NA&A'04: Third International Conference on Numerical Analysis and Applications

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NA&A'04

ABSTRACTS

Third International Conference on

Numerical Analysis and Applications:

NA&A'04

June 29 - July 03, 2004, Rousse, Bulgaria

Organized by

Division of Numerical Analysis and Statistics
University of Rousse "Angel Kanchev"

The main tracks of the conference are:

1. Numerical Linear Algebra.
2. Numerical Methods for Differential Equations.
3. Numerical Modelling.
4. High Performance Scientific Computing.

List of Keynote Speakers who accepted our invitation:

G. Akrivis (Greece), O. Axelsson (The Netherlands), F. Chaitin - Chatelin (France), I. Dimov (Bulgaria), E. G. D'yakonov (Russia), I. Farago (Hungary), B. S. Jovanovic (Serbia-Montenegro), M. Kaschiev (Bulgaria), R. Lazarov (USA), Z. Li (USA), V. Makarov (Ukraine), P. Matus (Belarus), S. Nicaise (France), I. V. Puzynin (Russia), H-G. Roos (Germany), L. Sevastianov (Russia), V. Shidurov (Russia), V. Thomee (Sweeden), E. Tyrtyshnikov (Russia), P. Vabishchevich (Russia)

Organizing Committee:

Chairmen: Lubin Vulkov
I. Angelova, I. Brayanov, J. Kandilarov, S. Karakoleva, M. Koleva, Z. Li, V. Pavlov, N. Strateva , K. Zlateva

Solving Volterra integro-differential and weakly singular Volterra integral equations by Laplace transform

Y. Amirian

We can solve linear Volterra integro-differential equations by using series solution, decomposition and modified decomposition methods and sometimes we can transform linear Volterra integro-differential equation to an integral equation or differential equation and these two mentioned equations can be solved by their methods. Weakly singular second-kind Volterra integral equations also can be solved by using decomposition and modified decomposition methods.
This paper presents an introduction for above methods and extends solving Volterra integro-differential and weakly singular second-kind Volterra integral equations by using Laplace transform.

Superclosure Between the Elliptic Ritz Projector and the Approximate Eigenfunction and Its Application to a Postprocessing of Finite Element Eigenvalue Problems

A. Andreev

An estimate confirming the superclosure between the elliptic Ritz projector and the corresponding eigenvectors, obtained by finite element method, is hereby proved. This result is true for a large class of self-adjoint $2m-$order elliptic operators. An application of this theorem to the superconvergence postprocessing patch-recovery technique for finite element eigenvalue problems is also presented. Finally, the theoretical investigations are supported by numerical experiments.

One-Dimensional Patch-Recovery Finite Element Method for Fourth-Order Elliptic Problems

A. Andreev, T. Dimov, M. Racheva

Interpolated one-dimensional finite elements are constructed, applied to the fourth-order self-adjoint elliptic boundary-value problems. A superconvergence posytprocessing approach, based on the patch-recovery method, is presented. It is proved that the order of convergence depends on the different variational forms related to the variety of the corresponding elliptic operators. Finally, the numerical results related to a problem with practical application are presented.

Modelling of the Deflection Curve for Twist Drill with Straight Shank Fixed in Three-jaw Chuck

A. Andreev, J. Maximov, M. Racheva

The aim of this study is to present a new approach for investigation of an important problem of mechanical engineering. Namely, the model of twist drill embeded in three-jaw chuck is discussed. This problem could be considered as a variant of a beam on the Winckler's foundation which is under the influence of a cross-force.

Our principal aim is to deduce the general mathematical model for this type of constructions. In order to determine the dynamic stresses of the drill using any variational numerical methods we present the corresponding variational formulations. These presentations are characterized by mixed formulation. So, the mixed finite element method is convenient for this kind of problems. The possibility for symmetrization of the weak formulation of the model problem is also discussed.

On the Solvability of the Steady-State Rolling Problem

T. Angelov

In this paper a steady-state rolling problem with nonlinear function, for rigid-plastic, rate sensitive and slightly compressible materials is considered. Its variational formulation is given and existence and uniqueness results,obtained with the help of successive iteration methods are presented. Considering the slight material compressibility as a method of penalisation , it is further shown, that when the compressibility parameter tends to zero the solution of the problem for incompressible materials is approached.

Numerical solution of elliptic interface problems using extrapolation methods

I. Angelova

In this work we develop and test Richardson extrapolation scheme of order higher then 3 for elliptic equations with discontinuous coefficients and singular sources. Supporting numerical experiments are discussed.

Comparison of Two Local Refinement Methods for Large Scale Air Pollution Simulations

A. Antonov

Two methods for Large Scale Air Pollution (LSAP) simulations over static grids with local refinements using the object-oriented version of the Danish Eulerian Model are compared.

The first method is a Galerkin finite element method over a static locally refined grid. We will call this algorithm Static Local Refinements Algorithm (SLRA). We compare SLRA and the Recursive Static-Regridding Algorithm (RSRA), in which regular grids with finer resolution are nested within a coarser mother grid.

RSRA and SLRA are compared how they solve the following air pollution problem: how to utilize more detailed emission and meteorological data over a region of the computation's domain. In this article they are compared on the translational and rotational cone tests, and simulations with real data. The drawbacks and advantages of the methods are discussed.

Relaxation Techniques for Nested Iterations in Finite Element Methods

M. Arioli, D.Loghin

Finite element methods represent an important source of sparse, generally nonlinear and non-symmetric systems of equations. For large problems, the solution is obtained through some nested iteration technique where the aim is to keep the computational load to a minimum through a judicious choice of stopping criteria. Invariably however, the theoretical or empirical convergence criteria use Euclidean norms of the residuals involved. However, finite element discretizations provide their own convergence criteria via matrix norms inherited from the functional setting of the original (weak) formulation. In this work we present an approach to relaxation based on norms induced by the underlying formulation. In particular, we provide approximations of these matrix norms based on the Krylov subspace information generated by methods such as GMRES, together with guidelines for their use inside nested iterations. We illustrate the resulting improvements on applications from fluid flow modeling.

Numerical studies of a singularity formation process in a coupled system of Yang-Mills-dilaton equations

E. Ayrjan, E. Donets, T. Boyadjiev, O. Streltsova

We present a detailed description of mathematical methods, used for numerical studies of a mixed type problem in a coupled system of nonlinear wave equations. These equations arise in the problem of interaction of spherically symmetric $SU(2)$ massless Yang-Mills fields with a dilaton field in $3+1$ Minkowski space-time. For the proposed finite-difference scheme, approximated the original problem, we use the corresponding energy identity which is a discrete analog of the energy conservation law. Based on this scheme, we studied the singularity formation process in the coupled system of Yang-Mills-dilaton evolution equations. The numerical analysis shows that if the initial data exceed some threshold value, then the solutions shrinking to $r = 0$ for finite time T. These solutions have universal asymptotic profile which is a stable self-similar solution of the system of evolution equations.

A Quasi-Monte Carlo method for an Elastic Electron Backscattering Problem

E.Atanassov, M. Durchova

The elastic electron backscattering is a problem that is important for many theoretical and experimental techniques, especially in the determination of the inelastic mean free paths. This effect arrises when a monoenergetic electron beam bombards a solid target and some of the electrons are scattered without energy loss.The description of the flow can be written as an integral equation and may be solved by Monte Carlo methods. In this paper we investigate the possibility of improving the convergence of the Monte Carlo algorithm by using scrambled low-discrepancy sequences. We demonstrate how by taking advantage of the smoothness of the differential elastic-scattering cross-section a significant decrease of the error is achieved.

Numerical Treatment of Fourth Order Singularly Perturbed Boundary Value Problems

B. Attili, Al-Ain

We will consider the numerical of fourth order singularly perturbed two point boundary value problems (BVP). The perturbation parameter which is a small positive parameter appears as the coefficient of the highest derivative. The method starts by transforming the BVP into a system of two second order ordinary differential equations with appropriate boundary conditions. The interval over which the BVP is defined will be subdivided into three disjoint regions. The system will then be solved separately on each subinterval. We combine the obtained solutions to get the solution of the BVP over the entire interval. For the inner regions, the boundary conditions at the end points are obtained through the zero order asymptotic expansion of the solution of the BVP. Examples will be solved to demonstrate the method and its efficiency.

Selection Strategies for Set-Valued Runge-Kutta Methods

Robert Baier

A general framework for proving an order of convergence for set-valued Runge Kutta methods is given in the case of linear differential inclusions, if the attainable set at a given time should be approximated. The set-valued method is interpreted as a (set-valued) quadrature method with disturbed values for the fundamental solution at the nodes of the quadrature method. If the precision of the quadrature method and the order of the disturbances fit together, then an overall order of convergence could be guaranteed. The results are applied to modified Euler method to emphasize the dependence on a suitable selection strategy (one strategy leads to an order breakdown).

SkyRadiance in the Limits of Totality: Numerical Modelling

K. Bakalova, D. Bakalov

Ground-based observations of the corona and of the spectral sky radiance within the totality region during a total solar eclipse are of significant interest because the contribution from direct and single scattered sun light is eliminated. Spectral images of the corona and measurements of the radiance in direction of the local zenith have already been performed in the frame of the Bulgarian National Scientific Programme for investigations during the total solar eclipse of 1999 August 11. In order to interpret the obtained data, numerical models of the propagation of single scattered coronal and of double scattered sun radiation had to be developed.

The early estimates of [1] involved many simplifications: the aerosol scattering was modelled with exponentially decreasing function of the altitude; the range of scattering angles was limited to 90°, etc. The sky brightness in the totality region was assumed to be mainly due to multiple scattered sunlight inside the umbra. The single scattered coronal radiation was neglected. The numerical approach developed in the framework of the National Eclipse Programme used instead a model of the atmosphere based on experimental data on the altitude stratification and spectral dependence of the aerosol phase function, and put no restrictions on the angle of scattering. Still, the evaluation of the zenith spectral sky radiance was based on the approximate model of flat earth-atmosphere system. As a whole, these results do not provide a satisfactory quantitative description of the double scattered sun radiation.

It has been shown recently that single scattered coronal radiation cannot be neglected: at angles beyond 4 solar radii from the axis of totality it dominates the direct flux from the corona [2]. The first numerical estimates show that along the axis of totality the single scattered coronal radiation exceeds the double scattered sun radiation, opposite to what was assumed earlier [3]. The questions therefore arise whether the multiple scattered sun radiation is really responsible for the sky brightness during a total solar eclipse, and whether it is possible to measure separately the double scattered sun radiation inside the umbra.

In the present paper we evaluate the radiance of double scattered sunlight and of single scattered coronal radiation during a total solar eclipse as a function of the direction of observation. We use a refined numerical model of the optical properties of the atmosphere, which is appropriate for our geographic region, and consistently account for the effects of the curvature of Earth. We also review critically the possibilities of measuring separately the double scattered sun radiation inside the umbra. The results can be applied not only to the interpretation of data accumulated in observations of the 1999 solar eclipse, but also - after minor updates in the atmospheric model - to data from any future total solar eclipse.

References

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Numerical Methods for the Landau-Lifshitz-Gilbert Equation

L. Baňas

The evolution of magnetization in a ferromagnetic material is governed by the Landau-Lifshitz-Gilbert (LLG) equation

Here consisting of several contributions, namely, anisotropy, exchange, magnetostriction and magnetic field. The LLG equation is the key equation in magnetic recording applications.

An important conservation property associated with LLG equation is everywhere in the ferromagnet. It is desirable that this property is preserved in the numerical approximations.

We will give a systematic overview of the numerical approaches which are usually used for the LLG equation when the magnetostrictive contribution is neglected. We will discuss numerical properties of the presented schemes such as stability and convergence. A few numerical examples will demonstrate the performance of specific methods.

When magnetostriction is included, the LLG equation has to be coupled with an equation of elastodynamics. We will briefly discuss the extension of existing methods towards this problem. Some recently obtained theoretical results in this field will also be presented.

Comparison Between Numerical Methods Applied to Experimental Data from Satellite B-1300

N.Bankov, M.Kaschiev

The experiments, used to meagure the cold plasma ionosphere parameters, generate mathematical problems, that usually are " ill posed". There are two basic approaches to solve such problems: deterministic, developed by Tickonov, and Hubber's "robust estimation". The results obtained from these two methods are compared with results obtained from modiffied Newton method. In this case we used the nonlinear Least Square Method. The numerical results show that the last method is stable and has a larger region for congevergence than other methods. Some important numerical calculations are given in the paper.

Prestressed Modal Analysis Using Finite Element Package ANSYS

R.Bedri, M.O. Al-Nais

It is customary to perform modal analysis on mechanical systems without due regards to their stress state. This approach is of course well accepted in general but can prove inadequate when dealing with cases like spinning blade turbines or stretched strings, to name but these two examples. It is believed that the stress stiffening can change the response frequencies of a system which impacts both modal and transient dynamic responses of the system. This is explained by the fact that the stress state would influence the values of the stiffness matrix. Some other examples can be inspired directly from our daily life, i.e., nay guitar player or pianist would explain that tuning of his playing instrument is intimately related to the amount of tension put on its cords. It is also expected that the same bridge would have different dynamic responses at night and day in places where daily temperature fluctuations are severe. These issues are unfortunately no sufficiently well addressed in vibration textbooks when not totally ignored. In this contribution, it is intended to investigate the effect of prestress on the vibration behavior of simple structures using finite element package ANSYS. This is achieved by first performing a structural analysis on a loaded structure then make us of the resulting stress field to proceed on a modal analysis.

Uniform Convergence of Monotone Iterative Method for Nonlinear Reaction-Diffusion Problem

I. Boglaev

This paper deals with a discrete monotone iterative method for solving the nonlinear singularly perturbed parabolic problem

$$\mu^2 \left(u_{xx} + u_{yy}\right) - u_t = f(x, y, t, u), \quad (x, y, t) \in Q,$$

$$Q = \Omega \times (0, t_F], \quad \Omega = \{0 < x < 1, 0 < y < 1\}, \quad f_u \geq 0,$$

$$u(x, y, t) = g(x, y, t), \ (x, y, t) \in \partial\Omega \times (0, t_F],$$

$$u(x, y, 0) = u^0(x, y), \ (x, y) \in \overline{\Omega},$$

where μ is a small positive parameter and $\partial\Omega$ is the boundary of Ω. For $\mu \ll 1$, the problem is singularly perturbed and characterized by boundary layers at the boundary $\partial\Omega$.

The monotone method (known as the method of lower and upper solutions) is applied to computing a nonlinear implicit difference scheme obtained after discretisation of the continuous problem. The monotone iterative method solves only linear discrete systems at each iterative step of the iterative process. The initial iteration in the monotone iterative method is either upper or lower solutions, which can be constructed directly from the difference equation without any knowledge of the exact solution, this method eliminates the search for the initial iteration as is often needed in Newton's method. This elimination gives a practical advantage in the computation of numerical solutions.

Uniform convergence of the monotone iterative method based on Shishkin- and Bakhvalov-type meshes is investigated and the rate of convergence is estimated. Numerical experiments are presented.

Semi-Lagrangian Semi-Implicit Time Splitting Two Time Level sScheme for Hydrostatic Atmospheric Model

A. Bourchtein

A semi-Lagrangian semi-implicit two time level scheme is considered for hydrostatic atmospheric model. The algorithm treats in different ways the principal fastest physical components and insignificant slowest modes. The former are discretized in semi-implicit manner with second order of accuracy and the latter are approximated by explicit formulas with the first order of accuracy and using a coarser spatial grid. This approach allows to reduce the computational cost with no loss of overall precision of the integrations. Numerical experiments with actual atmospheric fields showed that the developed scheme supplies rather accurate forecasts using time steps up to one hour and it is more efficient than three time level counterparts.

Modified Stabilizing Corrections Method for Hydrostatic Atmospheric Model

A. Bourchtein

A semi-Lagrangian semi-implicit stabilizing corrections scheme is described for hydrostatic atmospheric model. The standard splitting method is modified to reduce additional splitting truncation errors. The accuracy and stability of algorithm are investigated and analysis of truncation errors as function of time step is done for standard and modified versions. Applied approach allows to use extended time steps with no loss of accuracy and to keep simple design and computational efficiency of splitting algorithms. Numerical experiments with actual atmospheric fields showed that the developed scheme supplies rather accurate forecasts using time steps up to one hour and it is more accurate than standard splitting.

Nested Iterations and Strengthened Cauchy-Bunyakowski-Schwarz Inequalities

J. Brandts

In this presentation, we discuss new strengthened Cauchy-Bunyakowski-Schwarz inequalities in the context of finite element methods for elliptic partial differential equations. These inequalities serve to develop optimal order nested iteration schemes for the corresponding systems of linear equations. Our interest lies primarily in a superconvergent discretization of the Poisson equation in four space dimensions using simplicial linear finite elements and their refinements due to Freudenthal.

Second Order Uniformly Convergent Difference Scheme for Singularly Perturbed Problem of Mixed Parabolic-Elliptic Type

I. Brayanov

One dimensional singularly perturbed problem of mixed type is considered. The computational domain is partitioned into two subdomains. In one of them D^- we have parabolic reaction-diffusion equation and in other D^+ elliptic convection-diffusion equation. Decomposition into regular and singular part is constructed. The problem is discretized using an inverse-monotone finite volume method on Shishkin meshes. We established almost second-order in space pointwise convergence $O(\tau + N^{-2}\ln^2 N)$, that is uniform with respect to the perturbation parameter. Numerical experiments, that support the theoretical results are given..

New Perturbation Bounds for the Continuous-time H_∞-Optimization Problem

N. Christov, M. Konstantinov, P. Petkov,

A complete perturbation analysis of the H_∞-optimization problem for continuous-time linear systems is presented. Both local and nonlocal perturbation bounds are obtained, which are less conservative than the existing perturbation estimates.

Direct Methods on the Feyer Points for Solution Singular Integro- Differential Equations in the Complex Plane

I. Caraus

We have elaborated the numerical scheme of reduction method by Faber-Laurent polynomials for the approximate solution of system of singular integro-differential equations. The equations are defined on the arbitrary smooth closed contour. The theoretical foundation has been obtained in Hölder spaces.

Variational Approach for Restoring Random-Valued Impulse Noise

Ch. Hu, S. Lui

In this work we present a modified iterative method for removing random-valued impulse noise. This method has two-phase schemes. The first phase uses the Adaptive center-weighted median filter to identify those pixels which are likely to be corrupted by noise (noise candidates). In the second phase, these noise candidates are restored using a detail-preserving regularization method which allows edges and noise-free pixels to be preserved. This phase is equivalent to solving an one-dimensional nonlinear equation for each noise candidate. We describe a simple secant-like method to solve these equations. It converges faster than Newton's method to solve and requires less function or derivative evaluations.

On Finite Volume Discretization of Elliptic Interface pProblems with Perfect and Imperfect Contact

T. Chernogorova, R. Ewing, O. Iliev, R. Lazarov

A finite volume discretization of elliptic problems with discontinuous coefficients (interface problems) is presented. This approximation ensures second order truncation error for the fluxes. It uses a minimal stensil (5 points in 2-D and 7 points in 3-D) for the case when each interface is orthogonal to one of the coordinate axes on a grid that, in general, it not required to be aligned with interfaces.

Analysis of Riemann Wave Disintegration Problem for the Testing of the Numerical Methods

M. Chernyshov, P. Denisov, V. Uskov

Practical choice of numerical methods for hyperbolic systems requires the comparison of their results with analytical solutions of test problems. Solved tasks of voluntary discontinuity disintegration (Sod and Lax problems) are traditionally used for this goal in gas dynamics. We propose the test problem of centered Riemann wave disintegration and our parametrical analysis of its solution. It is non-stationary problem of gas compression caused by accelerating piston. All compression disturbances converge at the singular point and cause the resulting shock wave, contact discontinuity and reflected shock or centered rarefaction depending of the compression strength and the ratio of specific heats. Reflected wave is feeble comparing with the resulting shock, and ability to resolve it characterizes the method qualitatively. Numerical methods must also prevent the "smearing" of occurring discontinuities.

Unlike in Lax and Sod problems, mentioned discontinuities grow out of continuous initial data that allows us to analyze their origin. One also can investigate the different types of boundary solutions at mobile piston.

To characterize the numerical results, we worked out exact criteria defining the flow parameters at the every point of centered Riemann wave, speeds of all waves, type of the reflected disturbance, and conditions for reflection of "optimal" shock wave of maximal strength. To make the analysis more accurate for comparison with conservative schemes, we found all integrals $\int U_i(x)dx$ where $U = [\rho, \rho u, e]^T$ is a vector of conservative variables.

As an example, we studied the results achieved by Godunov, Courant-Isaacson-Rees, Roe, and Osher methods of the first, second, and fourth order. It turns out that first-order methods resolve the reflected wave quite unsatisfactory. We had to increase the order to prevent these wrong results.

An Adaptive-Grid Least Squares Finite Element Solution for Flow in Layered Soils

T. Chen, C. Cox, H. Merdun, V. Quisenberry

Groundwater flow in unsaturated soil is governed by Richards equation, a nonlinear convection-diffusion equation which may be written in the form

$$\frac{\partial\theta}{\partial\psi}\frac{\partial\psi}{\partial t}=\frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial\psi}{\partial z}-1\right)\right]$$

where $\theta(\psi)$ is the volumetric moisture content, ψ is the pressure head, and $K(\psi)$ is the hydraulic conductivity.

The process is normally convection-dominated, and steep fronts are common in solution profiles. The problem is further complicated if the medium is heterogeneous, for example when there are two or more different soil layers. In this paper, the least squares finite element method is used to solve for flow through 5 layers with differing hydraulic properties. Solution-dependent coefficients are constructed from smooth fits of experimental data. The least squares finite element approach is developed, along with the method for building an optimized, nonuniform grid. Numerical results are presented for the 1D problem. Generalization to higher dimensions is also discussed.

Conditioning and Error Estimaytes in the Numerical Solution of Discrete Matrix Riccati Equations

P. Petkov, N. Christov, M. Konstantinov

The paper deals with the condition number estimation and computation of residual-based forward error estimates in the numerical solution of the matrix Riccati equations. Efficient, LAPACK-based condition and error estimators are proposed involving the solution of triangular Lyapunov equations along with one-norm computation.

Progressively Refining Discrete Gradient Projection Method for Semilinear Parabolic Optimal Control Problems

I. Chryssoverghi

We consider an optimal control problem defined by semilinear parabolic partial differential equations, with convex pointwise control constraints. Since this problem may have no classical solutions, we also formulate it in relaxed form. The classical problem is then discretized by using a Galerkin finite element method with continuous piecewise linear basis functions in space and a theta-scheme in time, the controls being approximated by blockwise constant classical ones. We then propose a discrete, progressively refining, gradient projection method for solving the classical, or the relaxed, problem. We prove that strong accumulation points (if they exist) of sequences generated by this method satisfy the weak classical optimality conditions for the continuous classical problem, and that relaxed accumulation points (which always exist) satisfy the weak relaxed optimality conditions for the continuous relaxed problem. Finally, numerical examples are given.

Identification of a Nonlinear Damping Function in a Thermoelastic System

G. Dimitriu

In this paper we present an approximation framework and convergence results for the identification of a nonlinear damping function in a thermoelastic system. The approach starts from an abstract operator formulation consisting of a coupled second order hyperbolic equation of elasticity and first order parabolic equation for heat conduction. Well-posedness is established using monotone operator theory and nonlinear evolution systems in Hilbert spaces. A family of parameter identification problems is then defined involving mild solutions. It is assumed that the unknown damping function to be identified can be described by a maximal monotone operator which acts on the generalized velocity. The stiffness of the system is assumed to be linear and symmetric. Some functional techniques are used to demonstrate that solutions to a sequence of finite dimensional (Galerkin) approximating identification problems in some sense approximate a solution to the original infinite dimensional inverse problem. An example and numerical studies are discussed.

Some Generic Properties of Approximation of Control Problems

T. Donchev

In the paper we consider Bolza problem, given for differential inclusion. Using discrete approximations when the right-hand side is locally Lipschitz Morduhovich derived necessary optimal conditions in Euler-Lagrange form. Here we prove that the convergence of the optimal solution of the discrete problem to the optimal solution of the continuous problem is a generic property.

Filippov - Pliss lLemma and Some Applications (a Survey)

T. Donchev, E. Farkhi

The classical lemma of Filippov – Pliss claims that:

Let a Caratheodory multifunction $F : [0,1] \times R^n \to R^n$ with nonempty compact images, and satisfying the Lipschitz condition $D_H(F(t,x), F(t,y)) \leq L|x-y|$, be given. If $y(\cdot)$ is absolutely continuous with $dist(\dot{y}(t), F(t, y(t)) \leq f(t)$ ($f(\cdot)$ is nonnegative and integrable), then there exists a solution $x(\cdot)$ of the differential inclusion

$$\dot{x}(t) \in F(t, x(t)), \quad x(0) = x_0$$

such that for $t \in [0,1]$

$$|x(t) - y(t)| \leq e^{Lt}\Big(|x_0 - y(0)| + \int_0^t f(s)\, ds\Big).$$

We present some extensions and refinements of this lemma and discuss possible applications.

3D Modelling of Diode Laser Active Cavity

N. Elkin, A. Napartovich, A. Sukharev, D. Vysotsky

A menu-driven computer program is developed for numerical simulations of single-mode diode lasers operating well above threshold. Three-dimensional structures of typical single-mode lasers with the goal of efficient fibre coupling are considered. These devices have buried waveguides with high indices of refraction.

A beam propagation method being employed for the wave (Helmholtz) equation leads to the so-called round-trip operator which is non-linear due to gain saturation effects. Thus, the main problem for numerical modelling of lasing is the eigenvalue problem for the round-trip operator. Fox-Li iterative procedure is applied for calculation of a lasing mode.

A large size 3D numerical mesh is employed to discretize a set of equations describing (a) propagation of two waves using Pade approximation, (b) lateral diffusion of carriers within a quantum well, and (c) thermal conductivity. So, many important non-linear effects are properly accounted for: gain saturation, self-focusing, and thermal lens.

A serious problem arising for operation far above threshold is the appearance of additional lasing modes that usually cause degradation in optical beam quality. To calculate the electric current, at which additional modes appear, the software incorporates a subroutine that calculates a set of possible competing modes using gain and index variations produced by the oscillating mode, employing the Arnoldi method for linear eigenproblem.

Results of numerical simulations for typical experimental conditions will be presented.

Preconditioned Methods For The Matrix Exponential

J. van den Eshof, M. Hochbruck

The numerical solution of parabolic equations often involves the numerical approximation of the action of

$$e^{-\tau A}$$

with a vector. The matrix A represents a discretization of an elliptic operator. Often the product is approximated by using a suitable polynomial approximation, for example using the Lanczos method. Unfortunately, the degree of the polynomial to achieve a certain precision increases when the number of spatial grid points is increased.

Inspired by the vast amount of literature on preconditioning of iterative methods, we discuss in this talk different ideas for incorporating some form of preconditioning into the computation of the matrix exponential times a vector. A promising idea is to use a nested iteration where in each step we exploit a preconditioner to solve a suitable subproblem.

Operator Splitting Method with Applications

I. Faragó

In the modelling of complex time-depending physical phenomena the simultaneous effect of several different sub-processes has to be described. The operators describing the sub-processes are as a rule simpler than the whole spatial differential operator. Operator splitting is a widely used procedure in numerical solution of such problems. The point in operator splitting is the replacement of the original model with one in which appropriately chosen groups of the sub-processes, described by the model, take place successively in time. This de-coupling procedure allows us to solve a few simpler problems instead of the whole one.
In the talk several splitting methods will be constructed (sequential splitting, Strang splitting, weighted splitting). Using the semigroup context, the order of the operator splitting method and the convergence of the different splittings will be analyzed for the unbounded operators. We will discuss both the linear and nonlinear cases. We also examine the effect of the choice of the numerical method chosen to the numerical solution of the sub-problems in the splitting procedure.
As an important application, we consider the mathematical model of the transport of air pollutants, effected by the sub-processes of advection, diffusion, deposition, emission and chemical reactions. Numerical results will be presented in order to illustrate the effect of the choice of different splittings and numerical methods.

Ant Colony Optimization for Multiple Knapsack Problem and Model Bias

S. Fidanova

There are many NP-hard combinatorial optimization problems (COPs) for which it is impractical to find an optimal solution. Among them is the Multiple Knapsack Problem (MKP). For such problems the reasonable way is to look for algorithms that quickly produce near-optimal solutions. Ant Colony Optimization (ACO) is a Monte Carlo method with meta-heuristic procedure for quickly and efficiently obtaining high quality solutions to complex optimization problems. The ACO algorithms were inspired by the observation of real ant colonies. An important and interesting aspect of ant colonies is how ants can find the shortest path between food sources and their nest. ACO is the recently developed, population-based approach which has been successfully applied to several NP-hard COPs. One of its main ideas is the indirect communication among the individuals of a colony of agents, called "artificial" ants, based on an analogy with trails of a chemical substance, called pheromones which real ants use for communication. The "artificial" pheromone trails are a kind of distributed numerical information which is modified by the ants to reflect their experience accumulated while solving a particular problem. When constructing a solution, at each step ants compute a set of feasible moves and select the best according to some probabilistic rules. The design of a meta-heuristic is a difficult task and highly dependent on the structure of the optimized problem. In this paper we investigate the influence of model-based search as ACO. We present the effect of two different pheromone models for ACO algorithm to tackle the MKP. The results show the importance of the pheromone model to quality of the solution. The results obtained are encouraging and the ability of the developed models to rapidly generate high-quality solutions for MKP can be seen.

Finite Superelement Method for Elasticity Problems

M. Galanin, E. Savenkov, Yu. Temis

In our work we consider Fedorenko Finite Superelements Method (FSEM) for 3d elasticity problems with sharp nonhomogenities. We consider 3d composite media with a number of fibres. Diameters of fibres are greatly smaller then diameter of the whole body. Elasticity properties of the matrix and fibre are different.

We introduce variational equation which natural Petrov-Galerkin approximation leads to Fedorenko Finite Superelemet Method (FSEM). FSEM is considered as Petrov-Galerkin approximation of the certain problem for traces of boundary-value problem solution at the boundaries of some subdomains (superelements). We use Poincare-Steklov operators to construct variational equation for traces pointed above. Iterative methods of solution of the same problem are well known domain decomposition methods.

Some numerical results are presented.

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Finite Difference Schemes for Porp-Elastic Wave Propagation

F. Gaspar, F. Lisbona, P. Vabishchevich

We consider the fully dynamic poro-elasticity equations. They constitute a coupled mixed system (hyperbolic-parabolic), where the unknowns are displacements $u(x,t)$ and pressure $p(x,t)$:

$$\rho\frac{\partial^2 u}{\partial t^2} - \mu\triangle u - (\lambda+\mu)\mathrm{grad}\ \mathrm{div}\ u + \mathrm{grad}\ p = 0, \quad x \in \Omega$$

$$\frac{\partial}{\partial t}(\gamma p + \mathrm{div}\ u) - \frac{k}{\eta}\triangle p = f(x,t), \quad x \in \Omega, \quad 0 < t \leq T.$$

This system describes the wave propagation in an elastic, porous and permeable solid of density ρ , saturated by a viscous and slightly compressible fluid. Here λ and μ , are the Lame coefficients; $\gamma = n\beta$, with n the porosity and β the compressibility coefficient of fluid; k is the permeability of the porous medium and η the viscosity of the fluid.
For the numerical approximation of this equations, with Dirichlet boundary conditions, we use finite difference schemes. Energy stability estimates for the space semi-discrete and for the fully discrete equations are obtained and convergence results are presented. Some numerical calculations are given to illustrate the theoretical results.

Discretization Methods with Embedded Analytical Solutions for Convection Dominated Transport in Porous Media

J. Geiser

Higher order discretisation methods for convection dominated transport are studied. We present the discretisation of the convection-diffusion-reaction equation based on finite volume methods. The discretisation is derived with mass transfer for the convection-reaction term with embedded analytical solution of the mass. The method is based on the Godunovs-method. The exact solutions are derived for the one dimensional convection-dominant transport case. We use operator-splitting for the convection-reaction-term and diffusion- term and discretise the diffusion term with an implicit standard finite volume method. We present the explicit analytical methods for the convection-reaction term with Laplacian transformation and refer to special cases with equal retardation- and reaction-parameters. The higher order for this discretisation methods are confirmed with benchmark problems based on analytical solutions.

We apply our methods for complex examples in simulations for transported radionuclides in groundwater flow. Finally we discuss the methods and the convergence results compared with standard methods.

Element Preconditioning in MIC(0) Solution of Rotated Bilinear FEM Systems

I. Georgiev, S. Margenov

New results about preconditioning of non-conforming FEM systems in the case of mesh anisotropy are presented. This study is focused on the implementations of rotated bilinear elements, where algorithms $[MP]$ and $[MV]$ stand for the variants of the nodal basis functions corresponding to midpoint and integral mid-value interpolation operators. The considered model elliptic problem is associated with the bilinear form

$$a_h(u,v) = \sum_{e\in\omega_h} \int_e a(e) \sum_{i=1}^{2} u_{x_i} v_{x_i} de,$$

where ω_h is a decomposition of the computational domain Ω into rectangles denoted by e. The standard FEM algorithm leads to the linear system $A\mathbf{u} = \mathbf{f}$, where the symmetric and positive definite (SPD) stiffness matrix A is sparse. Our consideration is addressed to the case of large scale problem. The $MIC(0)$ preconditioned CG method is used for efficient iterative solution of the linear system.

To get a stable $MIC(0)$ factorization in the general case, we first substitute the stiffness matrix A by an auxiliary M-matrix. Element preconditioning techniques are implemented at this step. A local analysis is used to get estimates of the related spectral condition numbers.

This article is specially focused on the construction of optimal auxiliary M-matrix. The problem is formulated in the following general setting: for a given SPD matrix A we want to find SPD M-matrix B such that the condition number of the generalized eigenvalue problem,

$$A\mathbf{u} = \lambda B\mathbf{u}$$

is minimal. A locally optimized construction is presented. The included numerical tests well illustrate the behavior of the analyzed algorithms.

Restarted GMRES with Inexact Matrix–Vector Products

M. van Gijzen, G. Sleijpen, J. van den Eshof

There are many classes of linear problems for which the matrix–vector product must be calculated via an expensive approximation method. An important question is to what accuracy the inexact matrix–vector product must be approximated without compromising the final accuracy of the solution. In recent years this question has been studied for Krylov subspace methods by a number of authors. The general conclusion is that the accuracy to which the matrix–vector product is calculated can be decreased when the iterative process comes closer to the solution. This is usually called a relaxation strategy.

In the talk we will discuss startegies for controlling the accuracy of the matrix-vector products for *restarted* GMRES. Restarted GMRES is closely related to a nested method with Richardson's method as outer iteration, and unrestarted GMRES as inner iteration. It is well known that for *unrestarted* GMRES a relaxation strategy can be used. We will show, however, that at the moment of restart, a suitable strategy depends on the way the residual is calculated. If the residual at the moment of restart is updated via a recursion, a relaxation strategy can be employed. However, if the residual is calculated directly from the right-hand side and the current approximation for the solution, the accuracy of the matrix–vector product must be *increased* when the iterative process comes closer to the solution. Since restarted GMRES can be seen as a nested method, significant further savings can be obtained by lowering the accuracy in the inner loop.

Multiple Scale Procedure in Laplace Transform Space for Solution of Weakly Nonlinear Wave Equation

A. Golbabai

In this paper we formulate a Laplace-transform multiple scale expansion procedure to develop asymptotic solution of weakly non-linear partial differential equation. The method is applied to some general nonlinear wave and diffusion equations.

Order Reduction of Multi-scale Differential Inclusions

G. Grammel

In this paper we consider multi-valued differential equations of the form

$$\begin{aligned} \dot{x} &\in F(x,y,z), \\ \delta\dot{y} &\in G(x,y,z), \\ \delta\epsilon\dot{z} &\in H(x,y,z), \end{aligned}$$

where $\delta, \epsilon > 0$ are small parameters reflecting different time scales. We present conditions under which a re-iterated averaging procedure leads to a reduced order system representing the situation that both perturbation parameters vanish. Approximation rates are given as well.

Computing eigenvalues of the discretized Navier-Stokes model by the generalized Jacobi-Davidson method

G. Hechme, M. Sadkane

In this work the stability analysis of a 3D Navier-Stokes model for incompressible fluid flow is considered. Investigating the stability at a state leads to a special generalized eigenvalue problem whose main part of spectrum is computed by Jacobi-Davidson QZ algorithm.

A Modified Spectral Method for Stiff ODEs

M. Hosseini

It is well known that the eigenfunction of certain singular Sturm-Liouville problems allow the approximation of function in $C^{\infty}[a, b]$

where truncation error approaches zero faster than any negative power of the number of basic functions used in the approximation, as that number (order of truncation N) tends to infinity. This phenomenon is usually reffered to as spectral accuracy. The accuracy of derivatives obtained by direct, term-by-term differentiation of such truncated expansion naturally deteriorates, but for low-order derivatives and sufficiently high-order truncations this deterioration is negligible, compared to the restrictions in accuracy introduced by typical difference approximations.

Here, a modified spectral method is introduced which it is well applied for ODEs with non-analytic or impulse solution. Furthermore, with providing some examples, the aforementioned cases are dealt with numerically.

Adaptive Filters Viewed as Iterative Linear Equation Solvers

J.Husoy

Adaptive filtering is an important subfield of digital signal processing having been actively researched for more than four decades and having important applications such as noise cancellation, system identification, and telecommunications channel equalization. The various adaptive filtering algorithms that have been developed have traditionally been presented without a unifying theoretical framework: Typically, each adaptive filter algorithm is developed from a particular objective function whose iterative minimization gives rise to the various algorithms. This approach obscures the relationships, commonalities and differences, between the numerous adaptive algorithms available today. The objective of the present paper is to provide a novel unifying framework, briefly summarized in the next paragraph, based on stationary methods for the solution of iterative linear equations. It is believed that the new framework, based solely on numerical linear algebra, has the potential to further and unify the theory of adaptive filtering.

The highlights of our contribution can be summarized as follows: First we motivate a data dependent and time varying linear equation system

$$\mathbf{X}(n)\mathbf{W}(n)\mathbf{X}^T(n)\underline{h}(n) = \mathbf{X}(n)\mathbf{W}(n)\underline{d}(n), \tag{1}$$

where $\mathbf{X}(n)$ is a data dependent matrix of dimension $M \times L$, where, – depending on the situation, L may be smaller, equal to, or larger than M. $\mathbf{W}(n)$ is a weighting matrix, $\underline{d}(n)$ is a vector of data termed the desired signal, and $\underline{h}(n)$ is the time varying coefficients of the adaptive filter. By postulating a generic matrix splitting of the coefficient matrix $\mathbf{X}(n)\mathbf{W}(n)\mathbf{X}^T(n)$, we show that *all* classical and some new adaptive filter algorithms can be viewed as simple special cases of one simple iteration for the update of $\underline{h}(n)$. In addition to unifying and simplifying the derivation of adaptive algorithms, and providing a framework for the development new algorithms, we show how our theory facilitates a unified and common analysis of the properties of the various algorithms.

All the above is cast in the language of numerical linear algebra. This may facilitate future contributions to adaptive filtering from researches with other backgrounds than electrical engineering who, to the present time, have dominated the field.

Numerical Modeling of Laser Generation Propagation in the Atmosphere

I. Iliev, Gocheva-Ilieva, S. Georgieva

The application of lasers for treatment of materials incites a great amount of practical and theoretical problems. Due to the coupling of power into the focal spot an optical discharge arises which leads to partial absorption of radiation and low quality of laser beam. In this paper the conditions of appearance of a such optical discharge for the impulsive ruby laser with photon energy $\hbar\omega = 1,78$ eV are investigated. The main object was the determination of basic parameters: energy, wavelength and front increment of the laser impulse in the way that the loss of laser power is small. The presented model is based on the determination of the electron energy in the area of the focal spot as a solution of quasilinear heat conductivity problem with the equation of the form

$$\rho c_p \frac{\partial T}{\partial t} = \triangle(\lambda T) + I\mu$$

where ρ is air density, c_p is specific heat capacity, $\lambda = \lambda(T)$ is heat conductivity coefficient, I is laser radiation intensity and $\mu = \mu(T)$ is air absorption coefficient. For numerical solving of the problem an implicit difference scheme of order of accuracy $O(\tau + h^2)$ in spherical coordinates was applied. The calculations were carried out many times in order to establish the critical values of the electron energy while an optical discharge during the period of one laser impulse arises. Numerical experiments for different values of the laser parameters were explored too. At fixed values of the energy impulse some laser characteristics which guaranteed minimal loss of radiation were found. The obtained results are in good agreement with the experimental data. They can be used for further numerical investigation of the problems concerning the interaction of laser beam with the material and the improvement of the total efficiency of laser generation.

A Smooth Approximation for the Solution of a Special Non-Linear Second-Order Baundary-Value Problems Based on non Polynomial Splines

S. Islam, I. Tirmizi

Numerical Range of Weighted Composition Operators

R. Jabbarzadeh

In this paper we will consider the weighted composition operator $W = uC_\varphi$ between two different $L^p(X, \Sigma, \mu)$ spaces. We characterize the functions u and transformations φ that induce weighted composition operators between L^p-spaces by using some properties of conditional expectation operator, pair (u,φ) and the measure space (X, Σ, μ). Also, numerical rage and Fredholmness of these type operators will be investigated under certain conditions.

Finite Difference Approximation Of An Elliptic Interface Problem With Variable Coefficients

B. Jovanović, L. Vulkov

Interface problems occur in many applications in science and engineering (heat and mass transfer in composite materials, multi–phase flows, chemical reactions theory, colloid chemistry etc.). Mathematically, interface problems usually lead to differential equations whose input data have discontinuities across some interface and the solution or its derivatives satisfy some conjugation conditions on the interface. Many numerical methods designed for problems with smooth solutions do not work efficiently for interface problems.

In the present work we investigate an general elliptic interface problem in rectangular domain, crossed by curvilinear interface. By suitable change of variables problem is transformed into analogous one with rectilinear interface. For the numerical solution of transformed problem a finite difference scheme with averaged right–hand side is proposed. Convergence rate estimate in discrete W_2^1 norm, compatible with the smoothness of data, is obtained.

Immersed Interface Method via Rothe Time Discretizacion for a Diffusion Equation with Local Reactions

J. Kandilarov

A technique combined the Rothe method with the immersed interface method (IIM) of R. Leveque and Z. Li (SIAM J. Numer. Anal., V31,1994) for computation of numerical solution of a diffusion equation with nonlinear localized chemical reaction is developed. The equation is discretized by Rothe's method and elliptic equations with nonlinear singular source occur. The space discretization on each time level is performed by the IIM. The 1D and 2D numerical experiments are presented.

Using Hermite-Type 3-1 Elements for Solving Fredholm Integral Equations of the Second Kind

M. Karami

In this paper, we use the Petrov-Galerkin method for solving Fredholm integral equations of the second kind on [0,1] that the trial space is piecewise Hermite-type cubic polynomials and the test space is piecewise linear polynomials and for showing efficiency of method, we use numerical examples.

High Accuracy Algorithms for Solving the Bound States of Two-dimensional Schroedinger Equation

M. Kaschiev, M. Dimova

The proposed algorithms for solving the bound states of two-dimensional Schroedinger equation are based on the reducing of the given problem to solving the spectral problem for a system of ordinary second-order differential equations. Two reducing methods are used – the Bubnov-Galerkin method and the Kantorovich method. The high-order approximations of the finite element method are applied to the numerical solution of one-dimensional eigenvalue problem. Finite elements of order $p = 1, 2, \ldots, 10$ are implemented. As an example the bound states of the hydrogen atom in a strong magnetic field are calculated with an accuracy, approximately 10^{-8} a.e.

AN ECONOMIC METHOD FOR THE EVALUATION OF THE VOLUME POTENTIAL

Natalia Kolkovska

An approximation to the volume integral with a logarithmic kernel is obtained as a solution to a finite difference scheme. Exact integral representations of the discrete Laplacian are used in order to construct the right-hand side. The error estimates are obtained for functions in some Besov spaces.

Since the right-hand side of the discrete Laplacian equations includes evaluation of some integrals, appropriate quadratures for their calculations are used.

Nonlinear Optimal Control of Power System Via Approximate Solution of Hamilton-Jacobi-Bellman Equation Schroedinger Equation

M. Kharaajoo

In this paper, nonlinear H, control strategy is applied to speed control of permanent magnet synehronous motors. In order to obtain the nonlinear H, control law, some inequalities so-called Hamilton-Jacobi-Isaaes (HJI) should be solved. It is so difficult, if not impossible, to find an exact closed solution of HJI inequalities. However, there are some approximate solutions. One of these possible solutions is the use of Taylor Series expansion that will be used in this paper. Simulation results show better performance for higher order approximation controller that of lower order one in response to load torque variations and mechanical parameter uncertainty.

Higher Order Approximations of Smooth Control Systems

N. Kirov, M. Krastanov

A new approach for numerical approximation of trajectories of a smooth affine control system is proposed under suitable assumptions. This approach is based on expansion of solutions of systems of ordinary differential equations by Volterra series and allows to estimate the distance between the obtained approximation and the true trajectory.

A Property of Farey Tree

L. Kocić, L. Stefanovska

The Farey tree is a binary tree containing all rational numbers from $[0,1]$ in ordered way. It is constructed hierarchically, level by level, using the Farey mediant sum. Some numerical properties of the set of points $(p/q, p+q)$ and associated interpolating functions, where p/q belongs to the k-th level of the Farey tree are investigated.

Numerical Solution of Semilinear Parabolic Problems Using a Two-Grid Method

M. Koleva

A technique combined the Rothe method with two-grid (coarse and fine) algorithm of Xu [J. Xu, 1994] for computation of numerical solution of nonlinear parabolic problem with dynamical boundary conditions is presented. For blow-up solutions we use a decreasing variable step in time, according to the growth of the solution. We give theoretical results, concerning convergence of the numerical solution to the analytical one. Numerical experiments, presented below, demonstrate the accuracy of the algorithm for computation of bounded and unbounded solutions of the model problem.

Sensitivity Analysis of Generalized Lyapunov Equations

M. Konstantinov, P. Petkov, N. Christov

The sensitivity of the generalized matrix Lyapunov equations relative to perturbations in the coefficient matrices is studied. New local and non-local perturbation bounds are obtained.

An Algorithm to Find Values of Minors of Weighing Matrices

C. Kravvaritis, E. Lappas, M. Mitrouli

A $(0,1,-1)$ matrix $W = W(n,k)$ of order n satisfying $WW^T = kI_n$ is called a *weighing matrix of order n and weight k* or simply a *weighing matrix*. We consider the matrix $W(n, n-1)$. This is a matrix of order n, with one zero in each row and column and other entries ± 1, where the inner product of any distinct pair of rows or columns is zero. For the $W(n, n-1)$ since $WW^T = (n-1)I$ we have that $det(W) = (n-1)^{\frac{n}{2}}$. Write $W(j)$ for the absolute value of the determinant of the $j \times j$ principal submatrix in the upper lefthand corner of the matrix W. In the present paper we calculate the maximum minors $W(n)$, $W(n-1)$ and $W(n-2)$. We explore the use of a variation of a clever proof used by combinatorialists to find the determinant of a matrix satisfying $AA^T = (k-\lambda)I + \lambda J$, where I is the $v \times v$ identity matrix, J is the $v \times v$ matrix of ones and k, λ are integers to simplify our proofs. The determinant is $k + (v-1)\lambda(k-\lambda)^{v-1}$.

It is known that W is equivalent under permutation of rows and columns and multiplication of any row or column by -1 to a matrix, U, satisfying $U^T = (-1)^{\frac{n+2}{2}}U$. Using this fact, if we consider the first three rows of W we prove a distribution type lemma for weighing matrices

$W(n, n-1)$ concerning the number of columns starting with $(1,1,1)^T$ or $(-1,-1,-1)^T$, $(1,1,-1)^T$ or $(-1,-1,1)^T$, $(1,-1,1)^T$ or $(-1,1,-1)^T$, and $(1,-1,-1)^T$ or $(-1,1,1)^T$. Using this distribution lemma and the orthogonality properties of the weighing matrices, we develop an algorithm computing the $(n-j) \times (n-j)$ minors of $W(n, n-1)$. This algorithm can be used for the study of the growth problem for weighing matrices.

On an Stable Solution for a Cauchy Problem for Laplace Equation with Inexact Initial Conditions on an Approximately Defined Boundary

E. Laneev, M. Mouratov, E. Zhidkov

The paper considers an inverse problem stated in terms of the model describing stationary temperature distribution in a half-infinite rectangular cross section cylinder containing heat sources. On a surface S bounding the cylinder heat exchange with the surrounding environment obeys Newton's law. If we are given only temperature distribution on the surface - not knowing the sources distribution function - then inside the harmonicity domain we obtain the problem structurally similar to Cauchy problem for Laplace equation. Convergence theorem stating that in case of an approximately defined surface the stable approximate solution converges uniformly to the exact one is proved.

Numerical Methods for Moving Interface Problems and Applications

Z. Li

Moving boundary/interface problems are very challenge both theoretically and numerically. In this talk, I will introduce couple of examples including electrical migration, Stefan problems involving unstable crystal growth, and Hele-Shaw flow to summarize the challenges in the theory and the numerics. Then I will explain the numerical methods which I have employed to solve those problems.

One of the main components of the numerical methods is the immersed interface method used to solve the governing differential equations involving interfaces and discontinuities. Some recent developments including a fast immersed method for solving Poisson problems with large jumps, the weighted least squares interpolations technique, and the ADI method for parabolic equations will be briefly discussed.

Another major component in solving moving interface problems is how to update the interface. In our approach, the level set formulation is used because of the simplicity and robustness for problems involving topological changes and high dimensions. I am going to discuss some issues about how to use the level set method without affecting second order accuracy of the immersed interface method.

Finally, some numerical results and simulations will be presented with some physical explanations.

Computer Realization of the Operator Method for Solving of Differential Equations

B. Liepa, Z. Navickas, R. Marcinkevičius

Using operator computational method, exact descriptions of the phenomenon under investigation are obtained in the form of various operator expressions. So, qualitative object analysis results, obtained by replacing expressions at hand with slightly different structures (most often, with functional series), are available. The use of modern computers facilitates derivation of various digitized realizations of the said operator expressions.

In this case, the sought–for is written in the form of an operator series.

The solution $y(x; s_1, s_2, \ldots, s_{n-1}, v)$ of a differential equation

$y_x^{(n)} = P(x, y, y'_x, y''_x, \ldots, y_x^{(n-1)})$, $y\left(v; s_1, s_2, \ldots, s_{n-1}; v\right) = s_1$; $\left(y\left(x; s_1, s_2, \ldots, s_{n-1}, v\right)\right)'_x |_{x=v} = s_2$, $\left(y\left(x; s_1, s_2, \ldots, s_{n-1}, v\right)\right)''_x |_{x=v} = s_3, \ldots, \left(y\left(x; s_1, s_2, \ldots, s_{n-1}, v\right)\right)_x^{(n-1)} |_{x=v} = s_{n-1}$

can be presented in the form

$y(x; s_1, s_2, \ldots, s_{n-1}, v) = \sum\limits_{k=0}^{+\infty} p_k\left(s_1, s_2, \ldots, s_{n-1}, v\right) \frac{(x-v)^k}{k!}$,

$p_k(s_1, s_2, \ldots, s_{n-1}, v) = \left(D_v + s_2 D_{s_1} + s_3 D_{s_2} + \ldots + s_{n-1} D_{s_{n-2}} + P\left(v, s_1, s_2, \ldots, s_{n-1}\right)\right)^k s_1$, where $P(x, y, y'_x, y''_x, \ldots, y_x^{(n-1)})$ is an arbitrary polynomial or a function and D is a differential operator. When using computers, we restrict ourselves with an operator polynomial.

Taking polynomials of a sufficiently high degree one can find out and analyse various properties of the differential equations (systems) under investigation. In solving a more complicated differential equation (or, a system of differential equations), by means of two independent methods (for instance, numerical and operator), we avoid errors, and higher accuracy is obtained.

In solving ordinary differential equations, we escape problems associated with evaluation of symbolic differential expressions. The calculation time is made acceptable using (for parallelization) a particular computer network. So, the symbolic differentiation as well as graphical information is realized using Maple system, whereas the computer network is explored applying MPI tools.

Nonconvex Numerical Approach to the Seismic Soil-Pipeline Interaction under Instabilizing Effects

A. Liolios, K. Liolios, S. Radev, Y. Angelov

A numerical approach is presented for the unilateral contact problem of the seismic soil-pipeline interaction under second-order instabilizing effects. The problem is considered as an inequality one of structural engineering [1,2]. So, the nonconvex unilateral contact conditions due to tensionless and elastoplastic softening-fracturing behaviour of the soil as well as due to gapping are taken into account. The numerical approach is based on a double discretization, in space by FEM and /or BEM and in time, and on mathematical programming. So the number of the problem unknowns is significantly reduced and a nonconvex linear complementarity problem is solved in each time-step.

Parallel Performance of a 3D Elliptic Solver

I. Lirkov

It was recently shown that block-circulant preconditioners applied to a conjugate gradient method used to solve structured sparse linear systems arising from 2D or 3D elliptic problems have good numerical properties and a potential for high parallel efficiency. The asymptotic estimate for their convergence rate is as for the incomplete factorization methods but the efficiency of the parallel algorithms based on circulant preconditioners are asymptotically optimal. In this paper parallel performance of a circulant block-factorization based preconditioner applied to a 3D model problem is investigated. The aim of this presentation is to analyze the performance and to report on the experimental results obtained on shared and distributed memory parallel architectures. A portable parallel code is developed based on Message Passing Interface (MPI) and OpenMP (Open Multi Processing) standards. The parallel complexity of the algorithms is analyzed. The performed numerical tests on a wide range of parallel computer systems clearly demonstrate the high level of parallel efficiency of the developed parallel code.

Implicit Technique and Order Selection in Generalized Rayleigh Quotient Shift Strategy for QR Algorithm

Y. Liu, Z. Su

QR algorithm for eigenproblems is often applied with single or double shift strategies. To save computation effort, double implicit shift technique is employed. Watkins and Elsner introduced a generalized Rayleigh quotient shift strategy for higher-order shifts. In this paper, we give a generalization of the double implicit shift technique for this higher-order strategy, which includes only the computation of the first column of the shifted matrix. A heuristic criterion is given for selecting the optimal shift order and is verified by numerical experiments.

Accuracy eEstimates of Difference Schemes for Quasi-Linear Elliptic Equations with Variable Coefficients Taking into Account Boundary Effect

V. Makarov, L. Demkiv

While solving the elliptic equations in the canonical domain with the Dirichlet boundary conditions by the grid method, it is obviously, that boundary conditions are satisfied precisely. Therefore it is necessary to expect, that close to the domain boundary the accuracy of the corresponding difference scheme should be higher, than in the middle of the domain. The quantitative estimate of this boundary effect first was announced without proves in 1989 in the Reports of the Bulgarian Academy of sciences by the first author. There accuracy of the difference schemes for two-dimensional elliptic equation with variable coefficients in the divergent form has been investigated.

In this paper 'weight' a priori estimates, taking into account boundary effect, for traditional difference schemes, which approximate, with the second order, first boundary problem for quasi-linear elliptic type equation, which main part has a not divergent form, have been obtained.

The paper ends with numerical experiments, which testify to unimprovement, by the order, of the received 'weight' estimates.

Using Wavelet Petrov - Galerkin Method for Solving Integral Equations of the Second Kind

K. Maleknejad

WIn this paper, We use wavelet Petrov-Galerkin (WPG) method based on discontinuous orthogonal multiwavelets for solving Fredholm integral equations of the second kind that yields linear systems having numerically sparse cofficient matrices and their condition numbers are bounded. At least for showing efficiency of method, we use numerical examples.

Parameter estimation of Si Diffusion in Fe Substrates after Hot Dipping and Diffusion Annealing

B. Malengier

In this paper a general model is developed for the simulation of one dimensional diffusion annealing. Our main interest is determination of the diffusion coefficient from measured values at discrete space-time points within the sample. The method is based on a suitable reduction of the PDE to a system of ODEs by a second order finite difference space discretization. The inverse problem is solved by implementation of the Levenberg-Marquardt method. This allows the estimation of the parameters and the determination of Cramer-Rao lower bounds.

Stochastic Optimization of Tuned Mass Damper to Reduce Seismic Vibration

F. Manju, I. Anam

The applicability and use of passive and active mechanisms to control structural vibration due to dynamic loads like wind load and seismic vibration has been studied for many years. Among the various control devices, the use of the so-called optimized Tuned Mass Damper (TMD) is often considered to be a suitable option. The optimization of the TMD for seismic vibration is based on idealized spectra for the ground acceleration assuming it to be harmonic or White Noise, none of which truly represents the seismic vibration. Therefore the optimized properties of the TMD derived this way may not represent the best option in most practical situations, which depend on specific structural and site conditions. This paper studies numerically the suitability of the so-called optimized TMD in reducing the vibrations of different building structures subjected to real seismic ground motions like the El Centro (USA, 1940) and Kobe (Japan, 1995) earthquakes. The numerical simulations are carried out using probabilistic analysis, i.e., obtaining the expected response spectrum in the frequency domain and comparing with results from the Monte Carlo simulations in the time domain. The agreement obtained between the two results is found to be excellent, which validate the numerical model in the frequency domain. Thus validated, the frequency domain method is used to extend the study to obtain the true optimized TMD properties for the particular site conditions for El Centro and Kobe earthquake and the results are compared with the structural vibrations for the idealized optimizations

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Numerical Design of Optimal Active Control for Seismically-Excited Building Structures

D. Marinova, V. Marinov

Several control techniques have been recently developed as a possible way of reducing the vibrations of civil engineering structures during seismic excitations or strong wind gusts. Based on system control theory active control systems have been promoted requiring external energy for their operation on the building structures. Each structural control system should have appropriate optimal control algorithm suitable to the system's characteristics and its external loads. This paper presents a dynamic model of active control system for seismic-resistant building structures. A linear quadratic optimization problem is formulated. Two optimal performance indexes are considered. The first criterion is an integral index representing the balance between structural response and control energy and leads to control forces proportional to the structural response. The second criterion is a discrete time-dependent performance index in which the optimality is achieved at each instant time and leads to optimal control forces that are proportional to the time step and the structural response. For the later criterion the influence of the time step on the algorithm is investigated. The maximum structural response and maximum active control force versus control design parameter are studied. Numerical examples illustrate the effectiveness of the proposed algorithms in reducing structural response for an active control building under earthquake and wind excitations.

Additive Difference Schemes for Heat Conduction Equation with the Third Kind Boundary Condition

R. Martsynkevich

In the present talk, local one-dimensional (LOD) difference schemes of the second order of approximation and accuracy in space variables for multi-dimensional heat conduction equation with boundary conditions of the third kind are constructed by means of the approximation with respect to the off-designed (nonnodal) point $\overline{x}_i = (x_{i-1} + x_i + x_{i+1})/3$ in the half-integer nodes on the nonuniform grids in the multi-dimensional rectangular domain. The *a priori* estimates of the difference solution in the uniform norm C are obtained by means of the grid maximum principle.

Stability of Finite Difference Schemes for Nonlinear Time-Dependent Problems

P. Matus

In the present talk, a priori estimates of the stability with respect to the initial data of the difference schemes approximating quasi-linear parabolic equations and nonlinear transfer equation have been obtained. The basic point is connected with the necessity of estimating all derivatives entering into the nonlinear part of the difference equations. These estimates have been proved without any assumptions about the properties of solution of the differential equations and depend only on the behavior of the initial and boundary conditions. As distinct from linear problems, the obtained estimates of stability in the general case exist only for the finite instant of time $t \leq t_0$ connected with the fact that the solution of the Riccati equation becomes infinite. For example, for the nonlinear transfer equation this time $t_0 = \|u_0'\|_C^{-1}$ is connected with the behavior of the first derivative of the initial function and in the case of $u_0'(x) < 0$ fully coincides with the moment of the shock wave generation (gradient catastrophe). For the difference scheme approximating the quasi-linear parabolic equation the corresponding time $t_0 = \|u_0''\|_C^{-1}$ is already associated with the behavior of the second derivative of the initial function and coincides with the time of the exact solution destruction (heat localization in the peaking regime). A close relation between the stability and convergence of the difference scheme solution is shown. Thus, not only a priori estimates for stability have been established, but it is also shown that the obtained conditions permit exact determination of the time of destruction of the solution of the initial boundary value problem for the original nonlinear differential equation in partial derivatives. In the present talk, concrete examples confirming the theoretical conclusions are given.

Computing Transitive Closure Problem on Linear Systolic Array

I. Milovanović, E. Milovanović, B. Randjelović

A directed graph G is a doublet $G = (V, E)$, where V is a set of vertices and E is the set of direct edges in the graph. The graph which has the same vertex set V, but has a directed edge from vertex v to vertex w if there is a directed path (of lenght zero or more) from vertex v to vertex w in G, is called the (relexive and) transitive closure of G. A graph $G = (V, E)$ can be represented as an adjacency matrix A, whose elements $a_{ij} = 1$ if there is an edge directed from vertex i to vertex j, or $= j$; otherwise $a_{ij} = 0$. The transitive closure problem is to compute the adjacency matrix A^+ for $G^+ = (V, E^+)$ from A. Transitive closure is a technique for solving combinatorial problems thet are used in wide variety of applications in mathematics, computer science, engineering and business.

Computational tasks can be conceptually classified into two families: compute-bound computations and I/O-bound computations. For example, matrix multiplication represents compute bound computation. On the other hand, adding two matrices is I/O-bound task. A transitive closure problem falls into the category of compute-bound tasks. Speeding-up a compute-bound computations can often be accomplished in a relatively simple and inexpencive manner, that is by the systolic approach, without increasing I/O requirements. Systolic arrays (SA) are high-performance, special purpose architectures typically used to meet specific application requirements or to off-load computations that are especially taxing to general purpose computers.

In this paper we design a linaer systolic array for computing transitive closure for a given graph. The obtained array has optimal number of processing elements (PE) with respect to a problem size and the execution time is minimized for that number of PEs.

A Method Which Finds Maxima and Minima of a Multivariable Function Applying Affine Arithmetic

S. Miyajima, M.Kashiwagi

Fujii et al. proposed the method (Fujii's method) which finds maxima and minima of a multivariable function $y = f(x_1, x_2, \cdots, x_m)$ in the m dimensional region (the box) X applying interval arithmetic (IA). In this method, the maxima and the minima are calculated with guaranteed accuracy by means of dividing X into subregions recursively and bounding the ranges of f in the each subregion applying IA and discarding the subregions which don't possess the possibility of including the point that the maximum (minimum) value occurs.

However, this method possesses the serious problem that the large calculating cost is needed. To overcome this problem, more subregions have to be discarded in initial stage. One of the way which discard more subregions in initial stage is to overcome the overestimaton often observed in IA.

The purpose of this paper is to propose the new method which finds maxima and minima of a multivariable function applying affine arithmetic (AA). AA is a variant of IA and is able to overcome the overestimation. In this method, the ranges of f in the subregions are bounded applying AA instead of standard IA. Moreover, two algorithms are introduced into the new method to discard more subregions in initial stage. Outlines of these algorithms are as follows:

algorithm1

Lower bound (upper bound) of the maximum (minimum) value is pulled up (down) by utilizing the shape of the range boundary of f when AA is applied (in AA, the ranges are bounded in the shape of "linear approximation + error term"). By this operation, more subregions are able to be discarded than the Fujii's method.

algorithm2

The subregions are narrowed by utilizing the shape of the range boundary of f when AA is applied. Namely, the parts of the subregions are able to be discarded while they are not able to be discarded in the Fujii's method.

By applying the new method, the maxima and the minima, which are not able to be found in practical time when the Fujii's method is applied, are able to be found efficiently. And this paper includes some numerical examples to show the efficiency of the new method.

B-Spline Approximation of Set-Valued Functions with General Images

A. Mokhov, N. Dyn

We present in this paper some initial investigations of the approximation of set-valued functions with general compact images in R^n using B-splines. Linear operations on sets are usually understood in Minkowski sense (algebraic sum). If, however, the values of a set-valued function are nonconvex, then the approximating methods may fail. Therefore, in order to obtain an approximant the usual Minkowski average, which is appropriate for set-valued functions with convex images, is replaced by the metric average. We show that this approach can approximate multifunctions with general compact images in R^n in the Hausdorff metric.

Use of Richardson's Extrapolation in the Study by Finite Difference Method of Bending Thin Plates

I. Mura

The 'deferred approach to the limit' method, suggested by Richardson, is extremely useful when there is a reliable estimate of the discretization error as a function of the mesh lenght. It is of dubious value however near curved boundaries, near corners with interior angles exceeding 180 degrees, and near boundaries on which specified function values are not smooth.
Results obtained in the study of bending thin plates by F.D.M. are presented in the work.

The Conservative Finite-Difference Scheme for Solving the Dynamical Problems of the Theory of Elasticity in Two-dimensional Regions with an Arbitrary Shape

V. Patiuc , R. Galina

The numerical method for solving the dynamical problems of the theory of elasticity in two-dimensional regions that have the shape of arbitrary curvilinear quadrangle is proposed. The developed method consists of two main stages. The first stage of the method consists in numerical modeling of the conformal image of the arbitrary quadrangle region in the Cartesian co-ordinates Oxy to the square in co-ordinate system $O\xi\eta$. Towards this end two problems for Laplace's equations with mixed boundary conditions (that include the values of unknown functions and their derivatives) are formulated in $\xi\eta$ co-ordinates. These problems are efficiently solved by finite difference method since the definitional domain of the solution is a square. As the output of such solutions we obtain the discrete harmonic functions $x = x(\xi\eta)$, $y = y(\xi\eta)$ and inverse functions $\xi = \xi(x, y)$, $\eta = \eta(x, y)$ that determine desired conformal image. The obtained relationships allow us to construct the orthogonal difference grid in quadrangle region in Oxy co-ordinates. The second stage of the method consists in formulation of the equations of the theory of elasticity in arbitrary orthogonal co-ordinate system. The equations contain Lame's coefficients $H_k^2 = g_{kk}$, $k = 1, 2$, where the components of the metric tensor g_{kk} are expressed by means of difference derivatives from discrete functions $x = x(\xi\eta)$, $y = y(\xi\eta)$. In order to create the conservative difference scheme we use four types of difference grids: with integer, half-integer and mixed indexes. The application of such grids makes it possible to use central difference derivative that gives rise to getting the finite difference scheme with second order of accuracy. When creating the difference scheme we use the discrete analogue of potential energy, the transformation of which leads to receiving of self-conjugate positively defined difference operator and the approximation of boundary conditions that provides this self-conjugacy. So the difference scheme created in this manner is conservative as the fulfillment of the energy conservation law on the discrete level is an algebraic consequence of the obtained equations. Thus, the explicit three-layered difference scheme was constructed. By means of the a priori estimate method it was obtained the condition of stability of this scheme, that contains the physical and geometrical parameters of the initial problem. The condition of stability and the second order of approximation provide the convergence of the numerical solutions to the exact solutions of the differential problem with the second order of accuracy. The developed numerical method was applied for solving the problem of concentration of stresses in the vicinity of the elliptic hole and in vicinity of circular cylinder situated close to the boundary of half-space.

Fast Algorithm for Solving Fuzzy Relational Equations

K. Peeva, Y. Kyosev

We present two algorithms (conventional and fast) for solving fuzzy relational equations (FRE)

$$R \bullet S = T$$

over $[0,1]$, for one of the unknown relations on the left side, where $R \subseteq X \times Y$ and $S \subseteq Y \times Z$ are fuzzy relations, their composition is the fuzzy relation $R \bullet S \subseteq X \times Z$, and for all pairs $(x,z) \in X \times Z$,

$$(R \bullet S)(x,z) = \max_{y \in Y}(\min(R(x,y), S(y,z))).$$

Traditional linear algebra methods (Gaussian elimination), are not valid when solving FRE – for the operations max and min the inverse elements do not exist. Acknowledging the apparent inevitability of NP-hardness of the problem, we obtain as much improvements over straightforward exhaustive search as possible. We simplify the computation by pruning unnecessary paths in the search process. In this manner we reduce substantially the time complexity by making a more clever choice of the objects over which the search is performed.

The proposed algorithms are realized in MATLAB environment and they find the complete solution set. They may be implemented on the multiprocessor machines, realizing parallel computation of branches. The implementations in knowledge base engineering are given.

On Analytic Iterative Functions For Solving Of Nonlinear Equations

M. Petkov, G. Nedzhibov

An approach for establishing the convergence of iterative methods for solution of nonlinear (real or complex) equations is proposed.

Let we consider the system

$$z_1 = \varphi_1(z), z_2 = \varphi_2(z), \ldots, z_n = \varphi_n(z) \quad or \quad z = \varphi(z)\,,$$

where $z = (z_1, z_2, \ldots, z_n) \in C^n$- the n-dimensional vector space, where $\{z_s\}$ are complex numbers. Let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ be a fixed point of φ, i.e. $\alpha = \varphi(\alpha)$, localized in $C = \{z = (z_1, z_2, \ldots, z_n) : |z_s - \alpha_s| \leq r\,,\ r > 0\}$, $\varphi_s(z)$ are analytic in C and

$$\frac{\partial^k \varphi_s(\alpha)}{\partial z_1^{p_1} \partial z_2^{p_2} \ldots \partial z_n^{p_n}} \neq 0\,, k_1 + k_2 + \ldots + k_n = k \leq p - 1$$

and at least for one combination $(s; p_1, p_2, \ldots, p_n)$ we have

$$\frac{\partial^p \varphi_s(\alpha)}{\partial z_1^{k_1} \partial z_2^{k_2} \ldots \partial z_n^{k_n}} = 0\,, p_1 + p_2 + \ldots + p_n = p > 1\,.$$

Then the following result holds:
If $z_0 \in C$ and sufficiently close to α, then the iteration process $z_{k+1} = \varphi(z_k)\,,\ k = 0, 1, 2, \ldots,$ converges to α for $k \to \infty$ with order of convergence p.

We use this result to give new and simpler proofs for convergence of some known iterative processes. The same is shown for some new iterative processes too.

Numerical Modelling of the One-phase Stefan Problem by Finite Volume Method

N. Popov, S. Tabakova, F. Feuillebois

This paper is concerned with the problem of initially supercooled droplets immediately freezing after impact on solid surfaces. The droplets are assumed to be axisymmetrical with different shapes and are exposed to an ambient gas with constant thermal properties. Their freezing is modelled as a one-phase Stefan problem given in its enthalpy formulation. The droplet geometry is described by non-orthogonal body fitted coordinates, which are numerically generated by an elliptic generation system. The heat transfer equation written in these coordinates is solved using the finite volume method with linear interpolation. Third order (viz. mixed) boundary conditions are enforced between the droplet and the substrate surface on one hand and between the droplet and the ambient gas on the other hand, but with different parameters. The first order boundary conditions (viz. Dirichlet boundary conditions for the temperature) are also considered as a particular case. For first order boundary conditions with the ambient gas, the numerical results for the simple case of a spherical droplet touching a surface are well validated by a former 1D asymptotic analytical solution. In general, the evolution in time of the interface between the frozen part and the remaining liquid has a complicated behavior, for different combinations of the boundary conditions parameters. For all considered droplet shapes, the proposed method of solution is faster than a similar one using the ADI technique of a fully implicit conservative finite-difference scheme in cylindrical coordinates.

Numerically Study of Tooth Shape from Theoretical Exactly Epicycloidal Gears

P. Popovici, C.Cismas

In this paper it is presented the algorithm and calculus programme for to determine the tooth shape of theoretical exactly epicycloidal gears. The tooth shape calculus it is usefully for numerically study of gears, toothing tools and checking.

Numerical Modelling of the Copying and Rolling Gear-Cutters, for External Rotor of the Truninger System Pumps

P. Popovici, C.Cismas

High capacity pumps Truninger system, have parts of high wearing such as external rotors with internal teeth. The production of spare parts needs complicated shape tools. The algorithm and calculus programme conceived by the authors it's useful for the production of these tools.

On the Normwise Backward Error of Large Underdetermined Least Squares Problems

O. Pourquier, M. Sadkane

We propose an algorithm based on the Lanczos bidiagonalization to approximate the normwise backward error of large underdetermined linear system and discuss its theoretical and numerical aspects. Several numerical tests illustrate the theory. The tests show that the ratio of computational cost of a good approximation of the normwise backward error to the exact one is about three percent.

Adaptive Conjugate Smoothing of Discontinuous Fields

M.Ragulskis, V.Kravcenkiene

Conjugate smoothing of discontinuous fields is a problem of a high importance in hybrid numerical - experimental techniques when the results of experimental analysis are mimicked in virtual numerical environment. Typical example is the construction of digital fringe images from finite element analysis results imitating the stress induced effect of photoelasticity.

Conventional finite element analysis is based on interpolation of nodal variables (displacements) inside the domain of each element. Though the field of displacements is continuous in the global domain, the field of stresses is discontinuous at inter-element boundaries due to the operation of differentiation.

Construction of digital fringe images from finite element analysis results is a typical problem when discontinuous fields are to be visualized. Therefore it is important to develop numerical techniques enabling physically based smoothing applicable for visualization procedures.

The proposed strategy of smoothing parameter is based on the assumption that the larger smoothing is required in the zones where the discontinuity of the field is higher.

The finite element norm representing the residual of stress field reconstruction in the domain of the analyzed element is introduced. It can be noted that the calculation of element norms is not a straightforward procedure. First, the nodal stress values in the global domain are sought by the least square method minimizing the differences between the interpolated stress field from the nodal stress values and discontinuous stress field calculated directly from the displacement field. As the minimization is performed over the global domain and the interpolations are performed over the local domains of every element, direct stiffness procedure based on Galiorkin method is developed and applied to the described problem.

When the nodal stress values are calculated, the finite element norms are calculated for each element as the average error of the field reconstruction through the interpolation of those nodal values.

It can be noted that the first step of calculation of the nodal values of stress produces a continuous stress field of stresses over the global domain. Nevertheless that field is hardly applicable for visualization procedures as the derivatives of the field are discontinuous and the plotted fringes are broken. Therefore the augmented residual term is added to the previously described least squares procedure while the magnitudes of the terms for every finite element are proportional to the element norms.

Explicit analysis of the smoothing procedure for the reconstruction of the stress field is presented for a one-dimensional problem.

Digital images of two-dimensional systems simulating the realistic effect of photoelasticity are presented. Those examples prove the importance of the introduced smoothing procedure for practical applications and build the ground for the development of hybrid numerical experimental techniques.

The Finite Differences Scheme for the Euler System of Equations in a Class of Discontinuous Functions

M. Rasulov, T. Karaguler

The Cauchy problem given as below for the Euler system of equations describing the flow of perfect fluid is considered

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\nabla)\vec{u} = \vec{F} - \frac{1}{\rho}\nabla\rho, \tag{2}$$

$$\vec{u}(x,0) = u_0(x). \tag{3}$$

Here, $\vec{u} = (u, v, w)$ is the velocity vector, $\vec{F}$ is the body force on an elementary unit volume dv; p is the surface force (pressure) on a unit surface element ds; ρ is the density; and ∇ is the nabla operator; $u_0(x)$ is given vector function having a compact support and a positive and a negative slopes; $x = (x, y, z)$, and t is a time. For the sake of simplicity assume that $\vec{F} = 0$ and p is known function.

As it is known that if the initial profile has both a negative and a positive slopes, the solution of the problem (1), (2) includes the first type points of discountinuity (shock waves) whose positions are unknown beforehand. Therefore, the problem (1), (2) does not have a classical solution. In order to find the weak solution of the problem (1), (2) the following auxiliary problem

$$\frac{\partial \vec{\nu}(x,t)}{\partial t} + \frac{U^2}{2} + \frac{p}{\rho} = 0, \tag{4}$$

$$\vec{\nu}(x,0) = \vec{\nu}_0(x). \tag{5}$$

(4) is suggested. Here, $\vec{\nu}_0(x)$ are any continuous solutions of the following equations $\frac{\partial \vec{\nu}_0(x)}{\partial t} = \vec{u}_0(x)$, and $U^2 = u^2 + \nu^2 + w^2$. The auxiliary problem (3), (4) has some advantages, and the eq.(3) is called the Cauchy integral of (1).

Theorem. If a vector function $\vec{\nu}(x,t)$ is a smoother solution of the auxiliary problem (3), (4), then the vector functions

$$\vec{u}(x,t) = \frac{\partial \vec{\nu}(x,t)}{\partial x} \tag{6}$$

(5) are the weak solution of the problem (1), (2) in the weak sense.

Definition . The functions defined by

$$\vec{\nu}_{ext}(x,t) = \begin{cases} \vec{\nu}(x,t), & \vec{\nu}(x,t) < E(0), \\ E(0), & \vec{\nu}(x,t) \geq E(0). \end{cases} \tag{7}$$

are called the extended solutions of the problem (3), (4). Here, $E(0)$ is constant. From the theorem , for the weak solutions of the problem (1), (2), we have

$$\vec{u}_{ext}(x,t) = \frac{\partial \vec{\nu}_{ext}(x,t)}{\partial x}.$$

Since, the suggested auxiliary problem does not involve any derivatives of $\vec{u}(x,t)$ with respect to x, and t the numerical solution to the problem (1), (2) can be obtained with no difficulty through the numerical solution to the problem (3), (4).

Robust Attainability of a Closed Set for Nonlinear Control Systems under Uncertain Initial State Information

S. Rigal

In this paper, we investigate the existence of controls which allow to reach a given target through trajectories of a nonlinear control system in the case of a non exactly known initial state. For doing this, we use the key concept of invariant tubes and we give a new compactness property for invariant tubes with values in a prescribed collection of sets. We give some consequences of this property on the minimal time function to reach the target, and we prove a sufficient condition for the attainability of the target by invariant tubes of the considered system. If the attainability property is not satisfied, we characterize a subcollection of initial sets from which the attainability property holds true, and we provide an algorithm to compute it. This approach is illustrated through a basic example.

Semi-Lagrangian Semi-Implicit Time Splitting Two Time Level Scheme for Hydrostatic Atmospheric Model

R. Anchieta

A semi-Lagrangian semi-implicit two time level scheme is considered for hydrostatic atmospheric model. The algorithm treats in different ways the principal fastest physical components and insignificant slowest modes. The former are discretized in semi-implicit manner with second order of accuracy and the latter are approximated by explicit formulas with the first order of accuracy and using a coarser spatial grid. This approach allows to reduce the computational cost with no loss of overall precision of the integrations. Numerical experiments with actual atmospheric fields showed that the developed scheme supplies rather accurate forecasts using time steps up to one hour and it is more efficient than three time level counterparts.

Conservative Monotone Difference Schemes for Elliptic and Parabolic Equations with Mixed Derivatives

I. Rybak

For the development of difference schemes of the higher order of approximation it is important to save properties of both monotonicity and conservativeness because monotone schemes lead to the well-posed systems of algebraic equations, and iterative methods converge significantly better in the case of monotone matrices. Besides, for difference schemes the grid analogues of the conservative laws must be satisfied.

For elliptic and parabolic equations with mixed derivatives monotone and conservative difference schemes were proposed by Samarskii, Mazhukin, Matus and Shishkin, but only for constant-sign coefficients. If coefficients at mixed derivatives change their signs, differential equations were written in nondivergence form with first derivatives and monotone schemes were developed by means of the regularization principle. But in this case property of conservativeness was lost. In theory of difference schemes such situation is typical .

In this presentation for elliptic and parabolic equations with mixed derivatives new monotone and conservative difference schemes of the second order of approximation are proposed. The developed algorithms satisfy the grid maximum principle for both constant-sign and alternating-sign coefficients. For the proposed schemes the *a priori* estimations of stability and convergence in the grid norm C are obtained. Theoretical results are confirmed by the numerical experiments.

On a Cosmological Model Providing Oscillatory Mode of Expansion

B. Saha and T. Boyadjiev

The discovery of the cosmic microwave radiation has stimulated a growing interest in anisotropic, general-relativistic cosmological models of the universe. The choice of anisotropic cosmological models in the system of Einstein field equation enable us to study the early day universe, which had an anisotropic phase that approaches an isotropic one. On the other hand, though Big Bang theory is deep rooted among the scientists dealing with early day cosmology, it is natural to look back if one can model a Universe free from initial singularities. In doing so a nonlinear spinor field was introduced as a source of an anisotropic space-time given by Bianchi type cosmological models [1, 2, 3]. In this report a self-consistent system of spinor, scalar and BI gravitational fields is considered. Einstein field equations in account of the cosmological constant Λ and perfect fluid are studied. Solutions of the corresponding equations are given in terms of the volume scale $\tau(t)$ of the BI metric. It is shown that the problem can be reduced to the following second-order nonlinear multi-parametric equation

$$\ddot{\tau} = \mathcal{F}(\tau, p) \tag{8}$$

Here $\mathcal{F} \equiv 3\kappa \left[mC_0 + \mathcal{D}C_0 + \varepsilon_0(1-\zeta)/\tau^{\zeta}\right]/2 - 3\Lambda\tau$, and $p \equiv \{\kappa, \lambda, m, C_0, C, \varepsilon_0, \zeta, \Lambda\}$ is the set of the parameters. For $F = F(S)$, in account of $S = C_0\tau$ for $\mathcal{D}$ we have $\mathcal{D} = \lambda C^2 F_S/2\tau^2(1+\lambda F(S))^2$. From mechanical point of view the Eqn.(7) can be interpreted as an equation of motion of a single particle with unit mass under the force $\mathcal{F}(\tau, p)$. Then the following first integral exists

$$\dot{\tau} = \sqrt{2[E - \mathcal{U}(\tau, p)]}\,. \tag{9}$$

Here E is the integration constant and $\mathcal{U}(\tau, p)$ is the potential ($\mathcal{U}'_\tau = -\mathcal{F}$) of the force $\mathcal{F}$. We note that the radical expression must be non-negative. The zeroes of this expression, which depend on all the problem parameters p define the boundaries of the possible rates of changes of $\tau(t)$. We analyze Eqn. (8) for different choice of the interaction term as well as for different problem parameters p. It is shown that for a suitable choice of parameters, the Eqn. (7) admits oscillatory solutions which may be regular at any space-time point, thus giving rise to a singularity-free cosmological model.

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Stable Discrete Transform from Grid Values to Fourier Polynomial Coefficients

A. Sevastianov

In a number of applied problems appears a task of reconstructing a function $f \in W_2^l(G)$ as a finite segment of a generalized Fourier series $f \approx \sum f_i \varphi_j$ according to a full orthonormal system of functions $\varphi_j \in L_2(G)$ in case, when about f is known an inaccurate incomplete information on a finite grid $\{s^k\} = S \subset G$ as:

a) a perturbed restriction on a grid S of a function f;

b) a perturbed restriction on a grid S of a linear functional of partial derivatives of a function f.

In case of computer processing of experimental data $\{f(s^k)\}$ one may reconstruct coefficients $\{f_j\}$ of Fourier series in the space $L_2(G)$ with the help of a matrix F_j^k of a "discrete Fourier transform", which is searched by a variational regularization method of Tikhonov A.N. The stable approximate consistent in accuracy level of experimental data calculation of such matrix F_j^k was fulfilled earlier.

For a stable reconstruction of Fourier series coefficients $\{c_j\}$ in the space $W_2^l(G)$ from measured values of a function f on a grid $\{s^k\}$ we used the stabilization functional $||f||^2_{W_2^l(G)}$ which takes a form $\sum c_i c_j \langle \varphi_i, \varphi_j \rangle_{W_2^l(G)}$ according to a basis φ_j. The constructive method of calculation of the matrix $M_{ij} = \langle \varphi_i, \varphi_j \rangle_{W_2^l(G)}$ was presented earlier. For a serial computer processing of $\{f(s^k)\}$ we used the composition of matrices

$$(\delta_{ij} + \alpha M_{ij})^{-1} \circ F_j^k : \{f(s^k)\} \mapsto \{c_j\}$$

The last procedure after a simple modification allows to solve the problem b). The construction of this discrete transformation was made earlier.

We have fulfilled the accuracy consistent calculation of the matrices of the straight "discrete transformation" from the grid values to Fourier coefficients and of the inverse - from Fourier coefficients to the grid values.

Numerical Search for the States with Minimum Dispersion in Quantum Mechanics with Non-Negative Quantum Distribution Function

A. Sevastianov, V. Zorin, A. Belomestny

In quantum mechanics with non-negative quantum distribution function (QDF) the dispersion of physical quantity $A(x)$ is described by the functional

$$\Phi_A[\Psi] = \int (A - \langle A \rangle_F)^2(x) F_\Psi(x) dx,$$

where

$$\langle A \rangle_F = \int A(x) F_\Psi(x) dx,$$

or by the functional

$$\Phi_A[\Psi] = \frac{\langle \Psi | O(A^2) | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \left(\frac{\langle \Psi | O(A) | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right)^2.$$

States of minimal dispersion are described by the problem

$$\Phi_A[\Psi] \rightarrow_{\Psi \neq \vec{0}} \min. \tag{10}$$

The problem (9) while passing on to conventional quantum mechanics (CQM) is transformed into the problem

$$\hat{A}|\Psi^{(0)} = \alpha^{(0)}|\Psi^{(0)}$$

on eigenvectors and eigenvalues. These states in CQM possess minimal (trivial) dispersion.

One of the most important problems in quantum mechanics with non-negative QDF is the problem of optimization of all calculated results with respect to auxiliary functions $\{\varphi_k\}$. In case of the problem (9) it is formulated as

$$\{\Phi_A[\Psi] \rightarrow_{\Psi \neq \vec{0}} \min\} \rightarrow_{\{\varphi_k\}} \min. \tag{11}$$

It was shown earlier that the variational problems in our quantum mechanics are well stipulated in the basis of eigenvectors of corresponding problem in CQM. So one may pass on to coordinate representation of (10):

$$\left\{\left[\Big\{\sum_{j,k} C_j O_{jk}(A^2) C_k\Big\} - \Big\{\sum_{j,k} C_j O_{jk}(A) C_k\Big\}^2\right] \rightarrow_{\sum\limits_j C_j^2 = 1} \min\right\} \rightarrow_{\{\varphi_k\}} \min \tag{12}$$

where the vector $\{C_j\} \in l_2$ defines the expansion $|\Psi = \sum\limits_j C_j \Psi_j^{(0)}$.

It was also shown earlier that it is possible to look for the solution of the problem (11) near solutions of the corresponding problem in CQM, i.e. to look for the solution of (11) in the form $\Psi_k = \sum\limits_j (\delta_{jk} + \delta C_j)\Psi_j^{(0)}$. Then the linearized Euler-Lagrange equation of (11) takes the form

$$\sum_k \Big\{ O_{jk}(A^2) - 2O_{pp}(A)O_{jk}(A) - 2O_{jp}(A)O_{pk}(A) - \lambda_p \delta_{jk} \Big\} \delta C_k = 0$$

with $\delta C_p = 0$.

Numerical Solution of Integro-differential equations system by Block-pulse Functions

M.Shahrezaee

In this paper, we first introduce Block-pulse functions and then we use this functions for solving the Integro-differential equations. In the second step we generalized the method for solving a system of Integro-differential equations. Finally, theoretical analysis and numerical experiment provided to support the method.

Finite Difference Method for Thermal Analysis of Passive Solar System with Massive Wall

S. Shtrakov, A. Stoilov

The concept of passive solar systems is well-known method for using the solar energy, as a source of heating in buildings. Technical, economic, social and environmental analyses determine these systems, as the easiest way for solar energy utilization in buildings. The major impediments to increase market penetration for passive solar systems are the lack of available information and experience data. Experiments with passive solar systems with massive walls are very expensive and there are not enough test installations. Alternatively, mathematical treatment of massive wall systems is a very useful tool for investigation. The objectives of this work are to develop (and validate) a numerical solution model for predication of the thermal behaviour of passive solar systems with massive wall, to improve knowledge of using indirect passive solar systems and assess its energy efficiency according to climatic conditions in Bulgaria. Literature review shows that, the problem of passive solar system with massive wall (Trombe wall) is ordinarily modelled on using thermal and mass transfer equations. Main governing equation for heating processes is transient energy balance equations, which is parabolic partial difference equation. As a boundary conditions for the mathematical problem are used equations, which describe influence of weather data and constructive parameters of building on the thermal performance of the system. The mathematical model, composed for the massive wall performance, is usually very complicated and for solving the mathematical system of equations is needed to apply a different set of assumptions. The presented in this paper simulation scheme comprises three layers: a transparent cover (one or two glasses or plastic plates), massive wall (masonry, concrete) and air gap between transparent cover and massive wall. This scheme is modelled on governing partial difference equation and algebraic system of equations, as a boundary condition. Finite differences method is used to solve this mathematical system. Because of complicated boundary condition, a special improved solution procedure was developed. Computer program for simulation calculations is developed on the base of solution procedure. To verify the applicability of the above-proposed technique, extensive numerical experiments have been carried out. A good correspondence with published experimental data was received. The results of presented mathematical model would help us to increase our experience in passive solar systems. The designers of passive solar systems can use this model to select optimal constructive parameters of the massive wall. We expected, that this model and computer program would allow us to expand the scope of designers calculation methods (SLR - method, U-U - method) for different constructions of passive systems.

The Λ-Error Order In Multivariate Interpolation

D. Simian

The aim of this article is to introduce and study a generalization of error order in multivariate interpolation. Let $\Lambda = \{\lambda_1, \ldots, \lambda_n\}$ be a set of linear functionals, V apolynomial interpolation space with respect to conditions Λ and L_Λ the corresponding interpolation operator. We introduce the λ - remainder: $R_{\Lambda,\lambda}(f) = \lambda[(1 - L_\Lambda)(f)];\ f \in \mathcal{A}_0;\ \lambda \in \Pi'$. We name the λ - order of interpolation the largest k with $R_{\Lambda,\lambda} = 0$ forall polynomial of degree less then k. We derived the general form of λ - order of interpolation and then we studied it for many multivariate interpolation schemes. In the end we established an algorithm to determine λ - order of interpolation.

Computational Aspects in Spaces of Bivariate Polynomial of W-degree n

D. Simian, C. Simian, A. Moiceanu

Multivariate ideal interpolation schemes are deeply connected with H-bases. Any ideal interpolation space with respect to a set of conditions Λ, can be obtained like a space of reduced polynomials modulo a H-basis of the ideal $ker(\Lambda)$. The definition of a H-basis depends of the notion of degree used in the grading decomposition of the polynomial spaces. We studied, in the case of bivariate polynomials, a generalized degree, introduced by T. Sauer and named w-degree. This article give some theoretical results that allow us to construct algorithms for calculus in the space of bivariate polynomials of w-degree n and for reduction process modulo a H-basis. Analysis of this algorithms is done. We realize C++ programs using these algorithms. Taking into account the connection between H-bases and multivariate interpolation we studied also algorithmical and computational aspects of multivariate interpolation in polynomial spaces of w-degree n.

Effective Inner-Iterations in Jacobi-Davidson

G. Sleijpen, A. Stathopoulos

Jacobi-Davidson is an efficient method for computing part of the spectrum of large sparse matrices, either symmetric, or non-symmetric and even complex. The method is attractive since preconditioners can be exploited. It finds approximate solutions in a search subspace. The quality of the approximations is iteratively improved by an expansion of the search subspace (the outer loop). The expansion vectors are obtained from linear equations (the inner loop), so-called, correction equations. Exact solutions of these equations lead to quadratic convergence of the outer loop or cubic in case of symmetric matrices. Usually it is not feasible to compute the solutions exactly or to high accuracy. But, even with approximate solutions, there is often fast convergence. Nevertheless, more accurate solutions of the correction equations often results in faster convergence. More accurate solutions in the inner loop are obtained at higher computational costs and is not clear what strategy minimizes the overall costs for computing eigenvectors.

In this talk we first review the work by Notay and Stathopoulos for symmetric matrices: they provide an effective stopping criterion for the inner loop when certain iterative linear solvers have been used. Then, we discuss how their approach can be extended to more general matrices.

Quantum Macroscopic Coherence in Josephson Junction Networks with Non Conventional Architectures

P. Sodano

We shall focus on the interesting properties emerging in Josephson networks with non-conventional architectures showing, by means of explicit examples, how the networks topology and geometry may either lead to novel and unexpected coherent phenomena or be responsible for taming de- coherence in quantum Josephson devices. We shall also comment on some network s geometries leading to remarkable connections with gauge theories.

Anisotropic Adaptation Applied to Three Dimensional Unstructured Grids

A. Sorokin, N. Vladimirova

The anisotropic grid adaptation technique of thee dimensional unstructured grids is developed. The adaptation procedure identifies three directions of adaptation at each grid node, the refinement of grid edges aligned to these directions and reconnection. The directions of adaptations at the node are defined as a direction of minimal change of monitor function, a direction of maximal change and the direction orthogonal to the previous two. The interpolation based error indicator at an edge utilized in edge refinement is defined as a weighted sum of the first and second order derivatives of monitor function along an edge direction. The reconnection process aligns all edges to direction of minimal change of monitor function, except the ones aligned to the direction of maximal change of this function. The developed adaptation algorithm was applied to convection-diffusion problems. The solutions of these problems simulate three-dimensional curved viscous wakes with large gradients of Mach number. The explored dependencies of numerical errors on the number of grid nodes showed good correlations with theoretical predictions. The industrial application to the Euler transonic flow over a wing with wing tips is considered. In this problem the body geometry and initial isotropic grid was constructed with CAD system. The grid adaptation successfully resolved regions with large gradients of numerical solution at the shocks and leading edges.

Applications of Price Functions and Haar Type Functions to the Numerical Integration

S. Stoilova

By analogy with the theory of good lattice points for the numerical integration of rapidly convergent Walsh series, in the present paper the author use the Price functional system and Haar type functional system, defined in the generalized number system, for numerical integration. We consider two classes of functions, whose Fourier-Price and Fourier-Haar coefficients satisfy specific conditions. For this classes we obtain the exact orders of the error of the quadrature formula with good lattice points, constructed in the generalized number system.

Numerical Modelling of the Free Film Dynamics and Heat Transfer under the van der Waals Forces Action

S. Tabakova, G. Gromyko, L. Popova

In the present work a numerical model of the heat transfer of a hot free thin viscous film attached on a rectangular colder frame surrounded by an ambient gas is proposed. The film is assumed to be under the action of the capillary forces and attractive intermolecular van der Waals forces and to be symmetric to a middle plane. The heat transfer is due to conduction and radiation with the ambient gas and forced convection caused by the film dynamics. Since the film thickness is very small compared to the frame length, their ratio is expressed as a small parameter ε. The leading order terms of the asymptotic expansion in ε of the mass, momentum and energy balance equations are given with the appropriate boundary and initial conditions. Their one-dimensional form is solved numerically by a conservative finite difference scheme on staggered grid. The numerical results for the film shape, longitudinal velocity and temperature are obtained as depending on time for a large range of the process parameters: Reynolds numbers, dimensionless Hamaker constants and radiation numbers.

A High Order Parallel Method for Time Discretization of Parabolic Type Equations Based on Laplace Transformation and Quadrature.

V. Thomee

We consider the discretization in time of a parabolic equation, using a representation of the solution as an integral along a smooth curve in the complex left half plane. The integral is then evaluated to high accuracy by a quadrature rule. This reduces the problem to a finite set of elliptic equations, which may be solved in parallel. The procedure is combined with finite element discretization in the spatial variables. The method is also applied to some parabolic type evolution equations with memory.

Two-Stacked Josephson Junctions with Minimal Length

M. Todorov, T Boyadjiev

In the present work two-stacked homogeneous Josephson junctions are investigated numerically. Bound states of types “fluxon-fluxon” and “fluxon-antifluxon” are obtained. The affect of the interaction between stacks in the junctions, the boundary magnetic field, and the bias current upon minimal length is studied. The governing equations as a nonlinear eigenvalue problem with respect to the junction length are considered and by Continuous Analog of Newton Meth

Convergence Analysis for Eigenvalue Approximations on Triangular Finite Element Meshes

T. Todorov

The paper is devoted to the eigenvalue problem for second order strongly elliptic operator. The problem is considered on curved domains, which require interpolated boundary conditions in approximating finite element formulation. The necessary triangulations for solving the eigenvalue problem consists of isoparametric elements of degree n, where n is any integer greater than two.

An approximating numerical quadrature eigenvalue problem is the object of investigation in this paper. The considered convergence analysis is a crucial point for estimating of the error in approximating eigenvalues. An isoparametric approach is the basic tool for proving the convergence.

A definition and a Criterion for Pseudo Asymptotes and some Remarks on the Graphycs of the Curves with Psewdo Asymptotes and Asymptotes

A. Tomova

In this paper we describe a definition for pseudo asymptotes of differentiable functions and restrict the attention over the behaviors of some functions with pseudo asymptotes. We prove a criterion for existence of pseudo asymptotes and asymptotes for differentiable functions. Using the system for computer algebra MATHEMATICA 4.0 we obtain a set of elementary functions and an other set of special functions with pseudo asymptotes. We draw the graphics of such functions and make some conclusions.

Two Resultant Based Methods Computing the Greatest Common Divisor of Polynomials

D. Triantafyllou, M. Mitrouli

The computation of the Greatest Common Divisor (GCD) of two or more polynomials is one of the most frequent problems in several fields such as numerical analysis, linear and numerical linear algebra, control theory, matrix theory, statistics etc. Many numerical algorithms have been created to solve this problem.

In this paper we develop two resultant based methods for the computation of the GCD of two polynomials. Let a(s),b(s)$\epsilon R[s]$ be two polynomials, where a(s) is a monic polynomial of degree m, and b(s) a polynomial of degree n, with n ≤m. Let S be the resultant Sylvester's matrix of the two polynomials. If we apply Gaussian Elimination with partial pivoting or QR factorization to the previous matrix, the last non-zero row defines the coefficients of the GCD. If we modify matrix S to S^*, such that the rows with non-zero elements under the main diagonal, at every column, are gathered together, because of this special form of S^*, we do not need to zero all the elements under the diagonal and we do not have to update the whole (m+n-k+1)x(m+n-k+1) submatrix at every stage. We constructed modified versions of the LU and QR procedures which require only the $\frac{1}{3}$ of floating point operations than the operations performed in the general LU and QR algorithms. More precisely for a $2n \times 2n$ matrix the LU and QR procedures require $O\,(\frac{8}{3}n^3)$ and $O\,(\frac{16}{3}n^3)$ flops respectively whereas the modified LU and QR require only $O\,(\frac{5}{6}n^3)$ and $O\,(\frac{5}{3}n^3)$ flops respectively.

In practice the required flops are much less than the previous bounds. Finally, we give a bound for the error matrix which arises if we perform Gaussian elimination with partial pivoting to S^*. Both methods are tested for several sets of polynomials and tables summarizing all the achieved results are given.

Conservative Difference Scheme for Summary Frequency Generation of Femtosecond Pulse

V. Trofimov, A. Borhanifar, A. Volkov

As it is known, three-wave interaction of femtosecond pulses in optical fiber with quadratic nonlinear response is described by the following set of equations

$$\frac{\partial A_j}{\partial x}+\frac{1}{\nu_j}\frac{\partial A_j}{\partial t}+iD_j\frac{\partial^2 A_j}{\partial t^2}+F_j=0, \quad j=1,2,3, \qquad F_1=\gamma_1(iA_3A_2^*+\frac{1}{\bar\omega_1}\frac{\partial}{\partial t}(A_3A_2^*))e^{i\Delta x}, \tag{13}$$

$$F_2=\gamma_2(iA_3A_1^*+\frac{1}{\bar\omega_2}\frac{\partial}{\partial t}(A_3A_1^*))e^{i\Delta x}, \quad F_3=\gamma_3(iA_1A_2^+\frac{1}{\bar\omega_3}\frac{\partial}{\partial t}(A_1A_2))e^{-i\Delta x}.$$

To solve (12) let us introduce a new function E_j in the following manner

$$\frac{\partial E_j}{\partial t}+i\bar\omega_j E_j=A_j, \qquad j=1,2,3.$$

In this case, the set of equations (12) transforms to

$$\frac{\partial E_j}{\partial x}+\frac{1}{\nu_j}\frac{\partial E_j}{\partial t}+iD_j\frac{\partial^2 E_j}{\partial t^2}+\overline{F}_j=0, \quad \bar F_1=\frac{\gamma_1}{\bar\omega_1}(A_3A_2^*)e^{i\Delta x},$$
$$\bar F_2=\frac{\gamma_2}{\bar\omega_2}(A_3A_1^*)e^{i\Delta x}, \quad \bar F_3=\frac{\gamma_3}{\bar\omega_3}(A_1A_2)e^{-i\Delta x}.$$

Using the approach developing in our previous papers, we created the conservative difference scheme for the above set of equations with the second order of approximation $\Psi=O(h^2+\tau^2)$.

$$\frac{E_j(x+h,t)-E_j(x,t)}{h}+\frac{1}{4\tau\nu_j}\left[E_j(x,t+\tau)-E_j(x,t-\tau)+E_j(x+h,t+\tau)-E_j(x+h,t-\tau)\right]+$$

$$+i\frac{D_j}{2\tau^2}\left[E_j(x,t+\tau)-2E_j(x,t)+E_j(x,t-\tau)+E_j(x+h,t+\tau)-2E_j(x+h,t+\tau)+E_j(x+h,t-\tau)\right]+$$

$$+\frac{\gamma_j}{2\omega_j}\hat F_j=0,$$

$$\hat F_j=\frac{1}{4}\begin{cases}[(A_3(x+h,t)+A_3(x,t))(A_2^*(x+h,t)+A_2^*(x,t))]\,(e^{i\Delta(x+h)}+e^{i\Delta x}), & j=1,\\ [(A_3(x+h,t)+A_3(x,t))(A_1^*(x+h,t)+A_1^*(x,t))]\,(e^{i\Delta(x+h)}+e^{i\Delta x}), & j=2,\\ [(A_1(x+h,t)+A_1(x,t))(A_2(x+h,t)+A_2(x,t))]\,(e^{-i\Delta(x+h)}+e^{-i\Delta x}), & j=3,\end{cases}$$

$$A_j(x+h,t)=(E_j(x+h,t+\tau)-E_j(x+h,t-\tau))/(2\tau)+i\omega_jE_j(x+h,t), \qquad j=1,2,3.$$

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Comparison of some Difference Schemes for the Problem of Femtosecond Pulse Interaction with Semiconductor at Nonlinear Mobility Coefficient

V. Trofimov, Maria M. Loginova

The femtosecond pulse interaction with the semiconductor under certain conditions is described by the following set of dimensionless differential equations

$$\begin{aligned}
&\frac{\partial^2\varphi}{\partial x^2} = \gamma(n-N), \quad \frac{\partial N}{\partial t} = q_0 q(x)\delta(N,\varphi) - \frac{nN-n_0^2}{\tau_p},\\
&\frac{\partial n}{\partial t} = D\frac{\partial}{\partial x}\Big(\frac{\partial n}{\partial x} - \mu(x,t)n\frac{\partial\varphi}{\partial x}\Big) + q_0 q(x)\delta(N,\varphi)) - \frac{nN-n_0^2}{\tau_p}, \quad 0<x<L_x, \quad t>0,\\
&\frac{\partial\varphi}{\partial x}\Big|_{x=0,L_x} = \frac{\partial n}{\partial x}\Big|_{x=0,L_x} = 0, \qquad n|_{t=0} = N|_{t=0} = n_0
\end{aligned} \tag{14}$$

with following absorption and mobility coefficients

$$\delta(N,\varphi) = (1-N)\left\{e^{\beta|\varphi|},\, e^{\beta|E|},\, \cosh\beta\varphi,\, \cosh\beta E\right\}, \quad E = -\frac{\partial\varphi}{\partial x}, \quad \mu(x,t) = \mu_0/(1+|E|/E_{cr}).$$

In this report we deal with comparison of various difference schemes for the system (13). The evolution of semiconductor characteristics substantially depends on parameters values involving in the system (13) and on the nonlinear absorption coefficient. Particularly, there is a possibility of the forming of switching waves and as well development of oscillating regimes, which take place due to the system instability.

For the problem solution one can use the difference scheme proposed in [1]. But using the transformation $n(x,t) = \overline{n}(x,t)e^{\mu_0 F}$ it is easily to construct monotonous difference scheme regard to $\bar{n}$ [2]. After this transformation the initial system (13) can be reduced to the following form:

$$\frac{\partial E}{\partial t} = -\gamma D e^{\mu_0 F}\frac{\partial\overline{n}}{\partial x}, \quad \frac{\partial\varphi}{\partial x} = -E, \quad \frac{\partial N}{\partial t} = G - R \quad n = \frac{1}{\gamma}\frac{\partial^2\varphi}{\partial x^2} + N, \quad \frac{\partial F}{\partial x} = -\frac{E}{1+|E|/E_{cr}}, \tag{15}$$

$$0<x<L_x, \qquad t>0.$$

For problem (14) the difference scheme is created.

It should be stressed, that for some parameters values the iterative process in scheme proposed in [1] loses its convergence. Step decreasing does not change this situation substantially. But for the scheme, constructed on the base of system (14), there is no such problem.

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Soliton-like Regime of Femtosecond Laser Pulse Propagation in Bulk Media under the Conditions of SHG

V. Trofimov, T. Lysak

The report is devoted to the numerical investigation of soliton-like propagation of two interacting femtosecond pulses with high intensity in the bulk media. One of them is basic wave. The frequency of second pulse corresponds to doubling frequency of first wave. We discuss regime of pulses propagation for which the constant values of their intensities in the central part take place. However, the intensities can change essentially at the back and the front of pulses.

Similar propagation regime appears at the SHG under the condition of simultaneous action of quadratic and cubic nonlinearities. For this purpose, the phase mismatch has to be between interacting waves. Other condition concludes in special choosing of nonzero input amplitudes with certain phase difference between them. It should be stressed that the preceding condition, referring to phase shift between two pulses, cannot take into account for laser pulse propagation in layered media. For example, it is necessary to introduce in the special section of the media a certain phase shift between interacting waves.

To solve the problem, which is described of two NSE in two spatial coordinates and time with quadratic and cubic nonlinearities, we use conservation laws. In the long-time approximation for flat beam profile, the analytical solution of SHG problem is constructed. Using it, parameters of soliton-like propagation regime is calculated. Then, these parameters are used for numerical simulation, which is made on the base of conservative difference scheme, taking into account the conservation laws of the problem. For simplicity, we have assumed the radial symmetry of the media and input beames. Previous analytical investigation was proofed and soliton-like regime takes place.

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Computational Method for Finding Soliton Solutions of the Nonlinear Shrödinger equation

V. Trofimov , S. Varentsova

The propagation of the femtosecond laser pulse in an optical fiber in media with a cubic nonlinearity can be described by the dimensionless Shrödinger equation

$$\frac{\partial A}{\partial z} + i\frac{\partial^2 A}{\partial x^2} + i\alpha|A|^2 A = 0, \qquad z > 0, \qquad 0 < x < L \tag{16}$$

with the following initial and boundary conditions

$$A|_{z=0} = A_0(x), \qquad A|_{x=0,L} = 0,$$

where $A(x,z)$ is the complex amplitude of the pulse, normalized to its maximum value, x is the transverse coordinate measured in units of the initial beam radius, z is the longitudinal coordinate along which the laser beam propagates, α is the coefficient equal to the ratio of the input power of an optical beam to the characteristic power of the self-action, L is a size along the transverse coordinate. The self-action of the beam takes place, if $\alpha > 0$. For the opposite case $\alpha < 0$ the optical beam is defocusing.

The soliton solutions of equation (15) are given by

$$A(x,z) = \psi(x)e^{-i\lambda z}$$

with real functions $\psi(x)$ and real eigenvalues λ. For this case the equation (15) reduces to the form

$$\frac{d^2\psi(x)}{dx^2} + \alpha\psi^3(x) = \lambda\psi(x), \qquad 0 < x < L, \tag{17}$$
$$\psi(0) = \psi(L) = 0.$$

We propose a computational method for solving the nonlinear eigenvalue problem (16). It allows to find eigenvalues λ_k and eigenfunctions $\psi_k(x)$ with numbers $k \gg 1$ for any value of α with a special choice of the initial approximation to the solution of equation (16).

Computer experiments show that for the limited on x interval it is necessary to decrease the value of L in order to separate the eigenvalues when $|\alpha|$ increases in contrast to the case of the unlimited region $0 < x < \infty$ or $-\infty < x < \infty$. The possible way in computer simulation of the eigenvalue separation for big $|\alpha|$ consists on consecutive calculations with condensing meshes. At first we use the rough mesh. In this case we can define the first k eigenfunctions $\psi_k(x)$. Then it is necessary to decrease a mesh step and the next k' eigenfunctions can be found. If necessary, this procedure can be repeated once more.

This paper was supported partly by RFBR (grant N 02-01-727).

Numerical Method of a Solution of a Nonlinear Problem about the Static Instability of a Plate in a Supersonic Gas Flow

P. Vel'misov, S. Kireev

The static problem about deflection forms of a plate - band in a supersonic gas flow, described by the nonlinear differential equation

$$Dw'''' + Nw'' + \alpha w' + f(w) - \theta w'' \int_0^\ell w'^2 dx = 0, \quad \alpha = \frac{\alpha_0 \rho_0 V^2}{\sqrt{M^2 - 1}}, \quad M = \frac{V}{a} \tag{18}$$

with boundary conditions at $x = 0$, $x = \ell$

$$c_0 w''(x) = \sum_{k=1}^{n} c_k w'(x)^{2k-1}, \quad d_0 w'''(x) = \sum_{k=1}^{m} d_k w(x)^{2k-1}, \quad f(w) = \sum_{k=0}^{\infty} a_{2k+1} w(x)^{2k+1} \tag{19}$$

is considered. Here D is the deflection stiffness of the plate; V, ρ_0 are the velocity and density of the gas, a - the sound velocity of the homogeneous flow; N - the compressing (stretching) effort;M - the Mach number, a_j - coefficients, characterizing the stiffness of the ground; the integral term takes into account the nonlinear effect of the longitudinal stress; $\alpha w'$ - a term related to the aerodynamics effect, $\alpha_0 = 1 (\alpha_0 = 2)$ corresponds to one-side (two-side) flow along the plate; $w(x)$ - plate deflection; all coefficients of equations (17),(18) are constants. In (18) $c_i, d_j (i = 0 \div n, j = 0 \div m)$ are arbitrary, part of them must be equal to zero; the boundary conditions can be linear or nonlinear depending on the values of these coefficients. The value of the m and n must be equal ∞.

The numerical realization is that a boundary value problem is led to an initial Cauchy problem. Lacking initial conditions of a Cauchy problem are defined by means of parameters which are selected by the Newton's method help. The Cauchy problem is solved by the Runge-Kutta method of the sixth order with the pitch error monitoring. The Cauchy problem complexity is that the nonlinearity as an integrated item there is at the equation. The integrated item is defined by the help of the Newton-Cotes quadrature formula. The nonlinearity is solved by the constructed iteration process. The program is written by Delphi-6 language. The bifurcation diagrams which show dependence of the maximum sag of a plate from of the velocity of the gas flow are formed by means of this program.

Computer Modeling Waves in Anisotropic Crystals

V. Yakhno, H. Akmaz

This paper includes mathematical modeling and simulating the wave propagations in anisotropic solids and crystals with different structure of anisotropy. Dynamic mathematical models of elastic wave propagations in anisotropic media are described by the following system of partial differential equations

$$\rho \frac{\partial^2 u_j}{\partial t^2} = \sum_{k,l,m=1}^{3} C_{jklm} \frac{\partial^2 u_m}{\partial x_k \partial x_l} + f_j(x,t), \quad x \in \mathcal{R}^3, \quad t > 0,$$

$$u_j(x,0) = \varphi_j(x), \quad \left. \frac{\partial u_j(x,t)}{\partial t} \right|_{t=0} = \psi_j(x), \quad j = 1,2,3.$$

Here ρ is the density of the medium, $\mathbf{u}(x,t) = (u_1(x,t), u_2(x,t), u_3(x,t))$ is small amplitude vibrations, $\{C_{jklm}\}_{j,k,l,m=1}^{3}$ are the elastic moduli of the medium, $\varphi_j(x)$, $\psi_j(x)$, $f_j(x,t)$, $j = 1,2,3$ are given functions. We assume that ρ and C_{jklm} are constants.

An iterative procedure of finding a solution of this initial value problem with polynomial data is described in this paper. Wave fields for different anisotropic materials are simulated by this procedure. We have used Mathematica 4.0 to generate 3-D images and animated movies of elastic wave propagations in crystals. These images are collected in the library of images. This library can serve as a set of patterns and samples when we analyze the structure of anisotropic materials or evaluate the performance of numerical methods.

Parametrically Driven Dark Solitons: a Numerical Study

E. Zemlyanaya, I. Barashenkov, S. Woodford

The parametric driving is well known to be an efficient way of compensating dissipative losses of solitons in various media. In a number of applications the amplitude equation of the parametrically driven wave turns out to have the nonlinearity of the "defocusing" type. We consider the parametrically driven, damped nonlinear Schrödinger equation

$$i\psi_t + \frac{1}{2}\psi_{xx} - \mid \psi \mid^2 \psi + \psi = h\overline{\psi} - i\gamma\psi \tag{20}$$

where h is driver's srtength and γ is a dissipation coefficient.

The localized solutions forming in the defocusing media are domain walls, or kinks, also known as "dark solitons" in the context of nonlinear optics.

Our purpose is to numerically explore the stability and bifurcations of the dark solitons of Eq.(19) and their bound states. Results of the numerical analyzes are presented for both damped and undamped cases.

It is shown that unlike the bright solitons, the parametrically driven kinks are immune from instabilities for all dampings and forcing amplitudes; they can also form stable bound states. In the undamped case, the two types of stable kinks and their complexes can travel with nonzero velocities.

The remarkable stability of the damped-driven kinks and their bound states is in sharp contrast with stability properties of the bright solitons. The stable coexistence of two types of domain walls and their complexes in the undamped case is also worth emphasising; this multistability is not observed in the parametrically driven Klein-Gordon and Ginzburg-Landau equations.

Investigation of the Viscous Flow in a Chemical Reactor with a Mixer

I. Zheleva, A. Lecheva

Tank reactors with different mixers are very often used for many chemical and biological processes. For their effective use is necessary to know in details hydrodynamics and mass transfer which take place in them. For many practically important cases the experimental study of these processes is very expensive or impossible. This is why recently mathematical modeling of the complex swirling flows in such reactors becomes an effective method for investigation of the behavior of the fluids in these reactors. This paper presents mathematical model and numerical results for viscous swirling flow in a cylindrical tank reactor with a mixer. The model is based on the Navier-Stokes equations in cylindrical co-ordinate system which are written in terms of the stream function, vorticity and the momentum of the tangential component of the velocity. The flow is supposed to be stationary and axes-symmetric. A special attention is devoted to the correct formulation of the boundary conditions. A numerical algorithm for studying this motion of the fluid is proposed. The grid for the discretization of the equations is no uniform. Difference scheme of Alternating Direction Implicit Method for solving Navier-Stokes equations is used. Numerical results for the stream function, the velocity field and the momentum of the tangential velocity for different Reynolds numbers are obtained by this numerical algorithm. The results are presented graphically. They are discussed and compared with other authors results. It is observed a very good agreement between them.

Stability Analysis of a Nonlinear Model of Wastewater Treatment Processes

P. Zlateva, N. Dimitrova

Clean water is essential for health, recreation and life protection among other human activities. The activated sludge processes are most widely used biological systems in wastewater treatment. These processes are very complex due to their nonlinear dynamics, large uncertainty in uncontrolled inputs and in the model parameters and structure.

In this paper a nonlinear mathematical model of an activated sludge wastewater treatment process is considered. The Haldane law as the specific growth rate function is selected. Assuming that some of the model parameters are unknown but bounded, stability analysis of the steady states is carried out. Computer simulation results in Maple are also performed.

About One Iteration Method for Solving Difference Equations

G. Zverev

The numerical analysis of a wide range of applied problems of mathematical physics leads to necessity of solution of Linear Algebraic Equations System (SLAE), which arises at discretization of decision region and substitution of the differential operators by difference analogues. Despite of rapid progress in computing capacity, the problem of SLAE effective solution is one of the fundamentals in computational mathematics. Actuality of this problem at present is more increased in connection with wide propagation of numerical calculations and a rise in requirements to their accuracy and rate of realization [1].

In the given paper, a new iterative line-by-line method with a variable compensation parameter is proposed for solving a system of difference equations when arises from implicit approximation of two-dimensional differential elliptical and parabolic equations. It is further developments of modified and block line-by-line methods [2, 3]. The proposed computational technologies is convenient in practical application, maintain methodology of an alternating direction method and based on solution of one-dimensional three-point difference equations along grid lines.

The high efficiency of the method is conditioned by increasing ellipticity of its algorithm that answers the nature of a differential equation. The implicit consideration of a difference flux from other grid direction, a decrease of the iterative expression norm and application of variable compensation parameter (terminology [4]) allow to reach it. The values of a variable compensation parameter are evaluated in each grid node of calculation domain. The evaluation is based on an iterative expression minimum at definition of coefficients of two-point recurrence relations for a grid function. The physical interpretation of iteration algorithm is given. The method enables to apply a technology of parallel calculations.

The iteration method is approved on the test Dirichlet's problem for a Poisson's equation [1]. Calculations have showed that method's convergence rate is insensitive to variation of coefficients at high derivatives and weakly depends on grid's dimension. The application of new computational technology is especially effective on detailed grids and allows to reducing necessary number of iterations up to two orders of magnitude as compared with the line-by-line method [5] for solving SLAE.

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Three-level Difference Schemes on Non-Uniform Grids

E. Zyuzina

In this paper we consider three-level operator-difference schemes for the boundary value problems of mathematical physics of parabolic and hyperbolic type on the non-uniform in time grid:

$$Dy_{\bar{t}\hat{t}} + By_{\overset{\circ}{t}} + Ay = \varphi, \quad t \in \hat{\omega}_\tau, \quad y_0 = u_0, \quad y_1 = u_1,$$

$$\hat{\bar{\omega}}_\tau = \{t_n = t_{n-1} + \tau_n,\ n \in 1, 2, \ldots, N,\ t_0 = 0,\ t_N = T\} = \hat{\omega}_\tau \cup \{0, T\}.$$

Three-level difference schemes for the problems of mathematical physics on uniform grids are widely studied. Necessary and sufficient conditions of stability were already obtained in the sense of the initial data and the right-hand side in finite-dimensional Hilbert spaces. However for the problems with singularities the use of non-uniform grids both in space and in time is more advisable. In this work a priori estimates of stability of numerical solution with respect to the initial data and the right hand side on the non-uniform time grid are obtained.

While going over from uniform grid to a non-uniform one the order of local approximation decreases. Raising the order of local approximation is very important requirement for numerical solution of the mathematical physics problems on coarse grids. In presented paper new difference schemes with weights of the second order of approximation on the standard stensils are constructed and investigated for parabolic and hyperbolic problems on the non-uniform in time grids. All theoretical results are confirmed by computational experiments.

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