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8th Annual Meeting of the Bulgarian Section of SIAM
December 18-19, 2013
Sofia

BGSIAM'13

ABSTRACTS

HOSTED BY THE INSTITUTE OF MATHEMATICS AND INFORMATICS
BULGARIAN ACADEMY OF SCIENCES

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BGSIAM'13 Abstracts

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PREFACE

The 8th Annual Meeting of Bulgarian Section of SIAM (BGSIAM) takes part on December 18 and 19, 2013 and is hosted by the Institute of Mathematics and Informatics, Bulgarian Academy of Sciences, Sofia. The conference support provided by SIAM, as the major international organization for Industrial and Applied Mathematics, is very highly appreciated.

During the 8th Annual Meeting of BGSIAM (BGSIAM'13) a wide range of problems concerning recent achievements in the field of industrial and applied mathematics are presented.Main topics are: Numerical Methods and Algorithms; Control Systems and Applications; Partial Differential Equations and Applications; Neurosciences (Neural Networks); Equations of Mathematical Physics, etc. Following the established tradition, the conference provided a forum for exchange of ideas between scientists, who develop and study mathematical methods and algorithms, and researchers, who apply them for solving real life problems.

More than 50 participants from universities, institutes of the Bulgarian Academy of Sciences and also from outside the traditional academic departments participate in BGSIAM'13. They represent most of the strongest Bulgarian research groups in the field of industrial and applied mathematics. We are very glad to report that young researchers, Post Docs and Ph.D.students take part during BGSIAM'13. Organization of special sessions for young researchers is the main goal of BGSIAM in our future conferences.

During the 8th Annual Meeting of BGSIAM a special session is organized in order to present the problems and final reports of the 95th European Study Group with Industry (ESGI95) held in Sofia, Bulgaria, September 23-27, 2013. This study group was the first for Bulgaria and was organized by the Faculty of Mathematics and Informatics, Sofia University St. Kl. Ohridski in cooperation with the Institute of Information and Communication Technologies, Bulgarian Academy of Sciences (BAS) and the Institute of Mathematics and Informatics. The special session provided possibility for a new network between BGSIAM and European Study Groups with Industry.

Founded on January 18, 2007, the Bulgarian Section of SIAM was officially approved by the SIAM Board of Trustees on July 15, 2007. The activities of BGSIAM follow the general objectives of SIAM, as established in its Certificate of Incorporation: to further the application of mathematics to industry and science; to promote basic research in mathematics leading to new methods and techniques useful to industry and science; to provide media for the exchange of information and ideas between mathematicians and other technical and scientific personnel. The role of SIAM is very important for promotion of interdisciplinary collaboration between applied mathematics and science, engineering and technology in the Republic of Bulgaria.

LIST OF INVITED LECTURES:

- OLEG ILIEV
  Fraunhofer Institute for Industrial Mathematics, ITWM, Kaiserslautern, Germany, and KAUST, Saudi Arabia
  EFFICIENT ALGORITHMS FOR SIMULATION OF MULTISCALEPROCESSES IN POROUS ELECTRODES OF LI-ION BATTERIES

- VLADIMIR GEORGIEV
  Department of Mathematics, University of Pisa, Italy
  ON CONTINUITY OF THE SOLUTION MAP FOR THE CUBIC 1D PERIODIC NLW EQUATION

- ASSEN DONTCHEV
  Mathematical Reviews, American Mathematical Society and Department of Mathematics, University of Michigan, USA
  METRIC REGULARITY AND NEWTON'S METHOD

- PETAR POPIVANOV
  Institute of Mathematics and Informatics, Bulgarian Academy of Sciences,Bulgaria
  INVESTIGATION OF THE INTERACTION OF NONLINEAR WAVES VIA FIRST INTEGRALS

The present volume contains abstracts of the conference talks: Plenary Lectures (Part A), Contributed Talks (Part B) and list of participants (Part C).
I would like to thank to Dr. Roumyana Yordanova for her help with preparing this abstracts' booklet. Electronic version is available on the web site of BGSIAM: (http://www.math.bas.bg/IMIdocs/BGSIAM/index.html)

Angela Slavova
Chair of BGSIAM Section

Sofia, December 2013

PART A: INVITED LECTURES [1]

[1] Arranged alphabetically according to the family name of first author

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METRIC REGULARITY AND NEWTON'S METHOD

A.Dontchev

Mathematical Reviews, American Mathematical Society
and Department of Mathematics, University of Michigan, USA

After a brief review of metric regularity and its role in variational analysis, we introduce a version of Newton's method applied to generalized equations and discuss its convergence. Then we show how to extend the paradigm of the Lyusternik-Graves theorem to the framework of mappings involving Newton's sequences. We also present some recent results on superlinear convergence of Broyden's qiasi-Newton method.

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ON CONTINUITY OF THE SOLUTION MAP FOR THE CUBIC 1D PERIODIC NLW EQUATION

V.Georgiev

Department of Mathematics, University of Pisa,
Largo Bruno Pontecorvo 5, 56100 Pisa, Italy

We consider the Cauchy problems associated with the following two nonlinear equations

$$(\partial_t - |D_x|)u = \sigma|u|^2u \quad \text{for} \quad t \geq 0, \tag{1}$$

where $\sigma = \pm 1$. We shall assume that $u(t,x)$ is $2\pi-$ periodic in x. If we have solutions $u(t,x) \in C([0,T];H^s(0,2\pi))$, with $s > 1/2$, then the equation have at least two conservation laws

$$\|u(t)\|_{L^2(0,2\pi)} = const$$

and

$$\frac{1}{2}\||D|^{1/2}u(t)\|_{L^2}^2 + \frac{\sigma}{4}\|u(t)\|_{L^4}^4 = const. \tag{2}$$

Definition 1.
The problem (1) is well - posed in $H^s(0,2\pi)$ with $s \in (0,1)$ if for any $R > 0$ one can find $T = T(R) > 0$ so that for any data $u(0) = f \in H^s$ with $\|f\|_{H^s} \leq R$ one can define unique solution $u(t,x) \in C([0,T];H^s)$ so that the solution map

$$f \in B(R) = \{g \in H^s; \|g\|_{H^s} \leq R\} \to u(t,x) \in C([0,T];H^s)$$

is continuous.
A stronger property is the uniform continuity of the solution map.
Our main result is the following.
Theorem 1.
For any $s \in (1/3, 1/2)$ the Cauchy problem for

$$(\partial_t - |D_x|)u = |u|^2u \quad \text{for} \quad t \geq 0, \tag{3}$$

can not have uniformly continuous solution map in H^s.

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EFFICIENT ALGORITHMS FOR SIMULATION OF MULTISCALEPROCESSES IN POROUS ELECTRODES OF LI-ION BATTERIES

O.Iliev

Fraunhofer Institute for Industrial Mathematics, ITWM,
Kaiserslautern, Germany, and KAUST, Saudi Arabia

Li-ion batteries are widely used currently in automotive industry, in electronic devices, etc. In this talk we will discuss challenges related to the multiscale nature of batteries, mainly the treatment of the porous electrodes at pore scale and at macroscale. A mathematical model will be presented and FEM and FVM for its solution will be shortly discussed. A software tool for simulation of isothermal and non-isothermal processes in porous electrodes will be introduced. The pore scale simulations are done on 3D CT images of the porous electrodes, or on computer generated 3D microstructures which have the same characterization as real porous electrodes. Advanced mathematical techniques, such as homogenization, model reduction and reduced basis will be discussed in connection with numerical simulation of Li-ion batteries.
This is joint work with A.Latz (DLR), Y.Efendiev(Texas A&M) and M.Taralov, V.Taralova, J.Zausch, S.Zhang from Fraunhofer ITWM.

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INVESTIGATION OF THE INTERACTION OF NONLINEAR WAVES VIA FIRST INTEGRALS

P.Popivanov

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences,Bulgaria

This talk deals with the application of the first integral approach in investigating the interaction of several classes of nonlinear waves. They include resonant interaction of 3 waves and soliton (peakon) interactions. Applying Hirota direct approach one can study the resonant interaction of 2 or 3 nonlinear waves giving rize of new born waves. Those results are compared with the microlocal approach to conormal waves when new born singularity appears and propagates along the characteristic cone inscribed in the characteristic pyramide with vertex at the origin.

PART B: CONTRIBUTED TALKS [1]

[1] Arranged alphabetically according to the family name of first author

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CONTROL TECHNIQUES FOR COMPLEX CHAOTIC SYSTEMS[1]

G.Agranovich, E.Litsyn, A.Slavova

Dept. of Electrical and Electronic Engineering,
Ariel University Center of Samaria, 44837 Ariel, Israel
Department of Mathematics, Ben-Gurion University of the Negev,
Beer-Sheva, Israel
Institute of Mathematics, Bulgarian Academy of Sciences
Sofia 1113, Bulgaria

This paper is a survey of the results concerning stabilization of complex chaotic systems. First, receptor-based Cellular Nonlinear Network model with hysteresis is considered. Different mathematical models of hysteresis are presented. Dynamics and stability of the CNN model are studied from the point of view of local activity theory.Edge of chaos domain of the parameter space is found for the model. Numerical simulations and discussions about the pattern formation in such model are presented. Continuous feedback control is applied in order to stabilized the system.
Next we consider coupled FitzHugh-Nagumo neural system. First we construct Cellular Neural Network (CNN) discretized model of the system under consideration. Dynamical behavior of FitzHugh-Nagumo CNN model is investigated. Stabilization of the discretized model is proposed by feedback control which is simple for implementations. Computer simulations illustrate the obtained theoretical results.

[1]This paper is partially supported by the bilateral joint research project between Bulgarian Academy of Sciences and Israel Academy of Sciences

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TUNING FOR SCALABILITY ON HYBRID HPC CLUSTER

Emanouil Atanassov, Todor Gurov, Aneta Karaivanova, Sofiya Ivanovska, Mariya Durchova, Dobromir Georgiev, Dimitar Dimitrov

Institute of Information and Communication Technologies,
BAS Acad. G. Bonchev St., Bl.25A, 1113 Sofia, Bulgaria

The importance of the computing infrastructure is unquestionable for the development of modern science. In Bulgaria the Institute of Information and Communication Technologies in the Bulgarian Academy of Sciences play a central role in the provision of computing infrastructure and services for Bulgarian scientists and in the promotion of international collaborations in this area. In this work we present our approach in the installation and configuration of a high performance cluster with grid access at the institute, featuring state-of-the-art hardware and software for parallel computing. The cluster comprises of large pool of computational blades and two powerful GPGPU-enabled servers. Based on our analysis of the performance of the most widely used applications and use cases, we developed and tested services and techniques for optimizing the infrastructure utilization. We also present benchmarking results for the cluster and information about the main use cases and the observed usage of the cluster for scientific applications.

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THE COMPMATH COMPETITION

Stefka Bouyuklieva, Stoyan Kapralov, Mladen Manev, and Tsetska Rashkova

Technical University of Gabrovo
Gabrovo, Bulgaria

CompMath is a competition among university students in the field of Computer Mathematics. It serves as an excellent teaching tool for using computer algebra systems for solving mathematical problems.
Math education, and more generally the STEM (Science, Technology, Engineering, and Mathematics) education are of great importance to society. At the same time it is apparent that contemporary math education is in a deep crisis and that it requires a major shift from teaching manual calculation techniques towards computer-based solution techniques.
The Second National University Olympiad in Computer Mathematics (CompMath-2013) was held in October 2013 at the University of Ruse, Bulgaria. More than 80 students from 8 universities participated in the competition. They had to solve 30 math problems in 4 hours using a computer algebra system like Maple, Mathematica, MATLAB or MuPad. In accordance with the practice of the international high school student science olimpiads 50% of participants won medals.

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BICHARACTERISTIC CURVES IN 3D MODELLING OF THE LITHOSPHERE

Georgi Boyadzhiev

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences,Bulgaria

The geometrical properties of the bi-characteristic curves are employed in developing a new approach to 3D medelling of elastic piecewise homogeneous media, in particular Earth crust and upper Mantle. The method is based on tomography and the refraction, respectively, reflection, of the bi-characteristic curves at the layer boundaries of multi - layered media.

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PYTHAGOREAN TRIPLES AND QUADRUPLES VIA CONFORMAL TRANSFORMATIONS OF THE LIGHT CONES

Danail S. Brezov, Clementina D. Mladenova and Ivaïlo M. Mladenov

Department of Mathematics,
University of Architecture, Civil Engineering and Geodesy
1 Hristo Smirnenski Blvd., Sofia 1046, Bulgaria
e-mail: danail.brezov@gmail.com
Institute of Mechanics, Bulgarian Academy of Sciences
Acad. G. Bonchev Str., Bl. 4, Sofia 1113, Bulgaria
e-mail: clem@imbm.bas.bg
Institute of Biophysics,Bulgarian Academy of Sciences
Acad. G. Bonchev Str., Bl. 21, Sofia 1113, Bulgaria
e-mail: mladenov@bio21.bas.bg

In this article we propose an improved algorithm for generating primitive *Pythagorean* triples, based on a well-known construction by Barning and *Hall*. Interpreting the triples as integer points on the future light cone $\mathcal{L}_+$ in $\mathbb{R}^{2,1}$, we express the $\mathsf{O}(2,1)$ *Hall* matrices with their *vector-parameters* (or *Rodrigues' vectors*), which simplifies the calculations significantly. Similar construction is considered in the four-dimensional case of *Pythagorean* quadruples and the generalized case of relatively prime quadruples with the property $p^2+q^2=r^2+s^2$, this time involving a $\mathsf{O}(2,2)$-like analogue of the *Hall* matrices. At the end we briefly discuss some geometrical and physical aspects of the problem.

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AN ESTIMATE FROM BELOW FOR THE FIRST EIGENVALUE OF P–LAPLACIAN VIA THE HARDY INEQUALITY

Alexander Fabricant, Nikolai Kutev, Tsviatko Rangelov

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences, Sofia 1113, Bulgaria
rangelov@math.bas.bg

We consider the Dirichlet eigenvalue problem for the p–Laplacian

$$\begin{cases} -\Delta_p u &= \lambda |u|^{p-2}u \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{cases}$$

for $p > 1$ in a bounded domain $\Omega \subset R^n$, $n \geq 2$.
An approximation of λ is an important task due several applications in nonlinear eigenvalue problems and mathematical physics. Only in the case $p = 2$, i.e. p–Laplacian becomes Laplace operator, the value of λ is known with analytical formulae for domains Ω with simple geometry and with numerical approximation for more general domains.
If $p \neq 2$ the explicit value of λ is not known even for domains Ω like ball or square. Different methods for lower bound of λ are developed as isoparametric estimates or inverse power method by means of iterative techniques and corresponding numerical calculations.
In the present report we propose a new method for lower estimate of λ based on Hardy inequality with double singular kernels. For the case of a ball $\Omega = B_R$, the estimate for $p \neq n$ reads

$$\lambda(B_R) \geq \left(\frac{1}{Rp}\right)^p \left[\frac{(n-1)^{n-1}}{(p-1)^{p-1}}\right]^{\frac{p}{n-p}},$$

and was compared with known estimates obtained by other methods.

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PARALLEL ALGORITHM FOR FIELD FIRE SIMULATION

Stefka Fidanova and Pencho Marinov

Institute of Information and Communication Technologies,
BAS Acad. G. Bonchev St., Bl.25A, 1113 Sofia, Bulgaria

Every year a lot of hectares of forest are burn in Europe. Especially south part of Europe where the climate is hot and dry during the summer. Last decades with a climate change this part of the Europe becomes dryer and increase of the field fires is observed. The same problem arise in northern America. A model field fire spread can have several applications. The prevision of the fire front can help the fireman to optimize their work, and to reduce the damages. Another application is prevention. Possible scenarios can be played and the computer model can show the dangerous places. Existing models are fare to be satisfactory or they are very complicate and slow to be used in real time.
Our field fire model is based on game modeling using hexagonal cells and rules how the cell are changed during the time according neighbor cells and other conditions. We prepare parallel version of the algorithm which is run on Blue Gene supercomputer. We study the algorithm performance according number of processes and core distribution.

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APPLICATION OF NEURAL NETWORKS FOR EXPLODING MATERIALS CLASSIFICATION WITH BLASTING ACTION IN COHERENT SIGNALS EXPLOSURE

Valerij Dzhurov, Milena Kostova

University of Rousse
Rousse 7017, Bulgaria

The access control systems must have high reliability and speed. The use of neural network gives and opportunity for realization of these requirements. A neural network for classification of plastic and non-plastic materials with blasting action after explosure with coherent signals in optical range is offered.

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CUBATURE RULES FOR HARMONIC FUNCTIONS ON THE DISK USING LINE INTEGRALS OVER TWO SETS OF EQUISPACED CHORDS

Irina Georgieva

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences,
Acad. G. Bonchev, Bl. 8,
1113, Sofia, Bulgaria,
irina@math.bas.bg

Clemens Hofreither

Institute of Information and Communication Technologies,
Bulgarian Academy of Sciences,
Acad. G. Bonchev St., Bl. 25A,
1113 Sofia, Bulgaria,
chofreither@numa.uni-linz.ac.at

We consider an algebraic method for reconstruction of a function satisfying the Poisson equation with a polynomial right-hand side in the unit disk. The given data, besides the right-hand side, is assumed to be in the form of a finite number of values of Radon projections of the unknown function. We first homogenize the problem by finding a polynomial which satisfies the given Poisson equation. This leads to an interpolation problem for a harmonic function, which we solve in the space of harmonic polynomials using a previously established method. For the special case where the Radon projections are taken along chords that form a regular convex polygon, we extend the error estimates from the harmonic case to this Poisson problem. Finally we give some numerical examples.

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ON A FAMILY OF MKDV EQUATIONS RELATED TO $SO(8)$ ALGEBRA

V. S. Gerdjikov[1], D. M. Mladenov[2], A. A. Stefanov[2], S. K. Varbev[2]

[1] Institute of Nuclear Research and Nuclear Energy,
Bulgarian Academy of Sciences,
72 Tsarigradsko chausee, Sofia 1784, Bulgaria

[2] Theoretical Physics Department, Faculty of Physics,
Sofia University "St. Kliment Ohridski",
5 James Bourchier Blvd, 1164 Sofia, Bulgaria

We have derived a one-parameter family of MKdV equations related to the simple Lie algebra $so(8)$ using a Coxeter $\mathbb{Z}_6$ reduction. They admit a Lax pair

$$L\psi \equiv i\frac{\partial\psi}{\partial x} + U(x,t,\lambda)\psi = 0, \quad M\psi \equiv i\frac{\partial\psi}{\partial t} + V(x,t,\lambda)\psi = 0, \tag{1}$$

where

$$U(x,t,\lambda) = Q(x,t) - \lambda J, \qquad V(x,t,\lambda) = \sum_{s=0}^{2} \lambda^s V_s(x,t) - \lambda^3 K, \tag{2}$$

satisfying the reduction condition

$$CU(x,t,\lambda)C^{-1} = U(x,t,\omega\lambda), \qquad CV(x,t,\lambda)C^{-1} = V(x,t,\omega\lambda), \tag{3}$$

where C is the Coxeter automorphism of $so(8)$, $C^6 = \mathbb{1}$ and $\omega^6 = 1$. Next we analyze the grading of $so(8)$ introduced by the Coxeter automorphism. The corresponding one-parameter family is a system of four MKdV-type equations for the four independent coefficient functions of $Q(x,t)$. Their properties are briefly discussed.

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MKDV-TYPE EQUATIONS RELATED TO $SL(N)$ ALGEBRAS

V. S. Gerdjikov[1], D. M. Mladenov[2], A. A. Stefanov[2], S. K. Varbev[2]

[1] Institute of Nuclear Research and Nuclear Energy,
Bulgarian Academy of Sciences,
72 Tsarigradsko chausee, Sofia 1784, Bulgaria

[2] Theoretical Physics Department, Faculty of Physics,
Sofia University "St. Kliment Ohridski",
5 James Bourchier Blvd, 1164 Sofia, Bulgaria

We have derived systems of MKdV-type equations related to the simple Lie algebras $sl(n)$ using a Coxeter $\mathbb{Z}_n$ reduction. They admit a Lax pair

$$L\psi \equiv i\frac{\partial\psi}{\partial x} + U(x,t,\lambda)\psi = 0, \quad M\psi \equiv i\frac{\partial\psi}{\partial t} + V(x,t,\lambda)\psi = 0, \tag{1}$$

where

$$U(x,t,\lambda) = Q(x,t) - \lambda J, \qquad V(x,t,\lambda) = \sum_{s=0}^{2} \lambda^s V_{3-s}(x,t) - \lambda^3 K, \tag{2}$$

satisfying the reduction condition

$$CU(x,t,\lambda)C^{-1} = U(x,t,\omega\lambda), \quad CV(x,t,\lambda)C^{-1} = V(x,t,\omega\lambda). \tag{3}$$

Here C is the Coxeter automorphism of $sl(n)$ algebra, $C^n = \mathbb{1}$ and $\omega^n = 1$. Next we analyze the grading of $sl(n)$ algebra introduced by the Coxeter automorphism. The compatibility condition $[L, M] = 0$ reduces to a set of $n-1$ nonlinear evolution equations for the $n-1$ independent coefficient functions of $Q(x,t)$. Their integrability properties are briefly discussed.

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EXAMPLES OF G-STRAND EQUATIONS

Rossen Ivanov

Dublin Institute of Technology,
Ireland,

Darryl Holm

Imperial College London, UK

The G-strand equations are derived from the variational principle for a G-invariant Lagrangian, where G is at least two-parametric Lie group. The Lie group manifold is also the configuration space for the Lagrangian. The G-strand is the underlying map given by a general group element g(t; s), where t and s are the independent variables of the G-strand equations. The Euler-Poincar?e reduction of the variational principle leads to a formulation where the dependent variables of the G-strand equations take values in the corresponding Lie algebra and its co-algebra with respect to a pearing provided by the Lagrangian. In some cases the G-strand equations are completely integrable 1+1 Hamiltonian systems that admit soliton solutions. Our presentation is aimed to illustrate the construction with several simple but instructive examples, including G-strands with the following Lie groups: (i) SO(3)-strand equations for the so-called continuous spin chain. The equations reduce to the integrable chiral model in their simplest (bi-invariant) case. (ii) SO(3) - anisotropic chiral model, which is also integrable, (iii) Diff(R)-strand equations. These equations are in general non-integrable, however they admit solutions in 2 + 1 space-time with singular support (e.g., peakons). Peakon-antipeakon collisions can be solved analytically, and potentially can be applied in the theory of image registration.

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ON THE NUMERICAL SOLUTION OF TIME-FRACTIONAL BLACK-SCHOLES EQUATION

Miglena N. Koleva, Lubin G. Vulkov

University of Ruse, 8 Studentska St., 7017 Ruse, Bulgaria
e-mail:{mkoleva,lvalkov}@uni-ruse.bg

We consider the modified Rieamann-Liouville time-fractional derivative Black-Scholes model equation, with positive price of the stock S. The behavior of the solution is known for $S \to 0$ and $S \to \infty$, and the terminal price is also given. The usual change to forward time leads to right fractional derivative equation and given initial condition. Therefore, with or without change of time variable the relevant approach is based on simultaneously discretization of time and space variables and solving the full system of algebraic equations. We propose two finite difference schemes for the problem. Various numerical experiments are discussed.

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SERIES IN PRABHAKAR FUNCTIONS AND THE GEOMETRY OF THEIR CONVERGENCE

Jordanka Paneva - Konovska

Department of Applied Mathematics and Computer Science
Technical University of Sofia
1000 Sofia, Bulgaria

In 1971 Prabhakar introduced and studied a 3-index generalization of the Mittag-Leffler function. Here we consider series, defined by means of the Prabhakar functions. In studying the behaviour of such a kind of series we give their domains of convergence in the complex plane, and investigate the behaviour of the series on the boundaries of these domains. We determine where the series converges and where it does not, where the convergence is uniform and where it is not. We give analogues of the classical theorems for the power series like Cauchy-Hadamard, Abel and its converse Tauber and Littlewood, as well as Fatou type theorems. The established asymptotic formulae for the Prabhakar functions in the cases of "large" values of indices are used in the proofs of the convergence theorems for the considered series.

MSC 2010: 33E12, 31A20, 40E05, 40A30, 30B30, 30B50, 30D15, 30A10

Key Words and Phrases: Mittag-Leffler functions and generalizations, inequalities, asymptotic formula, Cauchy - Hadamard, Abel, Tauber, Littlewood and Fatou type theorems, summation of divergent series

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THEORETICAL AND NUMERICAL ASPECTS TO THE GENERALIZED SIXTH ORDER BOUSSINESQ EQUATION

N. Kutev, N. Kolkovska, M. Dimova

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences
Acad. Bonchev str., bl.8, 1113, Sofia, Bulgaria

We study the Cauchy problem to the generalized sixth order Boussinesq equation

$$\beta_2 u_{tt} - u_{xx} - \beta_1 u_{ttxx} + u_{xxxx} + \beta_3 u_{ttxxxx} = f(u)_{xx}, \quad x \in \mathbb{R},\, t \in [0,T),\; T \leq \infty, \tag{1}$$

$$u(x,0) = u_0(x), \quad u_t(x,0) = u_1(x), \qquad x \in \mathbb{R}, \tag{2}$$

where $\beta_1 \geq 0$, $\beta_2 > 0$ and $\beta_3 > 0$ are dispersive coefficients. The nonlinear term $f(u)$

$$f(u) = a|u|^p u + b|u|^{2p} u, \quad p > 0, \quad a, b = const \neq 0 \tag{3}$$

is known as generalized Bernoulli type nonlinearity.
This problem arises in a number of mathematical models of physical processes, for example in the modeling of surface waves in shallow waters and in the dynamics of nonlinear lattices.
The b.v.p. (1), (2) is completely investigated for all a and b in (3) by means of different methods. In case $b < 0$ we give a complete answer to the question about global existence or finite time blow up of the solution of (1), (2) by the well-known potential well method. In case $b > 0$, $a < 0$, $a^2 - \frac{(p+2)^2}{(p+1)} b > 0$ we suggest a new nonstandard potential well method based on new invariant sets and a new critical energy constant. For $a^2 - \frac{(p+2)^2}{(p+1)} b \leq 0$ the global existence of the solutions is obtained by the conservation law's method without any restriction on the initial energy.
The critical energy constants, crucial for the global solvability or finite time blow up in the framework of the potential well methods, are calculated explicitly.
A conservative finite difference scheme for the numerical solution of (1), (2) is proposed and studied. The performed numerical experiments illustrate and support our theoretical results.

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THREE-SOLITON INTERACTIONS FOR THE MANAKOV SYSTEM UNDER COMPOSITE EXTERNAL POTENTIALS

A. Kyuldjiev[1], V. S. Gerdjikov[1], M. D. Todorov[2]

[1]Institute for Nuclear Research and Nuclear Energy,
BAS, 1784 Sofia, Bulgaria
[2]Department of Applied Mathematics and Computer Science
Technical University of Sofia, 1000 Sofia, Bulgaria

We analyze the dynamical behavior of the 3-soliton train in adiabatic approximation of the perturbed Manakov system (MS)

$$i\vec{u}_t + \tfrac{1}{2}\vec{u}_{xx} + (\vec{u}^{\,\dagger}, \vec{u})\vec{u} = V(x)\vec{u}(x,t). \tag{1}$$

with composite external potentials of kind $V(x) = \sum_{s=1}^{N} c_s \mathrm{sech}^2(x - x_s)$ where x_s locate the positions of the small-amplitude ($|c_s| \ll 1$) wells/humps. We analyze the dynamics of 3-soliton trains of Cauchy problem composed by MS, Eq. (1) and the initial condition

$$\vec{u}(x, t=0) = \sum_{k=1}^{3} u_{k;1\mathrm{s}}(x, t=0)\vec{n}_k,$$

where $u_{k;1\mathrm{s}}(x,t)$ is the 1-soliton solution of the scalar nonlinear Schrödinger equation with given velocity, amplitude, phase, and position, and $\vec{n}_k$ is normalized polarization vector (for details see [1]).

We show that the dynamics of the 3-soliton train is modeled by a perturbed complex Toda chain for the train parameters which generalize the results of [1]. Cleverly combining the analytic and numerical approach we focus also on the perturbation effects on the asymptotically free behavior as well as on the bound state regime of the soliton trains. We conduct a big number of scenarios with $N = 13$, 17 and 33. The results obtained extend the ones in Refs. [2, 3].

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BINGO–BIOLOGICAL NETWORKS OF GENE OBJECTS WEB TOOL

Isaac Neuhaus, Roumyana Yordanova

Bristol-Myers Squibb, Hopewell, NJ, USA
isaac.neuhaus@bms.com
Institute of Mathematics and Informatics, BAS, Sofia, Bulgaria
ryordanova@math.bas.bg

An interactive web tool was developed to explore associations in networks built with Affymetrix transcriptional profiling data and other sources of genomics data. Partial correlation was used to filter the significant associations and discover direct edges between the genes in the networks. The tool enabled users to compare gene patterns across a large number of available experiments in an internal database. Similar methodology was developed to assess causality in genes sets whereby the K-Nearest Neighbors distance used in Fisher tests were used to judge associations.

The statistical calculations were encapsulated in an R package (RGraph). The direct relationships between the genes were modeled based on user defined parameters including the FDR level and a threshold for the probability that a partial correlation of an edge was significant in the network. In addition, mutual information was computed by discretizing gene expressions to capture nonlinear dependences. Furthermore, an outlier sampling procedure was applied to simulate knock-in/out scenario by dividing the samples based upon the expression of a gene. Networks were analyzed and targets prioritized by computing important characteristics of the graphs such as vertex connectivity, closeness, betweeness and other network characteristics.

A flexible and interactive JavasScript framework was built to visualize the networks and to allow data exploration. The visualizations included filterable and sortable data tables with multiple links to internal and external data resources. Similarly, the network visualizations counted with filterable widgets to explore what-if case scenarios. This framework will be made available in the future.

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MULTISCALE MODELING AND SIMULATION OF THE MECHANICAL PROPERTIES OF MINERALIZED BIOLOGICAL STRUCTURAL MATERIALS: THE EXAMPLE ARTHROPOD CUTICLE

S. Nikolov[1], H.-O. Fabritius[2], M. Friak[2] and D. Raabe[2]

[1] BAS, Institute of Mechanics,
Acad. G. Bonchev Str. Bl. 4,
1113 Sofia, Bulgaria
[2] Max-Planck-InstitutfurEisenforschung GmbH ,
Max-Planck-Str. 1,
40237 Dusseldorf, Germany

Biological structural materials (e.g., bone, arthropod cuticle and shells) represent hierarchical materials based on organic-inorganic nanocomposites. Understanding the underlying design principles promises the realization of a new generation of structural materials. By combining ab initio calculations at atomistic level with sequential homogenization at mesolevel and full-field 3D modeling at macrolevel, we propose a bottom-up multiscale approach that is able to describe how mechanical properties are transferred from the atomic scale through a hierarchy of specifically designed microstructures to eventually realize the outstanding mechanical properties of biological materials. To describe key concepts of this approach we choose the cuticle of the lobster Homarusamericanusas a model material. The cuticle consists of chitin in the form of crystalline nanofibrils (which serve as exoskeleton material for more than 90

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IMPROVED HIGH-PERFORMANCE IMPLEMENTATION OF A LARGE-SCALE AIR POLLUTION MODEL

Tzvetan Ostromsky

Institute of Information and Communication Technologies,
Bulgarian Academy of Sciences,
Acad. G. Bonchev St., Bl. 25A,
1113 Sofia, Bulgaria

The Danish Eulerian Model (DEM) is a powerful and sophisticated air pollution model, used successfully in different long-term environmental studies for the European region. Its main goal is to estimate accurately the concentrations of various dangerous pollutants and other closely related chemical species over a large spatial domain (a square with edge 4800 km.). For this purpose, the main physical, chemical and photochemical processes between the studied species, the natural and anthropogenic emissions, the quickly changing meteorological conditions, etc. should be taken into account. That is why numerous and huge data sets are to be processed along with the complicated calculations. With the rising power of the modern supercomputers and the novel developments in the up-to-date parallel implementation of the model (UNI-DEM), great improvement has been achieved in the speed of calculations. As far as the transfer and I/O processing of the huge data sets is concerned, this lately became a strong bottleneck for the overall performance of the code. A way to deal effectively with this problem is shown in this work. It is directed to minimization the number of file transfers and temporary work files on the price of some additional intensive MPI communications. The implementation requires some changes in the parallelization strategy in UNI-DEM. The effect of these improvements will be shown by test experiments on IBM BlueGene/P and IBM MareNostrum III, the most powerful parallel supercomputers in Bulgaria and Spain.

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STABILITY ISSUES OF A PARTITIONING ALGORITHM FOR TRIDIAGONAL AND BANDED LINEAR SYSTEMS

Velizar Pavlov

Department of Applied Mathematics and Statistics,
University of Ruse, 7017 Ruse, Bulgaria, vpavlov@uni-ruse.bg

This is a review paper where we present the main results of the componentwise stability analysis of Wang's parallel partition method for banded and tridiagonal linear systems. There are bounds on the equivalent perturbations depending on three constants, and bounds on the forward error as well depending on two types of condition numbers. It is shown that for some special classes of matrices, i.e. diagonally dominant (row or column), symmetric positive definite, and M-matrices, the algorithm is numericaly stable.

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ON THE STABILITY OF A PENTADIAGONAL SOLVER

Velizar Pavlov

Department of Applied Mathematics and Statistics,
University of Ruse, 7017 Ruse, Bulgaria, vpavlov@uni-ruse.bg

Linear systems with pentadiagonal matrices arise often when solving differential equations numerically. In this paper we present a roundoff error analysis of the LU-decomposition for linear systems with pentadiagonal matrices. In our approach we use the dependence graph of the algorithm and its parallel form. The equivalent perturbations of the inputs are relatively small for well-conditioned problems. Backward analysis needs much less computational time than forward analysis if we want to estimate the roundoff errors numerically.

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GRIDDING OF SUBSURFACE FORMATIONS WITH APPLICATIONS TO RESERVOIR SIMULATIONS

P. Popov and N. Simeonov

ppResearch Ltd.

Reservoir simulation in subsurface formations is a necessary step in the assessment and production phase of hydrocarbon reserves. It typically involves solving a complex set of partial differential equations in complex subsurface geometries. The domains of interest have a complex layered structure with very high aspect ratios. Their geometric description is further complicated by layer pinch-outs, faults, fracture networks, which lead to various discontinuities in the geological layering. It is often advantageous, when various fault and pinch-outs are present, to perform reservoir simulations on unstructured grids, compared to the standard approach of structured, topologically Cartesian, corner point grids. In this work we examine a practical approach to unstructured tetrahedral discretization of such geometries. Due to the many complexities, it is essentially impossible to mesh such geometries by standard mesh generators. We present a strategy, where individual layer interfaces are first meshed in 2D, followed by a scheme to "stitch together" an initial conforming 3D surface triangular mesh of very poor quality. A mesh improvement algorithm is then presented which converts this initial surface mesh into a good quality triangular grid. Special attention is paid gridding near pinches and care must be taken to avoid intersection of the final surface grid of different horizon surfaces. Once a valid surface mesh of good quality is produced, as a final step, a freely available mesh generator is used to produce good quality tetrahedral volume grids.

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IMPROVED ENCLOSURE FOR SOME PARAMETRIC SOLUTION SETS WITH LINEAR SHAPE

Evgenija D. Popova

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences
Acad. Bonchev str., bl.8, 1113, Sofia, Bulgaria

Consider linear algebraic systems $A(p)x = b(p)$ where the elements of the matrix and the right-hand side vector are linear functions of a number of parameters $p = (p_1, \ldots, p_K)^\top$ which are considered to be uncertain and varying within given intervals. Depending on the particular practical problem to be solved, we fix two disjoint index sets $\mathcal{A}$ and $\mathcal{E}$ for which the parametric AE-solution set of the system is defined by

$$\Sigma_{AE}(A(p), b(p), [p]) := \{x \in \mathbb{R}^n \mid (\forall p_{\mathcal{A}} \in [p_{\mathcal{A}}])(\exists p_{\mathcal{E}} \in [p_{\mathcal{E}}])(A(p_{\mathcal{A}}, p_{\mathcal{E}})x = b(p_{\mathcal{A}}, p_{\mathcal{E}}))\}.$$

We present some sufficient conditions for a general parametric AE-solution set to have linear boundary. Basing on these conditions a conversion theorem gives an equivalent representation of the parametric system where each parameter appears once in a diagonal matrix. The latter representation allows us to expand the scope of applicability of the best known so far interval method [1] for enclosing the parametric united solution set $\Sigma(A(p_{\mathcal{E}}), b(p_{\mathcal{E}}), [p_{\mathcal{E}}])$ and to generalize the method for systems where the parameter dependencies connect the matrix and the right-hand side vector. A generalization of the method for enclosing the parametric controllable solution set $\Sigma(A(p_{\mathcal{E}}), b(p_{\mathcal{A}}), [p_{\mathcal{A}}], [p_{\mathcal{E}}])$ will be presented, too. By some examples we demonstrate that parametric solution sets with linear boundary appear in various application domains and the generalized method improves the solution enclosure.

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CREATING GUI AND USING NNTOOL TO STUDY THE STATIC EQUATION OF LINEAR CNN

Victoria Rashkova

Department of Informatics,
University of Ruse,
7017 Ruse, Bulgaria
vkr@ami.uni-ruse.bg

The Neural networks are composed of simple elements operating in parallel. These elements are inspired by biological nervous systems. As in nature, the network function is determined largely by the relationships between elements. The coefficients defining relationships between cells are called, templates for feedback and control templates. The neural network can be train to perform a particular function by adjusting the values of the connections (called weights) between elements. Commonly neural networks are adjusted, or trained, so that a particular input leads to a specific target output. The article presenting graphical user interface created to study the static equation of linear CNN. GUI has a large variety of tools such as menus, toolbars, push buttons, radio buttons, edit text, static text, listbox, axes, pop- up menu and more. GUI is created using MATLAB tools can also perform any type of computation, read and write data files, communicate with other GUIs, and display data as tables or as plots. The GUI window has its own work area, separate from the workspace command line in Matlab . Thus, when using the GUI, you might export the GUI results to the (command line) workspace. Similarly you may want to import results from the command line workspace to the GUI. Presented are opportunities nntool. Presented simulation results for different values of the parameters too.
Key words: neural networks, neural network tool, templates, GUI, controls

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A STUDY OF SINGLE DOPANT SYSTEMS FOR APPLICATIONS IN QUANTUM COMPUTING

Jean Michel Sellier and Ivan Dimov

Institute of Information and Communication Technologies,
Bulgarian Academy of Sciences,
Acad. G. Bonchev St., Bl. 25A,
1113 Sofia, Bulgaria

Very recently, impressive advances in quantum computing devices based on Silicon material have been reported. Several novel architectures have been presented as eventual building blocks for actual quantum computers that have shown to work in laboratory experiments. These devices exploits, in some cases, the spin of a free electron and, in other cases, the charge distribution of a single electron. While it is not yet clear which architecture will eventually become the standard, it is evident that it will be based on Phosphorus atoms (single dopants) embedded in Silicon substrate, acting as attractors to conduction electrons. The experiments are advancing quickly but the same thing cannot stated for the theoretical comprehension of such devices. Only a few theoretical studies have been presented so far, based on stationary models unable to properly include phonon scattering effects (which are known to be relevant even at very low temperatures) and in the presence of open contacts (i.e. the physical leads). In this work, we present for the first time a three-dimensional, time-dependent, full quantum study of the building block of candidate quantum computing devices based on the Wigner-Boltzmann Monte Carlo method. We study the dynamics of an electron wave packet in proximity of one Phosphorus atom. In the aim to understand the physics of such phenomena, we perform simulations in different conditions related to the initial energy of the electron, the temperature of the Silicon crystal and the applied voltages on the open contacts. First we show how a wave packet behaves close to a single dopant (Phosphorus). We then present the effects of the crystal temperature which essentially destroys the information carried by a single electron.

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A MULTISCALE MULTILEVEL ALGORITHM USING ANALYTICAL COARSE OPERATOR APPLIED TO BONE TISSUE MODELING

R. Sviercoski and S. Margenov

Institute of Information and Communication Technologies,
Bulgarian Academy of Sciences,
Acad. G. Bonchev St., Bl. 25A,
1113 Sofia, Bulgaria

Complex multiscale problems related to computer simulation of deformable porous media are routinely encountered as a part of research and development activities in a number of engineering, environmental and biomedical fields. The studied bone tissue has complex hierarchical morphology in the sense that features ranges from the scales of nanometer to millimeter level. Predicting the mechanical behavior of such systems with hierarchical structures and multiple length-scales is very computationally demanding. The goal of this study is to propose an efficient numerical tool that reduces significantly the computational resources applicable to this class of problems, which will enable to perform predictive simulations as an integral part of osteoporosis treatment. To achieve that, a highly heterogeneous medium with trabecular bone tissue's characteristics is considered. The contribution of the fluid phase is interpreted in terms of almost incompressible material. The related linear elasticity problem is of high contrast and high frequency. The finite element method (FEM) is applied for discretization of the related linear elasticity problem. The multiscale system is obtained using a displacement decomposition method, and solved by using a block diagonal form as a preconditioner. The new feature here is that at the decoupled FEM elliptic systems we apply a multilevel technique that incorporates an analytical effective tensor of the respective heterogeneous elastic modulus into the block diagonal. We demonstrate numerically the efficiency and robustness of the solver near the incompressibility limit, when compared with other numerical methods for multiscale problems.

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SPATIOTEMPORAL STABILIZATION OF ULTRASHORT LIGHT PULSES PROPAGATING IN NONLINEAR IONIZED MEDIUM

T. P. Todorov (1), M. E. Todorova (2), M. D. Todorov (3) and I. G. Koprinkov (1)

(1) Department of Applied Physics,
Technical University of Sofia,
1000 Sofia, Bulgaria
(2) College of Energetics and Electronics,
Technical University of Sofia,
1000 Sofia, Bulgaria
(3) Faculty of Applied Mathematics and Informatics,
Technical University of Sofia,
1000 Sofia, Bulgaria

The spatiotemporal dynamics of high-intensity ultrashort light pulses is studied within a rigorous physical model. The pulse propagation is described by (3+1)D nonlinear envelope equation. The propagation and the material equations are solved self-consistently at realistic physical conditions. Self-compression of the pulse is found. At certain conditions, peak intensity, transversal width, time duration, and spatiotemporal shape of the pulse remain stable within given propagation range. This, to our knowledge, is the first simulation of stable propagation of high-intensity ultrashort pulses at realistic physical conditions.

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COMPARATIVE STUDY ON THE EFFICIENCY OF HYBRID LEARNING PROCEDURES USED FOR TRAINING OF FUZZY-NEURAL NETWORKS

Yancho Todorov, Margarita Terziyska

Institute of Information and Communication Technologies,
Bulgarian Academy of Sciences,
Acad. G. Bonchev St., Bl. 25A,
1113 Sofia, Bulgaria

This paper deals with the development of learning procedures, for training the parameters of a Takagi-Sugeno type fuzzy-neural network. A recurrent node is introduced by a global feedback, from the network output. To improve the predictions during the on-line process of network parameters adaptation, a hybrid training procedure based on Gradient descent and the fast converging Gauss-Newton and Levenberg-Marcquardt algorithms, is designed. To avoid possible model oscillations, the antecedent part of the fuzzy rules is scheduled at each sampling time by using the Gradient descent approach, while the rules consequent part is trained either by Gauss-Newton or Levenberg-Marcquardt approaches. A comparison is made with the classical case, when both groups of parameters are adjusted by the Gradient descent. The performance of the model using the proposed hybrid approaches is evaluated by simulation experiments for prediction of two commonly used chaotic time series Mackey-Glass and Rossler. The achieved results shows a better model performance when using the proposed hybrid learning procedures in contrast to the classical case of purely Gradient descent learning approach. A promising extension of the proposed approach is the inclusion of the designed models into model based process control shemes.

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ON A NONLOCAL NONLINEAR SCHRÖDINGER EQUATION

Tihomir Valchev

Dublin Institute of Technology,
Kevin Street Lower, Dublin 8, Ireland
e-mail: Tihomir.Valchev@dit.ie; tihov@yahoo.com

We consider a nonlocal version of nonlinear Schrödinger equation (NNLS) recently proposed by Ablowitz and Musslimani [1]. As the ordinary local NLS it is PT-symmetric which makes it useful for theoretical description of wave propagation in PT-symmetric coupled wave-guides and photonic crystals already been observed in experiments [2, 3, 4]. NNLS under study is integrable by means of inverse scattering method, i. e. it possesses a Lax pair, infinite number of integrals of motion and soliton-like solutions [1]. We aim here at presenting an alternative approach in deriving special solutions and integrals of motion. Possible generalizations of the considered NNLS which could be interesting in terms of physical applications will be discussed as well.

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LOCAL CRANK-NICOLSON METHOD FOR NONLINEAR OPTION PRICING PROBLEMS

R. Valkov

Department of Mathematics and Computer Science,
University of Antwerp, Belgium,
rvalkov@fmi.uni-sofia.bg

In this paper we solve numerically two strongly-nonlinear problems, modelling the replication of contingent claims in illiquid markets. The spatial discretization is standard centered-space as we investigate the stability, consistency and monotonicity properties of the semi-discrete solution. The full discretization is derived by the local Crank-Nicolson time stepping method. The resulting fully-explicit numerical scheme is shown to be unconditionally stable and consistent. Monotonicity and convergence properties of the numerical solution are also considered. Numerical experiments validate the obtained theoretical considerations.

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ON THE REMARKABLE APPLICABILITY OF 2-D ELASTIC CONTINUUM MODELS IN THE MECHANICS OF NANOSCALE STRUCTURES

Vassil M. Vassilev

Institute of Mechanics,
Bulgarian Academy of Sciences
Sofia, Bulgaria

In this report we will discuss the remarkable and somewhat surprising applicability of the continuum modelling of mechanical behaviour of two types of nanoscale objects: fluid lipid bilayer membranes and carbon nanostructures. The variational statement and associated Euler-Lagrange equations of a unified model based on the concept of two-dimensional (2-D) elastic continuum will be presented and used to handle tow different case studies. First of them consist in representing in explicit analytic form cylindrical and axisymmetric equilibrium configurations of single-wall carbon nanotubes and fluid lipid bilayer membranes subjected to uniform hydrostatic pressure. The second one is concerned with the mechanical behaviour of closed fluid lipid bilayer membranes (vesicles) adhering onto a flat homogeneous rigid substrate subjected to micro-injection and uniform hydrostatic pressure.

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INVESTIGATION OF TWO NUMERICAL SCHEMES FOR THE 2D BOUSSINESQ PARADIGM EQUATION IN A MOVING FRAME COORDINATE SYSTEM

Daniela Vasileva, Natalia Kolkovska

Institute of Mathematics and Informatics,
Bulgarian Academy of Sciences
Acad. Bonchev str., bl.8, 1113, Sofia, Bulgaria

The various variants of Boussinesq equation (BE) model surface waves in shallow fluid layer. One important feature of BE is the balance between the nonlinearity and dispersion, which leads to solutions of type of permanent waves (solitons).
A moving frame coordinate system helps us to keep localized structures in the center of the coordinate system, where the grid is much finer. It also reduces the effects of the reflection from the boundaries, allows us to use a small computational box and to compute the solution for very large times.
Here we investigate two difference schemes in a moving frame coordinate system for the time evolution of the solutions of the 2D Boussinesq Paradigm Equation (BPE). The first one of the schemes uses central finite differences for the mixed (v_{tz}) derivative, while the second one uses upwind finite differences. The grid is non-uniform and the truncation error is second order in space and time. The properties of the numerical methods corresponding to the linearized BPE are studied. It is proved that the proposed finite difference schemes are stable with respect to initial data, if the transformed BPE has elliptic right-hand side.
The numerical experiments use known stable 1D solutions in a 2D setting. The results demonstrate the second order of convergence of the schemes. Although the numerical schemes are stable, the solution of the 2D problem seems to be not stable – the waves preserve their shape in relatively long intervals of time (depending on the parameters), but after that the initial shape of the waves is changed. Such effects are not observed in the 1D setting – the 1D solutions preserve their shape for very large times.

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SOME PROPERTIES OF THE SPECTRAL DECOMPOSITIONS FOR THE RECURSION OPERATORS RELATED TO THE CAUDREY-BEALS-COIFMAN SYSTEM IN THE PRESENCE OF $\mathbb{Z}_R$ REDUCTIONS OF MIKHAILOV TYPE

A B Yanovski

Department of Mathematics and Applied Mathematics
University of Cape Town, 7700 Rondebosch, Cape Town, South Africa
E-mail: Alexandar.Ianovsky@uct.ac.za

We consider the spectral problem: $L\psi = (i\partial_x + q - \lambda J)\psi = 0$ (Caudrey-Beals-Coifman spectral problem) defined on an arbitrary simple Lie algebra. To the spectral problem $L\psi = 0$ is related the theory of Recursion Operators generating the soliton-type equations associated with L and the main tools for their investigation are the expansions over the so-called adjoint solutions of the Caudrey-Beals-Coifman problem. In case $\mathbb{Z}_r$ reductions of Mikhailov type are present the expansions show some interesting features that we are looking into. In particular, we pay special attention to the discrete spectrum terms.

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ON THE ASYMPTOTIC BEHAVIOR OF DISSIPATIVE WAVE EQUATIONS

Ryo Ikehata
Hiroshima University, JAPAN
ikehatar@hiroshima-u.ac.jp
Tuoc Phan
University of Tennessee-Knoxville, USA
phan@math.utk.edu
Petronela Radu
University of Nebraska-Lincoln, USA
pradu@math.unl.edu
Grozdena Todorova
University of Tennessee-Knoxville, USA
todorova@math.utk.edu
Borislav Yordanov*
Institute of Mathematics and Informatics-BAS, BULGARIA
byordanov@math.bas.bg

We discuss a series of results on the long-time behavior of solutions to dissipative wave equations in R^n or exterior domains. The so-called "diffusion phenomenon" gives simple asymptotics involving solutions to the corresponding diffusion equations, i.e., equations where the second-order time derivatives are absent. We can study this problem in abstract setting: A is a nonnegative self-adjoint operator in a Hilbert space H and $u(t)$ is a solution to a dissipative equation in $[0,\infty)\times H$, such as

$$u''(t)+Au(t)+u'(t)=0,\quad u(0)=u_0,\quad u'(0)=u_1$$

and

$$u''(t)+Au(t)+Au'(t)=0,\quad u(0)=u_0,\quad u'(0)=u_1.$$

The initial data are $(u_0,u_1)\in H\times D(A^{1/2})$. We can show that the leading term of $u(t)$ is determined by the semigroup e^{-tA} as $t\to\infty$. In most applications, A is an elliptic operator and the associated semigroup solves a parabolic equation.

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HEURISTIC APPROACHES TO GLASS CUTTING OPTIMIZATION

Biserka Yovcheva, Petar Ivanov, Valentina Dyankova

Faculty of Mathematics and Informatics
University of Shoumen
Universitetska str. 115, 9712 Shoumen

The aim of this work is to examine the case of a variation of the 2D bin-packing problem about placing rectangular glass objects with different sizes on a number glass bins with different sizes. An important additional limitation is induced by the nature of the glass cuts - objects must be cut sequentially from end to end (guillotine cuts). Bin-packing is a well known NP-hard problem and many heuristic approaches have been proposed. An overview of different approaches are examined including genetic algorithms, simulated annealing, gradient descent methods and greedy strategies. The quality measure which is being optimized takes into account the number of bins used and the number and sizes of the resulting unused glass parts. The possible cut procedures can be fully represented as a tree with specific glass objects and their rotation in the nodes. The examined algorithms are of an interest for the glass cutting industry.

PART C:
LIST OF PARTICIPANTS [1]

[1] Arranged alphabetically according to the family name of the author

G. Agranovich
Dept. of Electrical and
Electronic Engineering
Ariel University Center of Samaria
44837 Ariel, Israel

Emanouil Atanassov
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

Stefka Bouyuklieva
Veliko Turnovo University,
Veliko Turnovo, Bulgaria

Georgi Boyadzhiev
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Sofia, Bulgaria

Danail S. Brezov
Department of Mathematics
University of Architecture
Civil Engineering and Geodesy
1 Hristo Smirnenski Blvd.
Sofia 1046, Bulgaria
e-mail: danail.brezov@gmail.com

Dimitar Dimitrov
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

Ivan Dimov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria

M. Dimova
Institute of Mathematics and
Informatics,
Bulgarian Academy of Sciences
Acad. Bonchev str., bl.8,
1113, Sofia, Bulgaria

Assen Dontchev
Mathematical Reviews,
American Mathematical Society
and Department of Mathematics,
University of Michigan, USA

Mariya Durchova
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A,
1113 Sofia, Bulgaria

Valentina Dyankova
Faculty of Mathematics and
Informatics
University of Shoumen
Universitetska str. 115, 9712 Shoumen

Valerij Dzhurov
University of Rousse
Rousse 7017, Bulgaria

Alexander Fabricant
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Sofia 1113, Bulgaria

H. O. Fabritius
Max-Planck-
InstitutfurEisenforschung
GmbH, Max-Planck-Str. 1
40237 Dusseldorf, Germany

Stefka Fidanova
Institute of Information and

Communication Technologies,
BAS Acad. G. Bonchev St., Bl.25A,
1113 Sofia, Bulgaria

M. Friak
Max-Planck-
InstitutfurEisenforschung
GmbH, Max-Planck-Str. 1
40237 Dusseldorf, Germany

Dobromir Georgiev
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

Vladimir Georgiev
Department of Mathematics
University of Pisa
Largo Bruno Pontecorvo 5
56100 Pisa, Italy

Irina Georgieva
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Acad. G. Bonchev, Bl. 8
1113, Sofia, Bulgaria
irina@math.bas.bg

V. S. Gerdjikov
Institute of Nuclear Research
and Nuclear Energy, BAS
72 Tsarigradsko chausee
Sofia 1784, Bulgaria

Todor Gurov
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

Clemens Hofreither
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria
chofreither@numa.uni-linz.ac.at

Darryl Holm
Imperial College London, UK

Ryo Ikehata
Hiroshima University, JAPAN
ikehatar@hiroshima-u.ac.jp

Oleg Iliev
Fraunhofer Institute for
Industrial Mathematics
ITWM, Kaiserslautern, Germany
and KAUST, Saudi Arabia

Petar Ivanov
Faculty of Mathematics and
Informatics
University of Shoumen
Universitetska str. 115, 9712 Shoumen

Rossen Ivanov
Dublin Institute of Technology,
Ireland

Sofiya Ivanovska
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

Stoyan Kapralov
Technical University of Gabrovo
Gabrovo, Bulgaria

Aneta Karaivanova
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

Miglena N. Koleva
University of Ruse, 8 Studentska St.
7017 Ruse, Bulgaria
e-mail:mkoleva@uni-ruse.bg

Natalia Kolkovska
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Acad. Bonchev str., bl.8
1113, Sofia, Bulgaria

Jordanka Paneva - Konovska
Department of Applied Mathematics
and Computer Science
Technical University of Sofia
1000 Sofia, Bulgaria

I. G. Koprinkov
Department of Applied Physics
Technical University of Sofia
1000 Sofia, Bulgaria

Milena Kostova
University of Rousse
Rousse 7017, Bulgaria

Nikolai Kutev
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Sofia 1113, Bulgaria

A. Kyuldjiev
Institute for Nuclear Research
and Nuclear Energy
BAS, 1784 Sofia, Bulgaria

E. Litsyn
Department of Mathematics
Ben-Gurion University of
the Negev
Beer-Sheva, Israel

Mladen Manev
Technical University of Gabrovo
Gabrovo, Bulgaria

S. Margenov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria

Pencho Marinov
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

D. M. Mladenov
Theoretical Physics Department,
Faculty of Physics,
Sofia University "St. Kliment Ohridski"
5 James Bourchier Blvd
1164 Sofia, Bulgaria

Ivaïlo M. Mladenov
Institute of Biophysics
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., Bl. 21
Sofia 1113, Bulgaria
e-mail: mladenov@bio21.bas.bg

Clementina D. Mladenova
Institute of Mechanics,
Bulgarian Academy of Sciences

Acad. G. Bonchev Str., Bl. 4
Sofia 1113, Bulgaria
e-mail: clem@imbm.bas.bg

Isaac Neuhaus
Bristol-Myers Squibb
Hopewell, NJ, USA
isaac.neuhaus@bms.com

S. Nikolov
BAS, Institute of Mechanics
Acad. G. Bonchev Str. Bl. 4
1113 Sofia, Bulgaria

Tzvetan Ostromsky
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria

Velizar Pavlov
Department of Applied
Mathematics
and Statistics
University of Ruse
7017 Ruse, Bulgaria
vpavlov@uni-ruse.bg

Tuoc Phan
University of Tennessee-Knoxville,
USA
phan@math.utk.edu

Petar Popivanov
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Acad. G. Bonchev, Bl. 8
1113 Sofia, Bulgaria

P. Popov
ppResearch Ltd.
Bulgaria

Evgenija D. Popova
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Acad. Bonchev str., bl.8
1113, Sofia, Bulgaria

D. Raabe
Max-Planck-
InstitutfurEisenforschung
GmbH, Max-Planck-Str. 1
40237 Dusseldorf, Germany

Petronela Radu
Department of Mathematics
University of Nebraska-Lincoln, USA
pradu@math.unl.edu

Tsviatko Rangelov
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences
Sofia 1113, Bulgaria
rangelov@math.bas.bg

Tsetska Rashkova
University of Rousse
Rousse, Bulgaria

Victoria Rashkova
Department of Informatics
University of Ruse,
7017 Ruse, Bulgaria
vkr@ami.uni-ruse.bg

Jean Michel Sellier
Institute of Information and
Communication Technologies
BAS Acad. G. Bonchev St., Bl.25A
1113 Sofia, Bulgaria

N. Simeonov
ppResearch Ltd.
Bulgaria

Angela Slavova
Institute of Mathematics
and Informatics
Bulgarian Academy of Sciences
Sofia 1113, Bulgaria

A. A. Stefanov
Theoretical Physics
Department
Faculty of Physics,
Sofia University
"St. Kliment Ohridski"
5 James Bourchier Blvd
1164 Sofia, Bulgaria

R. Sviercoski
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria

Margarita Terziyska
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria

M. D. Todorov
Department of Applied
Mathematics and Computer Science
Technical University of Sofia
1000 Sofia, Bulgaria

T. P. Todorov
Department of Applied Physics
Technical University of Sofia
1000 Sofia, Bulgaria

Yancho Todorov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl. 25A
1113 Sofia, Bulgaria

Grozdena Todorova
Department of Mathematics
University of Tennessee-Knoxville,
USA
todorova@math.utk.edu

M. E. Todorova
College of Energetics and
Electronics
Technical University of Sofia
1000 Sofia, Bulgaria

Tihomir Valchev
Dublin Institute of Technology
Kevin Street Lower,
Dublin 8, Ireland
Tihomir.Valchev@dit.ie;
tihov@yahoo.com

R. Valkov
Department of Mathematics and
Computer Science
University of Antwerp, Belgium
rvalkov@fmi.uni-sofia.bg

S. K. Varbev
Theoretical Physics Department,
Faculty of Physics
Sofia University "St. Kliment Ohridski"
5 James Bourchier Blvd
1164 Sofia, Bulgaria

Daniela Vasileva
Institute of Mathematics and
Informatics
Bulgarian Academy of Sciences

Acad. Bonchev str., bl.8
1113, Sofia, Bulgaria

Vassil M. Vassilev
Institute of Mechanics
Bulgarian Academy of Sciences
Sofia, Bulgaria

Lubin G. Vulkov
University of Ruse,
8 Studentska St.
7017 Ruse, Bulgaria
lvalkov@uni-ruse.bg

A B Yanovski
Department of Mathematics and
Applied Mathematics
University of Cape Town
7700 Rondebosch
Cape Town, South Africa
Alexandar.Ianovsky@uct.ac.za

Borislav Yordanov
Institute of Mathematics and
Informatics
BAS, Acad. Bonchev str., bl.8
1113 Sofia, Bulgaria
byordanov@math.bas.bg

Roumyana Yordanova
Institute of Mathematics and
Informatics
BAS, Acad. Bonchev str., bl.8
1113 Sofia, Bulgaria
ryordanova@math.bas.bg

Biserka Yovcheva
Faculty of Mathematics and
Informatics
University of Shoumen
Universitetska str. 115, 9712 Shoumen