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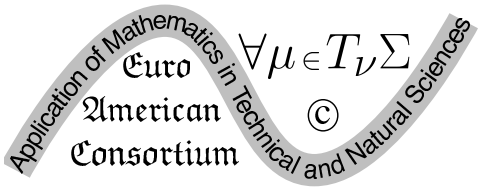
BOOK OF ABSTRACTS



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Unified Theory of Matter

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We are in front of the tremendous catastrophe in modern theoretical physics. Moreover, we have reached the revolutionary situation not only in physics but also 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. It is impossible to believe that in more than 300 years after Newton, we have the situation when 96% of matter and energy is of unknown origin. Recently the scientific community was convinced that the following physics development could lead only to rather small corrections in the modern theoretical physics. So to speak-4% corrections to 96% of the known results, but not quite the reverse! Now many scientists are aware that some way out will be achieved after creation of the unified theory of transport processes working from the structure of so-called elementary particles to the Universe evolution. This theory is really created and presented in particularly in [1-7]. As it is shown in these monographs and articles, the origin of difficulties consists in the total oversimplification inherent in local physics of the dissipative processes. In the latter part of twentieth century, two very important results were obtained:

(1) The Irish physicist John Stewart Bell (1928-1990) was to show that all local statistical theories of dissipative processes are wrong in principal.

(2) The Russian physicist Boris V. Alexeev was to show that the derivation of kinetic equation with respect to one-particle distribution function from the BBGKY equations (prior to introducing any approximation destined to break the Bogolyubov chain) leads to additional terms of the non-local origin, generally of the same order of magnitude, appear in the Boltzmann equation. Then the passage to the Boltzmann equation means the neglect of non-local effects. These additional terms cannot be omitted even in the limit cases of kinetic theory, therefore Boltzmann equation is only a plausible equation.

Therefore, the case in point is of unprecedented situation in physics, when the fundamental physical equation is revised. During my stay in Marseille as invited professor, A.J.A. Favre reminds me Henri Poincaré's phrase after the death of a great Austrian physicist – "Boltzmann was wrong, but his mistake is equal to zero." It is a pity, but the situation in kinetic theory is much more serious. 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;

9) Cold nuclear fusion;

10) Strict physical theory of levitation;

11) Time quantization and physical sense of the Nyquist-Shennon-Kotelnikov theorem.

Solution of all problems given above can be found by methods of non-local physics [5].

But what does it mean from the physical point of view – to create the unified theory of matter? It means:

(1) The concept of matter is the notion uniting the description of particles evolution, fields and physical vacuum.

(2) "Particles" can have the masses of rest which are equal (or not equal) to zero.

(3) The mathematical description can be realized in the frame of a unified mathematical apparatus for the tremendous scale diapason from the structure of so-called elementary particles to the Universe evolution.

It is well known that this problem was considered by A. Einstein but without success. Let us consider the genesis and evolution of the mentioned unified theory from the position of non-local physics. It is reasonable to divide the non-local theory evolution in two time periods. The first stage (conventional speaking) corresponds to the years 1982 (see [1])-2004 (see [4]). Main ideas of this period can be formulated as follows.

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 the 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 $f_{sm,2}(\mathbf{r}_1, \mathbf{v}, t)$ – 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 $f_{sm,2}(\mathbf{r}_1, \mathbf{v}, t)$ 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_1 and moves toward PhSV_2, introduces information about the DF $f_{sm,2}(\mathbf{r}_1, \mathbf{v}, t)$ 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 for example in [1-6].

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.

THE MAIN MISTAKE OF LOCAL PHYSICAL KINETICS CAN BE INDICATED AS FOLLOWS: This entire complex of the mentioned 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) fully ignores non-local effects and contains only the local collision integral J^B. The foregoing non-local 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. All of the known methods of deriving kinetic equation relative to one-particle DF f (including the method of many scales, the method of correlation functions, the iteration method) lead to appearance in the Boltzmann equation some additional fluctuation terms which cannot be omitted even in the limit cases of kinetic theory.

Now several remarks of principal significance:

1. All fluctuations are found from the strict kinetic considerations and tabulated [2-4]. The appearing additional terms in 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.

2. Fluctuations on the wall are equal to zero, from the physical point of view this fact corresponds to laminar sub-layer. Mathematically it leads to additional boundary conditions for GHE.

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 Euler equations in hydrodynamics. But 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. Many GHE applications were realized for calculation of turbulent flows with the good coincidence with the bench-mark experiments. GHE are working with good accuracy even in the theory of sound propagation in the rarefied gases where all moment equations based on the classical BE lead to unsatisfactory results.

5. The non-local kinetic effects listed above will always be relevant to a kinetic theory using one particle description - including, in particular, applications to liquids or plasmas, where self-consistent forces with appropriately cut-off radius of their action are introduced to expand the capability of GBE. The application of the above principles also leads to the modification of the system of the Maxwell electro-dynamic equations.

On this stage of investigation I used the terminology – generalized Boltzmann equation. Strictly speaking it was not still a unified theory of matter because the theory did not contain the description of very large physical system (including Universe) and very small systems (quantum mechanical systems). On the second stage the mentioned above systems were included in the consideration after 2004 (see for example [5]-[7]). Let us turn our attention to the quantum hydrodynamic

description of individual particles. The abstract of the classical Madelung's paper [8] contains only one phrase: "It is shown that the Schrödinger equation for one-electron problems can be transformed into the form of hydrodynamic equations." It means that evolution even a single electron can be "smeared" in hydrodynamics! The following conclusion of principal significance can be done from the consideration [5]:

1. Madelung's quantum hydrodynamics is equivalent to the Schrцdinger equation (SE) and leads to the description of the quantum particle evolution in the form of Euler equation and continuity equation. Quantum Euler equation contains additional potential of non-local origin which can be written for example in the Bohm form. SE is consequence of the Liouville equation as result of the *local* approximation of *non-local* equations.

2. Generalized Boltzmann physical kinetics leads to the strict approximation of non-local effects in space and time and *in the local limit* leads to parameter τ, which on the quantum level corresponds to the uncertainty principle "time-energy."

3. Generalized hydrodynamic equations (GHE) lead to SE as a deep particular case of the generalized Boltzmann physical kinetics and therefore of non-local hydrodynamics.

In principle GHE needn't in using of the "time-energy" uncertainty relation for estimation of the value of the non-locality parameter τ. Moreover the "time-energy"uncertainty relation does not lead to the exact relations and from position of non-local physics is only the simplest estimation of the non-local effects.

Really, let us consider two neighboring physically infinitely small volumes PhSV_1 and PhSV_2 in a non-equilibrium system. Obviously the time τ should tend to diminishing with increasing of the velocities u of particles invading in the nearest neighboring physically infinitely small volume (PhSV_1 or PhSV_2):

$$\tau = H/u^n. \tag{1}$$

But the value τ cannot depend on the velocity direction and naturally to tie τ with the particle kinetic energy, then

$$\tau = H/(mu^2), \tag{2}$$

where H is a coefficient of proportionality, which reflects the state of physical system. In the simplest case H is equal to Plank constant $\hbar$ and relation (2) becomes compatible with the Heisenberg relation. Possible approximations of τ – parameter in details are considered in monograph [5] and as well as the general principle of quantizations.

It is shown that non-local hydrodynamic form of equations is applicable to the description of the very large physical systems like Universe. The unified theory includes the effects:

1. Hubble expansion of Universe and Hubble expansions in so called Hubble' boxes;

2. Movement description in Black Holes;

3. Explosion (Big Bang) of physical vacuum.

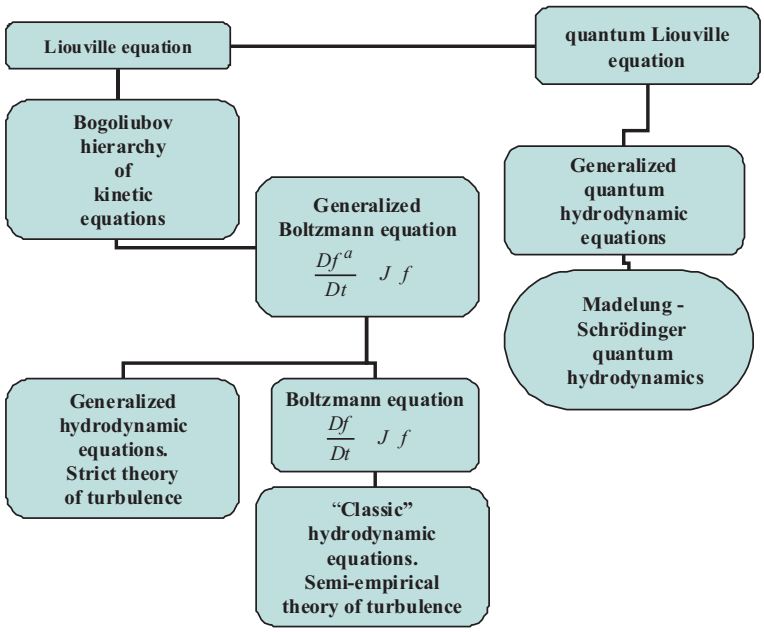
The relativistic generalization of the Unified Theory can be found in monographs [5,7]. As an example of the following theory development we demonstrate in our report the time quantization in the frame of non-local relativistic physics and connection with Shannon-Nyquist-Kotelnikov theorem [9-11]. It is shown:

1. Solutions of the relativistic non-local hydrodynamic equations are obtained for two kinds of distribution functions: δ- function (imitating the laser impulse) and Plank function. Both solutions have the character of the propagating waves without damping (for δ-function) and the propagating waves with damping (Plank function);

2. Non-local relativistic physics (in the frame of non-local relativistic hydrodynamics) leads to the time quantizing for photon gas;

3. The aim of the sampling theorem consists in obtaining a formula for reconstruction of the original signal using the special choice of the discrete time moments. The constructive proof of the theorem leads to an understanding of the aliasing that can occur when a sampling system does not satisfy the conditions of the theorem. From the first glance the sampling theorem has only mathematical content leaving aside the physical origin of the time quantization. It is shown that the sampling theorem is a consequence of relativistic non-local physics;

4. The mentioned above results do not depend on the choice of the non-local parameters. As an additional explanation we place on the figure the structure of the generalized transport theory.



References

[1] B.V. Alekseev, Matematicheskaya Kinetika Reagiruyushchikh Gazov (Mathematical Theory of Reacting Gases), Nauka, Moscow, 1982. [in Russian]
[2] B.V. Alexeev (1994) The Generalized Boltzmann Equation, Generalized Hydrodynamic Equations and their Applications, *Phil. Trans. Roy. Soc. Lond.* **349**, 417.
[3] B.V. Alexeev (1995) The Generalized Boltzmann equation, *Physica A***216**, 459.
[4] B.V. Alexeev, *Generalized Boltzmann Physical Kinetics*, Elsevier Amsterdam, The Netherlands, 2004, 368p.
[5] B.V. Alexeev, *Unified Non-local Theory of Transport Processes*, Elsevier Amsterdam, The Netherlands, 2015, 644p.
[6] B.V. Alexeev, Nelokal'naya fizika. Nerelyativiskaya teoriya, Lambert, Saarbrücken, 2011, 499p.
[7] B.V. Alexeev, I.V. Ovchinnikova, Nelokal'naya fizika. Relyativiskaya teoriya, Lambert, Saarbrücken, 2011. 406p.
[8]. E. Madelung (1927) *Zeitschrift für Physik* **40**, 322–326.
[9] H. Nyquist (1928) Certain topics in telegraph transmission theory, *Trans. AIEE* **47**, 617–644.
[10] V.A. Kotel'nikov, O propusknoj sposobnosti efira i provoloki v elektrosvyazi, Vsesoyuznyi energeticheskii komitet, Materialy k I Vsesoyuznomu sezdu po voprosam tehnicheskoj rekonstrukcii dela svyazi i razvitiya slabotochnoj promyshlennosti, 1933. Reprint stat'i v zhurnale UFN (Physics – Uspekhi) **176**(7) (2006), 762–770.
[11] C.E. Shannon (1949) Communication in the presence of noise, *Proc. Institute of Radio Engineers* **37**(1), 10–21.

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An Appropriate Method for Eigenvalues Approximation of Sixth-order Sturm-Liouville Problems by Using Integral Operation Matrix over the Chebyshev Polynomials

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In this study, we suggest an efficient and useful method using Chebyshev polynomials to approximate eigenvalues of a non-singular sixth-order Sturm-Liouville

equation. This method uses Chebyshev polynomials and integration operation matrix for approximating function and its derivations and we convert eigenvalues finding problem of Sturm-Liouville equation to problem of eigenvalues finding matrix. The obtained results demonstrate appropriate reliability and efficiency in proposed method.

Keywords: Six-order ordinary equation, Sturm-Liouville equation, Chebyshev polynomials; Eigenvalues, integral operation matrix, collocation method

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On the Stability of Equilibria in Cross-diffusion Systems

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We study a cross-diffusion model of species interaction. The model generalizes the model introduced in 1979 by Shigesada, Kawasaki and Teramoto for two species (SKT). All species are assumed to exhibit a functional response of the same form similar to SKT model. By constructing a Lyapunov functional of the system, we establish the global stability of the equilibrium, subject to some conditions on the cross-diffusion matrix and the diffusion vector. A sufficient condition is also derived for the coexistence of a large number of interacting species. Particular cases of the model for two species are considered extensively in the literature. Most of these results are shown to follow as consequences of the general theory developed here.

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Dynamics of the Driven Goodwin Business Cycle Equation

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We have considered the excitation of Goodwin's oscillations under the action of the periodic autonomous investment for the following models of the economic cycle

a) $\dot{Y}(t) = \frac{I(t)+I_a(t)-(1-\alpha)Y(t)}{\epsilon}, \quad \dot{I} = \frac{\varphi(\dot{Y}(t))-I(t)}{\theta};$

b) $\dot{Y}(t) = \frac{C(t)+I_a(t)-Y(t)}{\epsilon}, \quad \dot{I} = \frac{\varphi(\dot{Y}(t))-I(t)}{\theta}, \dot{C}(t) = \frac{\alpha Y(t)-C(t)}{\gamma};$

c) $\dot{Y}(t) = \frac{\varphi(\dot{Y}(t-\theta))+I_a(t)-(1-\alpha)Y(t)}{\epsilon}.$

Here $Y(t)$ is income, $I(t)$ is induced investment, $I_a(t)$ is autonomous investment, $\varphi(\dot{y})$ is nonlinear Goodwin's accelerator, $C(t)$ is consumption, t is time in years, $\varepsilon > 0$, $\gamma > 0$ and $t > 0$ are the time-lag of the dynamic multiplier, the consumption delay and the time-lag between the investment decisions and the resulting outlays (in years), α is the marginal propensity to consume, $0 \leq \alpha \leq 1$.

We assume that the autonomous component of investment is a periodic function of time [1]

$$I_a(t) = A(1 - \cos \omega t),$$

where the two parameters A and ω determine the amplitude and the frequency of investment respectively.

We have explored the dynamical features of the income oscillations depending on the parameters A and ω for the case $\omega T_G(A = 0) \approx \pi$ where $T_G(A = 0)$ is the period of Goodwin's oscillations if $A = 0$.

References

[1] S. Sordi, "The interaction between trend and cycle in macrodynamic models of the economy," in *The Theory of Economic Growth. A 'Classical' Perspective*, edited by N. Salvadori, Edward Elgar, Aldershot, UK, 2003, pp. 286–305.

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Evaluation of Stochastic Algorithms for Financial Mathematics Problems from Point of View of Energy-efficiency

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The recent developments in the area of high-performance computing are driven not only by the desire for ever higher performance but also by the rising costs of electricity. The use of various types of accelerators like GPUs, Intel Xeon Phi has become mainstream and many algorithms and applications have been ported to make use of them where available. In financial mathematics the question of optimal use of computational resource should also take into account the limitations on space, because in many use cases the servers are deployed close to the exchanges. In this work we evaluate various algorithms for option pricing that we have implemented for different target architectures in terms of their energy and space efficiency. Since it has been established that low-discrepancy sequences may be better than pseudo-random numbers for these types of algorithms, we also test the Sobol and Halton sequences. We present the raw results, the computed metrics and conclusions from our tests.

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Bilinear Supersymmetric Gardner Equation and Its Soliton Solutions

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A supersymmetric version of Gardner equation is discussed using the extension of Hirota bilinear formalism to superspace. This equation is a new one and cannot be obtained from super-mKdV equation with nonzero boundary. Following the steps to super-bilinear formalism we build the multisoliton solutions and prove integrability of super-Gardner equation.

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Numerical Modeling of Biosurfactants in Multiphase Flows

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Biosurfactants are microbially produced surface active substances. Being bioproducts, biosurfactants have important properties as lower toxicity, higher biodegradability and environmental compatibility, compared to their chemical/synthetic counterparts. Their application is in many fields, *e.g.*, environmental, food, crude-oil recovery, and in areas such as biomedicine and therapeutics.

A mathematical model and numerical method are developed to study the production of biosurfactants and their effect on the interfacial tension in multiphase flows. The model includes generalized reaction-advection-diffusion equations for the concentration of the substrate, the biomass and the biosurfactant. The reaction (bioprocess) is modeled using classical Monod kinetics. In the equation for the biomass transport the bacterial chemotaxis is taken into account using Keller-Segel model. On the interfaces the biosurfactant concentration is described by an advection-diffusion equation that takes into account the flux bulk-interface. The mathematical model includes also the interfacial tension dependence on the biosurfactant concentration and the related Marangoni stress.

Second order finite difference approximation on non-uniform meshes is used for the space discretization of the reaction-advection-diffusion equations in the fluid phases as well as on the interface. For the time integration explicit and implicit first and second order schemes are used with non-uniform time steps. Tests and comparisons are performed in order to investigate the accuracy and stability of the different numerical schemes. One and two-dimensional test problems are considered. Stokes equations are used to describe the flow in the two-dimensional axisymmetric case and are solved by a simplified version of Boundary integral method.

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On the Rayleigh-Stokes Problem for Generalized Oldroyd-B Fluids

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Fractional constitutive equations have been intensively used in linear viscoelasticity. This is due to the nonlocal character of fractional derivatives which makes them more suitable for modeling of phenomena with memory.

In the present work we study the initial-boundary value problem for the velocity distribution of a unidirectional flow of generalized Oldroyd-B fluid with fractional derivative model. It involves two Riemann-Liouville fractional derivatives in time. A theoretical analysis of the problem in a general abstract setting is presented first. Under appropriate conditions, well-posedness is proven and regularity estimates are obtained. In addition, some relations to other fractional evolution equations are established.

To study the flow evolution, special attention is paid to the behavior of the time-dependent components in the eigenfunction expansion of the solution. A numerical technique is developed and applied for the computation of these functions. Numerical experiments are performed for different values of the parameters and plots are presented and discussed. The results are compared to those obtained in the limiting cases of generalized fractional Maxwell and second grade fluids.

Acknowledgement: This work is partially supported by the Bulgarian National Science Fund under Grant DFNI-I02/9.

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Experimental and Computing Strategies in Advanced Material Characterization Problems

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The mechanical characterization of materials relies more and more often on sophisticated experimental methods that permit to acquire a large amount of data and, contemporarily, to reduce the invasiveness of the tests. This evolution accompanies the growing demand of non-destructive diagnostic tools capable to assess the safety level of components in use in structures and infrastructures, for instance

in the strategic energy sector. The information collected from nowadays commonly available full-field measurement techniques can be profitably exploited in combined experimental-numerical approaches. Advanced material systems that are not easily managed by traditional techniques can be characterized in this way. This is for instance the case of thin layered structures and of their adhesion on the relevant substrates.

In this context, reliable parameters identification involves the repeated simulation of the laboratory or in situ tests by sophisticated and usually expensive non-linear analyses while, in some situation, results would be required in real time. Contemporarily, most noises associated to both experimental and numerical processes should be eliminated. The filtering capabilities of reduced models based on decomposition and interpolation techniques can be profitably used to meet the above requirements. Some results recently achieved in this field will be summarized in this contribution.

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Investigation of the Influence of the Concentrations of Sn in Electrochemically Deposited CuSn Alloy Films on Their Mechanical Properties

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Mechanical properties of thin CuSn alloy films containing different concentrations of Sn (0.06-67.5 wt.%) were investigated by means of nanoindentation experiments, using Nanoindenter G200 (Agilent Technologies), equipped with Berkovich indenter tip. The films were electrochemically deposited on screen-intermediate Ni film with thickness about 3 μm electrodeposited on Cu or brass (Cu66Zn34) substrates with thickness respectively 300 μm and 500 μm. The thicknesses of investigated CuSn films varied from 0.138 to 5.47 μm. Mechanical properties of the Cu and brass substrates were investigated too. As a result of nanoindentation experiments, load-displacement curves were obtained and two mechanical characteristics of the substrate and investigated films – indentation hardness (HIT) and indentation modulus (EIT) – were calculated using Oliver & Pharr approximation method. Dependence of indentation modulus and indentation hardness on the depth of indentation, concentration of Sn, structure and phase composition of the alloy films

was investigated and discussed.

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A Sixth Order Generalized Boussinesq Type Equation using Hirota's Method

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We are using Hirota's bilinear operator

$$D_t^m D_x^n (f \cdot g) = \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial t'} \right)^m \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right)^n f(x,t) g(x',t')$$

and the bilinear form of the Boussinesq equation to render to a sixth order Boussinesq type equation (6BTE). We compare the new sixth order Boussinesq equation with the sixth order generalized Boussinesq (6GBE) equation. Both equations comprises solutions with monotone shapes and damped oscillatory tales, the so called Kawahara solitons. Localized solutions are obtained for both cases numerically using the Christov-Galerkin Spectral method.

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Transient Heat Transfer in Viscous Rarefied Gas between Concentric Cylinders. Effect of Curvature

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The thermoacoustic waves arising in cylindrical or planar Couette rarefied gas flow between rotating cylinders is studied in the cases of suddenly cylinder wall velocity direction turn on. An unlimited increase in the radius of the inner cylinder flow can be interpreted as Couette flow between the two flat plates. Based on the developed in previous publications Navier-Stokes-Fourier (NSF) model and Direct Simulation Monte Carlo (DSMC) method and their numerical solutions, are considered transient processes in the gas phase. Macroscopic flow characteristics

(velocity, density, temperature) and numerical results for the stress and heat flux at the "gas-cylinder wall" interface are received. The cylindrical flow cases for fixed velocity and temperature of the both walls are considered. The curvature effects over the wave's distribution and attenuation are studied numerically.

Keywords: Kinetic theory, rarefied gas, microfluidics, unsteady heat transfer, numerical methods, DSMC

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Nanomechanical Testing of Thin Composite Layers – Application to Pd-In Electrochemically Deposited Thin Films

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Pd-In thin films of various compositions were electrochemically deposited on brass substrates. Their mechanical properties (hardness and indentation modulus) were then determined using a nanoindenter G200 (Keysight Technologies) equipped with a sharp Berkovich tip. The main goal was to assess the effect of composition on the mechanical properties (indentation hardness and modulus) of the electrochemically deposited Pd-In thin films regardless the difference in the thickness and the significance of the surface roughness. It has been demonstrated that the mechanical properties of these films are highly compositionally sensitive and the surface roughness yields scatter in the results and introduces uncertainty in the obtained mechanical characteristics.

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The Numerical Solution of Navier-Stokes Equations for Viscous Incompressible Fluid by Semi-Lagrangian Approximation in the Finite Element Method

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The Navier-Stokes equations are of interest both itself and in combination with additional equations for more complex physical phenomena. At the same time, efficient and robust numerical methods for its solving is extremely challenged up to now.

In present talk the two-dimensional system of Navier-Stokes equations is considered for a viscous incompressible fluid in channel. On outlet boundary the modified "do nothing"boundary condition is imposed [1]. Its efficiency is shown by numerical experiments.

To construct a discrete analogue, we use a semi-Lagrangian approach (for approximation of the transport derivatives) in combination with a conforming finite element method (for approximation of other terms) [2]. Velocity components are approximated by bilinear elements and the pressure does by piecewise-constant elements on rectangles. Semi-Lagrangian approach provides unconditional stability. As a result of this combined approach, the stationary problem with a self-adjoint operator is obtained on each time level. This problem is numerically solved by the multigrid method which allows one to decrease the computational time.

The theoretical results are confirmed by numerical experiments.

Acknowledgement: The work is supported by Project 14-11-00147 of Russian Scientific Foundation.

References

[1] [1] R. Rannacher (2011) Incompressible Viscous Flow, *Encyclopedia of Computational Mechanics* **3** Fluids. – Chapter 6.

[2] O. Pironneau (1982) On the Transport-Diffusion Algorithm and Its Applications to the Navier-Stokes Equations, *Numerische Mathematik* **38**, 309–332.

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Numerical Approach of an Optimal Control Problem for a Model of Tissue Invasion by Solid Tumours

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An optimal control problem associated with a mathematical model of cancer invasion is considered. The mathematical model is defined by four partial differential equations and describes the growth of a generic solid tumour, which will assume has just been vascularised, *i.e.*, a blood supply has been established. The four state variables involved in tumour cell invasion represent tumour cell density (denoted by n), matrix-degradative enzymes concentration (denoted by m), macromolecules concentration (denoted by f) and oxygen concentration (denoted by c). Each of the four variables (n, f, m, c) is a function of the spatial variable x and time t. The target in the optimal control problem is that the state variables (n, f, m, c) to attain the desired states (nd, fd, md, cd) with a minimum cost. Numerical simulations of the optimal solution using the optimality system are presented.

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Numerical Methods for Hamiltonian Systems: Implementation and Comparison

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Some families of symplectic and symmetric numerical methods for solving the Cauchy problem for Hamiltonian systems of equations are analyzed and implemented. Their capabilities to conserve the important global properties of the exact solutions – conservation of the phase volume, the total momentum and the energy (in the absence of external forces), reversibility in time – are compared.

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On the Compositions of Rotations

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In this paper the problem of composition of two arbitrary rotations in $SO(3, R)$ given in their vector-parameter form is discussed. The cases when one or two half-turns are involved in the composition of two rotations or the resulting rotation is a half turn receive rigorous treatment. Systematization of the results is made and relying on the results, convenient computational method for composing rotations in vector-parameter form is proposed. Technically, this is done by lifting the problems to the covering group $SU(2)$.

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Numerical Simulation of Plasma Turbulence During the Injection of the Electron Beam

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The efficiency of generation of electromagnetic radiation in various nonlinear processes during the beam-plasma interaction has been studied on the base of computer simulation. This problem is actual for laboratory experiments on turbulent plasma heating in open traps, and for interpretation of various phenomena in space plasma (solar and gamma flares, radiation in magnetospheres of planets, generation of high-energy cosmic rays). The model of collisionless plasma is described by system of the Vlasov-Maxwell equations. We considered periodic boundary conditions and the beam injection in the region. The beam and plasma parameters were chosen close to the parameters in the experiment on the GOL-3 facility (BINP SB RAS).

The parallel numerical algorithm is based on the particles-in-cell method (PIC) with mixed Euler-Lagrangian domain decomposition. Various scenarios of the nonlinear evolution in a beam-plasma system, a transfer of energy from one unstable mode to another modes, and influence of an external magnetic field in the case of a low density beam were studied. Good agreement of the numerical and analytical solutions was obtained. Also, we consider the problem of excitement and evolution of plasma turbulence under the influence of the electron beam injected in plasma.

Calculations are performed on the Siberian Supercomputing Center of Institute of Computational Mathematics and Mathematical Geophysics SB RAS and the Supercomputing Center of Lomonosov Moscow State University.

Acknowledgements: The present work was supported by the Russian Foundation for Basic Research under Grant number 14-01-31220, and 14-01-00392 and by Russian Scientific Foundation grant 14-11-00485 "High performance methods and technologies of modeling the electrophysical processes and devices."

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Characterization of Perfluorinated Cation-exchange Membranes MF-4SC Surface Modified with Halloysite Nanotubes

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The electro-conductivity and diffusion permeability through perfluorinated cation-exchange membranes MF-4SC (Russian analogue of Nafion-type membrane), whose surface is modified by nanotubes of halloysite using short exposures of a low temperature microwave plasma, is theoretically investigated using the Nernst-Planck approach. The method of quantitative evaluation of physicochemical parameters (individual and averaged diffusion coefficients and averaged distribution coefficients of ion pairs in the membrane) of the systems 'electrolyte solution–bi-layer ion-exchange membrane–water/electrolyte solution,' which was proposed by us earlier, is further developed. The mentioned parameters of modified membranes on the base of MF-4SC and nanotubes of halloysite are obtained from both experimental data on electroconductivity and diffusion permeability for different concentration of NaCl and HCl solutions using theoretical calculations by the help of least squares method. New model of bi-layer membrane system can be used for refining calculated results with taking into account both diffusive layers. It is shown that grafting the layer of halloysite nanotubes onto the membrane surface noticeably affects exchange capacity as well as structural and transport characteristics

of the original perfluorinated membrane. In particular, such a membrane possesses a feature of asymmetry of diffusion permeability when changing its position inside a measuring cell. Hybrid MF-4SC/halloysite membranes can be productively used in fuel cells and catalysis.

Acknowledgement: This work is financially supported by the Russian Science Foundation, project no. 14-19-01045.

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Numerical Investigation of Unsteady Axisymmetric Stagnation-Point Flow

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It is known that on the solid surface there is always at least one point in which the components of the velocity vanish. This point is called stagnation or critical. The stationary stagnation-point flow of a viscous incompressible fluid is well studied. Numerical solutions of this problem were obtained for two-dimentional flows by Hiemenz (1911), for axisymmetric flow by Homann (1936). Study of the problem of the viscous incompressible fluid flow near the critical point, *i.e.*, the problem of flow near the wall set perpendicular to the flow direction, the subject of many works. However, unsteady flow is still weakly studied.

The goal of the present work is the investigation of the unsteady axially symmetric flow of a viscous incompressible liquid near the critical point. The results of numerical analysis show that if there are the counterflow zones in the initial data and the pressure gradient on the solid plane is negative, such zones disappear in finite time. We also consider the case when the pressure gradient is a periodic function of time. In this case both periodic process and blow-up solution in finite time are possible. The self-similar solutions describing the axisymmetric flow of a viscous incompressible fluid in the vicinity of the critical point are investigated too. The unsteady reversed stagnation-point flow is also considered.

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Extremely High-Precision Computations in Large-Scale Classical and Quantum Molecular Mechanics Simulation

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Molecular simulations are major modern computational challenge. The simulation technique must deal with: a colossal number of objects comprising the system under simulation – up to tens of millions and above; an exceptionally small iteration time steps – down to tenths of femtosecond and below; complicated interactions among simulated objects; difficult to obey constraints on the overall system behavior. In addition, current requirements demand simulation intervals longer than milliseconds. It is obvious that such a complex, above tera-times-iterating procedure will accumulate calculation inaccuracy, which, combined with inter-step dependencies, may lead to dramatic distortion of the trajectories of individual objects. This may not influence the statistical properties of the entire system for the entire simulation term, but when dealing with, *e.g.*, sophisticated biomolecules, the importance is often set on the single object's trajectory itself. This paper presents a thorough investigation on the effect of computational precision on molecular simulation. Though the subject may seem widely discussed for at least a decade, there has only been made an agreement that the adopted standards for floating point presentation are satisfactory, with not much of a detail. The obtained here results for trajectory deviation in dependence on precision show striking demand of extremely high precision.

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Advance Characterisation of Structure and Properties of Composites

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Industrial Computed Tomography is a modern technique for nondestructive testing and microstructure analysis of a wide class of objects, including composite and porous materials. By segmentation and image analysis, different features of the CT reconstructed volume can be visualized and studied. Based on the microstructure and the properties of the single components, the effective material

characteristics can be predicted using the technique of numerical homogenization. This is a computationally demanding procedure, since a series of large-scale problems with highly varying coefficients has to be solved.

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Merging and Energy Exchange between Optical Filaments

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We investigate two types of nonlinear interaction between collinear femtosecond laser pulses with power slightly above the critical for self-focusing. In the first case we study energy exchange between filaments. The model describes this process through degenerate four-photon parametric mixing (FPPM) scheme and requests initial phase difference between the waves. When there are no initial phase difference between the pulses, the FPPM process does not work. In this case it is obtained the second type of interaction as merging between two, three or four filaments in a single filament with higher power. It is found that in the second case the interflow between the filaments has potential of interaction due to cross-phase modulation (CPM).

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Manakov Soliton Trains and External Potentials: Criterium of Adiabaticity

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It is well known that the Complex Toda chain (CTC) models the N-soliton train dynamics for the Gross-Pitaevski solitons [1,2]

$$i\vec{u}_t + \tfrac{1}{2}\vec{u}_{xx} + (\vec{u}^{\,\dagger}, \vec{u})\vec{u} = V(x)\vec{u}(x,t). \tag{3}$$

An important ingredient here is the external potential, which could be of several types: a) harmonic potentials $V(x) = v_2x^2 + v_1x + v_0$, b) periodic potentials $V(x) = A\cos(\Omega x + \Omega_0)$ and c) shallow potential wells $V(x) = c_0(\tanh(x - x_{\rm f}) - \tanh(x - x_{\rm in}))$, $c_0 \ll 1$ and $x_{\rm in} < x_{\rm f}$.

Using analytical methods we propose a criterium which ensures that the combination of initial potential and the initial state of the soliton train comply with the adiabatic approximation. We demonstrate that the perturbed CTC adequately models the soliton train dynamics providing our criterium holds true [1,2].

References

[1] V.S. Gerdjikov, E.V. Doktorov, and N. P. Matsuka (2007) N-soliton Train and Generalized Complex Toda Chain for Manakov System, *Theor. Math. Phys.* **151**(3), 762–773.

[2] V. S. Gerdjikov and M. D. Todorov. "On the Effects of Sech-like Potentials on Manakov Solitons," in *5th AMiTaNS'13*, AIP CP1561, pp. 75–83, Melville, NY, 2013, http://dx.doi.org/10.1063/1.4827216.

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Classification of the Stratified Fluid Flows Regimes around a Square Cylinder

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The 2D density stratified (in vertical direction) viscous fluid flows around a square cylinder with diameter d (moving in horizontal direction with the velocity U) have been simulated on the basis of the Navier-Stokes equations in the Boussinesq approximation. For solving of the Navier-Stokes equations the Splitting on physical factors Method for Incompressible Fluid flows (SMIF) with hybrid explicit finite difference scheme (second-order accuracy in space, minimum scheme viscosity and dispersion, monotonous) has been used. The numerical method SMIF has been successfully applied for solving of the different problems: 2D and 3D separated homogeneous and stratified fluid flows around a sphere and a circular cylinder; the flows with free surface including regimes with broken surface wave; the air, heat and mass transfer in the clean rooms. At the present paper the original refined classification of 2D stratified viscous fluid flow regimes around a square cylinder at $\mathrm{Re} \leq 200$ has been obtained and the interesting fluid flows with two hanging vortices in the wake has been investigated in details at $\mathrm{Fr} = 0.1$, $\mathrm{Re} = 50$, where $\mathrm{Re} = U\Delta d/\nu$ is the Reynolds number, $\mathrm{Fr} = U/(N\Delta d)$ is the internal Froude, ν is the kinematical viscosity coefficient, N is the buoyancy frequency.

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Solitons and Protein Folding: An *in silico* Experiment

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Protein folding is the process of formation of a functional 3D structure from a random coil – the shape in which amino-acid chains leave the ribosome. Anfinsen's dogma states that the former is completely determined by the latter, but despite the progress in understanding the process rate and the success in folding prediction for some small proteins, with presently available physics-based methods it is not yet possible to reliably deduce the shape of a biologically active protein from its amino acid sequence. The protein-folding problem endures as one of the most important unresolved problems in science; it addresses the origin of life itself. Furthermore, a wrong fold is a common cause for a protein to lose its function or even endanger the living organism.

Soliton solutions of a generalized discrete non-linear Schrödinger equation (GDNLSE) obtained from the energy function in terms of bond and torsion angles κ and τ, provide a constructive theoretical framework for describing protein folds and folding patterns. Here we study the dynamics of this process by means of molecular-dynamics simulations. The soliton manifestation is the pattern helix-loop-helix in the secondary structure of the protein, which explains the importance of understanding loop formation in helical proteins.

We performed in silico experiment for unfolding the core structure of gp41 from the HIV envelope glycoprotein (PDB ID: 1AIK) by molecular-dynamics simulations with the MD package GROMACS. We analyzed 80 ns trajectories, obtained with one united-atom and two different all-atom force fields, to justify the side-chain orientation quantification scheme adopted in the studies and to eliminate force-field based artefacts. Our results are compatible with the soliton model of protein folding and provide first insight into the soliton-formation dynamics.

Keywords: protein folding, DNLSE, solitons, molecular dynamics simulations

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Using PCA and General Path Seeker Regression for Investigation of Air Pollution and CO Modeling

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The monitoring and control of air quality in urban areas is important problem in many European countries. The main air pollutants are observed and a huge amount of data is collected during the last years. In Bulgaria, the air quality is surveyed by the official environmental agency and in many towns exceedances of harmful pollutants are detected. The aim of this study is to investigate the pollution from 9 air pollutants in the town of Dimitrovgrad, Bulgaria in the period of 10 years based on hourly data. PCA is used to discover the patterns in the overall pollution and the contribution of the 9 pollutants. In addition the GPS method is applied to find dependence of CO (carbon monoxide) with respect to other pollutants and 6 meteorological parameters. It is reported that the CO concentrations are in continuously repeated quantities very harmful for human health.

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Numerical Solvers to the Stabilizing Solution of Perturbed Algebraic Riccati Equations in LQ Zero-sum Games

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We consider a generalized algebraic Riccati equation arising in stochastic control with indefinite quadratic part. It is well known Lanzon's approach (2008) for solving similar Riccati equations. Two matrix sequences are constructed. The focus of the iterative process is the computation the second matrix sequence. We consider a few iterative methods for computing the matrices of the second sequence, where each matrix is the stabilizing solution of the perturbed algebraic Riccati equation with definite quadratic part. Computer realizations of the presented methods are numerically tested and compared on the test of family examples. Based on the experiments some conclusions are derived.

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A Direct Multi-step Legendre-Gauss Collocation Method for High-order Volterra Integro-differential Equation

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The purpose of this study is to present a new direct method for approximate solution and approximate derivatives up to k of the solution for kth-order Volterra integro-differential equation with a regular kernel. This method is based on the approximation by shifted the original problem in to a sequence of subintervals. The Legendre-Gauss-Lobatto collocation method is proposed to solving the Volterra integro-differential equation. Numerical examples show that the approximate solution have a good degree of accuracy.

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Bi-quartic Parametric Polynomial Minimal Surfaces

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Minimal surfaces with isothermal parameters admitting Bézier representation were studied by Cosín and Monterde. They showed that, up to an affine transformation, the Enneper surface is the only bi-cubic isothermal minimal surface. Here we study bi-quartic isothermal minimal surfaces and establish the general form of their generating functions in the Weierstrass representation formula. We apply an approach proposed by Ganchev to compute the normal curvature and show that, in contrast to the bi-cubic case, there is a variety of bi-quartic isothermal minimal surfaces. Based on the Bézier representation we establish some geometric properties of the bi-quartic harmonic surfaces. Numerical experiments are visualized and presented to illustrate and support our results.

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Reduction of Linear Hamiltonian Systems of Ordinary Differential Equations

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In the paper, some approaches to numerical and analytical solution of linear boundary value problems for Hamiltonian systems of ordinary differential equations are discussed. These ways based on the idea of the reduction of the initial linear system of differential equations to the other more simple, in a sense.

Conservative numerical scheme with an arbitrary finite order of approximation to the exact solution is proposed for the numerical solution of linear Hamiltonian boundary value problems. The basis of this scheme is the reduction of the initial boundary value problem to a similar, but for a system with a constant nilpotent matrix and the right-hand side an unknown vector function; the last vector function satisfies the integral equation, the projection method is applied to get the numerical solution of the integral equation.

There are many articles devoted to analytical methods in the theory of Hamiltonian systems, but most of them are focused on nonlinear problems and used the technique of canonical transformations, as a rule. For linear problems, this method can be greatly simplified by using the Hamilton-Cayley transformation and the constructing asymptotic expansions for ordinary differential equations, described in the well-known monograph Wasow. Reduction algorithm of the original equations to two Hamiltonian systems of lower order was constructed.

Applications of these algorithms for the numerical analysis certain Hamiltonian systems of ordinary differential equations are in the paper.

Acknowledgement: This work was supported by the Russian Foundation for Basic Research (grant no. 14-01-00130).

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ANSYS CFX Wall-Function Approach for Modeling of Fully Separated Flow past a Circular Cylinder: Problems and Simulation Practical Guide

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The talk is to give a draft overview on a strategy elaborated for a reliable simulation of fully separated incompressible viscous flow past a circular cylinder by means of the commercial Software ANSYS CFX. It is motivated by its relevance to serve as a general flow prototype past a bluff-body, an issue of considerable engineering interest and aim to emphasize the computational specification. The flow separation is investigated by means of wall-function approach for Reynolds Averaged Navier-Stokes Simulations (RANS) method. Adequately to identify the separation characteristics the Shear Stress Transport model is employed. Fully to resolve the laminar viscous sublayer the wall function value up to 2 is taken to define the first layer thickness. Adequately to find out the vortex shedding structure and frequency the Strouhal number based time step is used. The calculated drag coefficient and periodicity of the vortex shedding reliable depict the experimental data.

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SKYTHIA: A Universal Multi-phase Analyzer

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SKYTHIA is a computer code for computational simulation of transient multi-phase flows based on three multi-component velocity fields in a porous structure that may change its geometry in time. The foundation of the computer code SKYTHIA allows applications for mathematical simulation of a variety of processes. From

- two-phase gas-plasma multi-component hydrogen detonation in pipe-network with dissociation of the gases;
- through condensation water-steam shock waves in complex pipe networks;
- gas solution and dissolution in liquids, dissolved gas release from water in pipe network and gas-slug formation and transport;

- pressure wave propagation, piping force computation and risk analysis in conventional island of 1700 MWe power plant including detailed models of the high pressure turbine;
- diesel injection problems;
- particles sedimentation in water;
- turbulent mixing and transport in a nuclear power plant sump;
- termite injection by high pressure steam-hydrogen mixture into air environment, melt-water interaction in postulated SWR 1000 severe accidents, alumina melt jet dropped into a subcooled water, Urania melt jet dropped in water;
- void formation in existing-;
- or future boiling water reactors;
- void fraction and velocity distribution in nuclear reactors with different thermal powers;
- modern steam generator simulation, thermal coupling of multi-phase nonequilibrium three fluid nonhomogeneous non-equilibrium flow inside the primary piping systems to complete 3D multi-phase nonequilibrium three fluid non-homogeneous nonequilibrium flow inside secondary systems with cyclones and dryers;
- volume fraction of steam in family of steam generators with different power;
- water velocities and void fraction in flooding reservoir for primary emergency condenser being operating on the secondary site as boiler; thermal coupling of multiphase non-equilibrium three fluid non-homogeneous flow inside the primary piping systems to complete 3D multi-phase non-equilibrium three fluid nonhomogeneous flow inside secondary systems;
- complete system for moisture separation of typical PWR, dynamic performance: multi-phase nonequilibrium three fluid non-homogeneous flow inside the secondary moisture separation system;
- local volume fractions of oxide and sodium liquid as a function of (r, z) in the vertical plane for a fast breeder reactor during melt water interaction; energetic interaction of molten reactor material with liquid sodium in argon environment;
- modern pre-heater (condenser) simulation, thermal coupling of single phase flow inside the primary piping systems to complete 3D multi-phase nonequilibrium three fluid non-homogeneous nonequilibrium condensing flow inside secondary systems, *etc.*

All these applications demonstrate the capability of single model architecture to handle different material systems, different intensities of interactions, and large variety of the spatial and temporal scales of the simulated processes.

This paper gives brief information about the basic principles used to build SKYTHIA, part of the validation procedure and illustrations of some very complex process simulations.

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Numerical computation of the critical energy constant for two-dimensional Boussinesq equations

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The critical energy constant d plays an important role in the theoretical and numerical study of the Boussinesq equations. For example, the qualitative behavior of the solution – global existence or finite time blow up – of problems with positive initial energy smaller than d is determined by the sign of the Nehari functional from the initial data.

The critical energy constant can be obtained as the value of a particular functional acting on the positive radially symmetric solution (ground state solution) to the problem

$$-\Delta u(x) + u(x) - f(u) = 0,\ x \in \mathbb{R}^n,\ |u(x)| \ \rightarrow 0 \ \text{ as } \ |x| \rightarrow \infty. \tag{4}$$

In the one-dimensional case problem (4) with a nonlinearity of the type $f(u) = a|u|^p$ or $f(u) = a|u|^{p-1}u$ possesses explicit solution, while in the multidimensional case the solution to (4) can be evaluated only numerically.

In this talk we present a numerical method for evaluation of the constant d in the one and two-dimensional cases. The positive symmetric solution to (4) is obtained by a proper modification of the shooting method, as the stability is a main point of concern.

The efficiency of the proposed method is demonstrated in the one-dimensional case, where the numerically computed value of the constant d differs from its exact value by 10^{-11}.

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Robust Ultrashort Laser Pulse Formation in Ionization Free Regime Propagation

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High-intensity ultrashort laser pulses propagation in bulk nonlinear medium is studied in ionization free regime. The propagation equation is (3+1)-dimensional cubic-quintic nonlinear envelope equation and the propagation medium is pressurized argon. A smooth pulse propagation dynamics free of abrupt changes of the pulse parameters is observed at realistic physical conditions. Twofold compression of the pulse in time is found. A smooth robust compressed pulse that propagates stably over few diffraction and nonlinear lengths, but still less than one dispersion length, is predicted based on numerical simulations. Such pulse can be considered as a partial spatio-temporal soliton.

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LQR Problem of Linear Discrete Time Systems with Nonnegative State Constraints

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In the paper linear quadratic regulator (LQR) problem of linear discrete time systems with nonnegative restrictions on the system state is considered. In this case the system trajectory must belongs to nonnegative orthant. Such kind of restrictions on the system determine the class of positive systems. They have big application in many fields like economics, biology, ecology, ICT and others. In this paper the nonnegativity of control is not considered.

There are very good developed methods for solving LQR problem, including with different type of constraints, but the nonnegativity (cone) constraints are not considered by now. For solving the problem we will use state feedback control determined by the solution of the Discrete time Algebraic Riccati Equation (DARE). In order to guarantee positivity of the closed-loop system we will consider only a restrictive set of initial states for which the state trajectory belongs to the nonnegative orthant. In other words, each initial state belonging to this set made nonnegative orthan invariant set.

In the paper we propose procedure for finding maximal admissible set of initial states which guarantee nonnegativity state constraints satisfaction. The illustrative example is given in case of admissible initial state.

The question arise what is the problem solution in case when the initial state does not belongs to the admissible set. In this case we apply concept of dual mode Model Predictive Control (MPC) until the trajectory enter in the admissible set. Then, the solution consists of two modes – the first mode for restriction satisfaction and the second mode for ensuring closed-loop stability and optimality.

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Decision Making in Prioritization of Required Operational Capabilities

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In the paper is described an expert heuristic approach for prioritization of required operational capabilities in the area of defense. On the basis of assessments by experts and by applying analytical-hierarchical method was developed methodology for their prioritizing. This methodology is applied to several practical studies - simulation games on decision making in resource management in the area of defense.

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Micromechanical (Microhardness) Testing of the Dentin Hybrid Zone Formed by Different Types of Adhesive Systems in Sound Human Dentin

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According to a fundamental clinical research encompassing a 30 year period on more than 2500 teeth from 257 patients, under a good plaque control, it was shown that the main reason for teeth loss is the fracture of the hard tooth tissues-around 62% (Axelsson *et al.*, 2004).

The modern restorative dentistry allows for a reconstruction of the hard tooth tissues, by using adhesive technology for the retaining of biomaterials in teeth (Van Meerbeck *et al.*, 2003).The formed biomaterial-tooth tissue interface includes the hybrid layer, which is formed at the border of adhesive material with dentin by monomer penetration and polymerization in situ. The success of teeth tooth restorations depends on the properties of this interface and for that reason includes the formed hybrid layer (De Munck *et al.*, 2003). A continuous hermetic seal at this interface without degradation and breakdown is important to avoid failure of the restoration.

Theoretically, the hybrid layer can provide marginal sealing of the cavity and resist acid challenge to prevent secondary caries.

Presently, there is a lack of published research on the dentin-material interface, which is formed by using dentin adhesive systems, as well as its relationship with the mechanical properties of human dentin.

In the present study, specimens made of dentin, treated with the most abundant adhesive materials will be used. Microhardness and moduli of elasticity of the hybrid zone will be estimated.

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Generalized Nehari Functional and Global Solvability of Boussinesq Equation

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We study the Cauchy problem to generalized Boussinesq equation

$$u_{tt} - u_{xx} - \beta_1 u_{ttxx} + \beta_2 u_{xxxx} = f(u)_{xx} \quad (t,x) \in \mathbb{R}^+ \times \mathbb{R}, \tag{1}$$

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

with nonlinear term

$$f(u) = a_1|u|^{p_1} + \sum_{k=2}^{l} a_k|u|^{p_k-1}u - \sum_{j=1}^{s} b_j|u|^{q_j-1}u.$$

Equation (1) arises in a number of mathematical models of physical processes, for example it describes the amplitude of surface waves in shallow water, dislocations of crystals, shape memory alloys, atomic chains and others.

A new generalized Nehari functional, invariant under the flow of (1)–(2), is introduced. By means of the sign preserving properties of the new functional, global existence of the weak solutions to problem (1)–(2) is proved. The results are an extension of the well-known potential well method in case of arbitrary high positive initial energy.

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Resonance of Brownian Vortices in Viscoelastic Shear Flows

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Diffusion of mesoscopic particles suspended in solvents, governed by Brownian motion, is one of the pillars of biological and soft condensed matter physics [1]. Although the behavior of Brownian motion in quiescent fluids has been investigated in detail, our understanding of thermally induced particle dynamics in viscoelastic shear flows is still far from complete in spite of its fundamental importance in microfluidic applications [2]. Motivated by the results of [3], we have considered the dynamics of an underdamped Brownian particle in an oscillatory viscoelastic shear flow using the generalized Langevin equation with a Mittag-Leffler memory kernel, focusing on the behavior of the mean angular momentum of particles. It should be noted that the Mittag-Leffler memory kernel includes a characteristic memory time, and thereby has more physical applications than the usually employed power-law type one. We have shown that the presence of a memory has a profound effect on the behavior of Brownian vortexes. Particularly, for case where an additive external noise dominates over internal noise, we have found double resonance of the mean angular momentum of "free" particles, trapped due to the cage effect, versus the shear flow frequency. One resonance peak is related to the presence of external noise and the other is related to the initial positional distribution of particles. The roles of the internal and external noises and the memory time in the behavior of the model are also discussed.

References

[1] F. Höfling and T. Franosch (2013). Anomalous transport in the crowded world of biological cells, *Rep. Prog. Phys.* **76**, 046602.

[2] L. Holzer, J. Bammert, R. Rzehak, and W. Zimmermann (2010) Dynamics of a Trapped Brownian Particle in Shear Flows, *Phys. Rev. E***81**, 041124.

[3] A. Rekker, K. Laas, and R. Mankin, "Resonant behavior of the spatial cross-correlation for particles embedded in viscoelastic shear flow," in *AIP CP***1561**, AIP, Melville, New York, 2013, pp.224–231.

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Recent Advances in Numerical Methods for Fractional Differential Equations

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We shall survey some resent results in numerical treatment of initial and boundary value problems for fractional differential equations involving both Riemann-Liouville and Caputo fractional derivatives. The issues of construction, analysis, stability, and error estimates that are optimal with respect to the regularity of the solution and expresses in terms of the data. Examples of such problems include fractional time dependent diffusion equation, multi-term transient diffusion equation, and distributed order fractional differential equations and their numerical treatment using semi-discrete and fully discrete schemes.

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Fluid Flow Structure around the Mixer in a Bioreactor with Mechanical Stirring

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Fluid flow structure around the mixer in a bioreactor with mechanical stirring is studied and numerical results are presented in this article. The calculations are made by a computer program, written in MATLAB. The complex structure of the flow around the mixing disk is described and commented.

Keywords: Navier-Stokes equations, mechanical mixing, boundary conditions, Reynolds number

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Molecular Modelling of the Interactions of Heparin-Derived Oligosaccharides, Human Interferon Gamma and Its Extracellular Receptors

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Interferon gamma (IFN-g) is a signaling molecule that is crucial for immunity against intracellular pathogens and for tumor control, but is also related to several autoimmune deceases. The cytokine binds to a specific extracellular receptor, the interferon gamma receptor (IFNgR). The biological activity of IFN-g can be controlled by interfering in the cytokine receptors binding. It is therefore important to understand this process in detail.

In order to study the formation of hIFN-ghIFNgR complex, we performed multiple molecular dynamics simulations. We found that the proper orientation of the hIFN-g molecule relative to the receptors is hindered by the strong interaction of the highly positively charged flexible C-terminal tails of the cytokine and negatively charged domains in the receptor molecules. This interaction prevents the binding sites from approaching each other, so that they remain separated in space. Therefore, we hypothesize that another participant is necessary for the cytokine receptor binding to occur.

In addition to IFNgR, interferon gamma is also known to bind to heparin-derived oligosaccharides. These are linear highly negatively charged carbohydrates, occurring at the basement membrane of all mammalian cells. There were no available force field parameters for the monosaccharide N-sulfated glucosamine in heparin, so we developed CHARMM compatible parameters using the Force Field Toolkit of the molecular visualization and manipulation program VMD. This allowed us gaining first insights into the interactions between hIFN-g, hIFNgR and heparin-derived oligosaccharides with various degree of polymerization.

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Solitary Waves for Non-Destructive Testing Applications: Delayed Nonlinear Time Reversal Signal Processing Optimization

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Over the last two decades, development of optimized signal processing methods for improving nonlinear Non Destructive Testing (NDT) methods and harmonic imaging derived from Nonlinear Elastic Wave Spectroscopy (NEWS) have been steadily intensified. Using symmetry invariance, nonlinear Time Reversal (TR) and reciprocity properties, the classical NEWS methods are supplemented and improved by new excitations (based on solitary waves) having the intrinsic property of enlarging frequency analysis bandwidth and time domain scales, with now both medical acoustics and electromagnetic applications.

One of the use of TR-NEWS methods is to focus ultrasonic wave energy in the tested medium. Using the proposed "delayed TR-NEWS," it will be possible to shape the focused wave as needed. The wave shape is important factor in solitary wave propagation. The applicability, ease of use and usefulness of the "delayed TR-NEWS" will be investigated with the prospect of using it to analyse the nonlinear and dispersive properties of the tested sample NDT applications using solitary waves. The physical experiments of "delayed TR-NEWS" have been done with glued aluminium sample and carbon fibre reinforced polymer samples. It has been found that the shaping of the wave works well in both of these materials. In terms of spectrum, the shaping is limited by the bandwidth of the transmitting transducer.

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Sign Reversals of the Output Autocorrelation Function for the Stochastic Bernoulli-Verhulst Equation

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The Bernoulli-Verhulst equation (also called the generalized Verhulst model (GVM)) is one of the classic models of self-organization in many natural and artificial systems, and as such is relevant to a wide range of situations including population dynamics in ecology, spread of viral epidemics, plasma physics, cancer cell growth, autocatalytic chemical reactions, social sciences, *etc.* [1,2]. Although the behavior of the deterministic and stochastic versions of the GVM has been intensively investigated, it seems that analysis of the potential consequences of the interplay between fluctuations of environmental parameters and self-regulation in the behavior of the output autocorrelation function (ACF) is still absent in literature. This is quite unjustified in view of the fact that information about the observed dynamical properties of population growth processes is widely extracted from the ACF of population sizes. Thus motivated, we consider a GVM where the effect of fluctuating environment on the carrying capacity of a population is modeled as colored dichotomous noise. Relying on the composite Fokker-Planck master equation an explicit expression for the ACF of a stationary growth process is found. On the basis of this expression a nonmonotonic decay of the autocorrelation function by increasing lag-time is shown. Moreover, in a certain regime of the noise parameters the ACF demonstrates anticorrelation as well as related sign reversals at some values of the lag-time. The conditions for the appearance of this highly unexpected effect are also discussed.

References

[1] M. Eigen, P. Schuster, *The Hypercycle: A Principle of Natural Self-Organization*, Springer, Berlin, 1979.

[2] A. A. Dubkov and B. Spagnolo (2008) Verhulst model with Lévy white noise excitation, *Eur. Phys. J. B***65**, 361-–367.

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Contact Boundary Value Problems and Nonlocal Problems in Mathematical Models of Heat Transfer

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In this paper the mathematical model in the form of nonlocal problems for the two-dimensional heat equation are considered. Communication nonlocal problem and boundary value problem, which describe the same physical process heating is investigated. Combining known solutions the nonlocal and boundary value problem, one can solve the inverse problem, which allows to determine the unknown characteristics of the thermal process. These problems arise during the study of the temperature distribution during annealing movable wire and strip permanent or periodically operating internal and external heat sources. When the temperature field is known at all points in the area, then the boundary value problem perfectly describes the temperature field. But if the temperature distribution is known only in the initial time and/or part of the boundary, to determine the temperature distribution in the whole area of heating it is necessary to specify additional conditions related to the balance of energy emitted in the heating zone. Knowing the amount of energy allocated in the whole area of heating allows to fully identify the temperature distribution. From a mathematical point of view, the determination of the temperature distribution in the field of heating under these conditions leads to the decision boundary and nonlocal problem for the heat equation. Stability and convergence of numerical algorithms for the solution of a nonlocal problem with piecewise monotone functions in the equations and boundary conditions is investigated. Conducted numerous experiments and plotted the temperature distribution in terms of internal and external heat sources. These experiments confirm the effectiveness of attracting non-local terms to describe the thermal processes. Expedience of bringing in to such models of integral terms of thermal balance is shown. This allows you to define the parameters of the process control heat and mass transfer, in particular heat source, concentration of the substance.

Optimal Sensor Location for Parameter Identification in Soft Clay

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Performing parameter identification prior to numerical simulation is an essential task in geotechnical engineering. However, it has to be kept in mind that the accuracy of the obtained parameter is closely related to the chosen experimental setup, such as the number of sensors as well as their location. A well considered position of sensors can increase the quality of the measurement and to reduce the number of monitoring points. This Paper illustrates this concept by means of a loading device that is used to identify the stiffness and permeability of soft clay. With an initial setup of the measurement devices the pore water pressure and the vertical displacements are recorded and used to identify the afore mentioned parameters. Starting from these identified parameters, the optimal measurement setup is investigated with a method based on global sensitivity analysis. This method shows an optimal sensor location assuming three sensors for each measured quantity, and the results are discussed.

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Robust AMLI PCG Iterative Solution Methods for Problems with Strongly Heterogeneous Coefficients

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The first part of the talk is devoted to construction and analysis of hierarchical basis algebraic multilevel iteration (AMLI) methods in the case of coefficient jumps which are aligned with the interfaces of the initial mesh. The condition number estimates are uniform with respect to both mesh and/or coefficient anisotropy, the coefficient jumps, as well as the size of the discrete problem. The computational complexity is proportional to the number of degrees of freedom.

Robust multilevel methods for high-frequency and high-contrast problems are presented in the second part. Some advantages of the nonlinear AMLI methods including the case of element-by-element approximation of the Schur compliment

are discussed. The last part of the talk is devoted to the recently introduced auxiliary space multigrid (ASMG) method for highly heterogeneous media based on preconditioning of the related weighted $H(\mathrm{div})$-norm.

The presented numerical tests demonstrate the robustest scalability of the developed multilevel methods and algorithms.

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High-order Artificial Compressibility for the Navier-Stokes Equations

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We introduce a generalization of the artificial compressibility method for approximation of the incompressible Navier-Stokes equations. It allows for the construction of schemes of any order in time that require the solution of a fixed number of vectorial parabolic problems, depending only on the desired order of the scheme. These problems have a condition number that scales like $O(\delta t h^{-2})$, with δt being the time step and h being the spatial grid size. This approach has several advantages in comparison to the traditional projection schemes widely used for the unsteady Navier-Stokes equations. First, it allows for the construction of schemes of any order for both, the velocity and pressure, while the best proven accuracy achievable by a projection scheme is second order on the velocity and 3/2 order on the pressure. Second, the projection schemes require the solution of an elliptic scalar problem for the pressure that has a condition number $O(h^{-2})$, in addition to a vectorial parabolic problem for the velocity. This makes them slower if iterative methods are used to solve the linear systems. Third, the artificial compressibility schemes of second or higher order based on a defect correction approach presented below have superior stability properties as compared to a second order projection scheme. Finally, the ability to construct higher order schemes allows to incorporate time step control techniques which greatly improves their efficiency.

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Study of Fiber – Reinforcement Self-Compacting Concretes

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Incorporation in concrete composition of dispersed reinforcement steel macro- and micro-fiber with structural function increases the degree of ductility of typical brittle cement containing composites, which in some cases can replace completely or partially conventional steel reinforcement in the form of rods and grids. Thus, reduced manufacture, detailing and placement of conventional reinforcement, which enhances productivity and economic efficiency of the building process.

In this paper are investigated six-fibre reinforced with different amounts of steel fiber cement containing self-compacting compositions. Presented are the results of some of their main strength-deformation characteristics.

Advance approach is proposed for the study of structural and material properties of this type composites using the methods of industrial computed tomography and nanoidentation. Received original tomography results for the microstructure and characteristics of individual structural components make it possible to analyze the effective macro-characteristics of the studied composites. Via possibilities and advantages of nanoindentation are defined their E-module and hardness. The resulting analytical data are relevant for the purposes of multi-dimensional modeling of these systems.

Multifactor structure-mechanical analysis of the obtained with different methods original scientific results is suggested There is conclusion of the capabilities and effectiveness of complex analysis in studies to characterize the properties of self-compacting reinforced concrete.

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Variations of (Pseudo-)Rotations and Quantum Mechanical Angular Momentum

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Here we derive the Lie derivatives of the scalar parameters in the generalized Euler decomposition with respect to arbitrary axes under left and right deck transformations. This problem can be directly related to the representation of the angular momentum in quantum mechanics. As examples, we calculate the angular momentum and the corresponding quantum hamiltonian for the Euler, respectively Bryan representation. Similarly, in the hyperbolic case, the Laplace- Beltrami operator is retrieved for the Iwasawa decomposition. The case of two axes is considered as well.

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Calculation of Geodesic Polygons with Strongly Dominant Angle Error

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A geodesic polygon is a sequence of points (stations) and vectors, defined by consecutive geodesic measurements between each two consecutive points. The polygon is closed if its initial and last points are the same. We consider closed azimuth polygons, in which the vectors directions are measured by a compass. Such polygons are often used to survey given geodesic object (by following its edges). If the object is flat (a lake, a piece of flat land/wood), then only distance and azimuth is measured for each vector (2D case). Otherwise, in the 3D case, the slope of each vector should be measured in addition.

If all the measurements are exact, then the sum of all vectors must be zero. In practice, however, this does not happen. Due to the limited precision of the

measurement instruments this sum (called here *displacement vector*) is not zero in general (causing a problem to place precisely all stations on the map).

There is a "classical" solution of the polygon closing problem, which is rather easy and straightforward – each vector of the polygon is adjusted by a part of the displacement vector, proportional to its length. This procedure changes both the lengths and the angles in the polygon. The new affordable laser meters made it easy to increase rapidly the precision of distance measurements, while this is not so for the azimuth measurements. Thus a new problem has arisen: how to close such polygons (2D and 3D) without changing the distances. A solution of the last problem will be given in this talk.

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A Tale of Two Tails: Investing with the Return Distribution

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Value at Risk (VaR) has become the standard risk management tool in Finance. It is a summary measure for market risk that captures the amount that can be lost over a certain time horizon at a given level of confidence. In recent years VaR has been extended to address other types of risk, such as credit, liquidity, and operational. In all its forms it has been seen as a risk measure and as such it focuses on the left tail of the return distribution of an investment, that is the on the possibility for large losses. In this paper we seek to explore the viability and the use of changing the framework of the application of VaR from a risk-management perspective to a risk-adjusted return on investment perspective. We incorporate the right tail of the return distribution, *i.e.*, the possibility of large profits, into a single measure capable of evaluating the level of expected profits per unit exposure to losses at a selected confidence level. We study the empirical distributions of different securities over different time scales. We apply several computational approaches to evaluate the expected tail return to risk ratio (RoR) – historical, analytical, and expected shortfall (ES). We compare the results for RoR to several popular risk-adjusted performance measures, including Sharpe ratio, and Sortino ratio. The results point out to the validity of this approach to investment, security selection, and trade strategy valuation. We conclude with a discussion for further research of the subject.

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High-Order Discontinuous Galerkin Methods for Coupled Thermoconvective Flows under Gravity Modulation

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In this work, we investigate convective flows in a rectangular cavity subject to both vertical and horizontal temperature gradients. The case of plane parallel flow with thermal relaxation for a Maxwell fluid and a fluid having variable viscosity is investigated. The whole cavity is subject to gravity modulation simulating microgravity environment. High accuracy and stability are required due to the sensitivity of the bifurcation flows making the use of a high-order accurate and efficient technique essential. To this end, high order discontinuous Galerkin methods with variable mesh sizes are developed and analyzed. The convergence of the underlying schemes is demonstrated and simulation results are provided. The schemes are validated by comparing to simplified models solved using a beam Galerkin spectral method.

Keywords: Convective flow, Maxwell fluid, Thermal relaxation, G-jitter, discontinuous Galerkin, high order, mesh refinement

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Recent Developments in Entropy Viscosity

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Maximum principle, entropy stability and convergence of viscosity approximations for scalar conservation laws have been established a long time ago. However, on discrete level the same questions sometimes are a lot harder and in most cases the results are proven on uniform/restricted meshes and only for first order schemes.

In the case of nonlinear systems, the scalar maximum principle is no longer valid and depending on the nonlinear problem one has different stability properties, for example invariant domain and entropy dissipation. In this talk, we will present two recent results. In the scalar case, we will derive a maximum principle preserving second order scheme based on entropy viscosity. The new method preserves maximum principle on a variety of finite element spaces. In the case of general hyperbolic systems, we will present a new class of numerical approximations and prove that they have an invariant domain property. This is the analog of maximum principle for systems. Numerical results obtained with entropy viscosity schemes based on this type of approximations will be presented.

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Mathematical Models of Polymer Solutions Motion and Their Symmetries

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We consider three mathematical models describing motion of aqueous polymer solutions. All of them are derived from equations of Maxwell type viscoelastic medium at small relaxation time. Distinction consists in the choice of time derivative in the rheological constitutive law. Namely, we can choose (a) connective, (b) partial or (c) objective derivative of the strain tensor in time. We found widest groups admitted by each of these models. Systems (a) and (c) admit the extended Galilei group containing four arbitrary functions of time while the group admitted by system (b) is rather poor. Wide classes of exact solutions are obtained and their behaviors are analyzed if the relaxation viscosity tends to zero. Asymptotic expansion in this parameter of solution describing the flow near a critical point in planar and axially symmetric cases is derived.

Analogs of the classical Poiseuille and Nusselt solutions are studied also. We found difference in the pressure distribution between solutions calculated on the

base of model (c) and two other models.

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More Applications of Fitzpatrick Functions for Solving Optimization Problems

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This talk presents more applications of Fitzparick functions for solving optimization problems. The main purpose of the present work is to introduce some new properties of the Fitzpatrick functions useful for solving optimization problems, using also their already presented specific properties, as the maximal monotonicity, proper, convex and lower semi-continuity.

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Influence of the Basset Force on the Resonant Behavior of an Oscillator with Fluctuating Frequency

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The harmonic oscillator is the simplest toy model for different phenomena in nature and engineering, and as such it is the typical theoretician's paradigm for various fundamental conceptions [1]. One of the objects of special attention in this context is a mesoscopic particle (a tracer) trapped by a harmonic potential in a particle-fluid-trap system, *e.g.*, like a particle trapped by optical tweezers in a microrheological experiment. The present work is focused on the influence of hydrodynamic interactions (Stokes and Basset forces [2]) on the dynamics of a harmonically trapped Brownian tracer. A generalized Langevin equation is used to

describe the tracer's response to an external periodic force and to dichotomous fluctuations of the stiffness of the trapping potential. Relying on the Shapiro-Loginov formula, exact expressions for the complex susceptibility and for the response function are presented. On the basis of these exact formulas it is demonstrated that an interplay of multiplicative colored noise and the Basset force induced memory effects can generate a variety of cooperation effects, such as multiresonance versus the driving frequency as well as stochastic resonance versus the noise amplitude. The conditions for the appearance of these effects are also discussed. We believe that the results obtained not only supply material for theoretical investigations, but also suggest some possibilities for reliable interpretation of experimental data, e.g. for particles trapped by optical tweezers in the cytoplasm of cells.

Keywords: Basset force, Shapiro-Loginov formula, multiresonance, stochastic resonance, Brownian particle

References

[1] C. C. Bloch, *Classical and Quantum oscillator*, Wiley, New York, 1997.
[2] J. D. Schieber, A. Córdoba, and T. Indei (2013) The analytic solution of Stokes for time-dependent creeping flow around a sphere: Application to linear viscoelasticity as an ingredient for the generalized Stokes-Einstein relation and microrheology analysis, *Journal of Non-Newtonian Fluid Mechanics* **200**, 3–8.

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The Use of Copulas to Practical Estimation of Multivariate Stochastic Differential Mixed-Effects Models

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A system of stochastic differential equations (SDE) with mixed-effects parameters and multivariate normal copula density function were used to develop tree height model for Scots pine trees in Lithuania. A two-step maximum likelihood parameter estimation method is used and computational guidelines are given. After fitting the conditional probability density functions to outside bark diameter at breast height, and total tree height, a bivariate normal copula distribution model was constructed. Predictions from the mixed-effects parameters SDE tree height model calculated during this research were compared to the regression tree height

equations. The results are implemented in the symbolic computational language MAPLE.

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Numerical Implementation of Mathematical Model of the Dynamics of a Porous Medium on Supercomputers of Cluster Architecture

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Parallel computational algorithm for analysis of the processes of elastic-plastic deformation of a porous medium under the action of external dynamic loads is developed. This algorithm is based on the mathematical model taking into account threshold nature of change in the strength of a material under collapse of pores. Such model is applicable, for example, to the simulation of porous metals - new artificial materials that find wide application due to their low density and good damping properties. Mathematical model is represented in the form of variational inequality, taking into account irreversible deformation of a medium. The von Mises yield condition is used for the description of plastic deformations. The change in resistance of a porous material to external mechanical impacts at the moment of pore collapse is taken into account by means of the von Mises-Schleicher strength condition. Explicit algorithm for numerical implementation of variational inequality is constructed on the basis of the splitting method with respect to physical processes. First at each time level the problem on deformation of an elastic porous medium is solved, and then the obtained solution is corrected to account for plastic properties. The algorithm is implemented in Fortran by means of functions of the MPI library. Parallelization of computations is performed at the stage of splitting the problem with respect to spatial variables. The computational domain may consist of an arbitrary number of blocks with curvilinear boundaries. Parallel program system has been tested on clusters in computations of the propagation of plane longitudinal shock waves of compression and in computations of the expansion of a cylindrical cavity in an infinite porous medium. The comparison of numerical results and exact solutions has shown their good qualitative and quantitative consistency.

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Mathematical Modeling of Deformation of a Porous Medium, Considering Its Strengthening Due to Pore Collapse

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Based on the generalized rheological method, the mathematical model describing small deformations of a single-phase porous medium without regard to effect of fluid or gas in pores is constructed. Such model is applicable, for example, to the simulation of porous metals – new artificial materials that find wide application due to their low density and good damping properties. The change in resistance of a porous material to external mechanical impacts at the moment of pore collapse is taken into account by means of the von Mises-Schleicher strength condition. In order to consider irreversible deformation, alongside with the classical yield conditions by von Mises and Tresca-Saint-Venant, the special condition modeling plastic loss of stability of porous skeleton is used. In the low-porous material with relatively high yield point, the collapse of pores under compressive stress takes place at the stage of elastic deformation, and plasticity shows itself only after compaction of a medium. In the material with low yield point and high porosity, plasticity appears before compaction. It is shown that the proposed mathematical model satisfies the principles of thermodynamics of irreversible processes. Phenomenological parameters of the model are determined on the basis of approximate calculation of the problem on quasi-static loading of a cubic periodicity cell with spherical voids. In the framework of obtained model, the process of propagation of plane longitudinal waves of compression in a homogenous porous medium, accompanied by plastic deformation of skeleton and collapse of pores, is analyzed. For the Tresca-Saint-Venant yield condition regardless of dilatancy in compacted state of a porous medium, the exact solution of the problem on propagation of shock waves under abrupt equally distributed pressure applied at the boundary of a porous half-space is constructed.

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Bulk Solitary Waves in Elastic Solids

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We consider the problem of nonlinear bulk wave generation and detection in structural basic elements - rods, plates and shells. The elements are exhaustively studied, and widely used in physics and engineering. However, it is mostly valid for linear elasticity, whereas dynamic nonlinear theory of these elements is still far from being completed. In order to show how the nonlinear waves can be used in various applications and in non-destructive evaluation, in particular, we studied the solitary elastic wave propagation along lengthy wave guides, rods and plates, and remarkably small attenuation of elastic solitons was proven in physical experiments. We demonstrated recently how the strain solitons can be used for non-destructive testing of laminated composites used nowadays for various applications, *e.g.*, in aerospace and automotive industries, and bulk strain solitons are among prospective instruments for NDT. Both theory and generation for strain soliton in a shell, were, however, remained unsolved problems until recently, and study of nonlinear bulk wave propagation in a shell attracts essential interest, being related to stability and NDT of thin-walled shells. We considered the axially symmetric deformation of an infinite nonlinearly elastic cylindrical shell without torsion. The problem for bulk longitudinal waves is shown to be reducible to the one equation, if a relation between transversal displacement and the longitudinal strain is found. However, the simplest hypothesis lead to unsatisfactory accuracy in the boundary conditions on free lateral surfaces. We refined the above mentioned relation, providing the validity of the boundary conditions with the desirable accuracy. We derived the only equation for longitudinal nonlinear strain wave and shown that the equation has, amongst others, a bidirectional solitary wave solution, which lead us to successful physical experiments.

We observed first the compression solitary wave in the duct-like polymer shell and proved, that there is no tensile area behind the wave, the bulk soliton propagates on a distance many times longer than its wave length, while both its shape and amplitude remain unchanged. Being aimed to propose the bulk strain solitons as an instrument for NDT in solids, we studied numerically the evolution of them in various wave guides with local defects, and shown that the strain soliton undergoes changes in amplitude, phase shift and the shape, that can be estimated. To sum up, now we are able to propose a new NDT technique based on bulk strain soliton propagation in structural elements.

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A Surface Generator

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Free-form surface modellers in Computer Aided Geometric Design are usually based on the representation of a surface as a construction of rectangular patches because of the relatively simple structures involved in their use. Unfortunately, it is sometimes impossible to model a surface as a mapping from a regular rectangular grid. Many surfaces require the insertion of patches which do not have four sides. A considerable amount of effort has been devoted to developing schemes for solving the problem of branching. These schemes can handle arbitrary topological meshes and are useful for precise surface modelling as in industrial design. However, they are computationally expensive or require complex constraints to maintain the continuity between two patches. Therefore, these methods are not suitable for interactive manipulation.

To date there does not exist a completely satisfactory method which generates surfaces of arbitrary topology and at the same time is able to produce fine detail on the surface. Most modelling is done by some combination of methods to produce the desired result, which is time consuming and can also be very complex.

This paper presents a method which constructs, at different steps, a new set of points with more vertices and smaller faces than the original set of points. After a number of iterations, this results in a smooth surface. The new points generated are divided into three categories:

- *new face points* – new points lying in the middle of the squares of the original mesh;
- *new vertex points* – new points corresponding to old control points; and
- *new edge points* – new points lying near the edges connecting original control points.

Each kind of new point is divided into different sub-categories. In fact in the case of curves there are two kinds of new vertex points and two kinds of new edge points, whereas in the case of surfaces there are three kinds of new face points, three kinds of new vertex points and four kinds of new edge points.

Mathematical and Numerical Modeling of the Pass of an Asteroid-Comet Body through the Earth's Atmosphere

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In the present talk, the mathematical model and the numerical algorithms are proposed for a modeling the complex of phenomena which accompany the pass of a friable asteroid-comet body through the Earth's atmosphere: the material ablation, the ionization, the dynamics and influence of shock waves. The proposed algorithms are constructed on the basis of the Navier-Stokes equations for viscous heat-conducting gas with the addition of an equation for a friable-dust mass and with the special coefficients of viscosity and ionization of materials. For physical model of the atmosphere, the distribution of density, pressure, and temperature in height is taken for the standard atmosphere. An asteroid-comet body is initially taken as a round body consisting of a heavy gas-dust mass with corresponding density and significant "viscosity" that models the strength index of this body. A numerical algorithm is proposed for solving the initial-boundary problem for the extended Navier-Stokes equations as the combination of the semi-Lagrangian approximation for Lagrange transport derivatives and the conforming finite element method for other terms [1]. The computational experiments were carried out for a wide range of the geometric and gas-dynamic parameters.

Acknowledgement: This work is supported by Project 14-11-00147 of Russian Scientific Foundation.

References

[1] V. Shaidurov, G. Shchepanovskaya, M. Yakubovich, "A Semi-Lagrangian Approach in the Finite Element Method for the Navier-Stokes Equations of Viscous Heat-Conducting Gas," in *AIP CP***1629**, AIP, Melville, New York, 2014, pp. 19–31, DOI: 10.1063/1.4902256.

Monte Carlo Approach for Studies of the Flows near Natural and Technogenic Objects in the Earth's Upper Atmosphere

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The gas flow near the surface of the space – natural or technogenic – body entering into the atmosphere is a very complicated problem because of the own surface outgassing. It is necessary to consider the gas mixture of outgassing and ambient atmospheric species, and the chemical reactions both on a space body surface and in the near-surface layer. It is known, that the flyby of the spacecraft with actively outgassing surface results in the formation of the slowly vanishing pollution plume which contains many radiatively and chemically active admixture species.

The considered physical system – the outgassing space body surface moving in the ambient atmospheric gas – is described by the system of nonlinear Boltzmann type kinetic equations [1], because the kinetics of the reactive collisions at hyperthermal velocities between atmospheric O atoms and water vapor in the bolide plume is a non-equilibrium one. The efficient analogue algorithms of kinetic Monte Carlo approach [1] are discussed in the report. This approach is used to investigate the input of chemical processes of the interaction of own external atmosphere of the entering body with the ambient atmospheric gas. Calculations show the formation of the transition region (or near-surface boundary layer) in which the interaction between the outgassing products and ambient atmospheric gas takes place. In particular, this transition region is characterized by the following features: (i) the effect of surface temperature shielding is increased for the stronger outgassing; (ii) the influence of chemical reactions mainly leads to the formation of new species in the spacecraft exhaust, some of them would be ecologically dangerous for both the Earth's atmosphere and the spacecraft surface.

Acknowledgement: The work was supported by the Russian Foundation for Basic Research, Grant No.13-07-00276.

References

[1] V.I. Shematovich *et al.* (2011) Influence of the hot oxygen corona on the satellite drag in the Earth's upper atmosphere, *Solar System Research* **45**, 231–239.

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Some New Estimates of the Modulus of Some Integrals of the Unit Circle in the Complex Plane

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In this paper, we make some new estimates bellow the modulus of some integrals of the unit circle in the complex plane.

Keywords: Modulus, integral, complex plane, increasing function, decreasing function, unit circle, polynomial

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The Influence of Inhomogeneity on the Behavior of Cracked Magneto-electro-elastic Materials

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Functionally graded materials are extensively used in modern industry. They are composite materials with continuously varying properties in one or more special dimensions, according to the specific purpose. In view of their applications, stress analysis of such materials is important for their structural integrity. In this study we will consider functionally graded magneto-electro-elastic materials with one or more cracks subjected to SH waves. We assume that the material properties vary in one and the same way, described by an inhomogeneity function. The boundary value problem is reduced to a system of integro-differential equations based on the existence of fundamental solutions. Different inhomogeneity classes are used to obtain a wave equation with constant coefficients. Radon transform is applied to derive the fundamental solution in a closed form. Program code in FORTRAN 77 is developed and validated using available examples from literature. Simulations show the dependence of stress, electric and magnetic field concentration on the frequency of the applied time-harmonic load for different types of material inhomogeneity and different disposition of the cracks.

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Modeling, Simulation and PDE Stability Analysis for Foreign Body Fibrotic Reactions

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The implantation of medical devices often triggers several immune responses, one kind of which is categorized as foreign body reactions. It is well established that macrophages and many other cells participate in the complex processes of foreign body reactions, and cause severe inflammations and fibrotic capsule formation in surrounding tissues. Mathematical models have been proposed to systematically decipher the behavior of this complex system of multiple cells, proteins and biochemical processes in wound healing responses.

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Upscaling the Coupled Water Flow and Heat Transfer near Subsurface – Comparison between Numerical and Field Data

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The simultaneous movement of liquid water, water vapor, and heat in the vadose zone plays a critical role in the overall water and energy balance of the near surface environment. Moisture near the soil surface is influenced by evaporation, precipitation, liquid water flow, and water vapor flow, most of which are strongly coupled. The demand for mathematical models that take into account spatial and temporal scales for the shallow soil are now-a-days more imperative given that: (a) the critical role that such processes play in the global water and energy balance; (b) the interplay between spatial and temporal scales in the near surface region

is not well understood. In this paper, the coupled model is revisited and some modifications are proposed aiming to represent the surface/subsurface interaction more accurately. The upscaled system is presented. The new contribution here is the comparison between numerical results of the fine-scale and upscaled models and data for both, moisture and temperature. The field data comes from a detailed controlled experiment from Riverside-CA, with measurements taken at at 2, 7 and 12 cm below the surface.

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Nonlinear Drainage of Some Non-Newtonian Free Films

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The behavior of Newtonian thin films have been studied theoretically in details by many authors because of their wide variety of applications in nature and industry. However, the thin films of non-Newtonian liquids have received much less attention, although their often occurrence, *e.g.*, as ceramic or polymer melts, liquid metals, suspensions, biological solutions, *etc.* The main difficulty is their nonlinear stress-strain relation, where the nonlinearity may be expressed in a very complicated manner. Most of these non-Newtonian fluids behave like Newtonian ones (with constant viscosity) at very high and very low shear rates. Such fluids are usually named shear thinning fluids, whose viscosity can be modeled by a nonlinear function of the shear rate or shear stress. One of the most common viscosity models, that are used, are: the power law and the Carreau model [1].

In the present work we apply the generalized lubrication approach (including inertial, viscous, capillary and van-der-Waals forces) [2] to study the dynamics of a free thin film of a non-Newtonian fluid, whose viscosity is described by the power and Carreau models. For planar films with fully mobile surfaces, this approach leads to a system of two nonlinear PDE for the film thickness and lateral velocity. This system is studied numerically in the case of laterally bounded free films. The calculations of the film shape and velocity are presented using data of some real liquids [1]. It is shown that the viscosity variations on the film drainage are significant, *i.e.*, the larger the viscosity, the slower the film thinning rate. The film shapes and velocities calculated by both viscosity models are almost the same.

References

[1] T. G. Myers (2005) Application of non-Newtonian models to thin film flow, *Physical Review E***72**, 066302, 11 p.

[2] S. Tabakova, "Dynamics and stability of free thin films," in *AIP CP***1301**, pp. 531–542, AIP, Melville, New York, 2010.

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Numerical Simulations of Two-fluid Flow Problems by an Energy-stable Lagrange-Galerkin Scheme

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We consider two-fluid flow problems, where each fluid is governed by theΓ́@Navier-Stokes equations and the surface tension proportional to the curvature acts on the interface. The domain which each fluid occupies is unknown, and the interface moves with the velocity of the particle on it. While numerical solution of one-fluid flow problems governed by the Navier-Stokes equations has been successfully established from the point of stability and convergence, it is not an easy task to construct numerical schemes solving the two-fluid flow problems. To the best of our knowledge there are no numerical schemes whose solutions are proved to converge to the exact one and there is very little discussion even for the stability of schemes. Recently we have developed an energy-stable Lagrange-Galerkin finite element scheme for the two-fluid flow problems. The scheme is an extension of the energy-stable finite element scheme proposed by us [1, 2] to the Lagrange-Galerkin method [3, 4]. Here we report some numerical simulation results of two-fluid flow problems of rising bubbles and falling droplets using this scheme. Those results show the robustness, the efficiency, and the applicability of the scheme.

References

[1] M. Tabata (2007) Finite element schemes based on energy-stable approximation for two-fluid flow problems with surface tension, *Hokkaido Mathematical Journal* **36**, 875–890.

[2] M. Tabata, "Numerical simulation of fluid movement in an hourglass by an energy-stable finite element scheme", in M. N. Hafez, K. Oshima, and D. Kwak (Eds), *Computational Fluid Dynamics Review 2010*, pp. 29–50, World Scientific, Singapore, 2010.

[3] O. Pironneau and M. Tabata (2010) Stability and convergence of a Galerkin-characteristics finite element scheme of lumped mass type, *International Journal for Numerical Methods in Fluids* **64**, 1240–1253.

[4] H. Notsu and M. Tabata (2015) Error estimates of a pressure-stabilized characteristics finite element scheme for the Oseen equations, *Journal of Scientific Com-*

puting, DOI:10.1007/s10915-015-9992-8.

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Nonlinear Absorption of Alfven Wave in Dissipative Plasma

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In the report, we study the absorption of Alfven waves on the basis of the exact solution of the two-fluid electromagnetic hydrodynamics equations (EMHD-equations) of the plasma with the electrons inertia fully taken into account. We investigate the temporal absorption of Alfven waves caused by the dissipative effects (magnetic and hydrodynamic viscosities and thermal conductivity of electrons and ions), and relaxation of electron and ion temperatures in the wave caused by their elastic interaction, based on the exact solution of the non-linearized magnetic hydrodynamic equations. The report shows that the analysis of temporal nonlinear absorption of Alfven wave is reduced to the study of a system of nonlinear ordinary differential equations (ODE) for the complex amplitudes of the wave parameters. The wave absorption does not depend on thermal conductivity of electrons and ions and is divided into two stages. With magnetic viscosity taken into account in the first stage, there is the rapid transformation of the magnetic energy and the large part of the kinetic energy into the thermal energy of electrons and ions, which is sharply accelerated by adding the hydrodynamic viscosities of electrons and ions. The conversion velocity of nonthermal energy sources into the thermal ones increases significantly with decreasing wavelength. The second stage is a much longer relaxation of the electron and ion temperatures, when the last part of the kinetic energy transforms into the thermal energy of the plasma components and magnetic energy does not change, and has a background value. The temperatures relaxation process in the second stage can be approximated (Harman-Grobman theorem) by solutions with sufficient accuracy of the linearized, near the singular point, ODE system for the complex amplitudes.

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Solving a Semilinear Convection-diffusion Problem by a Two-grid Method with Richardson extrapolation

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A boundary value problem for a second-order semilinear singularly perturbed ordinary differential equation is considered. We use Newton and Picard iterations for a linearization. To solve the problem at each iteration we apply the difference scheme with the property of uniform with respect to the singular perturbation parameter convergence. A modified Samarskii and central difference schemes on Shishkin mesh are considered. It is known that these schemes are almost second order accuracy uniformly with respect to the singular perturbation parameter (V.B. Andreev, I.A. Savin and V.B. Andreev, N.V. Kopteva). To decrease the required number of arithmetical operations for resolving the difference scheme, a two-grid method is proposed. According to the idea of the two-grid algorithm, at first, the problem is solved on a coarse mesh. Secondly, the found mesh solution is interpolated to nodes of the fine mesh and is used as the initial approximation for following iterations. It leads to reduction of the number of iterations on the fine mesh and also reduces the number of arithmetical operations. Note that the interpolation formula must be uniform with respect to the singular perturbation parameter else the accuracy of the found mesh solution may be lost. To increase the accuracy of difference scheme, we investigate the possibility to apply Richardson extrapolation using known solutions of the difference scheme on both meshes. The results of some numerical experiments are discussed. The comparison of Samarskii and central difference schemes is carried out.

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Numerical Solution of Differential-difference Equations in Large Intervals Using a Taylor Collocation Method

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In this paper, a collocation method based on Taylor polynomials is developed for solving systems linear differential-difference equations with variable coefficients defined in large intervals. By using Taylor polynomials and their properties in obtaining operational matrices, the solution of the differential-difference equation system with given conditions is reduced to the solution of a system of linear algebraic equations. We first divide the large interval into M equal subintervals and then Taylor polynomials solutions are obtained in each interval, separately. Some numerical examples are given and results are compared with analytical solutions and other techniques in the literature to demonstrate the validity and applicability of the proposed method.

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Appearance of Repeated Support Splitting and Merging Phenomena in a Porous Media Equation with Absorption

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The phenomena associated with interfaces in nonlinear diffusion have been of interest to applied mathematicians for a long time, and have enabled them to promote the development of numerical methods, which suggest interesting properties in the several fields of fluid dynamics, plasma physics and population dynamics. Among such properties, there appear interesting phenomena in the dynamical behavior of non-stationary seepage with the non-linear filtration; that is, a striking manifestation of "repeated support splitting and merging phenomena." Here the support means the region where the fluid exists. Such phenomena are caused by the interaction between the nonlinear diffusion and the penetration of the fluid from the boundary on which the flowing tide and the ebbing tide occur. To realize such phenomena we introduce a model equation written in the form of the initial-boundary value problem for some nonlinear diffusion equation, which is used to describe the flow through porous media with absorption.

From analytical points of view, Kersner [1] proved the appearance of "support splitting phenomena," but he did not show that "support merging phenomena" after the support splits.

To investigate such phenomena we tried numerical computation by our difference scheme, and obtained the following properties:

i) "Stabilization property," that is, the solution converges to the stationary solution as time tends to infinity, when the boundary value is constant;

ii) "Repeated support splitting and merging phenomena" appear, when the period imposed on the boundary value is very long;

iii) "Support splitting phenomena" never appear, when the period is sufficiently short in comparison with that in ii).

In this talk we state the proof of Properties i), ii) and iii).

References

[1] R. Kersner (1980) Degenerate parabolic equations with general nonlinearities, *Nonlinear Anal.*, 1043–1062.

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Modeling of the Interaction of Meteoroids with the Martian Atmosphere

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In this study, we develop the model which describes meteoroids entering the atmosphere of a planet, categorize the consequences of the collisions of cosmic bodies with the atmosphere and the surface and apply our results to the Martian atmosphere. Two types of results are considered: meteorite fall (a meteoroid fragment can be found on the surface), and full ablation (meteoroid does not reach the ground).

The model is based on the analytical solution of the classical equations of meteor body deceleration. The dimensionless solution for the mass-velocity dependence and the height-velocity dependence can be expressed using two main dimensionless parameters: the ballistic coefficient, which shows the ratio between the mass of the atmospheric column along the trajectory and the body's pre-entry mass, and the mass loss parameter, which is proportional to the ratio between the initial kinetic energy of the body and energy required to insure total mass loss of the body due to ablation and fragmentation. Every given meteoroid has a corresponding parameter pair.

The meteorite fall condition is established: the terminal mass of a meteoroid exceeds or is equal to a certain chosen value. Using the parameters, we get a boundary curve on the parameter plane and associate different events with the location of the point relative to this curve.

As an example, we take a chondrite with the entry velocity 10 km/s, and an iron meteoroid with the entry velocity 15 km/s. We show the impact consequences for several pre-entry mass values. We compare our results for the Martian atmosphere with the same meteoroid cases produced in the terrestrial atmosphere. For a certain range of pre-entry masses, a meteoroid entering the atmosphere of Earth would be fully ablated, while a meteoroid with the similar properties entering the atmosphere of Mars would result in a meteorite event.

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Numerical Investigation of a Space-fractional Model of Turbulent Fluid Flow

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The models that are based of fractional derivatives should be highlighted among promising new models to describe turbulent fluid flows. In the present work, a steady-state flow in a duct is considered under the condition that the eddy diffusion is governed by a fractional power of the Laplace operator. To study numerically flows in rectangular channels, finite-difference approximations are employed. For approximate solving the corresponding boundary value problem, the iterative method of conjugate gradients is used. At each iteration, the problem with a fractional power of the grid Laplace operator is solved. Predictions of turbulent flows in ducts at different Reynolds numbers are presented via mean velocity fields.

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Finite-difference Approximation for Two-dimensional Generalized Oldroyd-B Fluids

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An increasing attention has been devoted to the prediction of behaviour of viscoelastic non-Newtonian fluids in the recent years, due to their broad application in industry and biology (molten plastics, oils and greases, suspensions, emulsions, pulps, *etc.*). The generalized fractional Oldroyd-B constitutive model is frequently used for such viscoelastic fluids. It contains two Riemann-Liouville fractional time derivatives of orders α and $\beta \in (0, 1)$.

The two-dimensional Rayleigh-Stokes problem for a generalized Oldroyd-B fluid is considered in the present work. First and second order approximations of the fractional derivatives are implemented in the developed alternating direction implicit finite difference scheme. Extensive numerical experiments are performed in order to investigate the behaviour of the solutions for different values of the parameters α and β.

Acknowledgement: The work is partially supported by Grant DFNI-I02/9 from the Bulgarian National Science Fund.

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Modeling the Effect of Meteorological Factors on SO2 and PM10 Concentrations in SARIMA method and Model Refinement

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Numerous methods for time series analysis and forecasting allow for detailed study of processes, in particular the processes air pollution. The aim of this work is to explore empirically various aspects of the methodology of stochastic modeling approach such as ARIMA/SARIMA methods. Object of research is the pollution with two problematic pollutants SO2 and PM10 of Kardzhali, Bulgaria. There are built and examined various ARIMA models taking into account meteorological factors, influence of the transformations of the data, of outliers, of different horizons

selected to predict future concentrations and more.

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The Semi-Lagrangian Algorithm Based on an Integral Transformation for Three-Dimensional Advection Problems

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Nowadays many physical phenomena in transport processes are modeled by time-dependent advection equations. Semi-Lagrangian method (in some papers it is called as Eulerian-Lagrangian method or method of characteristics) profitably differs among other methods for numerical solving advection problems. In contrast to traditional Eulerian schemes, semi-Lagrangian algorithms provide unconditional stability in many cases and their efficiency makes them more and more popular. Now there are a lot of different versions of these algorithms. Most of them have no theoretical convergence justification of numerical solution to exact one. Nevertheless for two-dimensional advection problem, such algorithm is constructed with theoretical convergence justification [1]. It has the explicit form and the first order of accuracy. The theoretical results were confirmed by numerical experiments. But this version contains resource-intensive computations to get a numerical solution in each node of a numerical grid. To overcome this disadvantage, we have recently developed another semi-Lagrangian version [2]. The distinctive feature of this developed version consists in the technique of the computation for the integral at a previous time level with known functions. To compute it approximately, we make the integral transformation. The developed version helps to decrease resource-intensive computations and to reduce the computational time. In the present talk we extend these versions for three-dimensional advection problems.

Acknowledgement: The work is supported by Project 14-11-00147 of Russian Scientific Foundation.

References

[1] A. Efremov, E. Karepova, V. Shaydurov, A. Vyatkin (2014) A Computational Realization of a Semi-Lagrangian Method for Solving the Advection Equation, *Journal of Applied Mathematics* **2014**, Article ID 610398, 14 pages, doi: 10.1155/2014/610398.

[2] V. Shaydurov and A. Vyatkin, "The Semi-Lagrangian Algorithm Based on an Integral Transformation," in *AIP CP***1648**, 850041, AIP, Melville, New York, 2015,

doi: 10.1063/1.4913096.

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Some Features of CUDA Implementation of Semi-Lagrangian Method for an Advection Problem

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Nowadays there are a lot of algorithms of the semi-Lagrangian family for solving problems of computational fluid dynamics. These algorithms usually provide unconditional stability. The algorithm, presented in [1] for an advection problem, is based on a square grid, takes into account the boundary conditions, and has the first order of accuracy. Moreover, a discrete analogue of the balance equation holds when going from a known time layer to the next, calculated one. However, this algorithm is both compute- and resource-intensive. Therefore its parallel implementation is an actual task. Notwithstanding the algorithm is well-parallelizable (it is explicit with respect to time and data independence in the general space loop), direct attempts to use CUDA technology [1] faced severe restrictions of general-purpose GPU architecture.

In the present talk we have scrutinized the bottleneck of a direct sequential algorithm and its parallel versions and detected the primary causes of a poor CUDA performance. In this type of algorithm, the great part of computation consists in integration stage. The procedure of determining the mutual arrangement of a curvilinear quadrangle on a previous time level is especially resource-intensive. This code has many flow control instructions ("if" statements, mainly) and a deep nesting level of functions.

We have revised the integration stage at the previous time level in order to improve an efficiency of this algorithm. Numerical experiments corroborate a good CUDA performance of the new version of the algorithm. Note that we sacrifice a conservatism of the discrete analogue.

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References

[1] A. Efremov, E. Karepova, V. Shaydurov, A. Vyatkin (2014) A Computational Realization of a Semi-Lagrangian Method for Solving the Advection Equation, *Journal of Applied Mathematics* **2014**, Article ID 610398, 14 pages, doi: 10.1155/2014/610398.

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Multicriterial Analysis and Ontologically Represented Information

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The aim of our work is to attempt at designing a decision support system based on ontological representation of domain knowledge and semantic data processing. We assume that application of semantic data processing could increase the efficiency and adaptability of support provided to the user. Specifically, we consider the situation when the user describes her requirements as a class expression from an ontology, while the instances of (the same) ontology represent entities available in the system. The goal is to help the user to find the best option with respect to her requirements, while remembering that user's knowledge of the domain may be limited.

To solve thus stated problem we have considered multiple approaches based on semantic data processing, which require user interaction to different extend. First, we evaluated ontological matchmaking based on SPARQL queries and class expression, that allow finding entities matching criteria specified by the user. The resulting list of entities is not ranked and during the matchmaking process all criteria are treated as equally important.

The second approach was based on establishing semantic closeness between instances representing user requirements (constructed from the class expression) and instances representing entities in the ontology. This method is graph-based and the resultant list is ranked with respect to "similarity." For users with more in-depth knowledge, it is possible to extend this approach with weights that can be assigned to criteria; *i.e.*, user may indicate that a given feature of the required entity is more important than other features (note that, here, features map into the decision criteria). The last approach is based on multicriterial analysis and utilizes weights for decision criteria and expert domain knowledge (also ontologically demarcated). Specifically, the Analytical Hierarchy Process (AHP) is used to evaluate opinions

expressed by multiple experts with respect to user requirements and preferences regarding the importance of decision criteria. Finally, the system provides the user with recommendations on how to modify / extend requirements specified by the user in order to select the best option. This approach can be used by those who are not sure what they need, and from basic data that they put in the system, semantic analysis of expert knowledge would help them to "correct" the specification of the actual requirement. 1 The context of the work is provided by the Agents in Grid (AiG) project, which aims at development of an agent-semantic infrastructure for efficient resource management in the Grid. Decision support within the system should help the user with different level of expertise to choose optimal algorithm and/or resource to solve a problem from a given domain, and later to choose the best contract defining terms of collaboration with the provider of a resource used to solve the problem. However, the proposed approaches naturally generalize to other similar scenarios.

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Methods of Trajectories and Finite Elements in a Problem of the Supersonic Flow in the Asymmetrical Channel

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The flow in the two-dimensional channel with an expansion belongs to the simplest class of separated flows with the fixed separation point. A sudden expansion of the channel causes a separation of a stream and essentially changes its kinematic structure. Owing to the great practical importance, such flows were studied theoretically and experimentally both for laminar and for the turbulent modes for the movement of the incompressible and compressed mediums.

In the present talk, the mathematical model of two-dimensional supersonic gas flow in the channel with the backward step is treated [1]. The model of a flow is constructed on the basis of the modified Navier-Stokes equations for viscous heat-conducting gas. In the equations of mass and internal energy, the replacement of required functions is produced which transforms the conservation laws of mass and total energy from terms of L1-space to the Hilbert L2-space. It considerably simplifies justification of stability and convergence.

For approximation of a full (substantial) derivative in time, the method of trajectories is used in each equation. Discretization in space of other terms on each time level is carried out by finite element method with piecewise-bilinear basic

functions. The block Jacobi method with external iterations for nonlinearity is applied for solving the systems of the nonlinear algebraic equations received after discretization of a stationary problem at each time level. The received variation-differential scheme has the first order of accuracy on time and space.

By the constructed algorithm, the problem of a supersonic flow of gas in the channel with expansion in the form of a step is realized for various Mach and Reynolds numbers. Combination of the methods of trajectories and finite elements produces a stable and economic algorithm.

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References

[1] V. Shaidurov, G. Shchepanovskaya, M. Yakubovich (2012). Numerical modeling of supersonic flows in channel, *Russian Journal of Numer. Anal. and Math. Modeling* **27**(6), 585–601.

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Numerical Simulation of Photoexcited Polaron States in Water

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We consider the dynamic polaron model on the basis of a system of three nonlinear partial differential equations with appropriate initial and boundary conditions. A parallel numerical algorithm the solution of this system has been developed. A numerical simulation of the polaron states formation in water under the action of the ultraviolet range laser irradiation has been performed. The numerical results are shown to be in a reasonable agreement with the experimental data and the theoretical predictions.

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Numerical Study of Fluid Motion in Cylindrical Reactor with Two Mixers

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Numerical study of hydrodynamic behavior of a viscous fluid in bioreactor with multiple mixers is provided in the present paper. The calculations are made by a computer program, written in MATLAB. The fluid structure is described and numerical results are graphically presented and commented.

Keywords: Navier-Stokes equations, mechanical mixing, hydrodynamic characteristics of viscous fluid, Reynolds number