Editor

Jerzy Balicki

Advances in Applied *and* Pure Mathematics

Advances in Applied and Pure Mathematics

- Proceedings of the 2nd International Conference on Mathematical, Computational and Statistical Sciences (MCSS '14)
- Proceedings of the 7th International Conference on Finite Differences, Finite Elements, Finite Volumes, Boundary Elements (F-and-B '14)

Gdansk, Poland, May 15-17, 2014

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Preface

When one reads through the current literature on computer science, artificial intelligence, bioscience, and bioinformatics a common conclusion is: “the field of theses sciences is too young to be well defined, and its scope and limitations are still unknown”. So, this book grew out of a intense and fruitful discussion related to some observations from our volume about theory and practice of modern and advanced approaches. We realized that despite the interest in data bases, software engineering, distributed systems, knowledge engineering, neural networks, fuzzy systems as evident in the major scientific journals, there were no conferences of this subject in one place to intense exchange recent models, problems and techniques between scientists.

Moreover, the question of finite differences, finite elements, finite volumes, boundary elements is experiencing rapid development, which is manifested by a powerful increase in the number of applications in this field. It should be mentioned that mathematical, computational and statistical sciences complete themselves.

During
- the 15th International Conference on Neural Networks (NN '14)
- 15th International Conference on Fuzzy Systems (FS '14)
- 13th International Conference on Artificial Intelligence, Knowledge Engineering and Data Bases (AIKED '14)
- 13th International Conference on Software Engineering, Parallel and Distributed Systems (SEPADS '14)
- 7th International Conference on Finite Differences, Finite Elements, Finite Volumes, Boundary Elements (F-and-B '14)
- 2nd International Conference on Mathematical, Computational and Statistical Sciences (MCSS '14)
- 5th International Conference on Bioscience and Bioinformatics (ICBB '14)

in Gdańsk University of Technology, Poland in 2014, an extensive collection of models, methods, applications and instances were presented due to many benefits, including information technology, engineering, medicine, and education. This is particularly contemplated in this volume.

We do not claim this text is going to answer all questions about above sciences. Indeed, we see this very much as a first attempt and hopefully not the last one. We hope it will help to mature the field and inspire researches to gain a better understanding of such a new, rich, and exciting research area.

We would like to express our appreciation to all participants our conferences who contributed to this work. We are deeply grateful to professors from twenty five countries for creating a friendly atmosphere and favorable conditions during plenary lectures. Special thanks and appreciations go to supervisors of PhD students for supporting the work of them. Many valuable suggestions and proposals, which also contributed to enrich the content of this work, we have received from researchers during fruitful discussion.

To give the final shape of the work contributed some insightful and valuable comments from reviewers. Taking into account the shortcomings identified certainly allowed the authors of individual chapters for a fuller presentation of the test subject.

We do wish to thank our families for their great support during preparation of this work.

Jerzy Balicki
Gdańsk, May 2014

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Plenary Lecture 1

A Reduction of Dimensionalities in Quantum Information Systems through a Combined Spacetime Four-Manifold

Professor Gregory L. Light
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Abstract: The existing research in quantum information theories largely revolves around studies of the Clifford algebra. These pursuits are founded upon the probability interpretation of the quantum wave functions so that they easily involve dimensions more than four, devoid of any physical contents of energies. In our view, the waves are the classical electromagnetic waves carrying energies in a cosmic black hole, B, that is contained in a universe $M^{[2]}$ devoid of ordinary matter, and B coincides with the familiar universe of matter $M^{[1]}$. By virtue of the geometry of quotient spaces in B, information propagation is naturally entangled. That is, we model the Universe as one combined spacetime four-manifold of particle-waves in {(t+ti,x+yi,y+zi,z+xi)}. Thus, if our geometry of a particle at (t, x, y, z) in $M^{[1]}$ carrying its wave energy around (it, iz, ix, iy) in $B \subset M^{[2]}$ is correct, then the hitherto misspecified geometries will likely hamper the development of the technologies sought for. My talk will highlight the underlying logical flows of this model of a combined spacetime four-manifold.

Brief Biography of the Speaker: Dr. Gregory L. Light is a Professor of Finance of Providence College (PC), where he has been teaching Statistics, Operations Research, among other quantitative subjects. Passionate in his subjects and caring for his students, he was nominated for the 2005 - 2006 Joseph R. Accinno Faculty Teaching Award by the PC Students Congress. Equally engaged in has been his collaborative scholarly activities with his colleagues, opening new research avenues mutually. Dr. Light received his B.A. in Economics from National Taiwan University, M.B.A. from University of Illinois, Ph.D. in Business Economics and Public Policy from University of Michigan, followed by an M.A. in Mathematics by staying at UM-Ann Arbor and then a Ph.D.-ABD in Applied Mathematics from Brown University. The dual tracks of his pursuits evolved from his interests in Mathematical Economics, Dynamical Systems and Physics. In Economics, he has proposed the analytic methodology of “relative derivatives” as an integration of elasticities in Economics with derivatives in Mathematics. In Physics, he has recently connected his “combined spacetime four-manifold” with the Standard Model. He plans to continue his interest in mathematical modeling, extending his research and enriching his teaching.

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Plenary Lecture 2

Langlands Program, Related Representation and Applications

Professor Nikolaj Glazunov
Department of Electronics
National Aviation University
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Abstract: R. Langlands conjectured that some symmetric power L-functions extend to an entire function and coincide with certain automorphic L-functions. In our talk we will consider in the Langlands framework results on relations between motivic Galois group of a field and the ring of adèles of the field. Applications to Analytic Number Theory, Calabi-Yau type varieties and cryptography will be presented.

Brief Biography of the Speaker: http://www.researchgate.net/profile/Nikolaj_Glazunov/

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Plenary Lecture 3

Linear Relation of Signals with Shifting: An Application in Finance

Professor Edi Cahyono
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Abstract: We consider two signals defined in finite and closed interval of time to define a linear relation of the two with shifting. In general when one signal is expressed in a linear form of the other with shifting, they give an error. In this talk, we investigate the relative error and the condition where one signal can be approximated by the other in a linear form. We discuss geometric interpretation of linear expression. Moreover, we focus on the possibility of the applications in economics and finance. Especially, we apply to obtain the relation of two stock, currency and index dynamics. The linear relation with shifting of two signals can be applied to predict the stock, currency and index dynamics, based on the other. We note that predicting such dynamics is very difficult, especially for high frequency data.

Brief Biography of the Speaker: He was awarded a Doctor in Applied Analysis and Mathematical Physics University of Twente, the Netherlands in 2002. Upon completion of his PhD degree, he was appointed as a Lecturer in the Department of Mathematics, Universitas Halu Oleo, Kendari Indonesia. In 2010 he was promoted to Professor of Industrial and Applied Mathematics. His main research areas are focused on Partial Differential Equations and applications. For the case of diffusion equation, he has applied it for modeling of wood drying in an industry. Currently, he has been working on the relation of fundamental solution type with temporal probability density function of stock, currency and index dynamics.

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Plenary Lecture 4

Making an Analogy between a Multi Chain Interaction in CDW Transport and Wave Functionals to Form S-S' Pairs

Professor A. W. Beckwith
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Chongqing University
P. R. China
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Abstract: In this Plenary Lecture, we show through a numerical simulation that the massive Schwinger model used to formulate solutions to CDW transport in itself is insufficient for transport of solitons (anti-solitons) through a pinning gap model of CDW transport. We show that a model Hamiltonian with Peierls condensation energy used to couple adjacent chains (or transverse wave vectors) permits formation of solitons (anti- solitons) which could be used to transport CDW through a potential barrier. We argue tthere are analogies between this construction and the false vacuum hypothesis for showing a necessary and sufficient condition for formation of CDW soliton – anti - soliton (S-S') pairs in wave functionals This can be established via either use of the Bogomil'nyi inequality or maybe an experimental artifact which is due to the false vacuum hypothesis to obtain a 'distance between the S-S' 'charge centers'.

Brief Biography of the Speaker: http://xodusonefoundation.org/wordpress/2013/10/25/andrew-beckwith/

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Plenary Lecture 5

Obtaining Consensus of Multi-Agent Linear Dynamic Systems

Professor Maria Isabel Garcia-Planas
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Abstract: In this paper the consensus problem is considered for multi-agent systems, in which all agents have an identical linear dynamic mode that can be of any order. A generalization to the case all agents are of the same order but do not have the same linear dynamic.

Brief Biography of the Speaker: Professor Dr. Maria Isabel Garcia-Planas joined the Department of Applied Mathematics at the “Universitat Politecnica de Catalunya” Barcelona, Spain in 1981. Her work had been centered on Linear Algebra, Systems and Control Theory. She has authored over a hundred papers and serves on the referee on several scientific journals. She has been plenary Speaker in several WSEAS International Multi-Conferences as well to Euroment.

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Plenary Lecture 6

Efficient Evaluation of Sparse Jacobians by Matrix Compression

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Abstract: Many numerical methods in scientific computing require the evaluation of large sparse derivative matrices. It has been known since the seminal work of Curtis Powell and Reid (CPR) that once their sparsity pattern is known Jaconbians can be estimated on the basis of divided differences for a set carefully chosen directions. The number p of such seed directions and thus extra function evaluations can often be limited a priori to a smallish number, which is typically much smaller than the number of independent variables and unaffected by grid sizes and other discretization parameters. The cost factor p is bounded below by the maximal number of nonzeros per row, which is actually sufficient for Jacobian estimation using so-called Newsam-Ramsdell (NR) compression. The NR approach is numerically less stable than the CPR method, which was therefore preferred in practice as divided differences are strongly affected by truncation and round off errors. However now, using automatic or algorithmic differentiation, one obtains directional derivatives with working accuracy and can thus utilize the more economical NR approach. We show how this is done minimizing both the function evaluation costs and the number of arithmetic operations, while ensuring numerical stability.

Brief Biography of the Speaker: http://www.mathematik.hu-berlin.de/~griewank/

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Plenary Lecture 7

Equitability and Dependence Measures

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Abstract: Reshef et al. (Science, 2011) proposed the concept of equitability that dependence measures should satisfy: treating all types of functional relationships, linear and nonlinear, equally. Traditional measures such as Pearson's correlation prefer linear relationship and are inadequate to learn the complex structures in large data set. A novel measure, the maximal information coefficient (MIC), is proposed in Reshef et al. (2011). Recently, Kinney and Atwal (Proceedings of the National Academy of Sciences of the United States of America, 2014) showed that MIC is in fact not equitable under a strict mathematical definition. They showed that the equitability is satisfied by a fundamental quantity in information theory, the mutual information (MI). We discuss the equitability and other theoretical properties of several state-of-art dependence measures including MI, MIC and distance correlation (dcor). The relationship between equitability and copula based dependence measures is clarified. The mathematical properties of a new dependence measure, the copula correlation (Ccor), are studied and compared with existing measures. Ccor is equitable, and reflects correctly the proportion of deterministic relationships hidden in stochastic noise.

Brief Biography of the Speaker: Adam Ding received his Ph.D. degree from Cornell University in 1996. Since then, he has been a faculty member with the Mathematics Department of Northeastern University. He had hold visiting faculty positions in Harvard University and University of Rochester. His research focus on statistical methodology and applications in biostatistics, engineering and finance.

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Plenary Lecture 8

Wavelet Based Risk Measures

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Abstract: This research tests two wavelet based risk measures. The advantages of wavelet methodologies are multiple scale analysis and no need for a priori assumptions about the data distribution. While the first of the methodologies measures wavelet-based realized volatility at multiple time scale, the second additionally accounts for the higher order cumulants. A comparison of the two methods quantifies the horizon trade-offs for portfolio optimization. Wavelet-based estimators have been used very successfully for estimating scaling behavior. These estimators are blind to superimposed polynomial trends and are also very robust when the shape of the underlying distribution is changed (Abry et al.1998). The Wavelet Transform Modulus Maxima (WTMM) method allows us to build an estimator that is based on the local maxima of the continuous wavelet transform. This method has proven very efficient to compute the singularity spectrum of multifractal signals. And as shown by Audit et al. (2002) a WTMM estimator is a very good candidate for analyzing real data without any prior assumptions regarding the distribution type.

Brief Biography of the Speaker:
CEEL program in Adaptive Economic Dynamics, University of Trento 2012
MSRI Berkeley Workshop Percolation & Interactive Systems 2012
University of Brunei Darussalam/IBM Global Sustainability Summer School 2011
Santa Fe Institute & Institute of Theoretical Physics Beijing
Complex Systems Summer School 2007
Kent State University PhD Finance 2003
University of Pittsburgh, Katz Graduate School of Business MBA 1995
University Of Sofia Bulgaria; ABD microbiology 1991
Saint Petersburg State Medical Academy, Russia MD 1985

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Plenary Lecture 9

Kinetics of Structural Transformations in Nano-Structured Intermetallics: Atomistic Simulations

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Interdisciplinary Centre for Materials Modelling
M. Smoluchowski Institute of Physics
Jagiellonian University in Krakow
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Abstract: Kinetics of vacancy-mediated atomic ordering processes in nano-layered L10 and triple-defect B2 ordered intermetallics was the subject of extensive atomistic simulations. The two groups of systems differ substantially in their vacancy thermodynamics: very low and very high vacancy concentration is observed in L10 and triple-defect B2 intermetallics, respectively. Special attention was focused on the analysis of an effect of free surfaces on superstructure stability and defect concentration in the examined materials.
Two models of L10-ordered FePt intermetallic: Ising-type model with two-body interactions and a model with many-body interactions based on Analytic Bond-Order Potentials (ABOP) were simulated by the Quasi-Kinetic Monte Carlo (q-KMC) technique implemented with the vacancy mechanism of atomic migration. For the ABOP model the method was combined with Molecular Statics (MS). Simulation of “order-order” kinetics in [001]-oriented FePt nanolayers initially perfectly ordered in the c-variant L10 and modelled with two-body interactions revealed a tendency for superstructure transformation from c-variant (monoatomic planes parallel to the (001) free surface) to a- and b-variants (monoatomic planes perpendicular to the (001) free surface) (Fig.1) [1]. The transformation showed complex kinetics which, except for uniform (bulk-like) disordering, involved three processes: (i) nucleation of a- and b-variant L10 domains at the surface being initially a single atomic Fe layer, (ii) slow fluctuating growth of the nucleated a- and b-variant L10 domains inward the layer and (iii) relaxation of the microstructure of the surface domains. In sufficiently thin layers, a percolation of the a- or b-variant superstructure domain nucleated at the surface through the layered sample was observed.

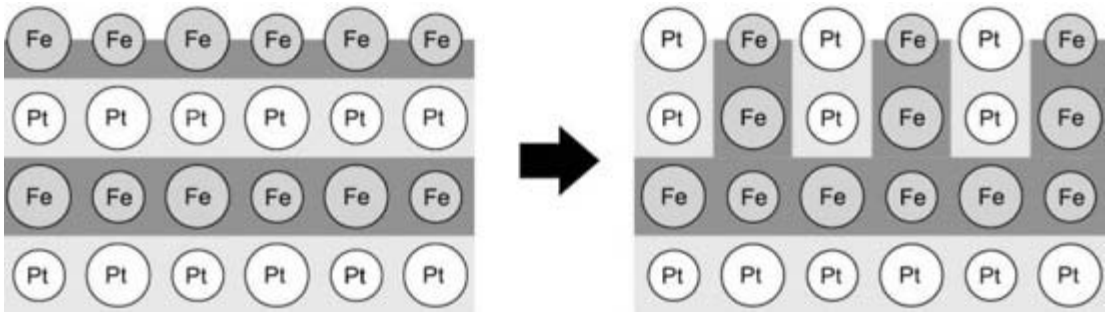

Fig.1. Scheme of an initial stage of L10 c-variant/a(b)-variant transformation in a FePt layer (atoms residing on two nn crystallographic planes are represented by small and big circles) [1].

MC simulations of ABOP-based model of the same L10 FePt layers revealed strong attraction of vacancies by free surfaces. Complex atomic ordering kinetics was observed. Initially fast partial disordering of an internal part of a layer was followed by surface disordering with no L10 c-variant to a(b)-variant transformation. The transformation, however, was observed in additional Monte Carlo/Static Relaxation simulations performed with the direct exchange algorithm [2,3].
The configurational energy of (001)-oriented FePt layers L10-ordered in c- and a(b)-variants was calculated with (i) an Ising-type model, (ii) an ABOP model and (iii) a DFT-based model. In all cases, a- and b-variants of L10 resulted in being energetically stable.
Remarkably, the L10 c-variant -> a(b)-vasriant transformation was experimentally observed in FePt epitaxially deposited multilayers [4].

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Triple-defect formation in B2-ordered NiAl intermetallic compound results from a strong asymmetry between the formation energies of Ni- and Al-antisite defects. Chemical disordering in the system is strictly correlated with vacancy formation, which is the reason for the very high vacancy concentration. As a consequence, Kinetic Monte Carlo (KMC) simulation of ordering occurring in the system and controlled by atomic migration via the vacancy mechanism must involve complete vacancy thermodynamics – i.e. the simulated system must contain an equilibrium concentration of vacancies. NiAl was modelled with an Ising-type Hamiltonian and the temperature-dependent equilibrium concentration of vacancies was determined by means of Semi Grand Canonical Monte Carlo (SGCMC) simulations [5], which assured consistency of the entire approach. The SGCMC simulations led to the evaluation of nearest-neighbour (nn) pair-interaction energies generating the triple-defect behavior of the system. The system generated and modelled in the same way as in the SGCMC was then simulated by KMC for “order-order” kinetics. The procedure required in addition the determination of saddle-point energies assigned to particular atomic jumps to nn vacancies. Their values were estimated in relation to the nn pair-interaction energies with reference to MS simulations performed for NiAl with embedded atom method (EAM) energetics.
The procedure was comparatively applied to bulk and nano-layered B2 AB systems. In both cases, the KMC simulations were started from a configuration with no antisite defects and vacancies (whose number resulted from SGCMC) distributed at random. The results elucidated the role of triple-defect formation as the atomistic-scale origin of the experimentally observed (surprising) low rate of “order-order” kinetics in bulk NiAl. The simulated “order-order” kinetics showed two stages: (i) extremely fast generation of triple defects – i.e. creation af A-antisite defects and related shift of almost all B-vacancies to A-sublattice; the process, which, however, did not lead the system to thermodynamic equilibrium, (ii) extremely slow continuation of the process towards thermodynamic equilibrium – i.e. equilibrium concentration and configuration of antiside defects and vacancies (Fig.2).

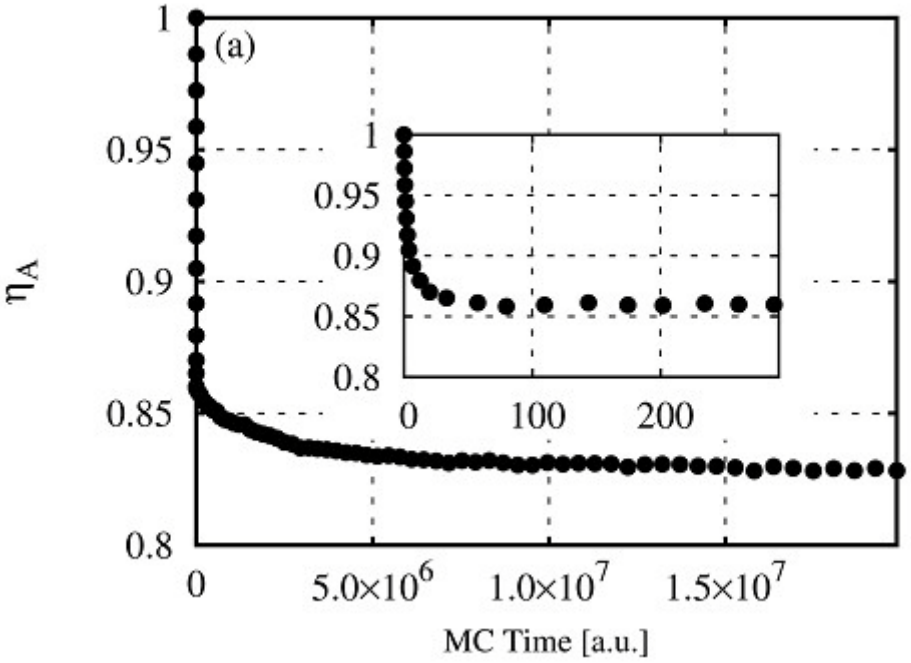

Fig.2. KMC simulated “order-order” kinetics in B2-ordering triple-defect binary AB system: ηA is a Bragg-Williams-type long-range order parameter [6,7].

It was shown that the slow rate of the stage (ii) was due to extremely low efficiency of disordering jumps of A-atoms, which were reversed with very high probability resulting from numerous vacancies residing on A-sublattice. It is claimed that only the stage (ii) of “order-order” kinetics is observed experimentally.
In nano-layers, an additional effect of vacancy segregation on free surfaces and its influence on ordering kinetics was modelled and compared with the related Molecular Dynamics results [8].

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Brief Biography of the Speaker: Prof. Rafal Kozubski academic carrier: 1984 Ph.D., Jagiellonian University in Kraków, 1987 - 1988 post-doctoral position, Strasbourg Institute of Physics and Chemistry of Materials (IPCMS), France, 1988, 1990, academic visitor, Institute for Applied Physics, Swiss Federal Institute of Technology, Zurich, Switzerland, 1993 - 1995 Lise-Meitner Fellow, Institute for Solid State Physics, University of Vienna, Austria, 1997 habilitation (DSc), Jagiellonian University in Kraków, 1997 - 2006 associate professor, 2006 - full professor in the Jagiellonian University, Kraków, 2006-2008 International Fellow, Queen's University in Belfast, 2007, 2008, 2009, 2010, 2011, 2012, 2013 Visiting professor L.Pasteur University in Strasbourg/University of Strasbourg. Research output: over 100 publications in international reviewed journals, over 140 communications on international conferences.

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Plenary Lecture 10

A Hybrid Deterministic/Probabilistic Solver for Modeling of Metal Vapor Transport in Near-Vacuum

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Abstract: Electron-beam physical vapor deposition (EB-PVD) is an established technology for producing unique material coatings for a variety of applications. In this process, a pre-selected metal ingot (the target) is vaporized in an evacuated chamber with a high power electron beam. The metal vapor flows across the high-vacuum chamber and is deposited on the component of interest (substrate). The process of vaporization and transport of metal vapors in near-vacuum involves a dense, region just above the target, which quickly expands and becomes rarefiedon route to the substrate.

This vapor transport process is characterized by increasing values of the Knudsen number, Kn, where Kn is a ratio of mean free path of atoms or molecules to a characteristic dimension, such as the target diameter (Kn = λ/D). The Knudsen number increases from a very low value on the order of 10^{-6} just above the evaporating target surface (the continuum regime), to a value around 0.01 to 10.0 (the reduced density transition regime), to Kn>10 near the substrate (the highly rarefied regime).Any attempt to create an optimal mathematical model of this processrequires successful descriptions of each of these regions. The continuum regime (around Kn< 0.01) is best described by Computational Fluid Dynamics (CFD), the deterministic solution of the Navier-Stokes equations. However, the transitional regime (around 0.01 10) is best described by a free molecular (FM) particle tracing methodology. In the modeling of the EB-PVD process, all three techniques may be needed due the extreme density gradient and highly non-ideal nature of the metal vapor.Such a solver is explored in this research.

This lecture will present ongoing research which seeks to create a hybrid code that can provide unique insights into rapidly rarefying flow fields, such asEB-PVD vapor transport. The primary goal is to gain a better understanding of the effect of model selection on predicted coating profiles in this process and determine methods to improve future modeling of this important manufacturing process. Research has concluded that the most uniform coatings are created in the transition density regime. It is due to the combination of open space to allow fast, unrestricted radial expansion and collisions to redistribute any dense regions of particles more evenly across the chamber.Results also show that extreme care must be taken when modeling EB-PVD processes for design purposes, as the incorrect choice of flow regime will yield inaccurate inlet criteria.

Brief Biography of the Speaker: Professor Kulkarni, Professor of Mechanical Engineering, joined the Department of Mechanical Engineering at The Pennsylvania State University in 1980 after completing Sc. M. and Ph. D. degrees (major: Fluid Mechanics, Minors: Applied Mathematics and Thermodynamics) from Brown University, USA. His academic areas of interest are energy, materials processing, computational fluid mechanics, indoor air pollution, and professional ethics. He also has served as the Professor-in-charge of Mechanical Engineering Graduate Program for eight years and project director for an NSF-funded Environmentally Conscious Manufacturing Graduate Research Traineeship program at Penn State among other positions. Currently, Dr. Kulkarniis a Fulbright Scholarat the Norwegian University of Science and Technology (NTNU), Norway, working on Indoor and Outdoor Fugitive Emissions in the Materials Processing Industry.

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Plenary Lecture 11

Mathematical Modeling from Algebraic Viewpoint

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Abstract: The advancement of informatization enabled the acquisition of many information via internet, and a lot of mathematical model had been proposed based on such information.
In this presentation, we introduce the method of mathematical modeling from algebraic viewpoint using Non-Negative Matrix Factorization (NMF).
The decomposition of NMF is not unique, but the effectiveness of NMF had been recognized in many field.
For this issue, we had investigated the mathematical structure of NMF, and proposed a feature extraction method using NMF in the data of network security.

Brief Biography of the Speaker: Takeshi Matsuda received Doctor of Science at Tokyo Institute of Technology in September, 2010. He was appointed as a lecturer in Faculty of Information Technology and Business, Cyber University from 2011 to 2013. And, He has been a lecture in the Department of Computer Science, Shizuoka Institute of Technology from 2013, and is engaging in the study of mathematical science, information security and educational engineering.

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Plenary Lecture 12

A Tribute to Sylvester: "Chemicographic" Representation of the Graph Matching Polynomial

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Abstract: The matching polynomial m(x) of a graph G^0 of order n, i.e. the generating function of the numbers mk of k-edge matchings of G^0, receives several types of applications in chemistry: considereing molecular graphs, it is thus invoked in either contexts of combinatoric analysis (definitions of indices for empirical structure-property relationships and chemoinformatic applications) or spectral analysis (generalization of the notion of "graph energy"). In the latter context, the matching polynomial has played a historical role by lifting the fuzziness of the notion of "aromaticity" (the effect of the cyclic character of the molecular graph on stability): in 1976, Aihara,[1] and Milun, Trinasjstic and Gutman[2] simultaneously showed that in the topological limit, aromaticity is exactly quantified by the "topological resonance energy", defined from the roots of the characteristic polynomial $P^0(x)$ of G^0, and those (all real) of the corresponding acyclic polynomial $P^{ac}(x) = x^n\, m(-x^{-2})$, for which a systematic graph interpretation was lacking.
From the Sachs theorem, the matching polynomial of a forest graph is the characteristic polynomial of a graph $G^{ac} = G^0$. A long-standing issue has thus been whether a similar representation of the acyclic polynomial could be generalized for cyclic graphs (with $G^{ac} \neq G^0$). After 36-years, the acyclic polynomial has been finally given an indirect interpretation -as a sum of characteristic polynomials-,[3] and a direct representation as the secular determinant of a "chemicograph" G^{ac}, in the Sylvester'definition of 1878.[4] G^{ac} is actually the graph of "twisting ring-opening-ring-closing metathesis product" of the molecule, resulting from "differential duplexation" ("roc product"®) and Möbius-twist (–1 edge-weighting) of G^0.[5]

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Brief Biography of the Speaker: After graduate studies in mathematics and chemistry, in 1988 he received a Ph.D. in chemistry and more precisely in the field of molecular chirality and asymmetric catalysis, under the supervision of Prof. H. B. Kagan in Orsay (France). He pursued as a post-doctoral fellow at MIT (USA) first, and then in Zürich (Switzerland) with Prof. A. Vasella. Back to France, he worked at the Roussel Uclaf company in Romainville, and by the end of 1993 came back to the academic research at the CNRS in Toulouse. In 1998, he was appointed full Professor at the Paul Sabatier University and launched a new research group at the Laboratory of Coordination Chemistry. Today author of 134 publications and running research in two different laboratories, he is involved in three experimental fields (organometallic chemistry of chiral phospho-carbon ligands, organic chemistry of functional carbo-mer molecules, organic synthesis of anti-tumoral compounds) and in several aspects of theoretical and mathematical chemistry. Beyond molecular modeling, his special focus on the continuous quantification of discrete qualitative properties (bonding, symmetry, chirality, aromaticity,...), led him to get involved in various domains of chemical mathematics, and more particularly today in spectral graph theory.

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Plenary Lecture 13

Detection of Changes in Dependent Processes: Learning from Algorithms, Simulations and Stochastic Inference

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Abstract: Many present day data are sequentially observed discrete-time processes, i.e. they represent data streams where the data associated to the nth time instant is available with negligible delay. The problem to design and study monitoring procedures which aim at detecting changes in the structure of the process has recently received substantial and growing interest. We provide an overview of recent advances in the construction of methods for change detection and their asymptotic distribution theory, which allows us to construct detection procedures with well-defined nominal statistical properties. A powerful and elegant mathematical approach is to establish limit theorems by showing that the detection algorithm of interest, often motivated by a statistical method of estimation applied to a specific distributional model, is induced (or can be approximated) by a smooth functional of a basic stochastic process such as the partial sum process or the characteristic process. In this way, one can obtain asymptotic results that hold true for rich nonparametric classes of time series. Further, we discuss simulation approaches that provide accurate distributional estimates for practical applications in cases where the asymptotic limit process is intractable. In this way, combining stochastic limit theory, simulation and applications provide a powerful approach to learn from data.

Brief Biography of the Speaker: Ansgar Steland received the M.Sc. and Ph.D. degrees in mathematics from the University of Gottingen Germany, in 1993 and 1996, respectively. He held positions as an assistant at the Technical University of Berlin, Berlin, Germany, as a consultant in industry, as a postdoc at the European University Viadrina of Frankfurt/Oder, Germany, and as a lecturer at the Faculty of Mathematics at the Ruhr-University Bochum, where he also led the statistical consulting services. Since 2006, he has been a Professor at RWTH Aachen University, Germany, where he holds the Chair of Stochastics at the Institute of Statistics. Dr. Steland has been member of several societies, headed the Department of Mathematics from 2010 to 2012, acts as the chair of the Society for Reliability, Quality and Safety, and also chairs the Working Group of Change-Point Analysis of the German Statistical Society. His current research interests are in nonparametric regression, signal and change-point detection, sequential analysis and quality control, applications to photovoltaics, empirical stochastic processes, econometrics, and time series analysis.

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Plenary Lecture 14

Explicit Finite Element Methods in Modelling of Crushing Process of FRP composite Absorbers

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Abstract: The delamination failure mode needs a three-dimensional representation of the constitutive equation and kinematics, and cannot be treated using thin shell theory. Thus, debonding and delamination are usually ignored when thin shell elements are used to model failure in composite modelling. In this research the delamination behaviour will be modelled with layers of shell elements in the box wall. Discrete non-linear spring elements will be also used to represent the through-thickness reinforcementinto the wall of composite absorbers.
Considering a real crashing scenario and the strain rate sensitivity of composite materials, various loading velocities will be applied to the rigid striker. The crushing process of stitched composite absorbers will be simulated by finite element software LS-DYNA and finally the numerical results will be verified with the relevant analytical and experimental results. The results will demonstrate the real behaviour of stitched composite box absorbers during a crash event. The critical crash loading will enable designers to improve the design of safety instruments as energy absorber components in vehicular structures to protect passengers during crash events.

Brief Biography of the Speaker: He was awarded a PhD in Composite Structures from Kingston University, London in 2009. Upon completion of his PhD degree, he was appointed as a Lecturer in Engineering Design at Kingston University London. In 2011 he was promoted to Senior Lecturer position in Composite Materials in the school of Aerospace and Aircraft Engineering. His main research areas are focused on the damage tolerance and failure modes in the laminated composite structures under various loading conditions such as buckling, post-buckling, fatigue, impact and crash. He has regularly published the outcomes of his research in more than 40 major international peer-reviewed multidisciplinary scientific journals and conferences. He is also member of EPSRC Peer Review College and acts as member of editorial board and scientific committees of international journals and conferences.

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Plenary Lecture 15

Finite Difference and Finite Element Approximations for One Nonlinear Partial Integro-Differential Equation

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Abstract: The nonlinear integro-differential equation arising in mathematical modeling of the diffusion process of an electromagnetic field into a substance is considered

$$\frac{\partial U}{\partial t}=a\left(\int_0^t\int_0^1\left(\frac{\partial U}{\partial x}\right)^2 dxd\tau\right)\frac{\partial^2 U}{\partial x^2},$$

where $a=a(S)$ is a given function defined for $S\in[0,\infty)$. If $a(S)=1+S$ the finite difference scheme and finite element method are studied for two types of initial-boundary value problems. The semi-discrete difference scheme is investigated for more general case $a(S)=(1+S)^p$, $0<p\le 1$. Some similar results for abovementioned type system are obtained in collaboration with Professors: Beny Neta, Zurab Kiguradze and Simeon Reich.

Brief Biography of the Speaker: Temur Jangveladze (Dzhangveladze) graduated from Ivane Javakhishvili Tbilisi State University (TSU) Department of Applied Mathematics and Cybernetics in 1977. He was Junior Scientific Researcher (1977-1983), Scientific Researcher (1983-1988), Senior Scientific Researcher (1988-1998), Leading Scientific Researcher (1998-present) of Ilia Vekua Institute of Applied Mathematics (VIAM) of TSU. Invited Professor (2009-present) at TSU, Professor (2010-present) at Caucasus University and Professor (2013-present) at Georgian Technical University. Since 1977 till now T.Jangveladze gives the lectures in Numerical Analysis, Numerical Solutions of Differential Equations, Nonlinear Partial Differential and Integro-Differential Models, Mathematical Modeling and etc. In 1984 he defended Ph.D. (candidate degree) thesis in specialty "Computational Mathematics". In 1998 he defended a thesis for a Doctor of Science (Habilitation) Degree in specialty "Theoretical Bases of Mathematical Modeling, Numerical Methods, Program Complexes". Field of his scientific interests is Nonlinear Differential and Integro-Differential Equations, Numerical Analysis, Nonlocal Boundary and Initial Value Problems, Mathematical Modeling and etc. The full list of his publications comprises more than 130 scientific papers and text books. He is editor and member of editorial board of several international scientific journals. He was the member of international program committee and the participant of many international scientific conferences. He is chair of the Enlarged Sessions of the Seminar of VIAM, Section of Partial Differential Equations. He is holder of various national and international grant awards. Recently he has been awarded of Fulbright Visiting Scholar Program.

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