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NUMERICAL ALGEBRA WITH APPLICATIONS

Abstracts of Lecturers and Young Scientists

Editors: Zhong-Ci Shi, Lev A. Krukier

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Second China-Russia Conference on Numerical Algebra with Applications (CRC-NAA'13) is organized by Computer Center and Faculty of Mathematics and Computer Science of Southern Federal University. It aims at bringing together researchers, scientists, engineers, and graduate students to exchange and stimulate ideas from different disciplines, at discussing the practical challenges encountered and the solutions adopted, and at learning about the recent developments on theory and numerical methods for numerical simulation about numerical algebra and scientific computing. The topics of CRC-NAA'13 include, but are not limited to: mathematical modeling; applicating of numerical methods and algorithms to solve problems of mathematical modeling; solving linear and nonlinear equations systems; preconditionining technique; parallel computing.

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Program
Second China-Russia Conference "Numerical Algebra with Applications"

June 25 (Tuesday)

Registration and Reception

June 26 (Wednesday)

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Departure

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Abstracts of Lectures and Invited Talks

A GLOBALIZED DIRECTIONAL DERIVATIVE-BASED NEWTON METHOD FOR INVERSE SINGULAR VALUE PROBLEMS

Bai Z.-J.

School of Mathematical Sciences, Xiamen University, Xiamen, China

In this paper, we give a regularized directional derivative-based Newton method for solving the inverse singular value problem (ISVP). The proposed method is also globalized by employing the directional derivative-based Wolfe line search conditions. Under some mild assumptions, the global and quadratic convergence of our method is established. To improve the practical effectiveness, we also propose a hybrid method for solving the ISVP. We show that the hybrid method converges quadratically and globally in the sense that a stationary point of a merit function for the ISVP is computed. Numerical tests demonstrate that the proposed hybrid method is very effective for solving the ISVP with distinct and multiple singular values.

TWO-STEP APPROXIMATION PRECONDITIONING METHODS FOR STEADY INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

Bai Z.-Z.

State Key Laboratory of Scientific/Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Beijing, China

When the artificial compressibility method in conjunction with high-order upwind compact finite difference schemes is employed to discretize the steady-state incompressible Navier-Stokes equations, in each pseudo-time step we need to solve a structured system of linear equations approximately by, for example, a Krylov subspace method such as the preconditioned GMRES. In this talk, based on the special structure and concrete property of the linear system we construct a structured preconditioner for its coefficient matrix and estimate eigenvalue bounds of the correspondingly preconditioned matrix. Numerical examples are given to illustrate the effectiveness of the proposed preconditioning methods.

SOME LOWEST ORDER NONCONFORMING MIXED ELEMENTS COUPLED WITH RAVIART-THOMAS MIXED ELEMENTS FOR STOKES-DARCY FLOWS

Chen J.-R.

School of Mathematical Sciences, Nanjing Normal University, Nanjing, China

In this paper, we study numerical methods for a coupled Stokes-Darcy model. This model is composed by Stokes equations involving the deformation tensor formulation in the fluid domain and Darcy's law in the porous media domain, coupling together through certain interface conditions. We use two lowest order nonconforming mixed finite elements choosing a nonconforming element for one velocity component of the Stokes flow and a conforming element for the other component in order to satisfy the Korn's inequality, and use the lowest order Raviart-Thomas elements for the Darcy law on triangular or quadrilateral meshes with nonmatching interface. By Boland-Nicolaides trick, the inf-sup condition of the discrete problem is proved. Moreover, we construct a new interpolation operator to derive the a priori error estimates of the proposed finite element method. Numerical examples are also given to confirm the theoretical results.

RATIONAL APPROXIMATIONS IN COMPUTATIONAL ALGORITHMS OF MATHEMATICAL PHYSICS

Gordin V.A.

Higher School of Economics, Hydrometeorological Centre of Russia, Moscow, Russia

1. Classical Pade approximations for gives us an approach to construction and classification of one-layer difference schemes. There is a generalization of the method that can be applied to multilayer difference schemes.

2. Two-point Pade approximation can be used to representations of solutions of boundary-value problems. The approach needs to be modified, when we approximate solutions of the differentiated equations (both ODE and PDE) at . We can estimate their asymptotics at and , but we need usually in the solution's approximation at "middle" time. The corresponding asymptotic series can divergent or convergent very slowly and are useless at the "middle" time. We have to generalize definition of Pade approximation for these purposes.

3. Compact difference schemes rather traditional ones (4-th order approximation instead of 2 July). Their construction is connected with Pade approximation of the symbol of the resolving operator corresponding to the differential problem.

4. The non-reflecting boundary conditions are desirable in various computing tasks of mathematical physics. They can be constructed as pseudo-differential operators on the boundary of the corresponding computational area. However, if we are going to construct such boundary conditions for some difference approximation, we must take into account the specific types of differential grid and difference approximation. "Memory" - the number of boundary points of the grid which are included in the boundary condition, is essential for the practical implementation of the algorithm. To minimize this "memory", a useful approach based on Z-transformation and Pade approximations.

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A PARALLEL ALGORITHM OF VORTEX-IN-CELL METHOD[1]

Govorukhin V.N.
Southern Federal University, Rostov-on-Don, Russia

In this talk the parallel algorithm of variant of vortex-in-cells method originally presented in [1, 3, 4] is developed. The governing equations are the 2D Euler equations in terms of stream function and vorticity or geophysical models of the atmosphere.

$$\frac{D\omega}{Dt} \equiv \omega_t + \psi_y\omega_x - \psi_x\omega_y = 0, \tag{1}$$

where ω is a vorticity, ψ is a stream function and D/Dt denotes the material derivative. Here $\psi_x = \partial\psi/\partial x$, $\psi_y = \partial\psi/\partial y$, $\psi_{xx} = \partial^2\psi/\partial x^2$, etc. The velocity of the fluid $v = (v_1, v_2)$ is expressed via the stream function ψ as

$$v_1 = \psi_y, \quad v_2 = -\psi_x, \tag{2}$$

In the most general case of two dimensional barotropic fluid dynamics on a sphere with allowance for the Coriolis force, the preserved quantity is the potential vorticity, which is related to the stream function as follows

$$\omega = -\Delta\psi + \Lambda^2\psi - \frac{1}{2}\gamma r^2. \tag{3}$$

Here, the Coriolis parameter near a pole is given by $f(r) = f_0 - \frac{1}{2}\gamma r^2 + O(r^4)$, where $\gamma = const$, $r = \sqrt{x^2 + y^2}$ is the polar radius, $\Lambda^2 = f_0^2/gh = const$, g is the acceleration due to gravity, and h is the thickness of the fluid layer.

The numerical method is based on vorticity field approximation using its values at a set of N fluid particles and the stream function computation using the Galerkin method. The flow domain is divided into rectangular cells. Vorticity in every cell is interpolated by a third order polynomial. The resultant piecewise continuous polynomial approximation of vorticity is employed to derive analytically Galerkin's coefficients of stream function expansion. Computed velocity field is used for fluid particles trajectories calculation as a solution of ODE system of hight dimension

$$\dot{x}_i = \psi_y(x_i, y_i), \qquad \dot{y}_i = -\psi_x(x_i, y_i) = v_2, \; i = 1..N \tag{4}$$

[1]Supported by RFBR Grant №11-01-00708

The effectiveness of integrator is important for the solution of (4). The set of different integrators is studied on a number of test problems of particles dynamics. As a result the most suitable methods are suggested. The algorithm of adaptive choice of integrator based on fluid particles locations is offered.

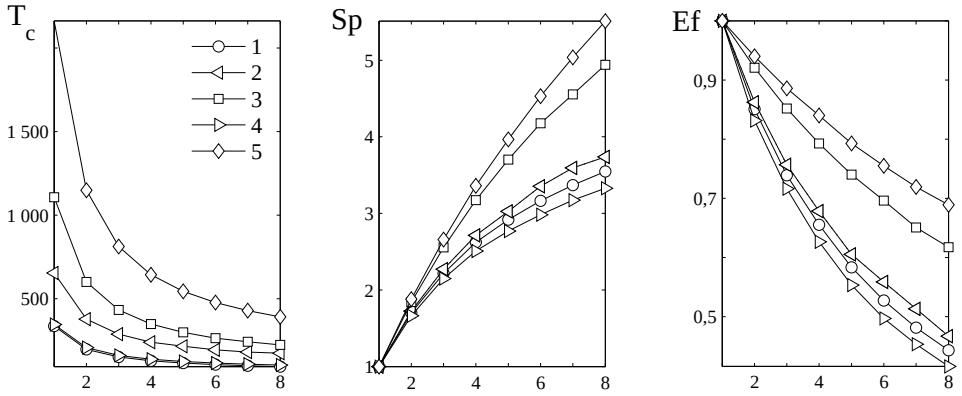

Fig. 1. Time of calculation (left), speedup (center) and efficiency (right) of the parallel algorithm with respect to the number of processors and for five sets of domain sizes and parameters of method.

The problem under consideration can be well parallelized and corresponding algorithm presented in the talk in detail. For the parallelization, the numerical method was modified using the OpenMP technology. Most of the computational cost of the flow calculation at each time-step corresponds to the finding stream function as a solution of equation (3). Several tests up to 8 CPUs have been performed to estimate performance of the parallel algorithm. The results of five calculations with different parameters of methods are presented in Figure.

The effectiveness of described numerical methods are illustrated by results of flows trough channel problem investigation [1, 2] and analysis of the multipoles vortex patch dynamics in geophysical flows.

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A NUMERICAL METHOD FOR SOLVING THE QUADRATIC MATRIX EQUATIONS

Gui B.

School of Science, Nanjing Forestry University, Nanjing, China

Nonlinear matrix equations have numerous applications in automatic control theory, signal processing, etc. Many methods have been developed for solving nonlinear matrix equations. Recently, Bai, Guo and Xu (Numer. Linear Algebra Appl. 13(2006) 655–674) proposed an alternately linearized implicit iteration method for computing its minimal non-negative solution of the algebraic Riccati equations. In this paper, we propose a new numerical method for solving the quadratic matrix equation associated with a nonsingular M-matrix by using the alternately implicit iteration method. Some numerical examples show that this method is effective.

MULTIPLICATIVE NOISE REMOVAL VIA A LEARNED DICTIONARY

Huang Y.-M.

School of Mathematics and Statistics, Lanzhou University, Lanzhou, China

Multiplicative noise removal is a challenging image processing problem, and most existing methods are based on the Maximum A Posteriori (MAP) formulation and the logarithmic transformation of multiplicative denoising problems into additive denoising problems. On the other hand, sparse representations of images have shown to be efficient approaches for image recovery. Following this idea, we propose in this paper to learn a dictionary from the logarithmic transformed image, and then to use it in a variational model built for noise removal. Extensive experimental results suggest that in terms of visual quality, PSNR and mean absolute deviation error, the proposed algorithm outperforms state-of-the-art methods.

HIGH PERFORMANCE COMPUTER SYSTEMS WITH RECONFIGURABLE ARCHITECTURE ON THE BASE OF FPGA TECHNOLOGY

Kalyaev I.A.

Southern Federal University, Rostov-on-Don, Russia

Until recently supercomputer technology had been developed according to large-block integration principles. Performance was provided due to technological achievements in the field of microprocessor design and communication systems development, but advantages of architecture and circuit design were not used. As a result, multiprocessor systems of cluster type designed on the base of widely-available computer nodes and communication networks became widespread during the last years. Cluster systems have relatively low price and simple programming methods. Software developed and debugged on personal computer may be rather easily adapted to such systems. However, cluster supercomputers generally provide high real performance only at solving loosely-coupled tasks when a number of data exchange operations is rather low. But if the solving tasks are tightly-coupled, performance of cluster systems considerably reduces and does not exceed 5-10% from the declared peak performance of the system. Besides, cluster system performance reduces when a number of processors in cluster supercomputer grows. This is the result of dissimilarity between task information structure and cluster supercomputer "fixed" architecture. Real performance of supercomputer decreases and burden sharply increases if the solving task is tightly-coupled and requires a great number of data exchange operations. The concept of multiprocessor computer systems with reconfigurable architecture had proved successful in solving specified problems of cluster supercomputers.

The essence of the concept is adaptation of reconfigurable computer system (RCS) architecture to the structure of information graph of the solving task. Usage of the principles of the concept can significantly reduce computational burden and increase system real performance.

Fixed unchangeable architecture is the cause of low real performance at solving specific problems. While mapping of a real task on such fixed architecture, large nonproductive time costs originate. The reason of the time costs is organization of computational process, but not performing of useful calculations. The main idea of reconfigurable computer systems creation is to give application programmer an opportunity to adapt computer architecture to the structure of the solving task. Time needed for computational process organisation is minimized and hence real performance is increasing.

The necessary element base is field programmable gate arrays (FPGA) of large-scale integration designed in the beginning of the XXI century. In contrast with standard integrated circuits with fixed internal structure defined on manufacturing stage, FPGA internal structure is programmable and may be varied by circuit engineer during operation. Consequently, FPGA may be used as reconfigurable co-processors for standard microprocessors. Nevertheless, using FPGA as co-processors is ineffective, because a single FPGA may contain computing structures providing several operations. Reprogramming of FPGA for each subsequent operation also needs time and leads to reducing of system real performance during the task solving.

FPGA may be considered as a component of a computational field within which multipipeline computing structures, realizing the entire graph of the algorithm, may be created. This concept provides fundamentally new opportunities of FPGA usage. The task is parallelized in the FPGA field according to the principle of fine-grain parallelization, time needed for computational process organization is minimized and hence high technical parameters of computer system, such as ratios "real performance/peak performance", "real performance/power consumption" and "real performance/volume", are provided.

RCS, designed for solving complicated problems, has to contain hundreds and thousands of FPGAs of large-scale integration, combined in the computational field. It is clear, that placing of such number of FPGAs on the one circuit board is impossible. This problem can be solved using a principle of modular design of the RCS computational field on the base of unified basic modules. Basic module is a board which contains a fragment of the FPGA computational field and auxiliary elements: intermodule data exchange interfaces, distributed memory blocks, secondary power units, synchronization subsystem, control nodes, network interfaces, etc. Basic module is a small-sized RCS which is able, along with a personal computer, to solve user's tasks. Several basic modules may be united into an RCS with the needed performance.

Process of software development for RCS greatly differs from the one for multiprocessor computer systems with cluster architecture. Software development for RCS may be divided into two parts: structural programming and procedural programming. The results of structural programming are computational structures within the field of FPGA logical cells, necessary for calculations. The sense of procedural programming is very similar to traditional programming and consists in creation of computational process in RCS. Structural programming of the FPGA computational field is the most

difficult for RCS programmer, because traditional programming consists only in creating computational process based on fixed hardware. For programming of computational structures, based on FPGA field, programmer needs quite different skills - skills of a circuit engineer.

FPGA-based reconfigurable computer systems are fundamentally new direction of high performance technique development. In contrast to cluster supercomputers, RCSs allow to create, within basic architecture, virtual special-purpose calculators with structure similar to the solving task structure. This provides high effectiveness of calculations and almost linear performance growth at computational resource expansion. General-purpose architecture of RCSs on the base of FPGA computational fields, which can be reprogrammed according to the structure of the solving task, offer unique opportunities of using RCS in problem domains which require:

- highly effective computer facilities, like special-purpose computer systems;
- ability of solving tasks from various problem domains.

RCSs with general-purpose basic architecture and ability of architecture reconfiguring entirely satisfy these requirements.

NUMERICAL ANALYSIS OF NONLINEARLY ELASTIC BEHAVIOR OF CIRCULAR MEMBRANES[1]

Karyakin M.I., Mostipan G.O., Ustinov Yu.A.
Southern Federal University, Rostov-on-Don, Russia

The paper presents a numerical-analytical algorithm for determining points of branching for circular membranes with arbitrary profile along the meridian. This class of structures includes a large number of corrugated membranes used as elastic elements in the devices of precision mechanics [1]. Spherical dome with a possible deviation from the ideal surface can be considered as a special case.

In the eighties of the last century, experiments conducted by S.Yamada [2], including high-precision measurements of the distribution of initial geometrical imperfections and vertical displacements in both subcritical and post-critical equilibrium states of a spherical dome showed the decisive influence of imperfections on the critical pressure and the shape of the stability loss. In this paper we show that by making targeted axisymmetric distortions in the shape of a spherical dome one can significantly reduce the impact of these defects.

Due to the need to allow distortions in the form of a spherical dome we consider the general problem for a circular shell of revolution of arbitrary profile and assume that the profile of such shell having a thickness h and radius $a \gg h$ is given by the function $z = f(r)$ in cylindrical coordinates.

To describe the large elastic strains of the membrane under hydrostatic pressure p we use two-dimensional nonlinear equations [3], based on the Kirchhoff's hypotheses. In addition to the detailed description of non-axisymmetric equations of the shell equilibrium, the boundary value problem for a ODE system describing the behavior of an axisymmetric shell is provided in [3]. The main method of numerical analysis of this two-point nonlinear boundary value problem was shooting method. The essential feature of its realization in comparison with [3] is associated with the impossibility to select the one loading parameter for the whole cycle of plotting the loading diagram, i.e. the dependence between force (say, applied pressure p) and geometric (e.g., deflection at the top of the dome w_0) characteristics. Traditionally, either pressure or deflection at the center of the membrane is chosen

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as such parameter, but in the case of a spherical dome (or shapes closed to it) one can encounter the situation where there is no functional relationship between these parameters: for non-shallow domes the loading diagram on the plane $p - w_0$ is a complex curve with self-intersections. To solve this problem a special algorithm was realized to automatically change and select the loading parameter. This algorithm is in some sense close to that of developed in [4].

The scheme for investigating of stability of the constructed axisymmetric solution is based on the bifurcation approach completely described in [3]. High density of intersected bifurcation curves for the perfectly spherical dome is manifested in the experiment as a high level of sensitivity of the stability of the dome to imperfections of its geometry and the impossibility to predict the specific form of the stability loss (e.g., number of dents).

In [5] for the manufacture of flapping safety membrane the concept and technology of "artification" was introduced. It involves special methods for manufacturing and refinement the membranes by introducing artificial imperfections in the spherical shape. The main purpose of these shape modulations is to eliminate (at least from some operational range of the membrane) the bifurcation points for nonaxisymmetric modes that introduce an uncertainty in the type and nature of the stability loss and post-critical behavior of the membrane. As an illustration, we present a simple model of such modulation scheme when the upper part of the dome is replaced by a flat portion. Calculations show that in addition to significant differences in the profiles of diagrams the important distinction is the absence of bifurcation points on the rising portion of the loading diagram for the modulated dome. In contrast to the comparable spherical domes the modulated membrane has no bifurcation points for modes with $n > 1$, and the point of bifurcation in the nonaxisymmetric mode $n = 1$ are located in the region of deep post-critical strains. The results presented here indicate, in particular, that for dome-shaped shells of the same thickness, equal the ratio of the arch height to the radius of the circle bearing and quantitatively similar profiles the behavior of the loading diagram of the axisymmetric loading as well as stability characteristics and the type of post-critical behavior can be qualitatively different.

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FORMS OF THE STEADY CONVECTION-DIFFUSION EQUATION AND CHOICE OF NUMERICAL METHODS[1]

Krukier L.A.

Southern Federal University, Computer Center, Rostov-on-Don, Russia

Steady convection-diffusion equation in 2-D domain can be written down in different forms. It was shown that choice of numerical methods for the solution convection-diffusion equation is strongly connected with choice initial form of equation. Using upwind schemes require non divergent form of initial equation, but central difference schemes prefer "symmetric" form. Theoretical results for different forms of convection diffusion equation have been presented.

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EFFECTIVE ITERATIVE METHODS FOR BLOCK-STRUCTURED LINEAR SYSTEMS[1]

Martynova T.S.

Southern Federal University, Rostov-on-Don, Russia

Effective algorithms for solution of a large saddle-point problem are considered. These methods are the modification of the Hermitian-Skew-Hermition iterations. Methods are applied for the solution of the constrained optimization problems. Numerical experiments have confirmed the effectiveness of this technique.

Considered indefinite linear system takes the form

$$\begin{pmatrix} M & E^T \\ E & 0 \end{pmatrix} \begin{pmatrix} u \\ \mu \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}. \tag{1}$$

The matrix $M = M^T$ is assumed to be $p \times p$, the matrix E is $q \times p$, where $q \leq p$. (Often $q \ll p$.) The matrix M is positive semidefinite , and the matrix E has full rank.

The problem that we shall consider will seek to minimize the quadratic objective functional $J(u) \equiv \frac{1}{2}u^T M u - u^T f$, subject to q linear constraints $Eu = g$. The Lagrangian functional $L(u, \mu) = J(u) + \mu^T(Eu - g)$ is associated with this constrained minimization problem, where μ denotes the Lagrange multipliers. Here M represents the Hessian of the quadratic function to be minimized, and E is the Jacobian of the linear constraints.

Our focus will be on iterative algorithms for solving (1).

We will consider cases where the $(1, 1)$ block in (1) is possibly singular or ill-conditioned. When M is singular, problem (1) may be well posed, provided M is positive definite in the subspace $Ker(E)$. In this case, minimizing $L(u, \mu)$ will not yield a unique minimum. If the augmented Lagrangian method is employed to construct an equivalent reformulation of the system , then matrix M will be replaced by a nonsingular matrix, and iterative algorithms can be applied to solve the augmented linear system [1]. The augmented Lagrangian approach is parameter-dependent and may be useful both when the $(1, 1)$ block is singular and when it is nonsingular.

We replace the $J(u)$ by $J_\gamma(u) \equiv J(u) + \gamma\|Bu - g\|^2_W$, where $\gamma > 0$ is a parameter and $W = W^T > 0$ is a weight matrix of size q. In the

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augmented system, matrix M will be replaced by the non-singular matrix $\tilde{M} \equiv M + \gamma E^T W E$ [2].

$$\begin{pmatrix} \tilde{M} & E^T \\ E & 0 \end{pmatrix} \begin{pmatrix} u \\ \mu \end{pmatrix} = \begin{pmatrix} f + \gamma E^T W g \\ g \end{pmatrix}. \tag{2}$$

For iterative solution linear systems (1) and (2) we apply the GSOR method [3] and new method GSTS (Generalized Skew-hermitian Triangular Splitting) [4], that becomes the PSTS (Product-Type Skew-Hermitian Triangular Splitting) iteration method [5] when equal iterative parameters are used.

Both GSTS and PSTS iterative methods based on the Hermitian / Skew-Hermitian splitting of the initial matrix.

Let $S = -EM^{-1}E^T$ is the Schur complement, and matrix Q be a nonsingular and symmetric matrix, an approximate (preconditioning) matrix of the S. We consider different variants for choosing Q and obtained the effective solvers for systems (1) and (2).

Numerical experiments are performed in MATLAB with a machine precision 10^{-16}. Optimal values for iteration parameters in GSOR are theoretical optimal values for parameters in [3]. The optimal iterative parameters for GSTS are choosing experimentally.

Numerical results show that the GSTS iterative method is effective for solving the constrained optimization problems and, in some cases, the GSTS method converges better then GSOR.

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MULTIGRID METHOD FOR THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

Muratova G.V.

Southern Federal University, Computer Center, Rostov-on-Don, Russia

We propose some approaches for solving the incompressible Navier-Stokes equations.

We consider classical formulation of the Navier-Stokes equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial P}{\partial x} - \frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f_1,$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial P}{\partial y} - \frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = f_2,$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = f_3,$$

where Re is Reynolds's number, $V = (u\ (x,\ y,\ t),\ v(x,\ y,\ t))$ is the velocity and P is the pressure.

To approximate the time derivative method of characteristics is used. Space discretization is carried out by finite element method. It's used a mixed formulation, when a combinations of simple finite elements – bilinear for velocities and constant elements for pressure are applied [1].

After discretization we obtain a linear algebraic equation system with a symmetric matrix which has a spectrum with alternating signs. We use multigrid method for solving this system. Multigrid methods are proving themselves as very successful tools for the solution of the algebraic equation systems associated with discretization of boundary-value problems. MGM is not a fixed multigrid algorithm. There is rather a multigrid technique fixing only the framework of the algorithm. The efficiency of the multigrid algorithm depends on the adjustment of its components to the problem in question [2].

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SOME ASPECTS OF FINITE ELEMENT APPROXIMATION FOR REISSNER-MINDLIN PLATES

Shi Z.-C.

State Key Laboratory of Scientific/Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Beijing, China

The Reissner-Mindlin plate model is one of the most commonly used models of a moderate-thick to thin elastic plate. However, a direct finite element approximation usually yields very poor results, which is referred to LOCKING phenomenon. In the past two decades, many efforts have been devoted to the design of locking free finite elements to resolve this model, most of these work focus on triangular or rectangular elements, the latter may be extended to parallelograms, but very few on quadrilaterals. In this talk we will give an overview of the recent development of low order quadrilateral elements and present some new results.

MULTISCALE COMPUTER MODELING OF THE ATOMIC AND ELECTRONIC STRUCTURE OF NOVEL MATERIALS

Soldatov A.V., Guda A.A., Soldatov M.A., Lomachenko K. A., Fain M.B., Suchkova S.A., Mazalova V.L.

Center for Nanoscale structure of matter, Southern Federal University, Rostov-on-Don, Russia

A technique for multi-scale computer modeling of nanoscale atomic and electronic structure of materials of nano-bio-medical technologies is described. Nanoscale local atomic structure determines most of unique properties of novel materials without long range order. To study its find details one has to use both computer nanodesign controlled by advanced experimental methods. An overview of results obtained by the use of supercomputing technology for computer modeling of nanoscale atomic and electronic structure of a wide range of materials for nano-bio-medical applications, such as complexes of gold and platinum, promising anti-cancer medicines, nanocatalysts, proteins with an active metal center and materials for hydrogen storage and materials for the electric current sources will be presented Molecular dynamics, density functional theory, the finite difference solution for the Schrödinger equation and the band theory were used for multiscale computer modeling. Re study made it possible to find the fundamental relationships between the local atomic, electronic and magnetic structures of the studied classes of active materials. The verification of the theoretical results on the basis of a comparison with the experimental spectroscopic techniques has been done. The ways of further development of the technique of multi-scale simulation using GPU computing technologies and involving technology of "cloud" computing is also discussed. The research is supported by the grants of Ministry of Science and Education of Russia and Southern federal university.

ADAPTIVE MODIFIED ALTERNATING TRIANGULAR ITERATIVE METHOD FOR GRID EQUATION SOLVING IN COASTAL COMPUTATIONAL HYDRODYNAMICS

Sukhinov A.I.

Institute of Technology of the Southern Federal University, Taganrog, Russia

Convection-diffusion equations are frequently required to be solved when it comes to applied problems such as finding numerical solutions to hydrodynamics, heat- and mass- transfer, geo-filtration, population dynamics, etc. problems. Implicit schemes used in such problems result in grid equations with a non – selfadjoint operator [1, 2]. In the class of two-layer iteration methods for grid equations with a selfadjoint operator, the alternating triangular method (ATM) is one of the most successful methods [1, 2], with a priori information on the boundaries of the spectrum of the grid operator used to select iterative parameters. An adaptive ATM version was developed later [3]. In [4] a modified iterative ATM for solving the Dirichlet problem for the Poisson equation is described along with the simple iteration method for the non-selfadjoint operator. In [5], a technique to improve the convergence rate of ATM with a priori information performed by refining spectral estimates of a preconditioned operator is given. Interesting results have been obtained by Professor Lev Krukier for special constructed precondition operator of grid equations [5]. In this work, we develop a version of the modified iterative alternating triangular method of minimal corrections for solving grid equations with the non-selfadjoint operator for the bounded Peclet grid number and estimate its convergence. The upper bound of the Peclet grid number is a natural consequence of the requirement of monotony of implicit difference schemes for hydrodynamics problems. Note also that the proposed variant of the method of minimal corrections is of independent interest. The developed algorithms were applied to solve grid equations resulting from approximation of the three-dimensional model of hydrodynamics of shallow water basins. We describe a parallel implementation of the algorithm of the adaptive modified iterative alternating triangular method of minimal corrections.

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MIMETIC FINITE-DIFFERENCE SCHEMES IN THE POROUS MEDIUM CONVECTION [1]

Tsybulin V.G.

Southern Federal University, Rostov-on-Don, Russia

The problems of fluid convection in a porous medium are under investigation because of different applications in geophysics and energetics. Many studies are based on direct simulation, so, the numerical schemes must be robust and inherit the key properties of governing equations. The mimetic finite-difference methods that provide the fundamental identities of vector calculus and partial differential equations have been successfully employed [1, 2]. Preservation of continuous and discrete symmetries of the underlying system is also important requirement for the numerical scheme. Among these properties, cosymmetry [3] plays an important role in Darcy or Lapwood convection. Lyubimov [4] found the branching off a family of steady states from the state of rest and Yudovich [3] explained this phenomenon using cosymmetry theory. It should be noted that the members of cosymmetric family of steady convective patterns have different spectrum of stability whenever in the symmetry situation all members of the family have the identical spectra.

Numerical studies for families of steady states in Darcy convection were carried out mainly for the case of rectangular enclosures and cartesian coordinates, see [5] and references here. Rather new theme concerns the problems in annular enclosures filled with a porous medium and the case of cylindrical coordinates [6].

We present here mimetic schemes to compute the family of steady convective fluid patterns in annular enclosures. The system of equations for stream function and temperature in the polar coordinates is discretized by the finite-difference method. Special attention is given to the approximation of the Jacobian as well as the buoyancy terms. This point was supported by computer algebra system Maple both for manipulation with nonlinear terms and realization of free parameters method. Derived scheme preserves the cosymmetry and discrete symmetry of the problem. Using the mimetic scheme, families of steady states are computed correctly for annular sectors and discs.

Our results show the non-uniform stability spectra for convective patterns belonging to the cosymmetric family of steady states. The continuation of the family up to the appearance of unstable states on it was done and the scenario

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with simultaneous instability in the finite number of points was found. So, these families are not the result of any symmetry group, this is due to the cosymmetric effect. It was shown that a non-mimetic scheme can destroy the family of steady states. The next issue is to consider the case of non-uniform polar meshes from the point of view cosymmetry and discrete symmetries preservation.

The case of a multicomponent fluid in the three-dimensional problem of porous medium convection is analyzed as well. We develop a mimetic finite-difference discretization of the Darcy equations in the primitive variables. This scheme is based on staggered grids with five types of nodes and a special approximation of nonlinear terms. Derived method is applied to the computer study of flows in a porous parallelepiped filled by two-component fluid and with two adiabatic lateral planes. We found that the stable continuous family of steady states exists in the case of rather thin enclosure. Destruction of the family of steady states under the non-mimetic approximation of nonlinear terms is found.

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MULTISPLITTING PARALLEL ITERATION METHODS BASED ON OPTIMIZATION FOR LINEAR SYSTEMS

Wen R.-P.

Department of Mathematics, Taiyuan Normal University, Taiyuan, China

In this report, we not only want to decrease the dificulty of constricting the multisplitting of the coefficient matrix, but also relax the constrains on the weighting matrices. We present two optimization models to modify parallel multisplitting iteration methods for solving positive definite (symmetric or nonsymmetric) linear systems.

SPLINE SMOOTHING METHODS FOR NONLINEAR PROGRAMMING AND MINIMAX PROBLEMS

Bo Yu

School of Mathematical Sciences, Dalian University of Technology, Dalian, China

In this talk, a constraint shifting spline smoothing homotopy method (CSSSH) for solving nonlinear programming and a smoothing Newton method for solving minimax problems will be introduced. They are global convergent under fairly weak conditions. The smooth spline approximation of the max-function, with m components, is used and, it involves only few components, hence the number of gradient and Hessian evaluation is reduced dramatically, so the proposed methods are efficient for problems with big m. Numerical tests with the comparisons to some other methods show that the proposed methods are very efficient.

BLOCK-SYMMETRIC AND BLOCK-LOWER-TRIANGULAR PRECONDITIONERS FOR PDE-CONSTRAINED OPTIMIZATION PROBLEMS

Zhang G.-F.

School of Mathematics and Statistics, Lanzhou University, Lanzhou, China

Optimization problems with partial differential equations as constraints arise widely in many areas of the sciences and engineering, in particular in problems of design. The solution of such kinds of PDE-constrained optimization problems is usually a major computational task. Because of the complication for directly seeking the solutions of PDE-constrained optimization problem, we transform it into the system of the linear equations of saddle-point form by using Galerkin finite-element discretizations. For the discretized linear systems, in this paper, we construct a block-symmetric preconditioner and a block-lower-triangular preconditioner for solving the PDE-constrained optimization problems. Both of the preconditioners exploit the structure of the coefficient matrix. The explicit expressions for the eigenvalues and eigenvectors of the corresponding preconditioned matrices are derived. Numerical implementations show that these structured preconditioners can lead to satisfactory experimental results of the preconditioned GMRES methods when the regularization parameter is suitably small.

MULTIPLICATIVE PERTURBATION BOUNDS OF G-INVERSE AND RELATED OBLIQUE PROJECTION

Zheng B.

School of Mathematics and Statistics, Lanzhou University, Lanzhou, China

In this paper, we obtain multiplicative perturbation bounds of the g-inverse and its related oblique projection under the spectral norm and the Frobenius norm. As the special g-inverse, the formulas of nearest perturbed least squares g-inverse and the multiplicative perturbation bounds of the least squares g-inverse are also given.

Abstracts of Young Scientists

GPGPU COMES TO MODERN LIFE

Agibalov O.I.

Southern Federal University, Computer Center, Rostov-on-Don, Russia

Modern graphics processing units or GPUs are represented with high-performance devices, which are also set up inside the practically all the modern PCs. There are two giant corporations that lead at the market of semiconductors: NVidia and AMD with their GeForce and Radeon GPUs relatively. At the last time the Intel corporation works on so-called APUs (accelerated processing units), that contain both CPU cores and GPU module. The performance of GPUs is incredible. So, the latest models may operate more than three thousand computing cores. And each of these cores works in parallel and independently from each other.

During the long time while GPUs exist the whole their power was applied for computing 3D and 2D graphics. But at the latest time new technologies of using graphical adapters for general purposes appear – so-called GPGPU (General-purpose Graphics Processing Units). Today there are many kinds of them. The leading GPGPUs are NVidia CUDA (Compute Unified Device Architecture), OpenCL, Microsoft DirectCompute amd AMD FireStream. They are similar in the common process of programming. Data is formed by CPU, then transmitted to GPU memory with a special bufferization stage. At the GPU it is processed by graphical card and transmitted back to RAM, where it becomes accessible for CPU again. And there is the main problem of all the similar technologies - necessity of transmitting and buffering data, which may last for a long time if we work with a high capacity of information. So, sometimes it is needed to choose between using slow CPU and fast GPU [1]. Nevertheless GPGPU technologies are extremely fast, faster than CPU in tens and even hundred times. This speed is reached due to absolutely parallel cores that compute independent data, but are able to cooperate and communicate with each other. Such communication is possible because of special common memory registers exist. For example, each thread had its own memory buffer, but the block of threads has such buffer too. Thus, the single thread cannot access memory slot of parallel thread, but it is able to use general memory of group of thread as well as another thread uses it [1]. It is clear that speed of GPU is provided not by the clock rate of any single core but by the principles of architecture themselves that allow to perform thousands of threads independently. And this architecture is what we call now GPGPU.

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INTRA-AORTIC SPIRAL WAVES MODELING[1]

Batishchev V.A., Petrovskaya D.S.
Southern Federal University, Rostov-on-Don, Russia

The spiral blood flow in the aorta of man and animals was discovered in the second half of the last century. Swirling flows of blood appear in the left ventricle of the heart and are transferred into the ascending aorta. The mechanism of occurrence of these flows is associated with morphological and functional features of the myocardium, including a contraction in opposite directions of various layers of cardiac ventricular muscle. The instability of the convergent flow of blood and bifurcation of rotation is possible. The long spiral waves arise in the aorta as a result of the elastic properties of blood vessels, but the waves are localized in the boundary layer near the wall of the aorta. The report presents a mathematical model of spreading the spiral blood flows in the ascending aorta. It is assumed that the spiral waves in the aorta are caused by a swirling stream of blood flow which comes to the input of the aorta from the left ventricle of the heart. Three types of spiral waves have been calculated - long and short spiral waves and quasi-stationary modes which are nearly independent of time. The aorta is modeled by a cylinder of a circular cross section which is limited by a thin elastic membrane. The blood flow is calculated on the base of the Navier-Stokes equations and dynamic equations of a thin membrane. It is known that in the aorta long longitudinal pulse waves spread. They were the subject of the intense research in the late nineteenth century. In the case of isotropic wall of the aorta, there are two longitudinal waves, the most powerful of which is measured in the experiment and called the pressure wave. In addition to the longitudinal waves in the aorta there extends the stationary flow, which is modeled by the Poiseuille flow. The spiral waves spread against these flows. The experimental studies have revealed the presence of thin boundary layers on the walls of the aorta and the left ventricle. Therefore, the method of the boundary layer is being used. Two small parameters were introduced, one of which is proportional to the thickness of the boundary layer. The second parameter is inversely proportional to the phase velocity of the longitudinal wavelength. The solution of the problem is constructed in the form of asymptotic series in powers of the second small parameter. The coefficients of these series are given with the boundary layers taken into account. It is shown that the long spiral waves are localized in the boundary layer near the wall of the aorta, and the short waves fill the entire cross section of the aorta. The cause of the long spiral waves are

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the elastic properties of the wall of the aorta and blood viscosity. It is shown that the transfer mechanism of short spiral waves is the stationary flow. The elastic properties of the membrane are shown for short waves only in the higher approximations. At low viscosity near the axis of the cylinder there is a thin critical layer. The solution of the problem in this layer is obtained both numerically and asymptotically. It is shown that some modes of short spiral waves are localized in the critical layer. The quasistationary modes, which in the main approximation are independent of the time and the elastic properties of the wall of the aorta, are calculated. The first quasi-stationary mode does not change the direction of rotation of the fluid either by time or by section. These modes are attenuated along the stream, and senior modes decay faster than the first modes. The dynamics of short spiral waves are investigated numerically. These waves are caused by the presence of the fluid rotation at the entrance to the aorta. The waves decay along the flow. It is shown that the circumferential velocity component reaches the highest value near the entrance to the aorta in the second half of systole. The systole is one of the phases of the cardiac cycle - the contraction. During the systole, the blood is pumped into the arterial system. It is shown that there are different variants of twists of blood flows in the systole. There may be one direction rotation of blood. The direction of rotation of the fluid may be reversed in a short period of time. This period can be close to any time point during the systole, and its duration comparing to the duration of systole is small. These results are confirmed experimentally. In the boundary layer near the membrane there dominate the long spiral waves.

THE EFFECT OF THE FLUID ROTATION IN THE MARANGONI LAYERS WITH NANOPARTICLES[1]

Batishchev V.A., Zaikin V.V.
Southern Federal University, Rostov-on-Don, Russia

The idea of the heat transport in the fluid with nanoparticles was offered by S.U.S. Choi and J.A. Eastman in 1995. Previously, Maxwell suggested putting metal particles of micron and millimeter sizes into the liquid to increase the thermal conductivity of the mixture. These models are based on the known fact that the thermal conductivity of some metals is hundreds times higher than the thermal conductivity of some liquids. Recently, many works on the transport of heat through the solid wall into the fluid with nanoparticles were published. The number of publications on the heat transport in the presence of free surfaces is very small. It is known that the heat flow through the solid boundary increases significantly with increasing of the concentration of nanoparticles in the liquid. However, at the thermocapillary flow of a fluid with a free surface (Marangoni effect) there appears the opposite effect. Thermocapillary effects in Marangoni layers have been intensively studied since the end of the last century in connection with the experiments in the space. Self-similar solutions were first obtained in Napolitano's works. At the axisymmetric liquid flow in a thin layer the Marangoni effect can lead to the rotation of the liquid layer. This rotation is the result of the bifurcation of the basic nonlinear condition, where the longitudinal temperature gradient on the free surface reaches the critical value. The report shows that for large Marangoni numbers in a fluid of infinite depth in the presence of nanoparticles the rotation only of a thin boundary layer near the free surface is possible. Outside this layer, the liquid does not rotate. The rotation can occur if the liquid cools on the free surface near the axis of symmetry. The rotation does not occur in the case of the local heating. To research the thermocapillary effects we use a single-phase model of the fluid with nanoparticles. The equations of the model are obtained from the Navier-Stokes equations by replacing thermal parameters for their effective values. These effective parameters were obtained by different authors in the last decade although the coefficient of effective viscosity of nanofluids was suggested by Brinkman back in 1952. The base of a single-phase model is founded on several hypotheses. For example, the slip between the nanoparticles and the liquid is neglected. The nanoparticles have spherical shape and

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the same size. The base fluid (water) is in thermodynamic equilibrium with the nanoparticles. Thermal parameters of the mixture (density, dynamic viscosity coefficient, thermal expansion coefficient, etc.) are considered to be permanent. We should note that the results of calculations for single-phase models are in good agreement with the experimental data, namely, the relative error of divergence is about ten percent. The boundary conditions at the free surface are obtained by replacing the thermophysical parameters for their effective values in the boundary conditions of the liquid without nanoparticles. In the report the effect of copper and titanium oxide nanoparticles on the thermocapillary effect near the free surface in the case of axisymmetric flow of nanofluids was investigated. It is shown that when the free surface near the axis of symmetry cools there occurs a rotation of a thin boundary layer near the border. However, outside the boundary layer the fluid does not rotate. With local heating of the free surface the rotation does not occur. The presence of nanoparticles in the fluid leads to the inhibition of the fluid flow. The speed of rotation of the boundary layer also reduces. The heat flow on the free surface decreases with the increasing of concentration of nanoparticles during the heating as well as the cooling of the free boundary. This fact was proved in the two-dimensional case, only for the local heating of the free surface and in the absence of rotation of the fluid. We should note that when the heat transfers into the fluid with nanoparticles through a solid surface, a contrary effect occurs, namely, the heat flow at the solid boundary increases with the concentration of nanoparticles in a liquid.

THE FORECASTS OF 3D ATMOSPHERIC FRONTS STRUCTURE AND PRECIPITATION

Bykov Ph.L., Gordin V.A.

Higher School of Economics, Hydrometeorological Centre of Russia

1. Atmospheric fronts are contact discontinues in continuum mechanics.
2. Direction-depended predictors (in particular, directional derivatives) are useful for lines on plane determination.
3. Correlation functions are suitable tool for quality assessment methods for the constructed fronts.
4. Our front construction algorithm use COSMO-RU7 model with 7 km horizontal resolution. Algorithm is based on model's forecasts with 1 hour resolution. Other version: global model NCEP with horizontal resolution.
5. Constructed atmospheric fronts associated with cloud on satellite imagery. This fact allows forecasters to have replacement satellite imagery in the forecast.
6. Satellite's precipitation data have strong positive connection with our predictor.

GENERATION OF OCTREE MESHES WITH CUT-CELLS FOR DOMAINS WITH MULTIPLE MATERIALS[1]

Chernyshenko A.Yu.
Institute of Numerical Mathematics RAS, Moscow, Russia

We present a robust octree mesh with cut-cells generation technology. This generator can be applied to complex domains with multiple materials. Such domains could appear from hydrodynamic, medical and other problems.

The main goal of the work is to produce a mesh which has most cells hexahedra whereas the remaining part are polyhedral cells. This is achieved by an octree mesh with cut-cells. The octree mesh may be locally refined and derefined easily whereas data interpolation between two consecutive octree meshes is efficient and straightforward. Appropriate refinement/derefinement can reduce the number of degrees of freedom preserving the basic approximation properties of the discrete solution. A cut-cell is a polyhedral cell produced by cleaving polyhedral pieces from a cubic cell. Cut-cells are used to recover geometric features and can approximate a domain boundary with the second order. The Cubical marhing squares algorithm [1] is used to produce a triangulation of a given surface which intersects a cube. The triangulation is used to cut cells, and resulting mesh with cut-cells belongs to the class of conformal polyhedral meshes. The developed methods of FV discretization are applicable to this class of meshes.

In some applications it is required to generate a mesh in a multi-material domain. For this purpose we use the modification of the Multiple material marching cubes algorithm [2]. The combination of this algorithm and the Cubical marhing squares algorithm provide an octree meshes with cut-cells generator which is applicable to multi-material domains. The resulting polyhedral mesh is weakly conformal in the sense that two cells can share more than one face.

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THE MATHEMATICAL MODEL OF THE FLOODING OF THE DON RIVER ESTUARY

Chikin A.L.*, Chikina L.G.**

* *Southern Scientific Center of Russian Academy of Sciences, Rostov-on-Don, Russia*

** *Southern Federal University, Rostov-on-Don, Russia*

According to the wind situation derived from the coastal forwarding base of the Southern Scientific Center of Russian Academy of Science on the coast of the Gulf of Taganrog for the period from 20 March to 26 March 2013 were modeled development surges in the delta of the Don River. To calculate the hydrodynamic parameters two-layer mathematical model was used. The model showed that a sharp change Drivings effect on Surges increases the rate of water flow, and, consequently, the amount of flooding.

CALCULATION OF THE ICE THICKNESS IN FRESHWATER TAGANROG BAY

Chikina L.G.*, Chikin A.L., Trepacheva A.V.***

* *Southern Federal University, Rostov-on-Don, Russia*

** *Southern Scientific Center of Russian Academy of Sciences, Rostov-on-Don, Russia*

Daily hydrometeorological observations are put in a basis of the real research from 2005 for 2012 on the coastal forwarding base of the Southern Scientific Center of Russian Academy of Science on the coast of the Gulf of Taganrog. The method of calculation of thickness of the ice, adapted for fresh-water Taganrog Bay is given. The Adjusted formulas in Taganrog Bay yields much more the best result in comparison with known formulas. It allows to claim that the offered technique rather adequately describes process of change of thickness of ice in Taganrog Bay. This can be used in a full mathematical model of ice formation.

AN IDENTIFICATION PROBLEM FOR INTENSITY OF ATMOSPHERIC POLLUTION SOURCE

Chubatov A.A.*, Karmazin V.N., Karmazin A.V.*****

* *Armavir State Pedagogical Academy, Armavir, Russia*

** *Kuban State University, Krasnodar, Russia*

*** *RheinMain University of Applied Sciences, Wiesbaden, Germany*

In present study a special case of the identification problem for intensity of the source is studied in application to the modelling of the transport of air pollution [1]. The considered approach uses as input parameters the set of known sensitivity coefficients and corresponding pollution measured in given locations $\bar{x}_j = (x_j, y_j, z_j)$: $c_{ji} = q(\bar{x}_j, t_i)$, $j = 1, \ldots, J$, $i = 1, \ldots, N$, where J is the number of sensors, N is the number of time steps. Then, the source identification problem is represented by the following approximate matrix equation

$$A_h \cdot g = f_\delta, \quad A_h \in \mathbb{R}^{M \times N}, \; g \in \mathbb{R}^N, f_\delta \in \mathbb{R}^M, \; ||A_h - A|| \le h, \; ||f_\delta - f|| \le \delta, \tag{1}$$

where $M = N \cdot J$, g is unknown intensity of the source, A_h, A are the approximate and the exact matrices of sensitivity coefficients [1] and f_δ, f are the approximate and the exact measured data written in terms of sensitivity, h and δ are the maximal allowable errors in approximations of A and f.

In the following the optimization problem for the residual of (1) $\mu = \inf \|f - A \cdot g\| = \|f - A \cdot g^*\|$ is considered. However, the presence of errors h and δ in (1) overdetermines ($\mu > 0$) the matrix equation of this ill-posed problem. It is more convenient to solve (1) with respect to its pseudo-solution determined as $g := g^* = \arg\min \|f_\delta - A_h \cdot g\| = A_h^+ \cdot f_\delta$, where $A^+ = (A^T \cdot A)^{-1} \cdot A^T$.

The equation (1) is transformed to the form $A_h \cdot g + r = f_\delta$, where $r = f_\delta - A_h \cdot g$ is the residual and both values g and r are unknown. Applying the least squares and considering that $A^T \cdot r = 0$ the following augmented system is obtained

$$R_\omega \cdot x = d, \qquad R_\omega = \begin{pmatrix} \omega \cdot E & A_h \\ A_h^T & O \end{pmatrix}, \quad x = \begin{pmatrix} \omega^{-1} \cdot \hat{r} \\ \hat{g} \end{pmatrix}, \quad d = \begin{pmatrix} f_\delta \\ 0 \end{pmatrix}, \tag{2}$$

where ω is the scaling factor, $\hat{r}$, $\hat{g}$ are the approximations of residual and intensity, $E \in \mathbb{R}^{M\times M}$, $O \in \mathbb{R}^{N\times N}$ are the identity and the zero matrices, respectively.

The matrix equation (2) is solved by applying the standard Tikhonov regularization [2] and by applying the method of an imaginary shift of the spectrum (using $R_\omega^T = R_\omega$) proposed by Faddeeva [3]. For the choice of the regularization parameter α two approaches are used here: a priori and a posteriori.

For numerical computation of the solution of ill-posed problem (2) the singular value decomposition (SVD) [4] is applied

$$A = U \cdot S \cdot V^T, \qquad A, S \in \mathbb{R}^{M\times N}, \quad U \in \mathbb{R}^{M\times M}, \quad V \in \mathbb{R}^{N\times N},$$

where U, V are the unitary matrices, $S = \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_N)$ is the diagonal matrix with singular values $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_N \geq 0$ on its diagonal.

Then the augmented system (2) is written as follows

$$R_\omega \cdot x = d, \qquad R_\omega = \begin{pmatrix} \omega \cdot E & S_h \\ S_h^T & O \end{pmatrix}, \quad x = \begin{pmatrix} \omega^{-1} \cdot \hat{\rho} \\ \hat{w} \end{pmatrix}, \quad d = \begin{pmatrix} b \\ 0 \end{pmatrix}, \tag{3}$$

where $w = V^T \cdot g$, $\rho = U^T \cdot r$ and $b = U^T \cdot f_\delta$. This system of equations can be solved efficiently since the matrix R_ω is sparse (tridiagonal matrix).

We use the fact proved by Morozov V.A. and Gilyazov S.F. [2] that $\|g(\alpha) - g^*\| = O(h + \delta)$ for $\mu = 0$ and $\alpha = h$. The a priori choice of α for which $\alpha_{apriory} = h$ guarantees the asymptotic convergence to the exact solution $g(\alpha) \underset{h,\delta\to 0}{\to} g^* = \bar{g}$, where $\bar{g}$ is the exact solution.

In the case of large fixed values of h and δ, parameter α is determined a posteriori using the generalized discrepancy principle as the root of equation corresponding to (3) $\varphi_\omega(\alpha) - \psi_\omega(\alpha) = 0$, where $\varphi_\omega(\alpha) = \sqrt{\|b - S_h \cdot w(\alpha) - \rho\|^2 + \left\|\omega^{-1} \cdot S_h^T \cdot \rho\right\|^2}$ and $\psi_\omega(\alpha) = \delta + \sqrt{2} \cdot h \cdot \sqrt{\|w(\alpha)\|^2 + \|\omega^{-1} \cdot \rho\|^2}$. The Newton method provides the fast convergence solving this root-search problem with the following initial approximation $\alpha_0 = 10 \cdot h$.

The quality of the choice of the parameter α is controlled using the value $\eta_{eff}(\alpha_{meth}) = \|g(\alpha_{meth}) - \bar{g}\| \,/\, \|g(\alpha_{best}) - \bar{g}\|$, where α_{best} is chosen as $\min\limits_{\alpha} \|g(\alpha) - \bar{g}\| = \|g(\alpha_{best}) - \bar{g}\|$.

The time-efficient algorithm developed and used in this work provides a stable numerical solution of the considered source identification problem.

The solution obtained by applying the regularization approach with singular decomposition (SVD) is numerically approved by authors considering numerical experiments. Two considered approaches for the choice of regularization parameter α are found to have following efficiency control parameters: $\eta_{eff}(\alpha_{apriory}) < 2$ for the a priori choice of α, $\eta_{eff}(\alpha_{apost}) < 1.3$ for the a posteriori choice of α.

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COMPUTER SIMULATION OF THE INDENTATION IN THIN MULTILAYER COATINGS[1]

Danilchenko S.A., Nasedkin A.V.
Southern Federal University, Rostov-on-Don, Russia

To examine the multilayer thin coatings, recently the method of micro and nanoindentation is extensively used. The method helps to analyse mechanical properties of such coatings at the micro and nano-levels, obtaining the values of microhardness, the stiffness moduli, etc. It has been widely adopted for practical use by railroad operators, who among other things need to examine anti-friction thin coatings applied on the rail.

In the present work for modeling the nanoindentation processes in multilayer thin coatings has examined both 2D axisymmetric, and 3D problems using a cone-shaped indenter and the Berkovich indenter. For every problem two modeling variants are considered to emulate an indentation into a coating sample, where the indenter was assumed to be a deformable solid body, and a non-deformable rigid boundary of preset geometry. Both options presumed that the coating sample is a deformable solid, and thus two contact problems between two deformable bodies and between solid indenter and deformable body were examined. The computing experiments were realized by using the mathematical modeling methods, the methods of contact mechanics, and the finite element technologies.

The package ANSYS was used as a tool kit for finite element modeling. The special software tools were in APDL ANSYS macrolanguage for solutions of the considered contact problems with various geometrical and physical input data. Solid models were built using the upward modeling technology with the following steps: setting of reference keypoints; building arcs and straight lines to connect the reference keypoints; generating areas by the lines and volumes by the areas. In accordance with the methodology of contact problem solution, in a similar manner [1-5], the fine finite element meshes were constructed around the contact zones. For this purpose, additional geometric subdomains were identified for which regular finite-element grids were built with smaller sizes compared to the remaining area. In areas occupied by elastic materials of the coating sample and the indenter (in case of contact between two deformable bodies), 2D eight-node serendipity finite elements PLANE82 with the axisymmetric option were used for the axisymmetric problems and 3D finite elements SOLID45 used for the three-dimensional

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problems. Contact interaction was simulated by using the elements CONTA175 and TARGE169.

By using the obtained finite-element models and numeric solutions of the the considered contact problems for different types of coatings there are calculated some important results: the distributions of contact stresses, the sizes of the contact zones, the distributions of equivalent von Mises stresses σ_{eqv} and strains ε_{eqv}, as well as plastic stresses and strains.

In addition to computer investigations, a series of NanoTest 600 measurements were used with analysis of the mechanical properties for different multilayer thin coatings on the micro and nano- levels.

Based on the main results of the following conclusions can be drawn. Comparison of the numerical results for the model of deformed indenter with the results for the model of rigid indenter was showed that the model of rigid indenter is gives a small error, but all trends of the changes of maximum stresses, stains and deformations are kept. Because the model of rigid indenter is more economical for computer resource costs, then it can be useful for analysis of the influence of input data changes for different multilayered coatings. However, the model of deformed indenter should be used for more precise calculations.

Moreover the comparison of the obtained data showed a sufficient agreement between numerical and experimental results of the indentation. Therefore we can conclude that the proposed finite element technologies are effective for considered elastic and elastoplastic contact problems.

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NUMERICAL MODELING OF BLOOD FLOW IN THE VESSEL NETWORK WITH PATHOLOGIES OR IMPLANTS

Dobroserdova T.K.

Lomonosov Moscow State University, Moscow, Russia

Modeling of blood flow in the vessel network with pathologies or implants is very useful nowadays. 1D model of global blood circulation can describe hemodynamics everywhere in the human body [1]. Two methods of taking into consideration influence of pathologies or implants are suggested.

State equation is a dependence between transmural pressure and the area of vessel cross section. It is the main description of elastic properties of the vessel wall in the model of global blood circulation. When pathology or implant appeares in the vessel, elastic properties of vessel wall change. New dependence is calculated using fiber model of elastic vessel wall or fiber-spring model of atherosclerotic arterial wall. In the first approach, the technology that import data between models has been constructed. Numerical experiments on modeling influence of atherosclerotic plaques on hemodynamics have been realized [2, 3, 4].

In the second approach, the vicinity with pathology or implant is considered to be three-dimensional. The blood flow in this domain is governed by the Navier-Stokes equations. New coupling boundary conditions for such multiscale model have been proposed. This boundary conditions guarantee the correct energy balance for the model. The splitting scheme with convergence of the second order for calculations has been constructed and tested. Accuracy of the scheme has been investigated on the problem with known analytical solution. Using this method some numerical experiments on modeling blood flow in the vessel network with cava-filter have been calculated [5].

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SPECIFICS OF RESIDUAL STRESS MODELING IN ELASTIC BODIES

Dudarev V.V., Nedin R.D., Vatulyan A.O.
Southern Federal University, Rostov-on-Don, Russia

The problems of solid mechanics involving residual stress (RS) are of great importance when estimating strength and stability of mechanical constructions. To describe the behavior of elastic bodies on the basis of material structure and hypotheses of residual stress origins, the linearized models were developed with differing types of constitutive equations. The progress in 3-dimensional linearized theories of deformable prestressed solids has been taking place since the beginning of XX century. In present the most demanded models describing the RS state in actual configuration are those which allow determining inhomogeneous RS state using the data on displacement or strain fields at the boundary of a body by employing methods of solving inverse problems and novel calculating schemes.

The most widespread mathematical models of RS being used at present in solid mechanics were proposed in the second half of XX century by V.V.Novozhilov, A.I.Lurie [1], C.Truesdell [2], A.N.Guz [3], K.Vasidzu, A.Hoger [4], L.Robertson. In spite of the fact that there are various continuous approaches to simulate RS state, today there is a strong scarcity of adequate review articles or monographs in the world literature providing the description of all the well-known RS models with their comparison and revealing the most appropriate one that could give practical recommendations based on boundary problems solutions.

According to the theorem on the general form of the Piola stress tensor $\underline{\underline{P}}$, the following representation takes place:

$$\underline{\underline{\Theta}} = \underline{\underline{P}}(\underline{\underline{C_0}}, \underline{\underline{T_0}}, \underline{\underline{\epsilon}}) + \underline{\underline{U}}(\underline{\underline{T_0}}, \underline{\underline{\epsilon}}, \underline{\underline{\omega}}) \tag{1}$$

where $\underline{\underline{T_0}}$ is RS tensor, $\underline{\underline{\epsilon}}$ is strain tensor, $\underline{\underline{\omega}}$ is rotation tensor, $\underline{\underline{P}}$ is symmetric tensor depending generally on the material constants $\underline{\underline{C_0}}$ in the reference configuration, RS and strain, $\underline{\underline{U}}$ is symmetric tensor depending on RS, strain and rotation [1, 5]. It is worth noting that whereas the tensor $\underline{\underline{U}}$ is uniquely defined by the formula

$$\underline{\underline{U}} = \frac{1}{2}\left(\underline{\underline{T_0}} \cdot \underline{\underline{\epsilon}} + \underline{\underline{\epsilon}} \cdot \underline{\underline{T_0}}\right) - \underline{\underline{T_0}} \cdot \underline{\underline{\omega}},$$

the structure of the symmetric tensor $\underline{\underline{P}}$ can be defined arbitrary due to the fact that the origins and the reason of RS state formation in a body or a mechanical construction are almost always unknown. The only one way to determine the form of the tensor $\underline{\underline{P}}$ for specific problem is the comparison with real experiments.

In the present research we view several groups of the most widespread RS models differing from each other by the constitutive relation binding together the nonsymmetric Piola stress tensor with symmetric RS tensor and strain gradient. On the basis of the representation (1) it is shown that all the models considered may be reduced to each other by varying the structure of the tensor $\underline{\underline{P}}$. According to the classical method of superposition of a small deformation on a finite one, the general form of the constitutive relation is obtained in terms of Piola stress tensor for an arbitrary form of elastic potential for an isotropic material.

The comparison of the statements and the solutions of the problems on steady-state vibration of beams and plates is occured for each of the RS models considered; the analysis of the effect of RS components on frequency response functions and natural frequency spectrum is made. The RS models considered are appraised in accordance with the data from the real experiments on determination of resonance frequencies of axially compressed beams. In addition, the important problem on vibrations of a pipe under axisymmetric RS state is investigated; the simple design formulas for resonance frequencies depending on the load value inside the pipe are obtained. On the basis of these formulas the RS identification is presented in the frames of the Lamé problem for a cylinder.

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A COMPUTER MODEL OF STEADY-STATE CROSS-SECTIONAL SHAPE OF LIQUID CYLINDRICAL INCLUSION MIGRATING THROUGH A CRYSTAL WITH ACCOUNT OF THERMAL GRADIENT DIRECTION AND ANISOTROPY OF INTERFACIAL ENERGY AND INTERFACE KINETICS

Garmashov S.I., Surnin V.I.

Southern Federal University, Rostov-on-Don, Russia

A cross-sectional shape of a liquid cylindrical inclusion migrating through a crystal under the action of a constant temperature gradient is determined by both interfacial surface energy and interface kinetics [1, 2]. In order to obtain information on the interfacial surface energy and the interface kinetics from analysis of experimental data on the inclusion shape, it is necessary to develop a mathematical model of the stationary non-equilibrium shape of the migrating cylindrical inclusion taking into account the interfacial surface energy and interface kinetics anisotropy.

One of such models has been proposed in the paper [1]. This model has been developed under the simplifying assumptions that the inclusion is confined by two singular (atomically flat) and two non-singular (atomically rough) parts of the liquid-solid interface, that the interfacial energy of the non-singular parts is isotropic and that the temperature gradient is normal to the singular parts.

In general case, it is important to take into consideration features of the interfacial surface energy and interface kinetics anisotropy and the temperature gradient orientaion. In order to solve this problem the technique described in [2] can be used. The essence of the technique is that the inclusion boundary is approximated by an array of flat facets. Each such facet is characterized by a given mechanism of crystallization (dissolution) (with given parameters) and a value of the interfacial energy γ_i in accordance with a given dependence $\gamma(\varphi_i)$, where φ_i is the angle determining the ith facet orientation.

Taking into account capillary phenomena, the interfacial surface energy and interface kinetics anisotropy and also the fact that the solution concentration distribution is to be flat in the steady-state regime of the inclusion migration driven by a constant temperature gradient [1], the system of nonlinear algebraic equations for the facet sizes can be composed. Solving the

system numerically allows calculating the stationary non-equilibrium shape of the inclusion cross-section.

A computer program (see Fig. 1) simulating the stationary cross-sectional shape of the migrating cylindrical inclusion as a function of both the interfacial surface energy and interface kinetics anisotropy and the thermal gradient direction is presented in this report.

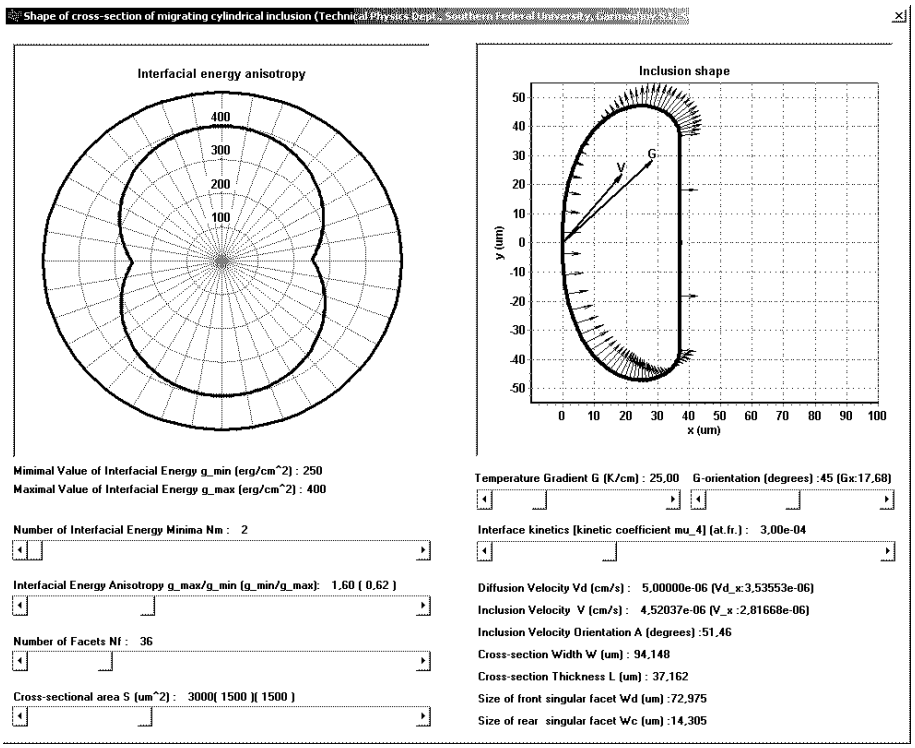

Fig. 1. The developed computer program calculating the stationary non-equilibrium cross-sectional shape of the cylindrical inclusion migrating through a non-uniformly heated crystal

The program allows varying the degree of anisotropy of the interfacial energy, the value and direction of the temperature gradient, the parameters of interface kinetics, the cross-sectional area and others parameters. The dependence of specific interfacial energy on the facet orientation is displayed at the left diagram of the program interface. The calculated shape of the inclusion cross-section is plotted at the right diagram.

The inclusion shapes calculated for the particular cases of the interfacial energy anisotropy considered in [1] are corresponded to the results presented in that work.

The proposed computer program is useful for detailed analysis of the influence of various parameters on the inclusion shape and can be used for

investigating kinetics of crystal growth (dissolution) by means of comparing the calculation results with experimental data on the cross-sectional shapes of inclusions migrating in non-uniformly heated crystals.

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ON CORRECTNESS AND DIFFERENCE METHODS FOR SOLUTION OF A NONLINEAR EVOLUTION PROBLEMS WITH A NONLOCAL SPACE OPERATOR

Glazyrina O.V., Pavlova M.F.

Kazan (Volga region) Federal University, Kazan, Russia

Let Ω be bounded domain in R^n, with the boundary Γ, $Q_T = \Omega \times (0,T)$. Consider the initial-boundary value problem in the domain Q_T

$$\frac{\partial u}{\partial t} - \sum_{i=1}^{n} \frac{\partial}{\partial x_i}(a_i(x,u)k_i(x,\nabla u, Bu)) = f, \tag{1}$$

$$u(x,0) = u_0(x) \quad x \in \Omega, \qquad u\,|_{\Gamma} = 0, \tag{2}$$

where B is the operator in the form

$$Bu(t) = \int\limits_{\Omega} g(x)\, u(x,t)\, dx\,, \tag{3}$$

g is known function.

Equations in form (1), for example, in the mathematical description of the diffusion of bacterial population under the assumption that the speed of spreading at a point is defined by the global state of the environment (see, for example, [1]).

We assume functions $a_i(x,\xi_0)$ and $k_i(x,\xi,\nu)$, $(i = 1,\dots,n)$, are continuous with respect ξ_0, ν and ξ, measurable with respect to x and satisfy the conditions which provide a boundedness, coerciveness and monotonicity of the operator

$$Lu = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}(a_i(x,u)k_i(x,\nabla u, Bu)),$$

acting from $\overset{\circ}{W}{}_p^1(\Omega)$ to $W_{p'}^{-1}(\Omega)$, $1/p+1/p' = 1$ with respect to the gradient of u.

The generalized solution of problem (1)–(2) is determined by relations

$$u \in L_p(0,T;\overset{\circ}{W}{}_p^1(\Omega)) \bigcap L_\infty(0,T;L_2(\Omega)),$$

$$u(x,0) = u_0(x) \quad \text{almost everywhere on } \Omega, \qquad \frac{\partial u}{\partial t} \in L_{p'}(0,T;W_{p'}^{-1}(\Omega))$$

and equation (1), understandable as an equality of elements in the space $L_{p'}(0,T;W_{p'}^{-1}(\Omega))$.

In paper [2] an existence for solution of problem (1)–(2) was proved when $f \in L_{p'}(0,T;W_{p'}^{-1}(\Omega))$ and $u_0 \in L_2(\Omega) \bigcap \overset{\circ}{W}{}_p^1(\Omega)$.

We proved the theorem of generalized solution uniqueness of the problem (1)–(2) when the L is the strongly monotone operator, with additional assumptions on coefficients of equation (1) and operator B (see also [3]).

In this paper for the problem (1)–(2) when the Ω is n-dimensional parallelepiped, we investigated explicit and implicit difference schemes on the uniform mesh. We proved the convergence for these difference schemes with minimal assumptions on the smoothness of initial data. For explicit scheme the theorem of convergence is valid when

$$\tau \le \begin{cases} c\dfrac{h^2}{4n^{2/p}}, & 1 < p < 2, \\ c\dfrac{h^{p+n(p-2)/2}}{2^p n}, & p \ge 2, \end{cases}$$

$$\tau\frac{n}{h^{p+n(p-2)/2}} \to 0, \quad \text{if} \quad p \ge 2, \qquad \tau\frac{n^{2/p}}{h^2} \to 0, \quad \text{if} \quad 1 < p < 2,$$

with $\tau, h \to 0$. Here is τ is the step on t, $h = \min\limits_{1\le i\le n} h_i$, h_i is the step on axis x_i.

Also we proved the existence of the solution for variational inequality which is arisen when we are searching the nonnegative solution of the problem (1)–(2).

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respect to the gradient. // Russian Mathematics (Iz.vuz.). 2012. Vol.56, No 3 P. 92–95.

FAST NUMERICAL ALGORITHMS FOR SIMULATION OF ELASTIC LAYERED PERIODIC STRUCTURES WITH DAMAGES

Golub M.V.*, Zhang Ch.**

* *Institute for Mathematics, Mechanics and Informatics, Kuban State University, Krasnodar, Russia*

** *Chair of Structural Mechanics, Department of Civil Engineering, University of Siegen, Siegen, Germany*

Physical phenomena in multi-layered structures of periodic, pseudo-periodic or stochastic nature have unique dynamic properties and important engineering applications. Periodic elastic composites or phononic crystals have many potential applications in the design of new devices, acoustic filters, control of vibration isolation, noise suppression etc. [1]. Elastic waveguides are susceptible to damages like cracks during the manufacturing or in service. Phononic crystals have often a quite complicated geometry due to the combination of elements of different materials. Accordingly, the numerical simulation of phononic crystals requires sophisticated computational methods and resources, when damages are introduced.

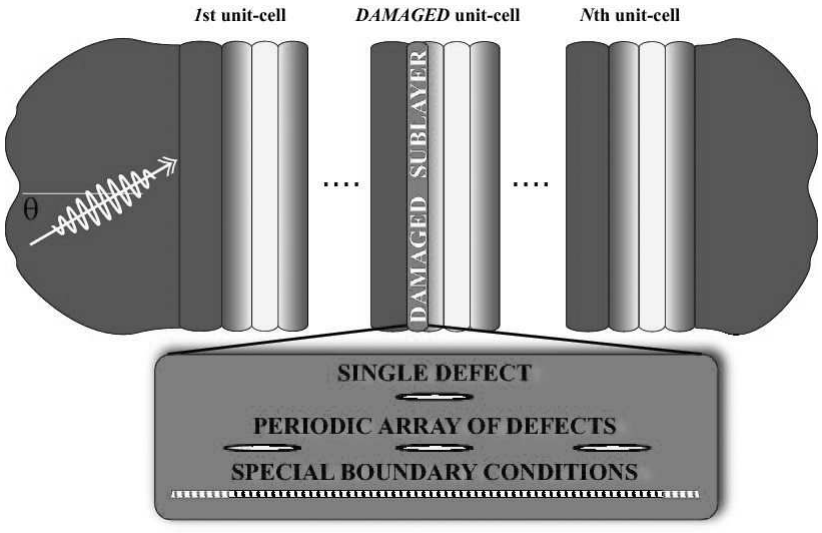

Fig. 1. Damaged periodic layered composite (phononic crystal)

To this end, efficient computational models based on a semi-analytical integral approach [2] are developed for precise and polyvalent analysis of phononic crystals and elastic composites of large, but finite number of layers.

It involves large linear algebraic systems and becomes very time-consuming. Moreover, for a qualitative research and to gain a deep insight into the nature of the physical phenomena many parameters (geometrical and physical) should be analyzed for a better prediction of the behaviour and for the optimal design of the periodic structure. The present investigation aims at the development and implementation of fast computational algorithms for multilayered composites with damages, see Fig. 1. Several models are developed here for the damaged zone: a single crack, a periodic array of cracks and a special kind of contact or boundary conditions [3].The wave fields are described by the integral representations [2, 4], where the wave fields in the structure are written as integrals along the real axis Γ_i in terms of the Fourier-transforms of Green's matrices K for periodic structures and the load exciting the waves $\mathbf{Q}$. A typical integral representation is

$$\mathbf{u}(x_1, x_2, t) = \mathrm{Re} \int_0^\infty \int_{\Gamma_1} \int_{\Gamma_2} K(\alpha_1, \alpha_2, \omega) \mathbf{Q}(\alpha, \omega) e^{-i(x_1\alpha_1 + x_2\alpha_2)} d\alpha_1 d\alpha_2 \; e^{-i\omega t} d\omega \tag{1}$$

The boundary value problem is solved by using a boundary integral equation method (BIEM), which needs the solution of a linear algebraic system. The implementation of BIEM requires the solution of the integral equations and the calculation of 3-dimensional arrays of integrals (1). The required computational time for the integrands in (1) increases in accordance with the total number of layers, which is quite large for the structures under investigation (the layer number is 50-1000). In order to provide a stable and fast computational procedure the algorithm given in [4] is used. The Laplace-transform in (1) can be calculated using a spline interpolation, and the calculations are time-consuming, especially when a wide range of frequencies is considered. Accordingly, the computer realization is carried out by a FORTRAN code, where all the steps during the simulation procedure are executed independently.

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MATHEMATICAL METHODS OF PROCESSING OF MEDICAL INFORMATION

Gordin V.A., Tokmakov M.A.

Higher School of Economics, Hydrometeorological Centre of Russia

1. We have processed the results of observations of chemical composition of blood (on 14 parameters), and evaluated eigenvalues and eigenvectors of the correlation matrix.

2. We have got linear and non-linear relations between these parameters of blood.

3. The level of possible influence of meteorological factors on these parameters of blood was evaluated.

4. We have considered the results of these assessments for the several groups of patients and compared the results with each other.

5. We have also evaluated the changes of the chemical parameters of blood during the treatment.

THE DRAG FORCES ON OSCILLATING PLATE IN A VISCOUS FLUID

Kamalutdinov A.M.

Kazan (Volga region) Federal University, Kazan, Russia

In this paper, we study drag forces on two-dimensional plate with height h and width b,which performs harmonic oscillations in a viscous incompressible fluid or gas, according to the law $x = Asin(\omega t)$, where A is the oscillation amplitude and ω is the radian frequency of oscillation.To determine drag forces of plate we use Morrison equation [1, 2, 3].According this equation, drag force can be expressed through inertia (C_M)and drag (C_D)coefficients of plate

$$P = -\frac{\pi}{4}\rho_\alpha b^2 C_M \frac{du}{dt} - \frac{1}{2}\rho_\alpha b C_D |u| u$$

where P is force which exerted on the plate by the fluid, ρ_α is density of fluid and u is speed of plate, for our case $u = A\omega cos(\omega t)$.

The inertia and drag coefficient generally depend on three non-dimensional parameters: relative thickness $\Delta = \frac{h}{b}$, Stokes frequency parameter $\beta = \frac{b^2\omega}{2\pi\nu}$, that plays the role of an oscillatory Reynolds number, and the ratio of the vibration amplitude A, multiplied by 2π, versus the width of the plate b, the so-called Keulegan-Carpenter (KC) number $KC = 2\pi\kappa = 2\pi\frac{A}{b}$. The theoretical results for drag coefficient C_D are known only for infinitely small value of Keulegan-Carpenter number [1, 4].

$$C_D = \frac{4.61}{\kappa\sqrt{\beta}}, \kappa \longrightarrow 0$$

Also approximation of experimental results is known for high value of Keulegan-Carpenter number [3]

$$C_D \approx \frac{6.2}{\sqrt{\kappa}}, \kappa > 1$$

We perform direct numerical simulation (DNS) of flow around a two-dimensional oscillation plate in the following range of parameters $\Delta \in [0.05, 0.3], \beta \in [50, 1000]$ and $\kappa \in (0, 3]$.We use open source package of computational fluid dynamics (CFD) openFOAM for direct numerical simulation. CFD package openFoam solves the Navier-Stokes equations by using the finite-volume method.There have been about 200 calculations. Each of

them consists in finding existing aerodynamic fields (velocity, pressure and vorticity) and forces on the plate over 40 periods of oscillation. We offer formula to determine the value of the drag coefficient on all range of value κ, which based on our numerical simulations and known approximations.

$$C_D = \frac{4.61}{\kappa\sqrt{\beta}} + \frac{6.2}{\sqrt{\kappa}}\frac{\xi^2}{(\xi^2+1.7)}, \xi = \kappa[2 + 1.78ln\Delta - ln\beta(0.54 + 0.88ln\Delta)]$$

This formula coincides exactly with the known approximations in extreme cases ($\kappa \longrightarrow 0$ and $\kappa > 1$). The results of this work can be applied to the study of the damping properties of materials.

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BIOELECTRICAL IMPEDANCE ANALYSIS AND MATHEMATICAL MODELLING, BASED ON REAL HUMAN ANATOMY

Kramarenko V.K.*, Danilov A.A., Vassilevski Yu.V.*,**, Rudnev S.G.**, Nikolaev D.V.*****

* *Moscow Institute of Physics and Technology*

** *Institute of Numerical Mathematics, Russian Academy of Sciences*

*** *Scientific-Research Centre MEDAS*

Segmental bioelectrical impedance analysis (segmental BIA) is commonly used for various purposes such as the assessment of body composition and abdominal adiposity, as well as for monitoring of body fluids redistribution under various physiological and pathological conditions [1]. For validation of existing measurement schemes, the development of new ones and for accurate interpretation, it is important to know relative contribution of tissues and organs to the result of bioimpedance measurements of the particular body segment. For this the segmented model of the Visible Human Project (VHP) man [2] containing 30 materials was constructed.

Partially segmented model of the VHP man torso [3] was initially used with the subsequent improvements as described in details in [4, 5] and with the addition of segmented head and extremities. Two schemes of segmental BIA were considered: an eight-electrode one with the placement of current and potential electrodes 5 cm apart on the dorsal surfaces of the wrists and ankles, and also ten-electrode scheme with an additional electrode pair located on the forehead [6]. After the addition of electrodes, an adaptive unstructured tetrahedral mesh was generated and post-processed in order to improve its quality using mesh cosmetics algorithms from the Ani3D library [7].

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APPROXIMATE METHODS FOR SOLVING THE PROBLEM OF RADIATION-CONDUCTIVE HEAT TRANSFER IN TWO-DIMENSIONAL PERIODIC STRUCTURE[1]

Kremkova A.A.

National Research University "Moscow Power Engineering Institute", Moscow, Russian Federation

In applications, it is of great importance to study the heat transfer process in periodic media containing vacuum interlayers or cavities through which the heat transfer is realized by radiation. A numerical solution of such problems requires considerable computational efforts and becomes, in fact, impossible for a large number of heat transferring elements, especially in the case of two-dimensional and three-dimensional structures. Therefore, it is important to construct effective approximation methods which, in particular, could be based on constructing special homogenizations of the problem under consideration. Such methods can be based on the construction of special semidiscrete or asymptotic approximations of the original problems.

Formal homogenized equations for such problems were constructed N.S. Bakhvalov [1, 2].

Special semidiscrete and asymptotic approximations for the one-dimensional problems of radiative-conductive heat transfer in the system of gray heat shields have been proposed and justified in [3], [4], [5].

We consider a nonstationary nonlinear initial boundary value problem describing the radiative-conductive heat transfer in the periodic system consisting of n^2 square heat-conducting elements separated by vacuum interlayers. The absolute temperature is unknown function. The heat transfer within each element is described by the heat equation. On the elements interface, there is radiative heat transfer. The heat flow supplied to the surfaces of elements through the mechanism of thermal conductivity equals to the difference of the absorbed and emitted energy. The existence and uniqueness of solutions to this problem follow from [6].

The idea of semidiscrete methods consists in the approximation of the energy balance of elements of the system. The temperature assumed to be a constant at each of the system elements. As a result, we come to the problem,

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which is discrete on a space variable and is continuous on a time variable. We constructed two semidiscrete methods which differ one from other by way of an approximation of the heat flux and by way of accounting the heat conductivity of the system elements. We also offer two asymptotic methods which may be considered as differential counterparts of the semidiscrete methods. The solutions of the semidiscrete and asymptotic problems are regarded as approximations to the solutions of the original problem.

Difference schemes have been constructed for all the approximations and a series of numerical experiments were conducted. The dependence of the errors of approximations on the size of the elements of the system, on the time and on the coefficient of thermal conductivity were studied. The experimental results [7] show that the second semidiscrete method has the smallest error, the first averaged method has the greatest error. The relative error for all approximations did not exceed 0.1%. The results show a sufficiently high efficiency of the proposed approximations. Currently, the work on the theoretical basis and estimates of accuracy of the offered approximations is carried out.

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SPECIAL PRECONDITIONERS FOR SOLUTION OF STRONGLY NON-SYMMETRIC LINEAR EQUATION SYSTEMS[1]

Krukier L.A., Pichugina O.A., Krukier B.L.
Southern Federal University, Rostov-on-Don, Russia

The system

$$Au = f \tag{1}$$

where A is non-symmetric positive real matrix, u is the vector of unknown, f is the vector of the right part is considered. Matrix A can naturally be expressed as a sum of symmetric matrix A_0 and skewsymmetric matrix A_1. If A_0 is a positive definite than matrix A is named positive real. We will name matrix A strongly non-symmetric if

$$\|A_0\|_* << \|A_1\|_*$$

where $\|\&\|_*$ is some matrix norm. It is well known, that difficulties to solve such linear equation systems grows up because matrix can lose property of diagonal dominant. Let us approach (1) by considering the iterative methods of the following form:

$$y^{n+1} = Gy^n + b, \quad G = B^{-1}(\omega)(B(\omega) - \tau A), \quad B_C = {B_C}^* \tag{2}$$

where $f, y_0 \in H$, H is an n-dimensional real Hilbert space, f is the right part of (1), A, $B(\omega)$ are matrices, A is given by equation (2), $B(\omega)$ is nonsingular preconditioner, y_0 is an initial guess, y_k is the k-th approach, $\tau, \omega > 0$ are parameters, u is the solution that we obtain, $e^k = y^k - u$ and $r^k = Ae^k$ denote the error and the residual in the k-th iteration, respectively. Consider the next choice of preconditioner B

$$B = (B_C + \omega K_U){B_C}^{-1}(B_C + \omega K_L), \quad B_C = {B_C}^* \tag{3}$$

where $K_L + K_U = A_1$, $K_L = -{K_U}^*$, $B_C = {B_C}^*$. Matrix B_C can be chosen arbitrarily, but has to be symmetric. This preconditioner is called two-parameters product triangular (TPT). Convergence iterative methods with TPT has been considered and proved before. We use TPT as preconditioner for GMRES(m) and BiCG and compare it with conventional SSOR preconditioner.

[1]Supported by RFBR, grant №12-01-00022_a and grant №12-01-31127_mol_a

The standard 5-point central difference scheme on the regular mesh has been used for approximation of the convection-diffusion equation with Dirichlet boundary conditions and small parameter at the higher derivatives in the incompressible medium. Its transformation by regular ordering to strongly non-symmetric linear equation systems have been made for the check of TPT behavior, as preconditioner. Matrix A can naturally be expressed in a sum of symmetric positive definite matrix A_0, which is a difference analogue of the Laplace operator and skew-symmetric matrix A_1, which is a difference analogue of the convective terms in the case of central difference approximation of the convective terms. Numerical experiments for different variants of strongly nonsymmetric systems have been executed. It was shown numerically and theoretically that the behavior of preconditioned GMRES(m) is the better then unpreconditioned in considered particular cases. Unpreconditioned BiCG is better work in number of cases than preconditioned BiCG.

ASPECTS OF THE NUMERICAL IMPLEMENTATION OF THE THREE-DIMENSIONAL TWO-PHASE MODEL OF FOREST FIRES[1]

Kuleshov A.A.*, Vinogradova S.A.**

* *Keldysh Institute of Applied Mathematics of Russian Academy of Science, Moscow, Russia*

** *Southern Federal University, Rostov-on-Don, Russia*

In recent decades mathematical modeling of forest fires, being an actual problem, develops quite rapidly. Currently, performance growth of supercomputers has made possible transition to the simulation of forest fires on the basis of full-scale three-dimensional models. The paper [1] suggests a three-dimensional two-phase model of forest fires, which is a generalization of the earlier two-dimensional two-phase models. This model reflects the fundamental physical laws of mass, momentum and energy conservation and takes into account all physical phenomena in the fire zone that are important for fire dynamics. Its distinctive feature is the $k-\varepsilon$ model, modified by including additional turbulence production and dissipation terms in the forest layer. The combustion rate in the gas phase is described by the Eddy Break-up Model which assumes that the combustion rate is limited by turbulent mixing rather than by reaction kinetics.

For numerical solution of the whole system of equations [1] the efficient algorithm of splitting by physical processes [2] has been used. A discretization in time $t_{n+1} = t_n + \Delta t$ is considered. At the time step $[t_n, t_{n+1}]$ the system splits to the following stages (input data for the each stage are obtained at the previous stage):

1. gas phase transfer;
2. accounting for the momentum and energy alteration due to changes in the phase volume fractions;
3. consideration of the impact of heat sources;
4. accounting for viscosity, thermal conductivity, diffusion and interphase energy exchange;

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5. accounting for the interphase friction;

6. accounting for interphase heat exchange and exchange by radiant energy;

7. accounting the pressure from the equation of state.

The problem is considered in the domain $\Omega = [0, L_1] \times [0, L_2] \times [0, L_3]$ with a regular mash. The listed subsystems of equations are solved by finite difference method. The equations of stages 2,3,5,6 are approximated by simple explicit difference schemes. The three-point difference scheme with Rusanov flux [3], which are also called the local Lax-Friedrichs flux [4], is applied to solve the subsystem of equations for the gas phase transfer stage.

An example of numerical implementation of the gas phase transfer stage is given. We solved the three-dimensional initial boundary value problem of the temperature dissemination from the hot cylindrical source. Changing of both the temperature profile and emerging gas flow was estimated. The obtained results show that the cloud of hot gas goes up and dissipates under the influence of its own flows, that corresponds to the actual physical process.

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HIGH-PERFORMANCE RECONFIGURABLE COMPUTER SYSTEMS BASED ON VIRTEX-6 AND VIRTEX-7 FPGAS

Levin I.I., Kalyaev I.A., Dordopulo A.I., Slasten L.M.
Scientific Research Institute of Multiprocessor Computer Systems at Southern Federal University, Taganrog, Russia

Today developers of highly-performance computer systems try to achieve record-breaking performance characteristics of supercomputers, and therefore they search new architectural solutions that could provide such results. During the last years multicore graphics microprocessors and programmable logic integrated circuits (FPGA chips) are used as computational nodes in addition to general-purpose microprocessors. In most FPGA-based computer systems, for instance, such as Jaguar - Cray XT5-HE [3], programmable chips are used as additions to microprocessors that perform laborious calculations or fragments of tasks that cannot be performed effectively.

At the same time, it is known [1, 2] that FPGAs have considerably higher computational capabilities, which can be entirely used in reconfigurable computer systems with a great number of FPGA chips that are used as principal computing elements [4, 5]. The idea of reconfigurability and adaptation of computer system architecture to the solving task was used in homogeneous computing media [6], systolic structures [7], systems with reconfigurable (programmable) architecture [8] [10]. However, in spite of numerous and various research several prototypes of these systems were designed, but the matter did not get any farther due to lack of element base satisfying requirements of the concept of reconfiguring of computer system according to the task structure.

New RCS designs of SRI MCS SFU, based on FPGAs of the Xilinx Virtex-6 and Virtex-7 families, use an open scalable architecture [1], owing to which many limitations of the lattice architecture can be omitted. The RCSs were designed according to the principles of open scalable architecture and consist of computational modules (CM) that contain Virtex-6 FPGAs. These systems are commercial products, which are produced in two modifications of computational modules: 6U Saiph and 1U Rigel. At the same time the team of scientists develops trend-setting products, based on Virtex-7 FPGAs: a reconfigurable computer system RCS-7 will contain a computation field of Virtex-7 FPGAs and will provide the peak performance up to 1015 fixed-point operations per second for a single 47U rack. Use of the Xilinx Virtex-7

FPGAs improves technical characteristics in about 1.7 times in comparison with those computational modules that are based on the Xilinx Virtex-6 FPGAs.

So, the new generation computational modules Saiph and Rigel, based on Xilinx Virtex-6 FPGAs, provide ample opportunities of creation of computer systems with higher performance and the same price in comparison with the Rigel-based RCSs [11]-[13]. At the same time, the computational modules are quite self-contained; as accelerators they can be easily combined with an IBM PC and used for solving of various tasks. The reconfigurable computer systems, designed in SRI MCS SFU, are programmed with the help of a high-level programming language COLAMO [2]. The language COLAMO is intended for description of parallel algorithms and for creation of special-purpose computing structure on the base of the principles of structural-procedural organization of computations [4] in RCS architecture. Such structure implies sequential change of structurally (hardwarily) implemented fragments of the information graph of a task. In addition, each fragment is an operand flow computational pipeline. So, the RCS application (task) consists of a structural component and a procedural component. The structural component is a set of hardwarily implemented fragments of computations. The procedural component is a control program which provides sequential change of computing structures and generation of data flows, and which is the same for all structural fragments. To provide such organization of computations, the language has a structure called "cadr" [4], which is an indivisible combination of the computing structure of the task fragment and a set of read/write operations of input/output data flows.

In the strict sense of the word, the cadr is a program-indivisible component, which is a set of operations that are implemented as arithmetic-logical operators and read/write instructions, performed by various functional units that are connected according to the informational structure of the algorithm.

The language COLAMO has no explicit descriptions of parallelism, and parallelization is provided by types of access to variables, and by indexing of array elements, which is typical for data flow languages. To access to data, it is possible to use two main access methods: parallel access (specified by Vector type) and sequential access (specified by Stream type). Granularity of parallelism is defined according to the minimum value of the parallelization parameter. For Stream access the granularity of parallelism is unity. For Vector access the granularity of parallelism is defined by the minimum value of the vector component of each array, used in computations. If data access is specified as parallel, it is possible to process all array dimensions of Vector

type simultaneously. As a result, we will need larger hardware resources for data processing, but the time of data processing will decrease.

Multidimensional data arrays can have many dimensions, each of which can have sequential or parallel type of access, specified by the keyword Stream or Vector, respectively. If arrays, involved in computations, have different access types, then the computing structure, developed by the user, may be unbalanced. As a result it will require additional hardware resource and decrease speed of data flow processing. Owing to variation of access type, the programmer can rather easily control granularity of parallelism of computations on the level of description of data structures, speed of data processing and used hardware resources. Owing to this, the programmer can describe various types of parallelism in rather succinct form. Besides the access type, each variable in the language COLAMO has a specified type of storage: memorial (Mem), register (Reg) and communication (Com).

Translation of the program, written in the high-level language COLAMO, consists in creation of the computer system circuit configuration (the structural component) and the parallel program (the stream and procedural components), which controls data flows. Creation of the structural component consists in generation of the computational graph of informational dependences between results, described with the help of the language COLAMO. Each operation, used in the program, has a correspondent special-purpose computing unit, designed according to the data type, the type of access to variables, and etc. Then the environment of computing structure development Fire!Constructor maps the synthesized computational graph of the task on the FPGAs of the RCS.

Like computational modules of previous generations, the next generation computational modules Saiph and Rigel use the same programming principles: all considered computational modules are programmed with the help of the integrated system software suit, which supports structural-procedural methods of organization of computations, and defines not only organization of parallel processes and data flows, but the structure of the computer system within the FPGA field as well.

The idea of reconfigurable computer systems with open scalable architecture based on macro objects is the original and new direction of design of high-performance systems. The principal elements of such RCSs are FPGAs which can be programmed according to the requirements of macro objects designed for various tasks of some problem area. Within basic architecture the macro objects are adjusted to execution of some task which is necessary to solve, and hence we get a virtual special-purpose calculator. Such calcu-

lator provides high real performance of the whole RCS owing to similarity between its architecture and the structure of the solving task.

The system software suit allows the application programmer to develop applications using a high-level programming language, without any knowledge of the RCS hardware structure or any help of the circuit engineer. As a result, it is possible to debug and modify applications very easily and quickly. The practical value is significant decrease (5-7 times) of the time needed for development of an application for such RCSs.

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THE INFLUENCE OF COSSERAT MATERIAL PARAMETERS IN THE PROBLEM OF DEFORMATION OF THE INCOMPRESSIBLE MICROPOLAR CYLINDER

Mayorova O.A.

Southern Federal University, Rostov-on-Don, Russia

A new wave of interest to the models of the Cosserat continuum mechanics is associated primarily with the needs of nanomechanics in such models of the elastic behavior of objects that can take into account the structure of the material; furthermore they are relevant in many areas of biomechanics. The main task of this study was to find such ways of influence on the elastic body which lead to stress-strain states significantly different in the classical theory of elasticity and in the theory of the Cosserat continuum.

We used semi-inverse method of nonlinear elasticity to study two problems, namely the problem of a nonlinear torsion and the problem of equilibrium of a cylinder with a wedge disclination. The problems differ in variants of semi-inverse representation of the displacements and in functions of the specific potential energy of the Cosserat medium, though in all cases the semi-inverse representation contains two functions to be defined, depending only on the one scalar parameter.

To study the equilibrium of the solid cylinder with wedge disclination at its axis within the framework of Cosserat continuum we used following representation of the deformation:

$$R = R(r),\ \Phi = \kappa\varphi,\ Z = \lambda z. \tag{1}$$

There are two known presentations for the orthogonal tensor of microrotations $\mathbf{H}$ used for modeling disclinations and dislocations [1, 2].

$$\mathbf{H_I} = \cos\chi(r)\,(\mathbf{e}_r\mathbf{e}_R + \mathbf{e}_\varphi\mathbf{e}_\Phi) + \sin\chi(r)\,(\mathbf{e}_r\mathbf{e}_\Phi - \mathbf{e}_\varphi\mathbf{e}_R) + \mathbf{e}_z\mathbf{e}_Z. \tag{2}$$

$$\mathbf{H_{II}} = \mathbf{e}_r\mathbf{e}_R + \cos\chi(r)(\mathbf{e}_\varphi\mathbf{e}_\Phi + \mathbf{e}_z\mathbf{e}_Z) + \sin\chi(r)(\mathbf{e}_\varphi\mathbf{e}_Z - \mathbf{e}_z\mathbf{e}_\Phi) \tag{3}$$

It was shown that though the presentation (2) could be used for the analysis of stresses and couple stresses distribution within the cylinder with disclination, it failed in the case of possible torsion of the cylinder as a whole. For this reason we used presentation (3) to study the possibility of macrorotation of the cylinder due to disclination.

We considered a series of specific strain energy functions for the Cosserat media with similar structure:

$$W_i = 2\mu\,\mathrm{tr}\,(\mathbf{Y}-\mathbf{I}) + \delta\left|\,\mathrm{tr}\left(\mathbf{L}\cdot\mathbf{L}^{\mathrm{T}(\mathrm{i}-1)}\right)\right| + \eta\,(\delta_{2\mathrm{i}}+\delta_{3\mathrm{i}}+\delta_{4\mathrm{i}})\left|\,\mathrm{tr}\left(\mathbf{L}^2\cdot\mathbf{L}^{\mathrm{T}(\mathrm{i}-2)}\right)\right| +$$

$$+\gamma\delta_{2i}\,\mathrm{tr}^2\mathbf{L} + \gamma\delta_{4\mathrm{i}}\,\mathrm{tr}\left(\mathbf{L}\cdot\mathbf{L}^{\mathrm{T}}\cdot\mathbf{L}\cdot\mathbf{L}^{\mathrm{T}}\right), \mathrm{i} = 1..4. \qquad (4)$$

where $\mathbf{Y}$ — strain measure, $\mathbf{L}$ — bending strain tensor [2], $\mu, \eta, \delta, \gamma$ — material parameters. To perform numerical calculations for their values we used data from [3] where energy function of type W_2 in (4) was used. In the case of absence of couple stresses all models (4) are reduced to the Bartenev-Khazanovich model of classical incompressible material [4]. By direct numerical computations and asymptotical analysis it was shown that it was possible to construct a model of an incompressible nonlinear elastic Cosserat pseudo-continuum, for which the formation of disclination is accompanied by macro-rotation of the cylinder — effect that is absent in classical nonlinear elasticity theory. To construct such material the terms with uneven degrees should be taken into account.

To study well-known nonlinear effect of changing the length of the cylinder due to pure torsion within the framework of Cosserat media we used following semi-inverse representation of deformation

$$R = R(r),\ \Phi = \varphi + \psi z,\ Z = \lambda z \qquad (5)$$

together with representation (3). In (5) ψ stands for the rotation angle per unit of the cylinder length. For the case of the hollow cylinder unknown functions in (3), (5) are given by expressions

$$P(r) = \sqrt{\frac{r^2+A}{\lambda}},\ \ \chi(r) = -\arctan\left(\frac{\psi R(r) r}{R(r)+\lambda r}\right)$$

where A — the constant of integration — should be determined from the boundary conditions.

The solutions related to material models (4) exhibited different behavior depending on the evenness of the polynomial terms. In the case of even degree terms pure torsion led to the elongation of the cylinder with an accuracy up to the fourth order in ψ. In the case of terms with odd degree the cylinder started to shorten after small elongation in contradiction to classical nonlinear elasticity theory.

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THE METHOD OF CHARACTERISTICS FOR SOLVING THE NAVIER-STOKES EQUATIONS

Muratova G.V., Andreeva E.M.
Southern Federal University, Rostov-on-Don, Russia

Mathematical model of hydrodynamics is the base for research of the various natural phenomena, technological processes and environmental problems. We propose some approach for solving the Navier-Stokes equations in hydrodynamics problems.

The system of Navier-Stokes two-dimensional non-stationary equations for two components of speed and pressure for an incompressible viscous fluid is considered. To approximate the time derivative and inertial first space derivatives a method of characteristics is used [3]. Space discretization is carried out by finite element method. This mixed method of approximation was suggested by O. Pironno in the 1980-th year and it's more often used in numerical researches now [2]. It's used a mixed formulation in the finite element method, when a combination of simple finite elements – bilinear for velocities and constant elements for pressure is applied. This combination provides stability of pressure calculation with additional application of a numerical filtration.

After discretization we obtain a linear algebraic equation system with a symmetric matrix which has a spectrum with alternating signs. We use multigrid method for solving this system.

We consider classical formulation of the Navier-Stokes equation in domain $\Omega = (0,1) \times (0,1)$ with boundary $\partial\Omega$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial P}{\partial x} - \frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f_1, \tag{1}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial P}{\partial y} - \frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = f_2 \tag{2}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = f_3, \tag{3}$$

$$\begin{array}{l} u\,(x,y,t) = g_1\,(x,y,t)\,, \quad v\,(x,y,t) = g_2\,(x,y,t) \quad on \quad \partial\Omega, \\ u\,(x,y,0) = u_0\,(x,y)\,, \quad v\,(x,y,0) = v_0\,(x,y)\,. \end{array}$$

where Re is Reynolds's number, and $V = (u(x,y,t), v(x,y,t))$ is the velocity, P is the pressure.

The modified method of trajectories (characteristics) approximating the transfer equation is developed for the solving Navier-Stokes system of the equations. The proved identity about exact equality of the masses located on the neighbour temporary layers and concluded in volumes (areas) with borders which are determined by trajectories of movement of particles back by time is the base of the method [2]. It is theoretically proved and experimentally confirmed that the offered numerical scheme has the first order of accuracy and converges in the discrete norm analog of L_1 space with the fixed relation of time step to space step. Numerical experiments and comparison with the upwind scheme showed that the maximum absolute errors for these schemes differ not considerably. Besides thanks using of trajectories (characteristics), the method allows to neglect a Courant-Friedrichs-Lewy stability condition and to formulate other restriction on a time step. It allowed to increase a step on time up to the size, by 10 times exceeding the maximum admissible value corresponding to a Courant condition in some numerical experiments. To increase the order of convergence to the fourth one the method of Richardson extrapolation is used.

Mixed formulation for the space discretization of the Navier-Stokes with combination of simple finite elements bilinear elements for velocity and constant ones for pressure is used in this research. As a result of the approximation we get the system of linear algebraic equations, which is solved by multigrid method.

The multigrid method (MGM) is one of the effective and enough universal iterative methods of the solving the systems of the linear algebraic equations [1], [4]. The multigrid method belongs to a class of quickly converging iterative methods. MGM has optimum of arithmetic operation number.

Multigrid method is not a fixed multigrid algorithm. There is rather a multigrid technique fixing only the framework of the algorithm. The efficiency of multigrid method depends on adjustment of its component to a considerable problem.

The results of some numerical experiments allow to conclude the efficiency of the suggested approach for solving the Navier-Stokes equations.

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ADMIXTURE SPREADING IN NATURAL STREAMS

Nadolin K.A.*, Zhilyaev I.V.**

* *Southern Federal University, Rostov-on-Don, Russia*

** *Southern Scientific Center of Russian Academy of Sciences, Rostov-on-Don, Russia*

The main goal of the presentation is to discuss the foundations, ideas, approaches and techniques for mathematical modelling of some natural phenomena on the base of their specific properties. As an example we use the admixture spreading process in natural streams, like rivers and channels and as a result build a set of simplified mathematical models for different types of stream-bed flows [2]. These models can be applied to the natural waterways that are characterized by a considerable difference in sizes of their length, width and depth. For example, the ratio between the characteristic depth and width for a typical lowland river varies from 1:10 to 1:200.

The formulation of the problem is as follow. An admixture spreads in an open turbulent flow of incompressible viscous fluid in some section of a channel. The channel bed is assumed to be known and quite smooth and the stream is assumed to be lengthy and shallow. So, the curvature of considered part of the stream is weak, the section's length is large with respect to the channel width and in this section the channel width is large with respect to its depth.

The admixture is assumed to be passive and its dissipation and diffusion are taken into account. The passivity of admixture means that the mathematical description of the process splits into two subsystems of equations. The first one – the "hydrodynamics subsystem" – allows to find fluid velocity and pressure fields and the second one – the "concentration subsystem" – allows finding the concentration of admixture in the stream with known velocity.

The objective of the investigation is to provide adequate mathematical models describing the admixture spreading process. These models should be reduced in space and simple enough for numerical or analytical solution, they should be adequate and provide acceptable accuracy, they should provide the opportunities for adjustment with experimental data and can be calibrated in accordance with available experimental data, and they should allow improvements and corrections.

As a result a set of mathematical models are derived by the small parameter technique, starting from the 3D Reynolds equations for the incompressible

fluid (coupled with Boussinesq turbulence hypothesis) and the diffusion equation for the moving medium.

In the framework of proposed classification of streams six kinds of the reduced models occurs: shallow and lengthy stream model; super shallow and lengthy stream model; shallow and super lengthy stream model; shallow and wide stream model; deep and lengthy stream model and essential 3D stream model. In the resulting set of equations the hydrodynamic part for the velocity field is balanced with the diffusion part for the concentration field.

The numerical results show that these reduced 3D models adequately describe the spreading processes in natural streams [1]. They provide acceptable accuracy and they allow improvements and recurrent correcting procedure.

It should be mentioned that the particular feature of these reduced models is that they take into account the stream cross-structure that allows us to study the contaminant spreading in a channel with varying width and depth more accurate than with depth-averaged models (for example, to catch the phenomenon of rising the near-surface opposite flow which may be caused e.g. by the wind action).

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FINITE-ELEMENT DETERMINATION OF THE EFFECTIVE PROPERTIES FOR POROUS PIEZOCOMPOSITE MATERIALS WITH DIFFERENT CONNECTIVITY[1]

Nasedkin A.V.*, Shevtsova M.S.**

* *Southern Federal University, Rostov-on-Don, Russia*

** *Southern Scientific Center of Russian Academy of Sciences, Rostov-on-Don, Russia*

Porous piezoelectric ceramics is relatively new and very promising class of piezocomposite materials used as the active elements in various piezoelectric devices. A peculiar property of the porous piezelectric ceramics is that its most important thickness characteristics are almost independent of porosity, when the respective longitudinal characteristics rapidly decrease with porosity growth. Experimental and theoretical studies have shown that the transducers on the basis of porous piezoceramics have high piezoelectric sensitivity, extended frequency bandwidth and significantly lower acoustic impedance compared to dense ceramics that provides a better matching with the acoustic medium. At the same time the available experimental data on the properties of the porous piezoelectric ceramics are rather contradictory. All this confirms the relevance of the theoretical determination and prediction of the effective properties for the piezocomposite materials, in particular, the porous piezoceramics.

In presented work the calculation of the effective properties for porous piezoelectric ceramics with different connectivity was conducted using the effective modules approach and the finite element (FE) modeling of the representative volume for porous piezocomposite material [1, 2]. For the numerical determination of the effective moduli using specially developed computer programs in the APDL ANSYS macro language, the set of static piezoelectric problems was solved for a representative volume with the different boundary conditions, ensured constant values for the stress and strain fields, electric field and electric displacement of a homogeneous body. The two methods: random method and the diffusion-limited aggregation (DLA) Witten-Sander method, were implemented in detached C++ programs, developed by V. Remizov, for the generation of representative volumes with their following transfer to the FE package ANSYS.

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To take into account the heterogeneity of polarization field the electrostatic problem for a dielectric composite was firstly solved, and the electric field that identifies the polarization field was determined. In total we had a representative volume of piezocomposite with inhomogeneous properties of piezoelectric matrix (generally near the pores).

As a result, the dependencies of the effective characteristics on porosity for piezocomposite material were obtained under the assumptions of uniform and non-uniform polarization of the piezoceramic matrix. It was found that the taking into account the polarization inhomogeneity in the pore vicinities provides better agreement between the obtained relationships and a number of known experimental data [3]–[6]. It was shown that the best adequacy to experimental data can be ensured by the DLA Witten-Sander method for generation of the porous piezoelectric material structure. The developed program tools allow to predict the effective materials constants for the wide range of porous PZT materials, thereby facilitating well grounded design of piezoelectric acoustic devices.

As an example of practical applications we investigate hydro-acoustic emitters made of solid ceramics with intermediate interjacent non-piezoelectric layers and piezoelectric emitter from porous piezoceramics without such layers . From the FE solutions of the coupled dynamic acoustopiezoelectric problems [7] we can conclude that porous piezoceramics is very effective material for different hydroacoustic ultrasonic applications.

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USING THE PRECONDITIONING TECHNIQUES FOR SOLVING CONVECTION-DIFFUSION PROBLEMS[1]

Pichugina O.A.

Southern Federal University, Computer Center, Rostov-on-Don, Russia

There are a lot of techniques for solving non-symmetric linear systems. However, strongly non-symmetric systems are studied not enough. We use special class of triangular and product triangular preconditioners [1] of Krylov subspace methods for solving strongly non-symmetric systems. They are easy to build and easy to invert because of the triangular structure. The new preconditioners make it feasible to solve strongly non-symmetric systems quickly and efficiently.

Numerical examples involving two-dimensional convection-diffusion equations with dominant convection are presented to demonstrate the convergence and accuracy of the new approach.

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THE SOFTWARE COMPLEX FOR CALCULATION RADIONUCLIDE AND DISTRIBUTION OF OIL POLLUTION IN WATER BODIES

Shabas I.N.

Computing Center of the Southern Federal University, Rostov-on-Don, Russia

A system of three-dimensional equations is considered. It describes the processes of transfer of multiphase materials in the environment. The resulting system is solved by finite difference methods using implicit schemes [4].

Reservoir with some radionuclide or oil contamination is considered as a test object. We use the model proposed by M.I.Zheleznyak [2] for describing the process of radionuclides distribution. Approach proposed in the works of a group of authors led by S.I.Dembitsky [3] are used for description of behavior of oil spills besides modeling the process of evaporation of oil. There are used the empirically derived formulas [1]. It's more accurately simulate the evaporation of oil from the surface of the water reservoir.

The paper presents a computer system that implements a three-dimensional mathematical model of multiphase transport of substances in the body of water [5]. It's implemented on high-performance computing systems using Web-based interface.

Counter modules are written in complex language FORTRAN-77. They use numerical methods of the package parallelized methods AZTEC. Free package Gnuplot are used for visualization of calculations.

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NUMERICAL COMPARISON OF METHODS FOR CALCULATING THE VOLUME OF OIL SPOTS EVAPORATION IN THE AZOV SEA

Shabas I.N., Chikina L.G., Burtyka P.B.

Southern Federal University, Computer Center, Rostov-on-Don, Russia

The process of evaporation of the oil slick from the surface of the water is considered. The comparison of the two approaches for the methods for calculating the amount of oil evaporated is interesting problem. The first approach is based on the idea that a mechanism of oil evaporation similar to the mechanism of water evaporation [1, 2]. The evaporation of oil on the basis of this assumption has been modeled in [1] for the first time. The second approach is based on the formulas derived from experimental studies [3]. It have been proposed empirical formulas for calculating the proportion of evaporation as a percentage of the total mass of oil poured out by the time t from the beginning of the spill [3]. We present a numerical comparison of the formulas [1, 3] for the types of oils spills are most likely to occur in the Azov Sea.

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NUMERICAL OPTIMIZATION OF DISTRIBUTED MODEL BASED THERMAL CONTROL FOR CURING OF COMPOSITE SRUCTURES[1]

Shevtsov S.N.*, Zhilyaev I.V.*, Wu J.-K.**

* *Southern Federal University, Rostov-on-Don, Russia*

** *National Kaohsiung Marine University, Kaohsiung city, Taiwan R.O.C.*

The high loaded composite structures made from fiber reinforcing with thermoset resin are produced by the autoclave and closed mould processes cure at which the consolidation of the fibers and matrix is done at the same time as the component is shaped. Full curing schedule include a pre-warming to the resin viscosity reaches a minimum, next applying of pressure to remove the gas bubbles and removal of excess resin, and finally vitrification of resin at elevated temperature to its full polymerization [1]. The change in the states of the composite should be made as possible uniformly across the thick-walled products. The main processing problems encountered in closed molding of articles with large variations in thickness include porosity, resin-rich areas, resin-dry areas, insufficient consolidation, degraded mechanical properties, and distortion which can arise from uneven cure. These problems can be resolved by correct timing of application of temperature and pressure. But the process control is complicated due to unobservability of the rheological state and temperature of material in a closed volume of a mould [2].

In this paper we propose a mathematical model for epoxy-based thick-walled composite structure curing. PDE system linking a kinetic equation of the resin cure with heat transfer equation, take into account heating caused by excessive exothermic reactions, a phase transition of resin from liquid to gel and further to the solid state, where required temperature field is supported by the independently controlled heat sources. In order to reconstruct the kinetic equation for the studied epoxy resin we used the Differential Scanning Calorimetry which implement the monitoring the thermal effects during polymerization [3]. Next the specific heat capacity and thermal conductivity at the phase transition from the liquid to gel and then solid states have been described by the empirical dependencies, which have been used in the heat transfer equation. The coupled kinetic and heat transfer equations have been solved for the domain geometry, imported from CAD model at the

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boundary conditions corresponding to the real system, where some boundaries are exposed to controlled heat flow. By the try and error method it has been established that good parameterizations for the one step heating (to the gelation or vitrification states) can be expressed as 4-parameters time dependence for each channel of the heating control, and these unknown parameters should be determined by some optimization technique [4]. As the cost function we used the weighted sum of averaged temperature, degree of cure, and its deviation, all calculated by integration which spread over the composite body at given reference time [5].

To synthesize the optimal control law we use the genetic algorithm which performs the transient analysis of the developed FE model on each iteration steps. Such coupled problem presenting PDEs in connection with control and optimization has been solved by live link Comsol Multiphysics FE tool with GA toolbox MATLAB. The pseudo optimal control laws were obtained at the population size equal to 10, and 20 generations of genetic algorithm, that required 3-5 hours on multi-core processors. Effectiveness and way to use in practice of the proposed model and its numerical implementation are illustrated on example of optimal control synthesis for the closed mould curing of composite spar, where the mould is heated by the controlled multiple independent heaters.

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THE INFLUENCE OF INTERNAL STRESSES ON EQUILIBRIUM AND STABILITY OF ELASTIC CYLINDER UNDER TENSION AND INFLATION [1]

Shubchinskaya N.Y.
Southern Federal University, Rostov-on-Don, Russia

In the present work we consider some issues of effects of internal stresses caused by defects of crystal lattice such as the wedge disclination and screw dislocation[1]. To describe the mechanical properties of a cylinder two constitutive models for compressible elastic solid were used: John material [2] and Blatz & Ko material [3].

The analysis of length changing of an unloaded cylinder due to the defect formation was performed. This changing is completely described by the dependence of γ (positive coefficient of the cylinder stretching or shortening) on the disclination parameter or the dislocation parameter at the absence of external load. It was shown numerically that it is nonlinear effect and the elongation $(\gamma > 1)$ or shortening $(\gamma < 1)$ depends on material parameters of the mechanical models. To verify the numerical results the asymptotic formula was obtained within the limits of the second-order effects theory [4]. Within this theory the relations for the length changing of the cylinder and for the twist angle ψ were obtained.

To analyze the stability of a cylinder with isolated defect under tension and inflation the bifurcation approach was used based on linearization of the equilibrium equations in the neighborhood of the solutions obtained by means of the semi-inverse representations Search of the bifurcation points is based on the analysis of the homogeneous linear boundary value problem of a six order, whose coefficients depend on radial displacement function found in the first stage. The bifurcation point is treated as such value of the "loading" parameter — it can be the parameter of the defect, or value of inflating pressure or axial force — for which the linearized problem has a nontrivial solution.

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MODELING OF RADIATION TRANSFER IN POWDER BEDS WITH MONTE CARLO METHOD[1]

Shumarov M.

National Research University "Moscow Power Engineering Insitute", Moscow, Russia

The moddeling of radiation transfer process is considered. Distribution of radiation intensity in a powder bed is under research. It is assumed that the powder is composed of spherical particles. The particles consist of a homogeneous absorbing scattering medium with extinction coefficient β, albedo factor λ and refractive index n. The external medium to the powder is also a homogeneous absorbing scattering medium with the parameters: β_e, λ_e, and n_e. Radiation on the surface of the particle is reflected and refracted according to geometrical optics laws in compliance with the Fresnel laws [1].

An algorithm based on the Monte Carlo method was proposed [2]. The algorithm was realized with creating a software package that allows to carry out numerical experiments using a multi-processor machines, including the MPEI cluster.

Dependance of transmission and reflection coefficients on the powder packaging structure and on the type of incident radiation (collimated or diffuse (Fig. 1)) is studied. A simple cubic packaging, the closest hexagonal and closest cubic packagings [3] are considered. Also the effect of changing of the particles radius on the distribution of radiation in a powder bed of a constant thickness is studied.

The results of numerical experiments show that the type of packaging and of the incident radiation affect the nature of radiation penetration significantly. Changing of the powder particles radius increases the absorptive properties of the powder bed when it has constant thickness.

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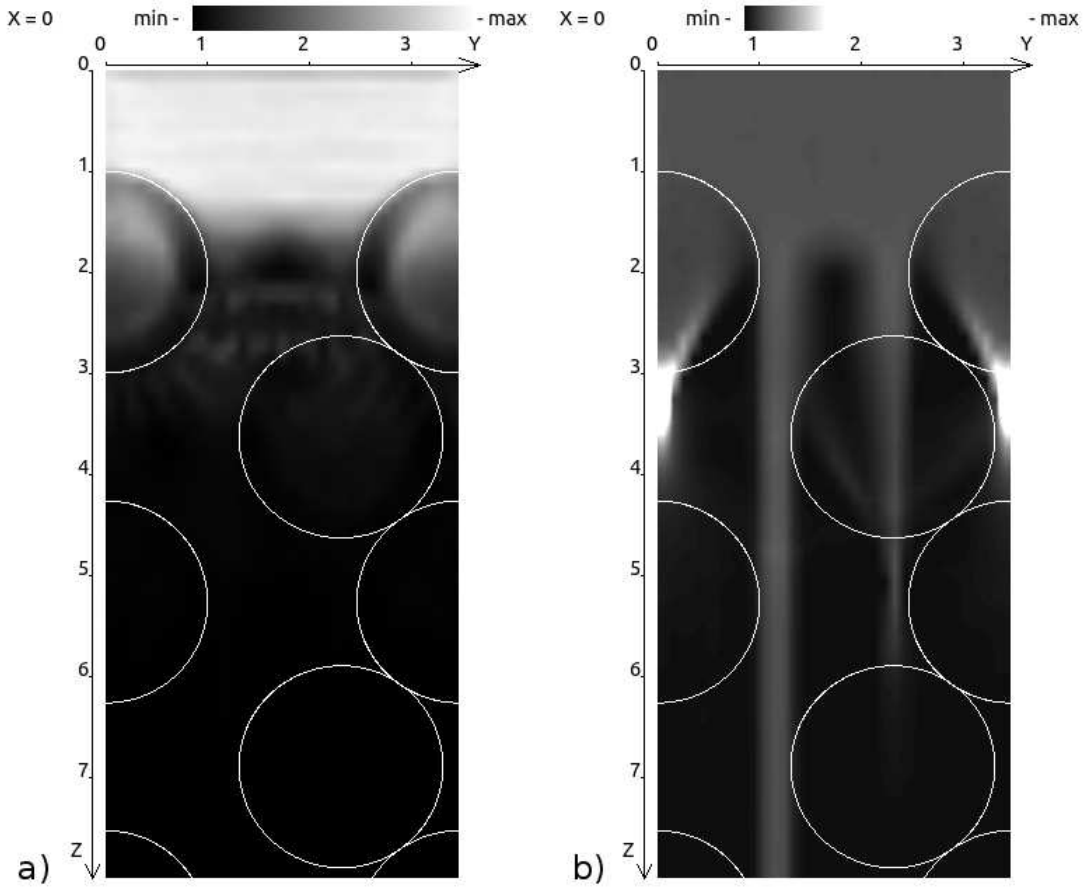

Fig. 1. Distribution of external diffuse (a) and collimated (b) radiation

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TWO-LEVEL MODEL FOR DESCRIBING SUPERPLASTIC DEFORMATION OF METALS[1]

Shveykin A.I., Trusov P.V., Volegov P.S.
Perm National Research Polytechnic University, Perm, Russia

The actual problem of nonlinear solid mechanics is the construction of mathematical models which can describe the evolution of meso- and microstructure of polycrystalline materials in inelastic deformation, including in the superplasticity mode. The modeling of the entry and outcome superplasticity regime of deformation is especially important. The development of the author's two-level model of inelastic deformation of polycrystalline metals [1] based on crystal plasticity with taking into account the characteristic mechanisms of superplastic deformation is proposed. The kinetic equations for describe the grain boundary sliding, diffusion creep, fragmentation and disruption of crystallites are formulated. For superplastic deformation description, which is characterized by local topology losing, and for desribing the input and output from this regime the measure of local topology saving and the measure of grains equiaxing and kinetic relations for this variables based on mesolevel model is included in the structure of the two-level model. Depending on the current state of the microstructure (local topology saving measure, grain morphology and defect structure) and the applied external influences at the current time certain physical mechanisms and inelastic deformation modes is "switched on". The developed model is included in the software package for solving boundary value problems with using multilevel constitutive models (in FEM-package Abaqus). The simulation results obtained for the materials processing, including the characteristics of the evolution of the internal structure, and are in satisfactory agreement with the experimental data.

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FAST SHEARLET TRANSFORM ALGORITHMS

Simonov K.V.*, Kirillova S.B. **, Cadena L. **

* *Institute of Computational Modeling SB RAS, Krasnoyarsk, Russia*

** *Siberian Federal University, Krasnoyarsk, Russia*

In the framework of solving spatial data analysis considered the principles of constructing a fast algorithm of discrete shearlet transform observational data which is based on the implementation of the algorithms are Fast Fourier transform. Following [1, 2] describes the continuous shearlet transform and then through the sampling parameters discrete shearlet transform. Shearlet considered on a cone this approach provides a good separation of the horizontal and vertical directions shearlet in the frequency domain.

Note that the problem of separation an image into morphologically different constituents recently received much attention due to its importance for critical applications. Successful computational techniques for efficient and accurate solution of this problem can be applied to a wide range of areas including the problems of spatial data visualization for diagnosis of complex phenomena.

Relatively recently introduced a system of representation of spatial signals (images) called shearlet system. Shearlet system is generated by the parabolic scaling, shear and translation parallel operators to the initial spatial observations. These are the same wavelet systems with binary scaling and translation functions but also includes profiles of focus, with an extra "The shear" operation (anisotropic scaling). This operation is, in fact, gives a more convenient approach for the analysis of trends. Thus, shearlet is a function that is similar to the wavelet along one axis and bump function on the other axis.

Consequently, shearlet transform requires a combination of the following operators: the operator to scale to create items in different scales; orthogonal operator to change direction, and the operator to translate of these elements in the 2D plane. Most important features of multi-dimensional problems of the studied data are concentrated in the varieties of small dimension. For example, in image processing, the edge is a one-size curve on which the image intensity changes dramatically.

Recently, a new approach shearlet system provided effective tools for the analysis of geometric features of the internal spatial signal using anisotropic and directed window functions. In this approach the orientation is achieved

by using integer powers of matrices shear and these operations preserve the structure of the integer lattice which is crucial for a digital implementation. The algorithm of discrete shearlet transform effectively implemented using fast Fourier transform algorithms. In the Matlab environment based on the considered algorithm the possibility shearlet transform for analysis in particular medical images.

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THEORETICAL SIMULATION APPROACHES AS POWERFUL TOOLS FOR THE COMPREHENSIVE ANALYSIS OF FUNCTIONALIZATION OF GOLD NANOPARTICLES BY LONG ALKYL CHAIN MOLECULAR LIGANDS

Suchkova S.A.*, Soldatov A.V.*, Dr. Eckart Rühl **

* *Department of Physics, Southern Fedaral University, Rostov-on-Don, Russia*

** *Institut für Chemie und Biochemie, Physikalische und Theoretische Chemie, Freie Universität Berlin, Berlin, Germany*

During past decades gold nanoparticles and their arrays are some of the most studied nanomaterials, with promising applications in many fields such as biology, medicine, electronics, optoelectronics and catalysis [1]. Bare gold nanoparticles need to be protected from aggregation. Therefore in order to manipulate the optical, electronic and catalytic properties of the gold core, as well as to control interfacial properties, the gold nanoparticles are generally capped by an organic layer. In our study protection of gold nanoparticles surface and functionalization are performed by amine- and thiol-containing long alkyl chain molecular ligands, accordingly, dodecylamine and mercaptoundecanoic acid. We analyzed the two groups of experimental data. For the free long alkyl chain molecular ligands and bonded to gold nanoparticles were measured N and S K-edge XANES spectra. Differences in the shapes of spectral curves for the free ligands and bonded to gold indicate changes of the local atomic and electronic structure around the absorbing Sulfur and Nitrogen atoms, i.e. chemisorbtion or physisorbtion. This difference needs to be explained by means of theoretical computational approaches to give understanding of functionalization of gold nanoparticles by long alkyl chain molecular ligands. The importance of joint theoretical and experimental analysis to perform a reliable interpretation of the observed properties of functionalized nanoparticles is enhanced by the issue that an extensive comprehension of the electronic structure of functionalized nanoparticles is essential to correctly interpret and exploit the mechanisms that underline their potential device applications. By means of application of theoretical simulation tools to the analysis of experimentally obtained data we determined the changes in local atomic and electronic structure of gold nanoparticles functionalized by the amine- and thiol-containing ligands that take place when ligands bond

to the surface of nanoparticles. In our work to understand and predict physical and chemical structures and reactivity of objects under investigation we use two accurate, parallelized, powerful computational physical and chemistry programs for theoretical simulation, they are ADF [2] and FDMNES [3] code. One of the most powerful methods in physics and chemistry to investigate the electronic structure of atoms, molecules and the condensed phases is Density Functional Theory [2]. This quantum mechanical modelling method allowed us to make analysis of bonding of amine- and thiol-containing ligands to the surface atoms of gold nanoparticles. The strength of chemical bonds formed between surface Au atoms and the nitrogen atoms of amine ligands and sulphur atoms of thiol ligands were studied. Theoretical simulation provides interpretation of the X-ray absorption near-edge structure spectroscopy (XANES) and analysis of the local atomic and electronic structure. XANES is proven to be a very powerful tool to investigate both the geometric and the electronic structure of wide range systems [4]. Theoretical simulation of the N and S K-edge XANES spectra was performed by means of Finite Difference Method Near Edge Spectrocopy (FDMNES code). The simulation of the spectra needs the calculation of the electronic structure around the absorbing atoms. Simulation of XANES spectra is performed using the density functional theory (DFT) with an exchange-correlation potential evaluated with the local electron density. In this approach, the calculation of the final states from the Schrödinger equation is performed in real space in the completely free potential shape. On the first stage of our investigation we construct the approximate model of ligand bonded to nanoparticle. We optimize geometry structure of the model by means of DFT ADF program. After the optimization we perform accurate precision calculation of electronic properties of the models. On the second step we use FDMNES program to simulate N and S K-edge XANES spectra. Then we compare simulated XANES spectra to experimental ones to corroborate consistency of obtained from DFT models of ligand bonding to gold surface. In the issue we receive comprehensive analysis of changes occurring on bonding of long alkyl chain molecular ligands to gold nanoparticles surface.

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LOCAL ATOMIC STRUCTURES OF MATERIALS FOR ELECTRONIC DEVICES: COMPUTER MODELING AND SPECTROSCOPIC DIAGNOSTICS

Sukharina G.B., Abdulvakhidov K.G., Soldatov A.V.
Southern Federal University, Rostov-on-Don, Russia

Computer modeling and spectroscopic diagnostic are very important tools for investigation of unique properties of nanomaterials. These properties depend on fine details of local atomic and electronic structure of materials. The possibility of studying structural parameters using combination of both computer modeling and experimental methods is described here. This complex technique allows to define not only interatomic distances with 0.02 Angstrom accuracy, but also bonding angles. That is 3D local atomic nanoscale geometry is determined. In this work we present the results of recent study of local atomic structure changes in the nanostructured ferroelectric ceramic $PbSc_{0.5}Ta_{0.5}O_3$ during the process of shear deformation. The ferroelectric materials are promising for electronic devices because they are used as active elements in such devices and have unique physical properties that depend on type of defects of local atomic structure. The main problems for preparation of functional ceramics are reproducibility and managing of physical properties. The changes of the concentration and type of structural defects that appear in the process of shear deformation. This is one of the possible ways to manage the physical properties. To study these materials multiscale computer modeling was performed on Linux clusters of Southern Federal University as well as using new Scientific Cloud Computing technology (CC) [1]. Analysis was employed based on experimental and theoretical methods: X-ray Absorption Near Edge Structure (XANES), X-ray diffraction (XRD), Scanning electron microscopy (SEM) [2]. The computer simulation of XANES was performed using both self -consistent full multiple scattering and finite difference methods realized FEFF 9 [3] and FDMENES [4] codes respectively. The computer modeling and experimental methods open possibility to predict and to study the nanoscale atomic structure of ferroelectric materials during the process of shear deformation.

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INCREASING EFFICIENCY OF SYMMETRIC SUCCESSIVE OVER RELAXATION METHOD BASED ON IMPROVED SPECTRAL ESTIMATES[1]

Sukhinov A.I., Shishenya A.V.
Southern Federal University, Rostov-on-Don, Russia

1. Introduction.

In some cases, taking into account the structural features of the matrix of the system of linear equations, it is possible to construct a specialized yet sufficiently efficient method to solve systems of such type [1, 2]. In this work, we consider a number of ways to improve spectral estimates for a preconditioned operator in the symmetric successive over relaxation (SSOR) method for SLAE with self-conjugate positive definite matrixes that rely on its specific properties.

2. Improved estimates of γ_1.

We consider the SSOR method for solving the equation

$$Ax = f, \tag{1}$$

with the self-conjugate positive definite matrix $A = A^* \geq 0$. We represent the matrix A of system (1) as $A = \alpha D + \tilde{A}$, where $\tilde{A} \geq 0$. Suppose $\tilde{A} = R + R^*$, where R is the upper-triangular part of the matrix $\tilde{A}$. We will use prior information from the following inequalities $(\delta - \alpha) D \leq \tilde{A}$, $R^* D^{-1} R \leq \frac{\Delta - \alpha}{4} \tilde{A}$, where we can take minimal and maximal eigenvalues of operator $D^{-1}A$ as δ and Δ respectively. Precoinditioner for SSOR takes form

$$B(\omega) = \left(D + \omega\left(\frac{\alpha}{2}D + R\right)\right)^* D^{-1} \left(D + \omega\left(\frac{\alpha}{2}D + R\right)\right).$$

It could be shown [3] that if $\omega \geq \frac{2}{\sqrt{\alpha\Delta}}$, the estimate for γ_1 takes form

$$\gamma_1 = \left(\frac{1}{\Delta} + \omega + \omega^2 \frac{\Delta}{4}\right)^{-1}. \tag{2}$$

It was shown theoretically [3], that the usage of the improved estimate (2) halves the number of iterations, which is confirmed in the numerical experiments.

3. Modified symmetric successive over relaxation.

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We consider the scheme that approximates the first boundary problem for the elliptic equation in the parallelepiped with the self-conjugate elliptic operator with strongly variable coefficients

$$-\sum_{\alpha=1}^{3}\left(a_{\alpha}^{+1}y_{x_\alpha}\right)_{\overline{x}_\alpha}+q\left(x\right)y\left(x\right)=\phi\left(x\right),x\in G, \tag{3}$$

$$y\left(x\right)=\mu\left(x\right),x\in\Gamma,$$

where $q\left(x\right)\geq 0,\ a_\alpha\left(x\right)>0,\ G=\{0\leq x_\alpha\leq l_\alpha,\alpha=1,2,3\}$ is a computational domain and Γ is it's boundary.

The scheme of the modified SSOR method for (3) takes the form

$$\left(D+\omega R_1\right)D^{-1}\left(D+\omega R_2\right)\frac{y^{n+1}-y^n}{\tau_{n+1}}+Ay^n=f,$$

$$R_1y=\sum_{\alpha=1}^{3}\left(\frac{a_\alpha}{h_\alpha}y_{\overline{x}_\alpha}+\frac{a_{\alpha x_\alpha}}{2h_\alpha}y+\frac{1}{6}qy\right),\ R_2y=-\sum_{\alpha=1}^{3}\left(\frac{a_\alpha^{+1}}{h_\alpha}y_{x_\alpha}+\frac{a_{\alpha x_\alpha}}{2h_\alpha}y-\frac{1}{6}qy\right)$$

In [4, 5] we developed an algorithm for computing optimal parameters ω and matrix of the operator D. We compare the modified SSOR method for the elliptic equation and the variant of the modified SSOR method constructed for the nonstationary heat conduction equation with strongly variable coefficients. In both cases the Chebyshev's acceleration is used. Given the restriction $\tau\leq O\left(\|h\|\right)$ it is shown that estimation of the number of iterations for modified SSOR with Chebyshev's acceleration is $n_0\left(\epsilon\right)=O\left(\frac{1}{\sqrt[4]{\|h\|}}\ln\left(\frac{2}{\epsilon}\right)\right)$, which is confirmed in the numerical experiments.

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COMPACT DIFFERENCE SCHEMES FOR LINEAR PROBLEMS OF MATHEMATICAL PHYSICS

Tsymbalov E., Gordin V.

Higher School of Economics, Hydrometeorological Centre of Russia

Compact difference schemes with high approximation order were developed for the following problems:

- Sturm-Liouville problem for linear 2^{nd} order ODE with 1^{st} or 2^{nd} kind boundary conditions.
- 1D heat and Schrodinger equation with periodic boundary conditions.
- 2D and 3D Poisson and Helmholtz equations with 1^{st} kind boundary conditions.

Some modifications of schemes and methods were considered:

- Two-step scheme for 1D heat equation with periodic boundary conditions.
- Staggered grids for 1D and 2D Poisson equations.
- Two-grid method with compact interpolation for 2D Poisson equation.
- Multigrid method with compact interpolation for 3D Poisson Equation.

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CFD ANALYSIS AND CALCULATIONS OF AERODYNAMIC CHARACTERISTICS OF HELICOPTER ROTOR

Vladimirova N.

Central Aerohydrodynamic Institute (TsAGI), Zhukovsky, Russia

At present in connection with the developments and the design of the new aerodynamic configurations of perspective high-speed helicopters the numerical methods of calculation of rotor characteristics are developed and applied intensively. Vortex models of rotor, based on the nonlinear vortex theory of the rotating blade, successfully used for the rotors under "vortex ring", the axial and oblique flow conditions, have been developed long ago and now are widely used for the calculations. However, vortex methods do not take into account the compressibility effects, viscous and separation phenomena caused by the rotation of the blade and specified for different sections of the rotor blades. Numerical studies of the these flow characteristics are performed using methods of computational fluid dynamics (CFD), based on the grid methods for solving the Navier-Stokes and Reynolds equations (RANS, URANS methods) and modern software systems of CFD analysis, which are intensively developed together with the swift increase of computer, supercomputers and cluster systems speed.

In the actual today problem of investigating the flow around the helicopter airfoils, which form the rotor blade rotating with the frequency of somewhat revolutions per second, the computational methods of unsteady aerodynamics are brought into the foreground. Creation of a databank of stationary and nonstationary aerodynamic characteristics of helicopter airfoils on the basis of developed numerical techniques and results of calculations becomes a basic task. Additional difficulties consist that carrying out test and verification experimental wind tunnel investigations and measurement of nonstationary airfoil characteristics in a free stream with high-frequency periodic change of the parameters, modeling highly periodic reciprocating oscillations of an airfoil in the direction of the incident flow is currently not possible.

In the first part of the work the calculation procedure is proposed and the results of calculations of stationary and nonstationary aerodynamic characteristics of NACA 23012 helicopter airfoil in a wide range of Mach numbers ($M = 0.3 \div 1.0$) are discussed.

In order to simulate special features of nonstationary flow of different sections of rotating helicopter rotor blades problem definition is proposed and

the technology of the calculation of the reciprocating flow around airfoil with a given periodic law of variation on time of the free velocity at the boundary of the computational domain is developed. The flow, with the Mach number variable according to the sinusoidal law from the time, around helicopter airfoil is examined. The calculation of nonstationary flow over two dimensional airfoil in this setting requires a very high quality meshes and enough small integration steps in time ($10^{-5} \div 10^{-4}$ s or less). As a result of numerical studies of nonstationary aerodynamic airfoil characteristics the phenomenon of the formation of hysteresis loop on the flow velocity is revealed.

In the second part of the work there is done a brief overview of recently published in the scientific journals results of three-dimensional flow calculations around helicopter propellers in the well-known commercial ANSYS FLUENT, ANSYS CFX CFD packages and other software systems.

In order to test the computational results obtained and verify them with the available experimental data the author have carried out the comparative calculations of the integral and local characteristics of the two-bladed helicopter rotor in the ANSYS CFX software package and in the new developed Russian LOGOS software package.

There are demonstrated examples and possibilities of newer approaches to the solution of a considered class of problems for the rotary-wing devices characterized by the presence of the revolving moving elements. This category of methods includes a relatively new developing XFlow code (developer is Next Limit Technologies company) based on meshless technology of Lagrange particles to solve Boltzmann's equations together with LES (Large Eddy Simulation) turbulence models within the framework of LBM method (Lattice Boltzmann Method).

TWO-LEVEL MODELS OF POLYCRYSTALS: HARDENING LAWS INFLUENCE ON THE MACRO EFFECTS OF COMPLEX CYCLIC LOADING AND DAMAGE ACCUMULATION[1]

Volegov P.S., Trusov P.V., Yanz A.Y., Shveykin A.I.
Perm National Research Polytechnic University, Perm, Russia

Changes in the physical and mechanical properties of the specimen during deformation in complex cyclic path is a consequence of a substantial restructuring of the micro- and mesostructure of the material, mainly - due to a significant evolution of the dislocation (wider - defective) material structure. Describing such processes is impossible without studying and establishing appropriate mathematical models that explicitly take into account the physical root causes of the microstructure evolution of the material under large deformations and can be applicable to the description of damage accumulation and fracture processes. The foregoing explains the considerable attention in crystal plasticity, which is paid to the modification of hardening laws. The goal is to study the effects produced by polycrystalline material under proportional and non-proportional cyclic loading (and the transition from one to another type of loading) as a consequence of changes occurring at the dislocation structure in the process of loading, and attempt to modify the hardening laws so that they can be transparently physically describe these changes and effects. In particular, there is attempt to justify and describe the known experimental effects, such as the dependence of additional cyclic hardening of the disproportionality of loading, cyclic softening the transition from non-proportional to proportional loading, transverse hardening, which manifests after proportional loading in one direction is followed by proportional loading in the other direction. We received both general and particular form of hardening laws of mono- and polycrystalline allows describing the formation and destruction of dislocation barriers, the annihilation of dislocations as well as additional hardening, resulting from the interaction of intragranular and grain boundary dislocations. Hardening is divided into "non-oriented" and "oriented". The first type describes the hardening regardless of the direction of deformation (under this definition, processes such as the formation of the intersection of dislocations, plaits, braids, dislocation barriers), and a hardening increases the critical shear stress at once on many slip systems (or

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even all at once). The second type is related to the accumulation of elastic energy to "pursed dislocations" (at different barrier) and this energy may be (fully or partially) released at the change the direction of deformation. The analysis of the possible mechanisms of interaction between carriers and the plastic deformation of the crystal lattice defects is executed; hardening laws that discovers a good agreement with experimental data are proposed. We also introduce the parameters characterizing the accumulation of damage and formulate fracture criterion using methodology of multilevel modeling.

ON APPLICATION OF COMPUTER-AIDED APPROACH TO SOLVING NONLINEAR ELASTIC PROBLEMS USING MODELS OF COMPRESSIBLE NONLINEARLY ELASTIC MEDIA

Zherebko A.I.

Southern Federal University, Rostov-on-Don, Russia

Materials that are capable to undergo large deformations and to keep elastic behaviour at the same time have been well-known in medicine and technology long ago. We speak about soft biological tissues and various grades of rubber widely applicable in modern engineering. There are a lot of different models describing the behaviour of such materials. Therefore the problem of choosing the model and its parameters that can adequately describe material behaviour is very relevant.

At the same time standard mechanical experiments: tension, compression, shear, bending, torsion – still remain important when determining material properties. Results obtained in the course of these experiments allow to determine such important characteristics of material as solidity, durability, viscosity, endurance, etc. One of the main requirements for all applied teqhniques in the area is creating so-called «nondestructive» testing teqhniques. It is a wide group of analysis techniques used in science and industry to evaluate the properties of a material without causing damage. Nowadays, the search of such techniques is conducted in modern mechanics. Some of them have already been applied in different areas – for instance, in noninvasive surgery and minimally invasive surgery [1]. However, since soft biological tissues have some particularities, samples that meet all the requirements of the experiment can not be produced. These circumstances lead to necessity of application tools of computer modeling. When solving nonlinear elastic problems the approach based on finite element method (FEM) has become widespread [2]. The approach certainly has a number of advantages: good flexibility of the method when building solution domains, wide range of different software implementing FEM (Ansys, Comsol, FlexPDE, FreeFem++, etc.), the relative simplicity in use. In spite of all advantages it is very difficult to analyze the results obtained with their help. For instance, the problem of choosing material model and its parameters that can describe behavior of the investigated material correctly, often occurs when modeling different mechanical experiments. It also could be necessary to estimate the influence of the shape and various material inhomogeneities (cavities, cracks, etc.). In

order to solve outlined problems the approach based on integration FEM and computer algebra system (CAS) has been performed.

Within the framework of computer algebra system Maple [3] and finite element modeling package FlexPDE [4] the program shell performing computer-aided approach to solving nonlinear elastic problems based on Saint-Venant′s semi-inverse method [5, 6] is presented. Several classes of 2D and 3D elastic problems are considered by applying the performed program shell. By using a number of compressible nonlinearly elastic media models [7] (Blatz & Ko model, Hadamard model, John semilinear model, Murnaghan model, Gent model, Tolokonnikov L.A. model) the problem of uniaxial extension of a rectangle with hard grips is solved. Tensile diagrams for linear and nonlinear cases are presented. Comparison and numerical analysis of the results obtained for mentioned models is given. The following classes of 3D elastic problems are considered: torsion of different height cylinders with inhomogeneity-containing structure, deformation of spherical caps with varying flatness, deformation of a thin plate. Boundary value problem of equilibrium for torsion of a cylinder with opposite moments is formulated. The ability of application the developed program shell to solving some elementary inverse problems is studied for the instance of identification unknown power characteristics. The influence of inhomogeneity on the tensile diagram of a cylinder is analyzed. Probable directions of further work are announced.

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NUMERICAL MODELLING OF THE ADMIXTURE SPREADING IN OPEN CHANNELS

Zhilyaev I.V.[*], **Nadolin K.A.**[**]

[*] *Southern Scientific Center of Russian Academy of Sciences, Rostov-on-Don, Russia*

[**] *Southern Federal University, Rostov-on-Don, Russia*

In this work some further results of numerical research of [1] are presented. Main goal of the study is to test simplified 3D mathematical models for admixture spreading process in shallow sheared flows which come from [2]. These models are geomechanics-oriented, so they can be applied to natural streams, for example, rivers and channels.

A passive admixture that spreading in the open turbulent flow of incompressible viscous fluid in the section of channel or river is studying with following assumptions: curvature of considered part of the stream is weak; the section's length is large with respect to the channel's width and the channel's width, in this section, is large with respect to its depth. The passivity of admixture allows to split the system of equations into two subsystems. The "hydrodynamics subsystem" could be solved independently and allows to calculate fluid velocity and pressure fields. Then the "concentration subsystem" could be solved for calculation of the admixture concentration within the stream with known velocity field.

In [2] a set of mathematical models are derived by the small parameter technique. These models are simple enough for numerical solution. For the verification of these models a number of calculations with finite-element package COMSOL was done.

The values of longitudinal velocity were calculated in the framework of reduced model formulas through numerical solution of the initial-boundary value problem for the free surface displacement function. These values were compared with data of laminar (figure 1) and $k-\varepsilon$ turbulent CFD COMSOL calculations (figure 2).

The computer experiments and calculations for concentration were made on the base of both COMSOL build-in model and elaborated computer program for reduced model. For the last one the coupled algorithm of Galerkin aproach and finite difference method on the base of the characteristic lines mesh was utilized.

The admixture spot spreading along stream is shown at the figures 3 and 4 where the concentration curves are presented. Figure 3 shows the results of

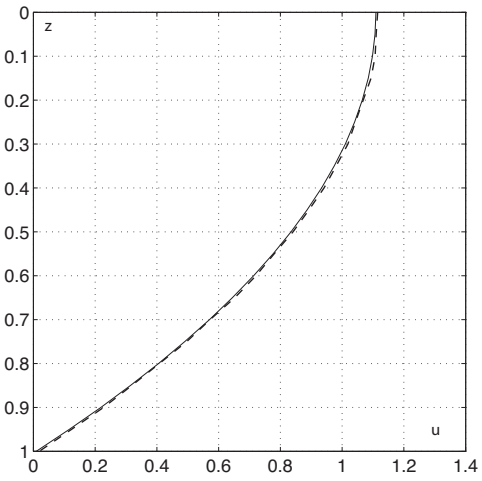

Fig. 1. Laminar flow

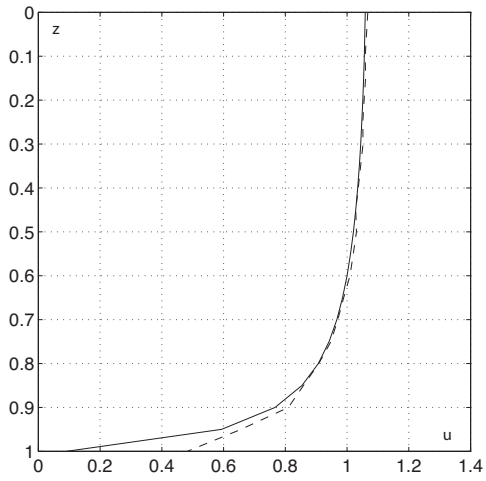

Fig. 2. Turbulent flow

COMSOL calculations and figure 4 — the numerical results for the reduced modelling. Each concentration curve depicts admixture distribution along stream near its' surface at the sequenced time moments.

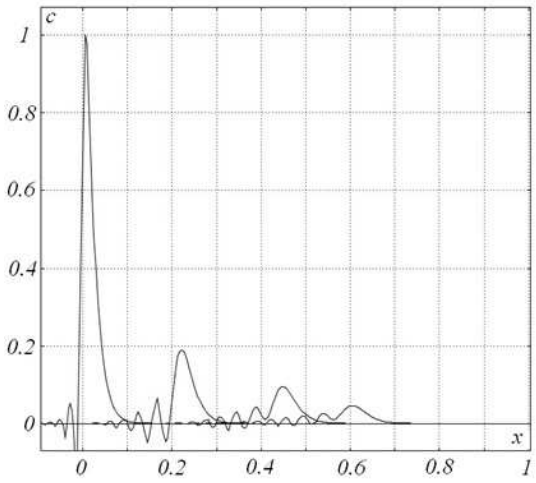

Fig. 3. COMSOL calculations

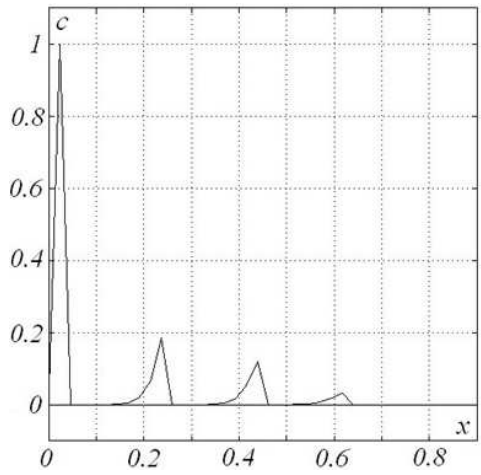

Fig. 4. Reduced model calculations

The obtaining results demonstrate that the hydrodynamics and admixture spreading in the shallow and lengthy bed-stream flow are described adequately by proposed reduced model.

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