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BOOK OF ABSTRACTS

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Postbuckling Behavior and Imperfection Sensitivity of an Elastic Compressible Rod whose Flexural Resistance Changes with Load

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This paper is concerned with the nonlinear behavior and imperfection sensitivity of a compressible elastic column whose flexural resistance changes with load [1-7]. A two-degree-of-freedom model of the column is analyzed. Imperfection is introduced into the system by assuming an initial rotation. Various types of load-stiffness relationships are considered. Post-buckling behavior under static unidirectional loads is investigated. Singularities of the equilibrium path of the column are classified according to the slenderness ratio of the column and the load-stiffness relationship of its support. It is shown that by including the compressibility, imperfections and stiffening of the supports, we can predict the buckling load of the column more accurately. It is also shown that the buckling load can be corrected by means of coefficients obtained from specific diagrams. Using a nonlinear finite element technique, numerical examples, illustrating the imperfection sensitivity of an elastic column in various ranges of slenderness ratios are also given. The results are qualitatively compared with those of a two-degree-of-freedom model.

Key Words: Geometric imperfection, Compressible column, Postbuckling behavior of a column, Euler load, Trifurcation point.

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A Sinc-Galerkin Approach for Systems of Conservation Laws of Mixed Hyperbolic-Elliptic Type

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A Sinc-Galerkin procedure is developed for systems of conservation laws of mixed hyperbolicelliptic type. Sinc approximations to both derivatives and the indefinite integrals reduce the system to an explicit system of algebraic equations. It is shown that Sinc-Galerkin approximations produce an error of exponential order, that considered to be an improvement over errors that are polynomials in h. Approximation by Sinc functions handles singularities in the problem, as well as changes in type of the system. Numerical results for the test problems presented sustain the exponential convergence rate of the method.

Modeling of an Elastic Sphere Hit on an Elastic-plastic Plate under a Continuing Action of an Outer Force

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Modeling of hitting processes at various properties of the colliding bodies is of particular theoretical and practical interest e.g. for modelling of plastic deformation processes. Best results regarding the parameters of the hitting processes (forces, tensions, deformations, duration of contact, etc.) are obtained by the final elements method (FEM).

This paper presents the results of FEM modeling of the hitting process after a free fall of a sphere on an elastic-plastic plate with specific dimensions with the added action of an outer force.

Two cases are described: of the action of an outer force only during the time of contact of the hitting bodies and during the whole time of movement of the sphere.

Correlations were obtained for the change of the strength of the hit, the tensions and deformations in time for the sphere and the plate. The deformations of the plate were defined for various values of the outer force. These results allow us to define the conditions, necessary to perform the so called 'Combined Hit.' This results in a significant change of the conditions in which the deformation processes flow in.

On Inversion of Radon Transforms from Partial Data

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A generalized Radon transform Rf puts into correspondence to a given function f(x) of n variables its integrals over a family of n-1 dimensional hypersurfaces (e.g., planes, spheres, etc.). Such transforms play a key role in various models of medical imaging modalities, radar and sonar imaging, industrial non-destructive testing, as well as in several areas of pure mathematics. The major problems related to these transforms are the existence and uniqueness of their inversion, development of stable numerical algorithms for inversion, and their range description.

Many of these problems have been extensively studied during the last couple of decades. In the case, when the Radon transform Rf is known for all surfaces in the given family, there are well developed theories now addressing most of the questions mentioned above. However, if Rf is known only for a part of the family of surfaces (partial data problems), many of these questions are still open.

Our talk will address some new results about the inversion of generalized Radon transforms from partial data. We use techniques of integral equations, integral transforms, and special functions theory to prove uniqueness and stability of the inversion in the case of limited data for spherical Radon transform.

Lower Bounds for Eigenvalues by Nonconforming FEM on Convex Domain

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In this work we analyze the approximations of second order eigenvalue problems (EVPs). The nonconforming piecewise linear finite element with integral degrees of freedom is used. We prove that the eigenvalues computed by means of this element on convex domain are smaller that the exact ones if the mesh size is small enough. Some numerical results are also given.

Richardson Extrapolation for Reaction-Diffusion Singularly Perturbed Interface Problems

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The accuracy of finite difference approximations can be increased either by using higher order finite difference approximations or Richardson extrapolation. However, a problem arise when the interface is treated. We propose different expressions for one-sided finite difference approximations on a line interface for a singularly perturbed reaction-diffusion equation in two-dimensions. Numerical experiments on fitted meshes (Bahvalov's, Shishkin's) illustrate the effect of the Richardson extrapolation.

A Case of Multi-vector and Multi-host Epidemiological Model: Bartonella Infection

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We consider a compartmental model for the Bartonella infection on rodents. More precisely, on the co-occurring populations of *Rattus rattus* and *Rattus norvegicus* where the vectors are two species of ectoparasites, namely ticks and fleas. As usual for such models a key stage is the modelling of the forces of infection. While the vital dynamics and the progression of the infection within each of the four species are sufficiently well know to determine the rest of the transfer rates, there is practically no data on the probability of infection. In order to determine appropriate values for the coefficients of the forces of infection we solve an optimal control problem where the objective function is the norm of the difference between the observed and the predicted by the model equilibrium infection prevalence rates in the four species. Within this setting the conjecture that the higher prevalence of the infection in *Rattus norvegicus* can be explained solely by their higher ectoparasite load is tested and disproved.

Analysis of Types of Oscillations in Goodwin's Model of Business Cycle

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We study numerically the properties of nonlinear oscillations of Goodwin's model of business cycle [1]

$$\begin{cases} \epsilon \dot{y}(t) + (1-\alpha)y(t) = \varphi(\dot{y}(t-\theta)) + l(t) + \beta(t), & t > 0\\ y(t) = \phi(t), & -\theta \le t \le 0. \end{cases}$$

Here y(t) is income, $\epsilon^{-1} > 0$ – the adjustment coefficient, α – the marginal propensity to consume, $0 \le \alpha \le 1$, $\phi(\dot{y}(t))$ – the induced investment function, θ is a lag in the investment function, l(t) is autonomous investment, and $\beta(t)$ is autonomous consumption,

$$\phi(z) = \begin{cases} \phi_+, & z > \kappa_1 \phi_+ \\ \kappa z, & \kappa_1 \phi_- \le z \le \kappa_1 \phi_+ \\ \phi_-, & z < \kappa_1 \phi_- \end{cases}$$

 κ is the acceleration coefficient, ϕ_{-} and ϕ_{+} are upper and lower limits of ϕ .

In simulating this model on an analog computer [2] was indicated the existence of Goodwin's limit cycle solution with a period much greater than θ and an infinite number of limit cycle solutions with periods θ , $\theta/2$, $\theta/3$,... Our calculations show that such cycles may be caused by high-frequency oscillations of the initial function $d\phi(t)/dt$. We have shown also that Goodwin's limit cycle solutions exist only in a limited range of θ , $0 \le \theta \le \theta_{\text{max}}$.

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On the Pulsating Strings in Sasaki-Einstein Spaces

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We study the class of pulsating strings on $AdS_5 \times Y^{p,q}$ and $AdS_5 \times T^{a,b,c}$. Using a generalized ansatz for pulsating string configurations, we find new solutions for this class in terms of Heun functions, and derive the particular case of $AdS_5 \times T^{1,1}$, which was analyzed in arXiv:1005.5334 [hep-th]. Unfortunately, Heun functions are still little studied, and we are not able to quantize the theory quasi-classically and obtain the first corrections to the energy. The latter, due to AdS/CFT correspondence, is supposed to give the anomalous dimensions of operators of the gauge theory dual $\mathcal{N} = 1$ superconformal field theory.

Stochastic Super-exponential Growth Model Describing Population Dynamics

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Observational data clearly suggest that the human population has grown faster than exponentially, exhibiting a super-exponential growth for most of the known history. The accelerating character of the growth rate describing the human population can be generalized as an inherent property of evolutionary processes. Based on the analogy with different evolutionary processes we have concluded that the human population is a dynamical system with non-linear positive feedback occurring between technological advancement and the abundance of a population. Behavior of a super-exponential function asserts that a population, growing at a super-exponential pace, will encounter a catastrophe within a finite time. This catastrophic event is mathematically described as a singular state, where population has exploded to infinity. In current paper the influence of the environmental noise to superexponentially growing population is considered. Ascribing stochastic nature to Malthusian parameter r, which denotes an influence of the environmental noise to a growth of a population, we consider a model that follows from the equation

$$\frac{dy}{dt} = -\alpha r + \sqrt{D}\zeta(t) \tag{1}$$

where t is time, α is a parameter describing the technological advancement of the population, D is the intensity of the Gaussian white noise $\sqrt{D}\zeta(t)$, interpreted in the sense of Ito. In equation (1) $y = p^{-\alpha}$, where p denotes the abundance (number of members or density) of a population. The corresponding Fokker-Planck equation is solved. The mean value and dispersion of the population density p as well as the average lifetime of the system together with its dispersion are calculated. Implications of the mathematical analysis of the stochastic super-exponential model on the biological system have also been examined. Various applications of the results of the analysis are discussed.

A Note on Interpolation Functions of the Frobenious-Euler Numbers

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The main purpose of this paper is to construct partial twisted zeta-type function, which interpolates q-generalized Frobenius-Euler numbers and twisted q-generalized Frobenius-Euler numbers. We give some applications related to this function.

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Key Words and Phrases. Euler Numbers, twisted q-Frobenius-Euler Numbers, twisted q-Frobenius-Euler polynomials, twisted q-zeta function, twisted q-l-function.

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Electromagnetic Scattering by Orthotropic Waveguides

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The talk will be devoted to the mathematical analysis of the scattering of time-harmonic electromagnetic waves by an infinitely long cylindrical orthotropic waveguide iris. This will be done by using an orthotropic Maxwell system in a cylindrical waveguide iris for plane waves, imbedded in an isotropic infinite medium. The corresponding 3D problem will be successfully reduced to a simpler 2D problem. The unique solvability of the associated boundary value problems will be proved and regularity of solutions will be obtained in Bessel potential spaces. Part of the talk is based on a joint work with R. Duduchava and D. Kapanadze.

The Need for a First-order Quasi Lorentz Transformation

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Solving electromagnetic scattering problems involving non-uniformly moving objects requires an approximate but consistent extension of Einstein's Special Relativity theory, which originally is valid for constant velocities only. For moderately varying velocities a quasi Lorentz transformation is presented. The conditions for form-invariance of the Maxwell equations, the so-called "principle of relativity," are shown to hold for a broad class of motional modes and time scales. A simple example of scattering by a harmonically oscillating mirror is analyzed in detail. Generally orbiting objects are discussed.

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In [1] the classical single factor term structure equation for models that predict non-negative interest rates is studied. For these models the authors proposed a second order accurate three - level finite difference scheme (FDS) using the appropriate boundary conditions at zero. For the same problem we construct a two-level second-order accurate (FDS). The flexibility of our FDS makes it easy to change the drift and diffusion terms in the model. A transform method that reduces the equation on a finite interval is also discussed.

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Modeling and Optimization of Locomotion for Multibody Systems

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Dynamical systems consisting of several rigid bodies can move progressively in a resistive medium, if these bodies perform certain relative motion with respect to each other. Different types of locomotion for multibody systems are analyzed, namely:

- snake-like locomotion along a plane of multilink systems whose links are connected to each other by cylindrical joints;
- fish-like locomotion of two-link and three-link systems in a fluid;
- locomotion of vibro-robots consisting of two rigid bodies that perform oscillations relative to each other.

The locomotion of multibody systems is controlled by actuators installed at the joints and occurs in the presence of different resistant forces acting upon the systems. The cases of Coulomb's dry friction forces, as well as forces that are linear or quadratic functions of the body velocity are considered.

Various modes of progressive motions are analyzed and simulated.

Special attention is given to the optimization of locomotion with respect to the system parameters and control of motion. As a result, the maximal possible speed of locomotion is evaluated.

Experimental data are presented that confirm the obtained theoretical results. These results are of interest for biomechanics and robotics, especially, for micro-robots that can move in a complicated environment and inside tubes.

Numerical Investigation of Boussinesq Equations with Saturation

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We consider Boussinesq type equations with saturated nonlinearity. The Proper Boussinesq equation with saturated nonlinearity (BPES) in one space dimension is of the form $u_{tt} = [u - \frac{u^2}{1+\gamma u^2} - u_{xx}]_{xx}$ and the analogous Paradigm Boussinesq equation is of the form $u_{tt} = [u - \frac{u^2}{1+\gamma u^2} - u_{xx}]_{xx}$.

To investigate these kind of problems we use a combination of Christov- Galerkin method and finite differences numerical schemes by introducing an auxiliary function $q = \frac{u^2}{1+\gamma u^2}$ to get $u_{tt} = [u - q - u_{xx}]_{xx}$. We solve the stationary problem and use its solution as initial condition for the time dependent problem. We use different values of the saturation parameter and investigate its impact in the total phase speed of the system. We examine thoroughly the phase shift of the solitons upon collision and evaluate numerically the mass and energy of the system and prove that the numerical scheme preserves the conservative properties.

$$\rightarrow \infty \diamond \infty \leftarrow$$

Modeling of Line Shapes Using Stochastic Processes

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Accurate calculations of line shapes are widely used by physicists to obtain information on the emitting gas or plasma. For the radiation emitted in such environments, the modeling of line shapes often asks for the solution of a stochastic differential equation describing the evolution of the emitter submitted to random perturbations. In plasma, the major perturbation is usually brought by the electric microfield created by the numerous charged particles moving around the emitter. Here the method consists of substituting the true electric field with an effective stochastic electric field, whose evolution is characterized by stepwise constant values separated by instantaneous jumps distributed according to a chosen dynamical process. Using the Continuous Time Random Walk theory (CTRW) [1], the standard Kangaroo process where the waiting time distribution between electric field jumps follows a Poisson distribution will be extended to various waiting time distribution including Lévy distributions. The standard Kangaroo process for the microfield have first been proposed several decades ago, using a Markov approximation for the microfield entering the emitters [2]. We will show that using the CTRW allows to retain non-Markovian effects. We will compare the previous and new results obtained with these models with profiles obtained by a plasma computer simulation coupled to a numerical integration of the Schrödinger equation.

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Cylindrical Couette Flow of Rarefied Gas between Two Cylinders Rotating with Different Velocities

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The cylindrical Couette flow of a rarefied gas is studied in the case of two cylinders rotating with different velocities. Velocity, density and temperature profiles are investigated by a Direct Monte Carlo Simulation method and a numerical solution of the Navier-Stokes equations for compressible flow is found. Noting by we have obtained for different values of D (at the variety velocity boundary conditions) numerical results for gas velocity and temperature at the walls. The gas lags or outstrips in comparison with the walls or it has the elastic rigid body behavior. These results are important for applications in non-planar microfluidic problems. The results obtained by both methods are in an excellent agreement at a small Knudsen number Kn = 0.02.

Keywords: Kinetic theory, Rarefied gas, Microfluidics, DSMC PACS: 51.20.+d

Interfacial Fluid Dynamics: Role of Surfactants

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Fluid dynamics involving interfaces is of wide interest from fundamental and application view points. There are many interesting questions associated with such problems some of which have been addressed experimentally, numerically and theoretically. We review some of these works including the author's and his co-authors' contributions in this area. In particular, we will first review, from the literature, experimental and computational results on the effect of surfactant on the thickness of thin films in Landau-Levich drag coating problem and Bretherton's bubble movement problem through a capillary tube. In both of these problems surfactant thickens the thin-film. Using lubrication approximation and asymptotic methods, we will prove these thickening effects. In the case of drag-out coating problem, the proof will be based on results on the upper bound of film thickness. However, in the case of motion of bubbles through a capillary tube the proof is somewhat along the similar lines. There are some open interesting problems that will also be discussed.

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Matrix-valued Polynomial Hermite Interpolation and the Cauchy-Riesz-Dunford Operator Integral in the Finite-dimensional Case

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We compute explicitly the Cauchy-Riesz-Dunford operator integral in the finite-dimensional case by a matrix-valued polynomial Hermite interpolant, where the projections onto the eigenspaces corresponding to different eigenvalues are shown to have the structure of matrix-valued fundamental Hermite basis polynomials. This construction generalizes the well-known explicit formula for the Cauchy-Riesz-Dunford operator integral in the particular case when all eigenvalues have multiplicity equal to 1 and the computation is in terms of a respective matrix-valued Lagrange polynomial interpolant. Several applications of the new formula are considered. We briefly discuss the possibility of extending this construction to compact operators in infinitely dimensional Banach spaces, where the construction needs essential upgrading.

Parametric Investigation of Static and Dynamic Regimes in Stacked Josephson Junctions

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The dynamics of Josephson phases in inductively coupled stacks of long Josephson Junctions is described by an initial boundary value problem for system of perturbed sine-Gordon equations. A detailed comparison analysis for the influence of the geometric parameters (number and length of junctions, coupling parameter) and the physical parameters (external current, external magnetic field and dissipation) on the solutions of this complicated nonlinear multiparametric problem is made. The regions of stability of the static solutions of the system with respect to the external current and the external magnetic field for different values of the geometric parameters are found. The cases of two, three and four stacked junctions are studied in detail and a comparison is made. Moving fluxons solutions are also investigated for different geometric parameters and dissipations. Finite Element Method and Finite Difference Method are used to solve numerically the dynamic and the corresponding static problems.

Thermodynamics of Scalar-Tensor AdS Black Holes Coupled to Nonlinear Electrodynamics

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We construct new numerical solutions describing charged anti-de Sitter black holes coupled to nonlinear Born-Infeld electrodynamics within a certain class of scalar-tensor theories and we study their thermodynamic phase structure. It is shown that for certain charge intervals phase transitions of zeroth and first order exist.

Methods for the Coupled Stokes-Darcy Problem

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The motion of particles in a viscous fluid close to a porous membrane is relevant for microfiltration applications. Here, particles are assumed to be large compared with the size of pores of the membrane. The hydrodynamic interactions of one particle with the membrane are considered here. The model involves Stokes equations for the fluid motion around the particle together with Darcy equations for the flow in the porous membrane and Stokes equations for the flow on the other side of the membrane. Boundary conditions at the fluid-membrane interface are the continuity of pressure and velocity in the normal direction and the Beavers & Joseph slip condition on the fluid side in the tangential directions. The no-slip condition applies on the particle. This problem is solved here by two different methods.

The first one is an extended boundary integral technique. A Green function is derived for the flow close to a porous membrane. This function is non-symmetric, leading to difficulties hindering the application of the classical boundary integral technique. Thus, an extended technique is proposed, in which the unknown distribution of singularities on the particle surface is not the stress, like in the classical boundary integral technique. Yet, the hydrodynamic force and torque on the particle are obtained by integrals of this distribution on the sphere surface.

The second method consists in searching the solution as an asymptotic expansion in term of a small parameter that is the ratio of the typical pore size to the particle size. The various boundary conditions are taken into account at successive orders: order (0) simply represents an impermeable wall without slip and order (1) an impermeable wall with a peculiar slip prescribed by Order (0); at least the 4th order is necessary to enforce all boundary conditions.

The methods are applied numerically to a spherical particle and comparisons are made with earlier works in particular cases.

Studying an Eulerian Computer Model Performance on Different High-performance Computer Platforms

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The Danish Eulerian Model (DEM) is an Eulerian model for studying the transport of air pollutants on large scale. Originally, the model was developed at the National Environmental Research Institute of Denmark. The model computational domain covers Europe and some neighbour parts belong to the Atlantic Ocean, Asia and Africa. If DEM model is to be applied by using fine grids, then its discretization leads to a huge computational problem. This implies that such a model as DEM must be run only on high-performance computer architectures. The implementation and tuning of such a complex large-scale model on each different computer is a non trivial task.

Here, some comparison results of running of this model on different kind of vector (CRAY C92A, Fujitsu, etc.), parallel computers with distributed memory (IBM SP, CRAY T3E, Beowulf clusters, Macintosh G4 clusters, etc.), parallel computers with shared memory (SGI Origin, SUN, etc.) and parallel computers with two level of parallelism (IBM SMP, IBM BlueGene/P, clusters of multiprocessor nodes, etc.) will be presented. The main idea in the parallel version of DEM is domain decomposition approach. Discussions according to the effective use of the cache and hierarchical memories of the modern computers as well as the performance, speed-ups and efficiency achieved will be done. The parallel code of DEM, created by using MPI standard library, appears to be highly portable and shows good efficiency and scalability on different kind of vector and parallel computers.

Phases of Soliton-like Solutions in the Scalar-tensor Theories of Gravity

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The aim of the present work is to investigate numerically phases of soliton-like solutions coupled to non-linear electrodynamics in the scalar-tensor theories of gravity. As a result of the numerical experiments new non-unique solutions of the corresponding boundary-value problem and their general properties were found.

Computations in Dynamics of Incompressible Nonlinear Elastic Medium by Using Near-front Ray Expansions of Solutions

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The present work deals with propagation curvilinear (cylindrical) shock waves in nonlinear elastic medium. As an example we consider one-dimensional problems concerning the anti-plane and twisted motion of an incompressible nonlinear elastic medium. Analytical solutions to these problems were obtained by the ray method. The latter lies in the fact that functions to be found behind the wavefront are represented in terms of series like Taylor's series [1,2]. The coefficients are the discontinuities in the strains and their derivatives on moving discontinuity surface. These coefficients are related to one another by the compatibility conditions for the discontinuities. The ray method modification for shock waves was proposed in [3]. The approximate solutions obtained in this way will be the closer to the exact solutions the smaller post-impact times considered. The subsequent shock loading process we computed numerically by use of a finite-difference method. The ray expansion of solution was applied to determine the wavefront position at every time step and to find a solution near the wavefront. The way of matching the near-front analytical solution and the numerical solution by the least-square technique is presented. Numerical solutions for the problems under study are illustrated graphically. In [4] this approach was implemented for plane shock waves.

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On Soliton Equations and Soliton Interactions

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I will describe an important class of nonlinear evolution equations in two-dimensional spacetime that are exactly integrable and find applications in nonlinear optics, hydrodynamics, plasma physics, superconductivity etc. Two important representatives of the soliton equations is the nonlinear Schrödinger equation (NLSE)

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + |u(x,t)|^2 u(x,t) = 0.$$

and the sine-Gordon equation (sGE):

$$\frac{\partial^2 v}{\partial x \partial t} = \sin v(x, t).$$

I will first outline the inverse scattering method that allows one to solve the NLSE and the sGE, and how to obtain explicitly their N-soliton solutions. Due to their stability they allow one to explain effects that can not be obtained by perturbation theory.

Then I will explain the soliton interactions and the effects of perturbations on them.

Finally I will address the generalizations of this theory to multicomponent NLSE related to symmetric spaces. Special attention will be paid to the system

$$\begin{split} &i\partial_t \Phi_1 + \partial_x^2 \Phi_1 + 2(|\Phi_1|^2 + 2|\Phi_0|^2)\Phi_1 + 2\Phi_{-1}^* \Phi_0^2 = 0, \\ &i\partial_t \Phi_0 + \partial_x^2 \Phi_0 + 2(|\Phi_{-1}|^2 + |\Phi_0|^2 + |\Phi_1|^2)\Phi_0 + 2\Phi_0^* \Phi_1 \Phi_{-1} = 0, \\ &i\partial_t \Phi_{-1} + \partial_x^2 \Phi_{-1} + 2(|\Phi_{-1}|^2 + 2|\Phi_0|^2)\Phi_{-1} + 2\Phi_1^* \Phi_0^2 = 0. \end{split}$$

which describes Bose-Einstein condensate of alcali atoms in the F = 1 hyperfine state and elongated in one direction.

Development of ROOT Services for Grid

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ROOT is platform independent, object-oriented framework used for solving the data analysis challenges of high-energy physics. Physical experiments like NA48, CMS, ALICE and ATLAS use g-Lite Grid infrastructure for data storage and analyzes and ROOT framework for interactive manipulation of tree objects and histograms of the analyzed data. It is strategically important ROOT to be used in Grid middleware. The intention of this research is to present methodology for exposing legacy ROOT functionality as services.

Recent Developments in Stability, Vibration and Control of Mechanical Structures

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This talk is devoted to the applications of the stability theory and modern control techniques to understand and to control the nonlinear behavior of a class of conservative, nonconservative, and time varying mechanical structures. To that end we first study the control problem of a spinning satellite in a gravitation field, then we study the full nonlinear behaviour of a pipe conveying fluid. Here we use the computed torque method to control the divergence, flutter and chaotic instabilities of this fluid-solid system. We will demonstrate that the fluid flow here can be used both for shape control and vibration control of a continuum. The last part of the talk is devoted to the long standing problem of periodic time varying systems. This has been a chalenge for more than a century since the time of Mathieu, Floqueut, Hill, Rayleigh, Lyapunov, and Poincare. The lecture is blended with some videos of recent experimental work to support theoretical results.

Efficient Gridification of Environmental Protection Applications with QoS

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The environmental protection was identified as a domain of high interest for South East Europe, addressing practical problems related to security and quality of life. The gridification of these applications faces several challenges:

- 1. These applications are usually resource intensive, in terms of both CPU utilization and data transfers and storage.
- 2. The use of applications for operational purposes poses requirements for availability of resources, which are difficult to be met on a dynamically changing Grid environment.
- **3.** The validation of applications is resource intensive and time consuming. This leads to a certain level of conservatism and requires the execution environment to be predictable and controlled by the developers of the applications. Such requirements preclude the use of some techniques that are acceptable for other areas. For example, the completion of the executable on-the-fly is not a viable option, even though in other areas it allows for the best performance.

The Job Track Service (JTS) is a grid middleware component which facilitates the provision of Quality of Service in grid infrastructures using gLite middleware. The service is based on messaging middleware and uses standard protocols like AMQP (Advanced Message Queuing Protocol) and XMPP (eXtensible Messaging and Presence Protocol) for real-time communication, while its security model is based on GSI authentication. It enables resource owners to provide the most popular types of QoS of execution to some of their users, using a standardized model.

In this work we describe a new version of the Job Track service offering application specific functionality, geared towards the specific needs of the Environmental Modelling and Protection applications. We used the modular design of the JTS in order to enable smoother interaction of the users with the Grid environment. Our experience shows improved response times and decreased failure rate from the executions of the application. In this work we present such observations from the use of the South East European Grid infrastructure. The new version of the JTS enables more collaborative and efficient use of the Grid resources and answers to the application requirements.

Analytical Kerr-Sen Dilaton-axion Black Hole Lensing in the Weak Deflection Limit

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We investigate analytical gravitational lensing by charged, stationary, axially symmetric Kerr-Sen dilaton-axion black holes in the weak-deflection limit. Approximate solutions to the lightlike equations of motion are present up to and including third-order terms of small parameter proportional to the black hole mass, to the black hole angular momentum and to the square of the black hole charge and inverse proportional to the impact parameter of the light ray. We compute the positions of the two weak field images, the corresponding signed and absolute magnifications up to post-Newtonian order. All of the lensing quantities are compared to particular cases as Schwarzschild and Kerr black holes as well as the Gibbons-Maeda-Garfinkle-Horowitz- Strominger black hole.

Unilateral Contact Problems for Hemitropic Solids – A Boundary Variational Inequality Approach

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In this talk we report on recent progress on the treatment of various contact problems for hemitropic elastic solids by boundary integral methods. This contribution is based on joint work with A.Gachechiladze, R.Gachechiladze, and D.Natroshvili from Tbilisi in Georgia.

Micropolar theory, by including intrinsic rotations of the particles, provides a rather complex model of an elastic body that can support body forces and body couple vectors as well as force stress vectors and couple stress vectors at the surface. Consequently, in micropolar theory all the mechanical quantities are written in terms of the displacement and microrotation vectors. A micropolar solid which is not isotropic with respect to inversion is called hemitropic, noncentrosymmetric, or chiral. Materials may exhibit chirality on the atomic scale, as in quartz and in biological molecules – DNA, as well as on a large scale, as in composites with helical or screwshaped inclusions, certain types of nanotubes, bone, fabricated structures such as foams, chiral sculptured thin films and twisted fibers.

Here we attack the nonlinear nonsmooth problems of contact without and with friction. We equivalently reduce these problems to boundary variational inequalities with the help of the Steklov-Poincaré type operator. Based on our boundary variational inequality approach we prove existence and uniqueness theorems for weak solutions. We include also the case, when the body is not fixed, but only submitted to force and couple stress vectors along some part of the boundary and is in unilateral contact with a rigid foundation. In this situation of a semicoercive boundary value problem we employ recession analysis and derive necessary and sufficient conditions of solvability.

Temperature Model of a New High-powered SrBr₂ Laser

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It has been established that laser generation with wavelength of $\lambda = 6.45 \mu$ m is widely applicable in the fields of medicine and biology. The main sources of this radiation were free electron lasers. Due to their high cost an alternative - SrBr₂ vapor lasers, which generate the same wavelength - was developed. They have a number of advantages – compact size, lower price, easy operation, longer tube service life. The operating temperature of SrBr₂ vapor lasers is 1000°C. This places special demands on the construction of new laser sources of this type. Up to this moment, the achieved laser output power is 4.26 W, with 90% of generation along the line $\lambda = 6.45 \mu$ m. In order to develop a new SrBr₂ vapor laser (with an expected output power 6-7 W), a preliminary evaluation of the temperature profile of the active laser medium and the laser tube is necessary. To this end, this paper utilizes a temperature model developed by the authors beforehand. Two types of laser tubes of similar geometric size but with different geometric structures of their cross-sections have been considered. For each of the two tubes, families of temperature profiles with variation of the input electric power, buffer gas pressure, and external wall temperature, have been developed.

Obtained results are part of the general preliminary studies for developing the new highpowered $SrBr_2$ vapor laser. They allow the evaluation of the electric supply, the optical resonator, and the mechanical construction. The application of statistical methods for the prediction of laser generation will be also stipulated. The optimal temperature profile of the future device and its geometric design can only be determined in the context of the general analysis.

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Accelerated Iterations for Finding the Soft-Constrained Stochastic Nash Games Equilibrium

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The following constrained weakly coupled system is considered [1]:

$$X_{1}(A_{0} - S_{2}X_{2}) + (A_{0} - S_{2}X_{2})X_{1} + A_{1}^{T}X_{1}A_{1} - X_{1}S_{1}X_{1} + X_{1}M_{1}X_{1} + \epsilon X_{2}S_{12}X_{2} + Q_{1} = 0$$
(1)
$$X_{2}(A_{0} - S_{1}X_{1}) + (A_{0} - S_{1}X_{1})X_{1} + A_{1}^{T}X_{2}A_{1} - X_{2}S_{2}X_{2} + X_{2}M_{2}X_{2} + \epsilon X_{1}S_{21}X_{1} + Q_{2} = 0$$

with the $m \times m$ unknown symmetric matrices X_1 , X_2 is called a set of cross-coupled stochastic algebraic Riccati equations (CSARE) under notations

$$S_{i} = B_{i}R_{ii}^{-1}B_{i}^{T}, \qquad M_{i} = EV_{i}^{-1}E^{T}, \qquad i = 1, 2,$$

$$S_{21} = B_{1}R_{11}^{-1}R_{21}R_{11}^{-1}B_{1}^{T}, \qquad S_{12} = B_{2}R_{22}^{-1}R_{12}R_{22}^{-1}B_{2}^{T}.$$

Mukaidani [1] has proposed the following stochastic algebraic Lyapunov iteration:

$$X_{1}^{(k+1)}\tilde{A}_{1,k} + \tilde{A}_{1,k}X_{1}^{(k+1)} + A_{1}^{T}X_{1}^{(k+1)}A_{1} + X_{1}^{(k)}S_{1}X_{1}^{(k)} - X_{1}^{(k)}M_{1}X_{1}^{(k)} + \epsilon X_{2}^{(k)}S_{12}X_{2}^{(k)} + Q_{1} = 0$$

$$X_{2}^{(k+1)}\tilde{A}_{2,k} + \tilde{A}_{2,k}X_{2}^{(k+1)} + A_{1}^{T}X_{2}^{(k+1)}A_{1} + X_{2}^{(k)}S_{2}X_{2}^{(k)} - X_{2}^{(k)}M_{2}X_{2}^{(k)} + \epsilon X_{1}^{(k)}S_{21}X_{1}^{(k)} + Q_{2} = 0$$

with $\tilde{A}_{i,k} = A_0 + S_1 X_1^{(k)} + S_2 X_2^{(k)} + M_i X_i^{(k)}$ for finding a positive semidefinite solution to (1). We propose a new iteration scheme for solving (1) and we compare a few iterations for com-

puting a positive definite solution to (1). We will compare the numerical effectiveness of the corresponding recursive procedures. Numerical examples are used to demonstrate the performance.

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Sensitivity Studies of a Large-scale Air Pollution Model in Grid Environment

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Variance-based approaches for sensitivity analysis have been applied and analized to study the sensitivity of air pollutants concentrations according to variations of rates of chemical reactions.

The Unified Danish Eulerian Model (UNI-DEM) has been used as a mathematical model simulating a remote transport of air pollutants. Plain and adaptive Monte Carlo algorithms for numerical integration have been applied to compute Sobol' global sensitivity indices. A comparison with sensitivity approaches implemented in SIMLAB software tool for sensitivity analysis has been done. Grid implementations of the UNI-DEM and the algorithms under consideration have been carried out.

Improved Sparse Fourier Transforms for Sparse Spectral Methods

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We study the problem of quickly estimating the best possible k-term nonlinear Fourier approximating for a given function. Randomized sublinear-time Monte Carlo algorithms, which have a small probability of failing to output accurate answers for each input signal, exist for solving this problem. In this paper we present a deterministic approximation scheme with accompanying error guarantees and uniformly bounded sampling requirements. Furthermore, we present a simple technique for reducing the estimation of high-dimensional functions to a related one-dimensional problem. The end result is a robust deterministic Fourier nonlinear approximation method for general functions. Empirical evaluations of our methods demonstrate their efficiency compared to both existing Monte Carlo Fourier methods and standard fast Fourier transform algorithms. Applications of these new algorithms to sparse spectral methods will also be discussed.

An Immersed Interface FEM for 1D Elastic Continuum Vibrations Under a Traveling Load

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In this paper we study the problem of a load, traveling along elastic structures, such as strings, beams or plates. The case of semi-active viscous dampers is also considered. The numerical method, based on the Immersed Interface Finite Element Method is developed. The presence of Dirac-delta function terms in the mathematical model leads to using of a special basis functions near the interfaces. Many numerical experiments are presented for different practical cases.

Hit of a Body into a Plate at a Continuous Action of an Additional Outer Force

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This paper discusses the case of the fall of a body with mass m from a height h on an absolutely rigid plate. At the very first moment of impact a constant outer force P_r begins action on that body. The value of rebound after the hit depends on the ratio between the force of rebound P_1 (which is a function of the mass m and the speed of the hit V_0) and P_r . From the basic equation of mechanics differential equations have been derived and solving them makes it possible to define V_0 for various resistances of the medium R for the case when this resistance starts to act after the passing of the distance h_* from the initial point of falling of the body. The formula to calculate the force $P_1(m, V_0, P_r)_R$ was derived based on those estimations. This is connected to the study on the value of the rebound of production machines with hammer action, propelled by a new type of engine. That engine can work during the vertical movement of the body (when we get acceleration of the falling parts up to $V_0 = 40$ m/s), and during and after the impact. Depending on the ratio between P_1 and P_r one can get various values of the rebound ('guided' or 'combined' hit) or no rebound ('sticking' hit).

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The Multi-index Mittag-Leffler Functions and Their Applications for Solving Fractional Order Problems in Applied Analysis

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During the last few decades differential equations and systems of fractional order (that is, of arbitrary one, not necessarily integer), begun to play an important role in modelling of various phenomena of physical, engineering, biological and biomedical, chemical, earth, economics, etc. nature. The so-called "Special Functions of Fractional Calculus" (SF of FC) provide an important tool of FC: In particular, they are often used to represent the solutions of the fractional differential equations in explicit form. Among the most prominent representatives of the SF of FC are the Wright generalized hypergeometric function ${}_{p}\Psi_{q}$, the more general Fox *H*-function, and the Inayat-Hussain \bar{H} -function. The classical special functions, among them the orthogonal polynomials and the ${}_{p}F_{q}$ -hypergeometric functions, can be represented as particular cases of the SF of FC.

In this survey talk, an overview of some properties and applications of an important class of SF of FC, introduced for the first time in our works, is given. For an integer m > 1 and the arbitrary real (or complex) indices $\rho_1, \ldots, \rho_m > 0$ and μ_1, \ldots, μ_m , the *multi-index (vector-index) Mittag-Leffler functions* are defined by:

$$E_{(1/\rho_i),(\mu_i)}(z) := E_{(1/\rho_i),(\mu_i)}^{(m)}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu_1 + \frac{k}{\rho_1}) \dots \Gamma(\mu_m + \frac{k}{\rho_m})} = {}_1 \Psi_m \begin{bmatrix} (1,1) \\ (\mu_1, 1/\rho_i)_1^m \\ \vdots z \end{bmatrix} .$$
(1)

The studies on these SF of FC were initialized in the monographs [1] and [2] and continued in a series of our papers till nowadays, some of them in collaboration with other colleagues from the family of the FC Analysts.

In the simplest case m = 1, the function (1) is reduced to the classical Mittag-Leffler (ML) function that is widely recognized nowadays as the Queen-function of FC. Other important particular cases of (1) are: the Wright function, the Bessel-Maitland, the Wright-Lommel, the Struve, the Lommel and the Airy functions, the Rabotnov and the Mainardi functions, the Lorenzo-Hartley R-function, the Dzhrbashjan function (ML function with 4 parameters, or function (1) for m = 2), the Delerue hyper-Bessel functions, etc. A lot of results connected with these and other special cases of (1) have been published recently in the journal [3].

In the talk, we survey some results on the analytical properties of the multi-index ML functions and their applications including a variety of their relations to the operational calculus and to the integral transforms, their asymptotics, distribution of their zeros, and some new integral and differential representations. The method used to derive many of these relations is based on the *H*-functions and the Generalized Fractional Calculus (GFC)-techniques. The functions (1) can be interpreted as the generating functions for a class of the Gelfond-Leontiev operators of the generalized integration and differentiation that are particular cases of the so-called multiple Erdélyi-Kober (EK) operators. Moreover, they are related to a Laplace type integral transform called the multiindex Borel-Dzhrbashjan transform, too. It can be shown that all SF of FC (in the sense of $_p\Psi_q$) can be represented in the form of the GFC operators acting on the three basic elementary functions and this fact suggests an unified approach to their classification into three classes. In particular, the multi-index ML functions (1) fall into the class of the trigonometric and the Bessel-type functions and can thus be seen as "fractional indices" analogues of the Delerue hyper-Bessel functions serving as solutions to differential equations of fractional multi-order $(1/\rho_1, 1/\rho_2, \ldots, 1/\rho_m)$.

Along with the analytical results for the functions (1), some examples of their applications in solving IVPs for the fractional differentiation equations with the multiple EK operators and in determining of the scale-invariant solutions of some partial differential equations of fractional order including the fractional diffusion-wave equation are presented.

Among the open problems we would like to attract the attention of the other researchers to, are the developments of reliable algorithms and computational procedures for evaluation of the functions (1) and other SF of FC. Some first results in this direction have been already obtained for the ML and the Wright functions, but the general problem is still waiting for its solution.

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Numerical Solution of Black-Scholes Equations with Non-differentiable Nonlinearities

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In this study we are concentrated with numerical solution of new Black-Scholes equations with the effect of transaction cost. Numerical algorithms based on the classical Newton method and the quasi-Newton method for nonlinear equations with nondifferentiable operators are developed. Numerical experiments are discussed.

Finite Difference Schemes for Multidimensional Boussinesq Equation

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We consider the Cauchy problem for the nonlinear Boussinesq equation

$$\begin{aligned} \frac{\partial 2u}{\partial u^2} &= \Delta u + \beta_1 \Delta \frac{\partial^2 u}{\partial t^2} - \beta_2 \Delta^2 u + \alpha \Delta f(u), \quad x \in \mathbb{R}^d, \quad t > 0, \\ u(x,0) &= u_0(x), \qquad \frac{\partial u}{\partial t}(x,0) = u_1(x), \end{aligned}$$

where α , β_1 , β_2 are positive constants and the solution u additionally satisfies the asymptotic boundary conditions $u(x,t) \to 0$, $\Delta u(x,t) \to 0$ as $|x| \to \infty$. Typically, the nonlinear term is $f(u) = u^2$.

For the numerical solution of this equation families of *conservative finite difference schemes* are constructed and studied theoretically.

Depending on the way the nonlinear term f(u) is approximated, we develop iterative and noniterative schemes, which are second order accurate in space and time. Our numerical experiments show clear advantage of the non-iterative schemes in precision and speed.

The schemes are implemented in fast, memory efficient and numerically stable methods. The extensive numerical experiments show good precision in real time computations and full agreement between the theoretical results and practical evaluation for single soliton and the interaction between two solitons.

Material Phase Causality or a Dynamics-statistical Interpretation of Quantum Mechanics

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Theoretical and experimental evidences of existence of a causal relation between the phase of the wave function and the dynamics of the quantum system are presented systematically for the first time. Theoretical arguments of spacial and general types are discussed in details. The special arguments arise from the study of the internal phase dynamics of a quantum system subject to interaction with an electromagnetic filed in presence of non-adiabatic factors that include amplitude and phase field time derivatives and dumping from the environment. Exact correspondence between the material phase behavior and the involved physical processes is found. General theoretical arguments for the relation between the phase of the wave function and the physical reality are presented based on the hydrodynamics presentation of quantum mechanics. Experimental evidences of observable dependence of the physical processes from the material phase are also discussed. Summarizing the theoretical and experimental arguments, a new dynamics-statistical interpretation of the quantum mechanics is proposed for the first time. A particle-wave duality picture incorporated in the wave function through its phase and amplitude is considered.

Application of the Fröbenius Method to the Schrödinger Equation

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The power series method is adapted to compute the spectrum of the radial Schrödinger equation $\left[-\frac{1}{2r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{2r^2} + V(r)\right]u(r) = Eu(r)$. Considering two ways of imposing the boundary condition at r = R, namely u(R) = 0 or $\frac{du(r)}{dr}|_{r=R} = 0$, we determine the lower and upper bounds for the eigenvalues as zeros of the calculable functions. This may be performed to arbitrary accuracy, since both functions are given by polynomials. For increasing R, the exact bound-state energy is approached from both sides monotonically. The generalization to the case of several coupled equations will be discussed and a few case studies will be presented for illustration.

Supercomputer Simulation of Radio-Frequency Hepatic Tumor Ablation

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The talk is in the field of large-scale computing in bio-medical engineering. A 3D voxel approach is used for finite element method (FEM) approximation of the involved partial differential equations. The discrete problem has hundreds of millions of degrees of freedom. The implementation of the computer model is done on supercomputer IBM Blue Gene/P.

We simulate the thermal and electrical processes, involved in the radio-frequency (RF) ablation procedure. RF ablation is a low invasive technique for the treatment of hepatic tumors, utilizing AC current to destroy the tumor cells by heating. The destruction of the cells occurs at temperatures of 45-50°C. The procedure is relatively safe, as it does not require open surgery. The surgeon places a RF probe inside the tumor and initiates RF current on it.

The mathematical model consists of two parts – electrical and thermal. The energy from the applied AC voltage is determined first, by solving the Laplace equation to find the potential distribution. After that, the electric field intensity and the current density are directly calculated. Finally, the heat transfer equation is solved to determine the temperature distribution. Heat loss due to blood perfusion is also accounted for.

The representation of the computational domain is based on a voxel mesh. Linear FEM in space is used for both partial differential equations. After the space discretization, the backward Euler scheme is used for the time stepping.

A parallel preconditioned conjugate gradient solver is used for the arising linear systems. As a preconditioner, we use BoomerAMG – a parallel algebraic multigrid implementation from the package Hypre, developed in LLNL, Livermore.

Parallel numerical tests run on the IBM Blue Gene/P massively parallel computer are presented. Some scalability issues are discussed.

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Ionization-free Filamentation in Gases

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The observation of plasma-free filamentation leads to challenge the role of plasma in laser filamentation. Up to now, no other process challenging plasma as the main defocusing process balancing the Ker self-focusing. We suggest here hew mechanism of filamentation on base of THz oscillation of the nonlinear refractive index in the femtosecond region. This oscillation is due to including of the offset frequency in the model. The equation obtained admits 3D+1 soliton solution.

Determination of Resonances by the Optimized Spectral Approach

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Spectral approach consists in representing a trial solution of the differential equation as a linear combinations of the basis functions. Under the name of the Rayleigh-Ritz, the procedure is popularly used in determining bound-state solutions of quantum-mechanical Schrödinger problems. Several ways of extending this approach to the determination of resonance states have been considered in the literature. Here we propose the application of the optimized Rayleigh-Ritz method to this end. The method consists in introducing nonlinear parameters into the basis functions and fixing their values so as to make the trace of the variational matrix stationary. We show that the optimized Rayleigh-Ritz scheme with complex parameters provides an effective algorithm for the determination of resonance energies and widths for particles trapped in various potentials. The obtained convergence rate compares favorably to other approaches.

Friction-induced Resonance of a Noisy Fractional Oscillator

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Mathematical models with fractional-order derivatives provide an excellent instrument for describing the memory and hereditary properties of various viscoelastic materials and processes. Thus motivated, the influence of the friction coefficient on the long-time behavior of the spectral amplification and the signal-to-noise ratio (SNR) for the output signal of a fractional oscillator with fluctuating eigenfrequency subjected to a periodic force is considered. The influence of the fluctuating environment is modeled by a multiplicative white noise and by an additive noise with a zero mean. The viscoelastic type friction kernel with memory is assumed as a power-law function of time. On the basis of exact formulas it is demonstrated that interplay of multiplicative noise and sufficient conditions for such a resonance of SNR versus the friction coefficient. The necessary and sufficient conditions for such a resonance effect are also discussed. Particularly, it is shown, that resonance-like behavior of SNR versus friction coefficient is qualitatively different in the cases of external and internal additive noise. The advantage of the effect of friction-induced resonance is that the control parameter is the damping coefficient, which can easily be varied in possible experiments as well as potential technological applications, e.g., in electric oscillator devices with circuit elements of a fractional type (i.e., tree or chain fractances).

The Wright Function: Its Properties, Applications, and Numerical Evaluation

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In this paper, some important elements of the theory of the Wright function ϕ defined by

$$\phi(\rho,\beta;z) := \sum_{k=0}^{\infty} \frac{z^k}{k! \Gamma(\beta + \rho k)}, \ \rho > -1, \ \beta \in \mathbb{R}, \ z \in \mathbb{C},$$

 Γ being the well-known Euler Gamma-function are first discussed. In particular, its representations through the other special functions of the hypergeometric type, different integral representations, and its asymptotical behavior are considered.

The Wright function – along with the Mittag–Leffler function – plays a prominent role in the theory of the partial differential equations of the fractional order that are actively used nowadays for modeling of many phenomena including, e.g., the anomalous diffusion processes or in the theory of the complex systems. This function appears there both as a Green function in the initial-value problems for the model linear equations with the constant coefficients and as a special solution invariant under the groups of the scaling transformations of the fractional differential equations. In this paper, both of these applications are shortly introduced.

Whereas the analytical theory of the Wright function is already more or less well developed, its numerical evaluation is still an area of the active research. In this paper, the numerical evaluation of the Wright function is discussed with a focus on the case of the real axis that is very important for applications. In particular, several approaches are presented including the method of series summation, integral representations, and asymptotical expansions. In different parts of the complex plane different numerical techniques are employed. In each case, the estimates for accuracy of the computations are provided. An implementation of the algorithms in the pseudo-code is included, too. The presentation is accompanied by a number of plots and pictures obtained with the algorithms discussed in this paper.

The ideas and techniques employed in this paper can be used with some small modifications for the numerical evaluation of other functions of the hypergeometric type.

Well-balanced Component-wise Scheme for Shallow Water System

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We present a high resolution scheme for approximating the solution of shallow water flows with non-flat bottom. The main difficulties in driving a convergent scheme can be due to solutions that vanish in nontrivial parts of domain or problematic for near steady states. The basic methodology is to avoid characteristic decompositions in spatial discretization and using a local hydrostatic reconstruction to derive a Component-wise well-balanced scheme.

Fractional Calculus Models for the Anomalous Diffusion Processes and Their Analysis

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In this invited lecture, the anomalous diffusion processes are modeled in terms of the partial differential equations of the fractional order that are then discussed in details. Anomalous diffusion can be characterized by the property that it no longer follows the Gaussian statistics and in particular one observes a deviation from the linear time dependence of the mean squared displacement. This is the case for many different phenomena including e.g. the translocation dynamics of a polymer chain through a nanopore, charge carrier transport in amorphous semiconductors, laser cooling in quantum optical systems to mention only few of them. In this lecture, we consider the case of the anomalous diffusion that shows a power-low growth of the mean squared displacement in time.

The starting point is a stochastic formulation of the model in terms of the random walk processes. Following this line, the continuous time random walk models that are mathematically expressed as a system of the integral equations of the convolution type for the corresponding probability density functions are introduced. These so called master equations can be explicitly solved in the Fourier-Laplace domain. The time- and space-fractional differential equations are then derived asymptotically from the master equations for the special classes of the probability density functions with the infinite first or second moments.

For the obtained model equations and their generalizations both the initial-value problems in the unbounded domains and the boundary-value problems in the bounded domains are discussed. A special focus is on the initial-boundary-value problems for the generalized time-fractional diffusion equation. For this equation, the maximum principle well-known for the elliptic and parabolic type PDEs is presented and applied both for the a priori estimates of the solution and for the proof of its uniqueness.

Mathematical Modeling of Magnetic Jets Acceleration Processes

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Mathematical modeling of space plasma acceleration in the vicinity of accretion disk leading to formation of subluminal jets in active galaxy nuclei and close stellar systems is one of the most complicated and theoretically important problems. The mechanism of acceleration including hydrodynamic, magnetohydrodynamic and radiative transfer models is being widely discussed for a long time but every model gives explanation only for a part of effects observed.

An 2D axial symmetric MHD model for the formation of a jet in the vicinity of a compact object surrounded by a thin accretion disk with a supersonic accretion regime is constructed, assuming that the plasma is perfectly electrically conducting and taking into account central compact body gravitation. Problem-oriented numerical code based on separative physical processes computation using unstructured triangular meshes is developed. The code uses natural approximation for both gas and magnetic parts of MHD equations system. The source of jet matter is described using boundary conditions.

A stable collimated jet of plasma along the z-axis symmetric about the plane of the accretion disk is obtained. The source of jet energy in the model is gravitational energy of central object. The jet is collimated by magnetized funnel which has form of Laval nozzle, flow parameters are continuous and smooth inside funnel. The funnel has optically thick hot unmagnetized walls. The parameters of the outflow are in good agreement with available observational data on the structure and properties of jets.

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Feigenbaum-Sharkovskii-Magnitskii Scenario of Transition to Turbulence in the Rayleigh-Benard Convection

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The problem of turbulence arose more than hundred years ago to explain the nature of chaotic motion of the nonlinear continuous medium and to find ways for its description; so far it remains one of the most attractive and challenging problems of classical physics. This problem is named by Clay Mathematics Institute as one of seven millennium mathematical problems [1] and it is also in the list of 18 most significant mathematical problems of XXI century formulated by S.Smale [2].

During several last years the universal unified transition mechanism of space-time chaos in nonlinear partial differential equations was theoretically and experimentally proven in number of papers of the author [3-6, etc.]. The mechanism is developing by FSM (Feigenbaum-Sharkovskii-Magnitskii) scenario through subharmonic bifurcation cascade of stable cycles or stable two dimens-ional tori. The purpose of this paper is to show that the universal FSM scenario is developing also in viscous incompressible 3D fluid motion in Rayleigh-Benard convection in transition from laminar to turbulent regimes. The analysis indicated that in different test series laminar-turbulent transition follows either the subharmonic bifurcation cascade of two- dimensional tori or the subharmonic bifurcation cascade of limit cycles. Cycles up to the third period were found in the system that indicated the end of the Sharkovskii cascade. Thus, it seems reasonable, that there is no unified laminar-turbulent transition scenario, but all scenarios lay in the frameworks of the FSM-theory.

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Simulations of Digital Communication Devices on Multicore Systems

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The purpose of this talk is to describe our experience in simulating digital communication systems in order to compare their performance when various methods for channel coding and modulation are implemented. Software simulations of digital communication systems are computationally intensive and run slow. They have to be performed for numerous values of signal-to-noise ratio, for various types of noise, and for very long input sequences. We have simulated communications trough AGWN and Rayleigh noisy channels and compare the combination of integer coded modulation and OFDM with the combination of trellis coded modulation and OFDM.

Computer simulation of a digital communication device possesses natural parallelism. The work of the different blocks can be carried out by different CPUs. Some of operations, (e.g., OFDM) are better performed by GPUs. We carried out the simulations on a multicore system as well as on a computational grid.

Parallel Numerical Simulations of Water Reservoirs

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The study of the water flow and scalar transport in water reservoirs is important for the determination of the water quality during the initial stages of the reservoir filling and during the life of the reservoir. For this scope, a parallel 2D finite element code for solving the incompressible Navier-Stokes equations coupled with scalar transport was implemented using the message-passing programming model, in order to perform simulations of hidropower water reservoirs in a computer cluster environment. The spatial discretization is based on the MINI element that satisfies the Babuska-Brezzi (BB) condition, which provides sufficient conditions for a stable mixed formulation. All the distributed data structures needed in the different stages of the code, such as preprocessing, solving and post processing, were implemented using the PETSc library. The resulting linear systems were solved using the projection method implemented by an approximate block LU factorization. In order to increase the parallel performance in the solution of the linear systems, we employ the static condensation method for solving the intermediate velocity at the vertex and centroid nodes separately. We compare performance results of the static condensation method with the approach of solving the complete system. In our tests the static condensation method shows better performance for large problems, at the cost of an increased memory usage. Performance results for other intensive parts of the code obtained in a computer cluster are also presented.

Total Robustness of Nonconforming Finite Element Methods

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The talk is in the field of large-scale scientific computing. The considered ill conditioned problems are described by partial differential equations (PDEs) with small parameters. The finite element method (FEM) is used for discretization. The total robustness means: a) robust finite element approximation; and b) robust solution of the arising FEM linear algebraic systems.

It is well known that the standard (conforming) finite elements don't provide stable approximation for certain ill conditioned problems. Here we consider the Crouzeix-Raviart (C-R) nonconforming elements as an alternative in such cases. The robustness of the C-R elements for elliptic problems in strongly heterogeneous media is explained by their equivalence to the mixed FEM discretization with lowest order Raviart-Thomas elements. We present also robust applications of C-R FEM for the following two strongly coupled ill conditioned PDEs: a) the Lame system of linear elasticity in the case of almost incompressible materials; and b) the time dependent equations of Navier-Stokes in the case of large Reynolds number.

The second part of the talk deals with the robustness of multilevel iterative solvers for the linear systems arising from the above described nonconforming FEM discretizations. The presented results are in the spirit of optimal order Algebraic MultiLevel Iteration (AMLI) methods (see, e.g., [1]). The theory of the AMLI methods is based on hierarchical decomposition of the FEM spaces where the constant in the strengthened Cauchy-Bunyakowski-Schwarz (CBS) inequality takes a particular role. Uniform estimates of the CBS constant are shown for the corresponding elliptic and parabolic problems. In addition to the problem related small parameters, the AMLI methods are robust with respect to mesh anisotropy.

The theoretical results are illustrated by a rich set of numerical tests.

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Biomathematics and Interval Analysis: A Prosperous Marriage

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- 1. Interval analysis briefly reviewed: Intervals and operations over intervals; interval arithmetic as a rigorous algebraic system; various aspects on interval arithmetic; interval arithmetic and interval analysis; main purpose of interval analysis; reliable/scientific computations; basic applications of interval analysis; the IEEE standartization of interval arithmetic.
- 2. Biomathematics: basic dynamical models and related mathematical problems. Case studies from population dynamics and enzyme kinetics. Parameter identification and model validation.
- **3.** Why interval analysis is an useful tool for modeling in biology:
 - i) uncertain (interval) data;
 - ii) (numerically) sensitive dynamical problems;
 - iii) need of model validation.
- 4. (if time allows) Brief history and references.

Cubic Convergence for Nonlinear Differential Equations with Initial Time Difference

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In this paper we have extended the method of generalized quasilinearization to nonlinear differential equations with initial time difference. Using natural lower and upper solutions under suitable conditions we obtained two sequences which converge uniformly and monotonically to the unique solution of the nonlinear differential equations with initial time difference. Furthermore, we prove that the rate of convergence is cubic.

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A new direction-splitting-based fractional time stepping for solving the incompressible Navier-Stokes equations will be discussed. The main originality of the method is that the pressure correction is computed by solving a sequence of one one-dimensional elliptic problem in each spatial direction. The method is unconditionally stable, very simple to implement in parallel, very fast, and has exactly the same convergence properties as the Poisson-based pressure-correction technique, either in standard or rotational form. The one-dimensional problems are discretized using central difference schemes which yield tri-diagonal systems. However, other more accurate discretizations can be applied as well. The method is validated on the lid-driven cavity problem showing an excellent parallel efficiency on up to 1024 processors.

Gauge and Rigid Symmetries of Light-cone Yang-Mills Classical Mechanics

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The Hamiltonian dynamics and symmetries of the light-cone version of SU(2) Yang-Mills classical mechanics, which originates from the light-cone version of the corresponding field theory under the supposition of the gauge potential dependence on light-cone time alone, is considered. According to the Generalized Hamiltonian formulation the light-cone model possesses a mixed system of first and second class constraints in contrast to its conventional counterpart, the instant form Yang- Mills classical mechanics. After a separation of the constraints of the model into sets of first and second-class constraints the generator of gauge symmetry group is constructed. It is found that the algebra of gauge symmetry is isomorphic to $su(2) \bigotimes u(1) \bigotimes u(1)$. The relation between the gauge and $SL(2,\mathbb{R})$ dynamical symmetry group of the light-cone SU(2) Yang-Mills classical mechanics is discussed.

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Some Explicit Solutions of the Shape Equation

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The consideration of the variational problem for the minimization of the bending energy of membrane surfaces under some natural geometric constraints leads to the so called general shape equation. The available analytical solutions of this equation including a new one are reviewed in some detail.

Rotating Black Ring on Kaluza-Klein Bubbles

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Using solitonic techniques we construct a new exact stationary axisymmetric solution to the 5D Einstein equations in vacuum in asymptotically Kaluza-Klein spacetime. The solution describes rotating black ring with a single angular momentum surrounded by two Kaluza-Klein bubbles. It is generated by applying a 2-soliton Bäcklund transformation on a static seed. The solution generation method is presented, the solution properties are discussed, and its physical characteristics, such as mass, tension, angular velocity and angular momentum, are derived.

Shallow Water Model Which Admits the Propagation of Shocks over a Dry Bed

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The equations of the first approximation of shallow water theory are widely used to model the propagation of hydraulic bores generated by total or partial dam breaks or by the impact of large sea tsunami-type waves on shallow beaches. The theory describes such bores as steady discontinuous solutions, which we will name shocks. However, the classical system of the basic shallow water conservation laws (which consist of the conservation laws of mass and total momentum) while correctly describing the parameters of hydraulic bores propagating in a fluid of finite depth, does not admit shock propagation over a dry bed. Exact solutions describing dry-bed water flows governed by this system, for example, solution of a dam break problem with a dry bed in the tail water, are continuous depression waves. At the same time, numerous laboratory experiments have shown that wave front velocity in continuous solutions is considerably overestimated and the wave front profile noticeably distorted. Experiments have shown that the wave fronts propagating over a dry bed are much steeper and exhibit breakdowns characteristic of hydraulic bores.

In the present work, a method for modeling the propagation of discontinuous waves over a dry bed using the first approximation of shallow water theory is proposed. The method is based on a modified conservation law of total momentum that takes into account the concentrated momentum losses due to the formation of local turbulent vortex structures in the fluid surface layer at a discontinuous-wave front. A quantitative estimate of these losses is obtained by deriving the shallow water equations from the Navier-Stokes equations with allowance for viscosity, which has a rapidly increasing effect in the turbulent flow regions described by discontinuous waves. As an example, a comparative analysis is performed of the solutions of the dam-break problem obtained for the classical and modified shallow water models.

A generalization of modified shallow water model for two dimensional case with variable bottom height is proposed. It is presented the numerical results obtained for the propagation over a dry bed of two dimensional shock caused by a partial dam break in a channel with variable bottom in the lower pool.

Convergence of Series in Mittag-Leffler Type Functions

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The Mittag-Leffler (M-L) functions are natural extensions of the exponential function and trigonometric functions like cos-function. Their basic properties are described yet in the Bateman Project "Higher Transcendental Functions" (Vol. 3), in a chapter devoted to "miscellaneous functions." The functions have been studied in details by Dzrbashjan [1]. The detailed properties of these functions can be found in the contemporary monographs [3], [4], [7]. The same functions, considered also in [5] and [8], are called M-L functions of vector index. Recently a class of special functions of M-L type, that are multi-index ana- logues of M-L functions, has been introduced and studied (see, e.g., [4]). Explicit solutions of some kinds of fractional order (or multi-order) differential and integral equations involving Erdelyi-Kober (E-K) operators are representable by means of series in M-L type functions like those considered in this work. Their domains of convergence are found. The series behaviour are studied on the boundary of these domains. Cauchy-Hadamard, Abel, Tauber and Littlewood type theorems for such series are given. Asymptotic formulae for "large" values of indices of these functions are also provided, used in the proofs of the convergence theorems for the considered series. In our previous papers [6] we studied series in systems of some representatives of special functions of fractional calculus (SF of FC) which are fractional indices analogues of the Bessel functions and also multi-index M-L functions (in the sense of Kiryakova |4|).

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2D Regimes of Non-Fourier Convection in a Rectangular Cavity

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In this work, we investigate the 2D flow in a rectangular cavity subject to both vertical and horizontal temperature gradients. The linearized model is studied and the effect of the relaxation of the heat flux in the law of heat conduction is examined. Two different implementations of the relaxation term are considered: a local time derivative (the so-called Maxwell-Cattaneo law), and a frame indifferent (Oldroyd) objective time rate. To this end, two spectral numerical models are created based on a Galerkin expansion. The basis is the cartesian product of systems of beam functions and trigonometric functions. Beam functions are used in the direction across the slot so that four boundary conditions are satisfied. Respectively, trigonometric functions are used in the vertical direction satisfying the periodic conditions.

The natural modes of the system are derived for both the Fourier and Non-Fourier models. The results are compared to the works of Bergholz and Elder for the plain Fourier law. The inclusion of an additional time derivative brings one more family of eigen-values. Our computations show that for the plain Maxwell-Cattaneo law, some of the modes of the new family have positive real parts, which means that the convective flow is unstable. For the same set of parameters, the frame-indifferent law exhibits only stable modes which are quantitatively different from the Fourier. The modes of heat conduction with relaxation of the flux decay slower than their purely Fourier counterparts, but their frequencies are higher. The new family of eigenvalues are strictly negative and correspond to rapidly decaying transients.

The present results seem to confirm the assertion that for fluids, the Maxwell-Cattaneo law without frame indifferent additions, leads to paradoxical results.

Mathematical Models and Distribution of the Zeros of the Duffing Equation and More General Equations

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Here we investigate the oscillation behavior of the equation:

$$\ddot{x}(t) + \delta \dot{x}(t) + \sum_{k=1}^{n} \beta_k (x(t - \sigma_k), t) + G(\ddot{x}(t), \dot{x}(t), x(t)) = f(t),$$

generalizing two recent results of Petrova. The Duffing equation is:

$$\ddot{x}(t) + \delta \dot{x}(t) + \alpha x(t) + \beta x^3(t) = f(t)$$

The common assumptions are that $\alpha > 0$, $\beta > 0$ and $\delta \in \mathbf{R}$ are constants and $f(t) \in C([T, \infty); \mathbf{R})$, T is a large enough constant. Also, in the general case we suppose that all the delays $\{\sigma_k\}_{k=1}^n$ are nonnegative constants as well as that $G(\ddot{x}(t), \dot{x}(t), x(t)) \in C(\mathbf{R}^3; \mathbf{R})$ and $\beta_k(x(t - \sigma_k), t) \in C(\mathbf{R}; \mathbf{R})$, $\forall k = 1 - n$, $n \in \mathbf{N}$.

Further, we make several approaches, concerned with the mathematical intuition based on the distribution of the zeros of wide classes of second order ordinary differential equations. The first one treats the bifurcation theory. The second one is connected with proper numerical methods.

Keywords: oscillation, the Duffing equation, limit cycle, numerical methods

A Distributional Investigation of Progressive Differential Operators

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The application of distributional techniques in a Schwartz-Sobolev space setting to the progressive differential operators are presented. The investigation starts with the standard (gradient, divergence, curl, Laplacian; time derivative) operators followed by the progressive (convective and Oldroyd derivatives) differential operators acting on the regular and singular components of a distribution. The regular components of a Schwartz-Sobolev distributions are described in the space of locally integrable functions in the Lebesgue sense, whereas the singular components are assumed to be constructed via the Dirac delta distributions of arbitrary order concentrated on a point, a regular surface and a regular space curve, respectively. By extending the definition of the standard spatial vector operators from the space of continuous functions to the space of distributions, their action on a field quantity in the Lebesgue space are described in a concise manner through a set of nine "generalized vector operators" first defined and used by Remus Rădulet in 1955 in his undergraduate textbook available only in Romanian language. We also provide commutative relations between the standard and progressive differential operators, which are the basic tools in construction of field theories based on material invariance (or frame indifference) principle.

Use of the Vector Finite Element Method for the Solution of Electromagnetic Problems

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The vector finite element method is formulated for the solution of time-harmonic Maxwell equations as applied to a wide range of electromagnetic problems including microwave circuits, high-frequency electronic packaging, scattering from various targets, and antenna radiation problems. A number of computational challenges often appear during the formulation of these problems ranging from proper excitation of the input/output ports to an accurate and effective truncation of the unbounded infinite space. A generalized eigenvalue problem is formulated at each of the ports in order to obtain the governing dispersive propagation characteristics and modes of the two-dimensional structure; these modal characteristics are subsequently used to properly excite/terminate the input and output ports of the three-dimensional structure. In the case of scattering or radiation problems, the unbounded infinite domain is properly truncated using first/second/higher-order absorbing boundary conditions, a perfectly matched layer, or an exact radiation condition based on a boundary-integral method. Numerical results on a number of practical engineering applications illustrate the power and effectiveness of the vector finite element method in solving complex electromagnetic problems.

A Splitting Scheme for Solving Reaction-Diffusion Equations Modeling Dislocation Dynamics in Material Subjected to Cyclic Loading

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Strain localization and dislocation pattern formation are typical features of plastic deformation in metals and alloys. Glide and climb dislocation motion along with accompanying production/annihilation processes of dislocations lead to the occurrence of of instabilities of initially uniform dislocation distributions. These instabilities result into the development of various types of dislocation microstructures, such as dislocation cells, slip and kink bands, persistent slip bands, labyrinth structures, etc., depending on the externally applied loading and the intrinsic lattice constraints. The Walgraef-Aifantis (WA) model is an example of a reaction-diffusion model of coupled nonlinear equations which describe microstructure formation of forest (immobile) and gliding (mobile) dislocation densities in the presence of cyclic loading. This paper briefly discusses two versions of the WA model and focus on a finite differences, second order in time Cranck-Nicholson semi-implicit scheme, with internal iterations at each time step, for solving the model evolution equations in two dimensions.

Partial L^1 Monge-Kantorovich Problem

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We consider the Monge-Kantorovich problem with transportation cost equal to distance and a relaxed mass balance condition: instead of optimally transporting one given distribution of mass onto another with the same total mass, only a given amount of mass, m, has to be optimally transported.

In this partial problem the given distributions are allowed to have different total masses and m should not exceed the least of them. We derive and analyze a variational formulation of the arising free boundary problem in optimal transportation [1]. Furthermore, we introduce and analyze the finite element approximation of this formulation using the lowest order Raviart-Thomas element. Finally, we present some numerical experiments where approximations to both the optimal transportation domains and the optimal transport between them are computed.

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Mathematical Models in Dynamics of Incompressible Viscoelastic Media

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A consistent model of incompressible viscoelastic Maxwell media is formulated. It corresponds to the choice of Jaumann rotational derivative in rheological relation. The determining system of equations has both real and complex characteristics. For this system, a solvability of initial-boundary value problem in the class of analytic functions is established, for its linearized variant the solvability was shown in the class of functions of finite smoothness. It was shown that the absence of short-wave instability was provided by smallness of non-diagonal terms of stress tensor. A wide class of exact solutions to motion of incompressible viscoelastic Maxwell medium is found. These solutions are partially invariant with respect to some subgroup of extended Galilei group which is admitted by equations of motion and their generalizations. With the help of obtained solutions there was described a deformation of viscoelastic strip with free boundaries, which moves either inertial or under the action of stretching or compressing longitudinal stresses, as well as shear stresses, applied to the free surface. A problem on spherical cavity filling in incompressible Maxwell medium under the action of constant pressure at infinity was considered. This is generalization of the classic problem for viscous incompressible liquid. In both cases cavity always converges to a point in a finite or infinite time. In case the surface tension differs from zero, the collapse happens in a finite time. Depending on the three dimensionless parameters (Reynolds number, capillary number and dimensionless relaxation time) both oscillatory and monotonic regimes of motion are possible. When the cavity radius becomes small, oscillations stop.

There was also considered a problem on spherical cavity filling in incompressible viscoelastic Kelvin-Voigt medium under action of constant pressure at infinity. On the contrary to similar problem for Maxwell medium, here both the cavity collapse and stabilization of its radius to a positive value with time are possible. It was shown that finiteness of deformations leads to new qualitative effects. There were revealed three different modes of boundary behavior, two of which stand for monotonous and oscillatory regimes of limit cavity radius achieving, while the third one stands for cavity collapse in a finite time.

Classical Couette problem analogues of incompressible viscoelastic Kelvin-Voigt and Maxwell media motion in the gap between two coaxial cylinders are investigated. External cylinder is fixed, while the internal one is either forcibly rotating with a constant velocity or inertially rotating. There was found analogy between propagation of acoustic cylindrical waves in viscous gas and transversal waves in Kelvin-Voigt medium which appear during its motion along circular trajectories. Asymptotes of solution stabilization to Couette motion in the first problem and inertial cylinder motion approaching to equilibrium state were studied. In the second problem for Maxwell motion there are also studied limit regimes of rotation retardation. In comparison to Kelvin-Voigt medium where both monotonous and oscillatory regimes of rest state approaching are possible, for Maxwell medium the velocity of rotation with time tends to zero in oscillatory regime.

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The Concepts of Polynomial Orthogonality and Their Applications

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Since the orthogonal polynomials have a lot of applications in mathematics (theory of special functions, fractional calculus, spectral operators, probability, analytic numbers and approximations) and other sciences (physics, mechanics, electrotechnics), they appeared numerous extensions of the concept of the standard orthogonality. We will discuss the concepts of quasi, almost and multiple orthogonality comparing their similarities and differences in: recurrence relations, differential properties, generating functions, Rodrigues formulas and zeros. As some of their most important applications, we will consider quadratures and approximations of functions. Especially, we will discuss almost orthogonal polynomials which are less known, but very useful in modeling of electronic systems which generate orthonormal basis. They are very suitable for analysis and synthesis of imperfect technical systems which are projected to generate orthogonal polynomials, but in the reality generate almost orthogonal polynomials.

As a next step, we plan to consider the relations of these new orthogonality's concepts to the operators of the fractional calculus, based on fractional order generalizations of the Rodrigues differential (or differintegral) formulas for the classical orthogonal polynomials.

Mathematics Subject Classification (MSC 2010): 33C45, 42C05, 26A33, 94A11.

Key words and phrases: Polynomials, Orthogonality (Regular, Quasi, Almost, Multiple), Quadrature, Approximation.

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Solution for the Mathematical Modeling of Population Growth by Spectral Methods

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Most populations of organisms tend to increase as far as their environment will allow. As a result, most populations are in a dynamic state of equilibrium. Their numbers increase in a delicate balance that is influenced by limiting factors. The Volterra model for population growth of a species within a closed system is given in terms of an integro-differential equation.

In the present work, we introduce a new computational method for solving the Volterra population model. The integro-differential equation is first converted to an equivalent nonlinear ordinary differential equation. The method is based on spectral methods in which the solution for nonlinear ordinary differential equation is approximated by the Nth degree polynomial, using Legendre-Gauss-Lobatto points as the collocation points, and Lagrange polynomials as trial functions. Properties of Legendre pseudospectral method are presented. These properties are then utilized to reduce the computation of the Volterra's population model to system of algebraic equations. Numerical examples are included to demonstrate the applicability and the accuracy of the proposed method and a comparison is made with the existing results.

On the Kernel Dimension of Singular Integral Operators with Weighted Shifts

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Singular integral operators with shifts appear in the modeling of several types of applied problems. In view of this, knowledge about the solvability of equations characterized by such operators is welcome. In this talk, we will concentrate in extracting information about the kernel dimension of certain singular integral operators with weighted shifts. Namely, bounds for the kernel dimension of Fredholm singular integral operators with continuous coefficients and involving a preserving-orientation weighted Carleman shift will be obtained. To attain such a goal, it will be fundamental to construct different types of auxiliary operators (through equivalence operator relations) and to use known Fredholm criteria for these operators.

2D Control Problem and TVD-Particle Method for Water Treatment System

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Analysis of the environmental impact of waste water discharges into aquatic media takes a great importance in the last years. The problem considered here is in the field water-quality improvement by varying the systems, such as flow regulation by means of reservoirs. The criterion functional to be minimized penalizes deviation of fecal coliform distribution from standard value. We address approximate controllability problems for a parabolic equation (evolution of pollutant concentration) associated with Dirac measures. From a practical point of view, a regularized version of the problem is considered. The simulation of the transport and fate of compounds within biological systems are done by an hybrid numerical approach combining particle method and finite difference technique. Symmetric TVD scheme [1] for the shallow water equations is provided to minimize numerical diffusion. The technique is a composed method that uses a second order flux in smooth regions but involves some limiting based on the gradient of the solutions so that near discontinuities it reduces to the monotone upwind method. A particle method is proposed to handle the parabolic equation. The difficulty is then to deal with a diffusion term and boundary conditions. The approximation of the diffusion operator is based on the introduction of boundary integral equation formulation [2]. In the minimizing algorithm, the gradient of the cost function is evaluated by adjoint techniques and a gradient type method as an iterative solution of the discrete control problem is chosen. The major issue of the numerical part relies on illustrating by direct simulation the effectiveness of this methodology when applied to the control of water quality problem. Relative merits and advantages of this approach are explored. The purpose of this talk is to present recent results which generalize those obtained in [1], [2] in the 2D case.

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Surface Generation from a Non-structured Set of Vertices

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A number of methods exist for curve and surface generation from a number of data points (vertices). These data points are called "control points," and they define the shape of the curve or surface. This is the reason why they have in their name the word "control" – they control the shape of the resulting curve/surface.

Spline methods are the most popular methods for describing curves and surfaces. They are parametric functions, piecewise functions, and they have k - 1 parametric continuity along the borders of adjacent pieces, where k is the degree of the polynomials. There exist two methods for defining the shape of curved surfaces. These are *interpolation* and *approximation*. In the case of interpolation the resultant surface passes through the control vertices whereas in the case of approximation the surface passes "near" the control vertices, approximating their shape.

This paper describes a recursive midpoint subdivision Bezier Spline. The method is derived from a standard cubic Bezier spline. At each step, it constructs a new set of points with more vertices closer to each other than the original set of points, resulting in a smooth curve/surface. Some of the new points lie near the edges connecting original control points, and these are called new edge points. The points corresponding to old control points are called new vertex points. In the case of surfaces some new points lie in the middles of the squares of the original mesh, and are called new face points. The importance of this method is that it is generalized to generate surfaces with an arbitrary topology of control points.

HPC Applications from Earth Science on Grid Infrastructures

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During the last six years of the European funded project Enabling Grids for E-SciencE (EGEE) a wide range of applications was ported on to the EGEE Grid infrastructure. Simulation codes from the different domains of Earth Science range from embarrassingly parallel multi jobs, which map easily to a Grid infrastructure, to MPI or OpenMP parallelized codes exhibiting fine-grained parallelism. These different fundamental characteristics pose a challenge for the scientist deploying the application, and demand different techniques to reach a certain level of productivity. Other applications have hard requirements on data management, need connections to existing data bases or services and as such make up for a different challenge again. We will present a sample of the simulation codes and discuss some of the typical problems arising when they are deployed on clusters in a grid infrastructure like EGEE.

Modeling Interfacial Fracture

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The talk will give an introduction to some basic concepts in Fracture mechanics. Materials that are fractured, no matter how small the fracture, act much differently than the same material without cracks. So it is of utmost importance to be able to understand and predict the behavior of a crack. Fracture mechanics is an area in solid mechanics that tries to explain under what conditions a crack begins, and how it grows.

The analysis of several fracture models based on a new approach to modeling brittle fracture will be presented. The considered modeling approach incorporates important nanoscale effects near the fracture surfaces into a continuum modeling framework. I will discuss the effects of ascribing constant and curvature-dependent surface tension to the fracture surfaces.

In the case of the classical Griffith crack (a crack of finite length in a single linearly elastic material, subjected to far filed tensile loading) we show that the proposed model leads to a cusp-like crack opening profile at the crack tip, in contrast to the blunt profile predicted by the classical theory of brittle fracture. Moreover, such models yield bounded stresses and strains. In particular, they do not suffer from the internal inconsistencies, characteristic of Linear Elastic Fracture Mechanics (LEFM), which is based on the assumption of small stresses and strains, but predicts singular stresses and strains in a neighborhood of a crack tip.

Further, the problem of interface fracture will be discussed briefly. Within the studied modeling approach, it leads to a system of four coupled singular integral equations, with a Cauchy-type singularity, which can be reduced to a four by four system of Fredholm integral equations of the second kind. We will discuss the implications of ascribing surface excess properties to the bimaterial interfaces.

Some Spectral Problems of Porous Media Acoustics

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The current talk concerns problems of finding natural frequency spectrum of media consisting of two fast alternating phases with different mechanical properties (e.g. elastic frame with channels filled with compressible or incompressible viscous fluid, mixture of two liquids with various viscosities and compressibilities, etc.). In a quite a number of cases macroscopic models of such media (they are usually called homogenized or effective models) are models of materials with dynamics described by integro-differential equations with integral terms of convolution product by time coordinate type. In the talk (a) there are exact statements on proximity between solutions of original boundary problems for two-phase models and solutions of corresponding boundary problems for the above integro-differential equations. In addition, (b) various natural oscillations spectra qualitative properties for the mentioned homogenized models are analyzed. It is shown that homogenized problem spectrum consists of two parts: real and complex. Complex part is a union of two complex conjugated sequences of complex numbers where real parts have a limit and imaginary parts tend to infinity or have finite limits. Real part of investigated spectrum is a union of a finite or countable number of limited sequences (lying on non-overlapping intervals of the real axis), each having a limit. Under some conditions it is possible for some interval to contain continuous spectrum.

Here we are stating a hypothesis of existence of a general operator model, with use of witch it could be possible to prove the existence of spectra of described above structure in all cases.

The presented results are new and original.

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Unsteady State Gaseous Flow past a Square Confined in a Micro-channel

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Micro mechanical devices are rapidly emerging technology, where new potential applications are continuously being found. A simulation of internal and external gas flows in or around these devices is important for their design. The gas flows are characterized with areas of low speed flows (low Reynolds numbers). The flows can go from high speed supersonic to very low speed regimes down to the incompressible limit. This made the pressure based numerical methods very suitable to be used for calculation of this kind of gas flows. In this paper we present a short review of a finite volume method, developed by the authors, and demonstrate its application for calculation of some unsteady state gaseous flows. We study a flow past square-shaped particle confined in a micro-channel filled with a hard-sphere monatomic gas. The problem is solved using the finite volume method SIMPLE-TS (a modification of SIMPLE created by the authors). The flow motion is described on the basis of the Navier-Stokes-Fourier compressible equations with diffusion coefficients determined by the first approximation of the Chapman-Enskog theory for the low Knudsen numbers. First order velocity slip and temperature jump boundary conditions are used. The target of the research is to find the Knudsen number (corresponding Reynolds number) for which the microflow becomes unstable and some effects of flow separation and Karman vortices appear. The investigation is accomplished for subsonic (Mach number M=0.1) and supersonic (M=2.43) speeds, leading to different regimes of the gas microflow.

Fredholm Characterization of Systems of Equations of Wiener-Hopf and Hankel Type Containing Piecewise Almost Periodic Elements

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The talk will be devoted to the study of operators which characterize systems of certain equations of Wiener-Hopf and Hankel type having so-called Fourier matrix symbols in the algebra of piecewise almost periodic elements. A main part of the talk will be addressed to identify conditions for obtaining the Fredholm property of those operators. In addition, the Fredholm index will be discussed as well. The systems under study appear in different types of applications (e.g., in problems of wave diffraction by wedges).

On the Solvability of a Problem of Wave Diffraction by a Union of a Strip and a Half-Plane

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We will consider a mathematical analysis of a problem of wave diffraction by a union of a strip and a half-plane which is characterized by a boundary-transmission problem for the Helmholtz equation, having higher order boundary conditions. The problem will be analyzed in an operator theory viewpoint. In particular, it will be possible to describe when the operators associated with the initial problem enjoy the Fredholm property. This is done by constructing several operator extension relations between different types of convolution type operators. The initial problem is considered within a framework of Bessel potential spaces, and the obtained properties are valid for a set of regularity indices of these spaces.

3+1 Representation of Maxwell Equation on Riemannian Manifold

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3+1 representation of Maxwell equations on Riemannian manifold have been carefully obtained using geometrical methods including decomposition of differential forms and operators. Natural definitions of *rot* and *div* are recovered by the dimensional reduction of the duality operator and the external derivative. As a result the time derivative for the electric and magnetic fields is turns out to be a bit complicated. In addition our 3+1 representation is a generalization for the case of noninertial reference frames.

On Analogs of Number π in q-Calculus

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Since the number π is introduced like quotient of circle circumference and diameter it occupies attention of whole scientific world. In the last century, q-calculus was made like a complete analogy of standard calculus. In that manner, the corresponding functions and operators (regular and fractional too) were introduced. Recently, the sequences of well-known special numbers (Fibonacci, Stirling) were found. It is interesting that the number e is present from the very beginning, but none mentioned number π . We noticed only two recent trials by R. Dyaz and S. Suslov. In this paper we will suggest a few new possible definitions and discuss their advantages and lacks in order to find the optimal one.

Mathematics Subject Classification: 11A67, 33D05

Key Words: number sequences, q-calculus, π

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Determining the Form of the Short Rate Volatility Using the Approximate Formula for Pricing Zero-coupon Bonds

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We consider a well known class of one-factor interest rate models, where the short rate is driven by a mean-reverting process with a volatility proportional to a power of the short rate. The whole term structure of interest rates is obtained from the bond prices, which are solutions to a parabolic partial differential equation. Except for the special cases, its solution is not known in a closed form. In [1], the authors proposed an analytical approximation. We derive the order of accuracy of this approximation. Then we use it to find the dependence of the volatility on the interest rate from the real market data. We solve an optimization problem where we consider the differences between the real interest rates and those obtained from the model.

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Relation between the Parameters of a Gravitational Lens and the Frequencies of Black-hole Quasi-normal Modes

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The characteristic modes of oscillation of black holes – the quasi-normal modes – are extensively studied since they carry information about the physical properties of the black holes and there is hope that they can be measured in near future gravitational wave experiments. In the current report an alternative method for the measurement of the frequencies of the quasi-normal modes through observations in the electromagnetic sector is proposed based on a relation between two processes – emission of gravitational waves and gravitational lensing.

Direct Simulation Monte Carlo Algorithms for Simulation of Non-equilibrium Gas Flows

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The emergence of Micro-Electro-Mechanical-Systems (MEMS) as a key enabling technology has led to the development of an increasing number of gas-phase microfluidic systems. Potential applications are numerous and include miniaturized heat exchangers, portable gas chromatography systems, miniaturized gas sensors and novel high-throughput gas flow cytometers. However, one of the most important issues influencing MEMS research is the growing realization that microflows are dominated by non-continuum or rarefaction effects. In this view, it becomes obvious that most of the classical fluid dynamics problems must be reconsidered when applied to flows through micro-channels or more complex micro-systems. Since the characteristic length of MEMS/NEMS is comparable with the mean free path of the gas molecules, the traditional computational fluid dynamics (CFD) methods, based on the Euler or Navier-Stokes equations, fail to predict the flows related with this devices. One of the most successful methods, developed for solving problems in rarefied gas dynamics and microfluidics, is the Direct Simulation Monte Carlo (DSMC) method, originally proposed by the Australian scientist G. Bird in 1963. Since then, DSMC has been applied to an impressive array of different problems ranging from hypersonic to subsonic flows.

The talk will report on some basic problems of the DSMC method concerning the accuracy estimation, the range of the numerical scheme parameters, within which correct results can be obtained, and some important parameter limits that restrict the method application. Several examples of application to rarefied dynamics and microfluidic problems taken from the author's practice will be given. The problems that will be considered belong to various application areas illustrating different flow regimes and requiring different degrees of rarefaction (Knudsen numbers), ranged from near-free molecular to near-continuum regimes. Some novel method modifications will be demonstrated.

Exploiting GRID for Model Estimates of Regional Climate Changes and Its Impact on the Air Quality of Bulgaria

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The main objective of the EC FP6 project CECILIA is to deliver a climate change impacts and vulnerability assessment in targeted areas of Central and Eastern Europe. Emphasis is given to applications of regional climate modeling studies at a resolution of 10 km for local impact studies in key sectors of the region. For the purposeq intensive long-term meteorological modeling took place in Bulgarian National Institute of Meteorology and Hydrology, in an attempt to determine climatic values for the main meteorological variables. The climatic version of the operational weather forecast model ALADIN was applied for simulating 3 time slices: 1960-2000 (Control Run, CR), 2020-2050 (Near Future, NF) and 2070-2100 (Far Future, FF), following the IPCC scenario A1B. The calculations are made for an area covering Bulgaria with resolution of 10 km. The created meteorological data base is used for two purposes.

First of all, calculation of the respective modeled climates took place. The comparison between CR results and the available measured climatic values shows in a categorical way that the increase of the resolution increases the preciseness of the simulation. The differences of climatic fields for the 3 periods are presented and interpreted.

The second use of the created meteorological database is to estimate the impact of climate changes on air quality. A respective modelling system was created on the base of US EPA Models-3 System (MM5, CMAQ and SMOKE) for a smaller region with resolution of 10 km covering Bulgaria. The TNO emission inventory for 2000 is used. The chemical boundary conditions are extracted from similar results of 50-km runs over Europe made in Aristotle University of Thessaloniki, Greece. Calculations for the period 1990-2000 (CR), 2041-2050 (NF) and 2091-2100 (FF) are performed, results presented and interpreted in the study. For year 2000, some scenarios are run, results compared with measuring data.

Dynamics and Stability of Free Thin Films

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The flows of thin films have been a subject of intense investigation for many years. The reason for this interest is the wide variety of applications of such flows, both natural and industrial. Free liquid films are thin liquid layers bounded by two interfaces between liquid and gas or liquid and two other liquids. Examples of such a configuration are the layers between two bubbles in a liquid or between two drops of different liquids suspended in a third liquid. Other examples concern the free thin films attached to frames surrounded by an ambient gas. A similar configuration can be found at the solidification of a thin film pulled from melt.

The modeling of the free thin film drainage and stability is usually performed in the framework of a generalized lubrication approach, including inertial, viscous, capillary and intermolecular surface forces. For films with fully mobile surfaces, this approach leads to a system of nonlinear PDE for the film thickness and lateral velocities. In the present work the 1D variant of this system is studied numerically at different dynamic and static boundary conditions in the case of a laterally bounded free film. A linear and non-linear stability analysis is performed for a free film attached on a frame, with a prescribed wetting angle on the frame, that generalizes the linear stability results obtained for a periodic free film by other authors. The results show that when the van-der-Waals forces are not active, the steady film shapes are stable. However, when the van-der-Waals forces are active, steady shapes do not exist for each value of the wetting angle and Hamaker constant (characteristics of the van-der-Waals forces) and some of the existing steady shapes are stable, while others are unstable.

Queuing Models for Vehicle Flow on Crossroads

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The limited road capacity and increasing traffic have become a severe problem in many countries. The paper presents the mathematical model describing movement of vehicles through adjustable crossroads. The model is based on the theory of queuing.

One direction vehicle flow throw an adjustable crossroads is considered as a multiserver system with changeable intensity of service, in case of a red light an intensity of service is equal to zero. We use a model with a bounded turn, the number of positions is equal to quantity of cars which can be located in a quarter on all strips. If all places in the turn are occupied then an approached car leaves system. Thus approach permit to obtain periodic steady-state distribution for arbitrary intensities of input flows. These are steady-state results assume that the arrival pattern remains the same throughout a period large enough to get steady-state conditions. Analytical model is proposed to estimate residual queues that exist at the end of red phase at traffic signal on fixed-time plan. The dependence of the basic parameters of work (the average length of turn, probability that the quarter is completely occupied, the probability of free movement) on values of entrance system parameters is investigated. These steady-state distributions are compared with those obtained through a simulation model.

Several performance criteria may be used to evaluate a signalized intersection, such as average number of stops per vehicle, average queue length, and average stop delay. The multicriteria problem of optimal duration of traffic light cycle is studied.

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On the Homogenization of a Damped Wave Equation

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The effective behavior of the solution of a wave equation with interior and boundary damping, defined in a periodically perforated medium, is analyzed.

We deal, at the microscale, with an ε -periodic structure obtained by removing from a bounded connected open set Ω in \mathbb{R}^n a number of closed subsets of characteristic size ε . As a result, we obtain a perforated domain Ω^{ε} , in which we consider a wave equation, with interior sources and damping and with dynamic boundary conditions imposed on the boundaries of the perforations.

Assuming suitable initial conditions, we prove that the asymptotic behavior, as the small parameter ε which characterizes the size of the perforations tends to zero, of the solution of such a problem is governed by a parabolic equation, defined on the entire domain Ω .

Key words: homogenization, wave equation, damping and source terms.

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Generation of Stable (3+1)-dimensional High-intensity Ultrashort Pulses

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The spatiotemporal dynamics of high-intensity femtosecond laser pulses are studied based on numerical simulations within an advanced physical model. Beside of the processes involved in the standard cubic nonlinear Schrödinger equation, additional processes describing some crossed space-time effects, quintic nonlinearity, ionization modification of the refractive index, and, for the first time in this model, ionization modification of the group velocity dispersion, are also taken into account. The pulse propagation is described by the nonlinear envelope equation that is capable to propagate ultrashort pulses reaching single-cycle regime. The propagation and the material equations are solved self-consistently. The evolution of the light and the material parameters are studied at realistic experimental conditions. Self-compression of the pulse down to almost single-cycle regime and dramatic increase of the pulse intensity is found. At suitably chosen conditions, the pulse intensity, transversal width and time duration, as well as the spatiotemporal pulse shape become stable with the propagation of the pulse. Such a behavior of the pulse closely resembles a soliton-like formation process. To the best of our knowledge, this is the first observation of stable (3+1)-dimensional propagation of compressed pulses around the single-cycle regime.

Uniqueness Theorem for Einstein-Maxwell Black Holes with Kaluza-Klein Asymptotic

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We prove a uniqueness theorem for stationary multi black hole configurations with Kaluza-Klein asymptotic in a certain sector of 5D Einstein-Maxwell gravity. We show that such multi black hole configurations are uniquely specified by the interval structure, angular momenta of the horizons, magnetic charges and the magnetic flux.

Physical Mesomechanics; Its Theoretical Basis and Applications

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Physical Mesomechanics is a recent theory of deformation and fracture of solid-state materials. The most intriguing feature of physical mesomechanics is its capability of handling all the stages of deformation, from the elastic stage to fracturing stage, on the same theoretical basis. This feature comes from the field (gauge) theoretical treatment that the theory is based on; physical mesomechanics views materials under deformation as a collection of finite volume elements (called the deformation structural element), as opposed to a point masses as the conventional continuum mechanics views, and allows each deformation structural element deform differently. At the same time, however, physical mesomechanics requests local (gauge) symmetry in the governing dynamics. This leads to field equations that describe all the stages of deformation comprehensively. The irreversibility of plastic deformation can be formulated as dynamics where elastic stress contributes to flow of defects, rather than elastic strain, causing the associated mechanical energy to be dissipated. Fracture can be interpreted as the final stage of plastic deformation where the material becomes completely dissipative. These ideas have led us to define physical mesomechanical criteria of plastic deformation and fracture. Using these criteria, it is possible to identify the plastic zone in the pre-fracturing stage and to infer the loading history of a material. Recent experiments show evidence that validates these criteria.

Optimal Flow over Body at Reynolds Great Numbers

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The power optimization problem of a body movement in a viscous medium at Reynolds great numbers is considered. Control forces for body motion from initial position to a given are required to be found. The case of great Reynolds numbers means transformation from stationary laminar flow to unstable flow in relation to small perturbations. In boundary layer flow over a body after a certain length of flow a laminar boundary layer become unstable. Instability at first arises in trace on some distance behind body and leads to slow fluctuations of trace of approximately sinusoidal form and then it comes nearer to body in the form of stationary vortex. These changes in the flow field are lead to changes of full drag force that is considered in the received equations of movement. Problem in view: to find the control forces to transpose the body for the given time with minimal expenses of energy on overcoming of drag force. Such problem is non-regular and its reduction to equivalent problem of non-smooth optimization therefore is offered.

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A New Method of Prompt Fission Neutron Energy Spectrum Unfolding

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A new method of prompt fission neutron spectrum unfolding was developed and tested with a 252 Cf(sf) source mounted on the common cathode of a twin double ionization chamber, used as a fission fragment spectrometer. The experimental method allowed the simultaneous measurement of two correlated fission fragment kinetic energies along with the determination of the angle of the fission axis in respect to the common cathode normal. Based on the neutron detector allocation along the ionization chamber axis, the kinematics of the neutron emission from the fission fragment was reconstructed in both laboratory and fission fragment reference systems. The neutron velocity was measured by the time-of-flight method as the time interval between the ionization chamber cathode and the neutron detector signals. The neutron time-of-flight distribution versus the neutron detector signal pulse height was investigated to obtain the neutron time-of-flight response function. The measured response function was then used for prompt fission neutron energy spectrum unfolding with the help of a special Monte-Carlo procedure.

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