continuous-Microflow Synthesis of Multiscale Materials based on Polymer Microparticles / Inorganic Nanoparticles Composites 135
Z. Chang, S. Li, M. Bouquey, I. Kraus, C. A. Serra, J. M. Kohler

Stabilization and Enhancement of Microcirculatory Video Sequences 140
Maher I. Rajab, Stephen P. Morgan, Ian M. Stockford, John A. Crowe

Investigation of Olive Oil as a New Photonic Liquid Crystal for Optical Communication Systems 144
Anwaar A. Al-Dergazly, Aqeel Fadhel

Results of UBV Photoelectric Observations of the Early-Type Eclipsing Binary System XZ Cep 150
M. I. Kumsiashvili, K. B. Chargeishvili, E. B. Janiashvili

Analysis of MWIR Infrared Pyroelectric Detectors Parameters 161
Genc Hyseni, Nebi Caka, Kujtim Hyseni

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CONTENTS

Diffusion Processes 4
Fractal Analysis 8
Gaussian and Related Processes and Random Fields 13
Generalized Renewal Processes 20
Information Security 23
Interacting Particle Systems 30
Limit Theorems for Stochastic Processes and Fields 34
Markov and Semi-Markov Processes 46
Mathematics of Finance 52
Queuing Systems 62
Risk Processes and Actuarial Mathematics 77
Statistics of Stochastic Processes 83
Stochastic Analysis 101
Stochastic Differential Equations 106
Stochastic Models of Evolution Systems 120
Author Index 130

combines an investigation of *the extended Poisson equation* $\mathcal{A}u = f$ (i.e. the equation that involves the extended generator $\mathcal{A}$ of the process X) and a calculus based on the extended version of the Dynkin formula.

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LIMIT BEHAVIOR OF SOLUTIONS OF STOCHASTIC EQUATIONS WITH UNBOUNDED COEFFICIENTS

Sergey Makhno

In the report we consider solutions of stochastic equations

$$\xi^\epsilon(t) = x + \int_0^t b^\epsilon(t, \xi^\epsilon(s))ds + \int_0^t \sigma^\epsilon(t, \xi^\epsilon(s))dw(s) + \int_0^t \int c^\epsilon(s, \xi^\epsilon(s), \theta)\tilde{\nu}(ds, d\theta).$$

In this equation $\xi^\epsilon(t)$ is a vector of dimension d, $w(t)$ is a $m-$dimensional standard Wiener process and $\nu(\tilde{t, A})$ is a centered Poisson process with parameter $t\Pi^\epsilon(A)$. We will study the convergence of family of measures corresponding to the processes ξ^ϵ on the Skorokhod space to the measure corresponding to the process

$$\xi(t) = x + \int_0^t B(s, \xi(s))ds + \int_0^t A^{1/2}(s, \xi(s))dw(s)$$

as $\epsilon \to 0$. The sufficient conditions for it will be formulated. Let's emphasize that it is not required the uniform boundedness of coefficients of the equation at parameter ϵ and at all (t, x). Next, we do not assume that the coefficients of equation have limits as $\epsilon \to 0$. Moreover, they may tend to infinity or may have not limits in general. For example,

$$b^\epsilon(t, x) = \frac{1}{\epsilon} b\left(\frac{t}{\epsilon^2}, \frac{x}{\epsilon}\right) + \frac{\epsilon^3|2t-1|}{[t(t-1)+\epsilon^2]^2} + \frac{\epsilon^{\frac{d}{4(d+1)}}}{(2\pi\epsilon)^{\frac{d}{2(d+1)}}} \exp\left\{-\frac{|x|^2}{2\epsilon(d+1)}\right\},$$

where $b(t, x)$ is a periodic function.

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GENERALIZED FRACTIONAL KINETIC EQUATIONS: ANOTHER POINT OF VIEW

David Márquez-Carreras

We deal with generalized fractional kinetic equations driven by a Gaussian noise, white in time and correlated in space, and where the diffusion operator is the composition of the Bessel and Riesz potentials for any fractional parameters. We give results on existence and uniqueness of solution by means of a weak formulation and study the Hölder continuity. Moreover, we prove the existence of a smooth density associated to the solution process and study the asymptotics of this density. Finally, when the diffusion coefficient is constant, we look for its Gaussian index.

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NONSMOOTH CONTROL AND STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS IN MODELLING COMPLEX SYSTEMS

Roderick V.N. Melnik

Stochastic partial differential equations (PDEs) arise frequently in the context of modelling complex systems under random perturbations, including random dynamical systems [1]. Some such systems need to be controlled and the resulting stochastic dynamic problems, that are usually reducible to partial differential equations by using Bellman's approach, lead to a number of challenges in modelling complex systems [2, 3]. Earlier, we analyzed in detail regularity assumptions on an adjoint process of such stochastic dynamics for nonsmooth control problems where the control was

allowed to be a discontinuous function [4]. Indeed, in situations like this (e.g., when we have to deal with interactive dynamics between macroscopic and microscopic scales of a dynamic process), the homogenization technique, widely used for parabolic equations [5], cannot be applied, and the Hamiltonian of the problem should be approximated accounting for consistent regularities of control and value functions [4]. In [2] it was shown how the original stochastic dynamics can be sequentially approximated by PDEs, the general form of which was derived by applying Steklov-Poincare operator technique.

In this contribution, we discuss the application of stochastic PDEs to modelling complex systems by exploring a connection between the training of artificial neural networks (via the dynamics of Markov chains) and the approximation of conservation law equations. The link between microscopic and macroscopic models for evolution of such systems is established via the concept of perturbed generalized dynamic systems. The discussion will be exemplified with a number of illustrative examples of network-based computational models treated here as Markov chain approximations.

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STABILITY OF A DAMPING MODE FOR QUASI-LINEAR PARABOLIC EQUATION WITH A STRONG STOCHASTIC SOURCE

S.A. Melnik

We consider such Cauchy problem

$$du(t,x) = au_{xx}(t,x)dt + bu^{\gamma}(t,x)dw(t), t \geq 0, x \in R^1, u(0,x) = u_0(x). \tag{1}$$

Here: $a > 0$, $b > 0$, $\gamma \in (1;3)$, $u_0(x) \geq 0$, $u_0 \in W_2^1(R^1)$, $w(t)$ – Brownian motion.
In this work it is proved that the space form of automodel damping solution is stable on initial function. In work [1] the automodel solution of this problem are constructed. It has such form:

$$\bar{u}(t,x) = \frac{r(t)}{v_0}\Lambda(2\alpha)^{1/(1-\gamma)}v\left(\frac{x}{2\alpha}\left(\frac{r(t)\Lambda}{v_0}\right)^{\gamma-1}\right).$$

Here: v_0, Λ, α – known constants, $v(y)$ is the solution of special ordinary differential equation and named the space form of $\bar{u}$. Dynamics of automodel solution is described by process $r(t)$ which is the solution of such problem:

$$dr(t) = Ar^{2\gamma-1}(t)dt + Br^{\gamma}(t)dw(t),\ r(0) = r_0 > 0.$$

Dynamics of non automodel solution $u(t,x)$ is described by the following theorem.

Theorem 1. *Let* $2A + B^2 < 0$, $B > 0$, $\gamma \in (1;3)$, $u_0(x) \geq 0$, $u_0 \in W_2^1(R^1)$ *and* $v(t,y) = r^{-1}(t)u\left(t, r^{1-\gamma}(t)y\right)$. *Then, for all* $t \geq 0$

$$\boldsymbol{M}\int |v(y) - v(t,y)|^2 dy \leq \int |v(y) - r_0^{-1}u_0(r_0^{1-\gamma}y)|^2 dy,$$

$$-2(2A+B^2)\boldsymbol{M}\int_0^t r^{2(\gamma-1)}(s)\int |v(y) - v(s,y)|^2 dyds \leq \int |v(y) - r_0^{-1}u_0(r_0^{1-\gamma}y)|^2 dy,$$

$$2a\boldsymbol{M}\int_0^t r^{2(\gamma-1)}(s)\int |v_y(y) - v_y(s,y)|^2 dyds \leq \int |v(y) - r_0^{-1}u_0(r_0^{1-\gamma}y)|^2 dy.$$

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Contents

Welcome	p6
2010 EvoStar programme chairs	p7
Invited speakers	p8-9
Best paper nominations	p10-12
EuroGP programme	p13-21
EvoCOP programme	p22-29
EvoBIO programme	p30-36
EvoCOMNET programme	p37-40
EvoCOMPLEX programme	p41-42
EvoENVIRONMENT programme	p43-44
EvoFIN programme	p45-47
EvoGAMES programme	p48-53
EvoIASP programme	p54-58
EvoINTELLIGENCE programme	p59-60
EvoMUSART programme	p61-65
EvoNUM programme	p66-70
EvoPhD programme	p71-72
EvoSTOC programme	p73-74
EvoTRANSLOG programme	p75-76
Lunchtime Activiites and Poster Session	p77
Social programmes	p78-81
Campus map	p82
Getting around Istanbul	p83
Metro map	p84

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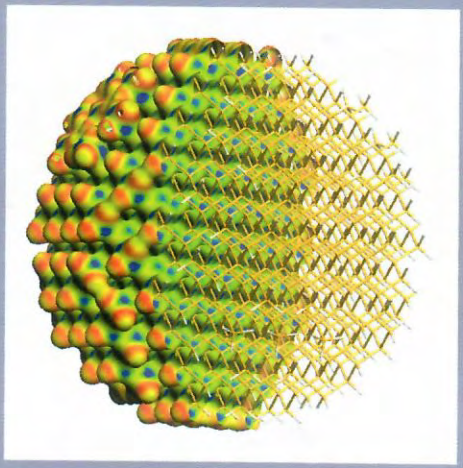

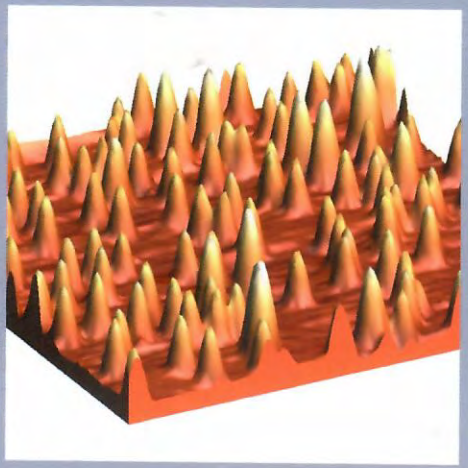

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Bandstructures of Quantum Dots and Coupled Thermo-electromechanical Phenomena

Roderick Melnik[1] **and Sunil Patil**[1]

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In a series of recent papers we demonstrated that *coupled* electro-mechanical effects can lead to pronounced contributions in bandstructure calculations of low dimensional semiconductor nanostructures (LDSNs) such as quantum dots, wires, and even wells [1,2]. Some such effects are essentially nonlinear [3]. Both strain and piezoelectric effects have been used as tuning parameters for the optical response of LDSNs in photonics and band gap engineering applications. However, thermal effects have been largely neglected. At the same time, thermal effects coupled with electric and mechanical fields in LDSNs are becoming increasingly important in many applications of LDSN-based optoelectronic devices, in particular where such devices face challenges for thermal management. Indeed, as thermoelectric and thermoelastic effects are often significant in LDSNs, it is reasonable to expect that the temperature may also be used as a tuning parameter in photonics and band gap engineering applications. In this contribution, by using the fully coupled model of thermoelectroelasticity, we build on our previous results [4,5] while analyzing the influence of these effects on optoelectronic properties of quantum dots. Results are reported for both III-V and II-VI group semiconductors with a major focus given to GaN/AlN and CdSe/CdS based quantum dot systems.

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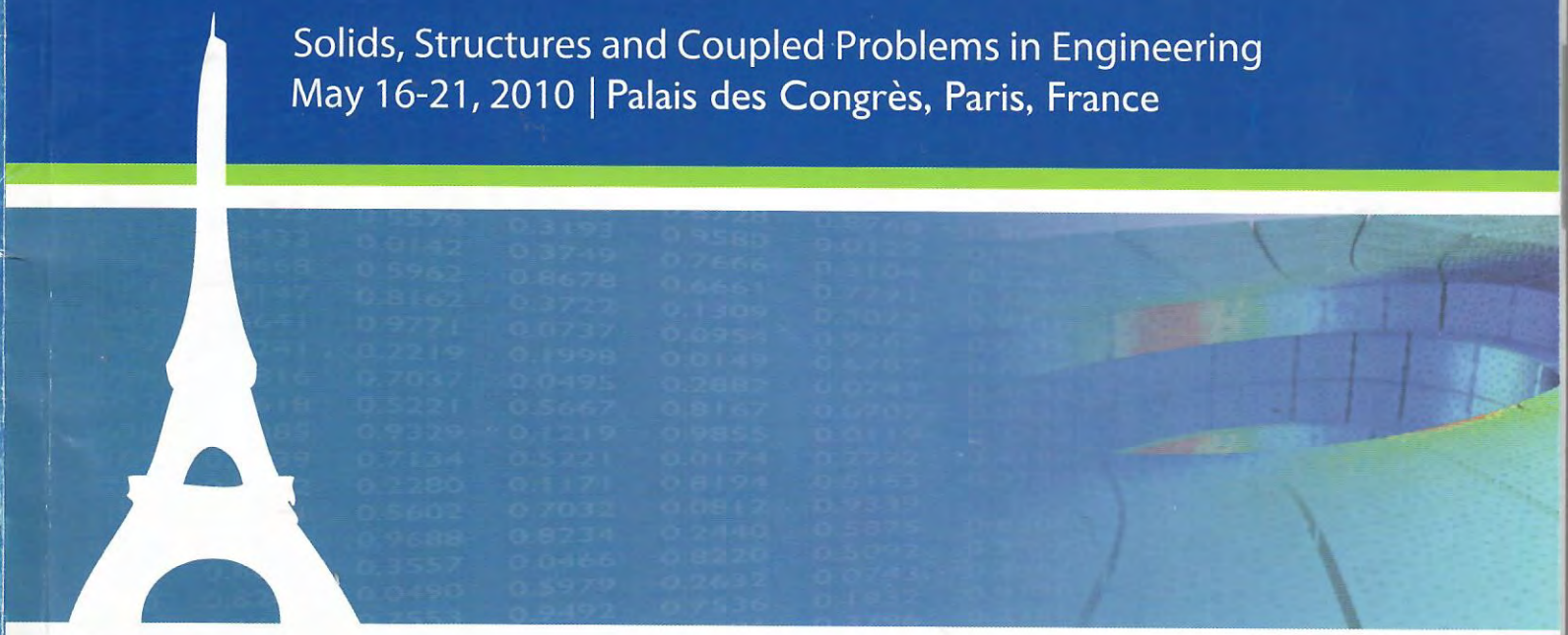

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Table of Contents

Conference organization	2
Plenary and semi-plenary lectures	8
Parallel sessions of Monday	10
Parallel sessions of Tuesday	30
Parallel sessions of Wednesday	46
Parallel sessions of Thursday	62
Parallel sessions of Friday	78
Access and conference rooms plans	85
Author index	88

Parallel sessions

Monday

17:20-18:40

MS 83 Chair: V. Sansalone **Amphithéâtre bleu**

Multiscale and multiphysics computational methodologies for complex materials

	ID	Authors	Title
17:20	1355	A. Nemov, A. Borovkov, D. Boso, B.A. Schrefler	Finite element simulation of the mechanical behaviour of multilevel composite iter cables
17:40	1448	B. Hugues	Numerical simulation of iter cable-in-conduit conductors mechanical behavior
18:00	25	A. Apicella, U. Heckenberger, G. Iannuzzo, G. Albertini	Integrated platform for design in aeronautics
18:20			

MS 77 Chair: L. Desvillettes **Room 242B**

Micro-macro scale-coupling and transition in solid and fluid mechanics

	ID	Authors	Title
17:20	553	V. Galkin, A. Galkin	The condensed structure in system of colliding particles
17:40	1530	L. Boudin, B. Grec, D. Yakoubi	We numerically investigate the relevance, in the aerosol-air model, of the strong coupling between both phases, in the framework of the respiratory system.
18:00	1439	L. Desvillettes, L. Chamoin	Control of simulation models used for kinetic equations
18:20			

MS 62 Chair: J. Murin **Room 243**

Computational structural stability

	ID	Authors	Title
17:20	28	K. Rzeszut	Initial imperfections and clearances in stability analysis of thin walled steel structures k. rzeszut, a. garstecki
17:40	1249	J. Xin, H. Mang	Conversion of an imperfection-sensitive into an imperfection-insensitive arch bridge
18:00	1655	I. Zuardy, P. Zahlen, W. Vöge, A. Herrmann	Stability behaviour of plain-curved cfrp sandwich panel with foam core under compression and shear loads
18:20	1334	K. Saavedra, O. Allix, P. Gosselet	Towards a multiscale domain decomposition method for the simulation of delamination and buckling interaction in composites

MS 67 Chair: A. Desimone **Room 252A**

Modeling and computational methods for the mechanics of biological systems

	ID	Authors	Title
17:20	1826	F. Fulga, C. Fulga, D. Nicolau	Multiobjective genetic algorithm for flexible filament model parameters extraction
17:40	715	S. Hossain, C. Nelson, T. Boulet, M. Arnoult, L. Zhang, A. Holmberg, J. Hein, N. Kleinschmit, E. Sogbesan	Material modeling and development of a realistic dummy head for testing blast induced traumatic brain injury
18:00	3	R. Miftahof	Dynamicsof the gravid uterus
18:20			

MS 153 Chair: F. Karaoulanis **Room 253**

Computational methods for structures

	ID	Authors	Title
17:20	1344	J.M. Battini, M. Hjiaj, Q.H. Nguyen	Geometrically non-linear finite element analysis of two-layer composite beams with interlayer slip
17:40	425	L. Komlanvi	Sensitivity analysis of solutions computed through the anm: application to the geometrical nonlinear behaviour of a laminated glass beam
18:00	669	T.R. Seong, T.Y. Yoon, H.M. Koh	Finite-element simulation of nonlinear behavior of ultra-thick plate joint with gap between plates
18:20	2036	T. Canor, V. Denoël	Patching asymptotic solution of a cable with a small bending stiffness

MS 27 Chair: F. Lebon **Room 341**

Mathematical and numerical modelling of microstructures in phase transformation and damaged materials

	ID	Authors	Title
17:20	240	F. Davi'	Singularities in landau-devonshire potentials for ferroelectrics phase-transitions
17:40	1535	R. Melnik	Numerical analysis of phase transformations in finite size nanostructures with mesoscopic models
18:00	1724	D. Indeitsev	Mathematical modeling of dynamical instability of surface and structure of materials
18:20	782	R. Rizzoni, F. Lebon	Asymptotic analysis of an elastic thin interphase with mismatch strain

MS 82 Chair: L. Muszynski **Room 342B**

Computational material modeling of wood and wood products

	ID	Authors	Title
17:20	1737	G. Turk	Semi-analytical buckling loads of timber columns subjected to fire
17:40	1121	J.L. Coureau	On the application of fracture mechanics for traditional connections design
18:00	1140	N. Dourado, S. Morel	R-curve estimate through an exact self-weight compensation method:wood
18:20	611	J. Cabrero, A. Heiduschke, P. Haller	Numerical and experimental investigation on wooden profiles with fiber confinement

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Numerical Analysis of Phase Transformations in Finite Size Nanostructures with Mesoscopic Models

R.V.N. Melnik[1], L. Wang[2], R. Dhote[3], J. Zu[3]

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[2] *Faculty of Mechanical Engineering, Hangzhou Dianzi University, Xiasha, Hangzhou, 310018, P.R. China*
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In a series of recent papers we developed several efficient methodologies to solve 2D models describing square-to-rectangle phase transformations in materials with memory, in particular the finite volume methodology [9] and a numerical reduction procedure based on the Proper Orthogonal Decomposition (POD) [8]. In this contribution we discuss the application of the models and numerical methodologies develoepd there to modelling finite nanostructures, in particular nanowires and nanoplates.

Our motivation for this study came from the fact that in gold (Au) nanowires, the energy as a function of lattice spacing exhibits two distinct minima that correspond to fcc and bct phases. These nanowires exhibit shape memory effects which has been confirmed computationally with such methodologies as tight-binding and density functional theory (e.g., [1]). A similar situation holds for ZnO nanowires and many other types of nanowires that show substantial potential for many applications in nano- and bio-nanotechnologies, including Cu, Ni, Al, Ag (e.g., [2] and references therein). Our major interests here include iron-based (FePd) and zinc-based oxide(ZnO) nanowires nanowires. The simulated results include nanowires in the length range of 30-200 nm for different diameter-length ratios as well as nanoplates. Typical test results obtained in the Comsol finite element package are given in Fig. 1 where we present microstructures of a nanowire and a nanoplate that are not observable in the corresponding bulk materials.

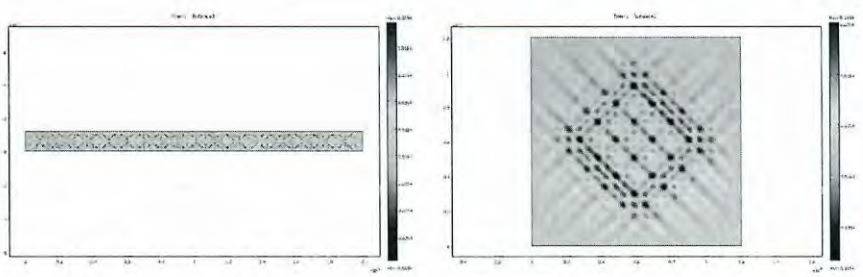

Figure 1: Evolution of microstructures in nanostructures (nanowire (left) and square nanoplate (right)).

We develop a relatively simple and computationally inexpensive model to study phase transformations in finite nanostructures. We build on the models describing shape memory effects at the mesoscopic level, in particular those described in [5, 3, 4]. We study the cubic-to-tetragonal transformations in which case the 2D analogue of the model describes the square-to-rectangle phase transformations. In particular, our considerations are based on a modification of the following coupled system of PDEs for the evolution

of displacements (u_1, u_2) and temperature T [8, 9]:

$$\frac{\partial^2 u_1}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x} + \frac{\sigma_{12}}{\partial y} + f_1, \quad \frac{\partial^2 u_2}{\partial t^2} = \frac{\partial \sigma_{12}}{\partial x} + \frac{\sigma_{22}}{\partial y} + f_2, \tag{1}$$

$$c_v \frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + a_2 T e_2 \frac{\partial e_2}{\partial t} + g \tag{2}$$

with

$$\sigma_{11} = \frac{\sqrt{2}}{2}\rho(a_1 e_1 + a_2(T - T_0)e_2 - a_4 e_2^3 + a_6 e_2^5) + \frac{d_2}{2}\nabla_x^2 e_2, \tag{3}$$

$$\sigma_{12} = \frac{1}{2}\rho a_3 e_3 = \sigma_{21}, \tag{4}$$

$$\sigma_{22} = \frac{\sqrt{2}}{2}\rho(a_1 e_1 - a_2(T - T_0)e_2 + a_4 e_2^3 - a_6 e_2^5) + \frac{d_2}{2}\nabla_y^2 e_2 \tag{5}$$

for the case of nanowire specific geometry. We discuss the contributions of the surface stress and in this context analyze the differences in modelling bulk and nanowires. One of the applications of the nanowires discussed in this presentation stems from their integration in biomolecular technologies and we highlight the importance of the contributions of entropic elasticity [6] in such cases. Finally, we provide details on the extension of the models discussed here to include nonlocal effects allowing to account for size-dependent properties of the nanostructures [7]. In the above model, T_0 is the reference temperature, c_v, a_i, i=1,2,3,4,6 and d_2 are material specific coefficients, while e_1, e_2 (the order parameter in the present model), and e_3 are dilatational, deviatoric, and shear components of the strain, respectively. A systematic procedure for the reduction of general 3D mathematical models describing shape memory effects to low dimensional models, initiated in [5] and developed further in a series of our papers, is discussed here in details in the context of modelling shape memory effects in nanostructures.

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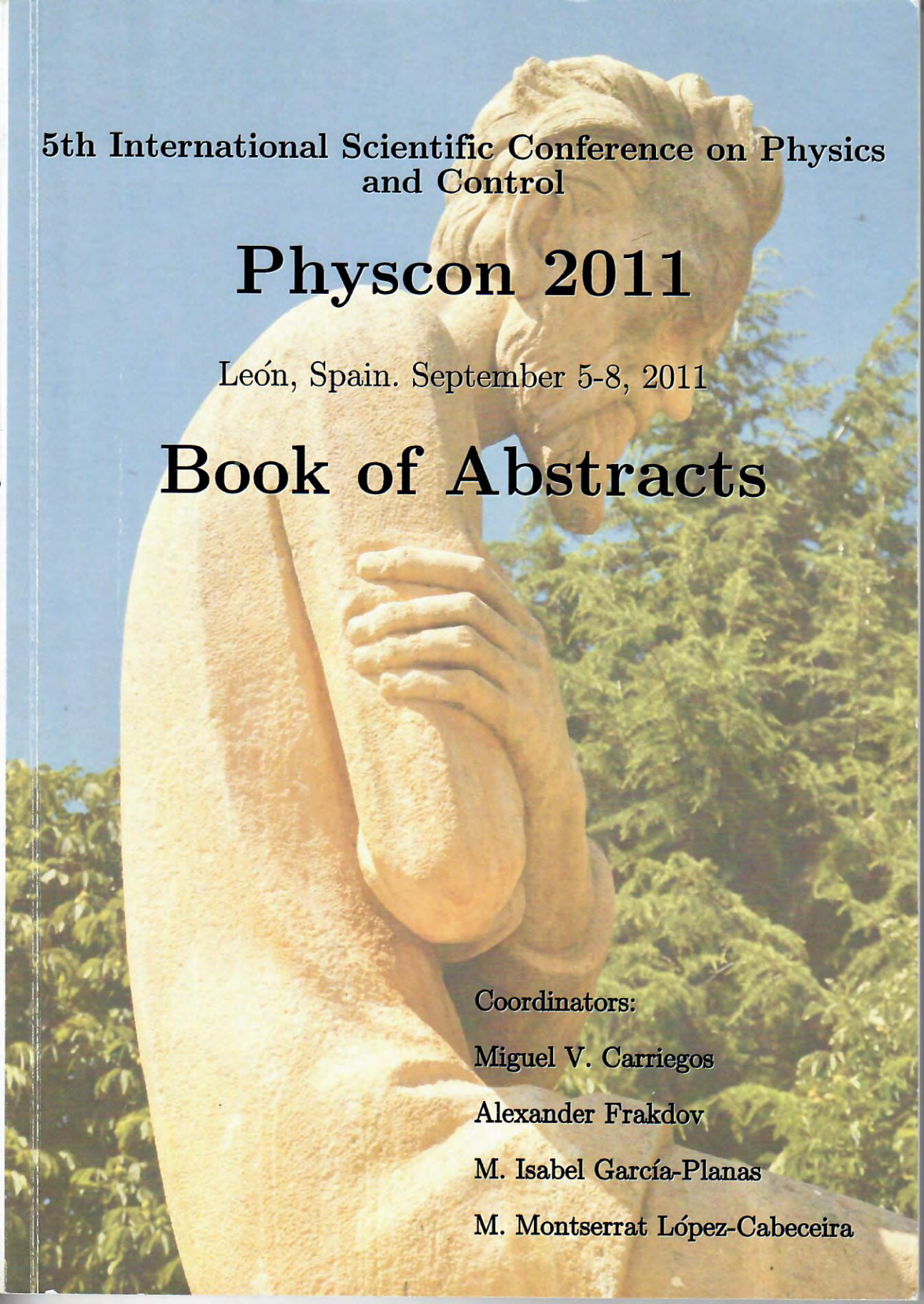

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Conten

Preface

Plenary lectur

Invited Lectur

Invited Minisy

Minisymposia

Regular paper

Posters

Authors index

Attractor Localization of Dynamical "Solar Wind-Magnetosphere-Ionosphere" Model

Kuznetsov N.V.*, Leonov Gennady A.*, Seledzhi S.M.*, Starkov K.E.†

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Abstract. The problem of localization of attractor of solar wind-magnetosphere-ionosphere (WINDMI) three-dimensional model has stimulated the development of method of conical nets. In the paper the development of this method is carried out and analytical estimates of the attractor of this model are obtained.

Gate control of single electron spins through Lande g-factor in InAs quantum dots

Sanjay Prabhakar, Roderick Melnik

Affiliation: Department of Mathematics, Wilfrid Laurier University, Waterloo, Ontario, Canada, sprabhakar@wlu.ca.

Abstract. We study the variation in the Lande g-factor of electron spins induced by an anisotropic gate potential in InAs quantum dots for potential use as non-charge based logic devices. In this paper, we present the numerical simulations of such spins in an electrostatically confined two-dimensional asymmetric gate potential forming a quantum dot system in a 2DEG. Using numerical techniques based on Finite Element Method, we show that the broken in-plane rotational symmetry, only due to Rashba spin orbit coupling in an asymmetric potential (induced by gate voltages), leads to a significant reverse effect on the tunability and control of the electron g-factor over a symmetric model potential (i.e. the derivative of the g-factor with respect to electric field has opposite sign in the two cases).

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ABSTRACTS

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In the book are presented reports abstracts of International Conference "Functional Materials" ICFM'2011. Conference is devoted to actual problems of physics, technology and applications of new materials and structures with the certain functional properties.

For scientists and graduate students in the field of physics, technologies and application of functional materials.

Abstracts are presented in author's edition.

Тези Міжнародної конференції «Функціональні матеріали» ICFM'2011, 3-8 жовтня, 2011 р. – Сімферополь, ДИАЙПИ, 2011. – 468 с.

У книзі представлені тези доповідей Міжнародної конференції «Функціональні матеріали» ICFM'2011. Конференція присвячена актуальним проблемам фізики, технології та застосування нових матеріалів і структур з певними функціональними властивостями.

Для учених та аспірантів, які працюють в області фізики, технології і застосування функціональних матеріалів.

Тези представлені в авторській редакції.

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Для ученых и аспирантов, которые работают в области физики, технологии и применения функциональных материалов.

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Table of Contents

Section 1. Fundamental Physics of Functional Materials 11

Section 2. Hard and Soft Magnetic Materials 93

Section 3. Spintronics. Transport phenomena. Multilayers 125

Section 4. Electrooptic and Magnetooptic Materials 159

Section 5. Piezoelectric and Magnetoelectric Materials. Multiferroics 201

Section 6. Magnetoelastic and Adaptive Materials 235

Section 7. Magnonics. Microwave Materials and Metamaterials 267

Section 9. Nanophysics & Nanotechnologies for Functional Materials 313

Section 10. Materials for Medical and Environmental Applications. Biosensors.. 371

Workshop LOD & Section 8. Luminescent and Radiation Sensing Materials.. 411

Author Index 456

Important Events for the Science of Functional Materials

100th Anniversary of A.I .Akhiezer (1911—2000)

A.I. Akhiezer

ALEXANDER IL'ICH AKHIEZER was the Soviet theoretical physicist, academician, known for his scientific contributions to quantum electrodynamics, nuclear physics, physics of plasma and solid state physics. He was one of the first PhD students of Nobel Price Laureate L.Landau . A.I. Akhiezer was the Head of the Department for Theoretical Physics at the Ukrainian Physical-Technical Institute (currently NSC KIPT). In 1996, on his initiative, the Institute for Theoretical Physics was created on the base of the Departments for Theoretical Physics of NSC KIPT. Now the Institute for Theoretical Physics is named after A.I. Akhiezer. A.I. Akhiezer, with V.G. Baryakhtar and S.V. Peletminskii, developed the theory of coupled magnetoacoustic waves and predicted a new effect-magnetoacoustic resonance.

100th Anniversary of Discovering the Superconductivity

H.K. Onnes

Heike Kamerlingh Onnes and Jacob Clay investigated the reduction of resistance at low temperatures. Onnes's research into the resistivity of solid mercury at cryogenic temperatures was accomplished by using liquid helium as a refrigerant. On April 8, 1911, 16:00 hours at the temperature of 4.19 K, he observed that the resistivity of mercury abruptly disappeared. Onnes disclosed his research in 1911, in a paper titled "On the Sudden Rate at Which the Resistance of Mercury Disappears". Onnes stated in that paper that the "specific resistance" became thousands of times less in amount relative to the best conductor at ordinary temperature. The next year, Onnes published more articles about the phenomenon. Initially, Onnes called the phenomenon "supraconductivity" (1913) and, only later, adopted the term "superconductivity". For his research, he was awarded the Nobel Prize in Physics in 1913.

The Nobel Prize in Physics 2010

A. Geim

K. Novoselov

The Prize was awarded jointly to Andre Geim and Konstantin Novoselov "*for groundbreaking experiments regarding the two-dimensional material graphene*". Graphene is a form of carbon. As a material it is completely new – not only the thinnest ever but also the strongest. As a conductor of electricity it performs as well as copper. As a conductor of heat it outperforms all other known materials. It is almost completely transparent, yet so dense that not even helium, the smallest gas atom, can pass through it. Geim and Novoselov extracted the graphene from a piece of graphite such as is found in ordinary pencils. Using regular adhesive tape they managed to obtain a flake of carbon with a thickness of just one atom.

With graphene, physicists can now study a new class of two-dimensional materials with unique properties. Graphene makes experiments possible that give new twists to the phenomena in quantum physics. Also a vast variety of practical applications now appear possible including the creation of new materials and the manufacture of innovative electronics. Graphene transistors are predicted to be substantially faster than today's silicon transistors and result in more efficient computers

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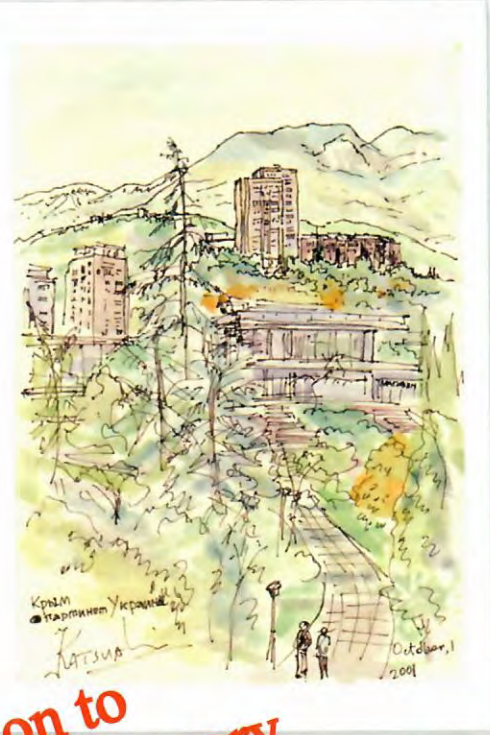

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EB-5L/1 Magneto-thermo-piezoelectric effects in quantum dots

Melnik R.V.N.[1,2] and Prabhakar S.[1]

[1]*M²NeT Laboratory, Wilfrid Laurier University,*
75 University Ave W., Waterloo, ON, Canada N2L 3C5
[2]*MIT Department, University of Javaskyla, Finland*
http://www.m2netlab.wlu.ca

Coupled effects play a fundamental role in predicting properties of low dimensional semiconductor nanostructures (LDSNs). Such coupled effects grow into a substantial factor to be accounted for in many current and potential applications of functional materials in LDSNs used for optoelectronic devices and other applications [1, 2, 3]. Furthermore, the influence of magneto-thermo-piezoelectric effects in the magnetic quantum dots (QDs) leads to their significant contributions in the bandstructures of these QDs.

In this presentation we analyze systematically the influence of magneto-thermo-piezoelectric effects on the strain and built-in piezoelectric field in three different types of quantum dots, namely (a) ferroelectric, (b) piezomagnetic, and (c) magnetoelectric. This analysis is carried out based on the fully coupled model of magneto-thermo-electroelasticity coupled with an effective envelope model for bandstructure calculation. In particular, we demonstrate that the influence of magnetic effects on the quantum dots can be significant and we quantify these effects in each case.

These findings are important from different perspectives. For example, wide band gap nanostructures studied here, such as AlN/GaN QDs doped with magnetic materials (e.g., Mn or Cr), have attracted significant attention in optical and electronic devices used in nano- and bionanotechnological applications [4]. In the meantime, ferroelectric nanostructures such as $BaTiO_3$ or PZT are important for the design of nonvolatile memory density devices, actuators and transducers [5].

In magnetic AlN/GaN quantum dots, we found that magneto-thermo-piezoelectric effects bring the localized eigenstates to the lower energy levels where we chose the flat band as a reference point. Due to these coupled magneto-thermo-piezoelectric effects, the spin splitting energy occurs at lower energy levels, compared to the case of electromechanical effects only, in the presence of external magnetic field along z-direction.

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CA-6O/4 **Laws of elasticity in the physical processes influence of parameters (TPH) on the properties and structural phase transitions**
Polyakov P.I.
Inst. For Phys. of Mining Processes, Donetsk, Ukraine

12.00-13.15 Oral Session CB.
Section 3. Spintronics. Transport phenomena. Multilayers

Chairmen: Ryabchenko S., Petrakovsky G.

CB-3L/1 (EB-5L/1) **Magneto-thermo-piezoelectric effects in quantum dots** *(Invited)*
Melnik R.V.N.[1,2] and Prabhakar S.[1]
[1]*M2NeT Laboratory, Wilfrid Laurier University, Waterloo, Canada*
[2]*MIT Department, University of Javaskyla, Finland*

CB-3O/1 **Magnetic, dynamic and transport properties of epitaxial Fe/MgO multilayers**
García-García A.[1,2], Vovk A.[3,4], Kakazei G.N.[4,5], Pogorelov Yu.G.[5], Golub V.[4], Salyuk O.[4], Pardo J.A.[6,7], Štrichovanec P.[6], Magén C.[6], De Teresa J.M.[1,2], Morellón L.[1,2,6], Algarabel P.A.[1,2], and Ibarra M.R.[1,2,6]
[1]*ICMA, Universidad de Zaragoza-CSIC, Zaragoza, Spain*
[2]*DFMC, Universidad de Zaragoza-CSIC, Zaragoza, Spain*
[3]*CFMC, Universidade de Lisboa, Lisboa, Portugal*
[4]*Institute of Magnetism, National Academy of Sciences of Ukraine, Kyiv, Ukraine*
[5]*IFIMUP and IN–INNanotechnology, Universidade do Porto, Porto, Portugal*
[6]*INA, Universidad de Zaragoza, Zaragoza, Spain*
[7]*DCTMFluidos, Universidad de Zaragoza, Zaragoza, Spain*

CB-3O/2 **Spin-wave and spintronic devices on the base of magnetic nanostructures**
Lutsev L.V.[1], Stognij A.I.[2], Novitskii N.N.[2], Shulenkov A.S.[3]
[1]*A.F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Peterburg, Russia*
[2]*Institute of Solid State and Semiconductor Physics, NAS of Belarus, Minsk, Belarus*
[3]*Minsk Research Institute of Radiomaterials, Minsk, Belarus*

CB-3O/3 **Positive magnetoresistance in granular magnetic films with perpendicular anisotropy**
Kalita V.M.[1], Timopheev A.A.[1], Lozenko A.F.[1], Ryabchenko S.M.[1], Los A.V.[2], Stognei O.V.[3], Sitnikov A.V.[3]
[1]*Institute of Physics of the NAS of Ukraine, Kyiv, Ukraine*
[2]*ISS Ltd. and Freescale Semiconductor Ukraine LLC., Kyiv, Ukraine*
[3]*Voronezh State Technical University, Voronezh, Russian federation*

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CB-3O/4 **Spin transfer in EuO:Fe/GaAs contact**
Borukhovich A.S.[1], Ignat'eva N.I.[2], Stognii A.I.[3], Yanushkevich K.I.[3]
[1]*Russian State Vocational Pedagogical University, Yekaterinburg, Russia*
[2]*Solid State Chemistry Institute of Ural Division of RAS, Yekaterinburg, Russia*
[3]*Joint Institute of Solid State and Semiconductor Physics, National Academy of Sciences of Belarus, Minsk*

CB-3O/5 **Experimental investigation of magnetic anisotropy of thin magnetic films**
Ubizskii S.B.[1], Pavlyk L.P.[1], Syvorotka I.I.[2]
[1]*Lviv Polytechnic National University, Lviv, Ukraine*
[2]*Scintific Research Company „Carat", Lviv, Ukraine*

9.00-13.00 Poster Session CP.
Section 4. Electrooptic and Magnetooptic Materials

Chairmen: Edel'man I., Belyaeva A.

CP-4P/1 **Research nanophotonics materials in terms of weakly-dissipative theory by Kolmogorov - Arnold - Moser**
Bogdanov R.I.[1], Demin A.V.[2]
[1]*Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, Russia*
[2]*All-Russin Research Institute for Optical and Physical Measurements, Moscow, Russia*

CP-4P/2 **On the laser-induced remagnetization of tunnel magnetic junctions**
Krupa M.M., Korostil A.M.
Institute of Magnetism NAS of Ukraine, Kyiv, Ukraine

CP-4P/3 **Optical activity of imperfect 1D-multilayer composite material**
Rumyantsev V.V., Fedorov S.A., Gumennyk K.V.
A.A. Galkin Institute for Physics and Engineering of National Academy of Sciences of Ukraine Donetsk, Ukraine

CP-4P/4 **The temperature- and geometry-dependent photonic band gap spectra of the photonic crystals with two superconducting defect layers**
Dadoenkova N.N.[1], Lyubchanskii I.L.[1], Lee Y.P.[2] and Rasing Th.[3]
[1]*Donetsk Physical & Technical Institute of the National Academy of Sciences of Ukraine, and Department of Physics, Donetsk National University, Donetsk, Ukraine*
[2]*q-Psi and Department of Physics, Hanyang University, Seoul, Korea*
[3]*Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, The Netherlands*

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COUPLED MULTIPHYSICS MODELS for THE ANALYSIS OF THE CONDUCTION and VALENCE BAND EIGENENERGIES in CYLINDRICAL QUANTUM DOTS

SANJAY PRABHAKAR, EDUARD TAKHTAMIROV, RODERICK MELNIK

M2NeT Laboratory, Wilfrid Laurier University, 75 University Ave W, Waterloo, Ontario, Canada, N2L 3C5

A new coupled multiphysics model has been developed for the analysis of conduction and valence band eigenenergy in quantum dots. This model has been applied to study the band structure of low dimensional semiconductor nanostructures (LDSNs) such as wurtzite AlN/GaN quantum dots in cylindrical coordinates in the presence of applied magnetic field along z-direction [1]. An algorithm for the solution of the resulting model has been based on the finite element method, and by using this algorithm eigenvalues and wave functions of cylindrical quantum dots of various sizes have been obtained. Details of the methodology of solution and appropriate boundary conditions have also been provided. A special attention has been given to the case of applied magnetic field along z-direction where we found localized eigenstates and wave functions in the conduction and valence bands for which our results open new possibilities for the design of such optoelectronics devices where the combination of electron-hole pairs can be used as tuning parameters.

References:

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Computational Methods for Coupled Problems in Science and Engineering V

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16:30 - 18:50 TECHNICAL SESSIONS

Numerical Methods in Coupled Problems V	WeE01 Room: Auditorium Chair: Vitoriano Ruas

A LS-DYNA/FLUKA coupling for the numerical simulation of high energy particle beam interaction with matter
M. Scapin, L. Peroni, V. Boccone and F. Cerutti*

Use of a BEM model to simulate unsteady coupled heat and moisture flow through porous solid
L. Škerget and A. Tadeu*

An iterative coupling approach to the simulation of elastic wave
J. António, A. Tadeu and P. Ferreira*

Iterative dynamic model to estimate thermal resistance of wall subjected to a transient heat flux
A. Tadeu, N. Simoes, I. Simoes, F. Pedro and L. Škerget*

Snap Through of Curved Structures in Thermal Environments
I. Stanciulescu and Y. Chandra*

Network models for the numerical solution of coupled ordinary non-lineal differential equations
I. Alhama, J.L. Morales and F. Alhama*

A new functional for improving cell area distribution
*P. Barrera, F.J. Domínguez-Mota and G. González**

Multiphysics Problems IV	WeE02 Room: R2 Chair: Robert L. Taylor

Keynote Lecturer: José Luis Pérez-Aparicio
Elastothermoelectric finite element analysis and optimization of pulsed thermoelectric
J.L. Pérez-Aparicio, R. Palma and J. Gómez-Hernández*

Coupled problems in analysis of quantum dots with multiband models
*S. Prabhakar and R. Melnik**

Coupled swelling and large strain model for hydrogels: Application to the nucleus pulposus of the intervertebral disc
V. Brulliard, S. Le Corre and E. Verron*

Inverse-motion-based form finding for electro-active polymers
R. Denzer, A. Ask, A. Menzel and M. Ristinmaa*

Numerical simulation for evaporation of chemical agent droplet
H. Hayakawa, M. Yamamoto, M. Kawai and K. Sakamoto

Numerical simulation of diffusion induced crack formation in solids
S. Hirobe and K. Oguni*

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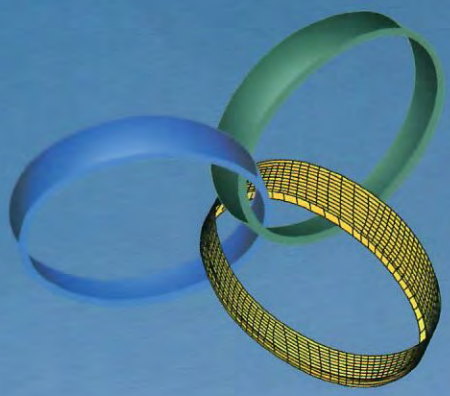

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(ELNANO)

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April 16-19, 2013
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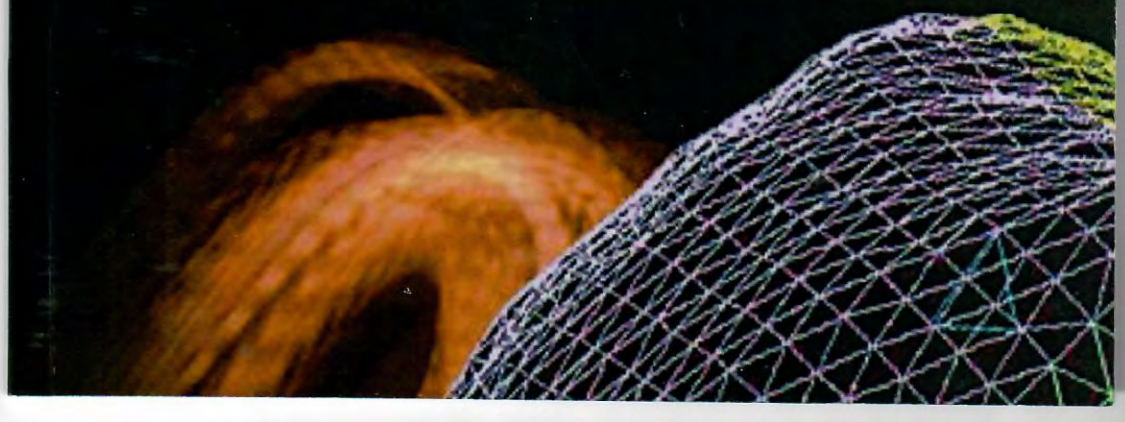

Friday 13 December 2013

14:00-15:30 **Session 2.3**
Materials & Nano-Technology

Chair: E A Al-Bahkali, King Saud University, Saudi Arabia

Rashba spin-orbit coupling effects in low dimensional nanostructures
R.V.N. Melnik and S. Prabhakar, M2NeT Lab, Wilfrid Laurier University, Waterloo, ON, Canada

An experimental and computational prediction for material characteristics of Jahgal Soil
Hirofumi IYAMA(1), Yoshikazu HIGA(2), Ken SHIMOJIMA(2), Shigeru TANAKA(3), Hironori MAEHARA(3) and Shigeru ITOH(2)
(1)Kumamoto National College of Technology.
(2)Okinawa National College of Technology.
(3)Kumamoto University.Ceramic powder compaction via elastoplasticity theory

Characterization of defect sizing in aluminum alloys by eddy current technique
Bennoud salim, Laboratory of Aircrafts, University of Saad Dahlab, Blida, Algeria

Some elastic parameters of zinc blende ZnS
E. Guler (1), M. Guler (1), E. Aldirmaz (2)
(1) Hitit University, Department of Physics, Turkey
(2) Amasya University,Department of Physics,Turkey

A comparative study for cubic elastic constants of fcc Ag, Au and Cu
M. Guler,E. Guler, H.Gunguneu and U. Alp, Hitit University, Department of Physics, Turkey

15:30-16:00 **Coffee Break**

Friday 13 December 2013

16:00-17:30 **Session 2.4**
Posters

A mathematical model for RTM process simulations in geometries with irregular shapes
B. G. Coutinho, M. F. Bezerra, S. R. Farias Neto, A. G. B. de Lima, Federal University of Campina Grande, Brazil

Cavitation Inception in Fuel Injector Nozzle: A CFD based Parametric Analysis
M. Mustafa Kamal (Department of Engineering, University of Cambridge, UK)

Drying of Ceramic Hollow Bricks in an Industrial Tunnel Drier: A Finite volume Analysis
Francisca Valdeiza de Souza Tavares, Severino Rodrigues de Farias Neto, Enivaldo Santos Barbosa, Antonio Gilson Barbosa de Lima, Federal University of Campina Grande, Brazil

Effect of Reversible Hydrogen Trapping on Crack Propagation in the API 5CT P110 Steel: A Numerical Simulation
J. P. Carrasco, E. T. da Silva, D. D. S. Diniz, A. A. Silva, J. M. A. Barbosa, Brazil

Evaluation of the contact switch materials in high voltage power supply for generate of underwater shockwave by electrical discharge
Katsuya Higa, Takumi Matsui, Soichiro Hanashiro, Osamu Higa, Shigeru Itoh, Okinawa National College of Technology, Japan

Evaluation of the effect of mechanical vibration on the levels of residual stresses in steel welded joints using an Interface Matlab based on Norm API 579
Rodrigues, Rmulo do Nascimento; Silva, Antonio Almeida; Maciel, Theophilo Moura; UFCG, Campina Grande-PB, Brasil

Multiphysics Investigation of Composite Shell Structures Subjected to Water Shock Wave Impact in Petroleum Industry
H. Khawaja and M. Moatamedi, Narvik University College, Norway

RASHBA SPIN-ORBIT COUPLING EFFECTS IN LOW DIMENSIONAL NANOSTRUCTURES

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R.V.N. Melnik and S. Prabhakar, M2NeT Lab, Wilfrid Laurier University, Waterloo, ON, Canada

The splitting of spin bands in low dimensional semiconductor nanostructures is a result of a combined (Rashba) effect of spin-orbit coupling and asymmetry of the potential. It plays an important role in the properties of such nanostructures. In this contribution, we analyze in detail the influence of Rashba spin-orbit coupling in several types of low dimensional nanostructures, focusing on nanowires modulated by longitudinal periodic potentials. If the modulation potential is obtained from a superlattice, the resulting structure is known as the nanowire superlattice. We demonstrate that the Rashba spin-orbit interaction induces the level crossing point in such nanowire superlattices. Finally, we study the phonon and electromagnetic field mediated spin transition rates in these structures for different values of Rashba spin-orbit coefficients.

Keywords: spin-orbit coupling effects, nanostructures, superlattices, coupled effects in quantum mechanical systems

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Morning session

09:00 - 09:30	Opening session J.Bonca, J.Stefan Institute, Slovenia *S.Kruchinin, BITP ,Kiev,Ukraine*
09:30 - 10:00	Transport properties of nanosystems *A.Balatsky, Los Alamos National Laboratory, USA*
10:00 - 10:30	Highly selective biochemical detectors *B.Vlahovic, North Carolina Central University, USA*
10:30 - 11:00	Electron transport in mesoscopic structures and nanowires *M.Mierzejewski, University of Silesia, Poland*
11:00 - 11:30	**Coffee break**
11:30 - 12:00	Spin echo dynamics in quantum logic gates and quantum in cryptography *R.Melnik ,Tier I Canada Research Chair, Canada*
12:00 - 12:30	Magnetic resonance study of nanocrystalline TiO_2 *N.Guskos, Athens University, Greece*

Afternoon session

14:00 - 14:30	Nanoscale aspects of phase transitions in copper based shape memory alloys *O. Adiguzel, ICMP, Turkey*
14:30 - 15:00	Andreev states in graphene/superconductor hybrids *L.Covaci, Antwerp University, Belgium*
15:00 - 15:30	**Coffee break**
15:30 - 16:00	Experimental detection of the spin-valve effect *A.Sidorenko, IEEN, Moldova*
16:00 - 16:30	Mechanical properties of micro-patterned carbon nanotube foams *L.Lattanzi ,California Institute of Technology, USA*
16:30 - 17:00	Control of electron correlations in perovskite superlattices: role of strain and interfaces *V. Moshnyaga, University of Goettingen, Germany*
20:00 - 22:00	**Poster session**

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CONTENTS

SCIENTIFIC PROGRAM **5**

LECTURES **11**

J. Freericks
Universal thermopower of bad metals 13

D. Logan
Some aspects of non-Fermi liquid phases incorrelated quantum impurity physics 14

M. Mierzejewski, T. Prosen, D. Crivelli, P. Prelovsek
Reduced density matrix for systems out of equilibrium 15

Y. Asano
Surface and interface states in topological superconductors and insulators 16

J.Y.T. Wei
Andreev nanoprobe of half metals and topological insulators 17

I.N. Zhilyaev
Nanostructure model for superconducting state of HTSC 18

L. Vidmar
Steady-state and relaxation dynamics of doped two-dimensional antiferromagnetic Mott insulators 19

B. Vlahovic, I. Filikhin
Localized-delocalized tunneling in double quantum dot: Effect of symmetry violation 20

R. Melnik, S. Prabhakar, L. Bonilla
Thermomechanics of ripples in grapheme 21

A. Maeda
Superconductivity fluctuation and dynamics of quasiparticles confined in nano space in cuprate and Fe-based superconductors 22

Y. Divin
Quest for ideal high-T_c Josephson junction 23

T. Tohyama
In-plane anisotropy and superconductivity in the antiferromagnetic phase of iron-based superconductors 24

T. Shibauchi
Exotic superconductivity of heavy electrons in artificial two-dimensional Kondo lattices 25

S. Feng
Interplay between superconductivity and pseudogap state in cuprate superconductors 26

J.D. Fan, Y.M. Malozovsky
Beyond the random phase approximation 27

M. Ishikado, K. Kodama, R. Kajimoto, M. Nakamura, Ya. Inamura, K. Ikeuchi, S. Ji, S. Wakimoto, M. Arai, S. Shamoto
Inelastic neutron scattering on iron-based supercondutor $Fe(Te_{0.5}Se_{0.5})$ to discriminate the origin of the "magnetic resonance mode" 28

V.V. Kabanov, V.V. Baranov, A.G. Balanov
Dynamics of resistive state in thin superconducting channels 29

J.Vinko
dc-SQUID magnetic measurements on PdHx (x > 1) 30

Thermomechanics of ripples in graphene

R. Melnik[1,*], S. Prabhakar[1], and L. Bonilla[2]

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It is well known that ripples are a typical feature of graphene sheets [1]. They are produced by long wavelength corrugations and may greatly affectelectronic properties of graphene-based systems and devices.

Several mechanisms of inducing such ripples in graphene have already been discussed in the literature. Among them is electron-induced rippling in graphene [2], as well as elasticity-induced rippling [3], that may, in the general case, include nonlinear effects. The origin of graphene rippling continues to be debated. In the meantime, there is substantial experimental evidence that in order to control such ripples, a pure eleasticity-based picture may not be sufficient [4] and thermal properties of graphene may also be essential.

In this contribution, for the first time we develop and apply a fully coupled model that describes thermomechanical processes in graphene sheets. Based on this model, we demonstrate that coupling between mechanical and thermal fields is an important factor in better understandingof the appearance of ripples in graphene. Next, we use a generalization of our multiband model [4] to analyze the effects of such thermomechanically-induced ripples on the electronic properties of graphene. Results of computational experiments are shown for different boundary conditions that allow controlling ripples.

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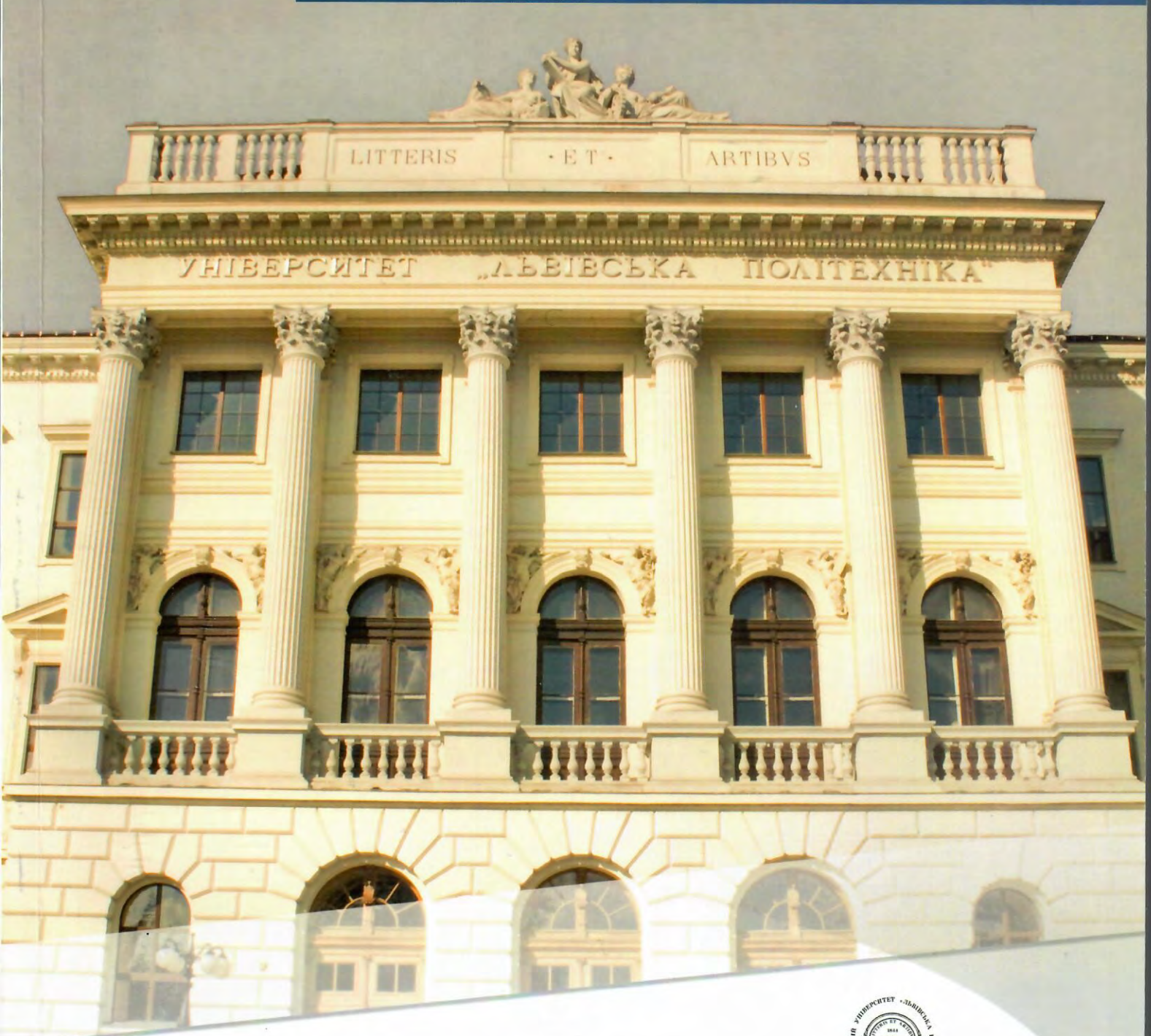

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Computational Analysis and Finite Element Modelling of Nanoscale Ripples in Graphene and Thermomechanical Effects

Roderick Melnik, Sanjay Prabhakar

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***Abstract* – The relaxed state of graphene nanostructures due to externally applied tensile stress along both the armchair and zigzag directions are analyzed in detail. The results, obtained with the Finite Element Method (FEM), demonstrate that the amplitude of ripple waves in such nanostructures increases with temperature. Details of the multiscale multiphysics computational procedure developed for this analysis are also provided.**

Key words – nanostructures, modelling, coupled processes, computer-aided design, nanotechnological applications.

I. Introduction

Graphene, a hexagon structure where the atomic layer of carbon atoms are arranged in a honeycomb lattice, is the thinnest material that can be found in the nature. It is poised to make a new breakthrough in nanotechnology due to the high mobility of charge and the potential interest to control its electronic properties by several different mechanisms such as gate controlled electric fields, magnetic fields and engineering the electromechanical properties via the pseudomagnetic gauge fields (see, e.g., [1] and references therein).

However, by now it is well known that the graphene sheets are not perfectly flat. They exhibit intrinsic roughening such that the surface normal varies by several degrees and the out-of-plane deformations reach to nanometer scale, known as ripples. In this contribution, we apply the computer-aided design methodology, based on FEM, to analyze such ripples.

II. Mathematical Model

We present a model that couples the Navier equations including thermomechanical effects to the electronic properties of graphene-based nanostructures. We start with the total thermoelastic energy density associated to the strain for the two dimensional graphene

$$U_s = \frac{1}{2} C_{iklm}\ \varepsilon_{ik}\ \varepsilon_{lm} - \beta_{ik}\ \Theta(x,y)\ \varepsilon_{ik}\ \delta_{ik},$$

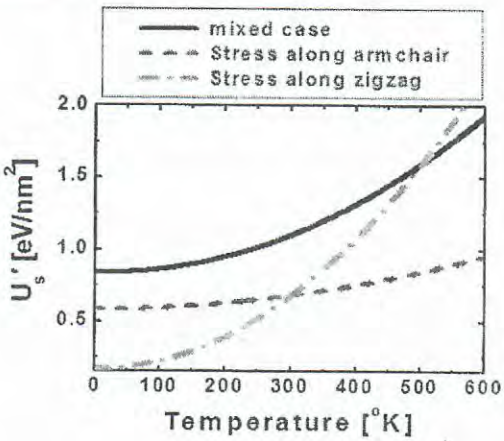
where C_{iklm} is the elastic modulus tensor of rank four, ε_{ik} is the strain tensor, β_{ik} is the stress temperature coefficients, Θ is the distribution of temperature in the graphene sheet that can be found by solving Laplace's equation for the temperature, assuming the Fourier law. As a result, we have to solve the coupled Navier equations for the graphene nanostructure. Ripples in graphene are described by an out of plane sinusoidal function on the sheet of graphene and we apply tensile edge stress along the armchair direction to induce the ripples so that the total edge energy per unit length is given by

$$Ue = \frac{1}{2}\tau_e\left(\frac{\partial u(x,0)}{\partial x}\right)^2 + \frac{1}{8}E_e\left(\frac{\partial u(x,0)}{\partial y}\right)^4,$$

where τ_e and E_e denote the edge stress and the elastic modulus of the edge along the armchair direction of the graphene sheet.

III. Computational Analysis and Modelling

We have developed a multiscale multiphysics computer-aided simulation technique, based on the Finite Element Method, to analyze thermomechanics of relaxed states of graphene nanostructures. Among other results, we will discuss the total thermoelastic energy density vs temperature (Fig. 1). Even though the optimal amplitude value of the ripple waves has been the same in all three cases studied here, the variation in the the total thermoelastic energy density is enhanced for the case of induced ripples due to applied tensile edge stress along zigzag direction (dashed-dotted line). This is due to the fact that the graphene sheet at one of the boundaries is connected to the heat reservoir that enhances the energy of the ripple waves along the y-direction. These differences affect also electronic properties of graphene nanostructures.



Conclusion

In this contribution we have analyzed thermomechanical behavior of nanoscale ripples in graphene by using the developed multiphysics FEM-based computational technique.

References

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Distributed Computing for Phase-Field Models

Rakesh Dhote[1,2], Roderick Melnik[1], Hector Gomez[3], and Jean Zu[2]

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Abstract – ***We summarize here our recent results on the implementation of the Isogeometric Analysis (IGA) code for phase-field modelling, cluster configuration and weak performance studies, focusing on distributed computing aspects. Main examples are given for phase-field models for materials with memory.***

Key words – distributed computing, NURBS basis functions, shape memory alloys, MPI communication time.

I. Introduction

The phase-field (PF) models provide a unified framework that can describe phase transformations in many areas of applications. They are well suited for the description of complex dynamics. Among other applications, these models have been used to study microstructures and mechanical properties of materials across different scales, including materials with memory such as shape memory alloys (SMAs). We highlight here our recent results on the application of the Isogeometric Analysis to such models and our implementation of the code in the distributed computing environment.

II. Mathematical Model

In [1] we applied for the first time the Isogeometric Analysis (IGA) to deal with complex dynamics of materials with memory, focusing on SMAs. IGA employs the complex non-uniform rational B-spline (NURBS) based geometry in a finite element analysis application directly. IGA offers unique advantages in solving problems involving higher-order PDEs such as higher order accuracy, robustness, two- and three- dimensional geometric flexibility, compact support, and higher-order continuity. In many cases, higher dimensional PF models are too complex (e.g., having highly nonlinear hysteretic behavior, strong thermo-mechanical coupling, and fourth-order spatial differential terms for SMA models). Hence, to solve them on a regular workstation is not always possible. We use the distributed computing environment for their numerical solutions. The model we use here, as an example, is based on the following coupled equations derived from the Gizburg-Landau theory

$$\dot{\mathbf{u}} = \mathbf{v},$$

$$\rho\dot{\mathbf{v}} = \nabla\cdot\boldsymbol{\sigma} + \nabla\cdot\boldsymbol{\sigma}' + \boldsymbol{\sigma}_g + \mathbf{f},$$

$$\rho\dot{e} - \boldsymbol{\sigma}^T : (\nabla\mathbf{v}) + \nabla\cdot\mathbf{q} = g,$$

where our notations here are identical to those in [1]. We convert the system of the governing equations into the weak formulation. The domain is discretized where we use NURBS for our basis functions, while the generalized-α method is used for time integration along with an adaptive time stepping scheme.

III. Computational Implementation

The numerical implementation of the 2D and 3D IGA models for SMAs using the distributed computing environment has been first reported in [1]. In this implementation, the IGA codes use a multiple instruction, multiple data (MIMD) architecture. The domain decomposition technique has been employed in the distributed computing. The domain has been decomposed spatially into smaller subdomains using a separate script. We have used the high-performance clusters of the Sharcnet computational facilities in Canada, in particular the simulations have been carried out on the Saw cluster (with each node having two 4-core Intel E5440 Quad Core Processors (2.83GH, 4 GB + 8GB FBD PC2-5300 Memory, and 120GB of local storage) with InfiniBand 4X DDR running Linux CentOS release 6.3). The simulations have been performed utilizing full nodes and the performance data has been collected.

We have also performed the weak scaling test with each MPI (message passing interface) task on a tile of spatial dimension 16 nm × 16 nm for the 2D model. The geometry has been chosen such that it confirms the multiple of $8n$ processors, where node n has been chosen as n = 1, 2, 3, 4 and 8 for the MPI studies. A number of examples have been calculated on which it has been shown that the microstructure evolution is in agreement with known results from the literature.

We have observed that there is an opportunity to improve the computational efficiency by changing the code implementation, which is being investigated. The scaling can be improved, e.g. by using the concept of Bezier extraction or PETSc-based implementations.

Conclusion

In this contribution we have highlighted the methodology of solution of the coupled non-linear Ginzburg-Landau type PF models for SMAs reformulated in a variational framework. The numerical solution has been based on the IGA and its implementation in the distributed computing environment.

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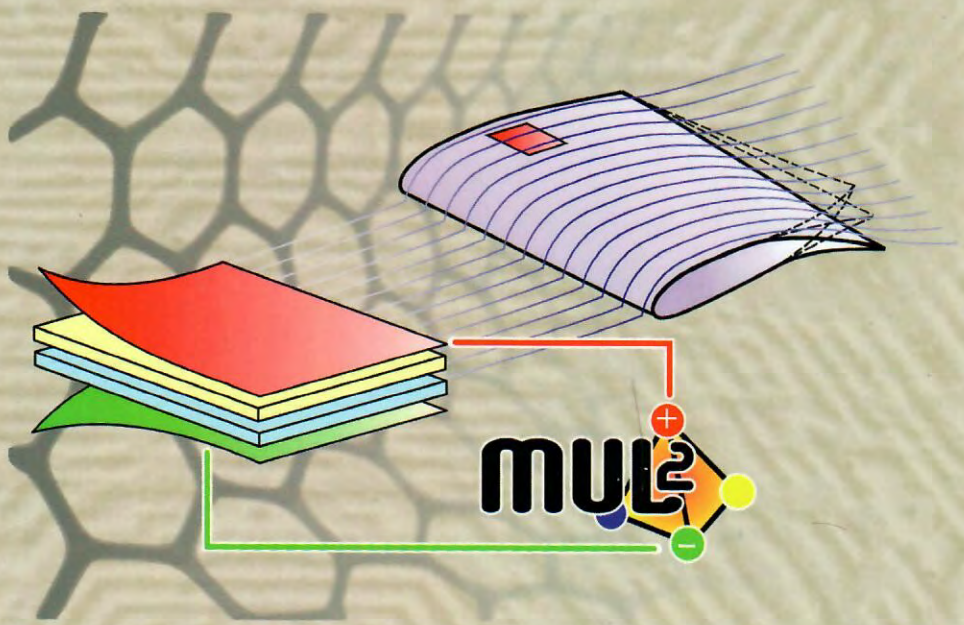

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ISOGEOMETRIC ANALYSIS IMPLEMENTATION OF THE PHASE-FIELD MODEL FOR 3D CUBIC-TO-TETRAGONAL TRANSFORMATIONS IN SHAPE MEMORY ALLOYS

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Key words: Shape memory alloys, Thermo-mechanical modeling, Isogeometric analysis, Phase-field model, Microstructure evolution.

Summary. *Shape memory alloys (SMAs) are a prime example of materials exhibiting multi-scale and multiphysics behaviors and complex microstructures. This contribution focuses on the multiphysics (thermo-mechanical) behavior of SMAs and has the dual objectives of model development and its numerical implementation. The phase-field model can describe the complex microstructure, stress and temperature induced phase transformations in the variational framework. The strain based order parameter 3D phase-field model is developed for the cubic-to-tetragonal transformations using the Ginzburg-Landau theory [1]. The developed model has a bi-directional coupling via strain, strain rate, and temperature. In addition to thermo-mechanical coupling it is characterized by inherent nonlinearity and higher (fourth) order differential terms. The bi-directional coupling has been usually neglected in a studies of SMA properties in the literature, and most of the model developments have been carried out under*

the assumption of isothermal phase transformations (e.g. [2]). The isogeometric analysis, a finite element methodology based on the non-uniform rational B-spline (NURBS) basis functions, offers several advantages in solving complex problems with higher order differential terms [3]. Here we report new results on microstructure evolution for the cubic-to-tetragonal transformations in SMAs. The tensile test on the 3D specimens has shown a significant impact of thermo-mechanical coupling on the mechanical properties.

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ECT- 65 Modelling of Heat Flow through a Three-Dimensional Crack in Thermoelasticity, J. Jaśkowiec

ECT- 66 The Influence of Thermo-Mechanical Effects on the Relaxed Shape Graphene S. Prabhakar, R. Melnik and A. Sebetci

ECT- 67 A Coupled Thermo-Mechanical Cohesive Crack Model in Three-Dimensional Crack Growth Analysis, J. Jaśkowiec

ECT- 68 Localization Analysis of an Anisotropic Damage Model M. Jirásek and F. Suárez

CST - Damage Mechanics

CST-245 Fully Coupled Moisture Transport in partially Damaged Materials J. Kruis and T. Koudelka

CTR10 - 1 **Invited Lecture:** Engineering Damage Mechanics: Review of Models and Formulations, M. Miñano and F.J. Montáns

10.30-11.00: Coffee

11.00-12.30: Chaired by: Professor J.B. Paiva and Professor EJ. Sapountzakis

CST - Boundary Element Methods

CST-191 Comparative study of Boundary Element Formulations for the Analysis of Pile-Soil Interaction, A.K. Rosa and J.B. Paiva

CST-192 Two Boundary Element Strategies for the Elastic Analysis of Raft Foundations on a Finite Layer Medium A.V. Mendonça, V.S. Almeida and J.B. de Paiva

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CST-194 Free Vibrations considering the Effects of Shear Deformation and the Geometric Non-Linearity in Plate Bending, L. Palermo Jr.

CST-195 A Numerical Study on Magneto-Hydrodynamic Mixed Convection Flow C. Bozkaya

CST-197 Composite Bars subject to Uniform Torsion with Deformable Shear Connection using the Boundary Element Method, V.G. Mokos and E.J. Sapountzakis

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P7.20 **Subsurface damaged layer reduction with atomic force microscope scratch nano machining on optical fiber end plane** **375V2**
S. Matsui[1], S. Umemura[1], and T. Sato[1]
[1]Department of Mechanical Science and Engineering, Chiba Institute Technology, Japan

P7.21 **Surface formation during micromilling of ultrafine grained low carbon steel** **379V2**
C.L.F. Assis, R.G. Jasinevicius, R.T. Coelho
University of Sao Paulo, Brazil

P7.22 **Proposal of high performance eco-friendly (water soluble) coolant utilizing strong alkali ion water** **383V2**
Manabu Iwai[1], Masahide Yamada[2], Haruhisa Yamada[2], Kiyoshi Suzuki[3]
[1]Toyama Prefectural University, Japan
[2]Yamada Machine Tool Co., Ltd, Japan
[3]K.Suzuki New R& D Office, Japan

P7.23 **A novel approach to cutting force modelling in diamond turning and its correlation analysis on tool wear** **387V2**
Worapong Sawangsri[1], Kai Cheng[1], Hui Ding[2]
[1]School of Engineering and Design, Brunel University, UK
[2]School of Mechatronic Engineering, Harbin Institute of Technology, China

P7.24 **Characterization of positive and negative pulses from a commerial RC based pulse generator in micro-EDM milling** **392V2**
J.Wang[1], E. Ferraris[1], M. Galbiati[2], J.Qian[1], D.Reynaerts[1]
[1]Department of Mechanical Engineering, University of Leuven, Belgium
[2]Sarix SA, Sant'Antonino, Switzerland

P7.25 **Friction controlled precision positioning** **396V2**
Oscar S. van de Ven, Jo W. Spronck, Robert H. Munnig-Schmidt
Delft University of Technology, The Netherlands

P7.26 **Tuning vibration frequencies with shape memory alloys in precision engineering applications** **400V2**
Roderick Melnik[1], Ali Sebetci[2], and Linxiang Wang[3]
[1]M[2]NeT Laboratory, Wilfrid Laurier University, Waterloo,Canada
[2]Department of Mechanical Engineering, Mevlana University, Konya, Turkeyy
[3]Department of Ocean Science and Engineering, Zhejiang University, China

P7.27 **A holistic approach for µEDM milling on SLMed steel** **404V2**
Jun Qian, Karolien Kempen, Jun Wang, Fei Yang, Dominiek Reynaerts
Department of Mechanical Engineering, KU Leuven, Belgium

Tuning vibration frequencies with shape memory alloys in precision engineering applications

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Keywords: shape memory alloys, vibration tuning, frequency adjustment, precision engineering, nanotechnological applications

Abstract

Shape memory alloys (SMAs) are used widely in a range of applications, including precision engineering, state-of-the-art bio-medical and nanotechnologies. In precision engineering, these materials are used, for example, for automatic alignment of optical systems. In SMA actuators, we often use hysteresis compensation for high-precision positioning, so that SMAs can be applied for control and vibration tuning of various structures. In vibration tuning in many of these applications, it is often necessary to apply supplementary oscillators to absorb the vibration energy input into the primary system. In this contribution we highlight how, due to the thermo-mechanical coupling, the vibration characteristics of the supplementary oscillator can be tuned by changing its temperature. The basis is our dynamic nonlinear model of SMA oscillator which has been simplified for the vibration analysis. At low temperatures, the SMA oscillator behaves as a regular damper by using its dissipation due to mechanically induced phase transformations.

1. Coupling primary and adaptive systems

The limitation of the linear mass-spring oscillator used for the vibration absorption and in similar technological applications lies with the fact that it only works when the excitation frequency is known and close (or, ideally, equal) to the natural frequency of the primary system. For many engineering structures, both such frequencies might not be known a priori [1,2]. In such cases, adaptive oscillators with adjustable stiffness would be beneficial in order to tune (and ultimately to control) the vibrations so that the natural frequency of the oscillator can be adjusted to match the resonance

frequency of the primary system. Due to their thermo-mechanical coupling properties, shape memory alloys are promising materials for these purposes.

These advanced materials have already been applied to the adaptive vibration absorption (e.g., [2,3] and references therein), in precision engineering, and in nanotechnological applications [4]. The unique properties of SMAs lead to hardening the elastic modulus of the material at higher temperature (in the austenite state) and to its softening at lower temperature (in the martensite state). When the temperature is continuously adjusted, the elastic modulus of the material will be changing accordingly. Therefore, the thermo-mechanical coupling of SMAs provides a way to adjust the frequency response of vibration absorbers for adaptive vibration tuning. Previous results on the technological applications of SMA (composite) beams showed that the frequency of the oscillator using such beams can be adjusted in a range of 15% (see [3] and references therein).

Up to date, most studies in this field relied on mono-frequency or harmonic assumptions. If one considers the vibration tuning in more realistic situations, where the excitation frequencies may not necessarily be mono-frequency or harmonic and the primary system itself may be nonlinear, then the adaptive vibration absorber designed according to the standard frequency analysis might not be a suitable choice. Indeed, in this case vibration tuning should be implemented by taking energy dissipation into account, ensuring stability and robustness of the system, because of the energy dissipation driven vibration attenuation. In order to exploit the application potential of SMAs in vibration tuning, precision engineering and similar applications, in this contribution we take into account both key SMA properties: the thermo-mechanical coupling and the hysteresis induced by phase transformations. The main ideas are explained on an example of a SMA rod with an end-mass as a vibration absorber [3]. We emphasize that when supplementary oscillators are used in the applications of interest here, we often have to deal with a situation where the primary vibration frequency is not known a priori. In such cases, we have to design a robust supplementary oscillator such that it is able to operate in a rather wide range of frequencies. A SMA-based oscillator is an ideal candidate for these purposes. Hence, we propose a dynamic nonlinear model and its numerical realization for using SMA oscillators as vibration absorbers and in other relevant applications. To model the vibration tuning, the vibration of the primary system and the attached oscillator

should be considered simultaneously. To do so, we formulate the governing equations for the entire system as in [3].

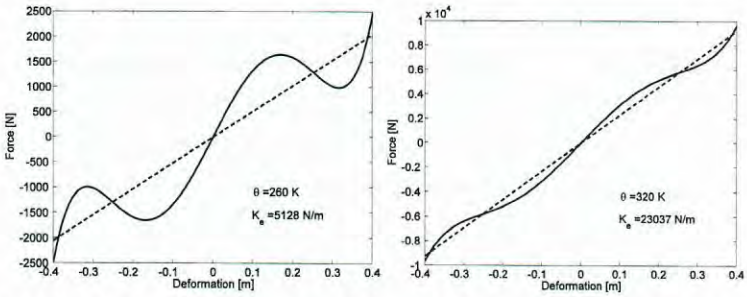

Fig. 1: Typical force-deformation relations of a SMA rod (260K and 320K).

2. Shape memory alloy dynamics for precision enegineering applications

In order to make the dynamic problem tractable in engineering applications, a dimensional reduction of the fully coupled dynamic three-dimensional model for shape memory alloys has been proposed (see [3] and references therein). The reduced model was approximated by a system of differential-algebraic equations and was applied to the modelling of SMA-based devices such as actuators.

The dependency of the dynamics of the mechanical field on the temperature is included in the proposed formulation. Recently we demonstrated that this model is able to capture the thermo-mechanical coupling effects and the first order phase transformations in SMA rods (see [3] and references therein). However, the main difficulty in applying this model to the analysis of vibration tuning in the context of our present problem is that the dynamic response simulation (accompanied by the simulation of phase transformations and wave propagations in the SMA rod) is computationally too costly for most engineering problems. Following [3], we explain here how to overcome this difficulty.

When the primary system is vibrating with unknown multiple frequencies, supplementary oscillators normally will not perform well by tuning their own natural frequencies in this case, because one supplementary oscillator can absorb only the vibration energy of a single frequency component which matches with the supplementary oscillator, with no effects (or very minor effects) on other frequency components. When the SMA oscillator is used in this case, it could be tuned to work

in its low temperature range in which the martensite transformations could be induced. However, such martensite transformations and martensite re-orientations are always accompanied by mechanical energy dissipation, and as a result, abroad-band vi- bration attenuation might be induced. In this case, the mechanism of vibration suppression will be different from that of attaching supplementary oscillators. The interested reader is referred to [3] (and references therein) for further discussion on vibration damping by using the mechanically induced phase transformations in SMAs in a situation described above.

The important results of our study include our proposed dynamic nonlinear model for SMA-based oscillators in the vibration absorption and precision engineering applications, as well as the evaluation of the performance of such oscillators. An essential part of such oscillators - the SMA rod - is modelled on the basis of the Ginzburg-Landau theory. The resulting nonlinear model accounts for both thermo-mechanical coupling and hysteresis effects induced by phase transformations. Numerical simulations, carried out for various excitation frequencies, demonstrate that the SMA vibration absorber could be adaptive in a sense that it could be adjusted to match different frequencies by changing its temperature. In particular, based on estimated values of temperature for the vibration absorption, our results show that the vibrations of the primary mass block are successfully attenuated by using the SMA absorber. In the general case, due to nonlinearity of the force-deformation relation (see Fig. 1), the best temperature for the vibration absorption should be found by using an appropriate optimization procedure. We conclude by a discussion of SMAs in nanotechnological applications in the context of [4].

Acknowledgments: RM and AS are grateful to TUBITAK for its support.

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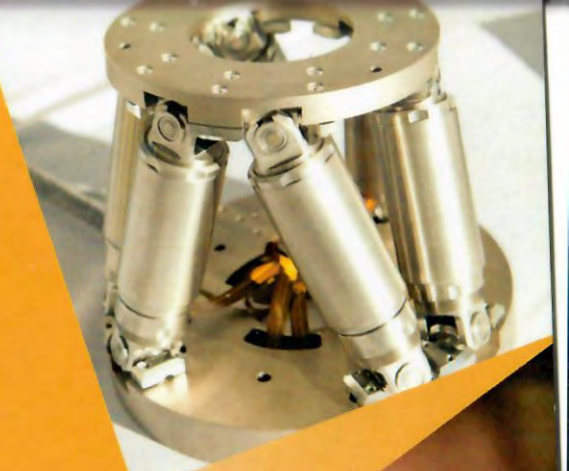

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Nanostructures with Shape Memory Effect: Modelling Coupled Dynamics

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***Abstract* — In this contribution we apply a phase-field (PF) modeling approach for the analysis of properties of shape-memory alloy (SMA) nanostructures, focusing on their complex microstructures and thermo-mechanical behavior. We have developed a model that includes domain walls, treated as a diffuse interface, which leads to a fourth-order differential equation in a strain based order parameter PF model. Arising numerical challenges have been overcome based on the isogeometric analysis (IGA). Microstructure evolutions for different geometries of SMA nanostructures under temperature- induced phase transformations have been studied and some typical examples are presented here.**

Keywords* — *Ginzburg-Landau theory; isogeometric analysis; phase- field models; nonlinear thermo-elasticity; low dimensional nanostructures; coupling

I. Introduction

There has been an increasing interest in using SMA nanotubes and other low dimensional nanostructures for nano-electromechanical (NEMS) and micro-electromechanical systems (MEMS), various engineering systems and devices, as well as for biomedical applications [1, 2]. These applications involve designing different geometries and using domain patterns for controlling distortions. In its turn, this motivates the need for a better of understanding of domain patterns and their thermo-mechanical properties in realistic and complex geometries for application development.

Among modeling approaches that have been used to study SMA dynamics [3, 4], we would like to especially emphasize the phase-field (PF) approach. Indeed, PF-based models have been used to study the phase transformations in SMA meso- and nano- structures [5, 6]. Broadly speaking, the PF models for SMAs can be divided into two groups. One is based on the kinetic model by using independent order parameter(s) (OPs). The second group combines the strain-based OP PF models. The implementation of models from the first group typically leads to models based on second-order differential equation(s) for microstructure evolution, while the implementation of models from the second group requires dealing with fourth-order differential equations in space. Due to strong (hysteretic-type) nonlinearities and coupling with structural and/or thermal physics, this leads to several computational challenges in both of these cases. The fourth order equations, in particular, introduce a number of especially severe numerical challenges such as restrictions on the time-step (for discretization) and stencil (or grid) size [7].

Most of the above studies were carried out using traditional numerical methods, such as spectral collocation or the finite difference method. These methods typically lack geometrical flexibility, and most of the simulations based on these methods were performed on a cubic domain with periodic boundary conditions. However, other geometries become increasingly important in applications of SMAs, and there is a need for more flexible methods which can allow to model complex bigger domains with different boundary conditions. Another difficulty we face when designing computational methods for strain-based OP PF theories is to find an efficient discretization procedure for fourth-order spatial differential operators. Due to its geometrical flexibility and the possibility of generating globally smooth basis functions, we propose isogeometric analysis (IGA) as an efficient numerical method to solve the fourth-order PF model on various geometries.

IGA is a new computational method originally developed to avoid mesh generation bottle-necks during engineering analysis. It uses non-uniform rational B-splines (NURBS), a back-bone of CAD and animation technology, as basis functions. The use of rich basis functions provides the IGA with a unique capability to model geometry exactly, in many instances, while field variables can be approximated with enhanced accuracy. The IGA provides unique attributes of higher-order accuracy and robustness with the C 1- or higher-order continuity necessary for solving higher-order differential equations. The IGA has been successfully used to solve models based on the PF theories and higher-order differential equations (see [8, 9, 10] and references therein).

In this contribution we apply the IGA to study SMA nanostructures. Our PF model has been developed on the basis of the Ginzburg-Landau theory and consists of coupled equations of nonlinear thermoelasticity. The governing laws are introduced in the IGA framework using the variational formulation.

II. Mathematical Model

All our results here are exemplified on the cubic-to-tetragonal phase transformations that occur in SMA alloys like

NiAl, FePd, InTl, etc. The cubic austenite phase is converted into tetragonal martensitic variants upon mechanical or thermal loadings (see Fig. 1).

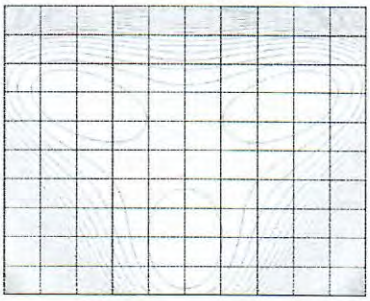

Fig. 1. Typical minima of the free energy function that corresponds to cubic-to-tetragonal phase transformation.

We have recently developed a mathematical model for the three-dimensional coupled thermo-mechanical analysis of SMAs [9, 10]. Our model has been derived from a free-energy functional using the Hamiltonian principle. Components of this functional in the 3D case are:

$$\begin{aligned}
\mathscr{F}_{nop/op} &= \frac{a_{31}}{2}\left[e_1 - E_0(e_2^2 + e_3^2)\right]^2 + \frac{a_{36}}{2}\left[e_4^2 + e_5^2 + e_6^2\right], \\
\mathscr{F}_{op/op} &= \frac{a_{32}}{2}\tau(e_2^2 + e_3^2) + \frac{a_{33}}{2}e_3(e_3^2 - 3e_2^2) + \frac{a_{34}}{2}(e_2^2 + e_3^2)^2, \\
\mathscr{F}_{gradient_{op}} &= \frac{k_g}{2}\left[(\nabla e_2)^2 + (\nabla e_3)^2\right],
\end{aligned}$$

where e_j are components of strain tensor and a_{ij} are material-specific coefficients.

The unknowns are the displacement field $u = \{u_1, u_2, u_3\}^T$ and the temperature θ. The problem is analyzed in the physical domain $\Omega \subset R^3$, which is an open set parameterized by Cartesian coordinates $x = \{x_1, x_2, x_3\}^T$. We use of the Cauchy-Lagrange infinitesimal strain tensor. The governing equations can be written as follows (see [9,10] for details):

$$\begin{aligned}
\dot{\mathbf{u}} &= \mathbf{v}, \\
\rho\dot{\mathbf{v}} &= \nabla\cdot\boldsymbol{\sigma} + \nabla\cdot\boldsymbol{\sigma}' + \boldsymbol{\sigma}_g + \mathbf{f}, \\
\rho\dot{e} - \boldsymbol{\sigma}^T : (\nabla\mathbf{v}) + \nabla\cdot\mathbf{q} &= g,
\end{aligned}$$

where the constitutive equations take the form:

$$\boldsymbol{\sigma} = \frac{\partial}{\partial e_{ij}}\left(\mathscr{F}_{nop} + \mathscr{F}_{op}\right), \qquad \boldsymbol{\sigma}' = \frac{\partial\mathscr{R}}{\partial\dot{e}_{ij}}, \qquad \boldsymbol{\sigma}_g = \frac{\partial}{\partial e_{ij}}\left(\mathscr{F}_{gradient}\right)$$

with the dissipation

$$\mathscr{R} = \frac{\eta}{2}\sum_{i=1}^{n}\dot{e}_i^2,$$

where v is the velocity and other notions are standard (see, e.g., [9, 10] and references therein).

III. Numerical Formulation

For its numerical implementation, the problem is reformulated in a weak form. We seek $S = \{u, \theta\} \in X$ such that $B(W, S) = 0$ for all $W \in X$, with

$$\begin{aligned}
B(W,S) = &\left(U, \frac{\partial u}{\partial t}\right)_\Omega + \left(V, \rho\frac{\partial v}{\partial t}\right)_\Omega + \left(\Theta, c_v\frac{\partial\theta}{\partial t}\right)_\Omega - (U, v)_\Omega \\
&+ (\nabla V, \sigma)_\Omega + (\nabla V, \eta v)_\Omega - (V, f)_\Omega + \left(V, \sigma_g\right)_\Omega \\
&+ (\nabla\Theta, \kappa\nabla\theta)_\Omega - (\Theta, g)_\Omega - (\chi_d)_\Omega,
\end{aligned}$$

where the interested reader can consult [9, 10] for additional details.

For the space discretization of the model we have used the Galerkin with the NURBS basis functions. We have also used the generalized-α method for time integration. This method has already found a wide range of applications in the computations where control over high frequency dissipation is useful, such as, for example, nonlinear structural dynamics and turbulence (e.g., [8] and references therein). We also note that it has been applied (in the IGA framework) for the computations of other nonlinear models such as the Cahn-Hillard equation and the isothermal Navier-Stokes-Korteweg equation. Here, we also take advantage of the fact that generalized-α methodpermits a straightforward one-step discretization of a coupled system of first- and second-order ordinary differential equations, which is precisely the structure of our semi-discrete form.

IV. Results And Discussion

In this section, we present numerical studies on nanostructured SMAs subjected to temperature induced loadings. The microstructure evolution and its effect on thermo-mechanical properties in SMA specimens have been analyzed. The developed thermo-mechanical model described has been rescaled in the spatio-temporal domains for numerical convenience, and the rescaled equations have then been converted into the rescaled weak formulation, as described in the previous section. The scaling constants for the spatial and temporal domains are 1.2645 nm, and 0.901 ps, respectively. All calculations presented here have been carried out for $Fe_{70}Pd_{30}$.

As mentioned earlier, applications exist where different geometries are required, often beyond cubic domains. While we carried out a series of numerical experiments for different nanostructured SMA geometries, we provide here typical examples for slab geometries. For the thermal physics, insulated boundary conditions have been used for all the simulations. We discretized the domains using B-spline or NURBS basis functions with C^k global continuity for $k \geq 1$.

Firstly, we performed a refinement study of the spatial mesh, holding the time step fixed at a sufficiently small value. The spatial mesh has been refined using the classical h-refinement and the new paradigm for mesh refinement introduced by IGA, k-refinement, in which the order of the basis functions is elevated, but their global continuity is likewise increased. The mesh convergence studies have been carried out on a cube with its side equal to 32nm, periodic boundary conditions and starting with initial random conditions. The cube was discretized using three meshes: two meshes with uniform

C^1-continuous quadratic B-spline with 34 and 50 basis functions in each direction and third mesh with uniform cubic C^2-continuous B-splines with 69 basis functions in each direction. Then, the cube was quenched to (non-dimensional) temperature corresponding to $\tau = -1.2$ and allowed to evolve for a sufficiently long time till it was stabilized. We analyzed the cut lines of OP deviatoric strains e_2 and e_3 along the normalized distance $\hat{x}$ between two points (0,15,15) nm and (32,15,15) nm on the opposite surfaces of the cube, for all three meshes. The maximum error of the coarsest mesh is 2 % with respect to the fine mesh, thus indicating that good results can be obtained by using the IGA even with the coarsest mesh.

Secondly, we analyzed the impact of the time step size on the solution holding the spatial discretization fixed. The simulations have been performed on a cube with its sides equal to 50 nm by using periodic boundary conditions and starting with an initial random condition. We have used three different fixed time steps 0.225 ps, 0.4505 ps, and 0.901 ps. Cut lines of the OPs e_2 and e_3 have been analyzed along the diagonal (0,0,0) – (50,50,50) nm, at time 0.427 ns, and the time evolution of the average temperature coefficient τ was studied. The maximum error in the OPs of the largest time step (0.901 ps) with respect to the smallest one (0.225 ps) is just 0.02 %. Hence, the largest time step can be safely used.

Finally, we generated a thermally induced microstructure in SMA specimens of different geometries, by quenching them to the temperature corresponding to $\tau = -1.2$ and allowing the system to evolve. All the simulations have been started with a small amplitude random initial condition, corresponding to the austenite phase, for the displacement vector u. Periodic, constrained or stress-free boundary conditions have been used on different surfaces for the structural physics. Our example is for a slab geometry which was discretized using uniform C 1- quadratic B-spline basis functions (while for other geometries, e.g. the cylindrical tube and tubular torus, we used the NURBS basis functions).

Now, if the domain size is reduced to half in one of the directions ($L_{x1} = L_{x3} = 60$ nm and $L_{x2} =$ nm) and microstructures are allowed to evolve in the slab domain, we obtain morphology evolution as shown in Fig. 2. The three variants exist in approximately equal proportions forming chevron patterns as shown in the last sub-plot of Fig. 2. The microstructure in slab domain (the last sub-plot) is morphologically different than the cube domain. The primary bands of M_1 and M_3 variants are prominent and intersected by a thin secondary band of the M_2 variant at 90^0. The width ratios of primary and secondary bands are in agreement with the cube specimen. These results clearly demonstrate the influence of geometry on microstructure evolution and morphology in SMA nanostructures.

Fig. 2. (Color online) Microstructure morphology evolution in a slab specimen with $L_{x1} = L_{x3} = 60$ nm and $L_{x2} = 30$ nm at time t (red, blue, and green colors represent M_1, M_2, and M_3 variants, respectively). (a) t = 0.036 ns, (b) t = 0.09 ns, (c) t = 0.18 ns, (d) t = 0.27 ns, (e) t = 1 ns

V. Conclusions

We have applied a newly developed phase-field model in the analysis of properties of shape memory alloy nanostructures, paying a special attention to complex microstructure evolution and coupled thermo-mechanical behavior. Since the model includes domain walls, treated as a diffuse interface, we had to deal with high order derivatives in our strain-based order parameter phase-field model. This led to a range of computational difficulties which were overcome by using the isogeometric analysis. Shape memory alloy nanostructures of different geometries were studied with the major focus given to microstructure evolution, and some typical examples of these studies were presented. These results can be used in coupling thermo-mechanical properties with band structure studies of shape memory alloy nanostructures, leading to more precise prediction of optoelectronic properties of these structures for application development.

Acknowledgement

RD and RM have been supported by NSERC and CRC program, Canada, and JZ by NSERC. RM and AS have been supported by TUBITAK. HG was partially supported by the European Research Council through the FP7 Ideas Starting Grant program (project #307201) and by Conseller´ıa de Educaci´on e Orde- naci´on Universitaria (Xunta de Galicia). Their support is gratefully acknowledged.

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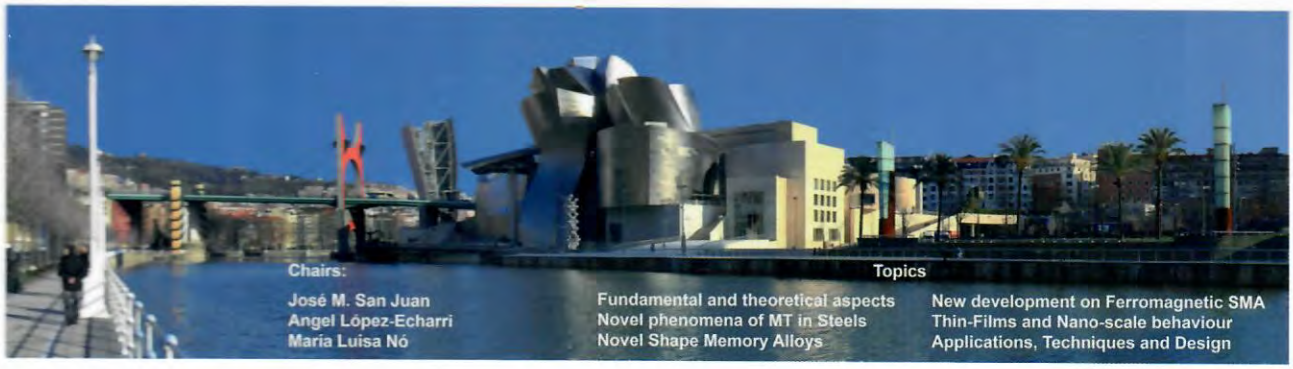

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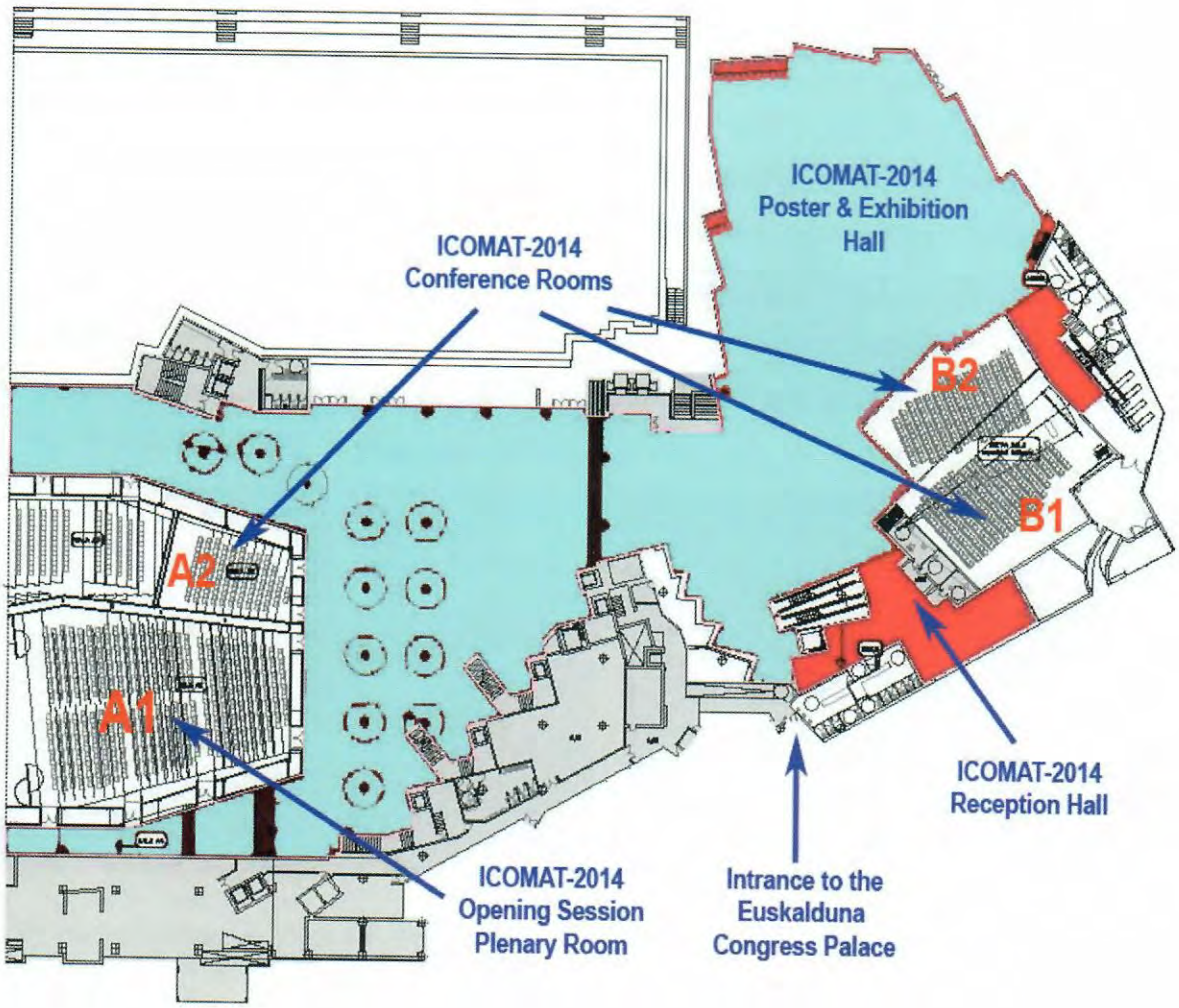

T8-O.06

(356)

Ti-Ta high-temperature shape memory thin films

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High temperature shape memory alloys (HTSMAs) are promising materials for actuators operating above 100°C, such as in aerospace, automobile, home appliances and energy industries. Recently, Ti-Ta based alloys have attracted attention as potential HTSMAs. These materials are in a group of β-type Ti based alloys with excellent cold workability; therefore they can be easily deformed into sheets, wires, springs and small objects suitable for a range of applications. Ti-Ta shape memory alloys were studied as bulk materials but their fabrication as thin films was not reported so far. In thin-film form, these materials could also be used as high-temperature actuators in micro-electro-mechanical systems (MEMS). In this study, Ti 30, 32, 33 and 45 at.% Ta films (~ 4μm) were fabricated by magnetron co-sputtering of pure Ti and Ta at room temperature. The formation of disordered α" martensite was confirmed in Ti 30, 32 and 33 at.% as-deposited thin films. For the first time, a reversible martensitic phase transformation and a shape memory effect at temperatures >100 °C were reported in Ti-Ta thin-films.

T8-O.07

(073)

Strain rates in SMA nanowires: 3D coupled model based on isogeometric analysis

R. Dhote[1,2], R.V.N. Melnik[2], H. Gomez[3], J. Zu[1]

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[2]*M2NeT Lab, Wilfrid Laurier University, Waterloo, ON, Canada*
[3]*University of Coruna, Coruna, Spain*
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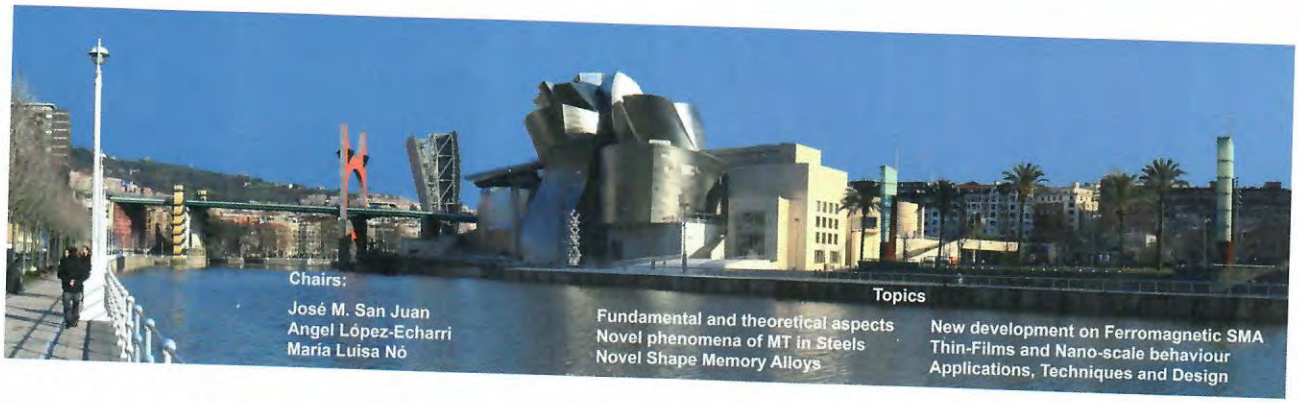
This contribution focuses on the thermo-mechanical behavior of shape memory alloy (SMA) nanowires subjected to different strain rates. We study the microstructure evolution and the properties of SMAs nanowires, as a function of microstructure, by using the developed 3D thermo-mechanical model [1]. The model, based on the phase-field approach and Ginzburg-Landau theory, has a strong material non-linearity, thermomechanical coupling, and higher-order differential terms and present substantial challenges for numerical simulation. We use the isogeometric analysis, that offers several advantages in solving complex problems with higher-order differential terms [2]. The SMA nanowires have been subjected to three different strain rates. The effect of strain rates on the thermo-mechanical behavior of the nanowires is observed due to the coupled dynamics, loading rate and motion of the domain walls. The transient microstructures and mechanical properties are in accordance with the crystallographic theory and experimental results.

[1] R. Dhote, H. Gomez, R. Melnik, and J. Zu, Isogeometric Analysis of Coupled Thermo-Mechanical Phase-Field Models for Shape Memory Alloys Using Distributed Computing, Procedia Computer Science, 18, pp. 1068–1076, 2013.

[2] R. Dhote, H. Gomez, R. Melnik, and J. Zu, 2014. Isogeometric analysis of a Dynamic Thermo-Mechanical Phase-Field Model Applied to Shape Memory Alloys, Computational Mechanics, to appear.



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	THURSDAY 10
Time	**Session 20 - Room B2** **Topic 8: Thin Films and Nano-scale behaviour** **Chairman:** Prof. Eckard Quandt. Christian-Albrechts-University of Kiel, Germany
8:30 – 9:10 **T8-I.01**	**Invited Lecture T8-I.01: Dr. Akira Ishida** **Application of the sputtering method in the study of shape memory alloys** National Institute for Materials Science, Tsukuba, Japan (27)
15:30 - 15:50 **T8-O.07**	**Strain Rates in SMA Nanowires: 3D Coupled Model Based on Isogeometric Analysis** *Rakesh P. Melnik, Roderick Melnik, Hector Gomez, Jean W. Zu* Wilfrid Laurier University, Canada (73)
9:30 - 9:50 **T8-O.08**	**Microstructure and martenstic transformation of nanocrystalline Ni-Mn-Ga-Gd high temperature shape memory alloy thin films** *Jian Yao, Wei Cai, Jiehe Sui, Z.Y. Yang* Harbin Institution of Technology, China (106)
9:50 - 10:10 **T8-O.09**	**Magnetic Properties of Ni-Mn-Ga Films Fabricated as Microdots** *Jeff Huntsinger, K. Wilson, A. Thompson, P. Lindquist, B. Knowlton, Peter Müllner* Boise State University, United States (273)
10:10 - 10:30 **T8-O.10**	**Thermomagnetic Actuation in Low Hysteresis Metamagnetic Ni-Co-Mn-In Films** *Marcel Gueltig, Makoto Ohtsuka, Hiroyuki Miki, Kohki Tsuchiya, Toshiyuki Takagi, Manfred Kohl* Karlsruhe Institute of Technology (KIT), Germany (208)
10:30 – 11:00	**Coffee Break**

11:00 – 13:00	Following: Session 23 - Room B2

Civil-Comp Proceedings: 105

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64 A Hybrid Grid System for a Spectral Wave Model
N. O'Brien and E. Ragnoli

Materials and Damage Modelling

65 Modelling of Heat Flow through a Three-Dimensional Crack in Thermoelasticity
J. Jaśkowiec

66 The Influence of Thermo-Mechanical Effects on the Relaxed Shape Graphene
S. Prabhakar, R. Melnik and A. Sebetci

67 A Coupled Thermo-Mechanical Cohesive Crack Model in Three-Dimensional Crack Growth Analysis
J. Jaśkowiec

68 Localization Analysis of an Anisotropic Damage Model
M. Jirásek and F. Suárez

Fluid Flow Problems

69 Application of Asymptotic Analysis to Derive a Time-Averaged Shallow Water Model
J.M. Rodríguez and R. Taboada-Vázquez

70 Classification of Regimes of the Stratified Fluid Flows around a Square Cylinder
P.V. Matyushin and V.A. Gushchin

71 Stabilized Galerkin-Characteristics Finite Element Schemes for Flow Problems
H. Notsu and M. Tabata

72 Acceleration of Sampling Methods for Uncertainty Quantification in Computational Fluid Dynamics
C.W.T. Thiem and M. Schäfer

73 An Experimental and Numerical Study of Gas Flow Laminar in a Thermal Reactor
A. Bellil, K. Benhabib, P. Coorevits, C. Marie, M. Hazi and A. Ould-Dris

74 Optimization of the GDI Engine Operation with Stoichiometric Mixtures using Numerical Modeling
S. Boccardi, F. Catapano, M. Costa, P. Sementa, U. Sorge and B.M. Vaglieco

75 Meshless Solution of Incompressible Flows in Complex Domains
G. Kosec

76 Leak Before Break Analysis using a New Enriched Finite Element
P.J. Gill and K. Davey

Fluid Structure Interaction

77 A Spectral-Element Simulator for Two-Dimensional Rigid-Body-Fluid Interaction Problems
L.-C. Chen and M.-J. Huang

78 Simulation of Cavitating Nonlinear Acoustic Fluid and Flexible Structure Interaction
F. Kalateh

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Paper 66

The Influence of Thermo-Mechanical Effects on the Relaxed Shape Graphene

S. Prabhakar[1], R. Melnik[1] and A. Sebetci[2]
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Keywords: armchair and zigzag graphene, electromechanical effects, finite element method.

In this paper, we consider a two-dimensional graphene sheet with armchair and zig-zag edges. We investigate the influence of temperature on the in-plane oscillations of the strain tensor in this graphene. We show that the in-plane oscillations of the strain tensor are enhanced with temperature.

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A. Cordero, R.G. Citarella, M. Stoschka, S. Mohasseb and J. Geiser

This book contains the summaries of the contributed papers presented at the Ninth International Conference on Engineering Computational Technology, held in Naples, Italy, 2-5 September 2014.

The full length papers are available online at: www.CTResources.info

Keyword and author indices are provided in this book.

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composition variation has been accompanied by the changes non-monotonously of the intensity and peak position of InAs QD emission. Numerical simulations of HR-XRD results have shown that the level of elastic strains and the composition of quantum layers vary none monotonously in studied QD structures as well. The numerical simulation of HR-XRD diagram has shown that the composition varies due to the process of Ga/In inter diffusion at the $In_xGa_{1-x}As$/InAs QD interface. Then the variation of the energy band gap due to the different levels of elastic strains in InAs quantum dots has been calculated and compared with the experimentally measured PL peak positions in studded structures. The physical reasons of the mentioned optical and structural effects and their dependence on capping layer compositions have been discussed.

S13-05

Manifestation of the anticrossing effect in the optic spectra of quantum dots PbS

Vladimir A. Gaisin[a] and **Boris C. Kulinkin**[b]

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[b]*First Pavlov State Medical University of St. Petersburg. Lev Tolstoy str., 6/8, Saint Petersburg, 1907022, Russia*

Quantum dots of the crystal PbS were studied. The absorption spectrum lines were divided into separate components. The dependences of the transition energy on the square of the quantum dots inverse radius were built. An anti-crossing effect was discovered. The lines are interpreted as a result of exaction transitions that are formed between the levels of dimensional quantization of the holes in state at n=1, 2… and the same state of the dimensional state of the electron at n=1.

S13-06
Computational Models for the Berry Phase in Semiconductor Quantum Dots

S. Prabhakar and **R.V.N. Melnik**

M2NeT Lab, Wilfrid Laurier University, 75 University Ave W, Waterloo, ON, Canada N2L 3C5

By developing a new model and its finite element implementation, we analyze the Berry phase low-dimensional semiconductor nanostructures, focusing on quantum dots (QDs). This phase is induced by letting the quantum dots to move adiabatically in a closed loop in the 2D plane along the circular trajectory. Therefore, we solve the Schr¨odinger equation

and investigate the evolution of the spin dynamics during the adiabatic transport of the QDs in the 2D plane along circular trajectory. Based on this study, we reveal that the Berry phase is highly sensitive to the Rashba and Dresselhaus spin-orbit lengths. We discuss the results of computational modeling of Berry phase low-dimensional semiconductor nanostructures and highlight why this work might be used for the realization of solid state quantum information processing.

S13-07

Modelling of efficiency of hydrophobic Drug encapsulation on Liposomes

C.R. González Vargas[1], L. Guzman Vargas[1], and J. Douda[1]

[1]*UPIITA – Instituto Politécnico Nacional, Othón Mendizábal S/N, La Escalera, 07320, México D. F., México*

In recent years liposomes have been used extensively for medical and pharmaceutical fields [1]. The efficiency of hydrophobic drug encapsulation on liposomes depends on various factors, like its hydrophobic bilayer volume for efficient water insoluble drug encapsulation, chemical and rheological stability of formed systems. The paper presents the study of lecithin and its poly-ethylene glycol (PEG) derivatives liposomes prepared for hydrophobic drug encapsulation. The liposomes have been investigated by microscopic and optic methods for evaluation of its capability for drug encapsulation. The modelling of efficient drug encapsulation on liposomes vas investigated.

S13-08
LIPOSOMES FOR QUANTUM DOTS ENCAPSULATION

J. Douda[a], C.R. González Vargas[a], and J.L. Casas Espínola[b]

[a]*UPIITA – Instituto Politécnico Nacional, 07320, México D. F., México;*
[b]*ESFM – Instituto Politécnico Nacional, México D. F. 07738, México*

Semiconductor quantum dots (QDs) have been extensively used for biomedical applications as efficient biomarkers. The liposome encapsulation presents an alternative method for quantum dots labeling to facilitate intracellular delivery of the QDs systems.
The semiconductor CdSe/ZnS core/shell quantum dots of two different emission wavelengths (530 and 640nm) were encapsulated with lecithin and its polyethylene glycol derivatives liposomes. The liposomes were prepared using a "chemically green" method: by sonication and freezing-unfreezing procedure and without organic solvents application. The liposomes were studied by atomic force microscopy (AFM) and photoluminescence (PL) spectroscopy before and after quantum dots encapsulation. The liposome encapsulation of core/shell quantum dots is effectively reflected in the changes of

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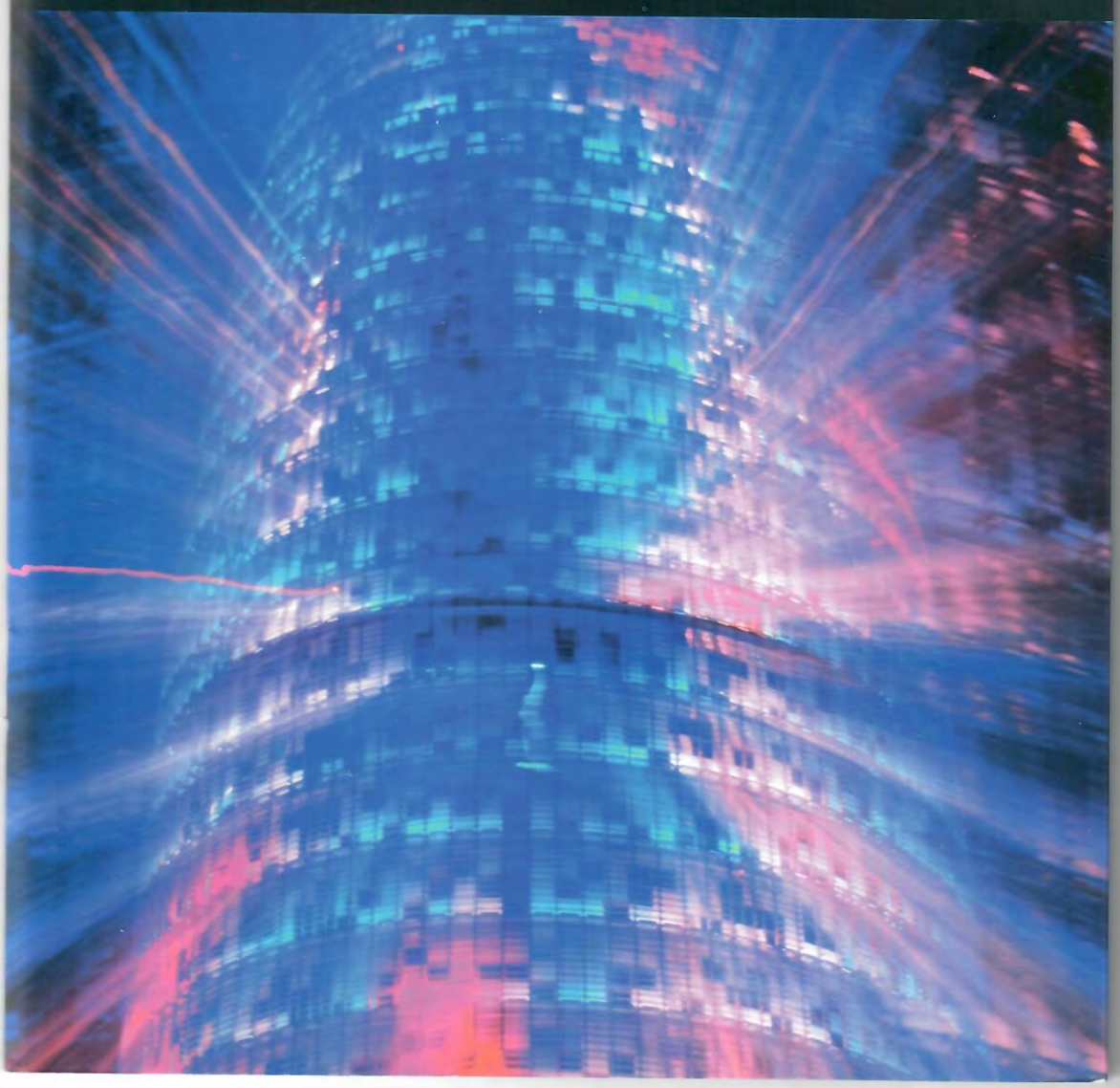

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Applications of Shape Memory Alloys in Structural Control (II)

(Special Session organized by Sara Casciati and Vicenç Torra)

WeE02
Room: VS213
Chair: Vicenç Torra
CoChair: Sara Casciati

Feasibility of Self-Post-Tensioned Concrete Bridge Girders using Shape Memory Alloys
O. Ozbulut, M. Sherif, R. Hamilton and A. Lanba

Coupled Multi-dimensional Models for Shape Memory Alloy Nanostructures: Microstructure Evolution in Nanofilms
R. Dhote, R. Melnik, H. Gomez, A. Sebetci and J. Zu

External Temperature Effects on the Hysteresis of NiTi Wires in Dampers for Stay-Cables
V. Torra, G. Carreras, C. Auguet and S. Casciati

Fatigue Performance of Ni-Ti SMA Wires
S. Casciati, L. Faravelli and M. Vece

Dynamics of Stress-Strain and Temperature Evolutions in Cyclic Phase Transition of NiTi Shape Memory Alloy: Experiment and Modelling
Q. Sun, H. Yin, M. Li and M. Chen

Simulation of Basic Properties of SMA by a Compact Macroscopic Phenomenological Model with Few Internal Variables
M. Evard, S. Mikhailova and A. Volkov

Advances in Data Acquisition and Processing Techniques for Health Monitoring of Civil Infrastructure (II)

(Special Session organized by Satish Nagarajaiah and Agathoklis Giaralis)

WeE03
Room: VS214
Chair: Jerome Lynch
CoChair: Eleni Chatzi

(INVITED Lecture) **Compressive Measurement Bounds for Wireless Sensor Networks in Structural Health Monitoring**
J.Y. Park, A.C. Gilbert and M.B. Wakin

Assessment of Compressive Spectral Estimation Techniques for Vibration-Based Structural System Identification and Condition Assessment Applications in the Presence of Noise
B. Tau Siesakul, K. Gkoktsi and A. Giaralis

A Hybrid Evolution Strategy approach to the Structural Identification Problem Via State-Space Models
V. Dertimanis and E. Chatzi

Data-Driven Approaches for Output-only Modal Identification, Damage Detection, and Data Compression and Cleansing by Blind Source Separation and Sparse Representation
S. Nagarajaiah and Y. Yang

Non-Destructive Evaluation of Chloride-Induced Corrosion in Reinforced Concrete: Electrochemical Impedance Spectroscopy Sheds New Light on the Performance of Commonly Applied Sensors
F. Pargar, D.A. Koleva, O. Copuroglu1, E.A. Koenders and K. van Breugel

PREFACE

This volume contains the Technical Program and full papers on CD Rom of the works presented at the Sixth World Conference on Structural Control and Monitoring, 6WCSCM, Barcelona, Spain, July 15 – 17, 2014.

6WCSCM is the 6th edition of the World Conference of the International Association for Structural Control and Monitoring (IASCM), hosted by the Universitat Politècnica de Catalunya-BarcelonaTech (UPC) under the auspices of the European Association for the Control of Structures (EACS).

The WCSCM is a premier leading conference devoted to the theoretical, numerical, experimental and practical advancements of monitoring and control technologies for dynamic structures in a wide range of civil, infrastructure, mechanical, aerospace and energy systems. This new edition will have gathered an international community contributing to the state of the art in such multidisciplinary scientific and engineering environment with new results, fresh ideas and future perspectives.

Previous editions of the conference were held in Pasadena - USA (1994), Kyoto - Japan (1998), Como - Italy (2002), La Jolla - USA (2006) and Tokyo - Japan (2010), with an increasing number of participants in each edition. 6WCSCM has attracted over 375 participants, coming from all over the world. All together around 400 lectures will have been presented, including 6 plenary lectures, which reflect the current state of the research and advances in the field.

The organizers would like to thank the authors for submitting their contributions and for their respect of the deadlines. Special thanks go to the colleagues who contributed to the organization of the 21 Special Sessions.

Barcelona (Spain) is a perfect environment for the 6WCSCM, being one of the most charming cities along the Mediterranean coast, which always offers the perfect environment for unforgettable events and plenty of enjoyable social, cultural and touristic opportunities.

In the name of the institutions and the human teams involved in the organization, we warmly hope the participants will have enjoyed the conference and the city. We also hope these proceedings will be a valuable open source of information and ideas for the future.

José Rodellar

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Barcelona, Spain

Alfredo Güemes

Univ. Politécnica de
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Eugenio Oñate, Xavier Oliver and Antonio Huerta (Eds.)

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CONTENTS

Greetings from the Co
Greetings from the Pr
Greetings from the Pr
Greetings from the Pr
Sponsors and Exhibit
Congress Venue .....
Organizers and Comm
Congress Information
Events .....
Moving Around in Bar
Scientific Program .....
Introduction .....
A short guide to the S
Program Overview.....
Invited Lectures .....
List of Minisymposia ..
List of Special Techno
List of Contributed Se
Poster Sessions.....
Technical Sessions....
Authors Index .....
Congress Schedule

25/07/2014 09:00 - 11:00
Computational Bioengineering II
Minisymposium organized by Suvranu De, Abdul I. Barakat, Sandra Rungonyi and Yusheng Feng

MS339B
Room: Business Centre II

An optimal design of artificial disc FE model for human Lumbar spine discs restoration
TaeKyeong Lee and JungHwa Hong

Development of robust elastic network model for predicting the experiment B-factor precisely
Min Hyeok Kim and Moon Ki Kim

Hemodynamic effects on tumor cell arrest at microvascular intersections
Peng Guo, Min Lei, Yang Liu and Bingmei M. Fu

Numerical analysis on two-phase vortex at microfluidic Y-junctions
Zhaomiao Liu and Likun Liu

Simulation of surgical cutting using a progressive cutting scheme and extended finite element method
Yi Ding, Stéphane P.A. Bordas, Paul Rosin and David Marshall

25/07/2014 09:00 - 11:00
Computational Modeling of Multiphysics/Multiscale Coupled processes in Biological and Nanotechnological Systems II
Minisymposium organized by Giovanna Guidoboni, Roderick Melnik and Riccardo Sacco

MS132B
Room: Sala de prensa I

Hemodynamics simulations in the cerebral venous network: Towards the understanding of blood flow in a complex geometry (Keynote Lecture)
Vincent Chabannes, Mourad Ismail, Christophe Prud'homme and Marcela Szopos

Retinal blood flow changes and vascular parameters and structure
Andrea Dziubek, Edmond Rusjan and William Thistleton

Theoretical analysis of the relationship between changes in retinal perfusion and tissue metabolic demand
Simone Cassani, Julia Arciero, Giovanna Guidoboni, Brent A. Siesky and Alon Harris

Mathematical modeling of bio-hybrid devices: Towards polymeric artificial retina
Matteo Porro, Sebastiano Bellani, Nicola Martino, Maria Rosa Antognazza, Maurizio Verri, Guglielmo Lanzani and Riccardo Sacco

Molecular dynamics studies of RNA nanotubes
Shyam Badu, Roderick Melnik, Maxim V. Paliy, Sanjay Prabhakar, Ali Sebetci and Bruce A. Shapiro

A two-layer model for drug delivery from a transdermal patch
Giuseppe Pontrelli

A mathematical model for an affinity-based drug delivery system
Martin Meere and Tuoi Vo

An innitiative of:

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In cooperation with:

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PROGRAMME

6th International Conference

PHYSICS OF LIQUID MATTER: MODERN PROBLEMS

PLM MP

Kyiv 2014

May 23-27, 2014
Kyiv, Ukraine

TOPICS OF THE CONFERENCE:

I Quantum liquids and solutions

II Molecular liquids, molecular solutions

III Ionic liquids, ionic solutions

IV Ion-electronic liquids (metals) and their solutions

V Polymer and biopolymer solutions

VI Mixtures of fullerenes, nanotubes, nanoplatelets with liquids

VII Colloid systems: fluids with self-organization, ferrofluids; clay suspensions

VIII Liquid confined systems. Liquids in porous media

IX Medical and biological aspects of physical properties of water and water solutions

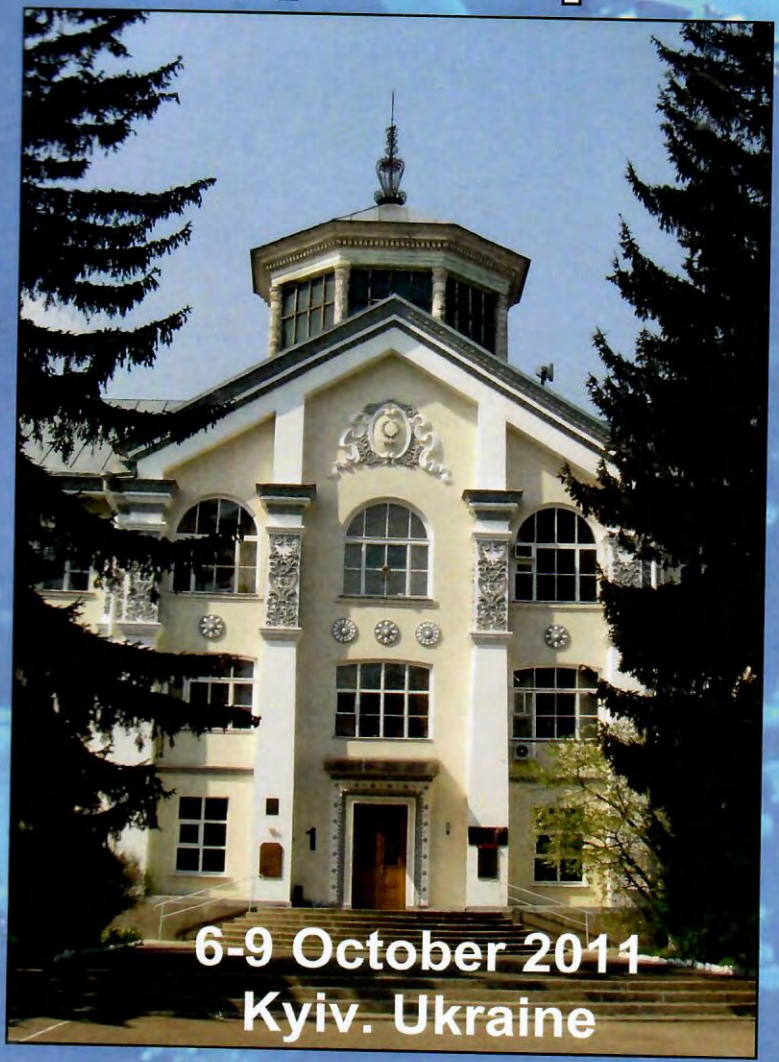
X Radiative aspects of the physics of liquid state

XI Critical and supercritical phenomena in liquids and liquid systems

XII Supercooled liquids. Glass transition

Second International Conference

Nanobiophysics: fundamental and applied aspects



6-9 October 2011
Kyiv. Ukraine

Second international conference

NANOBIOPHYSICS 2011: Fundamental and Applied Aspects

6-9 October 2011, Kiev, Ukraine

BOOK OF ABSTRACTS

Analysis of RNA Nanostructures with Coarse-Grained Models

M. Paliy[1], R.V.N. Melnik[1], A.V. Zhukov[1], B.A. Shapiro[2]

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[2] *Center for Cancer Research Nanobiology Program, National Cancer Institute, Frederick, MD 21702, USA*

Ribonucleic acid (RNA) has been proposed as a promising alternative to DNA and proteins for the design of the artificial self-assembled materials at nanoscale (see [1,2]). RNA offers a much greater variety of interactions, and great conformational flexibility of RNA structures make them a very promising functional nano-material for the design of the man-made molecular devices and systems in nano-biophysical and nano-biotechnological applications. Here, we first present a model based on all-atom Molecular Dynamics, demonstrating the stability and conformational dynamics of several simple RNA nanostructures. We explain the effect of the counterions and solvent, that are both known to modify strongly the stability and dynamics of RNA nanostructures, on the behavior of the "kissing loops". This effect is very important due to the fact that the "kissing loop" motif can be used as a basic constructional element to join the simplest building blocks into a symmetric structures with their spatial dimensions lying in the range of 10-20 nm. Then, we present several promising multiscale methodologies for simulation of biomolecular systems such as RNA nanostructures, focusing on our recent efforts in the development of a hierarchy of simplified coarse-grained mesoscopic models suitable for the description of these complex systems [3].

Finally, we extend our coarse-grained RNA model to describe other RNA nanostructures - ``RNA tectosquares" bearing the right-angle motifs, as well as ``RNA nanotubes" composed of stacked RNA nanorings. Such model extension requires incorporation of the new conformation classes found in the fore-mentioned nanostructures, as well as an improved scheme for treatment of the base-pairing and stacking interaction terms.

1. *Yingling, Y.G., Shapiro, B.A.* Computational design of an RNA hexagonal nano-ring and an RNA nanotube // Nano Letters-2007.-**7**.-2328.
2. *Paliy, M., Melnik, R., Shapiro, B.A.* Molecular dynamics study of the RNA ring nanostructure: a phenomenon of self- stabilization // Physical Biology.-2009.-**6**, N 4.-046003.
3. *Paliy, M., Melnik, R., Shapiro, B.A.* Coarse-graining RNA nanostructures for molecular dynamics // Physical Biology.-2010.-**7**, N 3.-036001.

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E-mail: lebovka@gmai
[2] *Unitŭ Transformation*
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Compiugne Cedex, Fra

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1. *Lebovka, N.I., Voro*
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2. *Vorobiev, E., Lebo*
Plants and Biomate
3. Lebovka, N.I., Vo
the Food Industry.

APMAS 2014

4TH INTERNATIONAL ADVANCES IN APPLIED PHYSICS AND MATERIALS SCIENCE CONGRESS & EXHIBITION

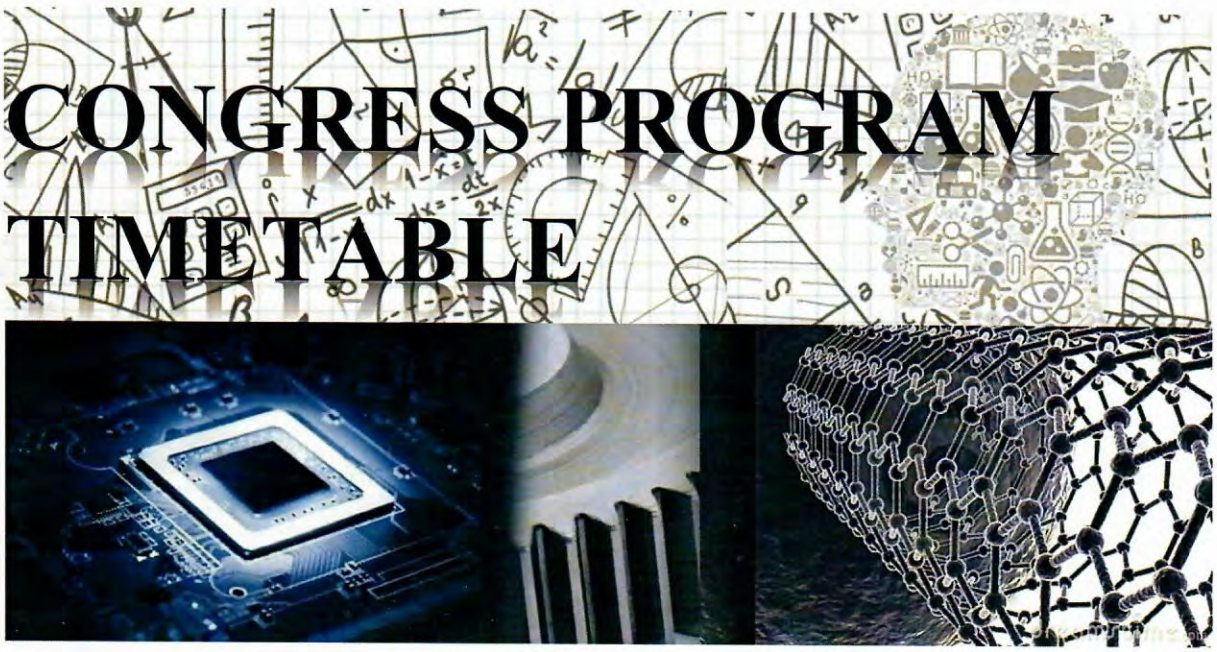
&

SCITEED 2014

INTERNATIONAL CONGRESS & EXHIBITION ON CURRENT TRENDS ON SCIENCE TECHNOLOGY EDUCATION

APRIL 24 – 27, 2014

Sentido Lykia Resort & Spa-Liberty Hotels Lykia, Oludeniz
MUGLA / TURKEY



28th European Conference on Modelling and Simulation

May, 27th - 30th, 2014, Brescia, Italy

ECMS 2014

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Fabio Baronio

Claudia Archetti

Marco Castellani

Honorary Chairs:

Andrzej Bargiela

Eugène J.H. Kerckhoffs

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PROCEEDINGS

28th European Conference on Modelling and Simulation ECMS 2014

May 27th – May 30th, 2014
Brescia, Italy

Edited by:

Flaminio Squazzoni

Fabio Baronio

Claudia Archetti

Marco Castellani

Honorary Chairs:

Andrzej Bargiela

Eugène J.H. Kerckhoffs

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Electrical and Electromechanical Engineering

Determination Of An Optimal Shape Of Rotor For The Synchronous Reactive Frequency Doubler

Aleksandrs Mesnajevs, Elena Ketnere 131

Modelling Of Broadband Electric Field Propagation In Nonlinear Dielectric Media

Matteo Conforti, Fabio Baronio 136

On The Processing Of The Recorded Data For The SF6 Circuit Breakers From The Transformation Substation 110/20/6kV Craiova South

Maria Brojboiu, Virginia Ivanov, Andrei Savescu 142

Design, Simulation And Testing Of Planar Spiral Coils For The Time-Gated Interrogation Of Quartz Resonator Sensors

Mohamad Farran, Marco Bau, Daniele Modotto, Marco Ferrari, Vittorio Ferrari 147

Applications Of The Graph Theory For Optimization In Manufacturing Environment Of The Electrical Equipments

Virginia Ivanov, Maria Brojboiu, Sergiu Ivanov 153

Current Control Of A VSI-FED Induction Machine By Predictive Technique

Sergiu Ivanov, Vladimir Rasvan, Eugen Bobasu, Dan Popescu, Florin Stinga 159

Modeling And Control Of Berry Phase In Quantum Dots

Sanjay Prabhakar, Roderick Melnik, Ali Sebetci 166

Efficient Modeling Of Graphene Based Optical Devices

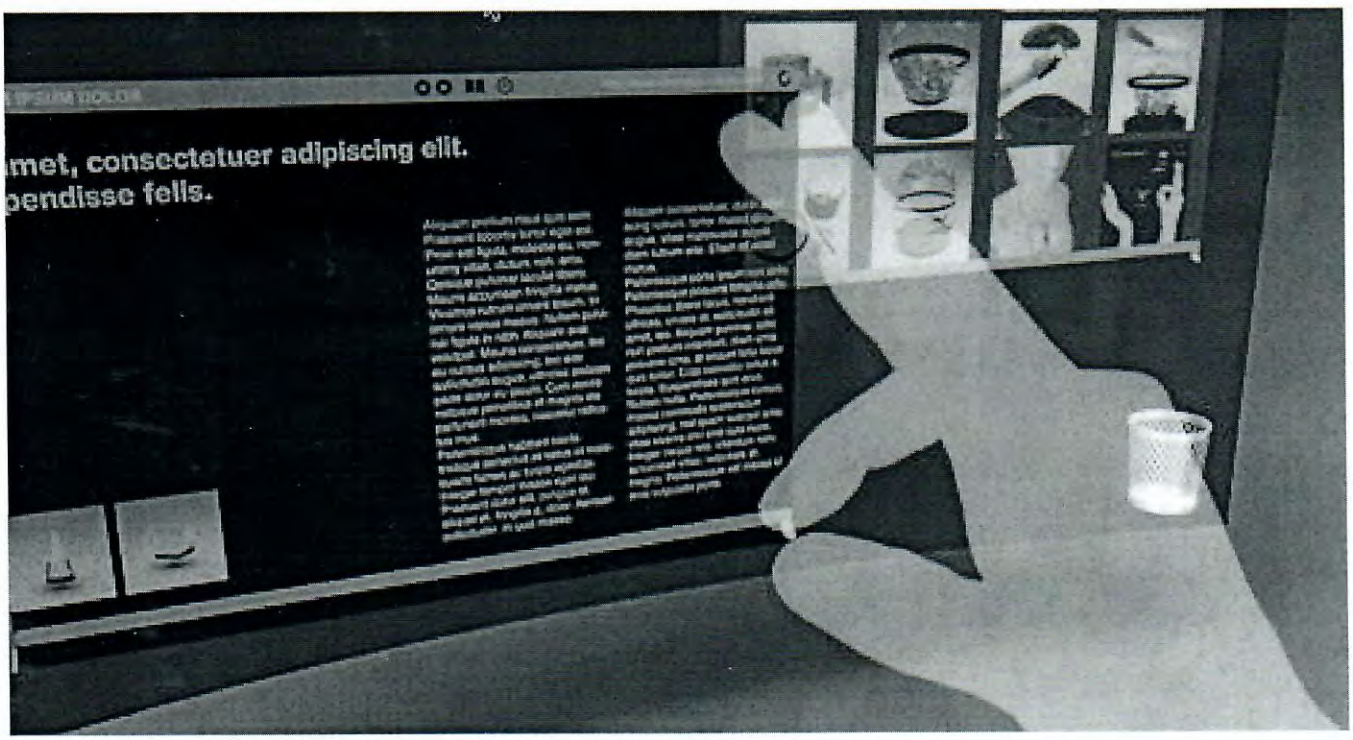
Costantino De Angelis, Andrea Locatelli 171

Collection of 2014 BARCELONA CONFERENCES

2014 7th International Conference on Computer Science and Information Technology (ICCSIT 2014)

2014 International Conference on Communications and Network Engineering (ICCNE 2014)

2014 International Conference on Artificial Intelligence (ICOAI 2014)



December 22-24, 2014
Barcelona, Spain

Boosting the Efficiency of First-order Abductive Reasoning Using Pre-estimated Relatedness between Predicates

Kazeto Yamamoto, Naoya Inoue, Kentaro Inui, Yuki Arase and Jun'ichi Tsujii

Clustering Approach of Device Interactions for Automatic Generation of Device Social Relation

Dong-oh Kang, Jang-Ho Choi, Joon-Young Jung and Changseok Bae

Artificial Neural Network Training via Markov Chains

Roderick Melnik

Artificial Neural Network Training via Markov Chains

Roderick Melnik[1]

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Email: rmelnik@wlu.ca

In this presentation, we review a general framework for the analysis of a connection between the training of artificial neural networks via the dynamics of Markov chains and the approximation of conservation law equations originally proposed in [1]. We consider computational aspects of the mathematical modelling of dynamic system evolution have been considered as a problem in information theory [2]. The developed framework allows us to demonstrate an intrinsic link between microscopic and macroscopic models for evolution via the concept of perturbed generalized dynamic systems. The main result is exemplified with a number of illustrative examples where efficient numerical approximations follow directly from network-based computational models, viewed here as Markov chain approximations. The approach also allows us to derive a stable approximation of the chain for the dynamic system evolution and provides the opportunity for analysing important limiting cases. In this context, stability and consistency conditions of the associated computational models are discussed. Finally, an intrinsic interconnection of constructive, sequential, and evolutionary approaches in related optimization problems is highlighted, along with open problems in this area.

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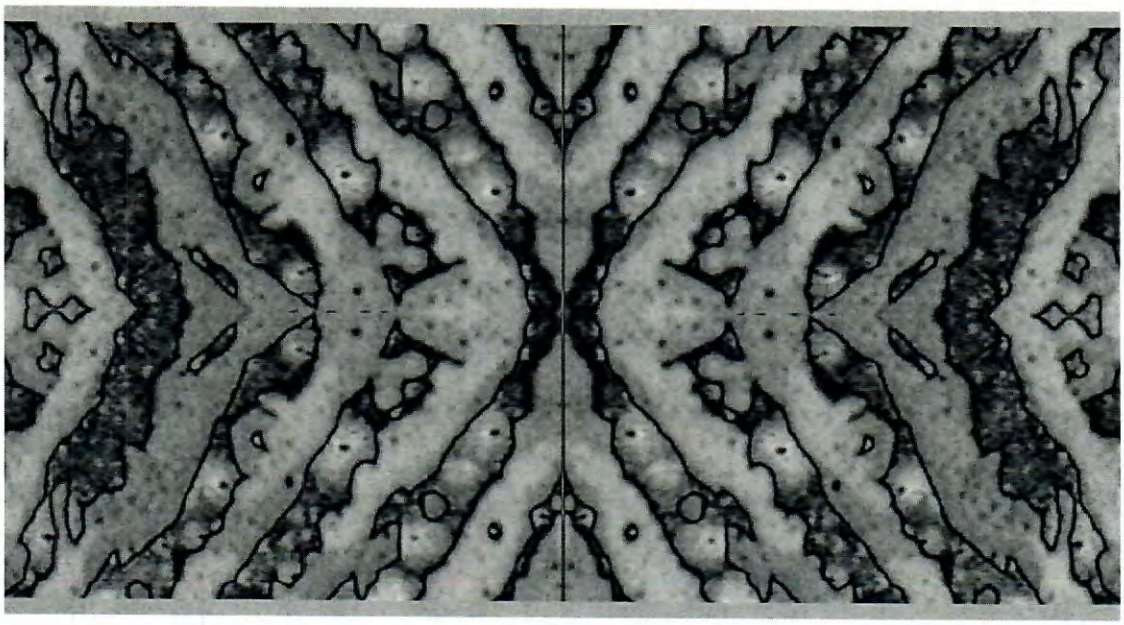
2. Melnik, R.V.N., Dynamic system evolution and Markov Chain Approximation, *Discrete Dynamics in Nature and Society*, 1998, 2, 7—38.

NanoSpain Conf 2016

March 15-18, 2016 Logroño (Spain)

Abstracts Book



		Page
Julia Jiménez López (Universidad de Granada, Spain) *Enhanced delivery of Paclitaxel using PLGA nanoparticles: therapeutic effect in lung cancer cell cultures*	POSTER	96
Marlene Klein (Ultra Traces Analyses Aquitaine (ADERA-UT2A), France) *Characterization of polymer based nanopharmaceuticals by Asymmetrical Flow Field Flow Fractionation*	POSTER	98
Frank Koppens (ICREA/ICFO, Spain) *Photons, Plasmons and Electrons meet in 2d materials*	INVITED Parallel Session	100
Lise-Marie Lacroix (LPCNO, UMR 5215 INSA-CNRS-UPS, France) *Nanoparticles with optimized properties: from chemical synthesis to assembly A bottom-up approach for nanostructured materials*	KEYNOTE Plenary Session	102
Rebeca Lara (Universidad de La Rioja, Spain) *Luminescent platinum systems based on the chromophore 2-phenylbenzothiazole*	POSTER	104
Fernando Ignacio López-Bara (Autonomous Barcelona University, Spain) *Dynamics of the spin-ice states with magnetic charges*	POSTER	105
Manuel López-López (Universidad de Huelva, Spain) *Do strong surfactant/swcnt-cooh interactions assure good dispersion quality?*	ORAL Plenary Session	106
Manuel López-López (Universidad de Huelva, Spain) *A thorough spectroscopic study about the interaction of surfactants with carboxylated singlewalled carbon nanotubes*	POSTER	107
Diego López-Torres (Public University of Navarre, Spain) *SnO_2 humidity interferometric sensor based on photonic crystal optical fiber and Fast Fourier Transform*	POSTER	108
Samuel Mañas-Valero (University of Valencia - ICMol, Spain) *Transition metal chalcogenides in the 2D limit: superconductivity in 2H-TaS_2*	ORAL Plenary Session	110
José Miguel Martín Martínez (University of Alicante, Spain) *Improvement of the toughness of PMMA-based acrylic resin for dental application by adding small amounts of graphene nanoparticles*	ORAL Parallel Session	111
Nicolas F. Martinez (ScienTec Iberica, Spain) *Bimodal HD-KFM and Resiscope Atomic Force Microcopy characterization of bidimensional materials and solar cells*	ORAL Plenary Session & Poster	113
Johann G. Meier (ITAINNOVA, Spain) *On the peculiar mechanical and tribological behavior of polymer nanocomposites with nanotubes of WS_2 and nanowires of $Mo_6S_2I_8$*	ORAL Plenary Session	114
Roderick Melnik (MS2Discovery Interdisciplinary Research Institute, Canada and BCAM, Spain) *Coupling, geometric phases, and properties of quantum dots: analytics and numerics for the Berry phase case*	ORAL Plenary Session	115

Coupling, geometric phases, and properties of quantum dots: analytics and numerics for the Berry phase case

Roderick Melnik, Sanjay Prabhakar

MS2Discovery Interdisciplinary Research Institute, WLU, Waterloo, 75 University Ave W, ON, Canada
BCAM - Basque Center for Applied Mathematics, Mazarredo 14, E48009, Bilbao, Bizkaia, Spain
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Recent experimental spin-based realizations of universal geometric quantum gates [1] open new exciting opportunities for practical applications and pose new challenges for theoretical research on geometrical phases. They clearly highlight the importance of geometric phases in nanotechnology in general and in the design and control of low dimensional nanostructures in particular.

In this contribution, we analyze and quantify the influence of such geometric phases on the properties of quantum dots. We focus on the Berry phase and demonstrate its high sensitivity to electric fields coming from the interplay between the Rashba and Dresselhaus spin-orbit couplings. The Berry phase is induced by letting the quantum dots to move adiabatically in a closed loop in the 2D plane along a closed trajectory [2]. We demonstrate that the accumulated geometric phase can be induced from other available quantum states that differ only by one quantum number of the corresponding spin state. Moreover, the sign change in the g- factor can be reflected in this phase. We carry out the analysis for typical spatial scales in such situations, namely for spin-orbit length, hybrid orbital length, and orbital radius, and determine the key characteristics of the Berry phase for these scales. The technique, developed for our analysis of spin dynamics evolution during the transport of quantum dots as describe above, is based on a combination of analytical and numerical tools. The timedependent Schrodinger equation is solved by applying the Feynman disentangling technique supplemented by the finite element methodology. It is shown that the superposition effect can be observed during the transport process, while the Berry phase for the pure Rashba and pure Dresselhaus cases are well separated at smaller values of the spin-orbit lengths. Finally, applications of the observed effects are discussed.

References

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7th International Conference
PHYSICS OF LIQUID MATTER: MODERN PROBLEMS

PLMMP 2016

http://plmmp.org.ua

PROGRAMME

May 27-30, 2016

Taras Shevchenko National University of Kyiv

Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine

Kyiv, Ukraine

7th International Conference

PHYSICS OF LIQUID MATTER: MODERN PROBLEMS

May 27-30, 2016

http://plmmp.org.ua

PLMMP 2016

ABSTRACTS

Taras Shevchenko National University Of Kyiv

Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine

Editor: Leonid A. Bulavin

Kyiv, Ukraine
2016

Section 10. Glass-forming liquids

Oral session

10-1.O

NON-PERTURBATIVE APPROACHES TO LATTICE MODELS, GLASS-FORMING LIQUIDS, AND BIOLOGICAL NANOSTRUCTURES IN SOLUTIONS

Roderick Melnik[1,2]

[1]*MS2Discovery Interdisciplinary Research Institute & M2NeT Laboratory, Wilfrid Laurier University, Waterloo*
http://www.m2netlab.wlu.ca || http://www.ms2discovery.wlu.ca
[2] *Department of Physics and Astronomy, University of Waterloo, BCAM, Spain*

There is an increasing interest in non-perturbative approaches. At the fundamental level, their development have been strongly stimulated by non-perturbative descriptions of quantum systems, but recent discoveries demonstrate a wider applicability of these approaches and their importance in other areas. For example, there is conclusive evidence of the existence of non-perturbative effects in spin glasses and the pronounced influence of such effects for phase transitions and critical phenomena in liquid systems. Here we review non-perturbative approaches applied to the lattice field theory defined on hypercubic lattices, as well as to classical spin systems. Among others, the 3D Ising, XY, n-vector and Heisenberg models will be considered, and corresponding correlation functions, universal ratios and Goldstone mode singularities will be discussed, as well as new estimations of correction-to-scaling exponents. We will conclude with examples of simulations of biological nanostructures in solutions and discuss their applications in biomedicine.

This is a joint work with Jevgenijs Kaupuzs.

In memory of Janis Rimshans.

10-2.O

QUANTITATIVE THEORY OF THE STRUCTURAL GLASS TRANSITION

Vassiliy Lubchenko *

[1]*University of Houston, Departments of Chemistry and Physics, Houston, TX 77204-5003, USA*
* Corresponding author e-mail: vas@uh.edu

The emergence of rigidity and many other phenomena accompanying the structural glass transition remain hotly disputed topics. We show that rigidity emerges in glassy liquids similarly to crystals, i.e., via a breaking of the translational symmetry. In crucial distinction from periodic crystallization, the free energy landscape of a glassy liquid is vastly degenerate, which gives rise to new length and time scales while rendering the emergence of rigidity gradual. We obviate the standard notion that to be mechanically stable a structure must be essentially unique; instead, we demonstrate that bulk degeneracy is perfectly allowed but should not exceed a certain value. The present microscopic description thus explains both crystallisation and the emergence of the landscape regime followed by vitrification in a unified, thermodynamics-rooted fashion. The present description allows one to quantitatively estimate, without using adjustable parameters, the key attributes of glassy liquids, viz., the relaxation barriers, glass transition temperature, and cooperativity size. The thermal, rheological, and electronic behaviors of glasses exhibit many universal features. I will explain how these can be understood quantitatively [1].

References

[1] V. Lubchenko, *Adv. Phys.*, **64**, 283-443 (2015).

8th ECCOMAS Thematic Conference on Smart Structures and Materials

6th International Conference on Smart Materials and Nanotechnology in Engineering

SMART 2017

5 – 8 June 2017, Madrid, Spain

PROGRAMME

A publication of:

International Center for Numerical Methods in Engineering (CIMNE)
Barcelona, Spain

CIMNE

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Structural Health Monitoring - II | We08O Room 2

Non-Destructive Evaluation of Delamination in Composite Material Based on Vibrational Approach
G. Serovaev, A. Shestakov and D. Oshmarin

Structural Health Monitoring By Combining Machine Learning And Data Assimilation Techniques
E. Lopez, G. Quaranta, E. Abisset-Chavanne and F. Chinesta

Investigation of the Electromechanical Impedance Changes related to the State of the Investigated Structures
P. Fiborek, P. Malinowski, P. Kudela, T. Wandowski and W. Ostachowicz

Scattering Analysis of Lamb Waves at Subsurface Cracks in Isotropic Plates
C. Humer, C. Kralovec and M. Schagerl

Modelling the Correlation between the Damage State and the Electrical Resistance Change in Symmetric Laminates
M. Zappalorto, M. Quaresimin, F. Panozzo, P. A. Carraro and N. De Rossi

Delamination Monitoring in Electrically Conductive Composites
M. Quaresimin, S.K. Nothdurfter, M. Zappalorto, F. Panozzo, A. Rullo and N. De Rossi

Energy Harvesting, Power and Storage | We08O Room 3

Phase-Field Study of Stress-Induced Polarization Switching for Vibration Energy Harvesting
D. Wang, R. Melnik and L. Wang

Jose Rodellar

Flywheel Proof Mass Transducer for Energy Harvesting Applications
A. Kras and P. Gardonio

Preliminary Investigation of the Energy Harvesting System Intended for use on an ORC Microturbine
T. Z. Kaczmarczyk, G. Żywica, E. Ihnatowicz, M. Lubieniecki and J. Roemer

Experimental Validation of a Porous Piezoelectric Energy Harvester
G. Martinez-Ayuso, H.H. Khodaparast, Y. Zhang, C.R. Bowen, M.I. Friswell, A.D. Shaw, H. Madinei and J.I. Roscow

Vibration Energy Harvesting with Electromagnetic and Piezoelectric Seismic Transducers: Experimental Results
L. Dal Bo and P. Gardonio (Udine)

Development of Li1.4Al0.4Ti1.6(PO4)3 Solid Electrolyte-Based Power Composites: Characterisation of Electrical Properties and Mechanical Properties
G. Liao, S. Geier, T. Mahrholz, P. Wierach and M. Wiedemann

Investigation of Interfacial Conditions for Li1.4Al0.4Ti1.6(PO4)3 Solid Electrolyte–based Multifunctional Energy Storage Devices
G. Liao, S. Geier, T. Mahrholz, P. Wierach and M. Wiedemann

An Asymptotically Correct Beam Type Piezoelectric Energy Harvester Model
S. Banerjee and S. Roy

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IEEE
UKRAINE SECTION

2017 IEEE First Ukraine Conference on

Electrical and Computer Engineering

UKRCON PROGRAM

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May 29 – June 2, 2017

http://ukrcon.ieee.org.ua

Track 4: Nanoelectronics & Photonics, Electron Devices & Embedded Systems

ORAL SESSION

Hall #10 of Library (14:30 – 15:30)

1	Shyam Badu and Roderick Melnik	NMR Properties of Fenna-Matthews-Olson Light Harvesting Complex: Photosynthesis and its Biomedical Applications
2	Denys Natarov	Lasing Thresholds of Plasmonic Modes of a Silver Tube Nanolaser with Active Shell and Core
3	Volodymyr Byelobrov	Lasing Thresholds of Plasmon and Grating Modes of Coated Silver Nanowire Gratings
4	Vitalii Shcherbinin and Anton Hlushchenko	Self-Consistent Effect of Ohmic Losses on Output Power of Gyrotron

POSTER SESSION

Library Floor (15:30 – 16:00)

1	Elena Velichko	Resonance Scattering and Absorption of Light by a Silver Circular Cylinder with Diameter Larger Than the Wavelength
2	Alexander Ye. Svezhentsev, Vladimir Volski, Sen Yan and Guy A. E. Vandenbosch	Shaped Nanoantennas on Cylindrical and Planar Substrate
3	Vira Tkachenko and Aleksandr Lipinskii	Mathematical Model of Volume Optical Interconnection Reconfiguration Utilizing Acousto-Optic Beam Forming
4	Yuriy Poplavko and Alexandr Borisov	Impact of Magnetic and Electrical Ordering on Resistivity: New Incite

ORAL SESSION

Hall #10 of Library (16:00 – 17:30)

1	Vadym Avrutov, Petro Aksonenko, Nadiya Bouraou, Patrick Henaff and Laurent Ciarletta	Expanded Calibration of the MEMS Inertial Sensors

31.05.2017

IEEE MILESTONE CEREMONY

Hall "Bilka" of Library,
Igor Sikorsky Kyiv Polytechnic Institute
(10:30 – 13:00)

Mr. Costas Stasopoulos,
Past Director of the IEEE Region 8 (Europe, Middle East and Africa), Director Member of the IEEE Board of Directors, Nicosia, Cyprus
Prof. Jozef Modelski,
2009-2010 Director of IEEE Region 8 (Europe, Africa and Middle East), IEEE Fellow, Warsaw University of Technology, Warsaw, Poland
Prof. Roberto Sorrentino,
EuMA Co-founder and President (1998 – 2009), IEEE Fellow, University of Perugia, Perugia, Italy
Prof. Andrew Tirkel,
Scientific Technology Co., East Brighton, Australia
Prof. Felix Yanovsky,
IEEE Ukraine Section Chair, Head of Electronics Department of the National Aviation University, IEEE Fellow, Kyiv, Ukraine
Prof. Alexander Nosich,
O. Ya. Usikov Institute for Radiophysics and Electronics of the NASU, IEEE Fellow, Kharkiv, Ukraine

IEEE MILESTONE

Zenit Parabolic Reflector L-band Pulsed Radar, 1938

The 1938 Zenit radar test at the Laboratory of Electromagnetic Oscillations of the Ukrainian Institute of Physics and Technology was a major advance in the development of radar. Designed by Abram Slutskin, Alexander Usikov, and Semion Braude, microwave scientists and magnetron pioneers, Zenit established the practicality of combining the pulsed method and a shorter wave band for determining precisely all three coordinates of airborne targets.

May 2017

IEEE

VII International Conference on Computational Methods for Coupled Problems in Science and Engineering

COUPLED PROBLEMS 2017

12 – 14 June 2017, Rhodes Island, Greece

PROGRAMME

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International Center for Numerical Methods in Engineering (CIMNE)
Barcelona, Spain

Coupled Problems in Bio-Medicine II	WeM07 Room: Nefeli A

Influence of mechanical stimuli in growth plate morphological evolution during long bone development
H. Castro-Abril, J.M. Guevara, S.J. Shefelbine and D.A. Garzón-Alvarado

Predicting age-dependent changes in human native heart valves due to growth and remodeling
P.J.A. Oomen, C.C.V.C. Bouten, E. Kuhl and S. Loerakker

Coupled nanostructures of ribonucleic acids: developing discrete-continuum models for large time-scale simulations
S. Badu and R. Melnik

Simulations of fluid and rigid bodies interaction for biomechanics problems
C. Samaniego, G. Houzeaux and M. Vázquez

A phase-field method in full Eulerian framework for fluid-structure interaction in biological systems
X. Zheng and G. Karniadakis

Flow-structure interaction simulations of the aortic heart valve at physiologic conditions: the role of tissue constitutive model
A. Gilmanov, H. Stolarski and F. Sotiropoulos

IS - Control, Uncertainty Quantification, and ROMs in Coupled Problems Invited Session organized by Hermann G. Matthies, Carlos Felippa, K. C. Park and Roger Ohayon	WeM08 Room: Nefeli B Chair: Hermann G. Matthies

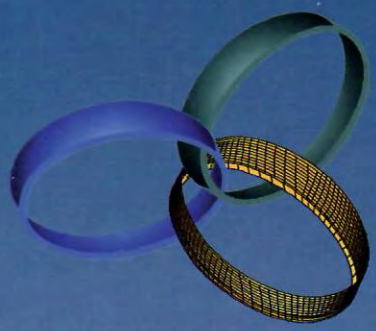
Reduced order model for fluid flow and transport of passive scalars in fluidized beds
S.R. Reddy, J. Chitale, P.G.A. Cizmas, G.S. Dulikravich, S. Gokaltun and D. McDaniel

Uncertainty quantification of coupled ODEs with stochastic Galerkin methods using adaptive higher order Runge-Kutta methods
J. Rang

Structure preserving Bayesian identification of a reduced order model for the control of the circular cylinder wake
N. Friedman, J. Vondrejc, R. Semaan and H.G. Matthies

Uncertainty analysis of the material properties of rock in hydrualic fracturing process
H. Garikapati, C.V. Verhoosel, E.H. van Brummelen and P. Díez

This volume contains the Technical programme of the papers accepted for presentation at the VII International Conference on Computational Methods for Coupled Problems in Science and Engineering, COUPLED PROBLEMS 2017
(12 - 14 June, 2017 - Rhodes Island, Greece)



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会刊 Conference Guide

Session 106: Next Generation MEMS, NEMS and Array Technologies
Time: 08:30-10:10, March 8, 2018 (Thursday); Place: Yamato-A, 5th Floor, Guest Room Tower, HRO

Chair	***Dr. Shane Bowen,*** Director, Scientific Research, Illumina Inc., USA
Co-Chair	***Dr. Viorel Dragoi,*** Chief Scientist, Wafer Bonding, EV Group, Austria
08:30-08:55	***Title:*** *Phase Shifted Fiber Bragg Gratings Is an Ideal Platform for Creating Special Sensors with Nano-Material / Technology* ***Mr. Peter Kung,*** President, QPS Photronics Inc., Canada
08:55-09:20	***Title:*** *Nanotechnology for a Genomic Revolution* ***Dr. Shane Bowen,*** Director, Scientific Research, Illumina Inc., USA
09:20-09:45	***Title:*** *High Performance SAW Resonator on New Multi-Layered Substrate and Applications* ***Mr. Tsutomu Takai,*** Manager, Murata Manufacturing Co., Ltd., Japan
09:45-10:10	***Title:*** *Wafer Bonding Technology for New Generations of MEMS Devices: Challenges and Promises* ***Dr. Viorel Dragoi,*** Chief Scientist, Wafer Bonding, EV Group, Austria

Session 107: Design, Development, Fabrication and Testing of Smart Structures and Systems
Time: 08:30-12:00, March 8, 2018 (Thursday); Place: Yamato-B, 5th Floor, Guest Room Tower, HRO

Chair	***Dr. Rafal Kozubski,*** Head, Solid State Physics Department, Jagiellonian Universityin Krakow, Poland
Co-Chair	***Dr. Aminul Islam,*** Associate Professor, Technical University of Denmark, Denmark
08:30-09:00	***Keynote Speech*** ***Title:*** *Dynamics and Applications of Smart Structures and Systems at the Nanoscale* ***Dr. Roderick Melnik,*** Director, MS2Discovery Interdisciplinary Institute, Wilfrid Laurier Universit, Canada
09:00-09:30	***Title:*** *Structural Transformations in Solid Materials: Power of Atomistic Monte Carlo Simulations* ***Dr. Rafal Kozubski,*** Head, Solid State Physics Department, Jagiellonian Universityin Krakow, Poland
09:30-10:00	***Title:*** *A Motivation and Game Approach to Enhance a Competence-based Open Distance Learning* ***Dr. Oleg Zaikin,*** Professor, Warsaw School of Computer Science, Poland
10:00-10:30	**Coffee Break**
10:30-11:00	***Title:*** *Design and Development of Smart Products by Moulded Interconnect Technologies* ***Dr. Aminul Islam,*** Associate Professor, Technical University of Denmark, Denmar
11:00-11:30	***Title:*** *High Pressure Synthesis of New Light Materials with Outstanding Properties* ***Dr. Yann Le Godec,*** CNRS Researcher, IMPMC, CNRS, UPMC Sorbonne University, France

Title: Dynamics and Applications of Smart Structures and Systems at the Nanoscale

Dr. Roderick Melnik*, Dan Wang, and Linxiang Wang
Director
MS2Discovery Interdisciplinary Research Institute
Wilfrid Laurier University
Canada

Abstract

In this contribution, we provide a survey of models for a large class of multidimensional coupled nonlinear systems with phase transformations, focusing on the analysis of dynamics and applications of smart structures and systems. Our exemplifications here are based on models describing coupled nonlinear phenomena in smart materials with memory, such as shape memory alloys, where we focus on cubic-to-tetragonal martensitic phase transformations in three dimensional settings under dynamic loading conditions. We will provide further insight into the application areas of these materials at the nanoscale, the development of computationally efficient reduction procedures for their 3D modelling, and the construction of fully conservative schemes for solving the associated problems. Next, we focus on a novel method for vibration energy harvesting based on stress-induced polarization switching, specifically in ferroelectric materials. Our analysis here has been carried out based on a Landau-type elastic Gibbs energy, giving a guidance for further investigations. The state-of-the-art phase field model is implemented to study the hysteretic nonlinear phenomena involved in the energy harvesting process. The influence of different materials is carefully compared and discussed. Furthermore, the combined effects of the bias electric potential and bias resistance in different materials are presented and discussed in the context of future real implementations.

Biography

Dr. Roderick Melnik has been Full Professor and Tier I Canada Research Chair in Mathematical Modelling in the Faculty of Science at the Wilfrid Laurier University in Waterloo, Canada since 2004. He is also affiliated with the Guelph-Waterloo Institute of Physics, University of Waterloo, and University of Guelph. Prior to his current appointment, Dr. Melnik held full Professorial positions at Louisiana Tech University in the USA and the University of Southern Denmark, where he was the Head of Mathematical Modelling and Engineering Mathematics. He received his M.Sc. degree in and Ph.D. degree from Kiev State University in 1985 and 1989, respectively. Starting his academic career in Europe, he continued it in Australia until in the late 1990s he took the position of senior scientist at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Sydney, working in the Division of Mathematical and Information Sciences. Dr. Melnik has published extensively in a variety of fields with his major focus on mathematical modelling for challenging problems in science and technology. Dr. Melnik is the recipient of many awards, including a number of prestigious fellowships outside of Canada, in Italy, Denmark, England and Spain. He has served on editorial boards of many international journals and book series. Currently, Dr. Melnik is the Director of the MS2Discovery Interdisciplinary Research Institute in Waterloo, Canada.

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						concrete elements: From mathematical modelling to assessment through structural
11:00-11:15			**[O2.24] Ensemble probabilistic forecasting in the microscale** A. Oliver*, L. Mazorra-Aguiar, E. Rodríguez, G. Montero *University of Las Palmas de Gran Canaria, Spain*	**[O3.23] Dynamic reliability analysis of nonlinear building structures subject to near-fault ground motions** D.X. Yang*, G.H. Chen *Dalian University of Technology, China*	**[O4.25] Numerical experimentation of global finite similitude scaling in die compaction process** M. Moghaddam[1], R. Darvizeh*[2], K. Davey[2,3], A. Darvizeh[1] *[1]University of Guilan, Iran, [2]The University of Manchester, UK, [3]University of Strathclyde, UK*	**[O5.24] Corrosion of steel bars in reinforced concrete columns: the effect of the cover concrete spalling on strength deterioration in axially loaded columns** R. Greco[1], M. Morga*[2] *[1]Technical University of Bari, Italy, [2]Anglia Ruskin University, UK*
			ECT2018: Crash and impact computational mechanics			
11:15-11:30	11:15-11:45	**[KEY6] Strain control of engineering band structures of graphene nanoribbons** **R. Melnik,** *Wilfrid Laurier University, Canada*	**[O2.25] On discontinuous boundary elements in the mechanics of solid bodies loaded by explosion** P.P. Prochazka*, M.J. Valek *Czech Technical University in Prague, Czech Republic*	**[O3.24] A new development of sequential approximation programming for reliability-based design optimization** P. Yi[1], G. Cheng*[1], M. Zhou[2], Z. Luo[2] *[1]Dalian University of Technology, China, [2]Altair Engineering, Inc., USA*	**[O4.26] Strain rate sensitivity in scaling of dynamic structural systems** H. Sadeghi[1], R. Darvizeh*[2], K. Davey[2,3], A. Darvizeh[1] *[1]University of Guilan, Iran, [2]The University of Manchester, UK, [3]University of Strathclyde, UK*	**[O5.25] Numerical modelling of chloride extraction from concrete structures with the help of electric field** J. Kruis*, J. Nemecek *Czech Technical University in Prague, Czech Republic*
11:30-11:45			**[O2.26] Study and characterization of abrasion phenomena for organic matrix composite and metallic materials in A/C emergency landing situations** L. Bigault[1,2], E. Deletombe*[1], Y. Desplanques[2] *[1]ONERA - The French Aerospace Lab, France, [2]University of Lille, France*	**[O3.25] Cohesive discrete element method to simulate Young's modulus variability effect on a natural fibre-reinforced composite performance** D. Moukadiri*[1], W. Leclerc[1], M. Guessasma[1], F. Druesne[2], E. Bellenger[1] *[1]University of Picardie Jules Verne, France, [2]University of Technology of Compiègne, France*	**[O4.27] Elastic-plastic formulation and damage prediction in forming processes with highly localized large strain** A. Vlasov[1], N. Biba*[2], s. Stebunov[1] *[1]QuantorForm Ltd, Russia, [2]MICAS Simulations, UK*	**[O5.26] Vulnerability assessment for the reinforced concrete beam exposed to monotonic loading using different damage indexes** M. Nasim*, S. Setunge *RMIT, Australia*
						CST2018: Artificial neural networks in computational mechanics
11:45-12:00	11:45-12:15	**[KEY7] An equation-free, nested, concurrent multiscale approach**	**[O2.27] The crash analysis of electric multiple unit driver's cab** P. Watroba, M. Pawlak*, D. Gasiorek	**[O3.26] Risk-based probabilistic seismic hazard analysis considering parameter uncertainties** L. Hofer*, M.A. Zanini, F. Faleschini, K. Toska, C.	**[O4.28] Investigating macrosegregation and inclusion-front interaction in continuously-cast steel slabs** S. Chaube *T.R.D.D.C, India*	**[O5.27] A comparative study of neural network model and LOLIMOT for self-compacting concrete containing supplementary cementitious materials**

ECT Keynote Speaker Biographies

Sondipon Adhikari
Swansea University
United Kingdom

Prof Adhikari is the chair of Aerospace Engineering in the College of Engineering of Swansea University. His research areas are multidisciplinary in nature and include uncertainty quantification in computational mechanics, dynamics of complex systems, inverse problems for linear and non-linear dynamics and vibration energy harvesting. He has obtained more than £1.5M of competitive research funding as a principal investigator, published four books, 275 international journal papers and over 175 conference papers in these areas. His works have been widely cited (over 10,000 citations and a H-index of 53 in Google scholar) in the scientific community. He was Wolfson Research Merit Award holder from the Royal Society, an Engineering and Physical Science Research Council (EPSRC) Advanced Research Fellow and winner of the Philip Leverhulme Prize (2007). He was a lecturer at the Bristol University and a Junior Research Fellow in Fitzwilliam College, Cambridge.nProfessor Adhikari is in the editorial board of 15 international journals, research grant reviewer of 20 funding councils and served in over 40 Scientific and Technical Committees. He is an associate Fellow of American Institute of Aeronautics and Astronautics (AIAA) and a Fellow of the Royal Aeronautical Society.

Fabio Casciati
University of Pavia
Italy

F. Casciati (born in Naples, January 16, 1949) had the degree in Civil Eng. cum laude on June 15, 1972, from the Univ. of Pavia, where he is Full Professor of "Scienza delle Costruzioni" since 1980.
He served as Institute and Department Chairman (1980-1983). He was member of the Faculty of the Ph.D Course on Structural Engineering ruled by the Polytechnic of Milan and the Univ. of Pavia in the period 1984-1994. Chairperson of the Civil Eng. Council in 1986-89, Responsible of the Infrastructure Engineering undergraduate school from 1993 to 2001, Coordinator of the Ph.D Course in Civil Eng. of the University of Pavia from 1994 to 2016.
He served as President of the European Association for the Control of Structures from 1993 to 2008, and as President of the International Association, IASC, from 2000 to 2004.
F. Casciati is editor of Smart Structures and Systems, and member of the Editorial Board of Structural Safety, J. of Structural Control & Health Monitoring, Computers & Structures, J. of Earthquake Engineering and Engineering Vibration.

Dominique Eyheramendy
Laboratoire de Mécanique et d"Acoustique (AMU-CNRS-ECM)
France

Dominique Eyheramendy, PhD is Professor of mechanics at Ecole Centrale de Marseille (France). He serves as Director of Laboratoire de Mécanique et d'Acoustique UMR7031 (Aix-Marseille Université, CNRS, Centrale Marseille). He formerly served as associate dean in charge of 1st and 2nd years curriculum. He graduated from the Ecole Normale Supérieure de Cachan (France) and received his PhD from the Swiss Federal institute Of Technology at Lausanne (Switzerland) in 1997. His main activities consist in developing models and methods at the border of numerical methods, software engineering and applications in mechanical engineering.

Roderick Melnik
Wilfrid Laurier University
Canada

Dr. Roderick Melnik has been Full Professor and Tier I Canada Research Chair in Mathematical Modelling in the Faculty of Science at the Wilfrid Laurier University in Waterloo, Canada since 2004. He is also affiliated with the Guelph-Waterloo Institute of Physics, University of Waterloo, and University of Guelph. Prior to his current appointment, Dr. Melnik held full professorial positions in the USA and Denmark. Starting his academic career in Europe, he continued it in Australia until in the late 1990s he took the position of senior scientist at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Sydney. Dr. Melnik has published extensively in a variety of fields with his major focus on mathematical modelling for challenging problems in science and technology. Dr. Melnik is the recipient of many awards, including a number of prestigious fellowships outside of Canada, in Italy, Denmark, England and Spain. He has served on editorial boards of many international journals and book series. Currently, Dr. Melnik is the Director of the MS2Discovery Interdisciplinary Research Institute in Waterloo, Canada.

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April 23 - 27, 2018
Mini-Course on Modeling Cellular Systems

April 30 - May 4, 2018
Workshop on Modeling Biological Phenomena from Nano to Macro Scales

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May 22 - 24, 2018
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May 28 - 31, 2018
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Bjorn Birnir - University of California, Santa Barbara
Ana Carpio - Complutense University of Madrid
Mitchell Luskin - University of Minnesota
Roderick Melnik - MS2Discovery Institute, WLU, Waterloo

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Focus Program on Nanoscale Systems and Coupled Phenomena: Mathematical Analysis, Modeling, and Applications

April 1 - May 31, 2018

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Physical and biological nanoscale systems and associated quantum phenomena are ubiquitous in nature and a man-made world. Today, they are becoming critically important in many key areas of human well-being, including environmental sustainability, alternative energy sources, and medicine. State-of-the-art approaches and methods of mathematics with the development and analysis of coupled mathematical models in this field provide a fundamental ingredient for our better understanding of such systems and their efficient applications. By bringing together some of the world's leading researchers in the field, this focus program is devoted to the study of such systems, their mathematical analysis, modelling, and applications.

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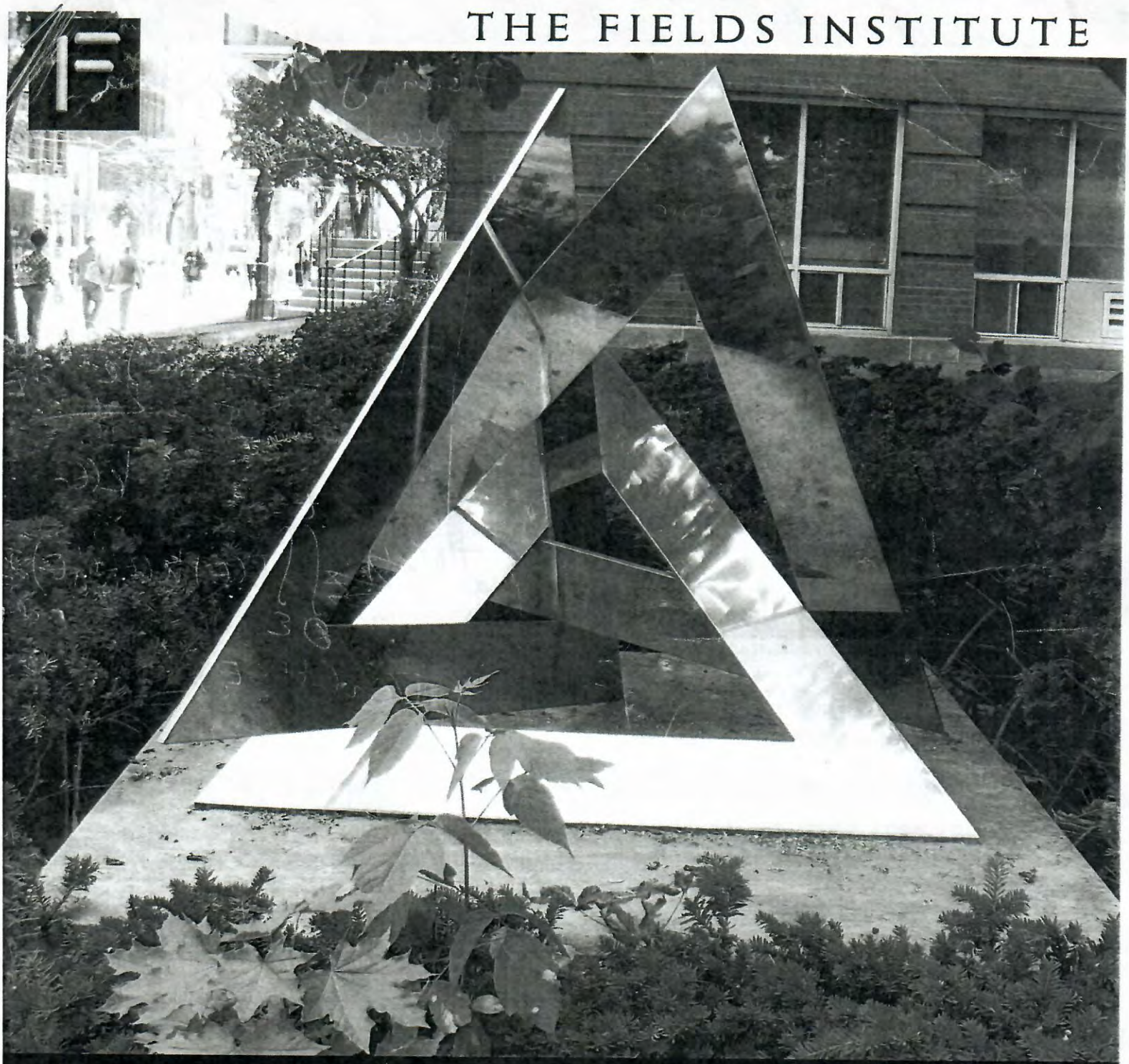

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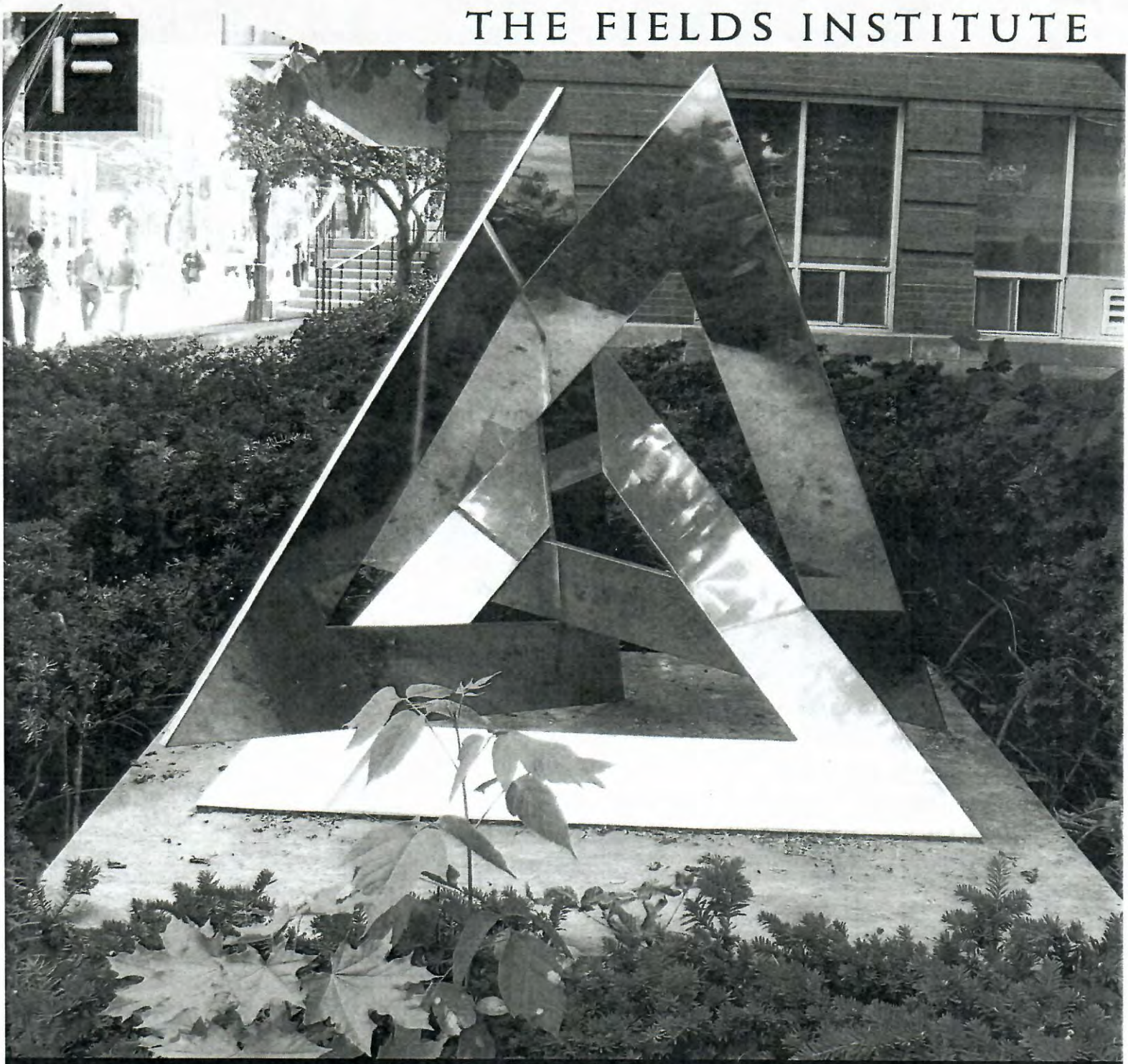

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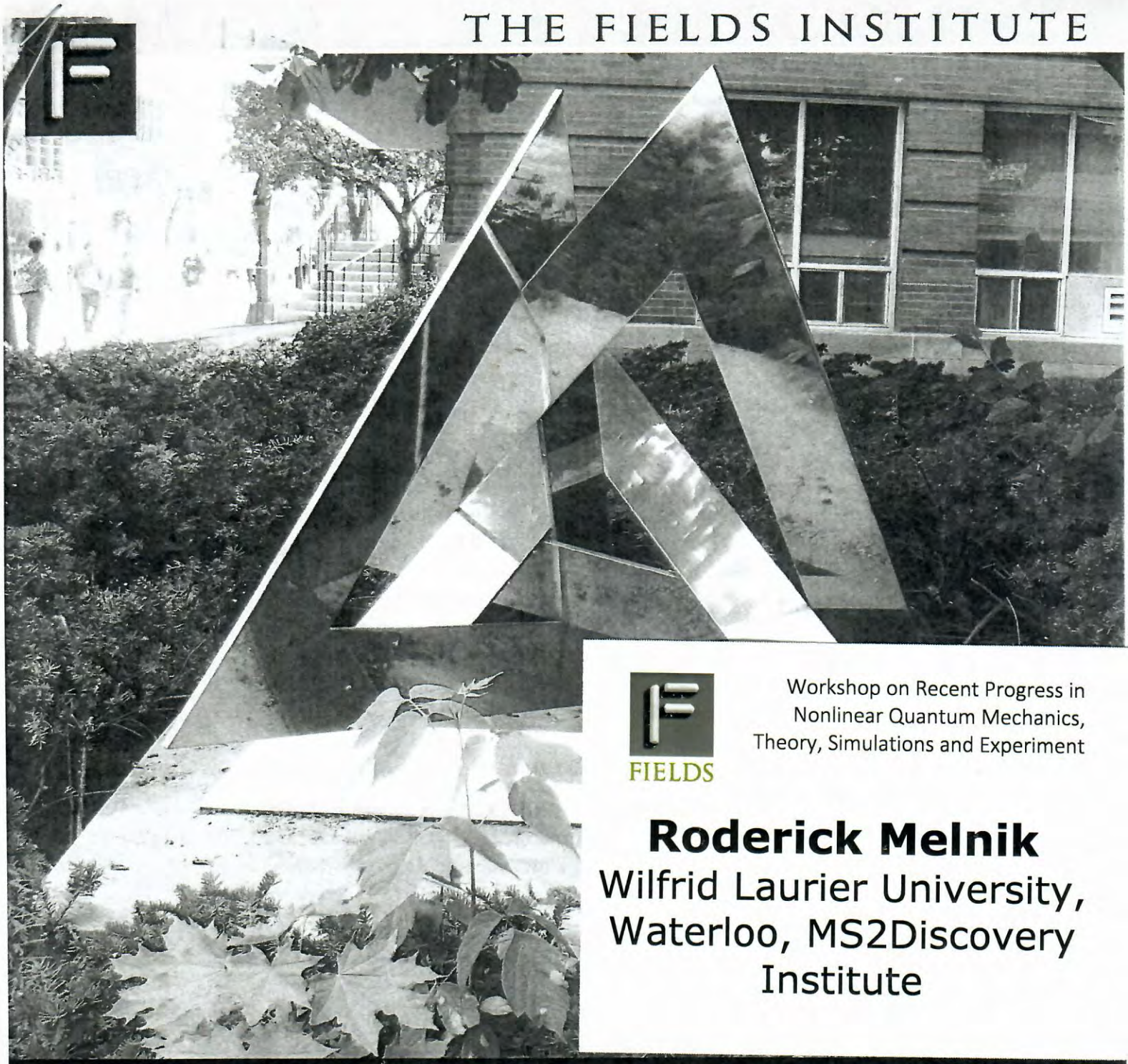

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Roderick Melnik

Wilfrid Laurier University, Waterloo, MS2Discovery Institute

Workshop on Recent Progress in Nonlinear Quantum Mechanics, Theory, Simulations and Experiment

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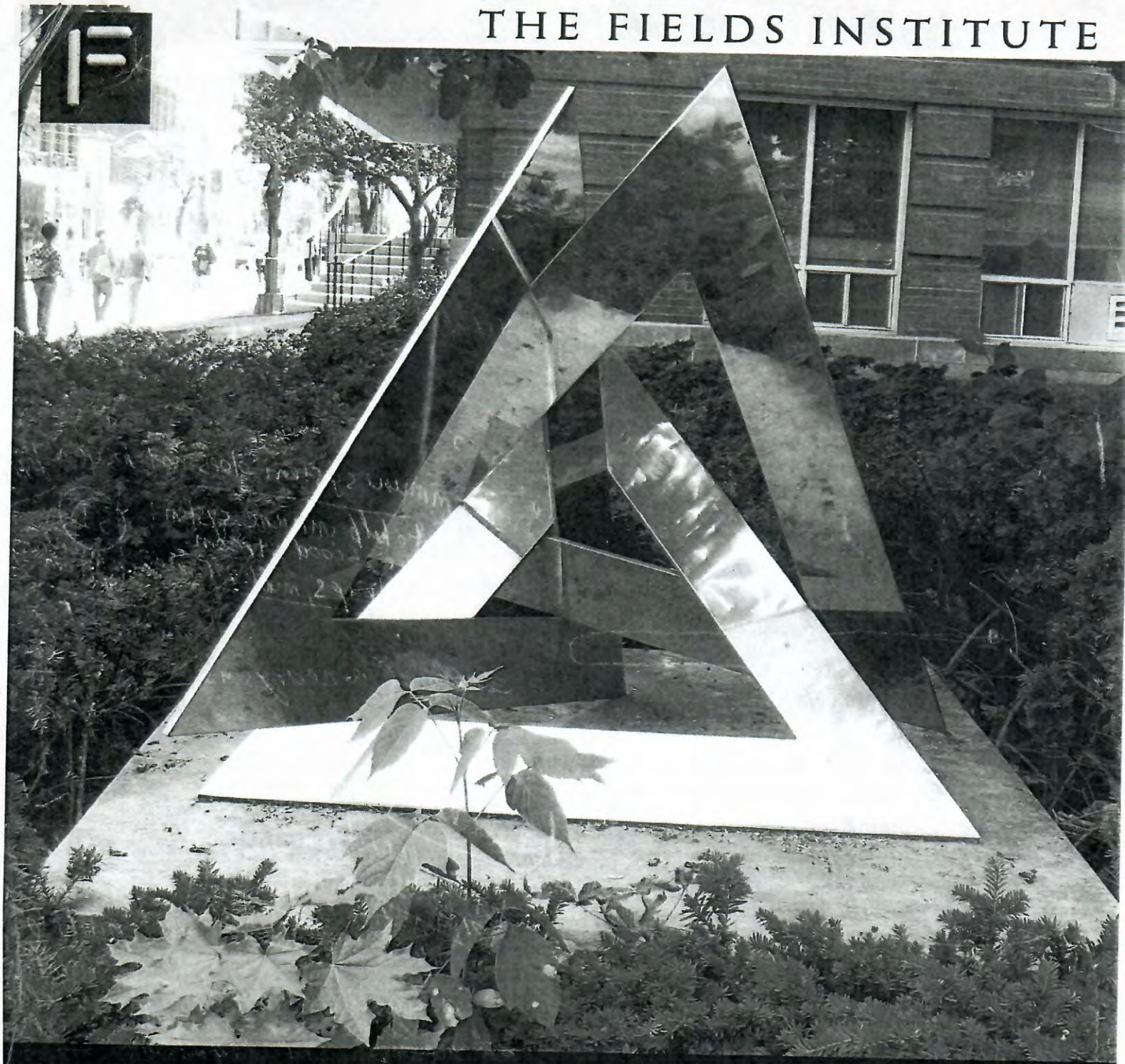

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Zoran Miskovic - University of Waterloo
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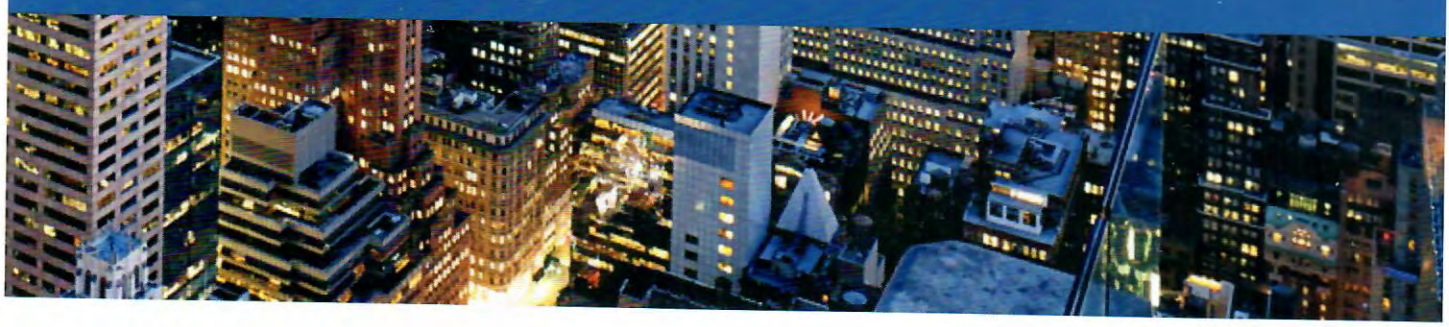

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510 Multidisciplinary Alliance in Biosciences: Modeling, Computing, Technology and Clinical Applications

***Riccardo Sacco**, Politecnico di Milano*
***Giovanna Guidoboni**, Indiana University and Purdue University at Indianapolis*
***Roderick Melnik**, Wilfrid Laurier University*

Life sciences are the crossroad for a multitude of disciplines: molecular biology, electrochemistry, mechanics, medicine, statistics, clinics, to name a few, so that a new winning vision for the next decade must rely upon a solid multidisciplinary alliance. Mathematical, statistical and computational modeling and methods have taken a leadership role in this alliance due to a number of factors: (1) mathematics is a universal language that makes the common denominator of scientific disciplines; (2) modeling based on solid biophysical and mathematical assumptions allows to design a virtual laboratory to investigate and compare different scenarios and solutions; (3) advanced computational techniques allow to numerically solve the formulated mathematical model producing the quantitative outcome to compare simulation and experimental data, answer open questions, assess or confute conjectures. In this minisymposium we aim at providing a forum in biosciences to facilitate: (a) break the barriers among disciplines; (b) confront different applications and related modeling approaches, including mechanistic and statistical formulations based on partial and/or ordinary differential equations, as well as other models; (c) illustrate the most recent and advanced computational methods; (d) validate models and methods in the simulation of complex problems. The organizers welcome contributions in all areas of modelling in biosciences and quantitative analysis in clinical applications and experiments. Subjects of this minisymposium comprise, but are not limited to: theoretical analysis and numerical approximation of differential systems and other models in biosciences and biotechnology; high-performance scientific computing and software implementation; imaging techniques and data analysis with statistical methods.

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TS 3: MONDAY EVENING, JULY 23

04:30 PM	04:50 PM	05:10 PM	05:30 PM	05:50 PM	06:10 PM
FLR 7: Liberty	**#MS501**	**Biomechanics and Mechanobiology of Soft Tissues, Chair(s): Chair 1: Rafael Grytz & Chair 2: Ellen Kuhl**			
Modelling the Biomechanics of the Eye after Strabismus Surgery	Investigating the Effect of Local Vision-Guided Scleral Remodeling on the Development of the Eye	A Versatile Hyperbolic Constitutive Framework for Soft Tissue Elasticity-Application to Skin Mechanics			
*Jorge Grasa, Begoña Calvo**	*Rafael Grytz*, Mustapha El Hamdaoui, Keyur Savla*	*Georges Limbert**			
FLR 6: Palace	**#MS504**	**Patient-Specific Computational Biomechanics: Clinical and Industrial Transfer, Chair(s): TBA**			
Three-dimensional Geometrical Characterization of Aneurysmal Location and Surface	Real-time High-Performance Robust Surgical Cutting Simulations	Automatic Constructions of Patient-specific Finite Element Models, Study of the Load Bypass Induced by TKR Implant Placement	Optimized Design of 3D Printed Trachea for Cancer Patients		
Masaharu Kobayashi, Marie Oshima, Katsuyuki Hoshina, Shu Takagi, Masaaki Shojima*	*George Turkiyyah*, Julien Abinahed, Ahmad Al-Ansari, Nicolas Haddad, Dinesh Manocha, Nikhil Navkar, Gorune Ohannessian, Zherong Pan, Georges Younes*	*Jean-Baptiste Renault*, Sébastien Parratte, Patrick Chabrand*	*Zhi Zhang*, Jaejong Park, Shaheen Islam, Alok Sutradhar*		
FLR 7: Times Square	**#MS509**	**Mechanobiology of Cells, Vesicles and Biomembranes, Chair(s): Shaofan Li**			
Multiscale Parametric Analysis of Strain Amplification in Cartilage under Different Loading and Tissue Conditions		Human Osteocyte Development during Bone Formation in a Bone-on-chip	Protein Transport in Curved Lipid Bilayer Membranes: An Extended Saffman-Delbruck Approach Incorporating Hydrodynamics in Curved Fluid Interfaces		
Vickie Shim, Sophia Leung, David Musson, Sue McGlashan, Iain Anderson, Jill Cornish*		*Elisa Budyn*, Nabila Gaci, Samantha Sanders, Morad Bensidhoum, Patrick Tauc, Bertrand Cinquin, Eric Schmidt, Herve Petite*	*Paul Atzberger, Ben Gross*, Misha Padidar*		
FLR 6: Music Box	**#MS510**	**Multidisciplinary Alliance in Biosciences: Modeling, Computing, Technology and Clinical Applications, Chair(s): Prof. Roderick Melnik**			
Photosynthesis and Its Biomedical Applications: NMR Properties of FMO Light-harvesting Complexes	Hydrodynamics and Nutrient Transport Inside a Cell-Seeded Hollow Fibre Membrane Bioreactor	Mathematical Modelling of Drug Delivery to the Targeted Organs through Bio-Absorbable Nanoparticles	Virtual Element Modeling of the Perfusion of the Lamina Cribrosa		
*Shyam Badu, Roderick Melnik**	*Prakash Kumar*, Raja Sekhar G. P.*	*Dasari Srikanth, J V Ramana Reddy*, Sint Sundar*	*Daniele Prada*, Silvia Bertoluzza*		

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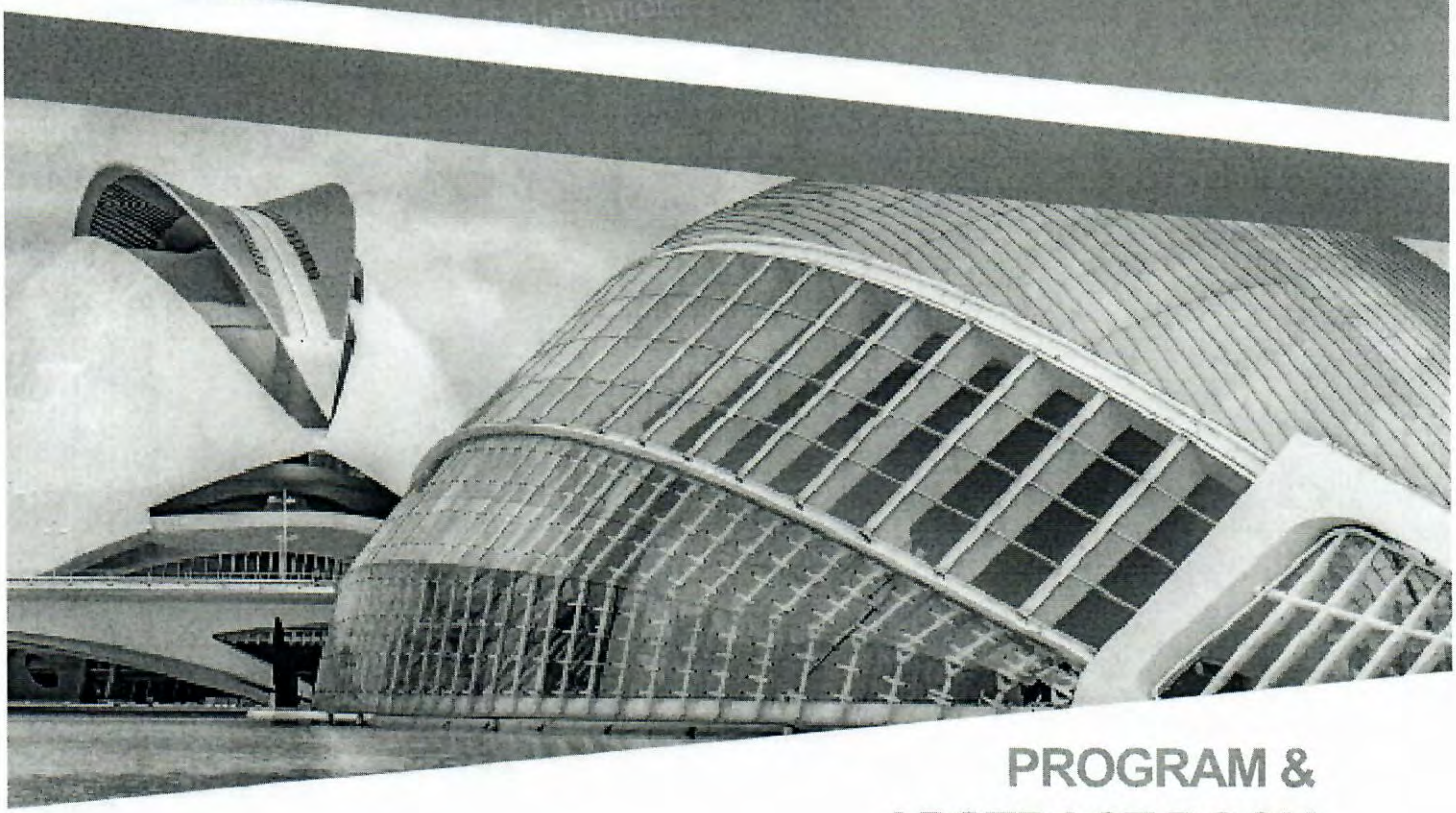

PROGRAM & ABSTRACT BOOK

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a currently challenging problem for multigrid. Emphasis will be place on the implementation aspects of the method for structured and partially structured meshes.

CP FT-1-7 4 17:00-19:00
Mathematical Topics and their Applications VI
Chair Person: Jagdish Prasad Maurya — Jorhat Engineering College

CP FT-1-7 4 1 17:00-17:20
Mathematical modelling of intensification of cyclonic wind
Jagdish Prasad Maurya — Jorhat Engineering College
Abstract: In this paper, we consider the general viscous model and present the analytical model of cyclonic winds and investigating how cyclonic winds intensify rapidly. Existence of double exponential terms are expected as the reason for the general form of viscosity. The azimuthal velocity rises fast with time close to the ground, but the rise is slower at a height little above the ground. We observe that pressure ascends with the vertical and radial distances.

CP FT-1-7 4 2 17:20-17:40
Spatial and Temporal Averaging Windows and Their Impact on Forecasting: Exactly Solvable Examples
YING LI — University of Wisconsin Madison
Samuel Stechmann — University of Wisconsin-Madison
Abstract: In making weather and climate predictions, the goal is often to predict quantities of temperature, wind speed, or rainfall after averaging in time and/or space instead of instantaneous, local value. What is the impact of spatial and/or temporal averaging on forecasting skill? Here this question is investigated using simple stochastic models that can be solved exactly analytically. Space averaging and time averaging are shown to have distinctly different impacts on prediction skill.

CP FT-1-7 4 3 17:40-18:00
Numerical Stability of s-step Enlarged Conjugate Gradient Methods
Sophie Moufawad — American University of Beirut
Abstract: In the aim of speeding-up the convergence of Krylov subspace methods on modern architectures, we present s-step enlarged Krylov subspace methods, whereby s iterations of enlarged Krylov subspace methods are merged; leading to faster convergence than Krylov methods in terms of iterations. Moreover, computing st basis vectors of enlarged Krylov subspace $K_{ks,t}(A|r_0)$ at each s-step iteration further reduces communication in parallel. We present several s-step enlarged CG versions (SRE-CG, MSDO-CG) and discuss their numerical stability.

CP FT-1-7 4 4 18:00-18:20
On time-optimal control in multibody dynamics
Philipp Eichmeir — Josef Ressel Center for Advanced Multibody Dynamics
Stefan Oberpeilsteiner — Josef Ressel Center for Advanced Multibody Dynamics
Thomas Lauß — Josef Ressel Center for Advanced Multibody Dynamics
Wolfgang Steiner — Josef Ressel Center for Advanced Multibody Dynamics
Abstract: Time-optimal control of multibody systems deals with the problem of finding control inputs minimizing the time. This task leads to a two-point boundary value problem, which is hard to solve and requires an initial guess close to the optimal solution. Instead of solving the underlying boundary value problem, we propose the adjoint-gradient method. Using the gradient information, a minimum of a cost function is found by applying the method of steepest descent or the BFGS-algorithm.

CP FT-1-7 4 5 18:20-18:40
Optimal design of piezoelectric transducers
David Ruiz — University of Castilla-La Mancha
José Carlos Bellido — University of Castilla-La Mancha
Alberto Donoso — University of Castilla-La Mancha
Abstract: The number of publications of the topic "Topology optimization" increases every year covering a wide range of applications such as: structural design, fluid-structure interaction, design of metamaterials, etc. This work presents chronologically the advances made by the research group OMEVA, from the beginning ten years ago, to the current lines. During this last decade, the works focused on piezoelectric microtransducers, working under the assumption of small deformation (static and modal analysis) and large deformation.

CP FT-1-7 4 6 18:40-19:00
Multiscale modelling of environmentally-friendly, high-performance 3D printable piezoelectric materials: challenges and applications
Andres Saez — University of Seville
Federico C. Buroni — University of Seville
Felipe Garcia Sanchez — University of Malaga
Anakkavoor K. Jagdish — Wilfrid Laurier University
Luis Rodriguez-Tembleque — University of Seville
Roderick Melnik — Wilfrid Laurier University
Abstract: We focus on the modelling of piezoelectric nanocomposites consisting of lead-free piezoelectric nanomaterials embedded in flexible matrices. The application of such materials is ranging from wearable piezoelectric energy harvesters to larger structures in civil infrastructures, replacing lead-based piezoelectrics. We develop and apply a new coupled electro-elastic model to bring together the effects of nanoscale and microstructural considerations in design of such 3D printable composites. We computationally investigate important aspects of piezoelectric composite design and performance.

SL03 19:15-20:00
The John von Neumann Prize Lecture
Chair Person: Lisa Fauci — Tulane University

19:15-20:00
A Hungarian Feast of Applied Mathematics
Margaret H. Wright — Courant Institute of Mathematical Sciences, New York University.
Abstract: If asked to name one Hungarian dish, almost everyone would say ``goulash'', even though there is no shortage of other traditional Hungarian foods. This relationship is reversed when mathematicians are asked to name John von Neumann's most important contributions. People tend to believe that his special interest was in their field, and they are often correct. The speaker will highlight a selection of areas in which von Neumann took a non-trivial interest, illustrating modern ramifications.

Wednesday sessions July, 17

IL07 08:30-09:15
Alfredo Bermúdez de Castro
Chair Person: Wil Schilders — TU Eindhoven

08:30-09:15
Some case studies in environmental and industrial mathematics
Alfredo Bermudez De Castro — Univ. Of Santiago de Compostela, Spain
Alfredo Bermúdez — Universidade de Santiago de Compstela and ITMATI
Abstract: Four case studies in environmental and industrial mathematics developed by the Mathematical Engineering research group in the University of Santiago de Compostela and ITMATI are shown. Two of them are related with fluid mechanics (submarine outfalls on the coast and gas transport in networks) and are modelled by nonlinear hyperbolic equations with source terms. The other two concern electromagnetism: magnetic hysteresis in simulation of nondestructive testing procedures and fast computing methods for electric machines.

IL08 08:30-09:15
Wolfgang Dahmen
Chair Person: Gitta Kutyniok — Technische Universität Berlin

08:30-09:15
High-Dimensional Operator Equations - Error Control and Complexity
Wolfgang Dahmen — University of South Carolina, USA
Cohen Albert — Sorbonne Universite
DeVore Ronald — Texas A & M University
Mula Olga — Universite Paris Dauphine

when groups of cells are prone to crowding and clustering. We propose a new model that accounts for clusters by determining a critical distance at which agents influence each other's actions. This model faithfully reproduces results from previously studied limiting cases and provides insight into clustering-prone parameter regimes.

CP FT-4-5 10 3 **15:10-15:30**

Dynamic changes in cells exposed to pulsed radiofrequency and focus on microtubules

Sundeep Singh — Wilfrid Laurier University
Roderick Melnik — BCAM - Basque Center for Applied Mathematics, Bilbao, Spain.Wilfrid Laurier University

Abstract: While pulsed radiofrequency (PRF) treatments are less destructive compared to their continuous counterparts, they can still adversely affect microtubules and microfilaments of the cells by both, directly (acting by PRF electric fields on their charged structures) and indirectly (causing damage to the mitochondria and degrading the microtubules and microfilaments). In this contribution we utilize a novel fully coupled thermo-electric mathematical model to quantitatively assess this phenomenon and discuss its consequences for medical applications.

CP A1-3-2 10 — 14:30-16:30

Numerical Analysis XVII

Chair Person: Antonio Pascau Llorente — EINA University of Zaragoza

CP A1-3-2 10 1 **14:30-14:50**

ENATE, a highly parallelizable scheme for transport equations

Antonio Pascau — EINA University of Zaragoza
Victor Javier Llorente — EINA University of Zaragoza

Abstract: ENATE, a numerical approximation to transport equations, has been presented to the scientific community in several papers. The scheme is exact in 1D and logically can also be employed in 2D and 3D problems. In the presentation the way to easily parallelize the scheme when used in several dimensions will be pointed out and several examples that underpin its great accuracy shown.

CP A1-3-2 10 2 **14:50-15:10**

WENO schemes using data bounded high order reconstructions.

Ritesh Dubey — Research Institute, SRMIST
Sabana Parveen — Research Institute, SRMIST

Abstract: In this work necessary conditions are deduced on non-linear weights to yield data bounded high order ENO/WENO reconstructions. These conditions are used to give data bounded region for non-linear WENO weights to be satisfied. Non-linear weights are constructed and used to construct WENO schemes up to 5th order. Numerical results show that proposed schemes captures the flow feature accurately without giving oscillations.

CP A1-3-2 10 3 **15:10-15:30**

Numerical Approximation of Nonlinear Second Order Boundary Value Problems via Hybrid Boundary Value Method

Grace O. ALAO — Covenant University
Raphael B. ADENIYI — University of Ilorin
Sheila A. BISHOP — Covenant University

Abstract: Hybrid Boundary Value Method (HyBVM) is a new scheme, based on the Linear Multistep Method (LMM). The LMM is constructed via interpolation and collocation procedures while utilizing data at both step and off-step points. The LMM is then implemented as HyBVM to approximate second order nonlinear Boundary Value Problems (BVPs) directly without necessarily converting them to their equivalent Initial Value Problems (IVPs). Also, the convergence and the stability theory of the new method are discussed.

CP A1-3-2 10 4 **15:30-15:50**

Accurate computations with h-Bernstein-Vandermonde matrices

ANA MARCO — UNIVERSIDAD DE ALCALÁ
JOSÉ-JAVIER MARTÍNEZ — UNIVERSIDAD DE ALCALÁ
RAQUEL VIAÑA — UNIVERSIDAD DE ALCALÁ

Abstract: An accurate and fast algorithm for computing the bidiagonal decomposition of strictly totally positive h-Bernstein-Vandermonde (hBV) matrices is presented. The hBV matrices are a generalization of the Vandermonde matrices obtained when replacing the monomial basis by the h-bernstein basis, a generalization of the Bernstein basis used in the area of CAGD. This bidiagonal decomposition is the initial step for solving in an accurate and efficient way several numerical linear algebra problems for these matrices.

CP A1-3-2 10 5 **15:50-16:10**

Bivariate polynomial regression by using the Bernstein basis

ANA MARCO — UNIVERSIDAD DE ALCALÁ
JOSÉ-JAVIER MARTÍNEZ — UNIVERSIDAD DE ALCALÁ
RAQUEL VIAÑA — UNIVERSIDAD DE ALCALÁ

Abstract: In this work, an algorithm for computing the bivariate regression polynomial in the bivariate tensor product Bernstein basis is given. The algorithm exploits the generalized Kronecker product structure of the Moore-Penrose inverse of the coefficient matrix of the linear system corresponding to the least squares polynomial fitting problem, and also the structure of the involved Bernstein-Vandermonde matrices. The numerical advantages of using the Bernstein basis instead of the monomial basis are shown.

CP A1-3-2 10 6 **16:10-16:30**

Accurate computation of the roots of orthogonal polynomials with totally positive Jacobi matrices

Ana Marco — Universidad de Alcalá
José-Javier Martínez — Universidad de Alcalá
Raquel Viaña — Universidad de Alcalá

Abstract: As we know from the work of Golub and Welsch, the roots of orthogonal polynomials can be computed as eigenvalues of the corresponding (symmetric and tridiagonal) Jacobi matrices. An important additional property of the Jacobi matrices, which arises in some families of orthogonal polynomials, is their total positivity. For this case it is shown how the use of algorithms for computing eigenvalues of totally positive matrices improves the accuracy of the computation of those roots.

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Session H14: Graphene: Magnetotransport

2:30 PM–5:30 PM, Tuesday, March 5, 2019
BCEC Room: 153C

Sponsoring Unit: DCMP
Chair: Erik Henriksen, Washington Univ

Abstract: H14.00010 : Aharonov-Bohm Phase and Valley Splitting in Strained Graphene P-N Junction*

4:18 PM–4:30 PM

← *Abstract* →

Presenter:
Rabindra Nepal
(University of Nebraska - Lincoln)

Authors:
Rabindra Nepal
(University of Nebraska - Lincoln)

Sanjay Prabhakar
(University of Nebraska - Lincoln)

Roderick Melnik
(The MS2Discovery Interdisciplinary Research Institute, Wilfrid Laurier University)

Alexey Kovalev
(University of Nebraska - Lincoln)

Veselago lens focusing on a graphene P-N junction is promising for the realizations of electron-optical devices such as electron lenses and electron beam splitters. We study two effects in a strained graphene layer with P-N junction: the Lorentz force due to fictitious magnetic fields and Aharonov-Bohm (AB) phase. In a strained P-N junction graphene layer, the strain induced magnetic field modifies the electron trajectories. Furthermore, the Lorentz force on electrons engenders the valley-splitting of electron beams as well as the shifting of caustics formed by refracted electron waves. We also calculate a non-zero AB phase associated with the electron beams due to a localized in-plane strain produced by a ripple. This non-zero phase is accumulated from the electrons that avoid traversing through the locally strained region and experience a non-vanishing vector potential associated with the fictitious magnetic field induced by the localized strain. We believe that these effects can be realized in a simple ballistic experiment and might be useful for mapping strain profiles by analyzing the interference pattern observed in electron-optical devices.

*NSF MRSEC Grant No. DMR-1420645, DOE DE-SC0014189, Canada Research Chair Program

IWBBIO 2019

INTERNATIONAL WORK-CONFERENCE ON BIOINFORMATICS AND BIOMEDICAL ENGINEERING

PROGRAM AND ABSTRACT

8-10 May, 2019
Granada (SPAIN)

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IWBBIO 2019

International work-conference on Bioinformatics and biomedical engineering Proceedings Extended abstracts 8-10 May,2019 Granada (SPAIN)

PROGRAM AND ABSTRACTS

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Analysis of gene regulatory networks inferred from ChIP-seq data 29
Eirini Stamoulakatou, Carlo Piccardi and Marco Masseroli

Entropy-based detection of genetic markers for bacteria genotyping 30
Marketa Nykrynova, Denisa Maderankova, Vojtech Barton, Matej Bezdicek, Martina Lengerova and Helena Skutkova

Flexible and Efficient Algorithms for Abelian Matching in Genome Sequences 30
Simone Faro and Arianna Pavone

Session B.9: Biomedical Engineering (Part III)

Analysis of the behavior of the red blood cell model in a tapered microchannel 30
Mariana Ondruov and Ivan Cimrk

A novel approach for evaluation of potential candidates for cancer therapy 30
Milena Georgieva, Bela Vasileva, Dessislava Staneva, Borislava Kukurina, George Miloshev, Kamelia Hristova-Panusheva, Milena Keremidarska-Markova, Tonya Andreeva, Giorgio Speranza, Dayong Wang and Natalia Krasteva

Radiofrequency Ablation for Treating Chronic Pain of Bones: Effects of Nerve Locations .. 31
Sundeep Singh and Roderick Melnik

Detection of Subclinical Keratoconus Using Biometric Parameters 31
Jose Sebastin Velzquez-Blzquez, Francisco Cavas-Martnez, Jorge Ali Del Barrio, Daniel G Fernndez-Pacheco, Francisco J.F. Caavate, Dolores Parras-Burgos and Jorge Ali

Relations Between Maximal Half Squat Strength and Bone Variables in a Group of Young Overweight Men 32
Antonio Pinti, Anthony Khwaja, Patchina Sabbagh, Jacques Prioux, Georges El Khoury and Rawad El Hage

Session A.10/B10: Poster Session

Therapeutic effects of melittin on atopic dermatitis in vivo and in vitro 32
H.Jin An, J.-Yeon Kim, Mi-Gyeong Gwon, Hyemin Gu, H.-Ju Kim and K.-Kyu Park

TGF-B1 and Smad oligodeoxynucleotide suppressed kidney fibrosis via regulation of epithelial/endothelial to mesenchymal transition in animal model of unilateral ureteral obstruction 33
Mi-Gyeong Gwon, Hyun-Jin An, Jung-Yeon Kim, Hyemin Gu, Hyun-Ju Kim and Kwan-Kyu Park

Bioinformatics analysis for predictions miR-15b, miR-22a, miR-20b, miR27b, miR-126, miR-130a, miR-210, miR-221, miR-222, miR-296 and Let-7f target genes and their relation with obesity and type 2 diabetes. 33
Adriana Mariel Gentile and Rajaa El Bekay Rizky

Interaction of biological systems with protein coated magnetic nanoparticles 34
Andreas Weidner, Christine Grfe, Paul Warncke, Moritz von der Lhe, Dagmar Fischer, Joachim H. Clement, Felix H. Schacher and Silvio Dutz

Correlations between sample entropy as well as atrial fibrillatory rate and CHA2DS2-VASc score in patients with atrial fibrillation 35
Rattapong Sungnoon and Narawudt Prasertwitayakij

conditions, cell begins to perform a certain type of repetitive motion. We focus on tank-treading and stretching. In this article we show that the model of red blood cell is capable of reconstruction these motions and we show quantitave and qualitative measures comparing the experimental and simulation data. We provide the analysis and description of these movements, and we study the effect of the cell's initial position on the type of motion to be performed.

A novel approach for evaluation of potential candidates for cancer therapy

Milena Georgieva, Bela Vasileva, Dessislava Staneva, Borislava Kukurina, George Miloshev, Kamelia Hristova-Panusheva, Milena Keremidarska-Markova, Tonya Andreeva, Giorgio Speranza, Dayong Wang and Natalia Krasteva

Abstract. Abstract: Nanotechnology together with the new advances in biomedical engineering has the potential to radically change the way we treat cancer. While traditional chemotherapeutics typically deliver around 0.1% of the injected drug to the tumour, nanoparticle therapies and moreover newly generated molecules for drug delivery have the potential to deliver greater amounts to the tumour by the proposed enhanced permeation and retention effect while minimizing toxicity. In this research we have evaluated the potential of novel nitrogen heterocyclic luminophores and amine-functionalized graphene oxide nanoparticles (GO-NH2) as new molecules for cancer therapy. For the purpose we have assessed the impact of a list of newly synthesized nitrogen luminophores and aminated graphene oxide (GO) sheets on the viability of different types of cancer cells, their potential to generate ROS and to influence cellular proliferation and survival. In order to elucidate their precise mechanism of action on the cellular systems we have probed their genotoxic and cytostatic properties, and compared them to control cells. Our results revealed that some of the newly synthesized nitrogen heterocyclic luminophores as well both GO samples have the potential to significantly contribute to cancer cell killing by enhancing the cytotoxicity effect exerted through the induction of ROS, subsequent DNA damage and apoptosis. Acknowledgements: The current work was supported by the National Research Foundation, bilateral project Bulgaria-China [Grant number DNTS/01/6/2016], by the Bulgarian National Research Fund [grant number: DN 19/11] and NATO Science for Peace and Security programme [grant number: NATO SPS MYP G5266]. The work was performed within the framework of COST Action CA15214 "An integrative action for multidisciplinary studies on cellular structural networks"

Radiofrequency Ablation for Treating Chronic Pain of Bones: Effects of Nerve Locations

Sundeep Singh and Roderick Melnik

Abstract. Abstract: The present study aims at evaluating the effects of target nerve location from the bone tissue during continuous radiofrequency ablation (RFA) for chronic pain relief. A generalized three-dimensional heterogeneous computational model comprising of muscle, bone and target nerve has been considered. The continuous RFA has been performed through the monopolar needle electrode placed parallel to the target nerve. Finite-element-based coupled thermo-electric analysis has been conducted to predict the electric field and temperature distributions as well as the lesion volume attained during continuous RFA application. The quasi-static approximation of the Maxwell's equations has been used to compute the electric field distribution and the Pennes bioheat equation has been used to model the heat transfer phenomenon during RFA of the target nerve. The electrical and thermo-physical properties considered in the present numerical study have been acquired from the well-characterized values available in the literature. The protocol of the RFA procedure has been adopted from the United States Food and Drug Administration (FDA) approved commercial devices available in the market and reported in the previous clinical studies. Temperature-dependent electrical conductivity along with the piecewise model of blood perfusion have been considered to correlate with the in-vivo scenarios. The numerical simulation results, presented in this work, reveal a strong dependence of lesion volume on the target nerve location from the considered bone. It is expected that the findings of this study would assist in providing a priori critical information to the clinical practitioners for enhancing the success rate of continuous RFA technique in addressing the chronic pain problems of bones.

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Computational Analysis of Pulsed Radiofrequency Ablation in Treating Chronic Pain

Sundeep Singh and Roderick Melnik

Abstract: In this paper, a parametric study has been conducted to evaluate the effects of frequency and duration of the short burst pulses during pulsed radiofrequency ablation (RFA) in treating chronic pain. Affecting the brain and nervous system, this disease remains one of the major challenges in neuroscience and clinical practice. A two-dimensional axisymmetric RFA model has been developed in which a single needle radiofrequency electrode has been inserted. A finite-element-based coupled thermo-electric analysis has been carried out utilizing the simplified Maxwell's equations and the Pennes bioheat transfer equation to compute the electric field and temperature distributions within the computational domain. Comparative studies have been carried out between the continuous and pulsed RFA to highlight the significance of pulsed RFA in chronic pain treatment. The frequencies and durations of short burst RF pulses have been varied from 1 Hz to 10 Hz and from 10 ms to 50 ms, respectively. Such values are most commonly applied in clinical practices for mitigation of chronic pain. By reporting such critical input characteristics as temperature distributions for different frequencies and durations of the RF pulses, this computational study aims at providing the first-hand accurate quantitative information to the clinicians on possible consequences in those cases where these characteristics are varied during the pulsed RFA procedure. The results demonstrate that the efficacy of pulsed RFA is significantly dependent on the duration and frequency of the RF pulses.

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University, China **15 min**	satisfying results.

B002
Roderick Melnik
MS2Discovery IRI, Wilfrid Laurier University, Waterloo, Canada
15 min

Effects of Heterogeneous Surroundings on the Efficacy of Continuous Radiofrequency for Pain Relief

Sundeep Singh | **Roderick Melnik**

This numerical study highlights the deviation between the predicted lesion volume of the homogeneous and heterogeneous models of the continuous radiofrequency (RF) procedure for pain relief. A three-dimensional computational domain comprising of a realistic anatomy of the target tissue has been considered in the present study. A comparative analysis has been conducted for three different scenarios: (a) completely homogenous domain comprising of only muscle tissue, (b) heterogeneous domain comprising of nerve and muscle tissues, and (c) heterogeneous domain comprising of bone, nerve and muscle tissues. Finiteelement-based simulations have been performed for computing the temperature and electrical field distributions during the continuous RF procedures for treating chronic pain. The predicted results reveal that the consideration of heterogeneity within the computational domain results in distorted electric field distribution and leads to the significant reduction in the attained lesion volume during the continuous RF application for pain relief.

Oral Session B-1

Tuesday, August 27th, 2019 **13:00-15:00** **Ponderosa 1001**

Conference Chair: Prof. Ian Robert McAndrew

Keynote Speech

13:00-13:45, Tuesday, August 27th, 2019

Ponderosa 1001, The University of British Columbia | Vancouver Campus

Title: Aviation Cybersecurity Issues for Unmanned Vehicles to fly Beyond the Visual Line of Sight

Prof. Ian Robert McAndrew

Capitol Technology University, Maryland, USA

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Simon Fraser University, Vancouver, June 17-19, 2019

Contributed and Invited Journal Presentations

CP1 Contributed session 1 **35**

CP1.1 Geometrical design of new auxetic 3D printable piezoelectric composite materials 35

CP1.2 Parallelized Neighbor Search with the Neighborhood Grid: A Computational Geometry Viewpoint 36

CP1.3 Volumetric Spline Parameterization for Isogeometric Analysis 37

CP1.4 Introduction to unstructured splines (U-splines) for use in computer-aided geometric design software 37

CP2 Contributed session 2 **37**

CP2.1 Dual Quaternion Surfaces 38

CP2.2 On the interference problem for ellipsoids: new closed form solutions 38

CP2.3 Rational developable surfaces 39

CP2.4 L1 splines: model, computation and recent advances 39

CP3 Contributed session 3 **39**

CP3.1 Variational Convergence of Discrete Elasticae 39

CP3.2 Quartic Bézier curves with rational offsets 40

CP3.3 Deformation of Pythagorean hodograph curves using rectifying control polygons 40

CP4 Contributed session 4 **41**

CP4.1 Rational Offsets of Regular Quadrics Revisited *(Invited CAGD 2018 Paper)* 41

CP4.2 Certified space curve fitting and trajectory planning for CNC machining with cubic B-splines *(Invited CAD 2019 Paper)* 41

CP4.3 Optimizing B-spline surfaces for developability and paneling architectural free-form surfaces *(Invited CAD 2019 Paper)* 42

CP5 Contributed session 5 **42**

CP5.1 Customization and Topology Optimization of Compression Casts/Braces on Two-Manifold Surfaces *(Invited CAD 2019 Paper)* 42

CP5.2 Automatic and high-quality surface mesh generation for CAD models *(Invited CAD 2019 Paper)* 43

CP5.3 Adaptive Slicing Based on Efficient Profile Analysis *(Invited CAD 2019 Paper)* 43

CP6 Contributed session 6 **43**

CP6.1 Support-free Elliptic Hollowing for 3D Printing via the Voronoi Diagram of Ellipses *(Invited CAD 2018 Paper)* 44

CP6.2 Curvature adaptive surface remeshing by sampling normal cycle *(Invited CAD 2019 Paper)* 44

CP7 Contributed session 7 **45**

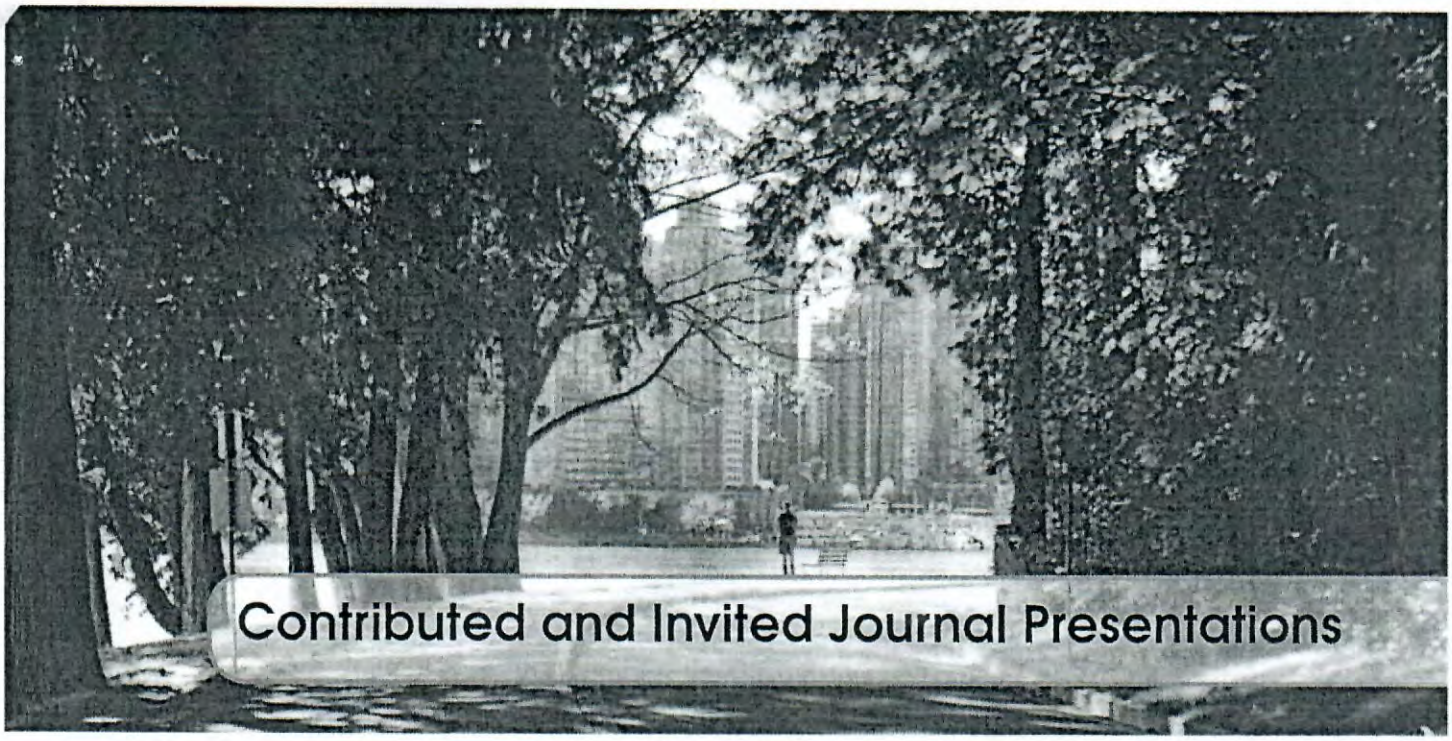
CP7.1 Discrete surfaces in sphere geometries 45

CP7.2 Bernstein-Bézier techniques for piecewise harmonic polynomials. 45

CP7.3 Shape preserving properties of weighted f-transformed systems 45

CP7.4 Convergence rates of iterative rational Hermite interpolants 46

Speakers and Organizers Index



CP1 Contributed session 1

Mon. h. 13:30-14:50 in JRS Centre 1420

Chair: Yongjie Jessica Zhang, Carnagie Mellon University, U.S.

CP1.1 Geometrical design of new auxetic 3D printable piezoelectric composite materials

Mon. h. 13:30-13:50 in JRS Centre 1420

Jagdish Krishnaswamy, Wilfrid Laurier University, Canada.
Federico C. Buroni, University of Seville, Spain.
Felipe Garcia-Sanchez, University of Malaga, Spain.
Roderick Melnik, Wilfrid Laurier University, Canada.
Luis Rodriguez-Tembleque, University of Seville, Spain.
Andres Saez, University of Seville, Spain.

3D printing has evolved as a promising manufacturing means to fabricate multiscale and auxetic materials by allowing a fine control over the micro-structured geometrical details [1]. An optimized micro-structured geometry can offer significant control over the effective properties of the macroscale material. Auxetic materials and structures have negative Poisson's ratio [2] and can offer unforeseen implications in the areas of transduction of mechanical energy. This is because of the complex interplay between the auxetic geometry of the material and its piezoelectric response. Here, we computationally explore the role of the micro-structured geometrical design of new piezoelectric composite materials. It is expected that the combination of optimized geometrical design and 3D printing can lead to the design and fabrication of auxetic piezoelectric materials with enhanced electro-elastic properties, important for novel applications in environmentally-friendly technologies [3]. The major focus of our effort is to use computational approaches to understand the complex relations between the micro-structured geometry of piezoelectric composites and the effective electro-elastic properties of the resulting auxetic materials.

References:

[1] F. Agnelli, A. Constantinescu, and G. Nika, "Optimal design of auxetic, additively manufactured, polymeric structures," arXiv preprint arXiv:1809.02467, 2018.
[2] J. Dagdelen, J. Montoya, M. de Jong, and K. Persson, "Computational prediction of new auxetic materials," Nature Communications, vol. 8, p. 323, 2017.
[3] A. K. Jagdish, F. C. Buroni, F. Garcia-Sanchez, R Melnik, L. Rodriguez-Tembleque, A. Saez, "Improving the performance of lead-free piezoelectric composites by using poly-crystalline inclusions and tuning the dielectric matrix environment" (under submission).

CP1.2 Parallelized Neighbor Search with the Neighborhood Grid: A Computational Geometry Viewpoint

Mon, h. 13:50–14:10 in JRS Centre 1420

Martin Skrodzki, Freie Universität Berlin, Germany.
Ulrich Reitebuch, Freie Universität Berlin, Germany.
Konrad Polthier, Freie Universität Berlin, Germany.

The neighborhood grid data structure has been introduced as a means for fast, parallelized computation of neighborhood approximations. It aims at contexts where speed is more important than an exact neighborhood relation. Given the wide availability of graphic cards including several hundreds or thousands of shaders, the ability for parallelization makes it well suited for applications like particle rendering, biological swarm models, or human crowd motion simulations. The data structure follows a simple building procedure. It takes a point set from some finite d-dimensional space and places each of the points in a separate cell of a cubical d-dimensional grid. Within this grid, a building algorithm sorts the cells lexicographically such that along any specific dimension neighboring cells grow monotonically when considering the entry of the included point in the dimension currently considered. The grid has reached a "stable state" when the above order relation is satisfied by all neighboring cells of the grid. When introducing the data structure, the authors gave an algorithm that iterates through all dimensions and performs a single step of a bubble sort by exchanging neighboring cells that violate the above condition. However, the authors did not prove convergence of their algorithm. In the talk, we will present this proof. More generally, we prove both an upper and a lower bound of $O(n\log(n))$ for any comparison-based building algorithm acting on n points. By providing such an algorithm, we also show its time-optimality. A previously published proof of this statement depended on the assumption that for any set of n points, a unique stable state exists. We show this assumption to be correct for n up to 9. However, we also prove it wrong for any larger n. Note that the popular data structure of k-d trees also has a building time of $O(n\log(n))$. However, at this point, parallelization plays its important role. Even with massive computing power, given n processors for n points, there is no algorithm known which builds $k-d$ trees in strictly less than $O(\log(n)^2)$. But given the same resources, the neighborhood grid needs building time of only $O(log(n))$. From a stable state of the neighborhood grid, neighborhood relations follow immediately. Given some point p in some cell in the grid, we declare all points in neighboring grid cells to be neighbors of p. This operation runs in constant time which provides an immense speed-up compared to other data structures like k-d trees, where a neighborhood look-up takes time $O(log(n))$. However, in general, the obtained neighborhood relations will not be correct. In the talk, we provide two worst-case examples: (1) two neighboring points reside at maximum distance in the neighborhood grid, (2) no two neighboring points lie within direct neighborhood relation in the neighborhood grid. The question

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COUPLED PROBLEMS 2019

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IS-Advances in Modelling Multiscale Systems and their Applications III
Invited Session organized by Roderick Melnik and Elena Akhmatskaya

MoE2
Room: Tramuntana 1+2
Chair: Elena Akhmatskaya
Co-Chair: Roderick Melnik

A Method to Solve Wave Equations with Multisingular Vortex Gaussian Initial Conditions
A. Ferrando and M.A. Garcia-March

Design of 3-D Printable Microstructured Lead-Free Piezoelectric Nanocomposites
A. Sáez, F. Buroni, L. Rodríguez-Tembleque, A. Jagdish, F. García-Sánchez and R. Melnik

Towards Effective Metabolic Engineering Using Multilevel and Probabilistic Modeling
T. Radivojevic, Z. Costello and H. Garcia Martin

Multiscale/Multiphysics Modeling of Ocular Physiology: the Eye as a Window on the Body
G. Guidoboni, L. Sala, C. Prud'homme, R. Sacco and A, Harris

IS-Algorithmic and Software Advances in Coupling Methods for Climate Models II
Invited Session organized by Pavel Bochev and Robert Jacob

MoE3
Room: Garbi 1
Chair: Kara Peterson

C-Coupler2: a Flexible and User-Friendly Community Coupler for Model Coupling and Nesting
L. Liu, C. Zhang, R. Li, B. Wang, G. Yang, C. Sun, X. Yu and H. Yu

Latest Developments of the OASIS3-MCT Coupler for Improved Performance
S. Valcke, L. Coquart, A. Craig, G. Jonville, E. Maisonnave and A. Piacentini

Flexible, Scalable, Conservative Spatial Coupling Infrastructure for Climate Models in E3SM
V. Mahadevan, I. Grindeanu, R. Jacob and J. Sarich

Data Transfer and Coupling of Native Fields with the Compadre Toolkit
P. Kuberry, M. Perego, N. Trask and P. Bochev

IS- Coupling FEA with Clinical Applications
Invited Session organized by Zohar Yosibash

MoE4
Room: Levant 1
Chair: Michael Roland

Failure Process in Metastatic Femurs by Accounting for Bone-Metastasis Interaction: a Patient-Specific Finite Element Study
C. Falcinelli, A. Gizzi, A. Di Martino and G. Vairo

An Experimental Testing Workflow for Individualized Osteosynthesis Systems
M. Roland, T. Tjardes, B. Bouillon and S. Diebels

Coupling FEA with Orthopaedic Oncology: A Fully Automated System for the Assessment the Risk of Fracture in Femurs with Metastatic Tumors
Z. Yosibash, N. Trabelsi, K. Myers and A. Sternheim

Finite Element-Based Periodic Homogenization of Cage-Like Microscaffolds for Tissue Engineering
V. Wittner, A. Ovsianikov and C. Hellmich

IS-Coupled Simulations for the Assessment of Environmental and Man-made Effects on Structures II
Invited Session organized by Roland Wüchner and Riccardo Rossi

MoE5
Room: Levant 2
Chair: Roland Wüchner
Co-Chair: Riccardo Rossi

Robustness and Challenges in 3D FSI Simulations with Chimera-Based Flow Solvers: Application to Flexible Structures in Environmental Flows
A. Ghantasala, N. K. Narayanan, R. E. Meethal, R. Wüchner and K.U. Bletzinger

Partitioned Coupling of Discrete Elements with Large Deformation Structural Finite Elements to Model Rockfall Impact on Flexible Protection Structures
K. B. Sautter, M.A. Celigueta, P. Bucher, K.U. Bletzinger and R. Wüchner

Automatic Generation of CFD Models for Wind Simulations
N Germano, G Camata, S Montelpare and R. Rossi

Fluid-Structure-Control Interaction (FSCI): General Algorithm and its Application to the Reduction of Wind-Induced Vibrations of Civil Engineering Structures
A. Winterstein, M. Péntek, K.U. Bletzinger and R. Wüchner

A 3D Two-Fluid Novel Technique for the Simulation of Free-Surface Environmental Flows
S. Wenczowski, J. Cotela, R. Wüchner, R. Zorrilla and R. Rossi

This volume contains the Technical programme of the papers accepted for presentation at the VIII International Conference on Computational Methods for Coupled Problems in Science and Engineering, COUPLED PROBLEMS 2019
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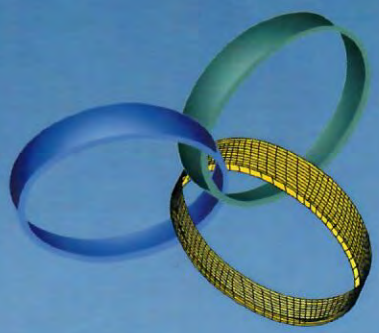

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MS10: Vibration Mitigation through Electromechanical Couplings III
Mini-Symposium organized by Boris Lossouarn and Andrea Bergamini

WeM04I02
Room: Amphi Esquillon
Chair: Boris Lossouarn
Co-Chair: Andrea Bergamini

Integration of piezostacks as frequency dependent stiffness elements in load bearing structures
J. Schmied and A. Bergamini

High voltage synthetic inductor in piezoelectric shunt to damp flexible vibrating structures
K. Dekemle, P. Van Torre and M. Loccufier

Suppression of delay-induced instabilities of digital piezoelectric vibration absorbers
G. Raze, A. Paknejad, G. Zhao, V. Broun, C. Collette and G. Kerschen

The use of negative capacitances to improve the vibration attenuation of piezoelectric resonant shunt
M. Berardengo, S. Manzoni, O. Thomas and M. Vanali

Hybridization of active control and passive resonant shunt
A. Paknejad, G. Raze, G. Zhao, M. Osée, A. Deraemaeker, F. Robert, G. Kerschen and C. Collette

Stick-slip oscillations in an electromechanical system
R. Lima and R. Sampaio

Uncertainty on joints of metamaterial assemblies undergoing flexural and longitudinal waves
A.T. Fabro, R. Sampaio and E.S. de Cursi

MS07: Modelling and Design of Smart Composite Structures I
Mini-Symposium organized by Aurelio Araujo and Filipa Moleiro

WeM04I03
Room: P3
Chair: Aurelio Araujo
Co-Chair: Roderick Melnik

Multi-dimensional models for the global-local analysis of smart layered structures. *E. Zappino and E. Carrera*

Environmentally-friendly Auxetic Piezoelectric Composites for Additive Manufacturing: Nonlocal and Nonlinear Effects
A. K. Jagdish, F. C. Buroni, F. Garcia-Sanchez, R. Melnik, L. Rodriguez-Tembleque and A. Saez

Process and Structural Health Monitoring of a "smart" Polymer-Matrix Composite using an in-situ piezoelectric sensor.
C. Tuloup, W. Harizi, Z. Aboura, Y. Meyer and K. Khellil (no ex-situ)

Design of Electro-Viscoelastic Sandwich Panels for Noise Reduction
F. Vieira and A.L. Araujo

Optimization of piezoelectric patches with passive shunted damping for noise reduction in sandwich panels. *A.L. Araujo and J.F.A. Madeira*

ACELAN-COMPOS Package for Finite Element Simulation of Active Composite Materials. *A. V. Nasedkin*

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Conference Archives

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VIEW CONFERENCE DETAILS

Cardiac tissue deformation and the efficacy of radiofrequency ablation

Sundeep Singh[1], Roderick Melnik[2]

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Minimally invasive radiofrequency cardiac ablation (RFCA) has emerged as one of the most promising and efficient modalities for treating certain types of cardiac arrhythmias. During RFCA, a catheter is navigated into the heart to locally heat and destroy tissue regions that generate or propagate arrhythmia. Computational modeling and simulations play a significant role in the design and development of new systems along with the improvement and optimization of the existing protocols of RFCA. Most modeling studies on RFCA reported till date have clearly neglected the influence of tissue deformation due to the insertion of the catheter. In a quest for minimizing the deviations between the numerically predicted and experimentally obtained lesion volumes during the RFCA, we report a fully coupled electro-thermo-mechanical model that accounts for the tissue deformation. The computational domain comprises of the cardiac tissue and the cardiac chamber in which the catheter has been inserted that is surrounded by the circulating blood (cardiac chamber). Moreover, in order to precisely predict the treatment outcomes during RFCA, temperature-dependent electrical and thermal conductivities, heat capacity, and blood perfusion rate have been considered. In this contribution, we quantify the effect of linearly elastic and hyperelastic models of myocardium tissue on the efficacy of the RFCA. We also systematically investigate the effects of blood flow, elastic modulus of myocardium tissue and tissue-catheter contact force on the lesion volume obtained from the fully coupled model of RFCA. The results obtained from this numerical study predict that the efficacy of RFCA is significantly dependent on the electro-thermo-mechanical parameters and the material models of the cardiac tissue.