

siam

11th Annual Meeting of the Bulgarian Section of SIAM
December 20-22, 2016
Sofia

BCSIAM'16

PROCEEDINGS

BCSIAM

BCSIAM



11th Annual Meeting of the Bulgarian Section of SIAM
December 20-22, 2016
Sofia

BGSIAM'16

PROCEEDINGS

Fastumprint

11th Annual Meeting of the Bulgarian Section of SIAM
December 20-22, 2016, Sofia

BGSIAM'16 Proceedings

©2016 by Fastumprint

ISSN: 1313-3357 (print)
ISSN: 1314-7145 (electronic)

Printed in Sofia, Bulgaria

PREFACE

The Bulgarian Section of SIAM (BGSIAM) was formed in 2007 with the purpose to promote and support the application of mathematics to science, engineering and technology in Republic of Bulgaria. The goals of BGSIAM follow the general goals of SIAM:

- To advance the application of mathematics and computational science to engineering, industry, science, and society;
- To promote research that will lead to effective new mathematical and computational methods and techniques for science, engineering, industry, and society;
- To provide media for the exchange of information and ideas among mathematicians, engineers, and scientists.

During BGSIAM'16 conference a wide range of problems concerning recent achievements in the field of industrial and applied mathematics will be presented and discussed. The meeting 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. The conference support provided by the SIAM is highly appreciated.

List of the Invited Speakers include:

- Vassil Alexandrov (Barcelona Supercomputing Center) "Data and Computational Science Methods Applied to Social Media"
- Krassimir Danov (Sofia University) "Modeling of Membranes with Complex Rheology: Computational Aspects"
- Oleg Iliiev (Fraunhofer ITWM) "Toward MLMC based exascale computations for Uncertainty Quantification for flow in porous media"
- Ivan Markovsky (Vrije Universiteit Brussel) "A low-rank matrix completion approach to data-driven signal processing"

The following special sessions are organized in the framework of the BGSIAM 2016 annual meeting:

- Biomedical Applications,
- Computational Mechanics (joint event with the Bulgarian National Section of GAMM), and
- Mathematics in Industry.

The present volume contains extended abstracts of the presentations (Part A) and list of participants (Part B).

Krassimir Georgiev
Chair of BGSIAM Section

Michail Todorov
Vice-Chair of BGSIAM Section

Ivan Georgiev
Secretary of BGSIAM Section

Sofia, December 2016

Table of Contents

Part A: Extended abstracts	0
<i>A. Alexandrov</i>	
Method and algorithm for WSN time synchronization based on Kalman filter and Fraser-Potter equation	2
<i>Vera Angelova</i>	
Local perturbation analysis of the stochastic matrix Riccati equation with applications in finance	4
<i>Teodor M. Atanacković</i>	
On a constitutive equation of heat conduction with fractional derivatives of complex order	6
<i>Emanouil Atanassov, Aneta Karaivanova, Todor Gurov</i>	
Advanced services for Virtual Research Environments	8
<i>Todor Balabanov, Maria Barova, Delyan Keremedchiev</i>	
Image construction with 2D ellipses by genetic algorithms optimization	10
<i>Todor Balabanov, Nikolai Manev, Walter Mudzimbabwe, Petar Tomov, Ilian Zankinski, Stela Zhelezova</i>	
Authenticity management algorithm for digital images	12
<i>M. Ben-Artzi, J.-P. Croisille, D. Fishelov</i>	
An embedded compact scheme for biharmonic problems in irregular domains	14
<i>Milen Borisov, Nikolay Kyurkchiev, Svetoslav Markov</i>	
On the formulation of population growth models by means of reaction networks	16
<i>Stefan Bushev</i>	
Industrial mathematics - phase transitions, scattering, structures	17
<i>Krassimir Danov</i>	
Modeling of membranes with complex rheology: computational aspects	20
<i>Svetoslav Enkov, Snezhana Hristova, Ekaterina Madamlieva</i>	
Approximate method for non-instantaneous impulsive difference equations with a periodic boundary condition	22
<i>Georgi Evtimov, Stefka Fidanova</i>	
Ant Colony optimization algorithm for 1D Cutting Stock Problem	24
<i>Atanaska Georgieva, Alben Pavlova, Iva Naydenova</i>	
Error estimate in the iterative numerical method for two-dimensional nonlinear Hammerstein-Fredholm fuzzy functional integral equations	26

<i>Stanislav Harizanov</i>	
Fast algorithm for solving ℓ^0-constrained graph-Laplacian minimization	27
<i>S. Harizanov, D. Dimov, N. Naidenov, S. Kostadinova</i>	
Multi-frame denoising of still images	28
<i>Stanislav Harizanov, Jaume de Dios Pont, Sebastian Ståhl, Dennis Wenzel</i>	
Denoising and feature extraction of 2D CT radiographic images	29
<i>D. Iankov, M. Datcheva, R. Iankov</i>	
Material parameter identification of thin film with diamond nanoparticles via nanoindentation	31
<i>Oleg Iliev, Jan Mohring, Nikolay Shegunov, René Milk, Mario Ohlberger</i>	
Toward exascale computations of uncertainty quantification for porous media flow using multilevel Monte Carlo	33
<i>N. Ilieva, E. Lilkova, P. Petkov, and L. Litov</i>	
Identification of structural units in large proteins for guided metadynamics investigations	35
<i>N. Ilieva, J. Liu, P. Petkov, J. He, and A. Niemi</i>	
Modular approach to large-scale biomolecule simulations	38
<i>Shpend Ismaili, Stefka Fidanova</i>	
Representation of civilians and police officers by generalized nets for describing software agents in the case of protest	40
<i>Tihomir Ivanov, Galina Lyutskanova, Dragomir Aleksov, Ognian Kounchev</i>	
Laboratory calibration of MEMS rate sensors	42
<i>Yonka Ivanova, Todor Partalin, Ivan Georgiev</i>	
Comparison of NDT techniques for elastic modulus determination of laminated composites	43
<i>Ivan P. Jordanov, Ivan N. Dushkov, Elena V. Nikolova, Nikolay K. Vitanov</i>	
Applications of time delay differential equations in dynamics of a system of three competing populations	45
<i>Dimitar Kisiakov</i>	
Water hammer in a multiple-supported penstock and earthquake-induced support excitation - coupled analysis of the axial load case	47
<i>Hristo Kostadinov, Nikolai Manev</i>	
About flash memories and error correcting codes	49
<i>Ralitza K. Kovacheva,</i>	
On the strong asymptotic of rows of classical Padé approximants	51

<i>Konstantinos Liolios, Vassilios Tsihrintzis, Krassimir Georgiev, Ivan Georgiev and Panagiotis Angelidis</i>	
Optimal mathematical model for the simulation of removal of pollutants in constructed wetlands: linear or non-linear procedures?	52
<i>Lubomir Markov</i>	
Some results involving Euler-type integrals and dilogarithm values	54
<i>Ivan Markovskiy</i>	
A low-rank matrix completion approach to data-driven signal processing	56
<i>Zlatogor Minchev</i>	
Future cyber risks landscape exploration: modelling, simulation, validation & verification	57
<i>Elena V. Nikolova, Ivan P. Jordanov, Zlatinka I. Dimitrova, Nikolay K. Vitanov</i>	
Nonlinear evolution equations for propagation of waves in arteries with aneurysms: exact solutions obtained by the modified method of simplest equation	58
<i>Ludmila Parashkevova, Pedro Egizabal</i>	
Modelling of light Mg and Al based alloys as "in situ" composites.	60
<i>P. Petrova, B. Petrova, E. Simeonov, Ch. Chilev</i>	
Theoretically sampling of reactive distillation using the RCM- method	62
<i>Stevan Pilipović</i>	
Complex fractional Zener model of wave propagation in viscoelastic media	63
<i>Evgenija D. Popova</i>	
Exact bounds for the unknowns in some interval FE models of structures	64
<i>Peter Rashkov</i>	
Emergence of hormesis in a simple enzyme kinetic model	66
<i>Peter Rashkov</i>	
Competition for resources and space contributes to the emergence of drug resistance in cancer	68
<i>Hassan Safouhi</i>	
<i>Joint work with: Philippe Gaudrea, Richard Slevinsky</i>	
Computation of energy eigenvalues of the Schrödinger equation with anharmonic oscillators	70
<i>Sonia Tabakova, Stefan Radev, Nilolay Kutev</i>	
Asymptotic study of the nonlinear velocity problem for the oscillatory	

non-Newtonian flow in a straight tube	73
<i>Margarita Terziyska, Yancho Todorov, Maria Dobрева</i>	
Efficient error based metrics for fuzzy-neural network performance evaluation	74
<i>Nikolay K. Vitanov, Kaloyan N. Vitanov</i>	
Box model of migration in channels of networks	75
<i>Evtim V. Zahariev</i>	
Modified coordinates for dynamics simulation of multibody systems with elastic bodies	77
Part B: List of participants	80

Part A
Extended abstracts¹

¹Arranged alphabetically according to the family name of the first author.

Method and algorithm for WSN time synchronization based on Kalman filter and Fraser-Potter equation

A. Alexandrov

The accurate and energy optimized clock synchronization is very important in Wireless Sensor Networks (WSN). Most of the sensor nodes in WSN are autonomous and battery powered. Therefore they have a limited power capacity and practically is not possible to achieve clock synchronization by unlimited passing information among sensor nodes.

Due to thermal, vibration and moisture environment and the quartz crystal degradation rate, the sensor module clock crystal frequency is not very precise and need a regular adjustment.

The clock frequency deviation can cause synchronization lost during the packets sending and sometimes can crash the communications in all the sensor network.

Most clock synchronization protocols as NTP, LTS, HRTS, ITR, TSync and etc. use stochastic methods, describing constant models, working in relatively permanent environment. These protocols work very well for compensation of the "white" noise and slow changes in the external environment. At the same time the real working conditions very often include, for example fast and extremely high or low environment temperature, which cause big clock frequency deviation.

The current paper describe method and algorithm for adaptive compensation of the deviations in quartz stabilized clocks, embedded in the wireless sensor modules. The method is effective in cases of dynamic change of external temperature, vibration and moisture.

The proposed method and algorithm are based on the Extended Kalman Filter, Central Limit Theorem and Fraser-Potter equation.

The diagram of Figure 1 illustrate the basic principles of the method.

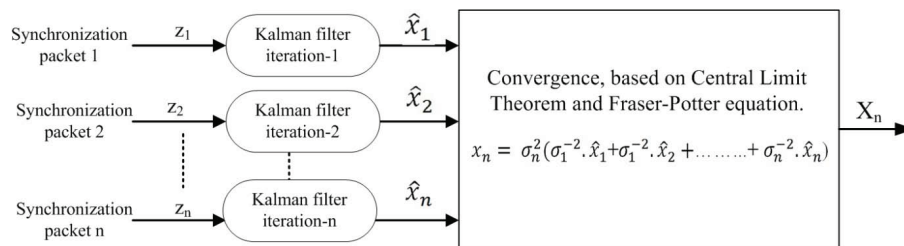


Figure 1

The paper describe two level iteration process, based on the data from network synchronization packets, to predict the size of the time compensation correction.

The first level use the Extended Kalman Filter and the second level use Central Limit Theorem and Fraser-Potter equation to smooth the correction curve.

The proposed method and algorithm lead to sensitive reducing of the traffic, generated from time synchronization packets in WSN's, builded on CSMA/CA and TDMA communication protocols. The other important benefit is the energy saving in battery powered sensor modules.

Local perturbation analysis of the stochastic matrix Riccati equation with applications in finance

Vera Angelova

Consider the stochastic matrix Riccati equation /SMRE/ with applications in linear quadratic optimization of stochastic finance models

$$A^T X + X A + Q + \sum_{j=1}^m C_j^T X C_j \quad (1)$$
$$- \left(X B + \sum_{j=1}^m C_j^T X D_j \right) \left(R + \sum_{j=1}^m D_j^T X D_j \right)^{-1} \left(X B + \sum_{j=1}^m C_j^T X D_j \right)^T = 0,$$

with $R + \sum_{j=1}^m D_j^T X D_j > 0$. The matrices Q , R , A , B , and C_j , D_j for $j = \overline{1, m}$ are constant matrices with appropriate dimensions and X is the unknown symmetric $n \times n$ real matrix.

The problem of existence and uniqueness of the solution of SMRE (1) is considered by Rami and Zhou in [2] and then extended by Ivanov and Lomev in [1], where two numerically effective iterations are proposed and compared with the approach based on the solution to a semidefinite programming problem.

In order to accurately and effectively solve equation (1) on a computer, an effective algorithm, as well as the knowledge of the sensitivity and the conditioning of the equation to perturbations in the data are needed. A measure of the conditioning of a computational problem are its condition numbers given by the ratio of the relative changes in the solution to the relative changes in the argument. The condition numbers are involved in the formulation of perturbation upper bounds of the error in the computed solution. In turn, the perturbation error bounds estimate the sensitivity of the computational problem and are one of the elements of the high-performance computations.

In this paper, the conditioning and the sensitivity of the stochastic matrix Riccati equation (1) are studied. Norm-wise absolute and relative condition numbers are proposed. For this purpose, equation (1) is rewritten in equivalent form using affine linear operators. Then the techniques of Fréchet derivatives are applied. Local perturbation bounds, based on the condition numbers are formulated as well.

References

- [1] I.G. Ivanov and B. Lomev. Numerical properties of stochastic linear quadratic model with applications in finance. *The Online Journal of Science and Trchnologu*, 2:41–46, 2012.

- [2] M. Rami and X. Zgou. Linear matrix inequalities, Riccati equations, and indefinite stochastic linear quadratic control. *IEEE Trans. Automat. Control*, AC-45:1131–1143, 2000.

On a constitutive equation of heat conduction with fractional derivatives of complex order

Teodor M. Atanacković

We study heat conduction with constitutive equation containing fractional derivatives of complex order. Motivated by the results of our previous works [1,2] in viscoelasticity, we propose a constitutive equation for the heat flux vector in the following form

$$q(x, t) + \widehat{a} {}_{t_0}D_t^\alpha q(x, t) + 2 {}_{t_0}\bar{D}_t^\gamma q(x, t) = -K_1 \frac{\partial T(x, t)}{\partial x}, \quad t > 0, \quad x \in (0, \infty).$$

Here T is temperature, ${}_{t_0}D_t^\alpha$ is a fractional order derivative, $\alpha \in (0, 1)$, given by

$${}_{t_0}D_t^\alpha q(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_{t_0}^t \frac{1}{(t-\tau)^\alpha} \frac{\partial q(x, \tau)}{\partial \tau} d\tau,$$

and ${}_{t_0}\bar{D}_t^{\alpha, \beta}$, $\beta > 0$ is combination of complex order fractional derivatives defined as

$$\begin{aligned} {}_{t_0}\bar{D}_t^{\alpha, \beta} q(x, t) &= \frac{1}{2} \left[\widehat{b} \mathbb{T}^{i\beta} {}_{t_0}D_t^{\alpha+i\beta} \frac{q(x, t)}{dt} + \widehat{b} \mathbb{T}^{-i\beta} {}_{t_0}D_t^{\alpha-i\beta} \frac{q(x, t)}{dt} \right] \\ &= \frac{1}{2} \left[\widehat{b} \mathbb{T}^{i\beta} \left(\frac{t^{-\alpha-i\beta}}{\Gamma(1-\alpha)} * \frac{q(x, t)}{dt} \right) \right. \\ &\quad \left. + \widehat{b} \mathbb{T}^{-i\beta} \left(\frac{t^{-\alpha+i\beta}}{\Gamma(1-\alpha)} * \frac{q(x, t)}{dt} \right) \right], \\ &t \geq t_0, \quad 0 < \alpha < 1, \quad \beta > 0, \end{aligned}$$

where $i = \sqrt{-1}$ and \mathbb{T} is a constant having the dimension of time, $\widehat{a}, \widehat{b} \geq 0$ are constants having dimension $(\text{time})^{1/\alpha}$. Both constants \widehat{a} and \mathbb{T} may be interpreted as relaxation times. Note that $q(x, t)$ is a real valued function of x and t .

The constitutive equation for q is a generalization of the classical Fourier law and the Cattaneo conduction law. Physically it shows thermal inertia of fractional type, i.e., thermal inertia with memory effects. Our central result in this work, are the restrictions on the coefficients in constitutive equation that are consequence of the entropy inequality

$$\int_0^d q(x, t) \frac{\partial T(x, t)}{\partial x} dt \leq 0.$$

Several known constitutive equations follow from our model as special cases. For a new constitutive equation we present a concrete example.

This is a joint work with Stevan Pilipović.

Acknowledgements: Partially supported by the Bilateral Research Project: “Mathematical Modeling by Means of Integral Transform Methods, Partial Differential Equations, Special and Generalized Functions, Numerical Analysis” between SASA and BAS.

References

- [1] T.M. Atanacković, S. Pilipović, B. Stanković, D. Zorica, Fractional Calculus with Applications in Mechanics: Vibrations and Diffusion Processes, ISTE - Wiley, London, 2014, <http://onlinelibrary.wiley.com/book/10.1002/9781118577530>;
- [2] T.M. Atanacković, S. Pilipović, B. Stanković, D. Zorica, Fractional Calculus with Applications in Mechanics: Wave Propagation, Impact and Variational Principles, ISTE - Wiley, London, 2014, <http://onlinelibrary.wiley.com/book/10.1002/9781118909065>.

Advanced services for Virtual Research Environments

Emanouil Atanassov, Aneta Karaivanova, Todor Gurov

The computational science have been long been considered as the third pillar of research, along with *theory* and *experimentation*. The growth in scale and depth of computational experiments lead to the establishment of large-scale research infrastructures comprising of supercomputers and large clusters complemented with huge storage capacities and advanced networking interconnections. Infrastructures built using Grid and Cloud technologies link resources from multiple institutions, while the actual computations are optimized to make full use of HPC technologies like multi-core programming, GPGPU, accelerators, etc. However, most researchers are only interested in achieving results and desire to be isolated from the details of the underlying hardware and middleware. The explosive growth of services at the top-level, which organize work into portals, hubs and databases, increases efficiency but also adds complexity and creates a risk of incompatibility between access and transfer protocols, identification etc. That is why the concept of the integrated Virtual Research Environment (VRE) has been developed, with the aim to provide scientists with integrated set of services that foster sharing and collaboration and take into account specific needs of the corresponding scientific discipline.

In the South Eastern Europe the need for collaboration and sharing of resources is palpable, because of the lack of economic resources and the danger of *brain drain* in general and especially in the scientific field. Through the years this lead to the establishment of Grid infrastructure and then to the HPC infrastructure that consists of some supercomputers and large clusters, with common policies and access protocols. The aim of the VI-SEEM project is to bring this collaboration to another level, by establishing VRE that offers top-level domain oriented services but also integrates the Grid, Cloud, HPC and storage resources of partners providing easy access to scientists from the target research communities in Life Sciences, climatology and digital cultural heritage.

Bulgaria has strong position in this consortium because of its leadership in the domain of High Performance Computing, after the provisioning of the supercomputer system Avitohol, which was deployed at the Institute of Information and Communication Technologies of the Bulgarian Academy of Sciences in 2015 and reached 332nd place in the Top500 list.

The challenges to the project come from the desire to offer transparent access to research data, organized using state-of-the-art technologies. In this work we illustrate how we can use different sources for authentication information and then how the different services are accessed. While the authentication information can be provided from stand-alone Identity Providers or from eduGAIN Identity Providers, or also from the VI-SEEM VHO, they all go the VI-SEEM Proxy Service. For the authorization we use VI-SEEM VHO and HEXAA AuthZ. Then the actual VRE services are divided into two main types – web-based services that use this information directly from the

VI-SEEM Proxy and more resourceful services like HPC, Grid, Cloud that use it through the token translator.

Some of these services required more work to be adapted to this framework while others are more straightforward. However, our goal is to create an extensible environment, so that new services that are requested by the scientists become easier to be added. Most of the domain-specific services that are requested are web-based. For example, the Clowder service is used throughout the Digital Cultural Heritage scientific community as a research data management system. Apart from the web front end, it provides RESTful web services and can do preprocessing or extraction services for extracting appropriate data and metadata.

Another example of domain-specific service is the ChemBioServer, which is used for effectively mining and filtering chemical compounds used in drug discovery. It allows for pre-processing of compounds prior to a computational search, as well as for post-processing of the best resulting molecules. The aim of this service is to increase the quality and efficiency of compound selection in order to save time and money during the more expensive experimental tests phase. Researchers can browse and visualize compounds along with their properties. It is obvious that such service aims to increase the effectiveness of the raw computational and storage services and to gain from the collaborative effort.

More complex service that offers powerful possibilities to researchers is the Scientific Application Environment, which is based on highly tuned, optimized and validated applications. Our experience shows that even well-known and widely researched applications can be hand-tuned to the particular hardware and software platform through changing parameters like compiler options, MPI and OpenMP launching options and by adding pragmas in *strategic places*. As an example, we modified the OpenFOAM source using an automated procedure and obtained about 50% overall improvement in speed, when using the Xeon Phi accelerators. In this way we made the case the using accelerators is faster than using the regular CPUs, even without modifying the sources through addition of vector intrinsic functions. The gradual extension of the Scientific Application Environment is a constant work in progress, but the current set of applications available already covers much of the needs expressed during our collection of requirements.

The Virtual Research Environment of the VI-SEEM project is an extensible set of services integrated through common authentication, authorization and accounting mechanisms. We plan to add more domain-specific services and later-on take other research communities on board of it, with special emphasis on the needs of the South East Europe's science and society.

Acknowledgments: This work was supported by EC programme HORIZON2020, Grant Agreement Number 675121, VI-SEEM project.

Image construction with 2D ellipses by genetic algorithms optimization

Todor Balabanov, Maria Barova, Delyan Keremedchiev

In Geometry there is a class of optimization problems called packing problems. It is an attempt to pack objects together into containers. In the most common case the goal is to pack a single container as densely as possible. For each packing problem there is a dual covering problem. In the covering problem it is asked how many of the same objects are required to completely cover every region of the container when, in the common case, objects are allowed to overlap. In this study a covering problem is presented where an image should be covered with regular ellipses with different colors and overlapping is allowed. The optimization objective function is strongly related to the composite picture and it is not so strongly related to the optimal packing. The criteria for good optimization is the Euclidean distance between the original image and the approximated image. The images are compared in HSV color space.

Some drawing devices are not capable to represent the visual information as pixels. For such devices the visual information should be transformed in a group of simple geometric shapes. This process of image data transformation is related to information reduction. The process is transformation of true colors image in a set of simple geometric shapes. This problem is very well known in literature and one of the most impressive implementations has been done with the image of Mona Lisa. The goal of this project was to approximate the picture of Mona Lisa by no more than 50 polygons. The colors and the points of the polygons were optimized by GAs.

The model proposed is based on Genetic Algorithms (GA). GA is applied over a set of shapes, represented by position and orientation. It is an unsupervised system which takes digital photographs as input and generates simplified, stylized vector data as output.

A raster image usually contains many details that are not relevant for a visual query and increase the cost of manipulations. Simplification of raster images is a process to eliminate the most useless elements, while retaining the perceptually dominant elements and shape. Simplification of raster images is a widely used process in the area of document analysis and recognition as a preprocessing step for high-level object recognition, such as optical character recognition (OCR) and graphic objects recognition. In image simplification and vectorization digital photographs are the input when generates simplified, stylized vector data are the output. The objective of image simplification by vectorization is to split the original image into simple geometric regions. In this process color reduction is also applied.

In this study ellipses were chosen as approximation shape, which to be used for image reconstruction. Each shape is described by its X,Y coordinates, angle of rotation and color. Each individual in the GA's population consists of an ordered set of shapes and fitness value. The ordered set of shapes is chosen so that the most used color in the picture is painted first. The less used colors are painted last. The fitness value is calculated as Euclidean distance between the approximate image and the original image.

The approximated image is assembled by shapes (in our case ellipses) with different colors given as a colormap at the input of the program. Color reduction is done in HSV color space. Each color from the original image is matched to a color in the given colormap. As an initial step GA population is initialized with randomly generated sets of shapes. For each shape X,Y coordinates and rotation angle are taken randomly. The color of each shape is not taken randomly. Color reduction is done from the color on the X,Y pixel coordinates in the original image instead. Such initialization creates approximated image very close to the optimal approximation. During GA's evolutionary process individuals are selected from the population, crossover, mutation, evaluation and survival are applied so that the image approximation is approved. In this study a binary crossover is chosen. Mutation is applied as X,Y shifting and color change of one shape in the individual. During evaluation phase the approximated image is compared with the original image. The result of the comparison is used as a fitness value of the individual. During the survival process it is decided which individual to be kept: the newly created or the already existing. The only stopping criteria used is the total number of image evaluations. Software implementation of the model proposed is absolutely free available, as open-source project, at GitHub repository (<https://github.com/TodorBalabanov/EllipsesImageApproximator/>). All experiments are done with an elitism rule, population size of 37 and maximum number of recombinations 10000. Initial population is assembled by randomly taken shapes according to the color of the pixel from the original image. An image of a flower is used for the experiments, but any other picture can be sent as input for the optimization program. Sixteen basic colors are used as colormap. The gaps in the image are getting smaller with the progress of the optimization procedure. The orientation of the basic shapes also gets better during the optimization process. Vectorized images can be produced by digital plotter with oil paint and can be presented as part of the concept for the digital home.

Experiments show that using GA may be very efficient and image approximation is pretty accurate in the limits of the color simplification. Optimization convergence is related to the probabilistic nature of GA. Image comparison is time consuming and slows down the optimization process. As further research, it could be interesting for GA to be implemented as distributed computing algorithm. Such distributed implementation is efficiently applicable for the class of evolutionary algorithms in which GA is. Set of ellipses can be treated as a multidimensional space and optimization can provide much better results.

Acknowledgements: This work was supported by private funding of Velbazhd Software LLC.

Authenticity management algorithm for digital images

**Todor Balabanov, Nikolai Manev, Walter Mudzimbabwe,
Petar Tomov, Ilian Zankinski, Stela Zhelezova**

Nowadays network services are gaining great attention. Image authentication is of great importance due to the large number of multimedia applications in various fields. Currently, the amount of digital images transmitted over non-secure channels is growing rapidly. Therefore, the protection of image integrity is of great interest.

The problem we consider is following. There is an image taken in an Android application. The application have to sign digitally the image without the user's knowledge in order to verify its origin. Apart from this, a digital watermark has to be added such that in case of tampering the modified part of the image is indicated. The application sends the image to the server where a corresponding algorithm part verifies the origin and the integrity of the image.

The initial restrictions with respect to this particular problem are:

- Size of the original image $n \times m$ pixels in Bitmap. Minimal size: 1024×768 . This is the worst case, because the hidden bits place is proportional to the image size.
- Content: interior and car pictures. The content is important in the connection with the hiding bits methods. If the image content is almost the same, i.e. the colors are evenly distributed hiding of information is much more difficult.
- The value of perceptual transparency is measured with Signal-to-noise ratio (SNR). SNR is used in science and engineering to compare the level of a desired signal to the level of background noise. It is defined as the ratio of signal power to the noise power:

$$SNR = 10 \cdot \log(MAX^2/MSE)$$

MAX - the expected pixel values,

MSE - the standard deviation of the pixel values between the original image (OI) and the watermarked image (WI) bits.

$$MSE = \frac{1}{m \cdot n} \sum_i \sum_j (O_{i,j} - W_{i,j})^2,$$

where $i \in \{1, \dots, n\}; j \in \{1, \dots, m\}$ are the dimensions of the original picture.

For the considered problem it is required $SNR > 30$.

Because of the particular case in which the watermarking is considered, we employ steganographic technique to embed data. The proposed authentication schema uses

spatial domain. Least Significant Bit (LSB) hiding is one of today's easiest techniques for image steganography. It imply adding some secret information in the least significant bits of the image pixel. The image quality is distorted for the number of bits embedded in a pixel greater than 3.

For the considered problem, the group propose an algorithm with client-server architecture. The chosen digital signature algorithm is based on image content and is according to latest NIST specifications.

The most common way to model color images in Computer Graphics is the RGB color model. We can use a packed ordering - the tree color components are placed together in a single array element. Next a matrix with zeroes in each bit which we will use later for hiding information is obtained. Then the "zerobits" image sequence ZBI_s is obtained according to a pixel permutation depending of a private key. User must not be involved in the signing procedure so as source of randomness the information about particular user, device and time parameters is used. Signing is performed applying SHA3-256withDSA. As a result the digital signature is embedded in 3-LSB of ZBI_s . To ensure tampering detection a blocking technique is used. The CRC16 is applied on each block. The relevant 16 bits codewords $CRC16$ are hidden in LSB. Only the signed and watermarked image sequence SWI_s is sent to the server part of the proposed algorithm.

In the server part of our algorithm the encoded public key is extracted. Next the digital signature for verification from the used 3-LSB and the CRC16 words for verification ($CRC16V$) from LSB also are extracted in order to remain the ZBI_s . It is used to verify the digital signature.

For a tampering detection the algorithm compare the extracted $CRC16V$ values and $CRC16$ words calculated on the received ZBI_s . If the image is not tampered the algorithm returns "true" else it changes the color of tampered blocks. As a result the matrix with zeroes in each used bit is obtained. It is not the original image, but perceptually indistinguishable.

The experiments with real data are needed in order to evaluate the lowest possible SNR for different parameters and to ensure the best performance of the algorithm. The real media environment have to be considered to supply the algorithm with error protection during the transmission.

The problem was considered during the 120 European Study Group with Industry, July 25-29, 2016, Sofia, Bulgaria.

An embedded compact scheme for biharmonic problems in irregular domains

M. Ben-Artzi, J.-P. Croisille, D. Fishelov

We consider in this contribution the biharmonic problem in a domain $\Omega \subset \mathbb{R}^2$ subject to Dirichlet boundary conditions:

$$\begin{cases} \Delta^2 \psi(x, y) = f, & (x, y) \in \Omega, \\ \psi(x, y) = \frac{\partial \psi}{\partial n}(x, y) = 0, & (x, y) \in \partial\Omega. \end{cases} \quad (1)$$

We present the design of a compact finite difference scheme for the problem (1), which is capable of handling irregular boundaries by an embedding method [2, 1]. The main properties of our scheme are the following:

- The grid is Cartesian with points $(x_i, y_j) = (ih, jh)$, where $h > 0$ is step size.
- At each point of the Cartesian grid, we attach a polynomial $P(x, y)$ of order 6:

$$P(x, y) = \sum_{p=1}^{19} a_p l_p(x, y), \quad (2)$$

where the 19 polynomials $l_p(x, y)$ are

$$\left\{ \begin{array}{l} l_1(x, y) = 1, \\ l_2(x, y) = x, \quad l_3(x, y) = x^2, \quad l_4(x, y) = x^3, \\ l_5(x, y) = x^4, \quad l_6(x, y) = x^5, \\ l_7(x, y) = y, \quad l_8(x, y) = y^2, \quad l_9(x, y) = y^3, \\ l_{10}(x, y) = y^4, \quad l_{11}(x, y) = y^5, \\ l_{12}(x, y) = xy, \\ l_{13}(x, y) = xy(x + y), \quad l_{14}(x, y) = xy(x - y), \\ l_{15}(x, y) = xy(x + y)^2, \quad l_{16}(x, y) = xy(x - y)^2, \\ l_{17}(x, y) = xy(x + y)^3, \quad l_{18}(x, y) = xy(x - y)^3, \\ l_{19}(x, y) = x^2 y^2 (x^2 + y^2). \end{array} \right. \quad (3)$$

The coefficients of $P(x, y)$ are calculated using values of the function and its first-order derivatives at neighboring points around (x_i, y_j) on a logically Cartesian 9 points stencil.

- The computational stencil is rectangular at regular interior points (x_i, y_j) . At near boundary points, the stencil is irregular, with Cartesian near-boundary gridpoints replaced by suitable boundary points. The discrete biharmonic is defined at the point (x_i, y_j) by

$$\Delta_h^2 u_{i,j} = \Delta^2 P(x_i, y_j). \quad (4)$$

mesh	17×17	Rate	33×33	Rate	65×65
e_∞	3.9014(-7)	4.49	1.7420(-8)	4.12	9.9940(-10)
$(e_x)_\infty$	3.5979(-6)	1.91	9.5902(-7)	3.39	9.1149(-8)
e_2	9.2739(-8)	4.75	3.4312(-9)	4.20	1.8602(-10)
$(e_x)_2$	1.5938(-6)	3.64	1.2719(-7)	4.02	7.7963(-9)

Table 1: Compact scheme for $\Delta^2\psi = 0$. $\psi(x, y) = x^2 + y^2 + e^x \sin(y)$ inside the star shaped domain given in Fig. 1. The domain is embedded in the square $[-1, 1] \times [-1, 1]$. We present e and e_x , which are the errors for the streamfunction ψ and for $\partial_x\psi$ in the l_2 and l_∞ norms.

Numerical results showing a remarkable accuracy even on coarse Cartesian grids (see Table 1 and Fig. 1) are reported and discussed.

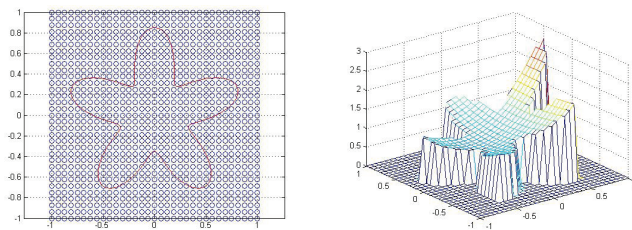


Figure 1: A star shaped domain (left) and the approximate solution (right) to the problem $\Delta^2\psi = 0$ with boundary data matching the exact solution $\psi(x, y) = x^2 + y^2 + e^x \sin(y)$. The grid is Cartesian 33×33 .

References

- [1] Ben-Artzi M., Croisille J.-P., Fishelov D., *Navier-Stokes equations in planar domains*, Imperial College Press, 2013.
- [2] Ben-Artzi M., Chorev I., Croisille J.-P., Fishelov D., A compact difference scheme for the biharmonic equation in planar irregular domains, *SIAM J. Numer. Anal.*, 47, 3087-3108.

On the formulation of population growth models by means of reaction networks

Milen Borisov, Nukolay Kyurkchiev, Svetoslav Markov

It has been recently demonstrated that some dynamical growth processes (e. g. logistic growth) can be formulated in terms of reaction networks. Such formulations suggest an insight on the intrinsic mechanisms of the physical (biological, biochemical, social) phenomena and thus can be useful for the interpretation and development of an adequate mathematical model. Another advantage of the reaction network presentation is that this presentation makes it easy for nonmathematicians to better understand the basic ideas behind the mathematical model. We elaborate further this idea by presenting various case studies of the realization of dynamical growth processes using suitable reaction networks. We especially focus on the time-course evolution of social processes following a logistic development and their possible interpretations. Numerical examples from social sciences are presented.

References

- [1] Borisov, M., N. Dimitrova, V. Beschkov, Stability analysis of a bioreactor model for biodegradation of xenobiotics, *Comp. and Math. with Appl.*, 64 (3) 2012, 361–373.
- [2] Markov, S., Cell Growth Models Using Reaction Schemes: Batch Cultivation, *Biomath* 2/2 (2013), 1312301.
- [3] Markov, S., Building reaction kinetic models for amyloid fibril growth, *Biomath* 5 (2016), 1607311

Industrial mathematics - phase transitions, scattering, structures

Stefan Bushev

The processes of structures formation are: phase transitions of I^{st} order (casting) and II^{nd} order (heat treatment); elastic and plastic deformation. The type of these structures is polycrystalline grains with size of macro-scale to $1\mu m$ or micro-scale below $1\mu m$ under a lattice parameter in A. The structure of all materials is a winner of its properties and the based interest of industries is: 1. improving the working properties of known materials; 2. creating new materials by structures design. Mathematical description of the phase transitions [1-7] presented by: the theory of thermal conductivity with the tasks of Stefan and Stefan - Schwartz; the fundamental equation of the formation of new phases of Kashchiev. On the Fig.1 we introduced castings technologies with different velocity of solidification and science support of micro-foundry.

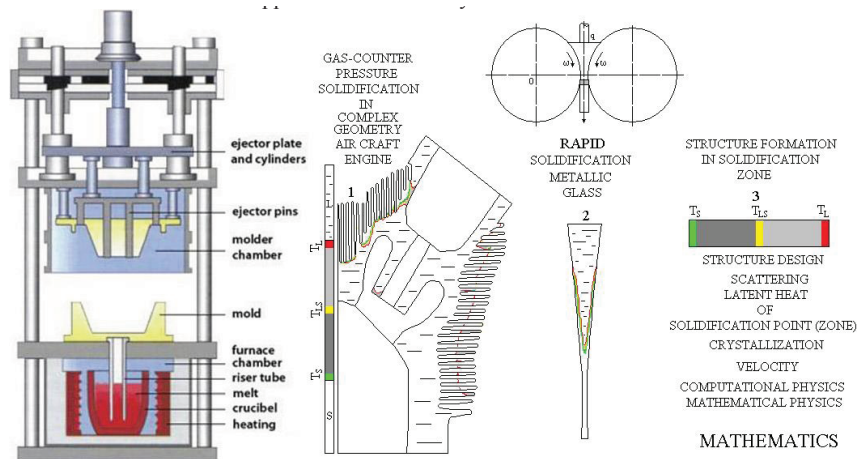


Figure 1: Industrial mathematics micro-foundry. Solidification process in temperature zone and character temperatures (T_S , T_{LS} and T_L , where solid S and liquid L): 1 air craft engine with complex geometry; 2 rapid solidification metallic glass; 3 scattering of latent heat of phase transition in solidification point (zone) - structure design, crystallization, velocity, computational physics, mathematical physics, fundamental and applied mathematics.

Electronic structure is origin of all properties of the metals and its alloys. For description the structures and properties of the metals and alloys are approach mathematics and mathematical physics. It will not be wrong to say that we need a nearly full knowledge i.e. tasks Stefan and Stefan-Schwarz must include mathematics and mathematical physics. This is done through mathematical tasks bridges between mathe-

mathematical fields and quantum mechanics. An example of such approach is the use of the results of the theory of scattering. In paper [2] is developed classical Stefan's problem. In Institute of Mathematics of Bulgarian academy of science are obtained great results about mathematical theory of scattering. The first base problem of scattering theory is proving existence of scattering operator. The second direction of development is inverse problem. It is well known, that thermodynamics driving force of the nucleation at phase transitions of 1^{-st} order (crystallization: liquid (L) \leftrightarrow solid (S)) is $\Delta\mu = \mu_L - \mu_S = Q_L \ln(T_m/T)$, where $\mu_{L(S)}$ are thermodynamics potentials of base (matter) and new phases; T_m and T are temperatures of transition and supercooling of the base (L) phase; Q_L - latent heat of melting. The supercooling is $\ln(T_m/T) = \Delta T_r + \Delta T_k + \Delta T_S$, where ΔT_r - supercooling effect radius of curvature, ΔT_k - supercooling for the transfer of atoms in the interface of liquid-solid phase; ΔT_S - supercooled liquid phase, which **scatter** heat of the phase transition. Received development task of Stephen with scatter theory [2] and assessments of supercooled melt ($\Delta T_S = 0, 1, 2, \dots, \max K$) in charge of literature [9]. Here many investigations are to be performed, but our opinion is that ΔT_S is a bridge to Quantum mechanics. The aim of this paper is to show methodological need to use the full modern knowledge required by the industry examples of casting and heat treatment.

References

- [1] S. Bushev, Thesis of PhD Controllability problems of crystallization process in casting, Technical University - Sofia.
- [2] S. Bushev, V. Georgiev, Developing the Solution of Stefan's Problem, Comptes rendus de l'Academie bulgare des Sciences, 47, No 3, 1994, 9-12.
- [3] S. Bushev, N. Miloshev, V. Todorov. Concept for Topological Model of New Phase Formation. Comptes rendus de l'Academie bulgare des Sciences, 53, 2000, No.9, 39-42.
- [4] S. Bushev, N. Miloshev, N. Stoichev, V. Todorov, Improvement of Mathematical Models of Phase Transition of First Order. J. of Materials Science and Technology, Vol. 12, 2004, No 1, p. 111-122.
- [5] S. Bushev, M. Dimitrov, N. Stoychev, Undercooling at the Crystallization Front in Stefan's Problem for Melt Rapid Solidification. Proc. of National Conference with international participation "Material Science and new materials", 4-5, December 2008, Sofia - Bulgaria, p. 288 - 293.
- [6] S. Bushev, N. Stoichev, N. Miloshev, M. Dimitrov, V. Todorov, Temperature Field and Crystallization During Solidifications of Liquids, Journal of Materials Science and Technology, v. 18, 2010, No 4, p. 228 - 239.
- [7] S. Bushev, Theoretical model of structure formation in die casting, Proceedings of XXII International scientific technical conference "Foundry 2015", 16-17.04.2015, Pleven, Bulgaria, p.60-63. ISSN: 1310-3946 (In Bulgarian)

- [8] S. Bushev, Computational physics - casting and heat treatment, Proceedings of "Fifth National Conference with International Participation Materials Science, Hydro- and Aerodynamics and National Security'2015".
- [9] M. C. Flemings, Solidification processing, Moscow, Peace, 1977. (In Russian)
- [10] V. Petkov, Representation of the scattering operator for dissipative hyperbolic systems, comm. in Part. Diff. Eq., 6, 1981, 993-1022.
- [11] V. Georgiev, High frequency asymptotics of the filtered scattering amplitudes and the inverse scattering problem for dissipative hyperbolic systems, I, Math. Nachr. 117, 1984, 111-128.

Modeling of membranes with complex rheology: computational aspects

Krassimir Danov

The mathematical and computational modeling of the equilibrium and dynamic behavior of membranes is a general problem in mechanics and biomechanics with a wide application to the medicine, pharmacy, foam and emulsion technologies, etc. The protein adsorption layers, phospholipid mono- and multilayers (biomembranes), floating thin polymer films, layers of nanoparticles on oil/water interfaces, monolayers of metal-organic complexes, etc. are modeled as 2D elastic membranes, which interact with the surrounding bulk phases.

We developed a theoretical model for 2D elastic continuum, which accounts for the complex rheology of interfaces. The parameters of the model are the surface (membrane) stretching and shear elasticity, Helfrich curvature elastic moduli. It is a special case of the general concept of Cosserat continuum with bending elasticity. The final result is a system of six strongly nonlinear partial differential equations, which expresses:

1. The surface balance of the linear momentum written for the pressure difference and surface stress tensor;
2. The surface balance of the angular momentum written for the surface torque and stress tensors.

To close the system of equations we use surface rheological constitutive relationships - the dependencies of the stress and torque tensors on the metric and curvature tensors of membrane surface. When one defines the necessary boundary conditions one should solve numerically the respective boundary value problem. For known physical constants the boundary value problem has many solutions and the criterion for the physical one is the minimization of the free energy of the system. For that reason original numerical methods are developed.

The model is applied to and verified with experimental data for different systems. In the case of biomembranes it is used to determine the membrane tension and adhesion energy of erythrocytes and the mechanism of stomatocyte-echinocyte transformations of red blood cells [1,2]. For elastic Langmuir layers and membranes the model is applied to calculate various shapes (nonharmonic oscillations, toothed profiles, and profiles with two characteristic wavelengths) and the bending elasticity [3]. Different numerical schemes for real time data processing of rotating axisymmetric drops are compared in Ref. [4]. The numerical procedures for calculation of experimental values of the components of stress tensors and energy of adhesion of drops and bubbles at different interfaces become a basis of the capillary meniscus

dynamometry (CMD) realized on commercial apparatuses.

References

1. K.D. Tachev, J.K. Angarska, K.D. Danov, P.A. Kralchevsky, *Colloids Surfaces B* 19 (2000) 61.
2. K.D. Tachev, K.D. Danov, P.A. Kralchevsky, *Colloids Surfaces B* 34 (2004) 123.
3. K.D. Danov, et al., *Langmuir* 26(1) (2010) 143.
4. K.D. Danov, et al., *Colloids Surfaces A* 489 (2016) 75.
5. K.D. Danov, et al., *J. Colloid Interface Sci.* 440 (2015) 168 and *Adv. Colloid Interface Sci.* 233 (2016) 223.

Approximate method for non-instantaneous impulsive difference equations with a periodic boundary condition

Svetoslav Enkov, Snezhana Hristova, Ekaterina Madamlieva

One of the powerful apparatus for discrete modeling of the dynamics of many real world processes are difference equations. They allow us directly to be implemented in computer programs. There are many processes and phenomena which are characterized by rapid changes in their state. In the literature there are two popular types of impulses:

– instantaneous impulses - the duration of these changes is relatively short compared to the overall duration of the whole process. The model is given by impulsive difference equations (see, for example, [2], [3], [4]);

– noninstantaneous impulses - an impulsive action, which starts at an arbitrary fixed point and remains active on a finite time interval. As a motivation for the study of these systems we consider the following simplified situation concerning the hemodynamical equilibrium of a person. In the case of a decompensation (for example, high or low levels of glucose) one can prescribe some intravenous drugs (insulin). Since the introduction of the drugs in the bloodstream and the consequent absorption for the body are gradual and continuous processes, we can interpret the situation as an impulsive action which starts abruptly and stays active on a finite time interval.

One of the problems in difference equations is approximate obtaining of the solution. It is very important specially in the case when the unknown function in the present time is involved in both side parts of the nonlinear equation. One of the approximate methods is based on the method of upper and lower solutions combined with a monotone - iterative technique (see [1], [3], [4], [5], [7]). This method allows us to be constructed two monotonous sequences of upper and lower solutions of the nonlinear noninstantaneous impulsive difference equation. These functional sequences converge monotonically to the minimal and maximal solutions of the nonlinear equation. Each term of the sequences is obtained as a solution of a periodic boundary value problem for linear non-instantaneous impulsive difference equation. An explicit formula for the successive approximations is given. Some comparison results are studied. Also, the existence result of extremal solutions of the boundary value problem for the nonlinear difference equation is obtained. The suggested algorithm is computerized. We developed a web-based tool in Javascript, which gives us flexibility to experiment in a platform-independent environment. We used two open-source libraries Math Parser by Matthew Crumley and Function Plot by Maurizio Poppe. Math Parser provides us with parsing text-based formulas, which allows us to define the formulas as text strings, without changing the code of our tool. We use Function Plot to visualize the functions. The tool provides input validation, compliance of the constants and steps of the algorithm, protection against loops, and calculation validation. Calculations are performed with a precision of 15 digits after the decimal point. The suggested

algorithm is illustrated on an example.

References

- [1] R. P. Agarwal, S. Hristova, A. Golev, K. Stefanova, Monotone-iterative method for mixed boundary value problems for generalized difference equations with "maxima", *J. Appl. Math. Comput.* 43, 1, (2013) 213–233.
- [2] H. Bereketoğlu, A. Huseynov, Boundary value problems for nonlinear second-order difference equations with impulse, *Appl. Math. Mech.* , 30, 8, (2009)1045–1054.
- [3] Z. He, X. Zhang, Monotone iterative technique for first order impulsive difference equations with periodic boundary conditions, *Appl. Math. Comput.*, 156, 3, (2004), 605–620.
- [4] S. Hristova, R. Terzieva, Monotone iterative technique with respect to initial time difference for initial value problem for difference equations with maxima, *AIP Conf. Proc.* 1690, 040018 (2015); <http://dx.doi.org/10.1063/1.4936725>.
- [5] P.Y.H. Pang, R.P. Agarwal , Monotone iterative methods for a general class of discrete boundary value problems, *Comput. Math. Appl.*, 28, 13, (1994), 243–254.
- [6] M. Peng, Oscillation theorems of second-order nonlinear neutral delay difference equations with impulses, *Comput. Math. Appl.*, 44,(2002), 741–748.
- [7] P. Wang, Sh. Tian, Y. Wu, Monotone iterative method for first-order functional difference equations with nonlinear boundary value conditions, *Appl. Math. Comput.* 203, 1, (2008), 266–272.

Ant Colony optimization algorithm for 1D Cutting Stock Problem

Georgi Evtimov, Stefka Fidanova

Every day different companies in industry have to solve many optimization problems. One of them is cutting out of linear materials, like steel or aluminum profiles, steel or wood beams and so on. It is so called cutting stocks problem (CSP). It is well known NP-hard combinatorial optimization problem. The accurate and fast cutting out is very important element from the working process. The aim in CSP is to cut items from stocks of certain length, minimizing the total number of stocks (wast). The computational time increases exponentially when the number of items increase. Finding the optimal solution for large-sized problems for a reasonable time is impossible. Therefore exact algorithms and traditional numerical methods can be apply only on very small problems. Mostly appropriate methods for this kind of problems are methods based on stochastic search or so called metaheuristic methods. Various metaheuristics have been applied on CSP. Some authors apply evolutionary algorithms including Genetic algorithm [4, 5, 6, 6] others apply Tabu search and Simulated annealing [4]. On this work we will propose a variant of Ant Colony Optimization (ACO) algorithm to solve CSP.

The first ACO algorithm was developed by Dorigo in his PhD thesis in 1992. During the years it has been improved several times and was created different variants of ACO algorithm. ACO was successfully applied on various combinatorial optimization problems. It is constructive method which does not need initial solution. ACO is very competitive method and outperforms others especially when it is applied on combinatorial optimization problems with strong constraints [1].

References

- [1] Dorigo M., Maniezzo M., Colorni A., *The ant system: Optimization by a colony of cooperating agents*, IEEE Transactions on Systems, Man, and Cybernetics B, Vol. 26(1), 1996, 29 – 41.
- [2] Falkenauer E., *A hybrid grouping genetic algorithm for bin packing*, Journal of Heuristics Vol. 2, 1996, 5 – 30.
- [3] Hinterding R., Khan L., *Genetic algorithms for cutting stock problems: with and without contiguity*, In X. Yao, editor, Progress in Evolutionary Computation, Berlin, Germany, Springer, 1995, 166 – 186.
- [4] Jahromi, M.H., Tavakkoli-Moghaddam, R., Makui, A. Shamsi A.. *Solving an one-dimensional cutting stock problem by simulated annealing and tabu search*, J. of Industrial Engineering International, Vol. 8(1), Springer, 2012, paper 24.

- [5] Reeves C. *Hybrid genetic algorithms for bin-packing and related problems*, Annals of Operations Research 63, 1996, 371 – 396.
- [6] Vink M., *Solving combinatorial problems using evolutionary algorithms*, 1997. Available from <http://citeseer.nj.nec.com/vink97solving.html>

Error estimate in the iterative numerical method for two-dimensional nonlinear Hammerstein-Fredholm fuzzy functional integral equations

Atanaska Georgieva, Albena Pavlova, Iva Naydenova

The concepts of fuzzy integrals and differential equations have been studied by many mathematicians and authors. The study of fuzzy integral equations begins with the investigations performed by Kaleva [1], Goetschel and Voxman [2] and others. The interest in fuzzy Fredholm integral equations is based primarily on its applications in fuzzy financial and economic systems [3].

In this work, we investigate the two-dimensional nonlinear Fredholm fuzzy functional integral equation

$$F(s, t) = g(s, t) \oplus f(s, t, F(s, t)) \oplus (FR) \int_c^d (FR) \int_a^b K(s, t, x, y) \odot H(x, y, F(x, y)) dx dy,$$

where $K(s, t, x, y)$ is an arbitrary positive kernel on $[a, b] \times [c, d] \times [a, b] \times [c, d]$, $g, F : [a, b] \times [c, d] \rightarrow \mathbf{R}_{\mathcal{F}}$ are continuous fuzzy-number valued functions and $f, H : [a, b] \times [c, d] \times \mathbf{R}_{\mathcal{F}} \rightarrow \mathbf{R}_{\mathcal{F}}$ is a continuous functions on $\mathbf{R}_{\mathcal{F}}$.

The existence and uniqueness of the solution is proven by Banach's fixed point theorem. We approximate the solution of equation using the quadrature formula of rectangles and the method of successive approximations we approximate solution of equation. The error estimation of the iterative method is obtained in terms of uniform and partial modulus of continuity, proving the convergence of the method. The error estimate obtained in this paper is expressed in terms of the modulus of continuity for g and K , which effect the statement concerning numerical stability. We illustrate the iterative method of numerical experiment by testing the convergence and the numerical stability with respect to the choice of the first iterations. Some numerical examples are included in order to confirm the theoretical results.

References

- [1] Buckley J., Eslami E., Feuring T., *Fuzzy Integral Equations*, in: *Fuzzy Mathematics in Economics and Engineering*, Studies in Fuzziness and Soft Computing, Springer, Physica-Verlag, Heidelberg, 2002, vol. 91, pp. 229-241.
- [2] Goetschel R., Voxman W., *Elementary fuzzy calculus*, Fuzzy Sets Syst., 1986, vol. 18, pp. 31-43.
- [3] Kaleva O., *Fuzzy differential equations*, Fuzzy Sets and Systems, 1987, vol. 24, pp. 301-317.

Fast algorithm for solving ℓ^0 -constrained graph-Laplacian minimization

Stanislav Harizanov

Let $\mathcal{G}_{\mathbf{u}}$ be a weighted graph associated to the discrete vertex set \mathbf{u} of cardinality \mathbf{n} , whose edge weights $\omega_{i,j}$ are non-negative, \mathbf{u} -dependent, and a priori computed. Denote by

$$J(\mathbf{v}) := \frac{1}{4} \sum_{i,j=1}^{\mathbf{n}} \omega_{i,j} (\mathbf{v}_i - \mathbf{v}_j)^2,$$

the (scaled) ℓ^2 norm of the discrete non-local gradient $\nabla \mathbf{v}$, related to $\mathcal{G}_{\mathbf{u}}$. This functional is directly related to the the graph-Laplacian operator Δ_{ω} via $J(\mathbf{v}) = \frac{1}{2} \langle \Delta_{\omega} \mathbf{v}, \mathbf{v} \rangle$. In this talk we consider the following ℓ^0 -constrained problem

$$\min_{\mathbf{v} \in \{0,1\}^{\mathbf{n}}} J(\mathbf{v}) \quad \text{subject to} \quad \mathbf{v}_i = \begin{cases} 1, & i \in L_1, \\ 0, & i \in L_0, \end{cases} \quad \|\mathbf{v}\|_0 = N,$$

that is applicable to nonlocal image and signal processing. The sets L_1 and L_0 are very small, fixed, and responsible for the uniqueness of the minimizer. The value $N < \mathbf{n}$ has certain physical meaning that depends on the application.

The counting measure ℓ^0 is non-convex while the admissible class of functions is discrete (namely, the vertices of the \mathbf{n} -dimensional unit cube), so the above optimization problem is NP-Hard and cannot be efficiently solved directly. We numerically study an iterative steepest-descent-type solver for it, based on the solution of the penalized continuous relaxation family

$$\min_{\mathbf{v} \in [0,1]^{\mathbf{n}}} J(\mathbf{v}) - \lambda \langle s, \mathbf{v} \rangle \quad \text{subject to} \quad \mathbf{v}_i = \begin{cases} 1, & i \in L_1, \\ 0, & i \in L_0, \end{cases} \quad \|\mathbf{v}\|_1 = N.$$

The penalizer λ and the direction s are free parameters that may vary from iteration to iteration. The proposed algorithm is theoretically convergent. Moreover, the conducted numerical experiments in the field of 2-phase image segmentation suggest that the algorithm always converges exponentially towards the true minimizer of the ℓ^0 -constrained problem. The efficiency of each iterative step is achieved due to a convenient change of basis in the image domain, for which the relaxed target function is decomposed element-wise. The most computationally expensive part is the generation of the weight matrix W , which needs to be done only once at the beginning and is part of the preprocessing.

Acknowledgements: The research of S. Harizanov is supported by the ‘‘Program for career development of young scientists, BAS’’ Grant No. DFNP-92/04.05.2016.

Multi-frame denoising of still images

S. Harizanov, D. Dimov, N. Naidenov, S. Kostadinova

During the 120th *European Study Group with Industry* (ESGI'120), the following problem was addressed by the company *MM Solutions AD*: A sequence of 8 images are captured quickly one-by-one while camera is held in hand and unintentional hand shake is present. When capturing in low light conditions ($< 20\text{Lux}$), the images appear blurred and noisy because the camera uses long exposure (1/15..1/5 sec) and high gain (ISO). The target is to combine multiple frames to produce an image with less noise and less (ideally no) blur. The processing algorithm should not be too computationally expensive. As usual in the image processing, the target is to get a good looking image, rather than removing the noise and the blur to achieve the ground-truth latent image.

In this talk we report the results of our study group that were achieved during and after the event. Two different denoising algorithms are proposed, implemented, and numerically investigated. The first one deals with aligned input data and is based on penalized regularization. The regularization term used in the target function is the mixed $\ell^{2,1}$ norm (also known as the *TV semi-norm*) of the discrete gradient of the output image. The data fidelity term used as a penalizer in the target function is the ℓ^2 norm of the offset vector between the output and a weighted convex combination of the 8 input frames. Our numerical solver of the above model is based on the *Alternating Direction Method of Multipliers* (ADMM). The conducted numerical experiments gave rise to convincing results, where both the quality of the output image and the time efficiency of the denoising process are satisfactory.

The second approach deals with unaligned input data and is based on *Inverse Noise Filtering*. Assuming that the motion between two chronologically consecutive frames \mathbf{f}_1 and \mathbf{f}_2 is linear and their misalignment $\Delta\mathbf{f}$ is known, we model the “dynamic” noise caused by the frame move, then reconstruct frame \mathbf{f}_1 from \mathbf{f}_2 , $\Delta\mathbf{f}$, and the “dynamic” noise, and finally extract information about the static noise level from the difference between \mathbf{f}_1 and its reconstruction. The implemented numerical algorithm uses direct and inverse FFT and performs all the computations in the Fourier domain, making the aligning process time efficient.

Combining the two different approaches into one is work in progress. There are also other aspects that needs improvement. Firstly, replacing the direct solver of a linear system in the ADMM algorithm step via an appropriate iterative one will increase the overall time efficiency. Secondly, apart from alignment, the Inverse Noise Filtering approach should take into consideration rotation, scaling, and rolling-shutter, which are also typical for CMOS cameras.

Acknowledgements: The research of S. Harizanov is supported by the “Program for career development of young scientists, BAS” Grant No. DFP-92/04.05.2016.

Denoising and feature extraction of 2D CT radiographic images

Stanislav Harizanov, Jaime de Dios Pont, Sebastian Ståhl,
Dennis Wenzel

In both industrial and medical applications the use of 2D radiography has increased in recent years as it offers in many cases a more reliable way of examining physical objects than performing quantitative measurements on them directly. The drawback of CT radiographic images is that they are generated by counting photons that penetrate the object of interest, thus they are often affected by measurement inaccuracies leading to generation of image noise. This reduces the amount of valuable information that can be extracted from the raw image as important structures might be dominated by the noise. In this talk we propose and analyze innovative image processing techniques that allow us to improve the data quality and to correctly extract most of the important structural information from it.

An obvious but ineffective way to deal with the presence of image noise is based on the central limit theorem: by averaging over an increasing number of different image instances the variance of the noise distribution tends to zero. The main problem of this approach is the need of a sufficiently large number of images. This causes additional problems, especially in medical applications where radiation exposure should be kept as low as possible for health reasons. The alternative is to develop more advanced image denoising techniques, suitable to the task specifics.

The first step of our research is a statistical analysis of the noise on real 2D CT data in order to find proper mathematical models for its removal. From the physical point of view we expect the noise to be a mixture of Poisson and Gaussian components but it is crucial for the design of effective methods to exactly know the noise parameters. The analysis is performed on various data sets of 8 to 16 images of the same object and the pixel-wise intensity relations between mean value and variance are studied.

Once the noise distribution has been determined, we examine two different approaches for its removal: the first one uses a variance-stabilizing transformation (VST) on the input image that transforms all the noise to a purely Gaussian one and afterwards standard additive white Gaussian noise (AWGN) denoising methods are applied, while the second one neglects the Gaussian component, works directly with the statistics of the dominant Poisson component and uses an iterative primal-dual algorithm directly on the input image. The first approach we consider makes use of the *generalized Anscombe transform*, which is designed to transform mixtures of Gaussian and Poisson noise into purely Gaussian noise, given the variance of the Gaussian part. The second approach we consider applies the *Alternating direction method of multipliers* (ADMM) to a constrained optimization problem with discrete gradient as regularization term and the *Kullback-Leibler divergence* as data fidelity term. Note that in the

ADMM algorithm there is a parameter to be chosen according to estimations. Underestimating this parameter leads to over-smoothing while over-estimations increase the intensity of the noise left after applying the algorithm.

The last step of the research is applying the denoising methods to two different real world CT radiographic images, one showing a 3D printed object and one showing an industrial metal welding. Especially the second example shows the need of effective denoising algorithms as the work piece contains small air bubbles in the weld seam possibly causing stability problems. In the original noisy image the bubbles are strongly overlaid by noise, making them almost invisible for the human eye, while they are very well visible in the denoised image.

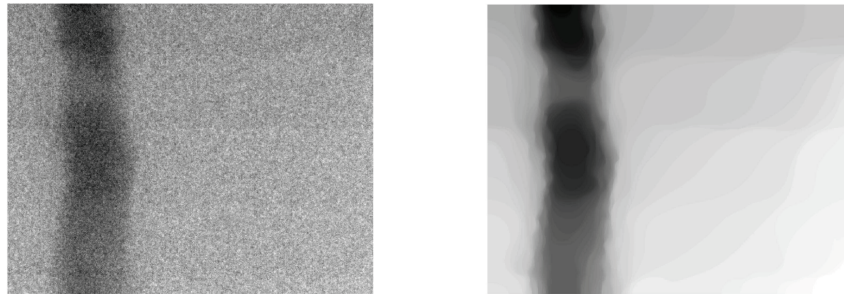


Figure 2: Noisy image (left), denoised image (right).

Acknowledgements: The research of S. Harizanov is supported by the “Program for career development of young scientists, BAS” Grant No. DFNP-92/04.05.2016.

Material parameter identification of thin film with diamond nanoparticles via nanoindentation

D. Iankov, M. Datcheva, R. Iankov

The basic aim of the present paper is to present an adequate model for numerical simulation of nanoindentation process of thin film with diamond nanoparticles deposited on Si substrate.

The goal of nanoindentation test is to extract elastic modulus and hardness (HIT) in a local point of the specimen employing the measured load-displacement curve (P-h curve). The elastic or indentation modulus EIT can be determined from the slope of the unloading part of the P-h curve [2]. The experiments on nanoindentation can be used to determine the mechanical characteristics of thin film and layers where the conventional test approaches fail. However, there are some limitations: (i) using nanoindentation we cannot determine the yield strength of the material because we have indirect information about the plastic properties by means of nanohardness. Moreover, the nanohardness value is highly dependent on the indenter tip geometry. This is also valid for homogeneous bulk materials but is more evident for thin coatings. (ii) It is uncertain to what extent the determined EIT and HIT for a system of thin film and substrate represent the properties of the thin film. (iii) The accepted in literature criterion to consider in determining the film characteristics only penetration depths up to 10% of the film thickness ([1]) is not applicable for all thin film-substrate system.

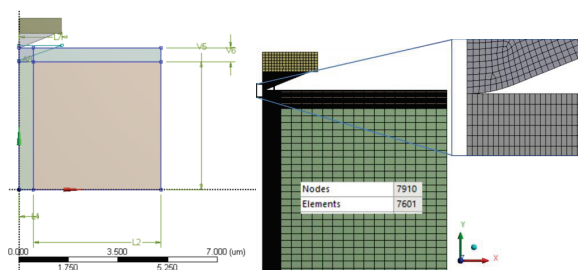


Figure 1: 2D BVP problem and FEM model.

The limitation of the interpretation of the nanoindentation results based solely on the P h curve as a geometric object can be overcome by numerical simulations of the experiment employing the contact analysis. Deformation process in the area of contact is a highly nonlinear problem due to the material nonlinearity, geometry nonlinearity (large deformation) and nonlinearity due to the friction and contact interfaces. The combination of finite element modelling and experimental data from nanoindentation tests can help to extract more information about the mechanical properties of the material and especially for the properties of thin coatings independently of the

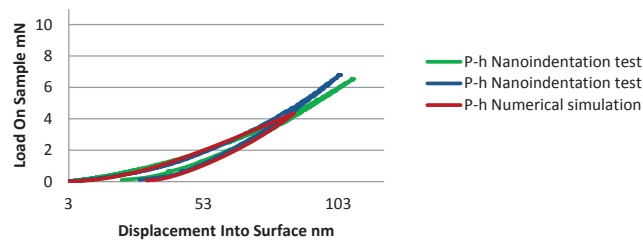


Figure 2: Comparison between experimental data and numerical simulation of indentation process.

substrate behaviour. Because such combination involves performing the back analysis and solving optimization problem, we need to have an adequate numerical and boundary value problem for the indentation process in order to ensure an efficient solution and reliable results.

In the case of isotropic materials the three-dimensional nature of the indentation problem with pyramidal indenter tip can be reduced to a 2D axisymmetric model [2]. In the figures such model is shown together with the fit to a real experiment on nanoindentation of very thin diamond film of silicon substrate.

Acknowledgments: Authors gratefully acknowledge the financial support of the Bulgarian National Science Fund under Grant No. T02-22/12.12.2014.

References

- [1] Anthony C. Fischer-Cripps , Nanoindentation, ISBN: 978-1-4419-9871-2, Springer Science+Business Media, LLC
- [2] M. Datcheva, S. Cherneva, D. Stoychev, R. Iankov, M. Stoycheva, Mater. Sci. Appl. 2 (2011) 1452-1464, doi:10.4236/msa.2011.210196.

Toward exascale computations of uncertainty quantification for porous media flow using multilevel Monte Carlo

Oleg Iliev, Jan Mohring, Nikolay Shegunov, René Milk, Mario Ohlberger

Uncertainty quantification (UQ) for porous media flow is of great importance for many societal, environmental and industrial problems. An obstacle to the progress in solving such problems, as well as in solving other stochastic PDEs, SPDEs, is the extreme computational effort needed for solving realistic problems. It is expected that the computers will open the door for a significant progress in this area. We shortly introduce the Distributed and Unified Numerics Environment DUNE [www.dune-project.org], and demonstrate how new features, developed in the last few years, can enable the handling of these computational challenges. In the frame of the DFG funded project EXA-DUNE, the software has been extended by multiscale finite element methods (MsFEM) and by a parallel framework for the multilevel Monte Carlo approach (MLMC). This is a general concept for computing expected values of simulation results depending on random fields, e.g. the permeability of porous media. It belongs to the class of variance reduction methods and overcomes the slow convergence of classical Monte Carlo by combining cheap/inexact and expensive/accurate solutions in an optimal ratio.

Let us discuss shortly different components of the considered algorithm and its implementation.

Different approaches have been developed for solving stochastic PDE. Perturbation methods, moment equations, generalized polynomial chaos and various Monte Carlo methods have been extensively studied. Our choice is an efficient variant of the Monte Carlo methods, namely Multilevel Monte Carlo method. As mentioned above, the idea of this method is to reduce variance by combining cheap/inexact and expensive/accurate solutions in an optimal ratio. Selection of the levels in MLMC is an open question and is subject of intensive research. For example, if one uses Karhunen-Loewe expansion to reduce the dimensionality in the stochastic space, the number of the terms in the expansion can be used to define levels in MLMC. Another approach for selecting levels in MLMC can be the number of the basis functions if reduced basis method is used. A more classical approach is to define levels by considering fine and coarsened grids. In the latter case when has to define the permeability on the coarse grid. In our talk we will elaborate on this last approach and will show results when renormalization is used to define the permeability on the coarser grids.

Another component of the algorithm is the generation of the permeability fields. This by itself is also a challenging computational task. Earlier we have reported on using

circulant embedding for this purpose, and in this talk we will shortly recall those results.

For each realization of the permeability field one gets a deterministic PDE with highly varying coefficients which has to be solved efficiently. To discretize this PDE we use two methods: FEM and FV. In both cases we exploit DUNE software, www.dune-project.org. In the case of FEM discretization, also Multiscale FEM, MsFEM, can be used, and MsFEM solution can also be used to define levels in MLMC. We will recall some results on this approach.

Finally, the software implementation also plays essential role in solving stochastic PDE. High performance computing is demanded for solving such problems. We will shortly discuss the parallelization approaches implemented in DUNE, and will show results from the tests performed on the cluster in Fraunhofer ITWM. Currently only CPUs are used in our computations. In parallel, partners are working on parallelizing DUNE for heterogeneous architectures, and a goal of our future work is to have efficient implementation of MLMC on heterogeneous architectures. In particular, we plan to use MLMC also for coarse grain parallelization of algorithms for solving SPDE on exascale computers.

References

- [1] Mohring, J., Milk, R., Ngo, A., Klein, O., Iliev, O., Ohlberger, M. and Bastian, P., 2015, June. *Uncertainty Quantification for Porous Media Flow Using Multilevel Monte Carlo*. In International Conference on Large-Scale Scientific Computing (pp. 145–152). Springer International Publishing.
- [2] Bastian, P., Blatt, M., Dedner, A., Engwer, C., Kloeckner, R., Ohlberger, M., Sander, O.: *A Generic Grid Interface for Parallel and Adaptive Scientific Computing. Part I: Abstract Framework*. Computing 82(2-3), 103–119 (2008)

Identification of structural units in large proteins for guided metadynamics investigations

N. Ilieva, E. Lilkova, P. Petkov, and L. Litov

The aim of this study is to develop a procedure for the selection of collective variables for metadynamics simulations of large biomolecules based on criteria reflecting the specifics of the investigated objects and processes. In particular, we assess the possibility of using the spatio-temporal multistage consensus clustering method (SMCC) as a guideline in this selection procedure. The SMCC method identifies compact groups of amino acid residues forming semi-rigid domains.

Protein-protein interactions (PPI) play a fundamental role in many biochemical processes and their study is a central problem in life sciences. A convenient approach to study the properties of such biocomplexes is Molecular Dynamics (MD), as obtaining detailed experimental data is usually difficult and sometimes even impossible. However, MD may often prove inefficient for PPI due to transitions with high free energy barriers or large-scale molecular rearrangements. Metadynamics is a powerful advanced sampling technique for computing free energy differences and barriers, reconstructing free energy surfaces and accelerating rare events in complex systems. The method is based on computation of the free energy of the system as a function of a small set of collective variables (CVs) by applying a history-dependent bias.

The reliability of metadynamics simulations depends significantly on the choice of CVs). They should comply with a number of criteria. Meeting all these criteria is a demanding task and there is no standard protocol for CV selection. Often a trials-and-errors approach is the only option, which is computationally very expensive, especially for large biomolecular systems.

The Spatiotemporal Multistage Consensus Clustering (SMCC) method is a post processing technique for analysis of MD trajectory data. It consists of initial spatial clustering performed on successive sub-segments of an MD simulation trajectory, followed by a temporal self-consistent consolidation of the results to generate domains that are stable over time. In the first step the C_α atoms are assigned in a preselected number k of spatial clusters by minimization of the variation of distances between pairs of C_α -atoms:

$$q(c) = \sum_{m=1}^k \sum_{i=1}^N \sum_{j=1}^N c_{im}c_{jm}S_{ij} \rightarrow \min \quad (1)$$

Here c_{im} is the cluster-membership coefficient of atom i in cluster m , for N atoms and k clusters. The standard deviations of distances d_{ij} between atom pairs (i, j) along a given trajectory are contained in the STDDV matrix

$$S_{ij} = \sqrt{\frac{L}{L-1} \langle (d_{ij} - \langle d_{ij} \rangle)^2 \rangle}, \quad (2)$$

where L is the number of frames (conformations) considered and the average is taken over the whole or a part of the trajectory. The procedure generates clusters of similar size.

The second step addresses the problem of cluster variation along different parts of the trajectory. In the temporal clustering, the number of clusters results from clustering itself and the procedure yields clusters of different size. The free parameters in the SMCC method are the number of segments into which the trajectory is divided, the number of spatial clusters for the first stage of the procedure and the dissimilarity index, which indicates the tolerance in the cluster assignment, that is, how often an atom is allowed to leave the cluster and still be considered a part of it. The values of these parameters depend strongly on the investigated object and the MD protocol.

We propose to apply the SMCC method to preliminary standard MD simulations of bimolecular complexes to identify semi-rigid domains in the structures. This information will then be used in the CVs selection for subsequent metadynamics simulations. The test system that was chosen is human interferon gamma (hIFN- γ) and its extracellular receptor. Three hIFN- γ analogues were used for the selection protocol development and calibration — the hIFN- γ wild type and two derivative proteins out of 100 random mutations in amino acids 86-88. They are typical cases of mutants in which the mutations preserved, resp. destroyed structure and activity, compared to the wild type. The domain identification protocol was tuned and validated by comparing results with unguided metadynamics analysis of the FES in the parameter space of Lys 86 backbone twist angles and antiproliferative activity competition bioassays.

In the calibration proteins the clustering procedure identified semi-rigid domains in the structures that are also associated with different functions. This suggests that the distances between centers of masses of certain amino acid residues groups, that were identified in the clustering process, may be suitable collective variables. The protocol will be applied in studying the hIFN- γ binding to its receptor, where all intuitive CV choices have not been successful so far.

Acknowledgements The simulations were performed on the HPC Cluster at the Faculty of Physics of Sofia University “St. Kl. Ohridski”. EL and NI acknowledge financial support under the programme for young scientists’ career development at the Bulgarian Academy of Sciences (Grant DFNP-99/04.05.2016).

References

- [1] D. Frenkel, and B. Smit (2002) *Understanding Molecular Simulation* (2nd ed.), Academic Press: San Diego.
- [2] L. Sutto, M. D’Abramo, and F.L. Gervasio (2010) Comparing the efficiency of biased and unbiased Molecular Dynamics in reconstructing the free energy landscape of met-enkephalin. *J. Chem. Theory Comput.* **6** 3640–3646.
- [3] A. Laio and M. Parrinello (2002) *Proc. Nat. Acad. Sci.* **99** 12562-12566.

- [4] G. Bussi, A. Laio, and M. Parrinello (2006) *Phys. Rev. Lett.* **96** 090601; DOI: 10.1103/PhysRevLett.96.090601.
- [5] A. Laio, and F.L. Gervasio (2008) Metadynamics: a method to simulate rare events and reconstruct the free energy in biophysics, chemistry and material science. *Rep. Prog. Phys.* **71** 126601.
- [6] M. Kenn, R. Ribarics, N. Ilieva, M. Cibena, R. Karch, W. Schreiner (2016) *Mol. BioSyst.* Advance Article, DOI: 10.1039/C5MB00879D.
- [7] R.G. Tsanev, I. Ivanov I. Immune Interferon: Properties and Clinical Application. (CRC Press LLC, USA, 2001), ISBN 0-8493-1148-9.

Modular approach to large-scale biomolecule simulations

N. Ilieva, J. Liu, P. Petkov, J. He, and A. Niemi

Biological molecules, being small in size (in the nanometer range), consist of a huge number of atoms, $10^4 - 10^6$ atoms. The time scale of the processes in which they are involved extends from picoseconds to hours, that is over 15 orders of magnitude. The purpose of any computational study is enabling the investigated system to explore sufficiently well its conformation space. No formal check whatsoever can prove that complete sampling has been achieved. This makes computational investigations of biomolecules and their interactions a challenging task, and explains the efforts for developing enhanced sampling techniques by using large ensembles of simulations or new algorithms to improve overall sampling quality, especially in the context of the exascale [1]. We address this problem by developing an advanced modular multiscale modelling technique stepping on synergistic protocols from complementary approaches, to tackle one of the major unresolved problems in science — the protein folding problem.

Protein folding is the process of formation of a functional 3D structure from a random coil. Despite Anfinsen’s dogma, which states that the native 3D shape (the tertiary structure) of a protein is completely determined by its primary structure (the amino acid sequence), with presently available physics-based methods it is not yet possible to derive the shape of a biologically active protein from the corresponding aa sequence. We analyse the structure formation during the folding process in terms of a complete set or order parameters — generalised bond and torsion angles $\{\kappa_i, \tau_i\}$, in the Frenet frames associated with the backbone $C\alpha$ atoms

$$\kappa_{i+1,i} \equiv \kappa_i = \arccos(\mathbf{t}_{i+1} \cdot \mathbf{t}_i) \quad (1)$$

$$\tau_{i+1,i} \equiv \tau_i = \text{sign}[(\mathbf{b}_{i-1} \times \mathbf{b}_i) \cdot \mathbf{t}_i] \arccos(\mathbf{b}_{i+1} \cdot \mathbf{b}_i), \quad (2)$$

where $(\mathbf{t}_i, \mathbf{b}_i, \mathbf{n}_i)$ are the unit backbone tangent, binormal and normal vectors, i numbers the aminoacid residues, $i = 1, \dots, N$ (see [2, 3]).

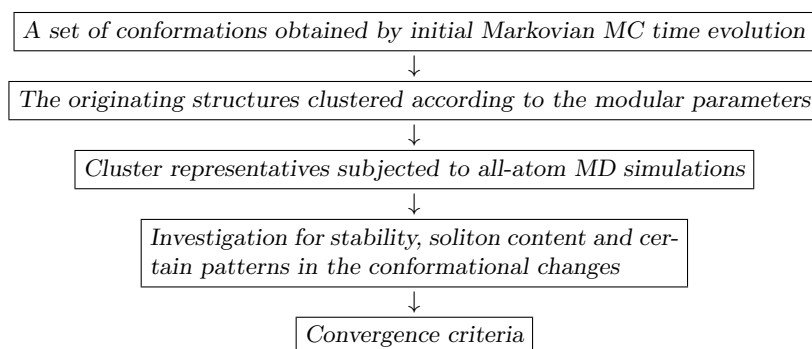
We aim at combining the strengths of the computational methods that are best suited for numerical investigations of large systems — molecular dynamics on the one hand and Monte-Carlo based methods on the other (see, e.g., [4]). The former, being deterministic, is the only one capable of delivering information about dynamical properties of the investigated system. The average values of the observables in this approach correspond to a microcanonical ensemble, which is not always convenient for comparison with the experimental data, while the second group of methods generates the average over a canonical ensemble

$$\langle \bar{A} \rangle_{MD} \simeq \langle A \rangle_{\text{microcanonical}} \quad (3)$$

$$\langle \bar{A} \rangle_{MC} \simeq \langle A \rangle_{\text{canonical}} \quad (4)$$

In MD, the system can easily get trapped in a potential well, while the MC-based methods, being stochastic in nature, and unsuitable for studying time- and momentum-dependent properties and phenomena, provide better coverage of the configuration space through tunneling between energetically separated regions.

Thus, we put forward a multistage procedure as follows [5]:



On the example of a protein which undergoes essential conformational transformations in its action we demonstrate that the protocol allows for accelerated sampling of the conformation space and faster convergence to the biological fold. It also sheds some light on the existence of exceptions from the Anfinsen dogma.

Acknowledgments This research was supported in part by Bulgarian Science Fund (Grant DNTS-CN-01/9/2014) and Intergovernmental S&T Cooperation Project at the Ministry of Science and Technology, P.R. China (2014-3).

References

- [1] S. Pall, M.J. Abraham, C. Kutzner, B. Hess, E. Lindahl. Solving Software Challenges for Exascale (Springer, Switzerland, 2015), pp.3–27.
- [2] A.J. Niemi, Theor. Math. Phys. **181** (2014) 1235.
- [3] J. Dai, A. Niemi, J. He, A. Sieradzan, and N. Ilieva, Phys. Rev. **E93**: 032409 (2016).
- [4] D. Frenkel and B. Smit, Understanding Molecular Simulation, 2nd Ed. (Academic Press, San Diego, 2002).
- [5] N. Ilieva, J. Liu, R. Marinova, P. Petkov, L. Litov, J. He, and A.J. Niemi, AIP Conf. Proc. 1773, 110008 (2016); <http://dx.doi.org/10.1063/1.4965012>

Representation of civilians and police officers by generalized nets for describing software agents in the case of protest

Shpend Ismaili, Stefka Fidanova

During some protest very important is the possibilities for crowd control and preventing and elimination of conflict situations. Very often there are factors which are difficult to predict, even when we expect that the crowd is well managed. In this case can appear conflict situations. It can cause mess and casualties. Crowd simulation is a very important research topic. Various approaches are applied for researching crowd behavior, fuzzy-theory-based method [5], bandit strategy [4], cellular automata [7], crowd motion simulation [6].

One of the simulation methods which is applied on modeling crowd behavior is agent-based. Multi-agent system consists of different kind of agents and environments. The interaction between the agents and change of the environment affect the individual agent and it can change his behavior. The agents can be passive or active and can react in different manner according the situation [8].

Agent-based modeling and simulation to solve difficult problems, becomes very popular last years. Predicting and preventing conflict situations are very actual now days. Therefore various mathematical techniques are used. One of them is application of multi-agent systems. The main element of the multi-agent systems is the software agent, which is an autonomous subject with a possibility to work together with other agents and environment. In our application the software agents represent civilians and police officers in protests.

Generalized Nets (GN) [1, 2, 3] are an efficient tool for modeling of various real processes. They are extension of Petri nets. The apparatus of the GN is very powerful and can be used for modeling in different areas like medicine and biology, economics, industry, description of algorithms and many others.

In this work we propose a model of the software agents with Generalized Nets. The Generalized Net is a very powerful tool for modeling processes and different situations. They are expandable and can represent a process in details. In this work we propose a model of the software agents with Generalized Net. Our agents model the behavior of the civilian and police officers in case of the protest.

We create more individuals which interact between them, to model civil violence. The structure consists of individuals, environment and empirical rules. Our software agents model polis officers and civilians. Accurate modeling of their attributes is crucial to the description which is as much as possible closer to human life and behavior in situations of unrest. Peaceful civilians are neutral participant, but they can react to external or internal stimulus. Police officers retain the order by the insertion of the activists in jail and through strategies that choose depends on the success of the management and control of violence. The police officers perform two tasks in a direct way: active arrest protesters and move in space.

Civilians are much more complex individuals, than the police officers. Civilian agent decides whether to be active or not. Typical of civilian agents is communication. The civilian agents can change from active to passive and from passive to active. The functioning of the system depends of the empirical rules. Empirical rules guide the interactions of agents and ensure the functioning of the system.

References

- [1] J. Alexieva, E. Choy, E. Koycheva, *Review and bibliography on generalized nets theory and applications*, In A Survey of Generalized Nets (E. Choy, M. Krawczak, A. Shannon and E. Szmids, Eds.), Raffles KvB Monograph No. 10, 2007, 207–301.
- [2] K. Atanassov, *Generalized Nets*, World Scientific. Singapore, London, 1991.
- [3] K. Atanassov *On Generalized Nets Theory*, Prof. M. Drinov Academic Publ. House, Sofia, 2007.
- [4] Chen H., Rahwan I., Cebrian M., *Bandit strategies in social search: the case of the DARPA red balloon challenge*, EPJ Data Science, Vol. 5(1), 2016, p.20.
- [5] Fu L., Song W., Lo S., *A fuzzy-theory-based method for studying the effect of information transmission on nonlinear crowd dispersion dynamics*, Communications in Nonlinear Science and Numerical Simulation, Vol. 42, 2017, pp. 682-698.
- [6] Li D., Yuan L., Hu Y., Zhang, X., *Large-scale crowd motion simulation based on potential energy field*, J. of Huazhong University of Science and Technology, Vol. 44(6), 2016, pp. 117-122.
- [7] Lubas R., Was J., Porzycki J., *Cellular Automata as the basis of effective and realistic agent-based models of crowd behavior*, Journal of Supercomputing, Vol. 72(6), 2016, pp. 2170-2196.
- [8] Salamon T., *Design of Agent-Based Models: Developing Computer Simulations for a Better Understanding of Social Processes*, ISBN 978-80-904661-1-1, Bruckner Publishing, 2011.

Laboratory calibration of MEMS rate sensors

Tihomir Ivanov, Galina Lyutskanova, Dragomir Aleksov,
Ognian Kounchev

We are interested in constructing a device that could measure two important angles in the borehole drilling—toolface and inclination. As far as miniature dimensions and full measurement range are concerned, the most advantageous solution is a sensor made of commercial microelectromechanical systems (MEMS) accelerometers, which employs measurements of the three Cartesian components of the vector of gravitational acceleration [3].

It is well-known, however, that MEMS accelerometers are subject to different sources of error that should be accounted for, before they can be used in practice. There are two main types of errors—deterministic and random. The deterministic error sources include the bias (offset) and the scale factor errors [2]. Another issue lies in the fact that the three axes of the MEMS accelerometers can never be perfectly orthogonal in practice.

The random errors include bias-drifts or scale factor drifts, and the rate at which these errors change with time. Furthermore, all the errors are sensitive to different environmental factors, especially to temperature variations [1].

We suggest a simple algorithm for compensating the deterministic errors. We use a classical linear relation, depending on 12 parameters, between the raw output from the sensors and the calibrated data, as well as a more complicated relation, derived from physical and geometrical considerations. We obtain the calibration parameters by formulating and solving a least-squares problem. Results of numerical experiments are shown to validate the proposed algorithm.

References

- [1] P. Aggarwal, Z. Syed, X. Niu, N. El-Sheimy, Thermal Calibration of Low Cost MEMS Sensors for Integrated Positioning, Navigation Systems, The Institute of Navigation National Technical Meeting (2007) 22–24.
- [2] P. Aggarwal, Z. Syed, X. Niu, N. El-Sheimy, A standard testing and calibration procedure for low cost MEMS inertial sensors and units. *Journal of navigation* 61 (2008) 323–336.
- [3] S. Luczak, W. Oleksiuk, M. Bodnicki, Sensing Tilt With MEMS Accelerometers, *IEEE Sensors Journal* 6 (2006) 1669–1675.

Comparison of NDT techniques for elastic modulus determination of laminated composites

Yonka Ivanova, Todor Partalin, Ivan Georgiev

The study of dependence of elasticity modulus on the type, shape and structure of the fillers in the composites is an important task. By theoretical point of view, different models are developed to describe the relation between geometrical, mechanical and physical parameters of the fillers and matrix with the macroscopic effective properties of composites [1, 2]. It is reasonable the Young's modulus of the composites to be determined both experimentally and theoretically. This work is a part of investigation on material characterization of laminated composites. In the present study non-destructive techniques are used for characterization of elastic modulus. NDT methods, namely, digital X-ray, ultrasonic and vibration methods are applied to find the relations between internal structure of composites and their elastic properties. A glass fiber laminated composite plate with thickness of 4 mm (GFC4) was chosen for the study. The plate was manufactured by hot pressing the glass cloth layers, impregnated with thermo-reactive phenolic and epoxy type resins. The glass fiber volume fraction was found to be 45 %. The material anisotropy was investigated by cutting the samples upon 0, 30, 45 and 90 degree on the length. Two methods are applied to characterize the elastic properties of laminated composite specimens. The dynamic methods, ultrasonic and vibration were applied to characterize the elastic properties of laminated composite specimens. Ultrasonic method includes different techniques for investigation by using ultrasonic longitudinal and shear waves and measuring their parameters as velocity and attenuation. Determination of the elastic moduli is based on the relation between ultrasonic longitudinal (C_L) and shear waves (C_S), density (ρ), Young's modulus (E) and the Poisson's ratio ν :

$$E = 4\rho C_S^2 \left[\frac{\frac{3}{4} - \left(\frac{C_S}{C_L}\right)^2}{1 - \left(\frac{C_S}{C_L}\right)^2} \right] \quad (1)$$

$$\nu = \frac{\frac{1}{2} - \left(\frac{C_S}{C_L}\right)^2}{1 - \left(\frac{C_S}{C_L}\right)^2} \quad (2)$$

Measured values of longitudinal and shear wave velocities are used in Equations (1)-(2) to calculate the elastic modulus in transversal direction of fiber-glass plate specimens. Resonant vibration method is promising for fast and accurate way for elastic modulus determination. The test specimen is mechanically vibrated in a torsional, transverse, or longitudinal vibration mode over a range of frequencies. Specific resonances are dependent on the elastic modulus, material density and geometry. For investigating of the elastic properties in different directions of composites we used a methodology

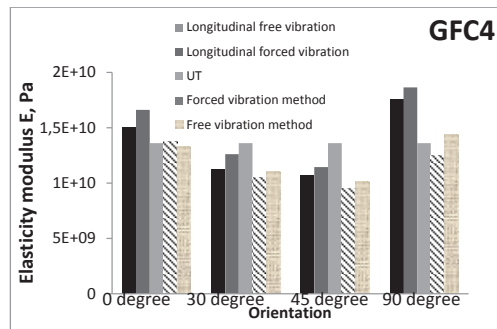


Figure 1

based on combination of different kind of vibrations. The bar shaped specimens are examined by free and forced longitudinal and flexural vibrations.

Forced excitation is realized by piezoelectric or electromagnetic actuators fed by a variable frequency generator. Vibration is detected by signal pickup piezoelectric transducer in direct contact with the specimen and analyzed. In free vibration method the impulse excitation is produced by striking the object and pickup transducer is acoustic microphone. The signal is addressed to personal computer and processed by signal processing methods in order to identify the values of the natural frequencies of vibration. The results obtained by longitudinal free and forced vibration method and those measured by flexural free and forced vibration tests are in a good agreement for the examined composites. The elastic moduli depend on the orientation of fiber cloth warp. The used NDT methods allow identification of anisotropy of material as shown in the Figure 1. The applied techniques demonstrate convenient, fast and accurate estimation of elastic properties.

References

- [1] Jones R.M., Mechanics of Composite Materials, Second Edition, Taylor & Francis, 1999. 2 Campbell F.C., Structural Composite Materials, Published by ASM International, Product Code: B-ASM-031, ISBN: 978-1-61503-140-5, 621 pages
- [2] Digilov R. M., H. Abramovich, Flexural Vibration Test of a Beam Elastically Restrained at One End: A New Approach for Young's Modulus Determination, Advances in Materials Science and Engineering, Hindawi Publishing Corporation, Vol 2013, Article ID 329530, 6 pages.

Applications of time delay differential equations in dynamics of a system of three competing populations

Ivan P. Jordanov, Ivan N. Dushkov, Elena V. Nikolova,
Nikolay K. Vitanov

Many processes in population dynamics are described by system of nonlinear ordinary differential equations. Such models are effective in the study of the evolution of systems over long periods of time. We know that the delay of the introduction of information into dynamic models may change generally their properties. In this article we will show that two population models (with and without delay) generate the same dynamics, if the delay is small enough. However, this is not true if the delay is greater. The theoretical conclusions are illustrated with well-known population model of Dimitrova and Vitanov [1, 2, 3], where a time delay is introduced. Thus we investigate a nonlinear dynamics of a system of populations in presence of time delay. The delay leads to an enrichment of the nonlinear dynamics of the system which is demonstrated by a discussion of new orbits in the phase space of the system, dependent on the time-delay parameters, as well as by an investigation of the influence of the delay.

In this paper we discuss a system of three interacting population systems for the cases with and without time delay. In the first case a for description of the system we use already known models [3, 4]. These models describe the phenomena of competition and adaptation that are two essential features of complex systems. The populations compete for resources and this competition often leads to significant changes in the environmental conditions. The populations react to changes by a greater or lesser adaptation. Those who adapt better, have better chances of survival. Clearly, it is important to model both processes simultaneously. In the model of Volterra the rate of growth and the rate of interaction are constants. But the change in the number of members of the population systems leads to a change in the number of meetings between them. This can lead to a change in the ratios of increase of the number of members of the populations and the coefficients of the interaction [2, 3]. This is a manifestation of adaptation to changing environmental conditions. The discussed model summarizes a number of classic models, such as the models of Volterra type. The system of model equations for this case is a system of ordinary differential equations. When time delays are introduced in these model equations, the resulting system describes the influence of delay on the respective evolution processes. In more detail we introduce a time delay and generalize a system of population dynamics model PDEs and then numerically solve the system with and without time delay. We use a modification of the method of Adams for the numerical solution of the system of model equations with time delay. By appropriate selection of the parameters and initial conditions we show the impact of the delay time on the dynamics of the studied population system. Finally, we will discuss the issue of sustainability in the behavior

of such population systems.

Acknowledgments. This work contains results, which are supported by the UNWE project for scientific researchers with grant agreement No. NID NI – 21/2016.

References

- [1] Z. I. Dimitrova, N. K. Vitanov, Influence of Adaptation on the Nonlinear Dynamics of a System of Competing Populations, *Physics Letters A* **272** (5), 368–380 (2000).
- [2] Z. I. Dimitrova, N. K. Vitanov, Dynamical Consequences of Adaptation of the Growth Rates in a System of Three Competing Populations, *Journal of Physics A: Mathematical and General* **34** (37), 7459–7453 (2001).
- [3] Z. I. Dimitrova, N. K. Vitanov, Adaptation and its Impact on the Dynamics of a System of Three Competing Populations, *Physica A* **300** (1), 91–115 (2001).
- [4] Z. I. Dimitrova, N. K. Vitanov, Chaotic Pairwise Competition, *Theoretical Population Biology* **66** (1), 1–12 (2004).

Water hammer in a multiple-supported penstock and earthquake-induced support excitation - coupled analysis of the axial load case

Dimitar Kisliakov

As a result of strong earthquakes, large hydropower plants are usually automatically shut down completely. This causes of course, the development of hydraulic transients in the supplying penstock(s). It is well known that the seismic response of buried penstocks is dominated by the developing ground displacements of the surrounding soil. The dynamic response of the multiple-supported penstocks, however, contains inertial effects which may not be neglected. The hydraulic transients in the hydropower penstocks have been intensively studied for all possible real operational and boundary conditions in the last few decades. As a result, highly sophisticated computational procedures have been developed and are available for the design of these facilities.

On the other hand, the problem of the earthquake-induced vibrations of a multiple-supported penstock on frictional stiff supports or support columns subjected to the simultaneous excitation of all three ground motion components was analysed in a series of works of the author in the last two decades. The structural model and the governing equations of motion of the considered pipeline part were discussed as well as their numerical solution based on appropriate approximations for all common types of support structures. All basic operational loads and the features of thermal strain compensators were taken into account, too. The dynamic interaction between the vibrating pipe and the flowing water inside it was also modelled by means of a special method developed by the author. Results from solved numerical examples with real structural data sets were discussed with corresponding conclusions drawn. As a result, the complete analysis procedure in the time domain was implemented in the ready-to-run computer program DREAMSuP.

To our knowledge however, there are only few works dedicated to the simultaneous development of both physical phenomena- the water hammer in the penstock and the earthquake-induced kinematic excitation of its support devices. These studies were developed in connection with very special tasks formulated either as fundamental problems or as ones arising from particular operation conditions in nuclear power plant piping systems. They all cannot be applied directly to the above mentioned operational conditions of a water power plant.

In the present work we pay attention to these actual physical phenomena developing in the penstock of a hydropower plant during a strong earthquake. We start here with the model of the most simple case - the simultaneous development of a water hammer and the axial seismic support excitation of the penstock. The water hammer is modelled in a simple penstock with the appropriate boundary conditions without taking into account the fluid-structure interaction, i.e. the so-called precursor wave. The numerical solution is carried out by means of the Method of characteristics (MOC). The axial dynamic structural response of the multiple-supported penstock is performed with the previously developed by the author above mentioned computa-

tional procedure. Since the material behaviour of the steel penstock is assumed in the linear-elastic range, superposition of the developed stress-strain conditions resulting from both impacts is justified. The results in terms of the cumulative stress-strain state of the penstock are discussed further as base for assessment of its structural capacity.

A numerical example with real penstock data has been solved as implementation of the proposed computational procedure for particular boundary conditions and excitation parameters. Finally, conclusions are drawn, and some following tasks for future research are formulated, as well.

About flash memories and error correcting codes

Hristo Kostadinov, Nikolai Manev

In this paper we show the flexibility of integer codes to correct type of errors instead of bits. New constructions of integer codes correcting asymmetric type of errors are presented. They can be applied in flash memories, where asymmetric errors are the most common.

Nonvolatile memory is computer memory that maintains stored information without a power supply. Flash memory is currently the dominant nonvolatile memory because it is cheap and, unlike punch cards and other more recent kinds of nonvolatile memory, can be electrically programmed and erased with relative ease.

A chip of flash memory contains an array of tens of thousands of cells, and we assume that each chip stores a bit string. Each cell on a chip of flash memory can be thought of as a container of electrons. In binary flash each cell has two states: if there are electrons in the container then the cell is in the state 1, and if there are no electrons in the container, the cell is in state 0. Until recently, binary flash was the only kind of flash available, but now a new kind of flash memory has been developed - multilevel flash. In a multilevel cell, it is possible to distinguish between several different ranges of charge, allowing for more than two states.

To transition between the states, it is necessary to add and remove electrons to and from the container. While it is easy to add electrons (i.e. to increase the state of the cell), it is impossible to remove electrons (i.e. to decrease the state of the cell) without first emptying the electrons from all the containers in a large selection of the chip. This process, called reset operation, is slow and, after many repetitions, wears out the chip. In multilevel flash, there are two types of mistakes that can occur when programming a cell: errors in which too many electrons are added ("overshoots") and errors in which too few electrons are added ("undershoots"). Because of the difficulty of removing electrons, overshoots are much bigger problem than undershoots.

Flash devices exhibit a multitude of complex error types and behaviors, but common to all flavors of flash storage is the inherent asymmetry between cell programming (charge replacement) and cell erasing (charge removal). This asymmetry causes significant error sources to change cell levels in one dominant direction. Codes for asymmetric limited-magnitude errors can be used to speed-up the memory access by allowing less-precise programming schemes that introduce errors in a controlled way. Asymmetric limited-magnitude error-correcting codes were proposed in [1]. These codes turn out to be a special case of the general construction method provided by Cassuto et al. [2].

In 2011, T. Klove and B. Bose [3] proposed systematic codes that correct single limited-magnitude systematic asymmetric errors and achieve higher rate than the ones given in [2]. Later T. Klove et al. [4] extended their result and gave a necessary and sufficient condition for existing a code over GF_p correcting a single asymmetric error.

In this work we shall propose two constructions of integer codes correcting single

asymmetric errors. We are going to give the exact form of the check matrix of an integer code correcting a single asymmetric 2-limited-magnitude error.

References

- [1] R. Ahlswede, H. Aydinian and L. Khachatrian: Unidirectional error control codes and related combinatorial problems. Proc. of the Eighth International Workshop on Algebraic and Combinatorial Coding Theory (ACCT), 6–9 (2002).
- [2] Y. Cassuto, M. Schwartz, V. Bohossian and J. Burck: Codes for Asymmetric limited-magnitude errors with application to multi-level flash memories. IEEE Trans. on Information Theory, Vol. 56 (4), 1582 – 1595 (2010).
- [3] T. Klove and B. Bose: Systematic, single limited magnitude error correcting codes for flash memories. IEEE Trans. on Information Theory, Vol. 57 (7), 4477 – 4487 (2011).
- [4] T. Klove, J. Lou, I. Naydenova and S. Yari: Some Codes Correcting Asymmetric Errors of Limited Magnitude. IEEE Trans. on Information Theory, Vol. 57 (11), 7459 – 7472 (2011).

On the strong asymptotic of rows of classical Padé approximants

Ralitza K. Kovacheva,

Given a power series $f(z) = \sum_{n=0}^{\infty} f_n z^n$ and a pair (n, m) of nonnegative integers ($n, m \in \mathbb{N}$), let $\pi_{n,m}(f) := \pi_{n,m}$ be the rational Padé approximant of f of order (n, m) . Recall that $\pi_{n,m} = p_{n,m}/q_{n,m}$, where $p_{n,m}$ and $q_{n,m}$ are polynomials of degree not exceeding n and m , respectively, and such that

$$f(z)q_{n,m}(z) - p_{n,m}(z) = O(z^{n+m+1}).$$

Set

$$\pi_{n,m} := P_{n,m}/Q_{n,m},$$

where $P_{n,m}, Q_{n,m}$ do not have common divisors and $Q_{n,m}$ is monic.

Suppose now that f is not a formal power series (i.e. $\limsup |f_n|^{1/n} < \infty$). Fix a number $m \in \mathbb{N}$ and let D_{R_m} be the largest disk, centered at $z = 0$, where f admits a continuation as a meromorphic function with no more than m poles (multiplicities included). By the classical theorem of Montessus de Ballore, generalized later by A. A. Gonchar, the sequence $\{\pi_{n,m}\}$ represents, as $n \rightarrow \infty$ and m is fixed, the function f in D_{R_m} , that is: $\{\pi_{n,m}\}$ converges in m_1 -measure to f on compact subsets of D_{R_m} .

We are interested in the behavior of the Padé approximants as $n \rightarrow \infty$ and m -fixed (the s.c. rows) outside the disk D_{R_m} .

As it is known, there is an infinite sequence of integers Λ such that

$$R_m \frac{|\pi_{n,m}(z)|^{1/n}}{|z|} \rightarrow 1 \text{ as } n \in \Lambda \text{ and } m \text{ fixed}$$

inside $D_{R_m}^c := \overline{\mathbb{C}} \setminus \overline{D_{R_m}}$ (uniformly in the max-norm on compact subsets).

The present talk is dealing with the strong asymptotics of the sequence $\{\pi_{n,m}\}_{n=0}^{\infty}$, m -fixed. We show that

$$R_m^n \frac{\pi_{n,m}(z)}{z^n} \rightarrow \chi(z)$$

inside $D_{R_m}^c$ through a sequence Λ , where χ is a function, holomorphic and different from zero in $D_{R_m}^c$.

Optimal mathematical model for the simulation of removal of pollutants in constructed wetlands: linear or non-linear procedures?

Konstantinos Liolios, Vassilios Tsihrintzis, Krassimir Georgiev, Ivan Georgiev and Panagiotis Angelidis

The use of Constructed Wetlands (CWs) for the wastewater treatment has been increased, especially in the last 20 years. The main advantage of these facilities is that they can remove various types of pollutants in an economical and ecological way, and so to improve the groundwater quality. Representative results of numerical simulation, concerning the removal of Biochemical Oxygen Demand (BOD) and Total Phosphorus (TP) by using Horizontal Subsurface Flow (HSF) CWs, have been presented in [1, 2], using mainly linear procedures. The aim here is to investigate which mathematical model, linear or non-linear, is the optimal one for the description of the removal procedure. The computer code Visual MODFLOW, based on the finite difference method, is used for the numerical simulation. A comparison between the computational results with available experimental data is realized, in order to select the optimal mathematical model. The general Partial Differential Equation which describes the fate and transport of a contaminant in 3-D, transient groundwater flow systems, is [3]:

$$\varepsilon R_d \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (qC) + q_s C_s + \sum_{n=1}^N R_n, \quad (1)$$

where ε is the porosity of the subsurface medium; $R_d = 1 + \left(\frac{\rho_b}{\varepsilon} \frac{\partial S}{\partial C} \right)$ is the retardation factor; ρ_b is the bulk density; C is the concentration of the dissolved pollutant; S is the adsorbed pollutant concentration; t is the time; D_{ij} is the solute hydrodynamic dispersion coefficient tensor; q is the Darcy velocity field; q_s is the volumetric flow rate of aquifer, representing fluid sources (positive) and sinks (negative); C_s is the concentration of the source or sink flux; and $\sum R_n$ is the chemical reaction term, dependent on C and S . This last term for an non-absorbable pollutant (e.g. BOD) is $S = 0$, and the usual linear reaction case is given by the formula [4]:

$$\sum R_n = -\lambda R_d C, \quad (2)$$

where λ is the first-order removal coefficient, which usually depends on the temperature, in a way either linear or non-linear [5]. Especially for the removal of an absorbable pollutant, e.g. TP, where adsorption S is present, there are two main equations which can describe this phenomenon [6], the linear Freundlich isotherm:

$$S = K_d \cdot C \quad (3)$$

and the non-linear Langmuir isotherm:

$$S = S_{max} \frac{K_L C}{1 + K_L C} \quad (4)$$

where K_d is the distribution coefficient, which expresses the distribution of the pollutant concentrations between solid and liquid phases, S and C , respectively; S_{max} is the maximum adsorption capacity; and K_L is the Langmuir constant. In order to select the optimal mathematical model concerning either eq. (3) or eq. (4), the following expression is formulated for each one of the two procedures:

$$E = \sum_{i=1}^N (C_{i,comp} - C_{i,exp})^2 \quad (5)$$

By $C_{i,comp}$ are denoted the values of concentration computed at selected points $i = 1, 2, \dots, N$ of the CW by using the procedure based on either the linear eq. (3) or the nonlinear eq. (4). By $C_{i,exp}$ are denoted the known experimental concentration values at the same points. The optimal mathematical model is that procedure which gives the minimum E value in eq. (5).

Acknowledgements: This work was supported by the Bulgarian Academy of Sciences through the "Young Scientists" Grant No. DFNP-97/04.05.2016.

References

- [1] Liolios, K.A., Moutsopoulos, K.N., Tsihrintzis, V.A.: Modeling of flow and BOD fate in horizontal subsurface flow constructed wetlands. Chem. Eng. J. 200-202, 681-693 (2012)
- [2] Liolios, K.A., Moutsopoulos, K.N., Tsihrintzis, V.A.: Numerical simulation of phosphorus removal in horizontal subsurface flow constructed wetlands. Desal Water Treat 56(5), 1282-1290 (2015)
- [3] Bear, J.: Dynamics of Fluids in Porous Media. Dover Publications, New York (1988)
- [4] Kadlec, R.H., Wallace, S.: Treatment Wetlands. 2nd Edition, CRC Press, Boca Raton, (2009)
- [5] Liolios, K., Tsihrintzis, V., Georgiev, K., Georgiev, I.: "Geothermal effects for BOD removal in horizontal subsurface flow constructed wetlands: A numerical approach", in Advanced Computing in Industrial Mathematics, edited by K. Georgiev et al. (Springer, 2016), accepted, ahead-of-print
- [6] Zheng, C., Bennett, G.D.: Applied Contaminant Transport Modelling, 2nd Edition, Wiley, New York (2002)

Some results involving Euler-type integrals and dilogarithm values

Lubomir Markov

Let $\zeta(z)$ be the Riemann zeta function and $\mathbf{L}(z)$ be the dilogarithm. In addition to the prominent place occupied by them in mathematics, both functions have increasingly appeared in modern physics (see for example [4], [5], [6]). At present, the evaluation of the dilogarithm in closed form is known to be possible only at eight values for z , the first four being the rational numbers $0, 1, -1$ and $\frac{1}{2}$. The remaining four are the irrational numbers $\frac{1}{\phi^2}, \frac{1}{\phi}, -\frac{1}{\phi}$ and $-\phi$, where $\phi = \frac{\sqrt{5}+1}{2}$ is the golden ratio. The evaluation of the first seven values has been performed by Landen [2] and is sometimes termed "Landen's list". We turn our attention to $\mathbf{L}(-\phi)$. It is almost incredible that the value for it circulating in the literature (see [3], [4], [5], [7], [8]) since at least 1958, namely $\mathbf{L}\left(-\frac{\sqrt{5}+1}{2}\right) = -\frac{\pi^2}{10} + \frac{1}{2} \log^2\left(\frac{\sqrt{5}+1}{2}\right)$, is wrong. For the correct derivation (cf. [3, pp. 1-7]), recall that one first obtains $\mathbf{L}\left(\frac{\sqrt{5}-1}{2}\right) = \frac{\pi^2}{10} - \log^2\left(\frac{\sqrt{5}-1}{2}\right)$. In Landen's functional equation: $\mathbf{L}(x) + \mathbf{L}\left(\frac{x}{x-1}\right) = -\frac{1}{2} \log^2(1-x)$, the argument x is taken to be $\frac{\sqrt{5}-1}{2}$. This yields $\mathbf{L}\left(\frac{\sqrt{5}-1}{2}\right) + \mathbf{L}\left(-\frac{\sqrt{5}+1}{2}\right) = -\frac{1}{2} \log^2\left(\frac{3-\sqrt{5}}{2}\right)$. Substituting $\mathbf{L}\left(\frac{\sqrt{5}-1}{2}\right)$, using the relations $\frac{\sqrt{5}-1}{2} = \frac{2}{\sqrt{5}+1}$, $\frac{3-\sqrt{5}}{2} = \left(\frac{2}{\sqrt{5}+1}\right)^2$ and simplifying gives the correct value:

$$\mathbf{L}\left(-\frac{\sqrt{5}+1}{2}\right) = -\frac{\pi^2}{10} - \log^2\left(\frac{\sqrt{5}+1}{2}\right).$$

As regards the evaluation of $\zeta(z)$, it is well-known that $\zeta(2) = \frac{\pi^2}{6}$, $\zeta(4) = \frac{\pi^4}{90}$, and in general $\zeta(2n) = \frac{(-1)^{n+1} B_{2n}}{2(2n)!} (2\pi)^{2n}$, where B_{2n} are the Bernoulli numbers. No such formula is known for the values of the zeta function at odd integers, and it is an open problem of the first importance whether $\zeta(2n+1)$ is expressible in terms of known constants. In a classical paper [1], Euler has derived the following representation for $\zeta(3)$ which he obviously considered of significant interest:

$$\zeta(3) = \frac{2\pi^2}{7} \log 2 + \frac{16}{7} \int_0^{\frac{\pi}{2}} x \log(\sin x) dx$$

His proof uses intricate manipulations of divergent and convergent series and takes up 16 pages. We shall give a very simple proof (perhaps the simplest so far) of this

formula and of several related results, for example

$$\zeta(3) = \frac{2\pi^2}{9} \log 2 + \frac{16}{3\pi} \int_0^{\frac{\pi}{2}} x^2 \log(\sin x) dx.$$

The integrals in the last two formulas may be termed Euler-type integrals. Such formulas involving $\zeta(3)$ have recently been found to be of importance in physics (see [7]).

References

- [1] L. Euler, Exercitationes analyticae, *Novi Comment. Acad. Sci. Imp. Petropol.* **17** (1772), 173-204
- [2] J. Landen, *Mathematical Memoirs*, London, 1780
- [3] L. Lewin, *Dilogarithms and Associated Functions*, Macdonald, London, 1958
- [4] L. Lewin, *Polylogarithms and Associated Functions*, Elsevier (North-Holland), New York/London/Amsterdam, 1981
- [5] L. Maximon, The dilogarithm function for complex argument, *Proc. R. Soc. Lond.* **459** (2003), 2807-2819
- [6] D. Schumayer and D.A.W. Hutchinson, Physics of the Riemann hypothesis, *Rev. Mod. Phys.* **83** (2011), 307-330
- [7] H.M. Srivastava and J. Choi, *Series Associated with the Zeta and Related Functions*, Kluwer Academic Publishers, Dordrecht/Boston/London, 2001
- [8] D. Zagier, The remarkable dilogarithm, *J. Math. Phys. Sci.* **22** (1988), 131-145

A low-rank matrix completion approach to data-driven signal processing

Ivan Markovsky

In filtering, control, and other mathematical engineering areas it is common to use a model-based approach, which splits the problem into two steps:

1. model identification and
2. model-based design.

Despite its success, the model-based approach has the shortcoming that the design objective is not taken into account at the identification step, i.e., the model is not optimized for its intended use.

In this talk, we show a data-driven approach, which combines the identification and the model-based design into one joint problem. The signal of interest is modeled as a missing part of a trajectory of the data generating system. Subsequently, the missing data estimation problem is reformulated as a mosaic-Hankel structured matrix low-rank approximation/completion problem. A local optimization method, based on the variable projections principle, is then used for its numerical solution.

The missing data estimation approach for data-driven signal processing and the local optimization method for its implementation in practice are illustrated on examples of control, state estimation, filtering/smoothing, and prediction. Currently, we are missing fast algorithms with provable properties in the presence of measurement noise and disturbances. Development of such methods will make the matrix completion approach for data-driven signal processing a practically feasible alternative to the model-based methods.

The talk is based on a technical report, available from:

<http://homepages.vub.ac.be/~imarkovs/publications/ddsp.pdf>

Future cyber risks landscape exploration: modelling, simulation, validation & verification

Zlatogor Minchev

Modern cyber world is constantly evolving towards a more intelligent mixed cyber-physical environment, generating numerous challenges for the new digital society resilience establishment [1]. The proper exploration in this context of future cyber threats & attacks prognosis is inevitably a cutting-edge issue, related to cyber intelligence, that is already successfully addressed in some recent industrial achievements [2], [3]. The work is presenting a probabilistic approach after [4], allowing uncertainty data coping, for future cyber risks landscape understanding, based on multi-dimensional matrix space (of both threats & attacks) exploration. The space is also combined with selected intrusions additional system modelling into an ad-hoc created software environment, following an agent-based representation. Supportive numerical simulations are performed for further model risk exploration and synthetic validation from probabilistic perspective. Dynamic verification of results is also discussed for low-dimensional non-linear systems with probabilistic coefficients, obtained from the validation. Being rather uncertain, due to futuristic nature of the obtained verification, some real log observations in mixed digital environment are further marked.

The material is based on ESGI 120 WG5 extended joint results with the industrial support of TechnoLogica Ltd.

References

- [1] Minchev, Z., Dukov, G. Emerging Hybrid Threats Modelling & Exploration in the New Mixed Cyber-Physical Reality, BISEC 2016, Belgrade Metropolitan University, October 15, pp. 13-17, 2016
- [2] Seven Ways to Apply the Cyber Kill Chain with a Threat Intelligence Platform, Lockheed Martin, 2015, Available at <https://goo.gl/UA3Bnd>
- [3] IT Executive Guide to Security Intelligence, IBM Security, 2015, Available at <https://goo.gl/4kPwBa>
- [4] Minchev, Z., Dukov, G., Boyadzhiev, D., Mateev, P. Future Cyber Attacks Modelling & Forecasting, In ESGI 120 Problems & Final Reports Book, 2016 (in press)

Nonlinear evolution equations for propagation of waves in arteries with aneurysms: exact solutions obtained by the modified method of simplest equation

Elena V. Nikolova, Ivan P. Jordanov, Zlatinka I. Dimitrova,
Nikolay K. Vitanov

The study of nonlinear waves is of large interest for many branches of science and technology [1, 2, 3]. In many cases these waves are modelled by nonlinear partial differential equations. The analytical exact solutions of the above model equations are of much interest as they can be used for test of computer programs that have to simulate the evolution of complex nonlinear waves and often the obtained exact analytical solutions describe solitons and soliton collisions.

In this study we shall consider propagation of nonlinear waves in biofluid systems. In more detail we shall focus on the propagation of small-but-finite amplitude waves in a blood-filled artery with a axially symmetric imperfection (an idealized aneurysm). We model this complex medium by a system of nonlinear partial differential equations which represent both the motion of arterial wall and the motion of blood. The aneurismal artery is considered as a prestressed, homogeneous, incompressible and thin hyper-elastic tube with a axially symmetric dilatation, as the longitudinal motion of arterial wall is assumed to be negligible. The blood is modeled as an incompressible Newtonian fluid, as the viscous effects are presented in an appropriate manner. By applying a reductive perturbation method to the basic quantities in the model equations, we derive two kinds nonlinear evolution equations (NLEEs) with variable coefficients (the extended Korteweg-de Vries-Burgers equation and its modified form) depending on the relation between initial stretch ratios. By employing an appropriate coordinate transformation we reduce the variable coefficient NLEEs to NLEEs with constant coefficients. Exact traveling-wave solutions of these equations are obtained by application of the modified method of simplest equation. This method is based on construction of exact solution of the solved complicated nonlinear partial differential equation on the basis of known exact solution of simpler partial differential equation called simplest equation. The modified method of simplest equation was proved to be very effective in obtaining particular exact solutions of many nonlinear partial differential equations that are non-integrable [4, 5, 6]. In our case we shall use the equation of Abel as simplest equation. In addition to the obtained exact solutions parameters of the model equation will be set equal to experimentally validated values and the variations of radial displacement and the blood pressure with the space coordinate are examined numerically, as the results are discussed in the context of arterial disease mechanics.

Acknowledgments. This work contains results, which are supported by the UNWE project for scientific researchers with grant agreement No. NID NI – 21/2016 and

References

- [1] T. K. Gaik, H. Demiray, Forced Korteweg-de Vries-Burgers equation in an elastic tube filled with a variable viscosity fluid, *Chaos, Solitons & Fractals* **38**, 1134–1145 (2008).
- [2] De-long Xiao, J. X. Ma, Yang-fang Li, Yinhua Xia, and M. Y. Yu. Evolution of nonlinear dust-ion-acoustic waves in an inhomogeneous plasma. *Physic of plasmas* **13**, 052308 (2006).
- [3] S. D. Yamigno. Propagation of dark solitary waves in the Korteweg-Devries-Burgers equation describing the Nonlinear RLC Transmission. *Journal of Modern Physics* **5**, 394–401 (2004).
- [4] N. K. Vitanov. Modified method of simplest equation: powerful tool for obtaining exact and approximate traveling-wave solutions of nonlinear PDEs. *Communications in Nonlinear Science and Numerical Simulation* **16**, 1176–1185 (2011).
- [5] N. K. Vitanov, Z. I. Dimitrova, H. Kantz. Modified method of simplest equation and its application to nonlinear PDEs. *Applied Mathematics and Computation* **216**, 2587–2595 (2010).
- [6] N. K. Vitanov, Z. I. Dimitrova, K. N. Vitanov. Modified method of simplest equation for obtaining exact analytical solutions of nonlinear partial differential equations: further development of the methodology with applications. *Applied Mathematics and Computation* **269**, 363–378 (2015).

Modelling of light Mg and Al based alloys as "in situ" composites.

Ludmila Parashkevova, Pedro Egizabal

Objectives. The present work is aimed to further elucidation of microstructure – properties relationship of a magnesium alloy from the system Mg-Al-Mn-Zn manufactured by gravity casting in a metallic die and reinforced with ceramic particles. Authors' attention is focused on modelling the elastic-plastic behavior of metal matrix composite (MMC) based on AZ91D alloy regarded as "in situ" composite, which is modified by TiC particles. Multilevel homogenization procedure is performed, accounting for size effects. In the model applied the supersaturated Mg matrix is considered as an elastic-plastic micropolar media, precipitation phase Mg₁₇Al₁₂ and the second hardening phase TiC are treated as conventional elastic/rigid, respectively. The preliminary

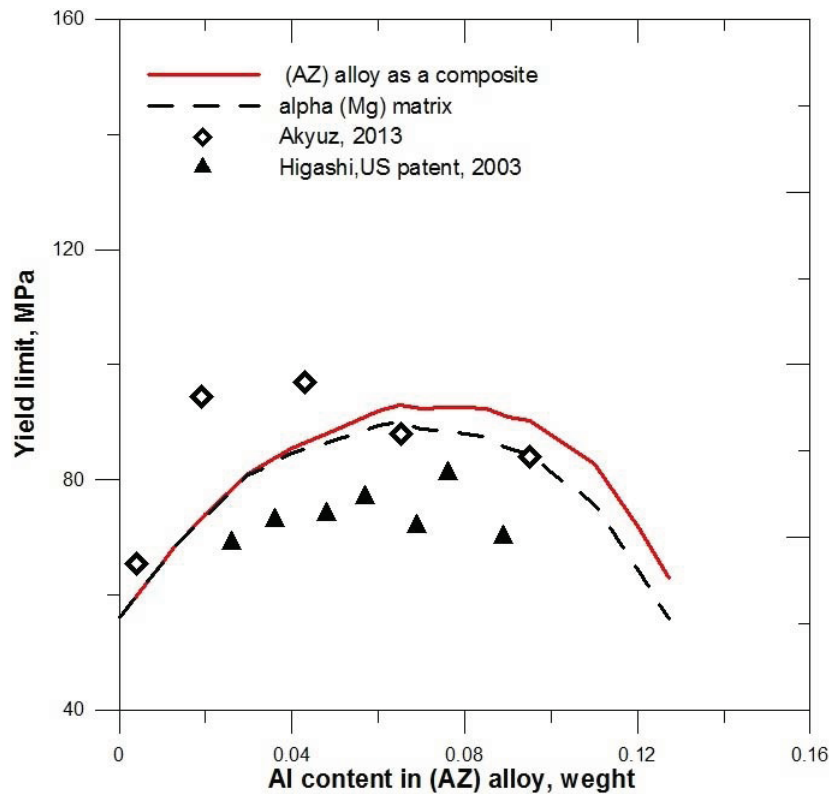


Figure 1

results show a different perspective on the influence of main microstructure, especially the precipitating mode of intermetallic phase (continuous or discontinuous) on

overall elastic moduli and composite initial yielding. Numerical procedures realizing the adopted homogenization approach are aimed to reveal the role of beta phase Mg₁₇Al₁₂ in the presence of one more hardening phase -TiC.

Results. A special formula has been presented which estimates the amount of the residual aluminum in alpha- phase depending on the intermetallic phase precipitated. Such a residual Al affects the properties of the matrix phase and of the MMC as a whole. For the case of continuous precipitations the chosen homogenization approach has been transformed into corresponding numerical subroutines. The elastic moduli and the initial yield limit of the three-phase MMC based on AZ91D alloy modified by TiC particles have been obtained. It was shown that further particle size refinement of TiC could not improve the overall composite strengthening since the ratio of particle size to the character size of the matrix phase remains much less than unity even at very fine grain crystallization of the alloy. Using temperature data from Al – Mg phase equilibrium diagram a phenomenological relation is presented coupling the quantity of residual Al in Mg matrix with amount of precipitated phase Mg₁₇Al₁₂. The model-calculated values of initial yield limit for different alloys of type AZ are in good agreement with experimental data found in the literature and are illustrated on Figure 1.

Theoretically sampling of reactive distillation using the RCM- method

P. Petrova, B. Petrova, E. Simeonov, Ch. Chilev

In this research RCM are theoretically generated. The application of reactive distillation may result in lower investment and operational costs. The chemical compound used as an example is n-propyl propionate. This product is a widely used solvent in industry and is synthesized by the heterogeneous catalyzed esterification reaction of 1-propanol (ProOH) and propionic acid (ProAc). The main objectives of this research are to describe the synthesis of n-propyl propionate and the thermodynamic and kinetic properties of the system. Based on the reactive residue curve maps, the reactive distillation concept for the production of ProPro tends to be technically feasible using one single column where an excess of alcohol is used in the feed. The resulting process is able to produce pure ProPro at the bottom and an azeotropic mixture of ProOH and water at the top of the column. Therefore, a non-reactive part should be installed at the bottom of the column to protect the catalyst from possible high temperatures in the reboiler. The methodology and mathematical models for the residue curve maps are described for the three following scenarios: non-reactive, chemical equilibrium and kinetically controlled. In case of a single feed the two reactants separate directly which results in low conversion levels. Therefore, ProOH is fed into the bottom and ProAc into the top of the reactive section to induce a countercurrent flow of the reactants. Another non-reactive part could be necessary in the top of the column to recover as much as possible ProPro that was distilled.

Acknowledgement: The authors would like to thank the Science & Research Programme of the UCTM - Sofia, contract No. 11568 for the financial support.

Complex fractional Zener model of wave propagation in viscoelastic media

Stevan Pilipović

Among the first applications of the differential operators of arbitrary real order was the theory of viscoelasticity, since fractional derivatives turned out to be quite appropriate for describing viscoelastic properties of materials.

In this talk we present complex order fractional operators for a class wave equations in order to capture some propagation phenomena occurring in viscoelastic materials.

Well-posedness of the complex fractional Zener wave equation will be discussed and the thermodynamical restrictions followed from the Second law of Thermodynamics will be derived. Especially, we will try to explain the existence and the uniqueness of a solution to an equation under consideration using a distributional framework.

More precisely, our particular interest is related to waves in a specific viscoelastic material described by a Zener standard model, given by a system of equations that correspond to isothermic motion. Now the system is considered on the whole real line with respect to space variable and with Cauchy data with respect to time.

Some details on these studies can be found in [1,2].

This is a joint work with Teodor Atanacković, Sanja Konjik and Marko Janev.

Acknowledgements: Partially supported by the Bilateral Research Project: “Mathematical Modeling by Means of Integral Transform Methods, Partial Differential Equations, Special and Generalized Functions, Numerical Analysis” between SASA and BAS.

References

- [1] T.M. Atanacković, S. Pilipović, B. Stanković, D. Zorica, Fractional Calculus with Applications in Mechanics: Vibrations and Diffusion Processes, ISTE - Wiley, London, 2014, <http://onlinelibrary.wiley.com/book/10.1002/9781118577530>;
- [2] T.M. Atanacković, S. Pilipović, B. Stanković, D. Zorica, Fractional Calculus with Applications in Mechanics: Wave Propagation, Impact and Variational Principles, ISTE - Wiley, London, 2014, <http://onlinelibrary.wiley.com/book/10.1002/9781118909065>.

Exact bounds for the unknowns in some interval FE models of structures

Evgenija D. Popova

Interval finite element methods (IFEM) name methods developed to handle finite element models where the uncertain parameters are described by given numerical intervals. The goal is to find as sharp as possible interval bounds for the unknown system response. A variety of solution techniques have been developed and applied to uncertainty models in structural mechanics, where complicated parameter dependencies cause overestimation of the solution set. For a review see, e.g., [4].

In a class of interval FE models, parameter dependency is reduced significantly by a special matrix reformulation based on an element-by-element technique and Lagrange multiplier method, cf. [1]. The obtained interval linear system of equations has the following structure

$$(A_0 + L \mathbf{D} R)x = b_0 + F \mathbf{b}, \quad (1)$$

where the interval parameters appear only once in the diagonal matrix \mathbf{D} and the vector \mathbf{b} . Then, an efficient and scalable interval method, proposed in [2], provides sharp bounds for the system response. To estimate the quality of the obtained outer solution enclosure, the latter is usually compared to the exact interval bounds obtained by the combinatorial approach (interval hull of the point system solutions for all combinations of the parameter end-points.) Combinatorial solution requires solving 2^K point linear systems, where K is the number of interval parameters, and therefore it is impractical for problems with big number of parameters. As an alternative, Monte Carlo simulations are applied. However, Monte Carlo simulations underestimate the true interval solution set hull.

It is well known that computing the exact range of response variables is an NP-hard problem in general. However, the exact interval bounds for a system response is an ultimate goal not only for comparison purposes. The quest for realism and accuracy in the model output also makes this goal highly desirable. We consider a class of interval FE models which reduce to solving interval linear system (1). It is proven in [3] that the solution set of (1) has linear boundary. For this class of problems we present a computationally feasible methodology for computing the exact range of the response variables even for large problems involving a big number (up to a few thousand) of interval parameters varying within large parameter intervals.

The proposed methodology is illustrated in example problems from structural mechanics and also to worst case analysis of electrical circuits.

References

- [1] Muhanna, R.L., Zhang, H., Mullen, R.L. (2007) Interval finite element as a basis for generalized models of uncertainty in engineering mechanics, *Reliable Computing*, 13(2):173–194.

- [2] Neumaier, A., Pownuk, A. (2007) Linear systems with large uncertainties, with applications to truss structures, *Reliable Computing*, 13:149–172.
- [3] Popova, E.D. (2014) Improved enclosure for some parametric solution sets with linear shape, *Comput. Math. Appl.*, 68: 994–1005.
- [4] Rama Rao, M.V., Mullen, R.L., Muhanna, R.L. (2011) A new interval finite element formulation with the same accuracy in primary and derived variables, *International Journal of Reliability and Safety*, 5(3-4):336–357.

Emergence of hormesis in a simple enzyme kinetic model

Peter Rashkov

Hormesis is a therapy response characterised by stimulation at low drug doses and inhibition at high drug doses [1, 2, 3]. It is also known as *biphasic dose response* in pharmacokinetics, and its dose response has the shape of an inverted U-curve. This paradox phenomenon is observed in application of multiple compounds: antibiotics, antifungals, cancer drugs, etc. In particular, it has been recently observed for the case of kinase inhibitors in cancer therapy, meaning that low drug doses actually stimulate tumour growth [4, 5, 6, 7, 8]. Despite the major consequences that hormesis has for cancer patients it remains poorly understood to this day.

In [9] a simple kinetic model based on the temporal dynamics of the MAPK signalling pathway is presented which demonstrates that hormesis can arise in a relatively simple setting. The change in steady states of substrate concentrations due to kinase inhibition is studied both analytically and numerically using Matcont [10], a package used for numerical bifurcation analysis of ODEs. Explicit necessary conditions on the reaction rates are given, and their importance is discussed in the context of flux at equilibrium concentrations. In particular, the model shows that the simplifying assumption of no flux at equilibrium concentrations used in theoretical models could mask the hormetic response. The model also suggests an explanation why hormesis arising from the proposed mechanism would be difficult to detect in population-level biochemical assays.

This is joint work with Ian Barrett and Claus Bendtsen (Innovative Medicines and Early Development, Discovery Sciences AstraZeneca, Cambridge, UK) and Ivana Gudelj (Biosciences, University of Exeter, UK).

References

- [1] E.J. Calabrese, L.A. Baldwin, *Chemotherapeutics and hormesis*, Crit. Rev. Toxicol. **33** 305–353, 2003.
- [2] E.J. Calabrese, *Hormesis: a revolution in toxicology, risk assessment and medicine*, EMBO Rep. **5** S37–S40, 2004.
- [3] H. Schulz, *Über Hefegifte*, Pflügers Arch. Gesamte Physiol. Menschen Tiere **42** 517–541, 1888.
- [4] C.A. Hall-Jackson, P.A. Eyers, P. Cohen, M. Goedert, F.T. Boyle, N. Hewitt, et al. Paradoxical activation of RAF by a novel RAF inhibitor, Chem. Biol. **6** 559–568, 1999.
- [5] P.I. Poulikakos, C. Zhang, G. Bollag, K.M. Shokat, N. Rosen, *RAF inhibitors transactivate RAF dimers and ERK signalling in cells with wild-type BRAF*, Nature **464** 427–430, 2010.

- [6] S.J. Heidorn, C. Milagre, S. Whittaker, A. Nourry, I. Niculescu-Duvas, N. Dhomen, et al. *Kinase-dead BRAF and oncogenic RAS cooperate to drive tumor progression through CRAF*, Cell **140** 209–221, 2010.
- [7] G. Hatzivassiliou, K. Song, I. Yen, B.J. Brandhuber, D.J. Anderson, R. Alvarado, et al. *RAF inhibitors prime wild-type RAF to activate the MAPK pathway and enhance growth*, Nature **464** 431–435, 2010.
- [8] M.C. Andrews, A. Behren, F. Chionh, J. Mariadason, L.J. Vella, et al. *BRAF inhibitor-driven tumor proliferation in a KRAS-mutated colon carcinoma is not overcome by MEK1/2 inhibition*, J. Clin. Oncol. **31** e448–e451, 2010.
- [9] P. Rashkov, I.P. Barrett, R.E. Beardmore, C. Bendtsen, I. Gudelj, *Kinase inhibition leads to hormesis in a dual phosphorylation-dephosphorylation cycle*, PLoS Comp. Biol., to appear.
- [10] A. Dhooge, W. Govaerts, Y.A. Kuznetsov, *MATCONT: A MATLAB package for numerical bifurcation analysis of ODEs*, ACM Trans. Math. Software **29** 141–164, 2003.

Competition for resources and space contributes to the emergence of drug resistance in cancer

Peter Rashkov

Experiments reveal targeted therapy of tumours promotes the spread of drug-resistant cancer cells in mixed sensitive-resistant tumours relative to vehicle treatment [1]. The hypothesis is that drug-stressed sensitive cells produce diffusible growth factors that stimulate the expansion of drug-resistant cells. A mathematical model employing simple ecological competition and a nonlinear motility law is able to reproduce the magnitude of observed expansion of the resistant population's volume without invoking production of diffusible growth factors. The model shows how the therapy-induced removal of the sensitive population alleviates the competitive pressure on the resistant for resources and space and confirms the *in vivo* experimental findings, and sheds light onto mechanisms behind the therapy-induced growth of the drug-resistant cancer.

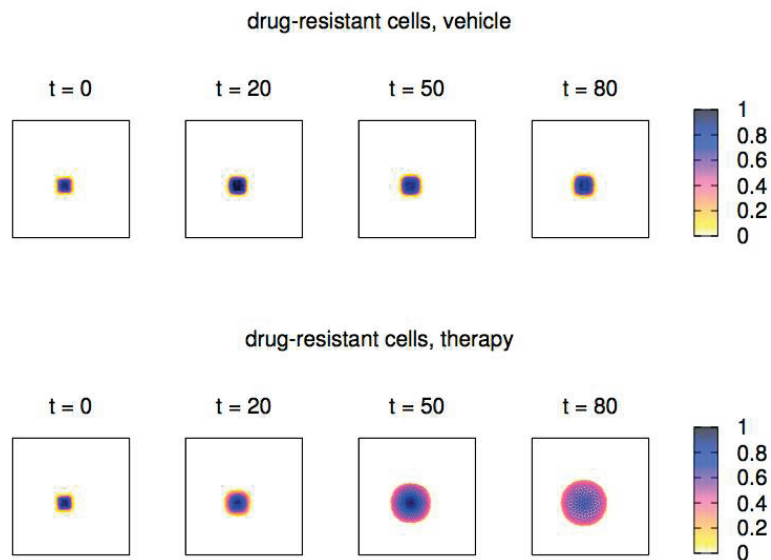


Figure 1: Simulations demonstrate that once the drug-sensitive cancer cells are eliminated by therapy, the reduced competition for resources and space inside the tumour mass accelerates the expansion of the drug-resistant cells. Because quantitative measurement of cell interactions *in vivo* is difficult, implicit factors related to the tumour microenvironment such as ecological competition and cell motility may be overlooked in an *in vitro* experiment [2], but can be quantified using mathematical modelling.

References

- [1] A. C. Obenauf, Y. Zou, A. L. Ji, S. Vanharanta, W. Shu, H. Shi, X. Kong, M. C. Bosenberg, T. Wiesner, N. Rosen, R. S. Lo and J. Massagué, 2015: Therapy-induced tumour secretomes promote resistance and tumour progression. *Nature*, **520**, 368–372.
- [2] K. Korolev, J. B. Xavier, and J. Gore, 2014: Turning ecology and evolution against cancer. *Nature Rev. Cancer*, **14**, 371–380.

Computation of energy eigenvalues of the Schrödinger equation with anharmonic oscillators

Hassan Safouhi
Joint work with: Philippe Gaudrea, Richard Slevinsky

The one dimensional anharmonic oscillator is of great interest to field theoreticians because it models complicated fields in one-dimensional space-time. A complete overview of quantum anharmonic oscillators would lead to a better understanding of the realistic analytic structure of field theory. Moreover, outside the realm of field theory, the one dimensional anharmonic oscillator also provides an approximation to more complicated quantum potentials near a stable stationary point. The study of quantum anharmonic oscillators as potentials in the Schrödinger equation has been on the edge of thrilling and exciting research during the past three decades [1, 2]. With advances in asymptotic analysis and symbolic computing algebra, the interest in developing more efficient methods was renewed recently [3, 4]. Several approaches have been used for computing efficiently and accurately the energy eigenvalues of the Schrödinger equation with the anharmonic oscillator. However, these methods are mostly case specific.

In [5], Rayleigh-Schrödinger perturbation series are used to evaluate the ground state energy for potentials $V = x^2 + \beta x^{2m}$ for $\beta \in [0, \infty)$ and $m = 2, 3, 4$. These series are strongly divergent for $\beta \neq 0$ and Padé approximants combined with nonlinear sequence transformations are used for their summation. In [1], Rayleigh-Schrödinger perturbation series are also used to evaluate energies of the ground state and the first excited state for potentials $V = x^2 + \beta x^4$. In [6], Rayleigh-Schrödinger perturbation series are used to evaluate energies of the ground state and the first four excited states for the Hamiltonian $\mathcal{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \lambda x^4$ in the limits $\lambda \rightarrow 0^+$ and $\lambda \rightarrow \infty$. In [7], exact soluble models are used to construct Rayleigh-Schrödinger perturbation series for the eigenvalues of the anharmonic potentials $V = \frac{1}{2}Ax^2 + Ex^4$. In [2], a study of Rayleigh-Schrödinger perturbation series is presented using the Wentzel-Kramers-Brillouin (WKB) method and a difference equation method. In [8], an averaging method is proposed to calculate energy eigenvalues for potentials $V = \lambda x^{2m}$ for $m = 2, 3, \dots$ with $\lambda > 0$, $V = \mu x^2 + \lambda x^4 + \eta x^6$ with $\eta > 0$ and $V = (ax^3 + bx)^2$ using a supersymmetric WKB approach. Their method yields appreciable accuracy for a variety of potentials and the accuracy increases as the energy level increases. In [9], the first seven coefficients of the WKB expansion for the energy eigenvalues of the potentials $V = x^4 + bx^2$ and $V(x) = x^6$ are presented. In [10], the WKB method and the Lanczos algorithm are used to calculate energy eigenvalues of the potential $V = \frac{1}{2}x^2 + \lambda x^{2m}$ with $m = 2, 3, \dots, 6$ to a high accuracy. Using a starting energy value from a WKB analysis, their shifted Lanczos algorithm is able to achieve 33 correct digits in three iterations or less for all energy states. In [11], the variational principle is used to calculate the first n energy eigenvalues using a Rayleigh-Ritz matrix for the perturbed Hamiltonian $\mathcal{H} = \frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\Omega^2 x^2 + \epsilon[\lambda x^4 + \frac{1}{2}(\omega^2 - \Omega^2)x^2]$. Utilizing the non-linear parameter Ω , this method becomes applicable when the parameter $\omega^2 < 0$.

Moreover, this method is able to find eigenvalues for several lower energy states even in deep double well potentials. Recently [3], an asymptotic expansion for the energy eigenvalues of the potential $V = \kappa x^{2q} + \omega x^2$, where $\kappa \in \mathbb{R}^+$, $\omega \in \mathbb{R}$ and $q \in \mathbb{N} \setminus \{1\}$ as the energy level n approaches infinity is derived using the WKB method and series reversion. In [4], the potential $V = ax^2 + \lambda x^4$ with $a < 0$ and $\lambda \geq 0$ is explored. Using asymptotic expansion of the Riccati equation solutions, an approximate solution is found which yields 9 to 10 significant digits for energy values. In [12], an asymptotic iteration method is used to calculate the energy eigenvalues of potentials of the form $V = Ax^{2\alpha} + Bx^2$.

As can be seen by the numerous approaches which have been developed to solve this problem, there is a beautiful diversity yet lack of uniformity in its resolution. While several of these methods yield excellent results for specific cases, it would be favorable to have one general method that could handle any anharmonic potential while being capable of computing efficiently approximations of eigenvalues to a high pre-determined accuracy.

The Sinc collocation method (SCM) has been used extensively during the last three decades to solve many problems in numerical analysis [13, 14]. Their applications include numerical integration, linear and non-linear ordinary differential equations, partial differential equations, interpolation and approximations of function derivatives. Recently, combination of the SCM with the double exponential (DE) transformation has sparked great interest [15, 16]. The double exponential transformation yields optimal accuracy for a given number of function evaluations when using the trapezoidal rule in numerical integration [17].

In [18], we used the SCM and the DE transformation to solve efficiently singular Sturm-Liouville eigenvalue problems. In the present work, we use this method to compute energy eigenvalues of anharmonic oscillators to unprecedented accuracy. The double exponential Sinc collocation method (DESCM) starts by approximating the wave function as a series of weighted Sinc functions. By substituting this approximation in the Schrödinger equation and evaluating this expression at several collocation points spaced equally by a specified mesh size h , we obtain a generalized eigensystem which can be transformed into a regular eigenvalue problem. For multiple-well potentials, the existing expression for the optimal mesh size h turns out to be not very effective. In such a case, we introduce an alternate mesh size \hat{h} by minimizing the trace of the resulting matrix using the principle of minimal sensitivity. After conducting an asymptotic study of this minimizing problem, we obtain the first order term in the asymptotic expansion of the alternate mesh size \hat{h} . The proposed method has numerous advantages over the existing alternatives. It can be applied to a large set of anharmonic potentials and is insensitive to changes in the potential parameters. The method is now shown to be efficient and accurate when dealing with multiple-well potentials. In addition, the DESCM has a near-exponential convergence rate and the matrices generated by the DESCM have useful symmetric properties which simplify considerably the computation of their eigenvalues.

References

- [1] J. Zamastil, J. Cížek, and L. Skála. Renormalized perturbation theory for quartic anharmonic oscillator. *Ann. Phys. (NY)*, 276:39–63, 1999.
- [2] P. Amore, A. Aranda, A. De Pace, and J. A. López. Comparative study of quantum anharmonic potentials. *Physics Letters A*, 329(6):451–458, 2004.
- [3] P. Gaudreau, R.M. Slevinsky, and H. Safouhi. An asymptotic expansion for energy eigenvalues of anharmonic oscillators. *Annals of Physics*, 337(0):261–277, 2013.
- [4] A.V. Turbiner. Double well potential: Perturbation theory, tunneling, WKB (beyond instantons). *International Journal of Modern Physics A*, 25:647–658, 2010.
- [5] E.J. Weniger. A convergent renormalized strong coupling perturbation expansion for the ground state energy of the quartic, sextic, and octic anharmonic oscillator. *Ann. Phys. (NY)*, 246:133–165, 1996.
- [6] P.K. Patnaik. Rayleigh-Schrödinger perturbation theory for the anharmonic oscillator. *Physical Review D*, 35:1234–1238, 1987.
- [7] B.L. Burrows, M. Cohen, and T. Feldmann. A unified treatment of Schrodinger’s equation for anharmonic and double well potentials. *Journal of Physics A: Mathematical and General*, 22(9):1303–1313, 1989.
- [8] R. Adhikari, R. Dutt, and Y.P. Varshni. On the averaging of energy eigenvalues in the supersymmetric WKB method. *Physics Letters A*, 131:217–221, 1988.
- [9] A. Nanayakkara. A new asymptotic energy expansion method. *Physics Letters A*, 289:39–43, 2001.
- [10] M.H. Macfarlane. A High-Precision Study of Anharmonic-Oscillator Spectra. *Annals of Physics*, 271(2):159–202, 1999.
- [11] A. Okopinska. Accurate energy levels and partition function of a quantum-mechanical anharmonic oscillator. *Physical Review D*, 36:1273–1275, 1987.
- [12] T. Barakat. The asymptotic iteration method for the eigenenergies of the anharmonic oscillator potential $V(x) = Ax^{2\alpha} + Bx^2$. *Physics Letters A*, 344:411–417, 2005.
- [13] F. Stenger. Summary of Sinc numerical methods. *Journal of Computational and Applied Mathematics*, 121:379–420, 2000.
- [14] P. Amore. A variational Sinc collocation method for strong-coupling problems. *J. Phys. A: Math. Gen.*, 39:L349–L355, 2006.
- [15] M. Sugihara and T. Matsuo. Recent developments of the Sinc numerical methods. *Journal of Computational and Applied Mathematics*, 164-165:673–689, 2004.
- [16] K. Tanaka, M. Sugihara, and K. Murota. Function classes for successful DE-Sinc approximations. *Mathematics of computation*, 78:1553–1571, 2009.
- [17] M. Mori and M. Sugihara. The double-exponential transformation in numerical analysis. *Journal of Computational and Applied Mathematics*, 127:287–296, 2001.
- [18] P. Gaudreau, R.M. Slevinsky, and H. Safouhi. The Double Exponential Sinc Collocation Method for Singular Sturm-Liouville Problems. *arXiv:1409.7471v2*, 2014.

Asymptotic study of the nonlinear velocity problem for the oscillatory non-Newtonian flow in a straight tube

Sonia Tabakova, Stefan Radev, Nilolay Kutev

The studies of non-Newtonian flows, such as the blood flow in arteries and polymer flows in tubes have very important applications. The non-Newtonian fluid viscosity is modelled by the Carreau model (nonlinear with respect to the viscosity dependence on the shear rate). This model is appropriate for shear thinning fluids, whose viscosities gradually decrease or increase with the shear rate increase or decrease reaching two different plateau values: upper and lower viscosity limits correspondent to small and high shear rates, respectively. If as a reference viscosity the upper limit is considered, then it is possible for some special fluids (for example, some polymer and biological solutions) to construct a small parameter entering in the nonlinear Carreau model function of viscosity.

In the present paper the oscillatory flow of Newtonian and non-Newtonian fluids in a straight tube is studied analytically and numerically. The flow in the tube is considered as 2D, which leads to a parabolic non-linear equation for the longitudinal velocity. The Newtonian flow velocity is analytically found, while the non-Newtonian velocity is found numerically by the finite-difference Crank-Nickolson method. In parallel, the non-Newtonian (Carreau) velocity is developed in an asymptotic expansion with respect to the small parameter. The first term of this expansion is exactly the Newtonian velocity solution. For the second term of the velocity expansion, a linear parabolic equation with a complicated right-hand side function is found. The solution is sought analytically in terms of higher order harmonics of time.

As an example the polymer solution (HEC 0.5%) is considered. It is shown that the obtained asymptotic solution and the numerical solution for the non-Newtonian (Carreau) velocity are close for different values of the small parameter. The disposal of this asymptotic solution will be very useful when some theoretical estimates of the difference between the non-Newtonian and Newtonian solutions are constructed.

Acknowledgment The third author has been partially supported for this research by the National Science Fund of Bulgarian Ministry of Education and Research: Grant DFNI-I02/9 and the other two authors - by Grant DFNI-I02/3.

Efficient error based metrics for fuzzy-neural network performance evaluation

Margarita Terziyska, Yancho Todorov, Maria Dobрева

Abstract: Predictive modeling is an essential approach in various application fields where signal and data processing are used to assess interesting data features needed for many up to date engineering tasks. The classification algorithms, the regression models and the factor analysis are well-known as predictive models. Recently, such algorithms have been transformed in the framework of machine learning, where the advantages of the fuzzy logic and neural networks give a more simple and transparent implementation. Both techniques have a proven advantage over the traditional statistical estimation and adaptive control approaches due to their possibility to deal with uncertain, imprecise, and noisy data streams. On the other hand, they can estimate or classify any function without the need of precise mathematical description between the input and target data. A special class of such models are the fuzzy-neural structures. The fusion of the fuzzy logic with the neural networks allows us to combine the learning and computational ability of neural networks with the human like IF-THEN thinking and reasoning of fuzzy system. Many fuzzy-neural networks are proposed in literature, but often is hard to be assessed their functional properties due the large number of error metrics used for any particular case. Along with the well-known Root Squared Error (RSE) and the Root Mean Squared Error (RMSE), the Mean Absolute Error (MAE), the Mean Absolute Percentage Error (MAPE), the Root Mean Square Percentage Error (RMSPE) and Mean Relative Absolute Error (MRAE) metrics are rarely discussed. This paper aims to investigate the effectiveness of different error metrics for an advanced fuzzy-neural network based on the frameworks of the theory of the intuitionistic fuzzy logic and the theory of the NEO-fuzzy neuron. The combination of these two theories allows to design a single architecture, which possess computational simplicity and it is able to handle uncertain data variations. The combination of these two theories allows to design a single architecture, which possess computational simplicity and it is able to handle uncertain data variations. A comparative studies in modeling of different chaotic time series under normal and noisy conditions are made in order to assess the information given by the different error metrics.

Box model of migration in channels of networks

Nikolay K. Vitanov, Kaloyan N. Vitanov

Statistical description of parameters and processes in social systems is interesting and leads to better understanding of properties of different complex systems [1, 2]. In this presentation we shall concentrate our attention on the migration of items in networks with application of the obtained results to international human migration. Migration processes became very actual because of the large migration of people directed to Europe in the last years. Migration flows lead to many social problems and changes and require important decisions that have to be supported by decision support systems based on mathematical models. Recently we [3, 4] have discussed one model of migration based on the treating of migration networks as system of channels that contain the migration flow. This model of the migration channels is further developed here.

We model the channels of the migration networks as follows. The channel consists of nodes of the network (nodes may be considered as boxes representing countries) and edges that connect these nodes and represent possible ways for motion of migrants. The boxes of the channel form a chain and each box has input and output gates. Migration flows enter the box through the input gates and leave the box through the output gates in the direction of the input gates of the next box (node) of the channel. In addition a "leakage process" may happen in any of the boxes. The leakage process corresponds to the change of the status of the migrant in the corresponding box. The status of migrant may change because of different reasons: the migrant may obtain permission to stay in the corresponding country, etc. The nodes (boxes) at the beginning and at the end of the migration channel are special ones. The situation at the first node of the channel chain of nodes (the entry country) is important as this situation influences the number of migrants that enter the channel. The situation in the last node of the channel chain of nodes (the final destination country) is important as the attractiveness of this location influences the amount of migrants that enter the channel. In addition the nodes close to the end of the channel (and especially the node corresponding to the final destination country) may be more attractive for migrants in comparison to the nodes around the entry node of the channel. Finally there may be different rates of "leakage" in the different nodes of the channel.

We model the traffic of migrants through the channel by a system of differential equations that account for the processes of (i) entering and leaving the nodes of the channels, and (ii) leakage that may happen in any of the nodes. The discussed channels may contain infinite or finite number of nodes. Two regimes of functioning of these channels are studied: stationary regime and non-stationary regime. In the stationary regime of the functioning of the channel the distribution of migrants in the countries of the channel is described by a distribution that contains as particular case the Waring distribution (for channel containing infinite number of nodes) or the truncated Waring distribution (for channel containing finite number of nodes). For the case of finite-size channel the migrants may tend to concentrate in the final

destination country if this country is very attractive. In the non-stationary regime of functioning of the channel one observes exponential increase or exponential decrease of the number of migrants in the countries of the channel. It depends on the situation in the entry country of the channel for which scenario will be realized. Despite the non-stationary regime of the functioning of the channel the asymptotic distribution of the migrants in the nodes of the channel is stationary.

References

- [1] Nikolay K. Vitanov, Marcel Ausloos. Test of two hypotheses explaining the size of populations in a system of cities. *Journal of Applied Statistics* **42**, 2686 - 2693 (2015).
- [2] Marcel Ausloos, Adam Gadowski, Nikolay K. Vitanov. Primacy and ranking of UEFA soccer teams from biasing organization rules. *Physica Scripta* **89**, Art. No. 108002 (2014).
- [3] Nikolay K. Vitanov, Kaloyan N. Vitanov. Box model of migration channels. *Mathematical Social Sciences* **80**, 108 - 114 (2016).
- [4] Nikolay K. Vitanov. Science dynamics and research production. Indicators, indexes, statistical laws and mathematical models. (Springer International, Switzerland, 2016).

Modified coordinates for dynamics simulation of multibody systems with elastic bodies

Evtim V. Zahariev

Theoretical basis of the Finite Element Theory (FET) for definition of deflection coordinates and deriving the mass and material properties of the discretized elastic bodies has been applied in many commercial software packages. On the other hand, the motion parameters of the FET cannot be effectively used to catch nonlinear effects of the large displacements and deformations. It was proven [1] that using the FET approach the dynamic equations are free of centrifugal and Coriolis accelerations and the corresponding inertia forces. Additionally, using FET approach the so called stiffening effects in non-isoparametric elements cannot be taken into account in case of large elastic deflections. To illustrate the problem the simple non-isoparametric beam element with two degree of freedom of each node is discussed. In Fig. 1(a) the beam element is presented with its possible deflections along the coordinate system axes Y and Z . In the figure with dotted line the idealized FET deflections are depicted where only transversal and the angular deflections are used. Actually this assumption is valid for very small deflections. With dashed line the actual deflections are shown where, as a result of the transversal and angular deflections, node 2 experience additional deflection w . That is the so called stiffening effect that is not taken into account in case of classical FET. In Fig. 1(b) a method for presentation of modified non-isoparametric coordinates is shown, in which the possible flexible deflections of the beam are modified by two rotational coordinates, virtual rotations, along the beam length. The stiffness properties of the beam, respectively the stiffness matrix, are presented by two spring coefficients k_1 and k_2 . The values of the coefficients k_1 and k_2 and the parameters l_1 and l_2 are free parameters and for the particular case they are fixed so that the distance between the virtual joints to be equal [2]. No other criteria for selections of these parameters are discussed in the previous papers of the author. As it could be seen from Fig. 1 (b) using the modified coordinates deflections along axis X is obtained in a natural way, i.e. the stiffening effect could be observed.

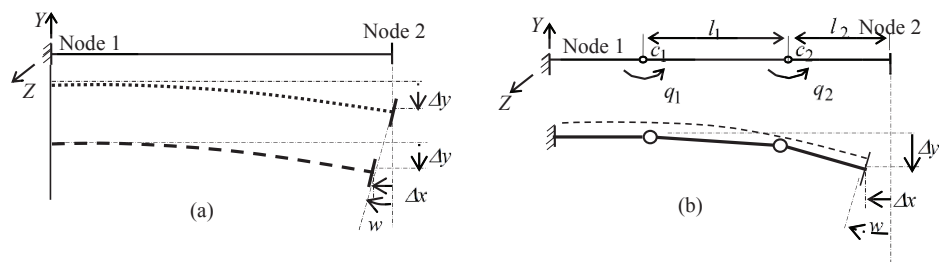


Figure 1: (a) flexible node deflections in FET and the real deflections; (b) modified coordinates and the corresponding real deflections

In the paper the problem for optimal selection of the modified coordinates and their position is defined as a nonlinear programming problem for which the general function is the quadratic form of minimal node deviations of the beam model with respect to the real large scale deviations. So with minimal number of coordinates the nonlinear effects in case of large elastic deflections are taken into account. The other problem for definition of the centrifugal accelerations of moving elastic bodies is solved using generalized Newton-Euler dynamic equations, derived by author [3]. The effectiveness of the method proposed is proven solving the example of the Kane's rotating beam [1] using only one elastic beam with two rotational coordinates.

References

- [1] T. R. Kane, R. R. Ryan, A. R. Banerjee. Dynamics of a cantilever beam attached to a moving rigid base, *AIAA Journal of Guidance, Control and Dynamics*, Vol. 10, pp. 139 - 151, 1987.
- [2] E. Zakhariiev, *Nonlinear Dynamics of Rigid and Flexible Multibody Systems, Mechanics of Structures and Machines*, MARCEL DEKKER INC, New York, Vol. 28, No. 1, pp. 105 -136, 2000.
- [3] E. Zahariiev. *Numerical Multibody System Dynamics, Rigid and Flexible Systems*, Lambert Academic Publishing GmbH & Co. KG, 2012

Part B

List of participants

Aleksander Aleksandrov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 2
1113 Sofia, Bulgaria
akalexandrov@iit.bas.bg

Vassil Alexandrov
ICREA-BSC
Carrer Jordi Girona 29
8034 Barcelona, Spain
vassil.alexandrov@bsc.es

Vera Angelova
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 2
1113 Sofia, Bulgaria
vangelova@iit.bas.bg

Teodor Atanacković
Faculty of Technical Sciences, University
of Novi Sad
and Serbian Academy of Sciences and
Arts (SASA)
21 000 Novi Sad, Serbia
e-mail: atanackovic@uns.ac.rs

Emanouil Atanassov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 25A
1113 Sofia, Bulgaria
emanouil@parallel.bas.bg

Todor Balabanov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 2
1113 Sofia, Bulgaria
todor.balabanov@gmail.com

Stefan Bushev
Institute of Metal Science, Equipment
and Technologies
with Center for Hydro and Aerodynamics
Bulgarian Academy of Sciences
Shipchenski prohod Str., 67
1574 Sofia, Bulgaria
stbushev@abv.bg

Jean-Pierre Croisille
Department of Mathematics, IECL, UMR
7502
Univ. de Lorraine
57045 Metz, France
jean-pierre.croisille@univ-lorraine.fr

Krassimir Danov
Department of Chemical and Pharmaceu-
tical Engineering
Faculty of Chemistry and Pharmacy,
Sofia University
James Bourchier Ave. 1
1164 Sofia, Bulgaria
KD@LCPE.Uni-Sofia.BG

Maria Datcheva
Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bontchev St., bl. 4
1113 Sofia, Bulgaria
datcheva@imbm.bas.bg

Georgi Evtimov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev str., bl. 25A
1113 Sofia, Bulgaria
gevtimov@abv.bg

Stefka Fidanova
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev str., bl. 25A
1113 Sofia, Bulgaria
stefka@parallel.bas.bg

Ivan Georgiev

Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 2
1113 Sofia, Bulgaria
ivan.georgiev@parallel.bas.bg

and

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

Krassimir Georgiev

Institute of Information and
Communication Technologies
Bulgarian Academy of Science
Acad. G. Bontchev str., bl. 25A
1113 Sofia, Bulgaria
georgiev@parallel.bas.bg

Stanislav Harizanov

Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., bl. 25A
1113 Sofia, Bulgaria
sharizanov@parallel.bas.bg

and

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

Snezhana Hristova

Faculty of Mathematics and Informatics
Plovdiv University
Tzar Asen Str., 24
4000 Plovdiv, Bulgaria
snehri@gmail.com

Roumen Iankov

Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bontchev St., bl. 4
1113 Sofia, Bulgaria
iankovr@yahoo.com

Oleg Iliev

Fraunhofer Institute for
Industrial Mathematics
Kaiserslautern, Germany

Nevena Ilieva

Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., bl. 25A
1113 Sofia, Bulgaria
nevena.ilieva@parallel.bas.bg

Shpend Ismaili

University of Tetovo
Tetovo, Macedonia
shpend.ismaili@unite.edu.mk

Tihomir Ivanov

Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 8
1113 Sofia, Bulgaria;
Faculty of Mathematics and Informatics,
Sofia University
5 James Bourchier
1164 Sofia, Bulgaria
tbivanov@fmi.uni-sofia.bg

Yonka Ivanova

Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., Bl. 4,
1113 Sofia, Bulgaria
yonka@imbm.bas.bg

Ivan P. Jordanov

University of National and World Economy
Studentski Grad "Hristo Botev"
1700 Sofia, Bulgaria
i.jordanov@email.bg

Dimitar Kisliakov

Dept. of Hydraulic Engineering and
Hydromelioration, UACEG
Hr.Smirnenski Blvd. 1
1046 Sofia, Bulgaria
kiss_fhe@uacg.bg

Hristo Kostadinov

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

Ralitzia Kovacheva

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

Elena Lilkova

Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., bl. 25A
1113 Sofia, Bulgaria
elilkova@parallel.bas.bg

Konstantinos Liolios

Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 25A
1113 Sofia, Bulgaria
kliolios@parallel.bas.bg

Nikolai Manev

USEA (VSU) "Lyuben Karavelov"
Suhodolska Str., 175
1373 Sofia, Bulgaria
and
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
Acad. G. Bonchev St., Bl.8
1113 Sofia, Bulgaria
nlmanev@math.bas.bg

Svetozar Margenov

Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., bl. 25A
1113 Sofia, Bulgaria
margenov@parallel.bas.bg

Lubomir Markov

Department of Mathematics and CS
Barry University
11300 N.E. Second Avenue
Miami Shores, FL 33161, USA
lmarkov@barry.edu

Svetoslav Markov

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

Ivan Markovsky

Department General Electricity
Vrije Universiteit Brussel
Pleinlaan 2, Building K
B-1050 Brussels, Belgium
ivan.markovsky@vub.ac.be

Zlatogor Minchev
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 25A
1113 Sofia, Bulgaria
zlatogor@abv.bg

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

Elena Nikolova
Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 4
1113 Sofia, Bulgaria
elena@imbm.bas.bg

Ludmila Parashkevova
Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 4
1113 Sofia, Bulgaria
lusy@imbm.bas.bg

Todor Partalin
Faculty of Mathematics and Informatics
Sofia University "St. Kliment Ohridski"
Blvd. James Bourchier 5
1164 Sofia, Bulgaria
topart@fmi.uni-sofia.bg

Albena Pavlova
Department of MPC
Technical University-Sofia, Plovdiv Branch
4000 Plovdiv, Bulgaria
akosseva@gmail.com

Polina Petrova
UCTM
Sofia University "St. Kliment Ohridski"
Bul. Kl. Ohridski 8
1756 Sofia, Bulgaria
polina.petrova1994@gmail.com

Stevan Pilipović Faculty of Sciences
University of Novi Sad
and Serbian Academy of Sciences and
Arts (SASA)
21 000 Novi Sad, Serbia
pilipovic@dmi.uns.ac.rs

Evgenija D. Popova
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
Acad. G. Bonchev str., block 8
1113 Sofia, Bulgaria
epopova@math.bas.bg
epopova@bio.bas.bg

Peter Rashkov
Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., Bl. 8
1113 Sofia, Bulgaria

p.rashkov@math.bas.bg

Hassan Safouhi Campus Saint-Jean,
University of Alberta
8406, 91 Street, Edmonton, Alberta T6C
4G9
Canada
hsafouhi@ualberta.ca

Sonia Tabakova
Institute of Mechanics,
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 4
1113 Sofia, Bulgaria
stabakova@gmail.com

Margarita Terziyska
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 2
1113 Sofia, Bulgaria
mterziyska@bas.bg

Yancho Todorov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 2
1113 Sofia, Bulgaria
yancho.todorov@iit.bas.bg

Nikolay K. Vitanov
Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 4
1113 Sofia, Bulgaria
vitanov@imbm.bas.bg

Yavor Vutov
Institute of Information and
Communication Technologies
Bulgarian Academy of Sciences
Acad. G. Bonchev Str., bl. 25A
1113 Sofia, Bulgaria
yavor@parallel.bas.bg

Dennis Wenzel
Dresden University of Technology
denniswenzel2012@gmail.com

Evtim Zahariev
Institute of Mechanics
Bulgarian Academy of Sciences
Acad. G. Bontchev str., bl. 4
1113 Sofia, Bulgaria
evtimvz@bas.bg