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Non-local Physics: Applications from the Universe Evolution to the Atom Structure in the Frame of the Unified Theory

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Non-local physics demonstrates its high efficiency in many fields – from the atom structure problems to cosmology [1-31, 35, 37-42]. As it is shown the theory of transport processes (including quantum mechanics) can be considered in the frame of the unified theory based on the non-local physical description. Only the main ideas and deductions of generalized Boltzmann physical kinetics and non-local physics are introduced here. For simplicity, we view the fundamental methodic aspects from the qualitative standpoint, avoiding excessively cumbersome formulas. Nevertheless some remarks and explanations should be done. A rigorous description is found, for example, in the monographs [1-4].

Transport processes in open dissipative systems are considered in physical kinetics. Therefore, the kinetic description is inevitably related to the system diagnostics. Such an element of diagnostics in the case of theoretical description in physical kinetics is the concept of the physically infinitely small volume (PhSV). The correlation between theoretical description and system diagnostics is well-known in physics. Suffice it to recall the part played by test charge in electrostatics or by test circuit in the physics of magnetic phenomena. The traditional definition of PhSV contains the statement to the effect that the PhSV contains a sufficient number of particles for introducing a statistical description; however, at the same time, the PhSV is much smaller than the volume V of the physical system under consideration; in a first approximation, this leads to local approach in investigating the transport processes. It is assumed in classical hydrodynamics that local thermodynamic equilibrium is first established within the PhSV, and only after that the transition occurs to global thermodynamic equilibrium if it is at all possible for the system under study.

Let us consider the hydrodynamic description in more detail from this point of view. Assume that we have two neighboring physically infinitely small volumes PhSV_1 and PhSV_2 in a non-equilibrium system. The one-particle distribution function (DF) $f_{sm,1}(\mathbf{r}_1, \mathbf{v}, t)$ corresponds to the volume PhSV_1, and the function $f_{sm,2}(\mathbf{r}_2, \mathbf{v}, t)$ – to the volume PhSV_2. It is assumed in a first approximation that $f_{sm,1}(\mathbf{r}_1, \mathbf{v}, t)$ does not vary within PhSV_1, same as $f_{sm,2}(\mathbf{r}_2, \mathbf{v}, t)$ does not vary within the neighboring volume PhSV_2. It is this assumption of locality that is implicitly contained in the Boltzmann equation (BE). However, the assumption is too crude. Indeed, a particle on the boundary between two volumes, which experienced the last collision in PhSV_1 and moves toward PhSV_2, introduces information about the $f_{sm,1}(\mathbf{r}_1, \mathbf{v}, t)$ into the neighboring volume PhSV_2. Similarly, a particle on the boundary between two volumes, which experienced the last collision in PhSV_2 and moves toward $PhSV_1$, introduces information about the DF $f_{sm,2}(\mathbf{r}_2, \mathbf{v}, t)$ into the neighboring volume $PhSV_1$. The relaxation over translational degrees of freedom of particles of like masses occurs during several collisions. As a result, “Knudsen layers” are formed on the boundary between neighboring physically infinitely small volumes, the characteristic dimension of which is of the order of path length. Then a correction must be introduced into the DF in the PhSV, which is proportional to the mean time between collisions and to the substantive derivative of the DF being measured (rigorous derivation is given in [1, 2]). Let a particle of finite radius be characterized as before by the position $\mathbf{r}$ at the instant of time t of its center of mass moving at velocity $\mathbf{v}$. Then, the situation is possible where, at some instant of time t, the particle is located on the interface between two volumes. In so doing, the lead effect is possible (say, for $PhSV_2$), when the center of mass of particle moving to the neighboring volume $PhSV_2$ is still in $PhSV_1$. However, the delay effect takes place as well, when the center of mass of particle moving to the neighboring volume (say, $PhSV_2$) is already located in $PhSV_2$ but a part of the particle still belongs to $PhSV_1$.

Moreover, even the point-like particles (starting after the last collision near the boundary between two mentioned volumes) can change the distribution functions in the neighboring volume. Adjusting of the particles dynamic characteristics for translational degrees of freedom takes several collisions. Therefore we experience a “Knudsen layer” effect between adjacent small volumes. This leads to fluctuations in mass and hence also in other hydrodynamic quantities. The existence of such “Knudsen layers” is not dependent on the choice of spatial nets and is fully defined by the reduced description for ensemble of particles of finite diameters in the conceptual framework of open physically small volumes, i.e., it depends on the chosen method of measurement.

This entire complex of effects defines non-local effects in space and time. The physically infinitely small volume (PhSV) is an open thermodynamic system *for any division of macroscopic system by a set of PhSVs.* However, the Boltzmann equation (BE)

$$Df/Dt = J^B \tag{1}$$

where J^B is the Boltzmann collision integral and $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}.\frac{\partial}{\partial \mathbf{r}} + \mathbf{F}.\frac{\partial}{\partial \mathbf{v}}$ is a substantive derivative, fully ignores non-local effects and contains only the local collision integral J^B. The foregoing nonlocal effects are insignificant only in equilibrium systems, where the kinetic approach changes to methods of statistical mechanics.

This is what the difficulties of classical Boltzmann physical kinetics arise from. Also a weak point of the classical Boltzmann kinetic theory is the treatment of the dynamic properties of interacting particles. On the one hand, as follows from the so-called “physical” derivation of the BE, Boltzmann particles are regarded as material points; on the other hand, the collision integral in the BE leads to the emergence of collision cross sections.

The rigorous approach to derivation of kinetic equation relative to one-particle DF f (KE_f) is based on employing the hierarchy of Bogoliubov equations. Generally speaking, the structure of KE_f is as follows:

$$\frac{Df}{Dt} = J^B + J^{nl}, \tag{2}$$

where J^{nl} is the non-local integral term. An approximation for the second collision integral is suggested by me in *generalized* Boltzmann physical kinetics,

$$J^{nl} = \frac{D}{Dt}\left(\tau \frac{Df}{Dt}\right). \tag{3}$$

Here, τ is the relaxation time proportional to the mean time t_m between collisions of particles, which is related in a hydrodynamic approximation with dynamical viscosity μ and pressure p,

$$\tau_{mt} p = \Pi\mu, \tag{4}$$

where the factor Π is defined by the model of collision of particles; for neutral hard-sphere gas, $\Pi = 0.8$ [32]. All of the known methods of deriving kinetic equation relative to one-particle DF f lead to the approximation (3), including the method of many scales, the method of correlation functions, and the iteration method. One can draw an analogy with the Bhatnagar-Gross-Krook (BGK) approximation for local integral J^B,

$$J^B = \frac{f^{(0)} - f}{\tau_r}, \tag{5}$$

(5) (in the simplest case $\tau_r \sim \tau$) the popularity of which in the case of Boltzmann collision integral is explained by the colossal simplification attained when using this approximation. The order of magnitude of the ratio between the second and first terms of the right-hand part of Eq. (2) is Kn^2, at high values of Knudsen number, these terms come to be of the same order. It would seem that, at low values of Knudsen number corresponding to hydrodynamic description, the contribution by the second term of the right-hand part of Eq. (2) could be ignored. However, this is not the case. Upon transition to hydrodynamic approximation (following the multiplication of the kinetic equation by invariants collision and subsequent integration with respect to velocities), the Boltzmann integral part goes to zero, and the second term of the right-hand part of Eq. (2) *does not go to zero* after this integration and produces a contribution of the same order in the case of generalized Navier-Stokes description.

From the mathematical standpoint, disregarding the term containing a small parameter with higher derivative is impermissible. From the physical standpoint, the arising additional terms proportional to viscosity correspond to Kolmogorov small-scale turbulence; the fluctuations are tabulated [2, 10]. It turns out that the integral term J^{nl} is important from the standpoint of the theory of transport processes at both low and high values of Knudsen number. Note the treatment of GBE from the standpoint of fluctuation theory,

$$Df^a/Dt = J^B, \tag{6}$$

$$f^a = f - \tau\, Df/Dt. \tag{7}$$

Equations (6) and (7) have a correct free-molecule limit. Therefore, $\tau\, Df/Dt$ is a fluctuation of distribution function, and the notation (6) disregarding (7) renders the BE open. From the standpoint of fluctuation theory, Boltzmann employed the simplest closing procedure

$$f^a = f. \tag{8}$$

Fluctuation effects occur in any open thermodynamic system bounded by a control surface transparent to particles. GBE (6) leads to generalized hydrodynamic equations [2-4], for example, to the continuity equation

$$\frac{\partial \rho^a}{\partial t} + \frac{\partial}{\partial \mathbf{r}} . (\rho \mathbf{v}_0)^a = 0, \tag{9}$$

where ρ^a, $\mathbf{v}_0$, $(\rho\mathbf{v}_0)^a$ are calculated in view of non-locality effect in terms of gas density ρ, hydrodynamic velocity of flow $\mathbf{v}_0$, and density of momentum flux $\rho\mathbf{v}_0$; for locally Maxwellian distribution, ρ^a, $(\rho\mathbf{v}_0)^a$ are defined by the relations

$$(\rho - \rho^a)/\tau = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} . (\rho \mathbf{v}_0),$$
$$\left(\rho\mathbf{v}_0 - (\rho\mathbf{v}_0)^a\right)/\tau = \frac{\partial}{\partial \tau}(\rho\mathbf{v}_0) + \frac{\partial}{\partial \mathbf{r}} . \rho\mathbf{v}_0\mathbf{v}_0 = \mathbf{I} . \frac{\partial \rho}{\partial \mathbf{r}} - \rho\mathbf{a}, \tag{10}$$

where $\mathbf{I}$ is a unit tensor and $\mathbf{a}$ is the acceleration due to the effect of mass forces. Finally, we can state that introduction of open control volume by the reduced description for ensemble of particles of finite diameters leads to fluctuations of velocity moments in the volume. This fact leads to the significant reconstruction of the theory of transport processes. Obviously the mentioned non-local effects can be discussed from viewpoint of breaking of the Bell's inequalities because in the non-local theory the measurement (realized in PhSV_1) has influence on the measurement realized in the adjoining space-time point in PhSV_2 and verse versa.

The equation (GBE) reads

$$\frac{Df}{Dt} = J^B + \frac{D}{Dt}\left(\tau \frac{Df}{Dt}\right). \tag{11}$$

Here τ is nonlocal parameter, in the simplest case it is the mean time BETWEEN collisions (for plasma τ is mean time between close collisions), for plasma in D/Dt should be introduced the self consistent force $\mathbf{F}$. For a multi species reacting gas, the generalized Boltzmann equation can be rewritten as

$$\frac{Df_\alpha}{Dt} - \frac{D}{Dt}\left(\tau_\alpha \frac{Df_\alpha}{Dt}\right) = J_\alpha^{B,el} + J_\alpha^{B,r}, \tag{12}$$

where f_α is distribution function for a particle of the αth kind, τ_α is nonlocal parameter for α species (in the simplest case τ_α is mean free time for a particle of the αth kind), and $J_\alpha^{B,el}$, $J_\alpha^{B,r}$ are the Boltzmann collision integrals for elastic and inelastic collisions, respectively. GBE (11) was derived in the theory of liquids, in this case τ is connected with the time of the particle residence in the Frenkel cell.

By the way derived by me GBE was presented in my lectures on physical kinetics given in Sofia University, Bulgaria, in the year 1987.

In the general case, the parameter τ is the non-locality parameter; in quantum hydrodynamics, its magnitude is defined by the "time-energy" uncertainty relation. The violation of Bell's inequalities [33, 34] is found for local statistical theories, and the transition to non-local description is inevitable.

Several extremely significant problems challenge modern fundamental physics, which can be titled as "Non-solved problems of the fundamental physics" or more precisely – of local physical kinetics of dissipative processes, namely:

1) Kinetic theory of entropy and the problem of the initial perturbation;

2) Strict theory of turbulence;

3) Quantum non-relativistic and relativistic hydrodynamics, theory of charges separation in the atom structure;

4) Theory of ball lightning;

5) Theory of dark matter;

6) Theory of dark energy, Hubble expansion of the Universe;

7) The destiny of anti-matter after the Big Bang.

8) A unified theory of dissipative structures - from atom structure to cosmology.

In appearance these old and new problems (including the problems 5 and 6 in the list) mean that we have reached the revolutionary situation not only in physics but in natural philosophy on the whole. Practically we are in front of the new challenge since Newton's *Mathematical Principles of Natural Philosophy* was first published in 1687. More than ten years ago, the accelerated cosmological expansion was discovered by the direct astronomical observation at distances of a few billion light years, almost at the edge of the observable Universe. This acceleration needs to be explained because mutual attraction of cosmic bodies can only decelerate their scattering. To accommodate this phenomenon, a new notion was introduced into physics: namely that there a 'new' force with the opposite sign that is called universal antigravitation. Many investigators believe that the physical source of this new force is dark energy that manifests itself only by providing antigravitation.

It was also postulated that the source of antigravitation is "dark matter" whose existence was inferred from the gravitational effects on visible matter. But from the other side, dark matter is undetectable by emitted or scattered electromagnetic radiation. This means that new notions - dark matter, dark energy - were introduced in physics only with the aim of accounting for the discrepancies between measurements of the mass of galaxies, clusters of galaxies and the entire universe as measured by dynamical and general relativistic means, based on the mass of the visible "luminous" matter. This might be reasonable if we were speaking about small corrections to our knowledge system of knowledge of today. But the above mentioned discrepancies lead to the claim that dark matter and dark energy constitute 96% of the total matter and energy in the Universe. In fact we could and should have anticipated this crisis of local statistical physics after the discovery of the fundamental Bell inequalities (Bell 1964).

These problems of the local physics lead to the questions:

1. Why is the concept of dark matter not significant in the solar system?

2. Why do the galaxy rotation curves have their characteristic flat form?

3. Is it possible to obtain the continuous transition from the Kepler regime to flat halo curves?

4. Why does the Hubble expansion exist with acceleration after the Big Bang explosion (or after the explosion in the Hubble boxes? (Nobel Prize 2011)

Mentioned problems constitute the circle of problems on the Universe scale. In this report the unified generalized non-local theory is applied for mathematical modeling of cosmic objects. For the case of the galaxies evolution the non-local theory leads to the flat rotation curves known from observations. The transformation of Kepler's regime into the flat rotation curves for different solitons is shown. The Hubble expansion with acceleration is explained as result of mathematical modeling based on the principles of non - local physics. Namely:

The main origin of Hubble effect (including the matter expansion with acceleration) is self-catching of expanding matter by the self-consistent gravitational field in conditions of weak influence of the central massive bodies.

Peculiar features of the rotational speeds of galaxies and effects of the Hubble expansion need not in the introduction of new essence like dark matter and dark energy. The origin of difficulties consists in the total Oversimplification following from the principles of local physics, [3, 41, 42].

The following problems belong to the "intermediate" macroscopic scales:

1) Kinetic theory of entropy and the problem of the initial perturbation in the Boltzmann kinetic theory, [2, 10, 11].

2) Strict theory of turbulence, [2, 3, 5, 10, 12-17, 21, 22, 37].

3) Theory of ball lightning [38].

4) The problem of the high temperature superconductivity, [39, 40]. Here these problems are re-considered in the framework of our unified non-local kinetic theory of dissipative structures. In particular the local theory of turbulence based on the Navier-Stokes equations now is in blind alley. Local statistical dissipative theories are wrong on principal (J. Bell, 1964). In the frame of the strict turbulence theory based on non-local description we have:

1. All fluctuations are found from the strict kinetic considerations and tabulated [2, 10]. The appearing additional terms in generalized hydrodynamic equations (GHE) are due to viscosity and they correspond to the small-scale Kolmogorov turbulence. The neglect of formally small terms is equivalent, in particular, to dropping the (small-scale) Kolmogorov turbulence from consideration and is the origin of all principal difficulties in usual turbulent theory. Fluctuations on the wall are equal to zero, from the physical point of view this fact corresponds to the laminar sub-layer. Mathematically it leads to additional boundary conditions for GHE. Major difficulties arose when the question of existence and uniqueness of solutions of the Navier - Stokes equations was addressed. O A Ladyzhenskaya has shown for three-dimensional flows that under smooth initial conditions a unique solution is only possible over a finite time interval. Ladyzhenskaya even introduced a "correc-

tion" into the Navier-Stokes equations in order that its unique solvability could be proved. GHE do not lead to these difficulties.

2. The problem of closure for senior moments does not exist in the turbulence non-local theory. Mild inlet and outlet conditions written for the average hydrodynamic values provide the stable calculations for flows with the open boundaries [19, 21, 22, 24].

3. It would appear that in continuum mechanics the idea of discreteness can be abandoned altogether and the medium under study be considered as a continuum in the literal sense of the word. Such an approach is of course possible and indeed leads to the Euler equations in hydrodynamics. However, when the viscosity and thermal conductivity effects are to be included, a totally different situation arises. As is well known, the dynamical viscosity is proportional to the mean time τ between the particle collisions, and a continuum medium in the Euler model with $\tau = 0$ implies that neither viscosity nor thermal conductivity is possible.

4. The application of the above principles also leads to the modification of the system of the Maxwell electro-dynamic equations (ME) [18, 23, 27, 28]. While the traditional formulation of this system does not involve the continuity equation (like (9) but for the charge density ρ^a and the current density $\mathbf{j}^a$), nevertheless the ME derivation employs continuity equation and leads to appearance of fluctuations (proportional to τ) of charge density and the current density. In rarefied media both effects lead to Johnson's flicker noise observed in 1925 for the first time by J.B. Johnson by the measurement of current fluctuations of thermo-electron emission.

Finally the following problems belong to the "microscopic" scales in applications:

1. Quantum non-relativistic and relativistic hydrodynamics, theory of the charges separation in the atom structure; [2, -4, 25-28, 30, 31].

2. The destiny of anti-matter after the Big Bang, [3, 29].

3. Application of generalized non-local quantum hydrodynamics to the calculation of the charge inner structures for particles including proton and electron, [3, 35]

Turn our attention to the quantum hydrodynamic description of individual particles. The abstract of the classical Madelung's paper [36] contains only one phrase: "It is shown that the Schrödinger equation for one-electron problems can be transformed into the form of hydrodynamic equations." In this case the unified non-local theory of dissipative structures leads to the conclusions:

1. Madelung's quantum hydrodynamics is equivalent to the Schrödinger equation (SE) and leads to description of the quantum particle evolution in the form of Euler equation and continuity equation. SE (and Madelung's hydrodynamics as well) are the non-dissipative theories and does not contain energy equation on principal.

2. SE is consequence of the Liouville equation as result of the local approximation of non-local equations.

3. Generalized Boltzmann physical kinetics leads to the strict approximation of non-local effects in space and time and after transmission to the local approx-

imation leads to parameter τ, which on the quantum level corresponds to the uncertainty principle "time-energy". On principal, GHE need not use the "time-energy" uncertainty relation for estimating the value of the non-local parameter . Moreover the "time-energy" uncertainty relation does not lead to the exact relations and from the position of non-local physics it is only the simplest estimation of the non-local effects.

4. GHE lead to SE as a deep particular case of the generalized Boltzmann physical kinetics and therefore of non-local hydrodynamics. From the very beginning SE was the simplest phenomenological non-local equation corresponding to the local approximation of non-local effects.

5. It is known that the Schrödinger-Madelung quantum physics leads to the destruction of the wave packets. The appearance in mathematics the soliton solutions is the rare and remarkable effect. *The soliton's appearance in the generalized hydrodynamics created by Alexeev is an "ordinary" oft-recurring fact.* From this point of view generalized non-local quantum hydrodynamics is Soliton quantum mechanics instead of Wave Schrödinger-Madelung quantum mechanics.

6. From calculations follow that proton and electron can be considered like charged balls (shortly CB model) which charges are concentrated mainly in the shell of these balls. The proton-electron collision in the frame of CB-model should be considered as *collision of two resonators.* In this case can be explained a number of character collisional features depending on the initial and final electron energies and the scattering angles.

7. Mathematical modeling (considered in [3, 26, 29]) for anti-matter particles leads to diminishing of the linear size of combined soliton in 2×10^3 times and cross sections in $\sim 4 \times 10^6$ times in comparison with atoms of regular matter. Now the conclusion of the principal significance. Matter and anti-matter atoms after creation in the Big Bang activity are involved in the process of the collisional relaxation. But the cross sections of anti-matter atoms and inversed atoms of regular matter have so small cross sections that they are leaving the physical system. Now anti-matter forms the outer edge of visible Universe.

In conclusion I should underline:

1. Boltzmann equation does not work on the distances of the radius of the particles interactions and cannot be applied to the modeling of nano-system even from this point of view.

2. Boltzmann equation belongs only to the class of plausible equations (B. Alexeev, 1982). The disaster with non-diagnostic dark energy and dark matter is obliged to the local statistical description, and finally

Physics of 21st century is non-local physics.

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On Periodic Solutions of Goodwin's Business Cycle Model with only Floor in Induced Investment

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Sasakura [1] obtained the excitation conditions of a time periodic oscillations of Goodwin's business cycle model for income in the form of second order ordinary differential equation [2]. According to Sasakura, under certain conditions the limit cycles solutions are possible even if the induced investment function is bounded only above or only below (that is, has a ceiling or a floor) [3]. We present an analytical solution of Goodwin's business cycle model in the form of delay differential equation for income [2] with fixed delay T and piecewise linear accelerator with only the floor (or the ceiling). We concluded that in this model a time periodic solutions do not exist. The solution looks very similar to the oscillation with a period T and its amplitude grows exponentially in time. We discuss also conditions for the existence of periodic solutions for Goodwin's model with fixed delay.

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Some Properties of Integro-Differential Equations from Biology

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We present some models of integro-differential equations from population dynamics, where the integral term describes the nonlocal consumption of resources. Fredholm property of the corresponding linear operators are useful to prove the existence of traveling wave solutions. For some models, this can be done only when the support of the integral is sufficiently small. In this case, the integro-differential operator is close to the differential one. One uses a perturbation method which combines the Fredholm property of the linearized operators and the implicit function theorem. For some other models, Leray-Schauder method can be applied. This implies the construction of a topological degree for the corresponding operators and the establishment of a priori estimates for the solution. Some biological interpretations follow from this study.

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Stabilization via Parametric excitation of Statically Unstable Systems

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The problem of the vibrational stabilization of statically unstable systems has a considerable attention in literature. Most of these studies, however, have been devoted to high-frequency stabilization, or specific, few d.o.f systems. Here the problem is investigated for general excitation frequency and general multi-d.o.f. systems.

A Hamiltonian linear statically unstable system close to the stability boundary is considered. Such system depends on a parameter, taken close to a critical value of which a static bifurcation occurs. Here the critical system possess a double-zero eigenvalue, while the remaining ones are purely imaginary in pairs. The system is parametrically excited by a harmonic forcing of low-amplitude and arbitrary frequency. Goal of the analysis is to investigate if and how the parametric excitation permits the statically unstable system to regain stability.

The solution of the problem is pursued by the Multiple Scale perturbation Method, as perturbation of a critical Hamiltonian system. Different asymptotic expansions are carried out, which are able to capture the long-term behavior of the system, for generic (non-resonant) values of the excitation frequency, resonant relations of 1:2, 2:1 and 1:1 type, between excitation and a selected natural frequency and combinations of natural frequencies.

It is shown that a proper ordering of the control parameters must be performed, and proper use of integer or fractional power expansions must be made, according to the resonance under study. A comprehensive scenario of the stabilization regions is given in which lower-bound as well as upper-bound curves are evaluated.

Inverted double- and triple-pendula are taken as sample systems to illustrate the theory. Asymptotic solutions are validated by comparison with exact numerical results furnished by Floquet theory of ordinary differential equations with periodic coefficients.

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Efficient Estimation of Heston Model Parameters

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The estimation of prices of options and other derivative assets is an important part of Financial mathematics. The model of Heston is one of the most widely used stochastic models for modelling the prices of the underlying assets. Various improvements to the Heston model have been proposed, generally leading to increased theoretical and computational complexity.

The evaluation of “exotic” options is based upon calibration of the Heston model parameters to the observed market prices of European call and put options. This process is computationally intensive and involves global optimization and many evaluations of the prices of European options.

The resulting parameters of the Heston model vary with time and are highly sensitive to daily market fluctuations. In this work we describe our theoretical and computational approach to mitigate the impact of these fluctuations and estimate efficiently the Heston Model Parameters. Numerical and timing results are shown, demonstrating the feasibility of our methods.

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Tilted Cosmological Model With Barotropic Fluid Distribution

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We investigated tilted Bianchi type I cosmological model for barotropic fluid with isotropic pressure p and matter density. To determine the complete solution, we have assumed the relation between metric potential as $A = BC$. To get model in terms of cosmic time t, we have also assumed some special condition. The physical and geometrical aspects of both the model are discussed.

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Numerical Simulation of Drop Coalescence in the Presence of Drop Soluble Surfactant

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A numerical method is presented for simulation of the deformation and drainage of axisymmetric film (gap) between colliding drops in the presence of surfactants soluble in the drop phase at small capillary and Reynolds numbers and small surfactant concentrations. The drops are considered to approach each other under the constant interaction force. The hydrodynamic part of the mathematical model is based on the lubrication equations in the gap between the drops and the Stokes equations in the drops, coupled with velocity and stress boundary conditions at the interfaces. A non-uniform surfactant concentration on the interfaces, related with the surfactant concentration in the drops, leads to a gradient of the interfacial tension which in turn leads to additional tangential stress on the interfaces (Marangoni effects). Both drop and interface surfactant concentrations, related via adsorption isotherm, are governed by a convection-diffusion equation. For the flow in the drops a simplified version of Boundary integral method is used. Finite difference method is used for the flow in the gap, the position of the interfaces and the surfactant concentration on the interfaces, as well as in the drops. For the hydrodynamic part of the model second order approximation of the spatial terms on adaptive non-uniform mesh is constructed in combination with Euler explicit scheme for the time discretization with automatically adaptive time step. For the convection-diffusion equation in the drops first order implicit and Crank-Nicolson time integration schemes are compared with respect to accuracy and stability. Tests and comparisons are performed to show the accuracy and stability of the presented numerical method.

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On a Nonlocal Boundary Value Problem for The Two-Term Time-Fractional Diffusion-Wave Equation

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Fractional calculus is a useful tool for modeling different physical processes where the memory effects of the complex or viscoelastic media should be taken into consideration. The time-fractional diffusion-wave equation describes important physical phenomena that arise in amorphous, colloid, glassy and porous materials, dielectrics and semiconductors, biological systems, polymers, random and disordered media, geophysical and geological processes.

We study a nonlocal boundary value problem for the spatially one-dimensional diffusion-wave equation with two fractional time-derivatives of different order. Thus, our model represents a generalized telegraph equation. The analytical solution of the problem is represented as a series expansion on the generalized eigenfunctions of a non-selfadjoint Sturm-Liouville problem. The time-dependent components of the solution are given in terms of the three-parameter Mittag-Leffler functions. It is known that, in the limiting case of the wave equation with nonlocal boundary conditions leading to multiple eigenvalues, the oscillation amplitude of the system increases with time. We study the effect of the fractional damping on such an oscillating system, establishing the asymptotic behavior of the solution. Some regularity estimates are also obtained. The proofs are based on the generalized eigenfunction expansion of the solution. To illustrate analytical formulas, results of numerical calculations and plots are presented.

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Motion of a Pendulum with Periodically Variable Length

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The paper is devoted to the study of regular and chaotic motions of the pendulum which length changes according a sinusoidal law. Asymptotic expressions for

boundaries of instability domains near resonance frequencies are derived. Domains for oscillational and rotational motions in parameter space are found analytically and compared with numerical study. Chaotic motions of the pendulum depending on problem parameters are investigated numerically.

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Creation of Parallel Algorithms for the Solution of Problems of Gas Dynamics on Multi-Core Computers and GPU

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The paper deals with a parallel algorithm for calculations on multiprocessor computers and GPU accelerators. The calculations of shock waves interaction with low density bubble results and the problem of the gas flow with the forces of gravity are presented. This algorithm combines a possibility to capture a high resolution of shock waves, the second-order accuracy for TVD schemes, and a possibility to observe a low-level diffusion of the advection scheme.

The algorithm is based on the AMR method – Adaptive Mesh Refinement of the computational grid. Utilization of AMR method can significantly improve the resolution of the difference grid in areas of high interest, and from other side to accelerate the processes of the multi-dimensional problems calculating. Parallel algorithms of the analysed difference models are built for the purpose of calculations on graphic processors using the CUDA technology.

New approaches to the doing science exponentially increasing computational requirements: in order to realistically describe and solve real-world problems, numerical simulations are becoming more detailed, experimental sciences use more complicated instruments to make precise measurements; and shift from the individuals-based science work towards collaborative research model now starts to dominate. Mathematical modeling forms a solid theoretical and applied basis in describing, simulating and studying the complex problems. Precise mathematical models are realizing by using parallel applications that requires high performance computational resources. Although new perfect high performance computational installations become available for researchers in many cases their resources are not sufficient for solving many practical problems.

Many complex problems of continuum mechanics are numerically solved on structured or unstructured grids. To improve the accuracy of the calculations is necessary to choose a sufficiently small grid (with a small cell size). This leads to the drawback of a substantial increase of computation time. Therefore, for the calculations of complex problems it is reasonable to use the method of Adaptive Mesh Refinement. That is, the grid refinement is performed only in the areas of interest of the structure, where, e.g., the shock waves are generated, or a complex geometry or other such features exist. Thus, the computing time is greatly reduced. In addition, the execution of the application on the resulting sequence of nested, decreasing nets can be parallelized.

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On Wave Diffraction Boundary Value Problems with a Crack Perpendicular to the Main Boundary

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We prove the unique existence of solutions for different types of wave diffraction boundary value problems with a crack perpendicular to the main boundary. Representations of the solutions are also obtained upon the consideration of some associated operators. This is done in a Bessel potential spaces framework and for complex wave numbers. The investigation is mostly based on the construction of explicit operator relations, the potential method, and certain factorizations.

The talk is based on a joint work with David Kapanadze.

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Homogenisation of Periodic Elastic Plates in Bending Regime

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We consider homogenisation problem of periodic elastic plate in bending regime. The thickness of the plate and the period of the plate structure are described by

two small parameters (h and epsilon correspondingly) which tend to zero simultaneously. We start from the fully non-linear elasticity setting. Bending regime corresponds to the energies of order h cubed. We consider the case when the thickness h is much smaller than the period. In the limit the homogenised energy is given by a quadratic (linearised) integral functional defined on the second fundamental form of the surface representing zero-thickness plate subject to a bending deformation. The key tools in our work are Gamma-convergence of functionals and the two-scale convergence of function sequences.

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A Parallel 3th Order Recursive Filter with Boundary Conditions in 3D-VAR Ocean Data Assimilation System

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In this paper we propose an improvements of the Ocean Variational Assimilation System 3D-VAR based on the 3rd order recursive filter (RF) with boundary conditions. The original model works with a 1rd order RF and it adopts ghost points for compute the model variables also in presence of discontinuities, represented by the land zone in the ocean. An advantage of the proposed modification is that time complexity can be substantially reduced with benefits on large scale simulations. For comparing the effectiveness between 1rd order RF with ghost points and 3rd order recursive filter (RF) with boundary conditions a set of experiments is showed by assimilating expendable bathythermograph (XBT) and ARGO data into Adriatic Sea. The numerical results prove the good preformance of a 3rd order recursive filter (RF) with boundary conditions and the overall computational time in the assimilation process is reduced by a 33% factor.

Moreover, the results in terms of model accuracy are comparable with those obtained by 1rd order RF and they prove that 3D-VAR, with 3rd order RF, is more suitable tool for operational numerical oceanic forecasting.

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An Optimal Control Problem of a Spatial Holling Type IV Nutrient-Phytoplankton-Zooplankton-Fish System

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An optimal control problem associated with a hybrid model of the spatio-temporally continuous nutrient-phytoplankton-zooplankton-fish reaction-diffusion system with Holling type IV predator response is considered. The parameter for fish predation is treated as a multiplicative control variable. Such models are especially suitable to examine the generic behavior of the aquatic systems and the eutrophication process of lakes. Numerical results of the optimal solution in two spatial dimensions are presented.

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Viscous Drag and Heat Transfer in Non-Stationary Gas Flow between Rotating Cylinders

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The viscous drag (wall shear stress) and heat flux on the both cylinder walls, as well as flow macroscopic characteristics (velocity, density and temperature) are numerically studied in non-stationary Couette gas flow between rotating cylinders. The results are obtained using Direct Simulation Monte Carlo (DSMC) method and numerical solution of a continual model based on the Navier-Stockes-Fourier (NSF) method. Three typical cases are considered: A) inner rotating – outer stationary cylinder; B) inner stationary – outer rotating cylinder; C) opposite rotating cylinders. These studies have been accomplished for fixed Knudsen numbers. The NSF results have been obtained by setting a local value of Knudsen number in the corresponding first order slip boundary conditions. Capabilities applications of continual model are estimated for several Knudsen numbers.

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Numerical Investigation of the Unified Model of Stacked Josephson junctions

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We study numerically the dynamics of multistacked Josephson junctions using the unified model of Machida and Sakai. This model takes into account simultaneously the inductive and the capacitive coupling between junctions. It occurs to be important for modeling of the intrinsic Josephson junctions. The influence of the capacitive coupling on the fluxon dynamics is analyzed and a comparison with the case of only inductive coupling is made. The corresponding system of coupled sine-Gordon equations is solved numerically by finite difference schemes. Different physical quantities that can be measured in real experiments are numerically calculated.

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New Class of Metastable Blow-Up Solutions of the Mathematical Model of Heat Structures

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The mathematical model of heat structures in an open nonlinear medium depends on two physical parameters: the first one (σ) determines the heat conductivity of the medium and the second one (β) - the self-generating volume source. Their ratio together with appropriate initial perturbations determines different kinds of structures and waves that may arise and preserve themselves for a finite period of time. We report about a new class of complex metastable waves in the case $\beta = \sigma + 1$.

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Collision Dynamics of Some Atomic States in Ne Hollow Cathode Plasma Using Time-Resolved Optogalvanic Signals

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The dynamic optogalvanic effect represents the change in plasma conductivity due to the absorption of a short (ns) laser pulse tuned to particular optical transitions in some of the plasma particles. The absorbed light would affect the population of the energetic levels involved in the optical transition illuminated and thus would change the effective ionization processes in the plasma [1]. The dynamic optogalvanic signals are more informative than the stationary optogalvanic signals (which originate from the continuous illumination) because they are characterized not only by their amplitudes and polarities, but also by time dependence. The time dependence of the optogalvanic waveforms contains information about the generations of excited and ionized particles and their quenching during with time [2].

The applications of the optogalvanic effect include spectrochemical analysis techniques, high-precision laser frequency stabilization, plasma diagnostics, high-resolution spectroscopy and isotope separation.

In the present work the dynamic optogalvanic effect from some neon atomic transitions and the associated time-resolved optogalvanic signals in a hollow cathode discharge lamp have been investigated both experimentally and theoretically. A system of rate equation including the various processes contributing to the generation of the optogalvanic signals is developed. It has been applied to analyze the experimentally registered time-resolved optogalvanic signals at different discharge current values and to identify the dominant plasma process most responsible for particular optogalvanic signal's generation. The decay rate constants of the levels contributing directly or indirectly to signal formation have been determined using non-linear fits of the experimentally measured dynamic optogalvanic signals with theoretically obtained function. The behavior of the optogalvanic signal waveform together with the decay rate constants as a function of the discharge current have been studied in detail. The procedure for deconvolution of registered optogalvanic signals and the instrumentation function is also demonstrated.

The structure of this model should be useful in determining ionization rates of electronically excited levels from optogalvanic measurements.

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Modeling for High Reynolds Number Flows with Generalized Hydrodynamics Equations (GHE)

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Generalized hydrodynamic equations (GHE) proposed by Alexeev (1994), have been successfully used for simulations of viscous flows for a wide range of problems and flow parameters, including high Reynolds numbers flows with thin boundary layers.

Spacial fluctuations (small flow scales) can be successfully captured with GHE, and the derived small scale of turbulent flow compares well with observed one in the experiments.

Analytical and numerical solutions using GHE for several viscous flow problems are presented and compared with experimental data for the cases we considered in the range of Reynolds number from $\mathrm{Re} = 10^{-6}$, to 3200, and to 1,000,000.

The solution methods are discussed and compared (analytical, numerical and measured data).

Comparison with the analytical asymptotic solution is provided for a boundary layer flow at high Reynolds numbers.

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Some Numerical Studies of the Atmospheric Composition Climate of Bulgaria

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Some extensive numerical simulations of the atmospheric composition fields in Bulgaria have been recently performed.

The US EPA Model-3 system was chosen as a modelling tool. The system consists of three components: MM5 – the 5th generation PSU/NCAR Mesometeorological Model used as meteorological pre-processor; CMAQ – the Community Multiscale Air Quality System CMAQ; SMOKE – the Sparse Matrix Operator Kernel Emissions Modeling System – the emission model.

As the NCEP Global Analysis Data with 1 degree resolution was used as meteorological background, the MM5 and CMAQ nesting capabilities were applied for downscaling the simulations to a 3 km resolution over Bulgaria.

The TNO emission inventory was used as emission input. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions. The biogenic emissions of VOC are estimated by the model SMOKE. The numerical experiments have been carried out for different emission scenarios, which makes it possible the contribution of emissions from different source categories to be evaluated.

The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behavior could be interesting. Therefore the Models-3 "Integrated Process Rate Analysis" option is applied to discriminate the role of different dynamic and chemical processes for the pollution from biogenic sources.

The obtained ensemble of numerical simulation results is extensive enough to allow statistical treatment – calculating not only the mean concentrations and different source categories contribution mean fields, but also standard deviations, skewness, etc. with their dominant temporal modes (seasonal and/or diurnal variations). Thus some basic facts about the atmospheric composition climate of Bulgaria can be retrieved from the simulation ensemble.

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Spherical Long Spirals

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Long spirals in the Euclidean plane have been introduced by A. Kurnosenko five years ago. Using a natural map of the shape sphere into the extended Gaussian plane we study spherical curves that are pre-images of plane long spirals. Applications to loxodromes and spherical spiral antennas are also given.

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Parametric Solitons

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When two or three optical pulses propagate in an isotropic media phase-matched conditions of the kind of $2\omega_1 - 2\omega_2 = 0$ or $2\omega_3 = \omega_1 + \omega_2$ could be satisfied. In this case terms connected with four photon parametric processes in the corresponding nonlinear evolution equations appear. These terms generate a periodical exchange of the energy between the optical waves. In the present work the existence of parametrically connected solitons is discussed.

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On the Spectral Properties of Lax Operators

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I will consider a class of Lax operators generalizing the Zakharov-Shabat system:

$$L\psi \equiv i\frac{d\psi}{dx} + (Q(x,t) - \lambda J)\psi(x,t,\lambda) = 0, \tag{1}$$

where $Q(x)$ and J take values in a simple Lie algebra $\mathfrak{g}$ and vanishes fast enough for $x \to \pm\infty$. Applying the inverse scattering method to L one is able to solve a number of important nonlinear evolution equations (NLEE) such as multicomponent nonlinear Schrodinger equations, N-wave equations, etc.

We will construct the fundamental analytic solutions of L and will show the important role they play in constructing the spectral decompositions of L. The FAS satisfy a Riemann-Hilbert problem, which allows one to use the dressing Zakharov-Shabat method for constructing the reflectionless potentials of L and the soliton solutions of the NLEE.

Another important field of applications of these results is in the quantum mechanics of multi-level atomic systems.

This method can be extended in several different directions. The first one is to treat Lax operators with deep symmetries. The second is to apply it to operators with polynomial dependence on λ, e.g.

$$L_{(2)}\psi \equiv i\frac{d\psi}{dx} + (Q_2(x,t) + \lambda Q_1(x,t) - \lambda^2 J)\psi(x,t,\lambda) = 0, \tag{2}$$

The third important direction is to study the spectral properties of the operators L and $L_{(2)}$ on the class of potentials with non-vanishing boundary conditions.

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Inversion of the V-Radon Transform

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The talk discusses a new class of Radon transform defined on V-shaped piecewise linear trajectories called the V-line Radon transform (also called broken-ray Radon transform). This transform appears in various mathematical models arising in nuclear medicine, homeland security, and astrophysics. We will present some new results about the inversion of V-line Radon transform. New simple explicit inversion formulae are presented in this case.

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Structure, Mechanics, and Remodeling Process of Bone: Biomechanics of Osteoporosis

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The significance rise in life expectancy we have achieved over the last century is a source of pride. Yet with it have come a number of new public health issues, such as the epidemic of fragility fractures in the elderly. Osteoporotic fractures occur in situations where healthy people would not normally break a bone; they are therefore regarded as fragility fractures. Typical fragility fractures occur in the vertebral column, rib, hip and wrist. Around 45reach the age of fifty will sustain at least one fragility fracture, and a quarter of men will have at least one fragility fracture during their lifetime. Despite these observations, there is no need to remain pessimistic as our knowledge of bone biology is improving rapidly.

Bone is a vital, dynamic connective tissue that gives form to the body, supporting its weight, protecting vital organs, and facilitating locomotion by providing attachments for muscles to act as levers under the control of CNS. It also acts as a reservoir for ions, especially for phosphate and calcium, the homeostasis of which is essential to life. These functions place serious requirements on the properties related to structural mechanics of bone, which should be strong enough to support the weight of body and unbreakable enough to prevent easy fracturing, as well as it should be able to be resorbed and deformed depending on the mechanical and biological requirements of the body. These requirements on the bone, coupled with its role in maintaining mineral homeostasis, strongly suggest that it is an organ of optimum structural design. To fulfill these structural and functional relationships adequately, bone is constantly being broken down and rebuilt in a process called remodeling. Bone has the potential to adapt its architecture, shape, and mechanical properties via a continuous process termed adaptation in response to altered loading conditions (Burr *et al.*, 2002; Yousefghahari & Guran, 2013). Under normal states of bone homeostasis, the remodeling activities in bone serve to remove bone mass where the mechanical demands of the skeleton are low, and form bone at those sites where mechanical loads are transmitted sufficiently and repeatedly. An early hypothesis about the dependence of the structure and form of bones, and the mechanical loads they carry, was proposed by Galileo in 1638, and was first described in a quantitative manner by Wolff in 1892. The adaptive response of bone has been a subject of research for more than a century and many researchers have attempted to develop mathematical models for functional adaptation of bone.

In this paper, we will first present a brief review of the bone structure, mechanics, and remodeling process. Then, the biomechanics of osteoporosis and its relation with bone remodeling process will be discussed. We close this article with a section on important issue of bone quality.

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Damage Diagnosis of the Tallest Pure-Brick Tower in the World Using a Robust Digital Image Analysis System

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In this talk we report on recent progress in the treatment of visual damage analysis of a historical monument by using a novel digital image analysis system. To that end we apply some imageprocessing techniques on taken images by a camera or obtained by photogrammetric methods.

Colored images acquired with a digital camera or photogrammetric methods were evaluated for damage identification and digital image processing techniques such as image enhancement and edge detection were used to identify affected textures. Also Several unsupervised classification and clustering algorithms were applied to evaluate and quantify structural damage in the tallest pure-brick tower in the world.

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Density Modeling Using Monte Carlo: Application in Risk Management

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In this work we consider the problem of simulation of unknown density based on a given sample. The described method includes B-spline approximation, least squares method and Monte Carlo method for calculating integrals. We apply this method to the problem of measuring the risk in a portfolio of assets. Simulation is useful in estimating the profit and loss distribution of a portfolio and thus in computing risk measures that summarize distribution.

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Statistical Algorithms for Estimation of Brown Bears' Population in Bulgaria

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The brown bear (Ursus arctos) is the most widespread bear in the world. It can be found across Europe, Asia and North America in habitats ranging from forests to dry deserts and tundra. Despite its adaptability, the species is protected in Bulgaria. That is why it is important to estimate habitat use and population dynamics of brown bears in the country.

In this work we study the population of brown bears in Bulgaria by statistical approaches, using data received from the National monitorings that were carried out in Autumn 2011/2012. We present some approaches and ideas for algorithms that should be integrated in a framework for modeling and estimation of brown bears' population in the country.

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Variational Modeling in Nonsmooth Mechanics and Stability Results

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This contribution surveys recent nonsmooth problems in diverse fields of mechanics ranging from unilateral contact without/with friction to Bingham fluids and Stokes flow with friction/leak boundary conditions. We discuss various variational modeling approaches including multi-field variational models in the steady-state case and dynamic case that lead to mixed (differential) variational inequalities (see

[1]). This motivates the study of well-posedness and stability of such variational inequalities with respect to perturbations of the data. This issue of stability is shown to be strongly connected with the convergence of higher order approximation in the numerical solution of those problems (see [2]).

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Finite Element Approximation of Higher Order for Nonsmooth Problems and Time Discretization by Implicit Runge-Kutta Methods

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In this talk we address higher order FEM approximation for unilateral problems including nonsmooth friction-type functionals. Such an approximation leads to a nonconforming discretization scheme. Then in contrast to previous related work we approximate such nonsmooth functionals using Gauss-Lobatto quadrature and take the quadrature error of the friction functional into account of the error analysis.

Moreover we are concerned with full space time discretization of related nonsmooth parabolic and evolutionary inequality problems employing implicit Runge-Kutta metods for time discretization. This talk is based on the recent work [1,2].

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User-Level Framework for Performance Monitoring of HPC Applications

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The analysis of performance monitoring of the High-Performance Computing (HPC) applications can be useful for the user as diagnostic for the overall performance of his applications. The existing monitoring tools for HPC provide to the user only aggregated information for all applications on the base of previously defined conditions by someone with administrative rights. Usually, the user does not have permissions to select only the relevant information for him and for his applications. In this article we present a framework for performance monitoring of the HPC applications. The framework provides standardized performance metrics, which the user can use in order to monitor his applications. Furthermore as a part of the framework a program interface is developed. The interface allows the user to publish metrics data from his application and to read and analyze gathered information. Publishing and reading through the framework is possible only with grid certificate. Therefore the user is authorized to access only the data for his applications.

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Nonlinear Second-Degree Model of Laser Efficiency of CuBr Laser

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Metal vapor lasers are widely applied in medicine, physics, chemistry, ecology, techniques and more. The essential increase of their output power provides the significant enlargement of their application. Along with pure experimental research,

a great number of analytical, statistical and numerical models continue to be of high interest.

A subject of study is CuBr laser, emitting in the visible spectrum – 510.6 nm and 578.2 nm developed in Georgy Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences. For the first time a second degree nonlinear parametric regression model is built on the basis of a great number of experimental data, showing the laser efficiency dependence on 10 independent input physical variables. Two types second degree regression equations are obtained – standardized and unstandardized equation. The adequacy of the obtained statistical model is checked by means of the unstandardized equation of laser efficiency used to compare the calculated model values with the known experimental data. The average relative deviation in the case of high power lasers is estimated to be 4.68%. New computer experiment is realized aiming the creation and development of new laser sources of higher efficiency. Laser sources with efficiency higher than the existing experimental data are obtained using new values of the independent physical variables. This allows significant decrease of time and means for development of this type of laser sources in future research. New estimation for the degree of influence of each one of the physical variables on laser efficiency is done using the standardized regression equation. Grouping of all quantities of the unstandardized equation and laser efficiency in three factors is realized using the method of factor analysis. In such a way the quantities having strong correlations with the laser efficiency are detected. A coincidence with the results from the standardized equation is obtained.

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Short-Time Air Pollution Forecasts Using Predictive Modeling Techniques

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Two type of predictive modeling techniques – seasonal ARIMA and a new Generalized PathSeeker Regularized Regression (GPS method) [1-3] have been used for modeling the data of ambient air quality. The models are built for measured data of primary air pollutants as particulate matter and sulphur in the town of Shumen, Bulgaria. The time series analysis was carried out based on hourly data with respect to six meteorological variables. The constructed models have been used for short-term forecasts. The obtained results demonstrate the advantages and applicability of the GPS method over seasonal ARIMA modeling. This gives a new perspective for preventing the possible pollution problems in urban areas.

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Euler-Poincaré Equations for G-Strands

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A G-strand is a map $g(t,s)$ from a domain $(t,s) \in \mathbb{R} \times \mathbb{R}$ into a Lie group G, that follows from Hamilton's principle for a G-invariant Lagrangian. G-strands on finite-dimensional groups satisfy evolutionary PDEs in $1+1$ space-time, defined on $\mathfrak{g} \times \mathfrak{g}^*$. Some of these G-strand equations are completely integrable Hamiltonian systems that admit zero-curvature representation (Lax pair) and soliton solutions. An example for SO(3)-strand is the chiral model. We give some more examples of G-strands for matrix Lie groups, as well as examples for Diff($\mathbb{R}$)-strand equations with solutions in $2+1$ space-time with singular support (e.g., peakons). One of the examples is a complexification of the Camassa-Holm equation. Investigations on the peakon solutions of the obtained equations is presented.

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Some Hierarchical Models for Cusped Elastic Prismatic Shells

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I.Vekua constructed hierarchical models for elastic prismatic shells, in particular, plates of variable thickness, when on the face surfaces either stresses (Model I) or displacements (Model II) are known. In the present paper other six hierarchical models for cusped, in general, elastic prismatic shells are constructed and analyzed, when on the face surfaces (i) a normal to the projection of the prismatic shell component of a stress vector and parallel to the projection of the prismatic shell components of a displacement vector (Model III), (ii) a normal to the projection of the prismatic shell component of the displacement vector and parallel to the projection of the prismatic shell components of the stress vector are prescribed. Hierarchical Models we will call Model V and Model VI, when on the one face surface conditions (i) and on the other one conditions (ii) are known. Besides we construct hierarchical model when on the upper face surface stress vector and on the lower face surface displacements (Model VII) and vice versa (Model VIII) are known. Moreover, other eight hierarchical models for prismatic shells with mixed conditions on face surfaces are constructed. In the zero approximations of the models under consideration peculiarities (depending on sharpening geometry of the cusped edge) of correct setting boundary conditions at edges are investigated. In concrete cases some boundary value problems are solved in an explicit form.

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Efficient Meshless Solutions to Multi-Dimensional Integral and Partial Differential Equations

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Radial basis functions (RBFs) can be seen as a major generalization of pseudospectral methods, abandoning the orthogonality of the basis functions and in return obtaining much improved simplicity and geometric flexibility. Spectral accuracy becomes now easily available also when using completely unstructured node layouts, permitting local node refinements in critical areas. With RBFs, we use

data location dependent expansion functions, and give up all orthogonality features. In exchange, it transpires that one can gain a wide range of advantages, including complete geometric .exibility with regard to both domain shapes and node layouts, as well as freedom from mesh generation. RBFs are means to approximate multivariable (also called multivariate) functions by linear combinations of terms based on a single univariate function or RBF. This is radialised so that in can be used in any dimension. They are usually applied to approximate functions that are only known at a finite number of points, so that then evaluations of the approximating function can take place efficiently.

A radial basis function, $\phi_j(\vec{\mathbf{x}}) \in \Re^d$, $d \geq 1$, is a univariate function that depend only upon the radial distance, $\|\vec{\mathbf{x}} - \vec{\mathbf{y}}\|$, $\vec{\mathbf{x}}$, $\vec{\mathbf{y}} \in \Re^d$. It shall be understood that $\phi_j(\vec{\mathbf{x}}) = \phi(\|\vec{\mathbf{x}} - \vec{\mathbf{y}}_j\|)$ is an RBF evaluated at $\vec{\mathbf{x}}$ having a data center at $\vec{\mathbf{y}}_j$. In numerical mathematics, there is the Platonic dilemma of the world of ideas and world of shadows. RBFs can be algebraic functions with com- pact support or transcendental C^∞ functions, both of which exist in the world of ideas. However, in computer applications (the world of shadows) transcendental functions are expressed as either Pade approximates or finite series expansions possessing finite order. Compactly-supported RBFs (CS-RBFs) are of order k and have limited bandwidth; their convergence rates increase as their band- widths increase or the order increases. Globally supported C^∞ RBFs possess exponential convergence rates that require global support or very broadbanded support. Exponentially convergent RBFs were chosen because they have the best potential to deal with the curse of dimensionality. C^∞ RBFs that have a set of associated shape parameters, σ_j, having the form $\phi_j(\vec{\mathbf{x}}) = \phi(\|\vec{\mathbf{x}} - \vec{\mathbf{y}}_j\|/\sigma_j^2)$.

Two of the most popular C^∞ RBFs are:

$$\phi_j(\vec{\mathbf{x}}) = [1 + (\vec{\mathbf{x}} - \vec{\mathbf{y}}_j)^2/\sigma_j^2]^k, \quad k \geq -\frac{1}{2} \quad \text{(generalized MQ)}, \tag{1}$$

$$\phi_j(\vec{\mathbf{x}}) = \exp\left[-(\vec{\mathbf{x}} - \vec{\mathbf{y}}_j)^2/\sigma_j^2\right] \qquad \text{(Gaussians)}. \tag{2}$$

where σ_j^2 are the shape parameters related to the dilation factors in wavelets. In fact, C^∞ RBFs are a class of non-orthonormalized wavelets, or prewavelets. Given N values of a continuous or or discontinuous dependent variable, $\vec{\mathbf{U}} = (U_1, U_2, ..., U_N)^T$ at evaluation centers, $\{\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2, ..., \vec{\mathbf{x}}_N\}$, then the interpolation or imposition of initial conditions is given by:

$$\sum_{j=1}^{N} \phi_j(\vec{\mathbf{x}})\alpha_j(t) = U(\vec{\mathbf{x}}, t) \tag{3}$$

It is recommended that the independent variables, $\vec{\mathbf{x}}$, $\vec{\mathbf{y}}$ be scaled to a unit cube in $\Re^d$. Domain decomposition methods (DDM) have the benefit of subdividing a large global problem, that is most likely ill-conditioned, into many smaller problems, each of which will have better conditioning. Consider a well-posed set of partial differential equations (PDEs) or integral equations (IEs) over a domain, Ω. Let $\mathfrak{L}$ be either a linear or nonlinear partial differential or integral operator on the interior, $\Omega \setminus \partial\Omega$ of both temporal and spatial operators over N_i points. Let β

be the well-posed boundary condition operator on $\partial\Omega$ over N_B points, such that $N = N_I + N_B$. The problem is thus stated as:

$$LU = \mathbf{f}(\vec{\mathbf{x}}_i) \quad \text{over} \quad \Omega \setminus \partial\Omega, \quad \forall i \in [1.N_I] \tag{4}$$

$$\beta U = \mathbf{g}(\vec{\mathbf{x}}_i) \quad \text{on} \quad \partial\Omega, \quad \forall i \in [1.N_B]. \tag{5}$$

where $\mathbf{f}(\vec{\mathbf{x}}_i)$ is the PDE forcing function, and $\mathbf{g}(\vec{\mathbf{x}}_i)$ represents the consistent Dirichlet, Neumann, or Robin forcing functions. A summary of the many applications and a discussion of the applications of MQ-RBFs to solve PDEs can be found in [1]. In this presentation, a survey of some applications of hyperbolic, parabolic, elliptic PDEs and weakly singular IEs will be given.

The main problem with multi-dimensional problems is the curse of dimensionality requiring increasingly more computer memory and speed. RBFs are meshless methods that readily treat scattered data problems over irregular domains by casting multivariate problems into univariate problems. C^∞RBFs possess exponential convergence and is combined with overlapping domain decomposition to solve the inviscid time-dependent Burgers' equations, see [2]. Using a power law distribution of shape parameters, it was observed that for increasingly .at shape parameters, the maximum eigenvalues of the time advance matrix tend toward unity from above. Thus two goals were accomplished: 1. Minimization of the number of discretization points; and 2. Stability of the time marching scheme. The domain, a unit cube in $\Re^4$, was decomposed into 16 overlapping subdomains. The exact solution of the inviscid Burgers' equations have either a cosine or exponential dependency. The max norm error average for each case was 0.002 and 0.0028 with a crude discretization pushing the MQ shape parameters to very flat limits. MQ-RBFs has the following properties: (1) They converge exponentially as ν^μ ($\nu < 1$, $\mu = c/h$), where c is the average shape parameter and h is the average data center separation, (2) C^∞ RBFs, because they are global in nature, can give rise to a badly conditioned set of equations. For computers with 32 bit chip, any solution, obtained with condition numbers above 10^{16} is unreliable due to round-off errors. Huang *et al.* [3,4] used the c-refinement method with C^∞ RBFs and used arbitrary precision arithmetic (APA) with a coarse discretization. They conclusively demonstrated that the roadblock to high accuracy and efficiency is the 32 bit chips having limited precision. MD problem that can lead to disease cures on the molecular and cellular level. String theory that may hold the key for unifying the laws of physics is a MD problem. Accurate modeling of turbulence with generalized Boltzmann kinetics (6D problem) is still an unsolved mechanical problem. These problems can be solved with APA modeling the governing equations with C^∞ RBFs.

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Randomized Quasi-Monte Carlo Algorithms Approximating Eigenvalues

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Randomized quasi-Monte Carlo (QMC) methods combine the advantages of Monte Carlo and quasi-Monte Carlo methods. They are based on scrambled low discrepancy sequences. The purpose of randomization in QMC is twofold. Primarily, it provides a practical method to obtain error estimates by treating each scrambled sequence as a different and independent random sample from a family of randomly scrambled sequences with low discrepancy. Thus, randomized QMC overcomes the main disadvantage of QMC while maintaining the favorable convergence rate of QMC. Secondarily, scrambling gives a simple and unified way to generate quasirandom streams for parallel and distributed computing environments. This motivated us to apply scrambled quasirandom sequences to approximate calculations of extreme eigenvalues. In this paper we review the scrambling approaches, describe a new algorithm for scrambling of Sobol sequence and study its use for solving the eigenvalue problem by quasi-Monte Carlo Power Iterations. We compare the performance and accuracy of the algorithm with other quasi-random and pseudo-random sequences.

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A Four-Level Conservative Finite Difference Scheme for Boussinesq Paradigm Equation

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A family of nonlinear conservative finite difference schemes for the multidimensional Boussinesq Paradigm Equation is considered. The schemes include values of the numerical solution on four consecutive time levels and have second order of approximation in space and time. A preservation of the discrete energy for the numerical solutions is proved.

The schemes have been tested on two one-dimensional models. The numerical experiments demonstrate the accuracy of the solutions and the preservation of the discrete energy in time.

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Propagation Behavior of Ultrashort High-Intensity Light Pulses

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Spatiotemporal dynamics of ultrashort high-intensity light pulses is investigated based on numerical solutions of (3+1)D nonlinear Schrödinger equation and (3+1)D nonlinear envelope equation. The physical models within the specified cases are presented. Some distinct propagations regimes are found. Pulse compression and generation of high-intensity ultrashort light pulses down to single-cycle regime is investigated. Correspondence between numerical and experimental results is discussed.

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Cryptanalysis of a Modified Encryption Scheme Based on Bent Boolean Function and Feedback with Carry Shift Register

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We propose a modified encryption scheme based on 128 bit bent Boolean function and Feedback with Carry Shift Register. We estimated the output bits properties by the NIST, DIEHARD and ENT test packages. The results of the cryptanalysis show that the new cryptographic scheme provides an exclusive level of data security.

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Broad-Band Laser Pulses. Linear and Nonlinear Regime

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Nano- and picocecond optics can be characterized as optics of narrow band pulses. The spectral width $\Delta\lambda$ of these pulses is much smaller than their carrying wavelength λ_0. Thus, paraxial spatio-temporal approximated equations well cover the linear and nonlinear evolution of nano- and picocecond optical waves in one isotropic media. Performing short femto- or atosecond pulses, their initial bandwidth can reach values of the order of the main wavelength ($\Delta\lambda \sim \lambda_0$). For such pulses new physical effects as λ^3 diffraction, filamentation, sub-THz coherent generation and others appear. These effects can not be described in the frame of a paraxial nonlinear theory and new non-paraxial evolution equations must be investigated. In the present work we will show that a non-paraxial nonlinear theory well covers these new physical effects.

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Global Existence to Generalized Boussinesq Equation with Combined Power-type Nonlinearities

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We prove global existence and finite time blow up of the weak solutions for the Cauchy problem to the generalized Boussinesq equation

$$\begin{aligned} &u_{tt} - u_{xx} - \beta_1 u_{ttxx} + \beta_2 u_{xxxx} = (f(u))_{xx} \qquad \text{for } x \in \mathbb{R},\ t \in [0,T),\ T \le \infty, \\ &u(x,0) = u_0(x), \quad u_t(x,0) = u_1(x) \qquad \text{for } x \in \mathbb{R}. \end{aligned}$$

The nonlinear term $f(u)$ has combined power-type nonlinearity

$$f(u) = \sum_{k=1}^{m} a_k |u|^{p_k - 1} u, \quad a_k = \text{const},\ a_m \neq 0, \quad 1 < p_1 < p_2 < \ldots < p_m,$$

and the dispersive coefficients are nonnegative, $\beta_1 \ge 0, \beta_2 > 0$. This problem arises in a number of mathematical models of physical processes, for example in the modeling of surface waves in shallow waters. In the original Boussinesq equation the nonlinear term is quadratic but in some models in the theory of atomic chains a cubic-quintic nonlinearities appear.

Under the main assumption guaranteing the existence of a nontrivial ground state solution to the stationary Boussinesq equation, we extend the method of potential wells for general combined power-type nonlinearities. For nonlinearities of the so called generalized Lienard (or generalized Bernoulli) type, i.e., $f(u) = a|u|^p u + b|u|^{2p} u$, we propose a nonstandard potential well method. As an application of the sign preserving properties of the Nehari functional we prove global existence or finite blow up of the weak solution to the generalized Boussinesq equation with subcritical initial energy, i.e., $E(0) < d$. The critical energy constant d is explicitly calculated. Some numerical experiments supporting these theoretical results are presented.

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Galerkin FEM for Inhomogeneous Time-Dependent Fractional Diffusion Equations

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We consider an initial boundary value problem for the inhomogeneous time-dependent fractional diffusion equations with a homogeneous Dirichlet boundary condition and a non-smooth right hand side in a bounded convex polyhedral domain. We study two semi-discrete schemes based on the standard Galerkin and lumped mass finite element methods. An almost optimal estimate is obtained for right hand side $f(x,t) \in L_\infty((0,T), \dot{H}^s)$, $-1 < s \leq 1$. For lumped mass method, an optimal L_2−norm error estimate is established for meshes that have some symmetry property. Finally, we present numerical experiments that confirm the theoretical results.

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Comparative Analysis of High Performance Solvers for Solving Stokes Equation

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We consider the time dependent Stokes equation on a finite time interval and on a uniform rectangular mesh, written in terms of velocity and pressure. A parallel algorithm based on a direction splitting approach is implemented.

We are targeting the massively parallel computer as well as clusters of many-core nodes. The implementation is tested on the IBM Blue Gene/P supercomputer and two Linux clusters.

We compared the results from the direction splitting algorithm with the results from Finite Element software package for solving of Stokes equation.

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Noise-Induced Transitions in a Generalized Verhulst Model with a Reflecting Boundary

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The Verhulst, Gompertz, Richards and Blumberg equations are widely used to describe demographic, biological, physical, economic and medical processes. A more generalized model for the evolution of population sizes, called the generic Verhulst (or generic logistic) equation, is introduced and discussed by Turner et al. [1]. However, this is a deterministic model and does not account of noises (fluctuations) which are inevitable in most natural processes.

Motivated by this circumstance, we have considered a particular subclass of the generic Verhulst model with a multiplicative white noise (fluctuating growth rate) in the presence of a reflecting boundary at the maximal size of the population. The exact formulae for the conditional probability density of the population size and for the probability density for the first-passage time are derived. Particularly, it is shown that an interplay of the self-regulation mechanism and the multiplicative noise can generate, by increasing the noise intensity, a phase transition between two qualitatively different shapes of the stationary probability density. The corresponding critical noise intensity as a function of other system parameters is found. Moreover, a transition of another type is also established: namely, there exists a critical value of an exponent characterizing self-regulation, which marks a transition between different regimes of the stochastical dynamics of the system. By unlimited increase of the noise intensity such a transition corresponds to an abrupt change of the coefficient of variation of population size from a divergent value to a nondivergent one. In the stationary case the analytical formulae for the first and second moments of the poulation size are presented and their behavior versus system parameters is analysed. Some possible applications of the model are discussed.

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Traveling Waves, Impulses and Diffusion Chaos in Autooscillating Media

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In the present work it is shown, that the Kuramoto-Tsuzuki (Ginzburg-Landau) partial differential equation with fixed parameters can have an infinite number of different stable wave solutions, travelling along the space axis with arbitrary speeds, and also traveling impulses and an infinite number of different states of spatiotemporal (diffusion) chaos. Those solutions are generated by cascades of bifurcations of stable two-dimensional tori and singular toroidal attractors according to the FSM (Feigenbaum-Sharkovskii-Magnitskii) theory in the four-dimensional system of ordinary differential equations, to which the Kuramoto-Tsuzuki partial differential equation can be reduced with a self-similar change of variables.

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Erasure Codes in Watermarking and Steganography

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We study the possibility of applying error-control and in partial erasure codes to watermarking and steganography. Our results show that the use of erasure codes in the proposed by us manner improves the robustness and increases the size of the embedded message.

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Large Amplitude Vibrations of Timoshenko Beams with Delamination

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Delamination is a major problem in multilayer composite structures. Due to this reason the development of adequate models describing the phenomena arising in the delaminated part of the structure is a very important topic for the practice.

In most of the dynamic behavior models of the beam with delamination the shear forces during the sublaminate interaction and the additional damping arising due to sliding between sublaminates are neglected. A model of the dynamic response of a composite Timoshenko beam which takes into account the above mentioned phenomena was recently developed in [1].

The goal of this work is to extend this model considering the large deflections of beams. Starting from the geometrical, constitutive and equilibrium equations of each layer the governing equations of the beam with delamination are deduced. The inertia terms in longitudinal directions are neglected. The contact phenomenon is modeled by considering each contacting sublaminate acting as a two-parametric elastic foundation on which the other contacting sublaminate is resting. However, the possibility of separation (opening of the delaminated area)and friction between the delaminated layers is taken into account.

Numerical calculations of the problems are done by using the finite differences method. The obtained ordinary differential equations in the time domain are solved by an iteration procedure using the Gears method.

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Traveling Wave Solutions of the Boussinesq Paradigm Equation

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The one-dimensional quasi-stationary flow of inviscid liquid in a shallow layer with free surface is described by the so-called Boussinesq Paradigm Equation [1]. This equation appears also in the theory of longitudinal (acoustic) vibrations of rods and in continuum limit for lattices. As it is well known [2], this equation admits a one-parameter family of traveling wave solutions expressed in an analytic form through the cosh function. The mechanism of evolution of interacting solitary waves with initial condition comprised by the superposition of two analytical cosh soliton solutions is investigated in [3]. In the present contribution new analytic solutions to this equation representing traveling waves are obtained. These solutions are expressed through Weierstrass and Jacobi elliptic functions, which in some cases reduce to elementary functions.

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Discrete Mathematical Model of Wave Diffraction on Pre-fractal Impedance Strips. TM Mode Case

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In this paper considering a TM wave diffraction problem on pre-fractal impedance strips. The overall aim of this work is to developed discrete mathematical model of boundary integral equations (IEs) and to perform numerical experiment with the help of an efficient discrete singularities method (DSM).

The model which is considered in this paper is an approximation of a real fractal antenna in 2D. Fractal antennas are used in a variety of modern mobile devices due to their compact size and broadband properties, which have made them essential in wireless communication, Bluetooth, Wi-Fi and GSM standards. Therefore, numerical analysis of diffraction problems of TM modes on pre-Cantor set of impedance strips on the [-l, l] interval are interesting, challenging and actual problem. To solve a 2D diffraction problem we calculate the total field which satisfies Maxwell's equations, supplemented with Shchukin-Leontovich impedance boundary conditions. Besides, the total field must also satisfy the Sommerfeld radiation conditions and the Meixner edge condition. In TM case the only non-zero component of magnetic field satisfies all the aforementioned conditions and also the two-dimensional Helmholtz equation off the metallic strips. The non-zero electric field components are expressed by Maxwell's equations.

Solving this problem with the mathematical theory of diffraction is a complicated task due to the involved integrals with logarithmic singularities in the kernels. This has raised an objective for us to develop a discrete mathematical model which would resolve these difficulties. We have successfully solved the boundary IEs with the help of a numerical DSM and special quadrature formulas. In this study we have developed an efficient discrete mathematical model and a wide numerical experiment of wave diffraction on strips, and highlighted the efficiency and performance of applied DSM.

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Numerical Simulation of Drop Coalescence in the Presence of Drop Soluble Surfactant

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The target aim of the reported work is development of fast and efficient numerical solution techniques for computer simulations of multiphase flow problems.

Multiphase, and especially, three-phase flows are present in many important application fields, for example, as the gas-oil-water system in porous media.

The phases are assumed immiscible, thus, they interact through sharp interfaces, which are in general difficult to simulate numerically. One possible approach to those problems is the so-called phase-field model, based on the assumption that interfaces between phases/components in a microstructure are diffused, and each phase can be represented by some smoothly varying function, referred to as the concentration. The basic idea is to let the concentration obtain a distinct value in each bulk phase of the mixture and then, sharply but smoothly change from one to another within the interfacial regions. In this way, the need to explicitly track the interfaces is avoided and, thus, also the difficult task to impose and handle proper boundary conditions on those interfaces. Creation, merging and destruction of interfaces, which are major obstacles in the sharp interface models, are implicitly built in the phase-field model.

In this work we consider the discrete structures (block matrices) arising in the numerical treatment of the above problem and propose a solution method that reduces the problem of solving the original very large scale system of algebraic equations to the problem of solving smaller sub-systems with 'easier' matrices, where off-the-shelf broadly available and efficient algorithms are directly applicable. The resulting iterative method exhibits optimal convergence and computational complexity properties.

The efficiency of the resulting solution method is illustrated via various numerical experiments, serial and in parallel, including large scale examples of 2D and 3D problems.

The work is done in collaboration with Owe Axelsson, Petia Boyanova, Minh Do Quang, Martin Kronbichler and Xunxun Wu.

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Green's Formula and Singularity at a Triple Contact Line. Example of Finite-Displacement Solution

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The various equations at the surfaces and triple contact lines of a deformable body are obtained from a variational condition, by applying Green's formula in the whole space and on the Riemannian surfaces. The surface equations are similar to the Cauchy's equations for the volume, but involve a special definition of the 'divergence' (tensorial product of the covariant derivatives on the surface and the whole space). The normal component of the divergence equation generalizes the Laplace's equation for a fluid-fluid interface. Assuming that Green's formula remains valid at the contact line (despite the singularity), two equations are obtained at this line. The first one expresses that the fluid-fluid surface tension is equilibrated by the two surface stresses (and not by the volume stresses of the body) and suggests a finite displacement at this line (contrary to the infinite-displacement solution of classical elasticity, in which the surface properties are not taken into account). The second equation represents a strong modification of Young's capillary equation. The validity of Green's formula and the existence of a finite-displacement solution are justified with an explicit example of finite-displacement solution in the simple case of a half-space elastic solid bounded by a plane. The solution satisfies the contact line equations and its elastic energy is finite (whereas it is infinite for the classical elastic solution). The strain tensor components generally have different limits when approaching the contact line under different directions. Although Green's formula cannot be directly applied, because the stress tensor components do not belong to the Sobolev space $H^1(\mathrm{V})$, it is shown that this formula remains valid. As a consequence, there is no contribution of the volume stresses at the contact line. The validity of Green's formula plays a central role in the theory.

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Sensitivity Study of a Large-Scale Air Pollution Model by Using High-Performance Computations and Monte Carlo Algorithms

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In this work we apply variance-based sensitivity analysis techniques to a large-scale air pollution model, the Unified Danish Eulerian Model (UNI-DEM) in particular. The main purpose of our study is to analyse sensitivity of ozone concentrations with respect to the rates of some chemical reactions as well as to several model input data sets, including the anthropogenic emissions and some meteorological conditions. The current sensitivity study is done for the areas of several European cities with different geographical locations, climate and population.

One of the most widely used techniques for sensitivity analysis, such as Sobol estimates and some their modifications, have been numerically implemented. A vast number of numerical experiments with a specially adapted for the purpose version of the Unified Danish Eulerian Model (SA-DEM) were carried out to compute global Sobol sensitivity measures. SA-DEM was created, implemented and run on IBM Blue Gene/P, the most powerful parallel supercomputer in Bulgaria. The refined (480×480) mesh version of the model was used in the experiments, which is a challenging computational problem even on such a powerful supercomputer like IBM BlueGene/P. Some optimizations with respect to the parallel efficiency and the memory use were performed in SA-DEM. Tables with performance results of numerical experiments on the IBM BlueGene/P are presented and analysed.

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Numerical Characterization of Nematic Liquid Crystal Microstructures under Applied DC Electric Fields

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In the current work we propose an efficient and accurate numerical approach to the problem of electrical characterization of Nematic Liquid Crystal (N-LC) microstructures under the influence of DC electric fields. N-LCs are anisotropic and their electrical properties are determined by the directors' tilt angles which in turn depend on the applied electric field. Therefore, the problem is governed by a coupled system of two-dimensional PDEs: A Poisson equation with variable coefficients for the electric potential and a highly nonlinear second-order equation for the tilt angle of the directors. Both equations are solved using finite-difference schemes with relaxation and the results are found to be in good agreement with the literature. Various 2-D geometries are considered and it is shown that a low DC voltage is sufficient to tune the average refractive index of the N-LC structures under consideration.

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Developing Semantic Representation of Computational Linear Algebra

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In the process of developing an agent-semantic infrastructure for the resource management in the Grid, we have reached the moment, when it became possible to consider support for the Grid users. Specifically, we are in the process of developing a decision support infrastructure that is going to help users in selecting the best

resources for their problems / jobs. The decision support is going to combine semantic data representation (and processing) with Saaty's AHP method.

In order to develop system capable of providing the needed support, it is necessary to ontologically represent knowledge pertinent to the domain(s) of interest. Here, we have selected computational linear algebra (CLA), for the development of the first prototype. To reach this goal, we have collected and taxonomically ordered information about problems, algorithms and libraries, in the selected sub-area of the CLA. In the development process we have involved a number of domain experts. Hence, we were able to capture not only their vision of the structure of the CLA, but also their opinions about appropriateness of different hardware and software combinations. Based on knowledge captured thus far, the aim of our presentation is to report our progress in development of ontology of computational linear algebra. Furthermore, we will illustrate how it can be used in decision support.

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A High Performance Computing Approach for the Simulation of Large-Scale Fluid-Solid Interaction Problems

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A high performance computing approach is described herein for the simulation of large scale Fluid-Solid Interaction (FSI) problems. In this approach, both fluid flow and rigid body dynamics are simulated in a Lagrangian framework, where general rigid body dynamics is coupled to Smoothed Particle Hydrodynamics (SPH) method via Lagrangian markers called Boundary Condition Enforcing (BCE) markers. A parallel simulation algorithm, relying on Graphics Processing Unit (GPU) is developed via CUDA library and is shown to scale linearly. By resolving the rigid-rigid contact via Discrete Element Method (DEM), the framework was implemented to simulate a confined flow containing tens of thousands of arbitrarily shaped rigid bodies. Simulation results for circular cylinder in plane Poiseuille flow, sphere in pipe flow, and transient Poiseuille flow are shown to agree with several experimental and numerical results.

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Open Formula of Runge-Kutta Method for Solving the Initial Value Problem of the Ordinary Differential Equation

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In this paper an open formula of Runge-Kutta method for solving the initial value problem of the ordinary differential equation is introduced, both the first type formula and the second type formula. One example will be illustrated.

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Special Case of the Cahn-Hilliard Equation

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A qualitative behavior of the Cauchy problem solution for the Cahn-Hilliard kind equation is analyzed. The sufficient condition of the global solution existence and its collapse for a finite time for the periodic function has been formulated. The examples of the stationary, self-similar and collapsing solutions are constructed.

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Application of Fitzpatrick Functions Satifying Relaxed One-Sided Lipschitz Conditions for Solving Optimization Problems

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The main purpose of this work is to solve equations and differential inclusions using multi-valued implicit Fitzpatrick functions that satisfy the relax one-sided Lipschitz conditions for solving nonlinear optimization problems. We use their specific properties such as to be maximal monotone, proper convex and lower semicontinuous.

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Resonant Behavior of the Spatial Cross-Correlation for Particles Embedded in Viscoelastic Shear Flow

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The Brownian motion of particles in a fluid is of central importance in chemical and biological physics as well as in material science and engineering [1,2]. Although the behavior of Brownian motion in quiescent fluids has been investigated in detail, little is known about the dynamics of Brownian particles and the hydrodynamic interaction effects in shear flows in spite of their fundamental relevance and importance in microfluidic applications [2].

Motivated by the results of [3] for a particle in Stokes shear flow, we have considered the dynamics of a Brownian particle in a fluctuating harmonic potential well, which is simultaneously exposed to an oscillatory viscoelastic shear flow using the generalized Langevin equation with a power-law-type memory kernel. The influence of a fluctuating environment is modeled by an additive internal fractional Gaussian noise. The exact expressions of the shear-induced cross-correlation between particle fluctuations along orthogonal directions as well as the mean angular momentum of the Brownian particle are found. As our main result we have established that an interplay of shear flow and memory effects can generate a multiresonance of the cross-correlation versus shear frequency and also a resonance of the mean angular momentum vs shear frequency. Specifically, a critical memory exponent is found, which marks a transition between different dynamical regimes of the system. Similarities and differences between the behavior of the models with Stokes friction and with a memory kernel are also discussed. Our results are verifiable in experiments analogous to the one described in [3].

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Weierstrass Transform Associated with the Whittaker Transform Integral

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We introduce Weierstrass transform associated with the Whittaker integral transform and we examine some of its properties. Using reproducing kernel theory, we introduce reproducing kernel related to the Whittaker integral transform.

Joint work with L.P. Castro and S. Saitoh (University of Aveiro).

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Nonequilibrium Transport Phenomena in a Tilted Ratchet Model Subjected to a Multiplicative Trichotomous Noise

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In the recent years, the net voltage and the DC current-voltage characteristics of electrical transport in superconducting junctions subject to noise have witnessed an increasing interest. A corresponding phase model for the equation of motion is applicable in a number of different problems, such as phase locking in electric circuits, mode blocking in ring lasers, motion of fluxons in superconductors, and the penetration of biological channels by ions. Although the influence of white and dichotomous noises on the dynamics of such phase models have been investigated in detail, little is known about the nonequilibrium transport phenomena in the cases of noises with a more general structure. Motivated by this circumstance, we have considered a tilted ratchet model with a sawtooth potential, which mimics the phase model, subjected to a multiplicative trichotomous noise and to an additive white noise. Note that the trichotomous noise (a three level noise) is a generalization of the colored dichotomous noise including as a control parameter the noise flatness the values of which can be varied in the interval $(1, \infty)$. The exact expression of the stationary probability flux W, which mimics the voltage across a Josephson junction, is found, and the dependence of the flux on the system parameters is analyzed. Asymptotic formulas for the flux for slow and fast noise limits are calculated and compared with the results of other authors. It is established that the differential mobility $m = dW/dF$ depends nonmonotonically on the values of tilting force F as well as on the noise parameters. Particularly, in some narrow regions of the tilting force the mobility and the flux as functions of noise parameters show a resonance-like behavior versus the noise flatness and also versus the noise switching rate.

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Mathematical Modeling of Impulsive Loading of Explosive Charge

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The impact of the shock wave from the detonation booster charge of cylindrical from with detonator was studied in this paper. The elastoplastic behavior of materials, formation and propagation of shock waves and other physical factors were taken into account. The experimental study of such objects is often difficult, needs significant resources or impossible. Meanwhile, the mathematical modeling with using modern computer facilities is the best approach to solving these problems.

To describe materials, composing the shell and the explosive substance we use elastoplastic model. We propose here a second order accurate finite-difference numerical scheme that is an extension of Wilkins scheme. This scheme based on the Lagrange coordinates description.

The charge is modeling as steel shell (R – radius, $2R$ – the length, $R/10$ – the thickness of the shell). The charge shell is filled with explosive material having parameters describing by state equation, which is modeling of TNT. The detonator ($R/10 \times R/4$) is in the top of the charge. The detonator is more sensitive to detonation than filling explosive. The impact loading is simulated by explosion of booster charge. The whole structure is surrounded by water saturated ground. The numerical investigations show that the geometry and location of booster charge strongly influences the nature and excitement of detonation of the shell.

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V.I. Arnold and Stability Problems in Solid Mechanics

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Stability problems represent an important field of mathematics having numerous applications in natural sciences and always attracting brilliant scientists. In 1960-70-80-ies Arnold made an outstanding contribution to stability theory. We recall his classical papers and books [1-6] directly or closely related to stability problems. In this paper we give a short review of the results of Arnold on stability problems with modern development and applications in classical and solid mechanics [7-12]. Below three instability problems for parametrically excited systems are considered with some extension to general systems with arbitrary finite degrees of freedom.

A problem of stabilization of a vertical (inverted) position of a pendulum under high frequency vibration of the suspension point is considered. Small viscous damping is taken into account, and periodic excitation function describing vibration of the suspension point is assumed to be arbitrary. A formula for stability region of Hill's equation with damping near zero frequency is obtained. For several examples it is shown that analytical and numerical results are in a good agreement with each other. An asymptotic formula for stabilization region of the inverted pendulum is derived. It is shown that the effect of small viscous damping is of the third order, and taking it into account leads to increasing critical stabilization frequency. The method of stability analysis is based on calculation of derivatives of the Floquet multipliers.

The swing problem is undoubtedly among the classical problems of mechanics. It is known from practice that to set a swing into motion one should erect when the swing is in limit positions and squat when it is in the middle vertical position, i.e. carry out oscillations with a double the natural frequency of the swing. However in the literature you cannot find formulae for instability regions explaining the phenomenon of swinging. In the present paper the simplest model of the swing is described by a massless rod with a concentrated mass periodically sliding along the rod axis. Based on analysis of multipliers the asymptotic formulae for instability (parametric resonance) domains in the three-dimensional parameter space are derived and analyzed.

The third classical problem is the problem of finding instability regions for a system with periodically varying moment of inertia. An equation describing small torsional oscillations of the system with periodic coefficients dependent on four parameters including damping is derived. Analytical results for instability (parametric resonance) regions in parameter space are obtained and numerical examples are presented.

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The Impedance Problem of Wave Diffraction by a Strip with Higher Order Boundary Conditions

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We will consider an impedance boundary-value problem for the Helmholtz equation originated by the problem of wave diffraction by an infinite strip characterized by 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 and Wiener-Hopf operators. The initial problem is considered within a framework of Bessel potential spaces. At the end, the solvability of the problem will be discussed for a range of regularity orders of the Bessel potential spaces.

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Solvability of a Receptor-Toxin-Antibody Interaction Model

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Coupled systems of PDEs and ODEs that are considered in the same domain are well known in theory of differential equations. Modeling of surface reactions leads to coupled systems of parabolic and ordinary or parabolic and integro-differential equations. The latter are determined on the boundary. We consider a coupled system which models a bulk reaction-diffusion and surface-reaction process in the cell receptor-toxin-antibody interaction and prove the existence and uniqueness theorem of a classical solutions. Numerical results will also be discussed.

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Modeling of Gas Flows Through Microchannel Configurations

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Gas flows are an inherent part of various technological processes and applications that are implemented in micro-electro-mechanical systems (MEMS. These microsystems touch almost every industrial field (e.g. fluidic micro-actuators for active control of aerodynamic flows, vacuum generators for extracting biological samples, mass flow and temperature micro-sensors, pressure gauges, micro heat-exchangers for the cooling of electronic components or for chemical applications, etc.). Single microchannels and more complex microchannel configurations are basic elements in such microsystem. In most applications, the flow regime in the microchannels is outside the continuum fluid dynamic description and kinetic theory models and methods must be applied for analysis of the gas flows. We will report on pressure and temperature driven flow simulation in 2D and 3D microchannels by using molecular Direct Simulation Monte Carlo (DSMC) method. Specific theoretical issues will be discussed and numerical results for microchannel confi-gurations with different geometry, such as single straight channel, vertical bend, T-shaped junction, will be presented

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Inverse Scattering Problems for Cracked Piezoelectric Media

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Scattering problems in cracked piezoelectric plane are studied. The solution is based on boundary integral equation representation of the scattered field in the frequency domain. The asymptotic of the fundamental solution and its derivatives in the far field are derived using the stationary phase method. Crack opening area and stress intensity factors (SIF) near the crack edge are determined uniquely by far field data. Numerical examples show the comparison between the identified and actual SIF.

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Stream Cipher Encryption Based on Bent Boolean Function and Chebyshev Polynomials

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In this paper, we study a symmetric cryptosystem based on two Chebyshev polynomials filtered with bent Boolean function. The novel derivative algorithm shows perfect pseudorandom properties established by number of statistical tests.

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Auxiliary Theorems About Some Estimates Above the Modulus of Integrals in the Complex Plane

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In this paper, we make some estimates above the modulus of some integrals in the complex plane. These results are connected to the similar ones, which are bellow the modulus of some integrals in the complex plane.

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A New Multiscale Multilevel Algorithm Applied to Bone Tissue Modeling

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Complex multiscale problems related to computer simulation of deformable porous media are routinely encountered as a part of research and development activities in a number of engineering, environmental and biomedical fields. The studied bone tissuehas have complex hierarchical morphology in the sense that features at scales from the nanometer to millimeter level. Predicting the bio mechanical behavior of such systems with hierarchical structures and multiple, often poorly separated length-scales, is very computationally demanding. In this work, we propose a method that reduces significantly the computational resources applicable to this class of problems.

To achieve that, a highly heterogeneous trabecular bone tissues are considered. The microstructure of the solid phase is extracted from a high resolution computer tomography image. The contribution of the fluid phase is interpreted in terms of almost incompressible material. The related linear elasticity problem is of high contrast and high frequency. The finite element method (FEM) is applied for discretization of the related linear elasticity problem. The efficient PCG iterative solution of such problems is a challenging topic of the numerical methods for large-scale scientific computing.

A separable displacement decomposition preconditioner of a block diagonal form is introduced for the considered 2D model problem. For the decoupled FEM elliptic systems we apply a multilevel technique that incorporates an analytical

effective tensor into the simulation avoiding costly numerical solutions of local problems that are inherent in some other multilevel methods for multiscale problems. The target of this study is to develop computationally efficient numerical tools that will enable to perform predictive simulations as an integral part of osteoporosis treatment.

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Downscaling of Bulgarian Chemical Weather Forecast from Bulgaria Region to Sofia City

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In the paper Bulgarian Chemical Weather Forecast System (BgCWFS), version 3, will be described end the respective end-user products will be demonstrated. Chemical Weather is understood as concentration distribution of some key pollutants in a particular area and its changes during some forecast period. In Bulgaria, a prototype of such a system was built in the frame of a project with the National Science fund. It covers a relatively small domain including Bulgaria that requires the use of chemical boundary conditions from similar foreign systems. The last version of the System is built in the frame of EU FP7 project PASODOBLE. Following its requirements, concentration data for a region of Bulgaria are provided by SILAM System of Finish Meteorological Institute. It operates over the whole European region but is able to provide data for any European sub-domain by its THREDDS service. The customer makes an Internet request containing all necessary parameters - sub-region dimensions, pollutants, period of forecast, etc. in a few minutes, the request is proceeded and all required data is downloaded as a single NetCDF file. This file is post-processed as to obtain the necessary boundary conditions. The new version of the system is built on the base of the nesting approach – two other domains with increasing resolution are nested in the Bulgaria ones downscaling to 1 km space resolution over Sofia city. The System is fully atomized. Computations start at 00 UTC every day and the forecast period is 72 hours. It is based on the well known models WRF (Mesometeorological Model) and US EPA dispersion model CMAQ (Chemical Transport Model). As emission input the 2010 inventory data prepared by Bulgarian environmental authorities is exploited. The results are presented in a respective web-site (http://www.niggg.bas.bg/cw3/)

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Uncertainty Quantification and Simulation in Reanalysis Procedures

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Structural dynamic reanalysis techniques can be defined as the methods by which dynamic behavior of a structure is improved by predicting the modified behavior brought about by adding modifications like those of lumped masses, rigid links, dampers, beams etc. or by variations in the configuration parameters of the structure itself. Such methods have roots in finite element models. Dynamic response of mechanical systems depends of structural parameters. The objective is to evaluate the structural response for successive modifications in the design avoiding the difficult solution of the modified equations. The structural modifications may be caused by external factors or by the designer in order to improve the characteristic of the response (eigenvalues and eigenvectors). Modification of dynamic characteristics means change of corresponding design variables to get desired dynamic behavior of structure. The design variables depend on the type of optimization problem. In the design of structural components, such as stiffened panels and cylinders, the design parameters represent the spacing of the stiffeners, the size and shape of the stiffeners, and the thickness of the skin. The thickness of plates, cross-sectional areas of bars, areas, moments of inertia, and torsion constants of beams represent sizes of the elements. Joints and members could be eventually added or deleted during the design process so that the geometry of the structures may be modified. Reanalysis methods can include next activities. (a) Modification in the geometry with no further change in the number of degrees of freedom. (b) Modification of design variables (mass, damping and stiffness). (c) Increase or reduction of the number of DOFs by changing of the supporting manner and addition or deletion of joints and members. (d) Alteration of kind of material on some places if is it modification possible. The main purpose of dynamic reanalysis is to provide numerical procedures to evaluate the structural response after modifications of design variables.

Most numerical simulations of physical systems are rife with sources of uncertainty. Uncertainty in simulations stems from the stochastic nature of geometric and physical parameters, indeterminate nature of intial/boundary conditions, and inadequacy of physical models coupled with discretization errors.

The paper will discuss about introducing a probabilistic treatment of important problem parameters.

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Modeling of Aircraft Vortex Wake Structure

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Currently, there is an intense increase in air traffic in the world. According to forecasts, by 2015, is expected to increase three times the volume of air transport by civil aviation aircraft. To ensure the necessary capacity of the air space is a complex and actual problem, requiring new approaches to air traffic management.

One of the main difficulties associated with increased airspace capacity, is the problem of vortex safety. Aircraft entering the vortex wake can lead to phenomena like the buffeting (frequency resonant excitation of the elements of the aircraft structure), bumpiness aircraft uncontrollable angular velocity of roll (-200 . 200 /s) with the loss of altitude (up to 150 . 200 m) as well as the loss of the aircraft controllability.

In this connection between the aircraft must provide a minimum distance of 4D-space, to avoid or minimize the effect of falling into the vortex wake in front of an airplane.

One way to increase throughput is to reduce existing separation minima between aircraft on the wake turbulence conditions imposed in the early 70's. According to many experts, the existing ICAO wake vortex separation rules don't fully meet modern requirements. However, to justify the restrictions on the possibility of changing the conditions of vortex safety it is necessary a deep understanding of the structure of the wake vortex and the evolution of the aircraft trail in a stratified atmosphere.

The most complex in terms of both the need to increase airport capacity, and from the point of view of vortex safety is the regime of landing. After landing the first aircraft it takes some time for the decay of the vortices formed and areas of turbulence. This waiting time depends on weather conditions as well as the structure of the vortex wake landing aircraft. The fact is that the regime of landing aircraft is flying with extended mechanization wing, leading to the formation of complex structures multi vortex wake. The dynamics of such a vortex structure is complicated by the fact that the evolution of the vortex trail is close to the earth's surface.

The proximity of the underlying surface causes the increasing role of the viscous wake vortex interaction with the boundary layer. In this work we analyze the formation mechanisms of the vortex wake structure for aircraft with different wing shape in the plan that are flying close to or away from the underlying surface with cleaned or released mechanization wing.

Studies based on direct numerical simulation (DNS) of the turbulent flow of a perfect, non-viscous, incompressible, weightless and non-heat-conducting gas. This model is valid for Mach numbers M¡0.3, which is consistent with the velocity of aircraft movement in landing mode. The use of direct numerical simulation allows to manage without recourse of near-wall functions which determine the characteristics of the flow profiles employed for the calculations on crude meshes.

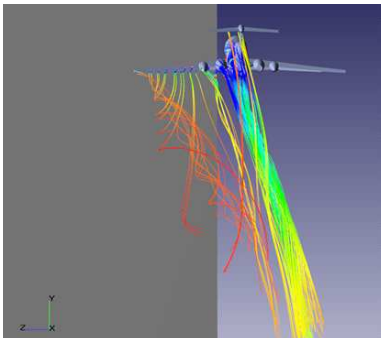
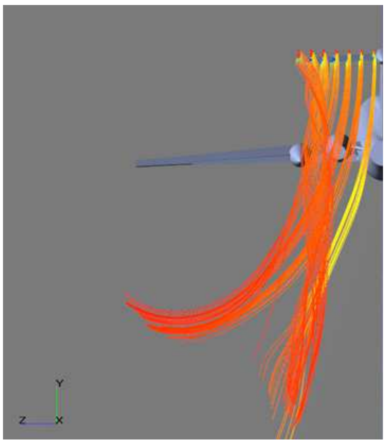


Figure 1



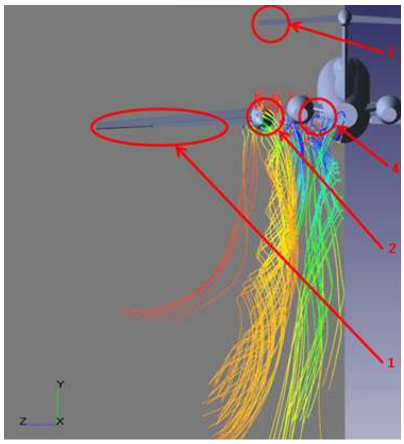
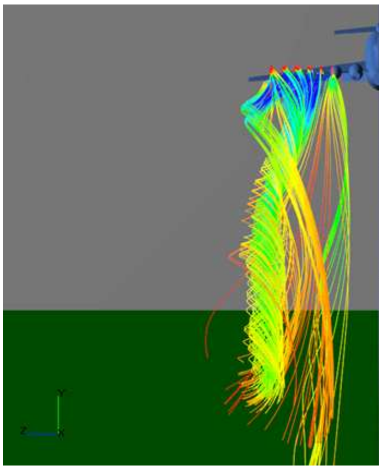


Figure 2 Figure 3

Scheme for solving the Navier-Stokes equations is based on a modification of the method of splitting on physical variables and allows calculations at any Mach number, including the incompressible flow. The calculations used absolutely steady implicit variant of the method of splitting. The equations approximation is based on the finite volume approach to accurately approximate the laws of conservation at the level of separated cells.

Figures 1-3 show as example the formation scheme of the vortex wake structure behind the aircraft Tu-154, that is flying away from the underlying surface with released at 10 degrees mechanization wing. You can see that the current streamlines ending with the tail goes right, and from the middle of empennage they are captured with wing tip vortices. It can be seen that the flap fluctuation has little influence on the formation of wake vortex, which is formed mainly due to the collapse of the vortex sheet, coming down from the end of the wing.



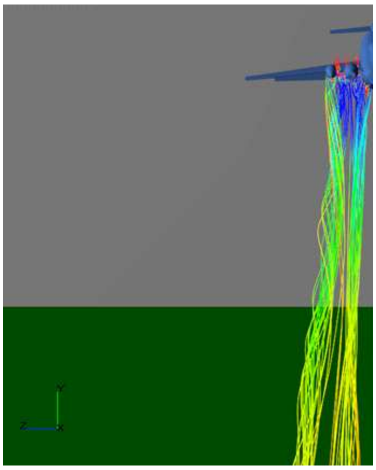


Figure 4 Figure 5

At the increase of the mechanization deviation angle the character of vortex trail formation behind the plane changes significantly (Figs. 4, 5, deviation angle of flaps is equal 45 degrees). Analysis of the results shows that the first bundle is formed due the vortex sheet coming down from the wing tip and the outer part of the flap. The second bundle is formed by the folding of the vortex sheet coming down from the inside of the flap.

Dynamics of formation of vortex wake is visually presented in Fig. 6, which shows that the emerging first multi vortex flow structure (section 1 in Figure 6) gradually by combining areas of vorticity is transformed to a two-vortex structure. Formation of a two-vortex structure of the flow is at a distance of 10 - 12 wingspan. It should be noted that the flight of an airplane at a sufficiently high altitude (more than the wingspan) the wake vortex interaction in the initial part of its evolution with the boundary layer of the earth does not occur, as it can be clearly seen in Fig. 6.

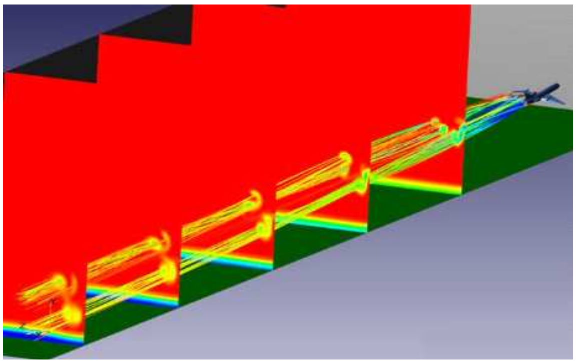
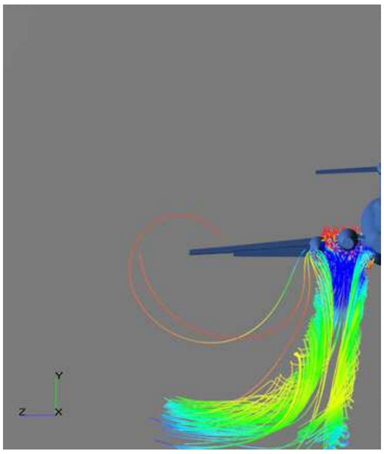


Figure 6



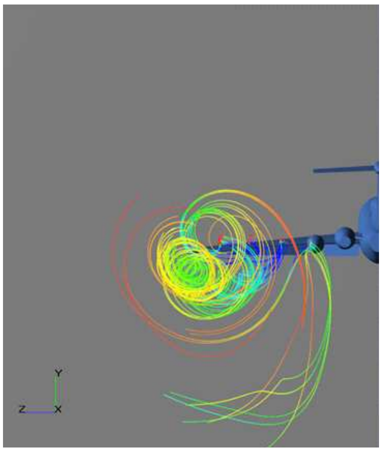


Figure 7

Figure 8

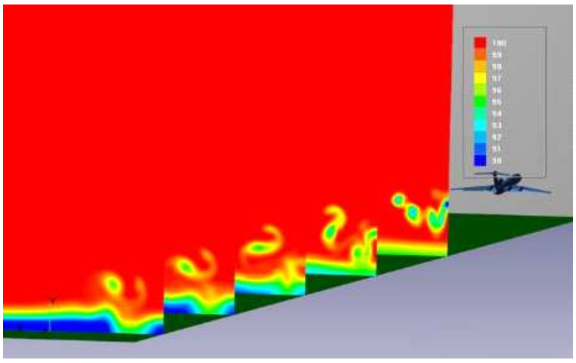


Figure 9

With decreasing aircraft altitude the wake vortex evolution after aircraft for the initial part is modified. On Figs. 7, 8 is set an example of structure formation vortex wake of an aircraft that is flying at a height equal to half the wingspan, with a deviation of 45 degrees mechanization.

You can see that a single vortex is mainly formed. This character of wake vortex formation at low altitude due, as shown in Fig. 9, intensive interaction with the boundary layer of the underlying surface.

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MARS Models of Laser Efficiency of Copper Bromide Laser

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New results of statistical modeling of data on laser efficiency of copper bromide lasers using the nonparametric method of multivariate adaptive regression splines (MARS). Linear and nonlinear models are built, based on original data of families of copper bromide lasers, developed in Laboratory of Metal Vapor Lasers of Institute of Solid State Physics of Bulgarian Academy of Sciences during the last 30 years. The obtained models are applied for estimating the values of laser efficiency, as well as for directing and predicting of future experimental studies in order to improve the laser performance.

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Evaluation of Fast Neutron Spectrum from IREN

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Fast neutron source IREN recently was commissioned in JINR. Neutrons was generated by the accelerated electron beam burst periodically (40 msec) impinging onto wolfram or natural uranium target at short time intervals about 100 ns.

Powerful bremsstrahlung radiation cause giant dipole resonance (GDR)in target nuclear creating neutron radiation. The neutron radiation was analysed using time-of-flight (TOF) technique with BC501 liquid scintillator located at approximately 60 meter flight path from the target. The digital pulse processing apparatus was implemented for neutron velocity measurements along with neutron pulse shape analysis. Digital pulse processing algorithms are presented and the source neutron spectrum evaluation is discussed in the presentation.

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