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Preface

This year the 12th WSEAS International Conference on MATHEMATICS AND COMPUTERS IN BIOLOGY AND CHEMISTRY (MCBC '11), the 12th WSEAS International Conference on MATHEMATICS AND COMPUTERS IN BUSINESS AND ECONOMICS (MCBE '11), and the 12th WSEAS International Conference on ACOUSTICS & MUSIC: THEORY & APPLICATIONS (AMTA '11) were held at the Transilvania University of Brasov, Romania, April 11-13, 2011. The conferences provided a platform to discuss mathematical models, modelling and simulation, experiments and computer analysis, statistics, optimization, advanced mathematics, computer science, computational intelligence, bio-engineering, chemical engineering, mathematical methods, computational techniques, statistical methods, simulation, mathematical or computer analysis of experimental methods, educational topics in business and financial management, acoustics, music etc. with participants from all over the world, both from academia and from industry.

Their success is reflected in the papers received, with participants coming from several countries, allowing a real multinational multicultural exchange of experiences and ideas.

The accepted papers of these conferences are published in this Book that will be indexed by ISI. Please, check it: www.worldses.org/indexes as well as in the CD-ROM Proceedings. They will be also available in the E-Library of the WSEAS. The best papers will be also promoted in many Journals for further evaluation.

Conferences such as these can only succeed as a team effort, so the Editors want to thank the International Scientific Committee and the Reviewers for their excellent work in reviewing the papers as well as their invaluable input and advice.

The Editors

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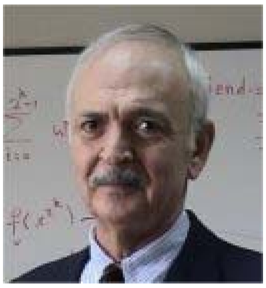
Keynote Lecture

Fluctuation Free Matrix Representation in Expectation Value Dynamical Issues and their Applications



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Abstract: Parabolic partial differential equations are encountered in many diverse fields of science and engineering and even managerial sciences, like classical or quantum wave propagations, nonequilibrium statistical mechanics, probabilistic and stochastic issues. In these aspects, they are unignorable components of the modellings in research areas like chemistry, biology, and even business and economy. These types of equations are generally first order in one coordinate which may be regarded as time and second order in some other coordinates which may be called space coordinates by following the most frequently encountered cases of modelling. Their first order temporal nature enforces them to be accompanied by an initial condition while certain boundary conditions should be imposed on spatial coordinates because of the ellipticity in their operator structures on spatial coordinates. Ellipticity means boundary value problem nature and therefore the expansions on certain orthonormal basis functions in appropriately defined Hilbert spaces can be used as the basic mathematical tools to construct the solutions. To this end the unknown solution can be considered as an infinite linear combination of the basis function varying in spatial coordinates only, with temporally changing linear combination coefficients. A complete set of basis functions in Hilbert space enables us to use the linear combination coefficients of a function as its matrix (or vector in a better terminology) representation. The linear operators mapping from the considered Hilbert space to the same space can also be given via their matrix representations. Matrix representations are important because they convert the abstractness of the Hilbert spaces to the concreteness of the Cartesian spaces. A mapping from a Hilbert space to itself can be described by an appropriately defined linear operator while its matrix representation arises as a tool mapping from a corresponding Cartesian space to itself. Thus elliptic PDE nature mapping from an appropriately defined Hilbert space to itself becomes a transformation by a matrix from a corresponding Cartesian space to itself by removing PDE related problematic issues from the scene and leaving us with the pleasent environment of the theory of matrices and linear algebra.

A parabolic PDE describes an evolution in one coordinate we call time, and therefore, it somehow defines a dynamical change, or in mechanical terminology, motion. When we use the matrix representation for the solution and elliptic part of the PDE under consideration time derivative of the unknown function becomes the time derivative of the vector coming from the unknown function's matrix representation whereas the elliptic part of that PDE becomes a time variant matrix when its matrix representation is used. Therefore the PDE and the accompanying boundary conditions define an infinite set of ODEs accompanied by an initial condition whose given vector function value at the beginning of the time comes from the matrix representation of the initial value function of the PDE. This infinite set of ODEs can be solved under the initial vector condition. However this may be considered as a formidable task because of the infinite dimensionality and we intend to truncate those ODEs appropriately to get an approximation. The numerical efficiency of this truncation based methodology completely depends on how the basis functions are constructed. This issue depends on rather modelling nature of the PDE under consideration.

What we have mentioned above is basically for the case of linear elliptic operator including PDEs. When the nonlinearity comes to the scene the matrix representations may become complicated and the tools of linear space may not work. Although there are of course some possibilities for these cases, they will be kept out of the content of this presentation.

Even in the linear case of ODEs the dimensionality may become an unpleasent problem if it grows undesiredly. Those cases can be treated in a different way by using fluctuation free matrix representation and the dimensionality growth can be suppressed accordingly in many cases. The fluctuation free matrix representation is based on fluctuationlessness theorem conjectured and proven by the presenter. It states that the matrix representation of an algebraic function operator which multiplies its operand with the function under consideration in the operator definition, is equivalent to the image of the universal matrix which is the matrix representation of the independent variable operator multiplying its operand by the independent variable, under the abovementioned function, over the same basis function set. This equivalence holds when the set is complete to span entire Hilbert space wheras any

incompleteness coming from the usage of a subset of the complete basis function set destroys this equivalence. However, even in the case of incompleteness, the deviation from the equivalence come from the fluctuation terms which are related to the differences of the matrix representations of powers of the independent variable from the same power of the matrix representation of the independent variable alone. These fluctuation terms may tend to quite rapidly vanish when the considered set approaches or gets close to the whole basis set. Hence theorem dictates the equivalence for all cases when all fluctuations are ignored. This theorem enables us to simplify the matrix representation of the PDE's elliptic part at the threshold of fluctuation free representations and therefore to construct good quality approximations. Talk will be about these issues up to certain details which can be given as much as time allows.

Brief Biography of the Speaker:
Metin Demiralp was born in Turkey on 4 May 1948. His education from elementary school to university was entirely in Turkey. He got his BS, MS, and PhD from the same institution, Istanbul Technical University. He was originally chemical engineer, however, through theoretical chemistry, applied mathematics, and computational science years he was mostly working on methodology for computational sciences and he is continuing to do so. He has a group (Group for Science and Methods of Computing) in Informatics Institute of Istanbul Technical University (he is the founder of this institute). He collaborated with the Prof. Herschel A. Rabitz's group at Princeton University (NJ, USA) at summer and winter semester breaks during the period 1985–2003 after his 14 months long postdoctoral visit to the same group in 1979–1980. Metin Demiralp has more than 90 papers in well known and prestigious scientific journals, and, more than 170 contributions to the proceedings of various international conferences. He gave many invited talks in various prestigious scientific meetings and academic institutions. He has a good scientific reputation in his country and he is one of the principal members of Turkish Academy of Sciences since 1994. He is also a member of European Mathematical Society and the chief–editor of WSEAS Transactions on Computers currently. He has also two important awards of turkish scientific establishments. The important recent foci in research areas of Metin Demiralp can be roughly listed as follows: Fluctuation Free Matrix Representations, High Dimensional Model Representations, Space Extension Methods, Data Processing via Multivariate Analytical Tools, Multivariate Numerical Integration via New Efficient Approaches, Matrix Decompositions, Multiway Array Decompositions, Enhanced Multivariate Product Representations, Quantum Optimal Control.

Plenary Lecture 1

On the Present Status of High Dimensional Model Representation as a Function Decomposer

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Abstract: High Dimensional Model Representation (HDMR) is a function decomposition method basically developed in the last two decades. Although it was first proposed by I. M. Sobol, there has been quite important contributions from H. A. Rabitz and his group. Further developments and various new varieties of HDMR were made in the Group for Science and Methods of Computing in ?Istanbul (Demiralp, Baykara, Tunga et. al.). HDMR is basically for continuous multivariate functions even though very recently linear and multilinear arrays to be decomposed. The roots of those efforts lie in the earlier studies, but not all that comprehensively.
Most prominent versions of HDMR are the Plain, Cut, Multicut, Factorized, Logarithmic, Hybrid ones. There are various successful applications of these on the practical problems coming from Engineering, Science and Physical Chemistry. The general intention is to truncate the HDMR up to and including at most the bivariate terms, although univariate truncation is preferable. The quality of this truncation increases when it dominates in the norm square of function under consideration. This urges the methodologists to develop methods for maximizing this quality via certain appropriately chosen flexibilities. Certain fruitful methods to this end have been developed. Amongst these, Transformational HDMR is the first important step. The most prominent aspect of this approach (THDMR) is the choice of appropriate transformation whose inverse is rather easily obtainable. The Logarithmic HDMR can be thought as the most elementary version of THDMR where additivity and multiplicativity can be interchanged. One of the other approaches within this framework is the affine transformation where the constancy optimization reduces certain rational approximants which can be more efficiently applicable in practice compared to Pad/e approximants. Quite recently conic transformations are brought under focus enabling comparisons with the Hermite–Pad/e approximants by utilizing approximants involving square roots. Another important flexibility to be optimized is the weight function. Univariate and multivariate cases have been investigated and quite non-linear algebraic equations have been obtained. These equations could have been approximated efficiently by using Fluctuation–Free matrix representations, and then, a perturbation expansionhas also been developed to get corrections. What is mentioned above is not the full story of the issue. There have been various interesting developments also, amongst which Enhanced Multivariance Product Representation (EMPR) and its varieties, Generalized HDMR, Discrete and Continuous HDMR and EMPR together with applications to multilinear array decompositions. The presentation will outline all this within the time limitation.

Brief Biography of the Speaker:
N. A. BAYKARA was born in Istanbul,Turkey on 29th July 1948. He received a B.Sc. degree in Chemistry from Bosphorous University in 1972. He obtained his PhD from Salford University, Greater Manchester, Lancashire,U.K. in 1977 with a thesis entitled “Studies in Self Consistent Field Molecular Orbital Theory”, Between the years 1977–1981 and 1985–1990 he worked as a research scientist in the Applied Maths Department of The Scientific Research Council of Turkey. During the years 1981-1985 he did postdoctoral research in the Chemistry Department ofMontreal University, Quebec, Canada. Since 1990 he is employed as a Staff member of Marmara University. He is now an Associate Professor of Applied Mathematics mainly teaching Numerical Analysis courses and is involved in HDMR research and is a member of Group for Science and Methods of Computing in Informatics Institute of Istanbul Technical University. Other research interests for him are “Density Functional Theory” and “Fluctuationlessness Theorem and its Applications” which he is actually involved in. Most recent of his concerns is focused at efficient remainder calculations of Taylor expansion via Fluctuation–Free ?Integration, and Fluctuation–Free Expectation Value Dynamics.