

NAA'12: Fifth Conference on
Numerical Analysis and Applications

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Organized by
Department of Mathematics and Informatics
University of Rousse "Angel Kanchev"

Main tracks: Numerical Approximation and Computational Geometry; Numerical Linear Algebra and Numerical Solution of Transcendental Equations; Numerical Methods for Differential Equations; Numerical Stochastics; Numerical Modeling; High Performance Scientific Computing.;

List of Keynote Speakers who accepted our invitation:

I. Farago (Hungary), M.J. Gander (Switzerland), B. S. Jovanovic (Serbia), N. Kopteva (Ireland), R. Lazarov (USA), Ch. Markidakis (Greece), P.Matus (Belarus), G. Milovanovic (Serbia), P. Minev (Canada), V.Nistor (U.S.A), E. O'Riordan (Ireland), A.K.Pani (India), B. Popov (U.S.A), M.Razzaghi (U.S.A), H.-G. Roos (Germany), V.Rukavishnikov (Russia), G. Shishkin (Russia), V. Shidurov (Russia), M.Stynes (Ireland), P. Vabishchevich (Russia).

Organizing Committee:

Chairmen: Lubin Vulkov

Ivanka Angelova, Tatyana Chernogorova, Juri Kandilarov, Miglena Koleva

Unconditionally stable schemes for non-stationary convection-diffusion-reaction equations

N. Afanasyeva, P. Vabishchevich and M. Vasilyeva

Convection-diffusion problem are the base for continuum mechanics. The main features of these problems are associated with an indefinite operator the problem. In this work we investigate the stability of difference schemes with weights for convection-diffusion problems with different forms of the operator of convective transport. We construct unconditionally stable scheme for non-stationary convection-diffusion equations, which are based on use of new variables. Also, we consider these equations in the form of convection-diffusion-reaction and construct unconditionally stable schemes when explicit-implicit approximations are used with splitting of the reaction operator. Similar schemes we use for pressure equation in the multiphase filtration problem.

Nonconforming Rectangular Morley Finite Elements

A. Andreev and M. Racheva

We analyze some approximation properties of modified rectangular Morley elements applied to fourth-order problems. Degrees of freedom of integrals type are used which yields superclose property. Further asymptotic error estimates for biharmonic solutions are derived. Some interesting and new numerical results concerning plate vibration problems are also presented.

Numerical simulation by finite volume approach of viscous incompressible fluid flow in cone-cylinder gap

V. Arkhipov and E. Kornaeva

In this paper we study laminar flow of viscous incompressible fluid in the gap between static outer cone (stator) and rotating inner cylinder (rotor). The mathematical model is based on Navier-Stokes and continuity equations. The simulation model is based on finite volume approach. The simulation results are studied in comparison with some results of other authors and with analytical solution in asymptotic cases.

High order accurate difference schemes for hyperbolic ibvp

A. Ashyralyev and O. Yildirim

The abstract Cauchy problem for the hyperbolic equation

$$u''(t) + Au(t) = f(t), 0 < t < T, u(0) = \varphi, u'(0) = \psi$$

in a Hilbert space H with the self -adjoint positive definite operator A is considered. The third and fourth orders of accuracy difference schemes for the approximate solution of this problem are presented. The stability estimates for the solution of these difference schemes are established. A numerical method is proposed and results of numerical experiments presented in order to support the theoretical statements.

A note on the modified Crank-Nicholson difference schemes for ultra parabolic equations with Neumann condition

A. Ashyralyev and S. Yilmaz

Mathematical models which are formulated in terms of ultra parabolic equations are of great importance in many natural phenomenons, for instance in age-dependent population model, in the mathematical model of Brownian motion, in the theory of boundary layers, etc.

In this paper, we focus on studying the stability of second order difference scheme for the approximate solution of the initial boundary value problem for ultra parabolic equations

$$\begin{cases} \frac{\partial u(t,s)}{\partial t} + \frac{\partial u(t,s)}{\partial s} + Au(t,s) = f(t,s), & 0 < t, s < T, \\ u(0,s) = \psi(s), & 0 \leq s \leq T, \\ u(t,0) = \varphi(t), & 0 \leq t \leq T \end{cases}$$

in an arbitrary Banach space E with a strongly positive operator A . For approximately solving this problem, r-modified Crank-Nicolson difference schemes of the second-order of accuracy

$$\begin{cases} \frac{u_{k,m} - u_{k-1,m-1}}{\tau} + Au_{k,m} = f_{k,m}, & 1 \leq k, m \leq r, \\ \frac{u_{k,m} - u_{k-1,m-1}}{\tau} + \frac{A}{2}(u_{k,m} + u_{k-1,m-1}) = f_{k,m}, & r+1 \leq k, m \leq N, \\ f_{k,m} = f(t_k, s_m), t_k = k\tau, s_m = m\tau, & 1 \leq k, m \leq N, N\tau = 1, \\ u_{0,m} = \psi_m, \psi_m = \psi(s_m), & 0 \leq m \leq N, \\ u_{k,0} = \varphi_k, \varphi_k = \varphi(t_k), & 0 \leq k \leq N \end{cases}$$

are presented. The stability estimates for the solution of these difference schemes is established. In applications, the stability in maximum norm of difference shemes for multidimensional ultra parabolic equations with Neumann condition is established. Applying the difference schemes, the numerical methods are proposed for solving one dimensional ultra parabolic equations.

**Bifurcations in long Josephson junctions with second harmonic in the current-phase relation:
Numerical Study**

P. Atanasova and E. Zemlyanaya

Critical regimes in the long Josephson junction (LJJ) are studied within the frame of a model accounting the second harmonic in the current-phase relation (CPR). Numerical approach is shown to provide a good agreement with analytic results. Numerical results are presented to demonstrate the availabilities and advantages of the presented numerical scheme for investigation of bifurcations and properties of the magnetic flux distributions in dependence on the sign and value of the second harmonic in CPR.

Multiple moving cracks in a non-homogeneous orthotropic half-plane under shear deformation

M. Ayatollahi , R. Bagheri and R. Moharrami

This paper provides a theoretical investigation of the behavior of multiple moving cracks in a non-homogeneous orthotropic half-plane under anti-plane deformation. The distributed dislocation technique is used to carry out stress analysis in a non-homogeneous half-plane containing moving cracks under anti-plane loading. The Galilean transformation is employed to express the wave equations in terms of coordinates that are attached to the moving crack. Finally, the solution of a moving screw dislocation is obtained in a non-homogeneous half-plane by using the Fourier transform. The stress components reveal the familiar Cauchy singularity at the location of dislocation. The solution is employed to derive integral equations for a half-plane weakened by several moving cracks. Numerical examples are provided to show the effects of material properties, crack size and the speed of cracks propagating on the stress intensity factors of crack tips.

Keywords: Non-homogeneous material; Screw dislocation; Multiple moving crack; Dynamic stress intensity factor;

A modified quadratic hybridization of Hestenes-Stiefel and Dai-Yuan conjugate gradient methods

Saman Babaie-Kafaki

Conjugate gradient methods comprise a class of unconstrained optimization algorithms characterized by low memory requirements and strong global convergence properties which made them popular for solving large-scale problems. In a recent effort to take advantage of the nice computational performance of the Hestenes-Stiefel (HS) conjugate gradient method and the strong global convergence properties of the Dai-Yuan (DY) conjugate gradient method, by an extension of Andrei's approach of hybridizing the conjugate gradient parameters convexly, Babaie-Kafaki [S. Babaie-Kafaki, A hybrid conjugate gradient method based on a quadratic relaxation of the Dai-Yuan hybrid conjugate gradient parameter, Optimization, DOI: 10.1080/ 02331934.2011.611512]

proposed a hybridization of the HS and DY methods, globally convergent for uniformly convex objective functions, based on a quadratic relaxation of a hybrid conjugate gradient parameter suggested by Dai and Yuan. In this study, in order to achieve the global convergence for general objective functions, we apply Powell's approach of nonnegative restriction of the conjugate gradient parameters and make a modification on the quadratic hybrid conjugate gradient parameter suggested by Babaie-Kafaki. We show that if the line search fulfils the strong Wolfe conditions, then our method is globally convergent for general objective functions. Numerical results demonstrating the efficiency of our method in the sense of the performance profile introduced by Dolan and Moré are reported.

Numerical and analytical modeling of orthotropic circular plate deformations under normal pressure

S. Bauer and E. Krakovskaya

The stress state of an orthotropic circular plate under normal pressure is analyzed. The shell material is considered to be cylindrically orthotropic or transversely isotropic. Different numerical and analytical methods are applied to study the effect of material parameters on the plate deflection.

The results obtained in the frameworks of different shell theories such as Kirchhoff–Love, Timoshenko–Reissner, Ambartsumyan and Rodionova–Titaev–Chernykh theories and also results of numerical analysis of 3D problem with the applied package ANSYS are compared. The comparison shows that the Rodionova-Titaev-Chernykh theory provides the results, which are the closest to exact (3D) solution. The difference between solutions obtained with different approximate (2D) methods goes down as the plate thickness decreases.

The results obtained could be used in analysis of some biomechanical problem, for example, strain fields in Lamina Cribrosa under glaucoma. The Lamina Cribrosa (LC) is a part of eye shell (sclera), where the optic nerve fibers pass through and where the layer of sclera becomes thinner and more than 400 little pores appear. Consequently the LC is simulated as continuous nonuniform orthotropic plate under uniformly distributed intraocular pressure.

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On unsymmetrical buckling of nonuniform orthotropic circular plates

S. Bauer and E. Voronkova

This work is concerned with the numerical and analytical study of unsymmetrical buckling of clamped orthotropic plates under uniform pressure. The effect of material heterogeneity on the buckling load is examined. The refined 2D shell theory is employed to obtain the governing equations for buckling of clamped circular shell.

The unsymmetric part of the solution is sought in terms of multiples of the harmonics of the angular coordinate. The lowest load value, which leads to the appearance of waves in the circumferential direction, is obtained numerically. It is shown that if the elasticity modulus decreases away from the center of a plate, the critical pressure for unsymmetric buckling is sufficiently lower than for a plate with constant mechanical properties. The folds in the narrow zone at the periphery of the Lamina Cribrosa (LC) — a part of eye shell (sclera), where the optic nerve fibers pass through — could be explained by the bucking of the axisymmetric state of LC in the nonaxisymmetric state.

A Petrov-Galerkin pype stabilization for unsteady convection diffusion equation on rectangular grids

O. Baysal

An enrichment finite element method is proposed for parabolic equation modeling convection diffusion process in two dimensional space. We first discretize the problem in space with Petrov-Galerkin type stabilization. More precisely trial and test spaces are enriched by bubble and multiscale functions, which are independent of time variable, on rectangular grids. These functions however require the solution of steady convection diffusion equation that makes the method quite expensive. In order to simplify algorithm, we instead use their cheap and comparable approximations in each element. Then time integration is performed by the generalized Euler scheme (θ - method). Numerical tests validate the accuracy of the algorithm.

Numerical modeling of the supersonic air flow with transverse injection of helium jet using WENO schemes

A. Beketaeva, A. Abdalla and Ye. Belyayev

The flow field generated by transverse injection of helium through a slot into supersonic air flow is numerically simulated. The numerical algorithm is developed for solution of the Favre-Averaged Navier - Stokes equations for two-dimensional supersonic multi-species flows. The fourth order implicit WENO scheme (Weighted Essentially Non oscillatory scheme) has been used to approximate the inviscid fluxes terms of the system. Computer code was validated by solution of the problem and comparison with experimental data in terms of surface pressure profiles, flow structures at the upstream and downstream of the jet.

Numerical investigation of the stability of convective flow in cylinder

V. Bekezhanova and V. Andreev

The problem of convective flow of viscous heat-conducting liquid with complex rheology in radiative heating conditions was investigated in the framework of the Oberbeck–Boussinesq model. Exact solution describing the stationary flow in a cylinder with large radius was obtained

$$\mathbf{u} = (u, v, w), \quad u = u(z)r, \quad v = 0, \quad w = w(z), \quad p = p(z) + ar^2/2, \quad \theta = \theta(z),$$

where u, v, w are the radial, azimuthal and axial velocity components, respectively; p is the pressure, θ is the temperature, parameter a is to be defined.

The original problem is divided into consequently solved problems for u, w, p, θ . The basic one of them is the boundary problem for $u(z)$ function

$$u_{zz} + 2u_z \int_0^z u(z)dz - u^2 + a = 0, \quad 0 < z < 1,$$
$$u(0) = u(1) = 0, \quad \int_0^1 u(z)dz = 0,$$

which can be reduced to the operator equation $u = Au$, where A is a strongly nonlinear operator satisfying the Schauder theorem in $C[0, 1]$. The iterative procedure for finding the a parameter and obtaining the radial velocity component was suggested. Three different values of the a parameter were found in the domain of the problem's physical parameters.

The linear stability of the three classes of solutions with regard to small perturbations was investigated numerically. The instability mechanism is changed and restructuring of neutral curves occurs depending on the a value.

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An improved numerical scheme for the generalized Burgers–Fisher equation

A. Bratsos

Fisher proposed the well-known equation, encountered in various disciplines, as a model for the propagation of a mutant gene displaying the density of advantage. Henceforth this equation has been used as a basis for a wide variety of models for different problems.

The most general form of the Fisher's equation is the so-called generalized Burgers-Fisher (BgF) equation, which has the form

$$u_t + \alpha u^\delta u_x - u_{xx} = \beta u (1 - u^\delta); \quad 0 \leq x \leq 1, \quad t > 0$$

with appropriate initial and boundary conditions.

The main aim of this paper is to solve the BgF equation explicitly with a direct method. To this attempt, a third order in time numerical method is used. The solution of the resulting nonlinear system is given by expressing the unknown vector component wise and updating each component

as soon as its value becomes available. This process, which is known as a modified predictor-corrector (MPC) method, opposite to the iterative classical predictor-corrector (P-C) one is always *explicit* and is applied *once*, has also been applied successfully in other PDE's with various other approximations in time giving an improvement in the accuracy over the P-C method. The results from the experiments are analyzed and compared with the known ones for the BgF equation, while conclusions for the efficiency of the MPC over the P-C method and comparisons with the known analogous methods are going to be given.

ADI fitted finite volume method for the Black-Scholes equation in stochastic volatility models

T. Chernogorova and R. Valkov

In this paper we develop numerical schemes for the two-dimensional Black-Scholes equation in stochastic volatility models. In order to obtain a method, that provides efficient approximations of the mixed derivative and the degeneration we combine a fitted finite volume method spatial discretization and a fractional step method for the time variable. Some numerical examples, confirming the expected behaviour of the method, are presented.

Two splitting methods for a fixed strike asian option

T. Chernogorova and L. Vukov

The valuation of Asian Options can often be reduced to the study of initial boundary problems for ultra-parabolic equations. Two splitting methods are used to transform the whole time-dependent problem into two unsteady subproblems of a smaller complexity. The first subproblem is a time-dependent convection-diffusion, the finite volume difference method of S. Wang is applied for its discretization. The second one is a transport problem and is approximated by monotone weighted difference schemes. The positivity of property of the numerical methods is established. Numerical experiments are discussed

On the numerical simulation of unsteady solutions for the 2D Boussinesq paradigm equation

C. Christov, N. Kolkovska and D. Vasileva

Boussinesq equation (BE) is the first model for surface waves in shallow fluid layer that accounts for both nonlinearity and dispersion. The balance between the steepening effect of the nonlinearity and the flattening effect of the dispersion maintains the shape of the waves. In the 60s it was discovered that these permanent waves can behave in many instances as particles and they were called *solitons*. A plethora of deep mathematical results have been obtained for solitons in the 1D case, but it is of crucial importance to investigate also the 2D case, because of the different phenomenology and the practical importance. The accurate derivation of the Boussinesq system

combined with an approximation, that reduces the full model to a single equation, leads to the Boussinesq Paradigm Equation (BPE):

$$u_{tt} = \Delta [u - F(u) + \beta_1 u_{tt} - \beta_2 \Delta u], \quad F(u) := \alpha u^2 \quad (1)$$

where u is the surface elevation, $\beta_1, \beta_2 > 0$ are two dispersion coefficients, and α is an amplitude parameter. The main difference of Eq. (1) from BE is that in the former one more term is present for $\beta_1 \neq 0$ called “rotational inertia”.

It has been recently shown that the 2D BPE admits stationary soliton solutions as well. Even though no analytical formula for these solutions is available, they can be accurately constructed using either finite differences, perturbation technique, or Galerkin spectral method. Virtually nothing is known about the properties of these solutions when they are allowed to evolve in time and it is of utmost importance to answer the questions about their structural stability.

In order to devise a numerical time-stepping procedure we recast Eq. (1), as the following system:

$$v(x, y, t) := u - \beta_1 \Delta u, \quad v_{tt} = \frac{\beta_2}{\beta_1} \Delta v + \frac{\beta_1 - \beta_2}{\beta_1^2} (u - v) - \alpha \Delta F(u).$$

We design an implicit time stepping scheme for the above coupled system and solve it by the Bi-Conjugate Gradient Stabilized Method with ILU preconditioner. The scheme is second order accurate in space and time and unconditionally stable. We perform all standard tests to validate the algorithm: three different spatial grids and different time increments. The results from our numerical experiments show that for some values of the phase speed and relatively small times the unsteady solutions have a solitonic behaviour, although for large times the solution either transforms into a diverging propagating wave or blows-up. The threshold for the value of phase speed for which blow-up is observed depends mildly on the resolution of the grid, because a rougher grid has additional numerical dispersion that acts to diminish the role of the nonlinear terms.

A finite difference approach for the time-fractional differential equation with concentrated capacity

Al. Delić

In this paper we consider finite-difference scheme for the time-fractional differential equation with Caputo fractional derivative of an order $\alpha \in (0, 1)$ with the coefficient at the time derivative containing Dirac delta distribution. Estimate for the rate of the convergence compatible with the smoothness of the solution is obtained.

SMP parallel implementation of finite element method for elliptic-type problem

E. Dementyeva and E. Karepova

Nowadays high-performance cluster systems with hybrid architecture are wide spread. Generally, computational node in such systems is multicores or multiprocessors (SMP) and usually is equipped with general-purpose graphics processing units with massively parallelism (MPP GPGPU). As a result, while implementing the parallel programs the problem of efficient using of multilevel hierarchy of memory and many computational devices arises.

The most prevailing paradigm of coding for SMP-nodes clusters is MPI and OpenMP technologies joint use for multithreads MPI-process launching on each node. For GPGPU programming CUDA technology should be added to those described above.

This work is devoted to selected issues of efficient using of cluster systems with hybrid architecture by way of example of finite element method for elliptic problem implementation. While solving this very type of problems we faced some difficulties concerning the reaching of a high speedup of a parallel program. Thereby, a subsidiary research on the impact of a set of factors on speedup and efficiency of parallel implementation was made: ratio of time for the calculation itself and time for the data communications, for fork/joint threads and its synchronize; special features of memory access with multithreads program run, characteristics of GPGPU using and, finally, characteristics of compiling optimization conjointly with parallel libraries linked.

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Symplectic numerical schemes for stochastic Hamiltonian equations

J. Deng, Y. Wong and Cr. Anton

We propose a new method to develop high order symplectic schemes for Hamiltonian stochastic differential equations. This approach is an non-trivial extension to the stochastic case of the methods based on generating functions for deterministic Hamiltonian systems. We consider the stochastic differential equations in the sense of Stratanovich:

$$dP = -\frac{\partial H^{(0)}(t, P, Q)}{\partial Q} - \sum_{r=1}^m \frac{\partial H^{(r)}(t, P, Q)}{\partial Q} odw_t^r, \quad P(t_0) = p \quad (1)$$

$$dQ = -\frac{\partial H^{(0)}(t, P, Q)}{\partial P} + \sum_{r=1}^m \frac{\partial H^{(r)}(t, P, Q)}{\partial P} odw_t^r, \quad Q(t_0) = q, \quad (2)$$

P, Q, p, q are n -dimensional vectors, and w_r^t , $r = 1, \dots, n$ are independent standard Wiener processes. The equations (1)(2) represent a stochastic Hamiltonian system for which the stochastic flow $(p, q) \rightarrow (P, Q)$ is symplectic. We associate the following stochastic partial differential equation with the system (1)-(2):

$$dS_w^1 = H^{(0)} \left(P, q + \frac{\partial S_w^1}{\partial P} \right) dt + \sum_{r=1}^m H^{(r)} \left(P, q + \frac{\partial S_w^1}{\partial P} \right) odw_t^r. \quad (3)$$

The map $(p, q) \rightarrow (P(t, \theta(t)w), Q(t, \theta(t)w))$ defined by $p = P + \frac{\partial S_w^1}{\partial q}(P, q)$, $Q = q + \frac{\partial S_w^1}{\partial P}(P, q)$ is the flow of (1)-(2). We use this relationship between the generating function S_w^1 and the solutions of the system (1)-(2) to construct symplectic numerical schemes based on approximations of the solutions of the partial differential equation (3). By construction these schemes preserve the symplectic structure. We illustrate the excellent long term accuracy of the proposed schemes on several examples with additive and multiplicative noise.

On the asymptotic stabilization of a bioprocess model

N. Dimitrova and M. Krastanov

One of the main drawbacks in the modeling and control of a biological process lies in the difficulty to monitor on-line the key biological variables of the process and to obtain explicit analytic expressions for the growth rate functions. For this reason to control a bioprocess is a delicate problem since the corresponding nonlinear kinetics is in fact unknown.

In the present talk we present a result for asymptotic stabilizability of a nonlinear model of a bioprocess.

Metamodeling and Monte Carlo Algorithms for variance-based sensitivity analysis of the unified Danish Eulerian model

I. Dimov, R. Georgieva, Tz. Ostromsky and Z. Zlatev

The problem of representing in a direct way the relationship between input factors and the model output is essentially a task of model approximation or metamodeling. It is an important step during the procedure of variance-based sensitivity analysis studies. Various approximation techniques for presenting mesh-functions have been studied and applied during the metamodeling process of a large-scale air pollution model (Unified Danish Eulerian Model, UNI-DEM). A comparison of their efficiency has been done.

A number of new numerical experiments with UNI-DEM have been carried out to compute Sobol' sensitivity measures in order to analyze sensitivity of ozone concentrations according to variations of rates of a larger number of chemical reactions. The reactions are taken from the standardized scheme for air-pollution chemistry CBM-4. Various Monte Carlo algorithms have been applied for numerical integration of multidimensional integrals.

An application of the finite element method in modeling the magnetic field in the earth's magnetosphere

P. Dobрева

The capabilities of the finite element method in modeling the magnetic field in the stationary 3D magnetosphere are demonstrated. The whole magnetic field in the magnetosphere consists of a) the Earth's dipole field, b) the field of the magnetopause currents, c) the field, due to various currents systems in the magnetosphere - the cross-tail, ring and Birkeland currents, presented here by the data-based model of Tsyganenko. The object of calculation is the field, due to the magnetopause currents, for which Neumann boundary value problem is solved by the use of the finite element method. In order to approve the solution the grid refinement is applied. Magnetic field line configurations in the magnetospheric cavity are also presented.

Harmanli fire (Bulgaria) 2009, simulation on blue gene/P

N. Dobrinkova and G. Jordanov

During the last years in Bulgaria the number of forest fires has increased and the need of computer based tools also. The team in BAS has focused its efforts in creation of methodology for simulations in parallel mode the fire propagation by using the WRF-Fire model (recently renamed to SFIRE). We have run simulation with real data about forest fire near by the village of Leshnikovo, region of Harmanli, that occur from 14 to 17 August 2009 by using US supercomputer. Now our team will run the model and the created data for the real case in Harmanli region on the Bulgarian Blue Gene/P architecture and will compare the results from the parallel computations.

Modal properties of vertical cavity surface emitting laser arrays under the influence of thermal lensing

N. Elkin, A. Napartovich and D. Vysotsky

Modal behavior of an $n \times n$ array of vertical cavity surface emitting lasers (VCSEL) was studied numerically. Thermal lensing was simulated by the temperature profile set as a quadratic function of a polar radius. Mathematical formulation of the problem consists of self-consistent solution of the 3D Helmholtz wave equation and 2D non-linear diffusion equation as the material equation of the active laser medium. Complete formulation of the problem contains boundary conditions and an eigenvalue to be determined. Bidirectional beam propagation method was taken as a basic for numerical algorithms. In calculations, both Fourier and physical spaces description of beam propagation was combined. Above-threshold operation of laser array was simulated using round-trip iterations similar to the Fox-Li method. In addition, the Arnoldi algorithm was implemented to find several high optical modes in a VCSEL array with gain and index distributions established by the oscillating mode. The partial eigenvalue problem for a linear non-hermitian operator of large dimension was solved in this case.

Calculations were made for various spacing length between elements and a size of the array. Array optical modes having different symmetry properties were found. They include in-phase mode with constant phase over the array, out-of-phase mode with alternating phase between elements and modes with mixed symmetry. Conditions are found for favorable lasing of the in-phase mode providing high laser beam quality.

Well-posedness of the right-hand side identification problem for a parabolic equation

A. Erdogan and A. Ashyralyev

We consider the inverse problem of reconstructing the right side of a parabolic equation with an unknown time dependent source function. Numerical solution and well-posedness of this type problem is considered previously by A.A. Samarskii, P.N. Vabishchevich and V.T. Borukhov.

In this paper, we focus on studying the stability of the problem. A stable algorithm for the approximate solution of the problem is presented. With the results of numerical experiments presented, the theoretical statements are supported.

Numerical and analytical modeling of buckling of the cylindrical shell under axial compression with use of non-classical theories of shells

A. Ermakov

The problem of stability of a cylindrical shell under axial compression by means of new non-classical shell theories is studied. To solve it the local approach is used. According to it the buckling deflection is sought in the form of a doubly periodic function of curvilinear coordinates. Well-known solutions obtained with the use of classical shell theories of Kirchhoff–Love and Timoshenko–Reissner are compared with the results of improved nonclassical shell theories of Rodionova–Titaev–Chernykh and Paliy–Spiro. For the PS and RTCH theories of anisotropic shells of moderate thickness the stability equations were elaborated with linearization of nonlinear equilibrium equations.

Analytical and numerical results which were obtained with the use of 3D theory by the FEM code ANSYS11 were also compared. As an example, the steel tube under axial compression is modelled with 3D 20–nodes elements Solid186. During mesh construction the tube thickness was splitted for five elements.

Richardson Extrapolation in Actions

I. Faragó

For the numerical modelling of different nature the ordinary differential equations are typical and widely used tool. To their numerical handling, in general, we apply different Runge–Kutta methods. To increase the efficiency of the method, to increase the order of convergence we apply the Richardson extrapolation, which is an efficient general tool to enhance the accuracy of time integration schemes. In this talk we investigate the convergence of the combination of any diagonally implicit (including also the explicit) Runge–Kutta method with active Richardson extrapolation and show that the obtained numerical solution converges under rather natural conditions. We also investigate some other qualitative properties of the combined schemes, particularly the A-stability of the schemes. We give an elementary proof of the convergence of the implicit Euler method for the scalar equation.

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Thermodynamic modeling of the reciprocating compressor with using AGA8 state equation

M. Farzaneh-Gorda, A. Niazmand and M. Dashtebayz

In this study, a thermodynamic modeling for investigation of gas properties inside reciprocating compressors usable at pressure enhancing stations has been represented. Interior space of compressor cylinder and its inside gas were considered as control volume and respectively. The first thermodynamic law, mass conservation law and AGA8 state equation were used to obtain required thermodynamic properties for modeling. Valve dynamic models approximate on based of a single vibration mode. The gas leakage of compressor was ignored. Temperature, pressure, mass flow rate as well as movement of suction and discharge valves were curved versus crank angle. Further, the results were compared with ideal gas. The result show that there are no noticeable differences between ideal and real gas models at studied pressures, while there are difference between temperature and mass flow rate. The results show a good agreement with previous studies where applicable

Modification of boundary element method for mathematical physics problems

V. Fedotov

Boundary Element Method (BEM) is one of the most popular methods for the solution of problems elasticity, heat transfer, diffusion, vibrational motions and so on. However a further development of this method for nonlinear and connected problems causes difficulties relating to the calculation accuracy and the computational speed. In the paper the Modification Boundary Element Method (MBEM) is presented. It is based on an exception of labor intensiveness and often incorrect operations of numerical differentiation and integration. Preliminary analytical integration of Green's functions on a base element is for this purpose used. For analytical integration the block "a motionless basic element - the mobile point of influence" is offered instead of the classical block "a motionless point of influence - a mobile limiting element". Distinctive features of the approach offered by the author are a use of analytical integration and ideology of parallel calculations at algorithm level.

Simulation of non-Newtonian pseudo-plastic blood flow in arteries

I. Fernandes and M. Gokhale

Numerical blood flow simulation is a vital tool during treatment of cardiovascular diseases associated with abnormal blood flow. This paper presents simulation of Casson model for non-Newtonian (shear-thinning) blood flow in arteries which has potential applications in treatment of diseases like aneurysm. Blood with small shear rates $\dot{\gamma} \leq 10s^{-1}$ and hematocrit less than 40 percentage is considered. The D2Q9 model of Lattice Boltzmann method (LBM) is used to simulate the flow with expansion geometry, taking into consideration the nature of the human artery. Two kinds of boundary conditions are investigated: Bounceback boundary and Von-Neuman boundary conditions. The geometry is considered such a way that an artery with local expansion can be simulated. The velocity and shear rate profiles are presented and compared with Newtonian flow to validate the use of LBM as the numerical technique.

Influence of the parameters A and B on ant colony optimization start strategies

S. Fidanova and P. Marinov

Ant Colony Optimization (ACO) is a stochastic search method that mimic the social behavior of real ants colonies, which manage to establish the shortest rout to feeding sources and back. Such algorithms have been developed to arrive at near-optimal solutions to large-scale optimization problems, for which traditional mathematical techniques may fail. On this paper semi-random start is applied. Estimation of start nodes of the ants are made and several start strategies are prepared and combined. There are several parameters which manage the algorithm performance. In this work we focus on influence of parameters A and B (percentage of good and bad solutions respectively) on the quality of achieved solutions. This new technique is tested on Multiple Knapsack Problem

(MKP). Benchmark comparison among the strategies are presented in terms of quality of the results. Based on this comparison analysis, the performance of the algorithm is discussed. The study presents ideas that should be beneficial to both practitioners and researchers involved in solving optimization problems.

Numerical and asymptotic modeling of annular plate vibrations

S. Filippov

Free axisymmetric flexural vibrations of an annular elastic thin plate are studied. Numerical solutions of eigenvalue problem for various boundary conditions are obtained. The plate can be used as a model of the supporting frame of a shell. In this connection the boundary conditions at the attachment line connecting the plate with the shell of revolution are also analyzed. The plate is called narrow if the ratio of its width to the radius of the inner edge is small. For vibrations analysis of a narrow plate new asymptotic methods are elaborated. Simple approximate formulas for evaluation of natural frequencies and vibrations modes are found. Comparison of the asymptotic and numerical results shows, that the errors of the approximate formulas rapidly decrease down with the plate width.

Projection methods for solving incompressible flows with weighted ENO schemes

J. Frutos and Julia Novo

One of the difficulties in the numerical simulation of incompressible flows is the coupling between the velocity and the pressure. The so called projection methods offer the possibility to find approximations of decoupled equations for the velocity and the pressure in the time integration of incompressible flows. In this work, we study the performance of projection methods in time for the incompressible Navier-Stokes equations combined with finite differences WENO schemes in space. In a recent paper by Volker John and Julia Novo (J. of Computational Physics (2012)) the good performance of the spatial discretization based on WENO schemes is shown for evolutionary convection-reaction-diffusion equations in two and three spatial dimensions. The schemes are combined with explicit total variation diminishing Runge-Kutta time integrators. The resulting schemes are specially suited to approach the equations in the convection dominated regime. In the present work we show that the use of WENO schemes in space and projection methods in time produce suitable approximations for high Reynolds numbers. The influence of the use of different projection methods in the time integration is study.

Numerical study of the atmospheric composition in Bulgaria

G. Gadzhev, K. Ganev, N. Miloshev and D. Syrakov

The present work aims at studying the local to regional atmospheric pollution transport and transformation processes over Bulgaria and at tracking and characterizing the main pathways and processes that lead to atmospheric composition formation in the region. The US EPA Models-3 system is chosen as a modelling tool. As the NCEP Global Analysis Data with 1 degree resolution is used as meteorological background, the MM5 and CMAQ nesting capabilities are applied for downscaling the simulations to a 9 km resolution over Balkans and 3 km over Bulgaria. The TNO emission inventory is used as emission input. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions. The study is based on a large number of numerical simulations carried out for four emission scenarios with all the emissions and with biogenic emissions, emissions from energetics and road transport excluded. Some results from the numerical simulations concerning the main features of the atmospheric composition in Bulgaria and the contribution of the different emission categories are demonstrated in the paper. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behaviour could be interesting. Therefore the Models-3 Integrated Process Rate Analysis option is applied to discriminate the role of different dynamic and chemical processes for the atmospheric composition formation. The processes that are considered are: advection, diffusion, mass adjustment, emissions, dry deposition, chemistry, aerosol processes and cloud processes/aqueous chemistry.

Stabilization of convection-diffusion problems by Shishkin mesh simulation. Recent advances

B. García-Archilla

Standard numerical methods are liable to perform poorly in convectiondiffusion problems, particularly on convection-dominated situations, where spurious (unphysical oscillations) are likely to pollute the numerical approximation. Several techniques have been developed in the past 30 years to flatten the unwanted oscillations, although no clear winner has turned up yet. Among the most successful ones are the use of Shishkin meshes, their disadvantage being the difficulty of designing them on nontrivial geometries. We present a technique to simulate Shishkin meshes without the need to build them. The technique is applicable to irregular grids and on nontrivial geometries. The numerical approximation obtained present similar accuracy and lack of oscillations as real (not simulated) Shishkin meshes. Problems with exponential and parabolic boundary layers can be treated, as well as problems with interior layers.

Numerical analysis of a mathematical model used in cancer research

B. Garkova and M. Kolev

During several last decades mathematical models have been shown to be helpful in the collaboration between biologists, immunologists, doctors, computer specialists and mathematicians. Our paper is an application of mathematical modelling approach in the field of cancer research. We consider a model of chemotaxis, which describe the migration of cancer cells through healthy tissue. Their motion is governed by diffusion and gradients of matrix degradative enzymes.

The purpose of the paper is to develop and apply efficient numerical scheme for solving the system of reaction-diffusion-chemotaxis equations. Numerical results of the model are presented. The role of some parameters of the model and analyzed from the point of view of cancer research. Analysis of the properties of the approximate solutions is performed.

A 3D surface finite element method for modeling biological cell shape and morphology dynamics

J. Genoff

The enormously complex biological systems are researched by modeling at various levels of abstraction. A fundamental one is the cell as the basic unit of life. Several software packages implement the most adopted theoretical apparatus that tries to explain the intra-cellular operation and extra-cellular interaction. This paper focuses on modeling the 3D shape of the cell and proposes a finite-element method for surface representation with an appropriate mixture of chemo-electro-mechanical concepts to determine surface shape and dynamics. Besides, these concepts are introduced without any simplifications aiming at abstraction or performance effects. A special attention is given to the computational precision and scaling issues. It is shown that avoiding simplifications and using very high precision computation gives strikingly different results compared to those obtained by more ordinary settings. An assessment of the performance costs is presented.

The method is tested against modeling the shape of realistic neurons in developmental simulation of neural network in glial environment.

Mesoscopic simulation approach to non-newtonian fluid flow in porous media

M. Gokhale and I. Fernandes

This paper presents numerical simulation of non-Newtonian fluid flow in porous media. The Carreau-Yasuda viscosity model is used to represent non-Newtonian (shear-thinning) fluid with index $n < 1$. Lattice Boltzmann method (LBM) is used to simulate the micro-channel flow by considering Bounceback boundaries (BB). The walls of the channel are considered to be solid for appropriate application of BB. The D2Q9 model of LBM for 2D flow is used to investigate the pressure drop along the channel. The effect of pseudo-plasticity (shear-thinning) is investigated on the velocity profiles and the shear stress distribution. The fundamentals of LBM are presented with a brief discussion on its advantages over other macroscopic numerical techniques. The method is validated by comparing the results with a Poiseuille flow in a duct. The comparison is done for the case of Newtonian flow and pseudo-plastic fluids. The Carreau-Yasuda model prevails over the shortcomings of power law model at high gradient and potentially infinite viscosity. It is demonstrated that this method is suitable for simulation of the non-Newtonian pseudo-plastic fluid in channel flow.

Formulas and algorithms for quantum differentiation of quantum bernstein bases and quantum bezier curves based on quantum blossoming

R. Goldman and P. Simeonov

We use a new version of the blossoming-the quantum blossoming, to derive formulas and recursive evaluation algorithms for the quantum derivatives of quantum Bernstein bases and quantum Bezier curves.

Crank-Nicolson scheme for the oldroyd model of order one

D. Goswami and A. Pani

In this talk, we would like to analyze Crank-Nicolson scheme for the equations of motion arising in the Oldroyd model of order one with the forcing term independent of time or L^∞ in time. This model can be considered as an integral perturbation of Navier-Stokes equations. We would focus mainly on the difficulties due to the presence of the integral term. A priori error estimates in L^2 -norm are derived for the discrete problem which are optimal in nature.

A singularly perturbed reaction–diffusion problem with a discontinuity between the boundary and initial data

J. Gracia and E. O’Riordan

Singularly perturbed reaction-diffusion parabolic problems with a discontinuity between the initial and boundary conditions are examined. A finite difference scheme is considered which utilizes a special finite difference operator on a special rectangular fitted mesh. The fitting coefficient is defined using the error function and the fitted mesh is a piecewise uniform mesh, which is fine in the layer region. Numerical results in the pointwise maximum norm are presented for both nodal and global convergence using bilinear interpolation

Method SMIF for incompressible fluid flows modeling

V. Gushchin and P. Matyushin

For solving of the Navier-Stokes equations describing 3D incompressible viscous fluid flows the Splitting on physical factors Method for Incompressible Fluid flows (SMIF) with hybrid explicit finite difference scheme (second-order accuracy in space, minimum scheme viscosity and dispersion, capable for work in wide range of Reynolds (Re) and Froude (Fr) numbers and monotonous) based on Modified Central Difference Scheme and Modified Upwind Difference Scheme with special switch condition depending on the velocity sign and the signs of the first and second differences of transferred functions has been developed and successfully applied (*Gushchin V.A., Konshin V.N. 1992. J. Computers and Fluids. V. 21. No. 3, 345-353*). For the visualization of the 3D vortex structures in the fluid flows the isosurfaces of β have been drawing, where β is the imaginary part of the complex-conjugate eigen-values of the velocity gradient tensor.

The numerical method SMIF has been successfully applied for solving of the different problems on supercomputers: 2D fluid flows with a free surface, 3D separated homogeneous and stratified fluid flows around a sphere and a circular cylinder; the air, heat and mass transfer in the clean rooms. For example in the case of the homogeneous fluid the detailed formation mechanisms of vortices in the sphere wake at $200 < Re < 1000$ have been described in (*Gushchin V.A., Matyushin P.V. 2006. Fluid Dynamics. V. 41. No. 5, 795-809*). In the case of the stratified fluid the classification of flow regimes around sphere at $Fr < 10, Re < 500$ has been refined (*Gushchin V.A., Matyushin P.V. 2011. Comput. Math. and Math. Physics. V. 51. No. 2, 251-263*).

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Finite element simulation of nanoindentation

R. Iankov, M. Datcheva, S. Cherneva and D. Stoychev

In last years there is an increasing interest to design new materials whose microstructure is controlled. For example nanostructured materials, functional graded materials, thin layers, compositionally graded coatings and etc. Because the microstructure is the main target of the designer for all these materials there is a need of evaluation of their mechanical properties in a local area using small volumes. However in most cases conventional macro experiments cannot be carried out due to e.g. the geometry, the size and the build-up of the specimen. Nanoindentation, where a sharp indenter is pressed normal onto the surface of the specimen and penetration depth is measured in nanometers, had been proven within the last decade to be a promising technique to investigate the mechanical properties of small volumes and thin films. During such tests the global variables load and displacement are continuously monitored and the mechanical properties such as indentation modulus and hardness are estimated based on these data.

However the indentation modulus and hardness are not sufficient to characterize the material behaviour in case of numerical simulation of constructions and details whose components are fabricated using materials with controlled microstructure. To overcome this shortage a technique for material model parameter identification using instrumented indentation test data together with a finite element simulation was intensively developed in recent years. In this paper a finite element model of nanoindentation on thin film and substrate employing nonlinear material model is presented. The numerical model and the obtained numerical solution are discussed in details and the simulated force-displacement curve is compared with data from real nanoindentation tests. Conclusions on the applicability of the used material model are done.

Runge-Kutta method with equation dependent coefficients

L. Ixaru

The family of the simplest three-stage explicit Runge-Kutta methods is examined by a conveniently adapted form of the exponential fitting approach. The unusual feature of the new versions is that their coefficients are no longer constant, as in the standard version, but depend on the equation to be solved. Two valuable mathematical properties emerge from this. Firstly, although in general the order is three, that is the same as for the standard method, this can be easily increased to four by a suitable choice of the position of the stage abscissas. Secondly, the stability properties are massively enhanced. Two particular versions of the new type and order four are A-stable, a fact which is quite unusual for explicit methods. This recommends them as efficient tools for solving stiff differential equations.

Analysis of the semidiscrete FEM

B. Jin, R. Lazarov and Z. Zhou

We consider the initial boundary value problem for the homogeneous time-fractional diffusion equation $\partial_t^\alpha u - \Delta u = 0$ ($0 < \alpha < 1$) with the initial condition $u(x, 0) = v(x)$ and a homogeneous Dirichlet boundary condition in a bounded polygonal domain Ω . We shall study two semidiscrete approximation schemes, the Galerkin FEM and lumped mass Galerkin FEM, by using piecewise linear functions. We establish optimal with respect to the regularity error estimates, including the cases of smooth initial data, $v \in H^2(\Omega) \cap H_0^1(\Omega)$, and nonsmooth initial data, $v \in L_2(\Omega)$.

For semidiscrete Galerkin finite element method on for quasi-uniform meshes and $t > 0$ we have derived the following family o

$$\|u_h(t) - u(t)\| + h\|\nabla(u_h(t) - u(t))\| \leq Ch^2 \ell_h t^{-\alpha(1-\frac{q}{2})} \|v\|_q, \quad \ell_h = |\ln h|,$$

where $\|\cdot\|_q$ is the norm in the space $H^q(\Omega)$, $0 \leq q \leq 2$. Obviously, for $q = 0$ the convergence rate deteriorates for $t \rightarrow 0$.

For the lumped mass method we have established similar results. However, the optimal L_2 -norm error estimate is valid only under additional assumption on the mesh, which in two dimensions is known to be satisfied for symmetric meshes. Finally, we presents numerical experiments that shed insight into the reliability of the theoretical study.

Boundary value problems for fractional PDE and their numerical approximation

B. Jovanović, L. Vulkov and A. Delić

The use of fractional partial differential equations in mathematical models has become increasingly popular in recent years. Such equations are used for the description of large classes of physical and chemical processes that occur in media with fractal geometry, disordered materials, amorphous semiconductors, viscoelastic media as well as in the mathematical modelling of economic, biological and social phenomena.

Because of the integral in the definition of the fractional order derivatives, it is apparent that these derivatives are nonlocal operators. This explains one of their most significant uses in applications: noninteger derivatives possess a memory effect which it shares with several materials such as viscoelastic materials or polymers. On the other side, this feature of the fractional derivatives makes the design of accurate and fast numerical methods difficult.

In this paper we present some examples of fractional PDE and highlight the main theoretical and numerical problems appearing. In particular, we emphasize some interface and transmission problems related with fractional PDE.

Mathematical modeling of refraction anomalies on the higher-order aberrations

A. Kachanov, V. Kornikov and T. Kaunenko

The higher-order aberrations in emmetropic eyes and eyes with keratoconic are analyzed. Aberration functions can be represented as expansion in power series or in orthogonal Zernike polynomials. Statistically significant differences between eyes with keratoconic and all other groups are revealed. Higher-order aberrations and coma-like aberrations, especially Zernike polynomials $Z(3, 1)$ are significant higher in the keratoconic eyes.

Method of lines and finite difference schemes with exact spectrum for solving some problems of mathematical physics

H. Kalis, S. Rogovs and A. Gedroics

We study linear initial-boundary value problems of mathematical physics with different types of the homogeneous boundary conditions (BCs), using for the space discretization the finite difference scheme of the second order approximation (FDS) and the finite difference scheme with exact spectrum (FDSES). The solution in the time (the method of lines) is obtained analytically and numerically with continuous and discrete Fourier methods. Using the spectral method for BCs of the third kind are obtained new transcendental equation and algorithm for solving the last two eigenvalues and eigenvectors of the finite difference scheme. This algorithm depends on the parameter $Q = \frac{l\sigma_1\sigma_2}{\sigma_1+\sigma_2}$, where σ_1, σ_2 are the heat transfer coefficients and l is the length. We define the FDSES method with the finite difference matrix A in the form $A = WDW^T$ (W, D are the matrices of the finite difference eigenvectors and eigenvalues), where elements of the diagonal matrix D are replaced with the first $N + 1$ (number of grid points) eigenvalues of the differential operator. The advantages of the FDSES in the case of the first kind and periodical BCs are demonstrated via several numerical examples in comparison with well-known methods of finite difference schemes.

The numerical solution of the inverse problem for the shallow water models

E. Karepova and E. Dementyeva

Shallow water models adequately describe a large class of natural phenomena such as large-scale free surface waves arising in seas and oceans, tsunamis, flood currents, surface and channel run-offs, gravitation oscillation of the ocean surface.

In this paper the problem of long-wave propagation in a large water area is considered. The mathematical model of the shallow water equations on a spherical surface is used. The boundary of numerical domain consists of the coastline ("hard") part and open-water ("liquid") part. In general case the influence of the ocean through the open-water part of the boundary is uncertain. Therefore the boundary conditions contain special unknown function at "liquid" part of boundary which to be determined together with velocity and free surface level. Thus, the ill-posed inverse problem to the reconstruction of the boundary function is considered.

To solve this problem we use additional information, e.g. observation of free surface level on a part of the boundary. We investigate some approaches to regularization of our ill-posed problem using adjoint operators and optimal control theory. The advantages and disadvantages of each regularizer are researched. As a result, the solving of the inverse problem is iterative process on alternate solutions of direct and adjoint equations. The differential problems are reduced to algebraic ones by the finite element method. Parallel software using MPI is developed.

Numerical experiments of data recovery are carried out on the sea of Okhotsk region. We use the model observation data of different smoothness - smooth, with white noise, with gaps.

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The collocation method in the problem of bickling of plates with a hole

S. Kashtanova and N. Morozov

The collocation method is used to study buckling under uniaxial loading of an infinite plate weakened by circular hole taking into account the effect of surface stresses. It was shown previously that the global energy minimum in considered problem is lower than in the classical Kirsch problem. Here the collocation method is applied to find the approximate eigenvalue and to solve the buckling problem.

Numerical solution for nonlinear fourth order boundary value problems based on non-polynomial sextic spline

P. Khandelwal and A. Khan

In this paper, non-polynomial sextic spline function is used for the numerical solution of fourth-order nonlinear problems two-point boundary value problems. Spline relations are derived and direct methods of order two, four and six have been obtained. Convergence analysis of methods has been discussed. The proposed method is tested on linear and nonlinear problems. Comparisons are made to confirm the reliability and accuracy of the proposed technique.

A software tool for modelling of three-phase mass transition with an application in atmospheric chemistry

N. Kochev and A. Terziyski

A software tool for modelling of mass transfer physicochemical processes is presented. It is a Java based library for simulation of sorption processes occurring in the atmosphere. The main goal of the software is to provide an efficient theoretical frame for interpretation of the results obtained from Coated Wall Flow Tube (CWFT) reactor experiments. The numerical calculations are based on Langmuir adsorption theory and second Fick's law, which describes the diffusion processes. Additionally the library provides functionality for interfacing ice surface adsorption/desorption processes with the ice bulk diffusion. We describe different numerical approaches for modelling the mass transfer through the surface area. The system can be applied to simulate the processes occurring in a CWFT reactor or for detailed investigation in a small closed segment. The main usage of the system is to estimate the basic kinetic rate constants that characterize the processes. Estimation is obtained by fitting the laboratory measurements from the reactor with the simulated curves.

Application of Numerical Analysis in Virology

M. Kolev and A. Benova

During several last decades mathematical models have been successfully used in biology and medicine. Our paper is an application of mathematical modelling approach in the field of virology. Viruses are among the main agents causing various diseases, some of which are very dangerous like AIDS, Hepatitis B and C, T cell leukemia virus (HTLV-1) etc. We study the influence of increased body temperature due to viral infection on humoral immune response by the use of a mathematical model of Boltzmann-type. The humoral immunity together with cellular immunity are the main defensive mechanisms of the organisms to fight infections. Humoral immunity is performed by antibodies produced by B cells.

The model considers the activities of the main interacting populations. The aim of the paper is to develop an effective numerical procedure for solving the complicated system of partial integro-differential equations. Numerical results of the model are presented. The role of some parameters of the model and analyzed from the point of view of virology.

Two positivity preserving flux limited, second-order numerical methods for a Haptotaxis model

M. Kolev, M. Koleva and L. Vulkov

Two numerical methods for a one-dimensional haptotaxis model, that exploit the use of van Leer flux limiter are developed and analyzed. Conditions for mesh spacing, time step size and flux limiting are given for such formulation that ensure the non-negativity of the discrete solution (positivity of the corresponding ODE system) and second-order accuracy in space. Another advantage is that we avoid solving a large nonlinear systems of algebraic equations. The discrete preservation of conservation/evolution integral laws of the continuous solution is also verified for the numerical solution. Numerical results concerning accuracy, convergence rate, positivity and conservation properties are presented and discussed. Because of the efficient way in which they determine the space discretization, the methods can be also implemented for the corresponding two or three-dimensional problems.

A multicomponent alternating direction method for numerical solving of boussinesq paradigm equation

N. Kolkovska and K. Angelov

We study the Cauchy problem for Boussinesq Paradigm Equation (BPE)

$$\frac{\partial^2 u}{\partial t^2} = \Delta u + \beta_1 \Delta \frac{\partial^2 u}{\partial t^2} - \beta_2 \Delta^2 u + \alpha \Delta f(u), \quad x \in \mathbb{R}^2, \quad 0 < t \leq T, \quad T < \infty$$

on the unbounded region \mathbb{R}^2 with asymptotic boundary conditions

$$u(x, t) \rightarrow 0, \quad \Delta u(x, t) \rightarrow 0, \quad |x| \rightarrow \infty.$$

We construct and analyze a multicomponent alternating direction method for the numerical solution of this problem. In contrast to the standard splitting methods, at every time level a vector of two discrete solutions is found. The method provides full approximation to BPE and is efficient in implementation.

A conservation law and the unconditional stability are proved for the difference scheme of the linearized BPE. We also prove that the error of the discrete solution of the nonlinear problem is of second order of convergence in space and of first order in time.

The method is implemented numerically. The numerical tests confirm the theoretical rate of convergence.

Maximum norm a posteriori error estimates for classical and singularly perturbed parabolic equations

N. Kopteva and T. Linss

For classical and singularly perturbed semilinear parabolic equations, we give computable a posteriori error estimates in the maximum norm, which, in the singularly perturbed regime, hold uniformly in the small perturbation parameter. The parabolic equations are discretized in time using the backward Euler, Crank-Nicolson and discontinuous Galerkin methods. Both semidiscrete (no spatial discretization) and fully discrete cases will be considered. The analysis invokes certain bounds for the Green's function of the parabolic operator. When dealing with the full discretizations, we also employ the elliptic reconstruction technique.

In the final part of the talk, we shall briefly discuss our current work on a posteriori error estimation for moving-mesh methods in the context of singularly perturbed parabolic equations.

Controls twist in the numerical model flow continuum

V. Korobitsyn

In the modern practice of mathematical modeling of physical processes of continuum, discrete operators, forming schemes for oblique moving grids do not satisfy the identity $\mathbf{ROTGRAD} = 0$ for the discrete operator \mathbf{GRAD} included in the momentum equation. The consequence is not the fulfillment of the discrete level, the theorems of conservation of circulation, and the potentiality of irrotational flow. Discrete models, complying with the identity $\mathbf{ROTGRAD} = 0$ is called a "potential" or vortex agreed. Note that for a regular rectangular, uniform grids, this problem does not arise.

The fundamental problem is defined as the construction of vortex agreed difference schemes for oblique 2D grids. The relations of the discrete vector analysis $\mathbf{ROTGRAD} = 0$ performed for the discrete operator \mathbf{GRAD} in the discrete momentum equation and the the range of value for is coincide with the domain of the discrete operator \mathbf{ROT} . The need to establish such schemes follows from the hypothesis that a vortex approximation has a significant impact on the unphysical distortion (tangling and spurious vorticity) of the Lagrangian computational grid cells. The solutions obtained on the basis of "potential" of difference schemes for 2D oblique grids will serve to confirm or refute this hypothesis.

The main aim is to create effective of vortex agreed numerical algorithms inherit the basic properties of approximated differential equations in partial derivatives, and performing the discrete analogue of the relationship $\mathbf{ROTGRAD} = 0$, as a continuum relations $\mathbf{rotgrad} = 0$ for the operator \mathbf{GRAD} in the discrete momentum equation. Checking the efficiency of the numerical solutions of nonlinear problems in mathematical physics. Model calculations of irrotational flows.

Modified method of characteristics combined with finite volume element methods for incompressible miscible displacement problems in porous media

S. Kumar

The incompressible miscible displacement problem in porous media is modeled by a coupled system of two nonlinear partial differential equations, the pressure-velocity equation and the concentration equation. In this paper, we present a mixed finite volume element method (FVEM) for the approximation of the pressure-velocity equation. Since modified method of characteristics(MMOC) minimizes the grid orientation effect, for the approximation of the concentration equation we apply a standard FVEM combined MMOC. A priori error estimates in are derived for velocity, pressure and concentration. Numerical results are presented to substantiate the validity of the theoretical results.

Numerical and analytical modeling of elliptic thin plate vibrations

A. Lebedev, A. Smirnov and E. Zhukova

Free vibrations of an elliptic thin plate with an elliptic cut-out are modeled by means of analytic and numerical methods. The analytic solution for an elliptic plate with co-centric elliptic hole is obtained in Mathieu functions. The obtained characteristic equation is solved numerically and asymptotically for the small ratio of plate and hole sizes. The analytical results and the results of FEM analysis are compared. Finally an elliptic plate with cutout of other types is studied numerically.

GOES system - general description

V. Marinov

The GOES project is funded under the Civil protection financial instrument launched by DG ECHO of EU, which aims to increase preparedness, awareness and maximum cooperation between public authorities of different member states through quick and effective responses in crisis situations. The authorities involved in the GOES project are: Province of Ancona (Lead partner), Marche region, Local Police of Valencia, Municipality of Sofia and the Institute of Information and Communication Technologies Bulgarian Academy of Sciences. The common idea for the project consortium is fast and better response to emergency situations avoiding the disorganization, delays or deficiencies in communication between local actors involved in emergency management. The system designed under GOES project framework is done in a way to share information on some issues, related to traffic management. The system will allow the interaction between mobile groups on the roads and devices called "mobile" such as PDA or tablet, and Server based environment to exchange data via the web application and support the everyday work of the responsible authorities. This is developed with various services available as open source including those communication, management and publication of information in a geographic context. The software architecture is 3-layer based and its components are used to create user friendly environment for data collection, data exchange and data storage. Sofia municipality will implement the software tool as pilot project in its department for civil protection and citizen's safety.

On a research of hybrid methods

G. Mehdiyeva, V. Ibrahimov and M. Imanova

As is known, the use of hybrid methods for solving applied problems dates from the mid-twentieth century. Construction of multi-step methods of hybrid type and their application to solving the ODE is associated with the names Gere and Butcher, one-step methods of hybrid type with the names Hamer and Hall. Given the high accuracy of hybrid methods, the experts examined the use of hybrid methods for solving integral and integro-differential equations. The use of hybrid methods for solving integral equations belongs to Makroglou. Here, developing the idea, explored a more general hybrid method applied to solving Volterra integral equations and constructed a concrete method with the degree $p = 8$. However, the appropriate known methods are of level $p \leq 4$. Consider to numerical solution of the following Volterra integral equation:

$$y(x) = f(x) + \int_{x_0}^x K(x, s, y(s))ds, \quad x \in [x_0, X]. \quad (1)$$

We assume that equation (1) has a unique solution defined on an interval $[x_0, X]$. To determine the numerical solution of equation (1), we divided the segment $[x_0, X]$ with a constant step into equal parts and define the terms of partitions in the form $x_i = x_0 + ih$, ($i = 0, 1, \dots, N$).

The method applied by Makroglou to solving nonlinear Volterra integral equation is as follows:

$$\sum_{i=0}^k \alpha_i y_{n+i} = h \sum_{i=0}^k \beta_i g_{n+i} + h\beta_m g_{n+m}, \quad (y' = g(x, y), \quad m \in 0, 1, \dots, k). \quad (2)$$

Two grid decoupling method for parabolic transmission problem on disjoint domain

Z. Milovanović

In this paper we investigate a two-grid decoupling method for solving parabolic problems on disjoint domain. A priori estimates for weak solutions in appropriate Sobolev-like space are proved. A finite difference scheme approximating this problem is proposed and analyzed.

A direction splitting algorithm for flow problems in complex/moving geometries

P. Mineev

An extension of the direction splitting method for the incompressible Navier-Stokes equations proposed in earlier, to flow problems in complex, possibly time dependent geometries will be presented. The idea stems from the idea of the fictitious domain/penalty methods for flows in complex geometry. In our case, the velocity boundary conditions on the domain boundary are approximated with a second-order of accuracy while the pressure subproblem is harmonically extended in a fictitious domain such that the overall domain of the problem is of a simple rectangular/parallelepiped shape.

The new technique is still unconditionally stable for the Stokes problem and retains the same convergence rate in both, time and space, as the Crank-Nicolson scheme. A key advantage of this approach is that the algorithm has a very impressive parallel performance since it requires the solution of one-dimensional problems only, which can be performed very efficiently in parallel by a domain-decomposition Schur complement approach. Numerical results illustrating the convergence of the scheme in space and time will be presented. Finally, the implementation of the scheme for particulate flows will be discussed and some validation results for such flows will be presented.

Finite element method for the stratified liquid internal wave equation

M. Moskalkov and D. Utebaev

In the paper, the spatial and time schemes of the finite element method for solving the combined boundary value problem for the stratified liquid internal wave equation are proposed and analyzed. For the problem under consideration, the estimates of accuracy of the corresponding schemes are obtained. The comparison of the analyzed schemes with the known schemes is performed by using variance analysis.

Hybrid numerical scheme for singularly perturbed problems of mixed parabolic-elliptic type

K. Mukherjee and N. Srinivasan

Here, we consider the following class of singularly perturbed mixed parabolic-elliptic problems posed on the domain $G^- \cup G^+$, $G^- = (0, \xi) \times (0, T]$, $G^+ = (\xi, 1) \times (0, T]$:

$$\left\{ \begin{array}{l} \left(\frac{\partial u}{\partial t} - \varepsilon \frac{\partial^2 u}{\partial x^2} + b(x, t)u \right) (x, t) = f(x, t), \quad (x, t) \in G^-, \\ \left(-\varepsilon \frac{\partial^2 u}{\partial x^2} - a(x, t) \frac{\partial u}{\partial x} + b(x, t)u \right) (x, t) = f(x, t), \quad (x, t) \in G^+, \end{array} \right.$$

where $0 < \varepsilon \ll 1$ is a small parameter and the coefficients a, b are sufficiently smooth functions and the source term f is sufficiently smooth on $G^- \cup G^+$ such that $a(x, t) > 0$, $x > \xi$, $b(x, t) \geq 0$ on $\bar{G} = [0, 1] \times [0, T]$, with suitable initial boundary conditions and the interface condition at $x = \xi$.

To solve this problem, the time derivative is discretized by the classical backward- Euler method, while for the spatial discretization a hybrid finite difference scheme is proposed. The proposed method is analyzed on a layer resolving piecewise-uniform Shishkin mesh and is shown to be ε -uniformly convergent with almost second-order spatial accuracy in the discrete supremum norm. Finally numerical results are presented to validate the theoretical results.

Simulation of interactions solid particles and gases in the planar channel

A. Naimanova and T. Usseanova

The characteristics gas-solid turbulent flow, heat transfer, devolatilization particles and combustion process in the planar channel is simulated. Mathematical models involve two stages, where, the gas phase flow in Eulerian, particles in Lagrangian approaches is modeled correspondingly. The gas flow is described by Reynolds-Averaged Navier-Stokes system of equations, closed by $\kappa - \varepsilon$ model turbulence and is solved using control volume method numerically. The constructed computer code allows to make the detailed analysis of coal combustion in two-dimensional channel of complex shapes.

Localization and formation of stationary internal layers in nonlocal reaction-diffusion-advection problems

A. Nikitin and N. Nefedov

Problems for nonlocal reaction-diffusion-advection equations describe many important practical applications in chemical kinetics, synergetics, astrophysics, biology, etc. In many important cases the solutions of these problems feature internal layers. We consider initial boundary value problem for integro-parabolic the equation

$$\varepsilon \frac{\partial u}{\partial t} = \varepsilon^2 \frac{\partial^2 u}{\partial x^2} - \varepsilon A(x, \varepsilon) \frac{\partial u}{\partial x} - f(u) - \int_0^1 G(u(x, t), u(s, t), x, s, \varepsilon) ds, \quad 0 < x < 1, t > 0,$$

$$\frac{\partial u}{\partial x}(0, t) = \frac{\partial u}{\partial x}(1, t) = 0, \quad u(x, 0) = u^0(x),$$

where $\varepsilon > 0$ is a small parameter. The main results of work are

1. We have received the equation to find localization points of moving fronts and stationary internal layers. We show how to use this information for numerically-analytic investigation of the problem.
 2. We have constructed uniform asymptotic of solutions with an internal layer and estimate the accuracy of this asymptotics.
 3. We have found essentially the domain of attraction of the stationary solution - a set of initial functions $u^0(x)$ such that the stable stationary internal layers are formed from this initial functions. The example from applications described by activator-inhibitor system will be presented.
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Boundary value problems on polyhedral domains and applications to numerical methods

V. Nistor

I will first review some of the issues and earlier results on boundary value problems on polyhedral domains. The main lesson is that there is a 'loss of regularity' for boundary value problems on singular domains if the usual Sobolev spaces are used. This is inconvenient however in practical applications such as the Finite Element Method. An alternative approach is to use 'weighted Sobolev' spaces. Then one can then restore full regularity for elliptic problems on such domains under the additional condition of that there are no 'Newmann-Newmann' corners or edges (this result is joint result with Bacuta, Mazzucato, and Zikatanov). The case of 'Newmann-Newmann' corners requires some additional ideas. I will then present some results in this case in two dimensions and how they can be used to construct sequences of Finite Element Spaces that provide quasi-optimal approximation rates for transmission and pure Neumann problems (joint work with Mazzucato and Li). This method is then generalized to three dimensions.

Numerical experiments with a Shishkin numerical method for a singularly perturbed quasilinear parabolic problem with an interior layer

E. O' Riordan and J. Quinn

Abstract. In Russ. Acad. Dokl. Math., 48, 1994, 346352, Shishkin presented a numerical algorithm for a quasilinear time dependent singularly perturbed differential equation, with an internal layer in the solution. In this paper, we implement this method and present numerical results to illustrate the convergence properties of this numerical method.

Verified solutions of sparse linear systems

T. Ogita

To solve linear systems is ubiquitous since it is one of the basic and significant tasks in scientific computing. Floating-point arithmetic is widely used for this purpose. Since it uses finite precision arithmetic and numbers, rounding errors are included in computed results. To guarantee the accuracy of the results, there are methods so-called verified numerical computations based on interval arithmetic.

In this talk algorithms for calculating verified solutions of sparse linear systems are proposed. The proposed algorithms are based on standard numerical algorithms for a block LDL^T factorization and error estimates for specified eigenvalues by Lehmann's theorem. Numerical results are presented for illustrating the performance of the proposed algorithms.

A new block second derivative backward differentiation formula with symmetric quadratures for initial value problems in ordinary differential equations

S. Okunuga , J. Ehigie and A. Sofoluwe

Continuous multistep schemes derived from multistep collocation technique have been used extensively in the literatures- to derive a large family of numerical methods for the solution of ODE, ranging from linear multistep to Runge-Kutta methods. In this paper, a block second derivative backward differentiation formula with symmetric quadratures as hybrid points is derived from continuous multistep schemes. Some properties such as the linear stability analysis of the linear multistep formulae is investigated as a block and the region of absolute stability is presented. The Block method is implemented such that the problem is transformed to a system of non-linear equations, thereby obtaining numerical solutions at several points concurrently. Some standard problem are solved to show the effectiveness of the method. 1

Multiscale convection in one dimensional singularly perturbed convection–diffusion problems

E. O’Riordan and J. Quinn

Linear singularly perturbed ordinary differential equations of convection diffusion type are considered. The convective coefficient varies in scale across the domain which results in interior layers appearing in areas where the convective coefficient decreases from a scale of order one to the scale of the diffusion coefficient. Appropriate parameter-uniform numerical methods are constructed and their numerical performance is discussed.

High performance computing of data for a new sensitivity analysis algorithm, applied in an air pollution model

T. Ostromsky, I. Dimov, R. Georgieva, P. Marinov and Z. Zlatev

Variance-based sensitivity analysis approach has been proposed for studying of input parameters’ error contribution into the output results of a large-scale air pollution model - the Danish Eulerian Model in its recent unified version (UNI-DEM). It is a powerful air pollution model, used to calculate the concentrations of various dangerous species over a large geographical region (including whole Europe). The model takes into account the main physical and chemical processes between these species, the actual meteorological conditions, emissions, etc. . Among the input data sets of UNI-DEM, the antropogenic emissions are some of the most important and expensive to be evaluated precisely. On the other hand, strong and costly measures are recently being taken in most developed countries to cut off these emissions, which results in a stable trend to reduction (with uneven rate for the different countries and species). That is why it is important to know with more certainty the effect of various emission changes on the expected output concentrations and particularly on those of the most dangerous pollutants. The sensitivity analysis study discussed in this paper would help to get more definite answers to that questions as well.

A 3-stage sensitivity analysis approach, based on analysis of variances technique for calculating Sobol global sensitivity indices and computationally efficient Monte Carlo integration techniques, has recently been developed and successfully used for SA study of UNI-DEM with respect to several chemical reaction rate coefficients. As a first stage it is necessary to carry out a set of computationally expensive numerical experiments and to extract the necessary multidimensional sets of sensitivity analysis data. A specially adapted for that purpose version of the model, called SA-DEM, was created, implemented and run on IBM Blue Gene/P , the most powerful parallel supercomputer in Bulgaria. Its capabilities have been extended to be able to perturb the 4 different input data sets with antropogenic emissions, either separately or altogether. The refined (480 x 480) mesh version of the model is used in our current experiments, which is more challenging computational problem even on such a powerful supercomputer like IBM BlueGene/P and required optimization of the parallelization strategy, as well as the memory use. Tables with performance results of our numerical experiments on IBM BlueGene/P will be presented and analysed.

The increasing power of the computational grid structures is also quite attractive for such kind of problems. We prepared also a grid version of the extended abilities SA-DEM version. Performance results from the Grid implementation will be also presented, analysed and compared to these on the supercomputer.

Application of error-free transformation for matrix multiplication

K. Ozaki and T. Ogita

This talk is concerned with accurate computations in numerical linear algebra. If a problem is ill-conditioned, then it is difficult to obtain an accurate solution of the problem by finite precision arithmetic such as floating-point arithmetic. To overcome this problem, some iterative algorithms with higher precision arithmetic for matrix computations have been developed, for example, accurate matrix inversion by Rump and accurate matrix factorization by Ogita. The algorithms require a routine for accurate matrix multiplication.

Recently, the authors developed an error-free transformation for matrix multiplication. It transforms a product of two matrices into a sum of floating-point matrices. This transformation is useful for accurate matrix computations. We specialize the transformation and apply it to the iterative algorithms by Rump and Ogita. Finally, we present numerical examples to illustrate the efficiency of our algorithms.

Condition and error estimates in kalman filter design

P. Petkov, M. Konstantinov and N. Christov

Kalman filters play a key role in the solution of the main linear optimal control and estimation problems. The Kalman filter design consists in finding the filter gain matrix determined by a matrix Riccati equation. As it is well known the numerical solution of this equation may face some difficulties. First, the equation may be ill conditioned, i.e. small perturbations in its coefficient matrices may lead to large variations in the solution. Therefore, it is necessary to have a quantitative characterization of the conditioning in order to estimate the accuracy of solution computed. The second difficulty is connected with the stability of the numerical method and the reliability of its implementation. It is well known that the methods for solving the Riccati equations are generally unstable. This requires to have an estimate of the forward error in the solution. The paper deals with the computation of condition numbers and residual-based forward error estimates pertaining to the numerical solution of Riccati equations arising in the continuous-time Kalman filter design. Efficient LAPACK-based condition and error estimators are proposed involving the solution of triangular Lyapunov equations along with one-norm computation.

Numerical methods for evolutionary equations with delay and software package PDDE

V. Pimenov and A. Lozhnikov

In the paper the grid-based numerical algorithms for solving the evolutionary equations (parabolic and hyperbolic) with the effect of heredity on a time variable are considered. The algorithms are based on the idea of dividing the discrete prehistory into past and present parts. By the present part (current state of required function) we construct the full analogs of the algorithms, known for objects without delay. To take into account the past part we use interpolation with preset properties. This approach leads to the systems of difference equations with the effect of heredity. The main problems associated with nonlinear dependence of difference equations from prehistory of discrete model are overcome by earlier proposed approach to construction of a general scheme of the numerical solution of the functional-differential equations, which allows us to investigate a local error, stability and convergence of systems with heredity.

From uniform positions we construct analogs of schemes with weights for the one-dimensional heat conduction equation with delay of general form, analog of a method of variable directions for the equation of parabolic type with time delay and two spatial variables, analog of the scheme with weights for the equation of hyperbolic type with delay. For the one-dimensional heat conduction equation and the wave equation we obtained conditions on the weight coefficients that ensure stability on the prehistory of the initial function.

Numerical algorithms are implemented in MATLAB in the form of a software package Partial Delay Differential Equations (PDDE) toolbox. The package contains the programs of numerical solution of parabolic equations with one and two spatial variables and equations of hyperbolic type. These equations can contain lumped variable delays as well some types of distributed (integral) delays.

Numerical and asymptotic modeling of vibrations of a beam with variable parameters

E. Pomytkina and A. Smirnov

Free vibrations of a prismatic beam with arbitrary varied geometrical and material parameters are analysed. Natural vibrational frequencies are sought in the first and second approximations with the help asymptotic technique. As an example the perturbations of linear and quadratic types are considered. The obtained asymptotic results are compared to the numerical (FEM) results.

Convergence of the Nessyahu-Tadmor scheme for bounded initial data

B. Popov

Non-oscillatory high-order schemes are widely used in numerical approximations of nonlinear conservation laws. It is well known that their typical representatives do not satisfy the so-called strict cell entropy inequalities and therefore convergence results for such schemes are difficult to obtain. Using the theory of compensated compactness, we show that in the case of a scalar strictly convex conservation law with bounded initial data, the second order Nessyahu-Tadmor (NT) scheme based on a MAPR-like limiter converges strongly on compact sets to the unique entropy solution of the conservation law.

Numerical method for a singularly perturbed quasilinear parabolic problem with an interior layer

J. Quinn

In [G.I. Shishkin, Difference Approximation of the Dirichlet Problem for a Singularly Perturbed Quasilinear Parabolic Equation in the Presence of a Transition Layer, *Russian Acad. Sci. Dokl. Math.*, (1994) **48**(2) 346-352.], Shishkin presented and analysed a numerical method for the following type of singularly perturbed parabolic problem

$$\begin{aligned}(\varepsilon u_{xx} - uu_x - bu - u_t)(x, t) &= f(x, t), \quad (x, t) \in G := (-1, 1) \times (0, T] \\ b(x, t) &\geq 0, \quad (x, t) \in \bar{G}, \quad u(x, t) = \phi(x, t), \quad (x, t) \in \bar{G} \setminus G, \\ \phi(0, t) &> 0, \quad \phi(1, t) < 0, \quad \phi(d, 0) = 0, \quad \phi = \phi_0 + \phi_1, \\ \|\phi_0'\| &\leq C, \quad \left| \frac{\partial^k}{\partial x^k} \phi_1(x, t) \right| \leq C\varepsilon^{-k} e^{-C|d-x|/\varepsilon}, \quad 1 \leq k \leq 5, \quad (x, t) \in \bar{G} \setminus G.\end{aligned}$$

In this paper, we implement this method and present numerical results to illustrate the convergence properties of the method in practice.

Numerical computation of basic hypergeometric functions

P. Rajković, S. Marinković and M. Stanković

Basic numerical functions, like analogies of the corresponding elementary functions, has a lot of nice properties and satisfy the cognizable identities. But, because of finite and infinite products presence, their numerical evaluation requires careful research. The special attention will be devoted to q -shifted power

$$(a; q)_n = \prod_{k=0}^{n-1} (1 - aq^k), \quad (n \in N_0 \cup \{\infty\}), \quad (a; q)_\lambda = \frac{(a; q)_\infty}{(aq^\lambda; q)_\infty} \quad (\lambda \in C).$$

The numerical methods for infinite products are based on the Euler identity, Jacobi's triple product identity or recursive formulas. Also, a method interpolation type for the functions with two variable is developed. Hence we will consider evaluation of basic hypergeometric functions

$${}_r\Phi_s \left(\begin{matrix} a_1, \dots, a_r \\ b_1, \dots, b_s \end{matrix} \middle| q; z \right) = \sum_{n=0}^{\infty} \frac{(a_1, \dots, a_r; q)_n}{(b_1, \dots, b_s; q)_n} \left((-1)^n q^{n(n-1)/2} \right)^{1+s-r} \frac{z^n}{(q; q)_n}.$$

Based on it, computation problems for q -analogs of the elementary functions will be discussed.

Finally, we will expose a few methods for numerical solving of equations with so introduced functions.

Interior layers in coupled system of two singularly perturbed reaction-diffusion equations with discontinuous source term

S. Rao and Sheetal Chawla

We study a coupled system of two singularly perturbed linear reaction- diffusion equations with discontinuous source term. A central difference scheme on layer-adapted piecewise-uniform mesh is used to solve the system numerically. The scheme is proved to be almost first order uniformly convergent, even for the case in which the diffusion parameter associated with each equation of the system has a different order of magnitude. Numerical experiments are conducted to support the theoretical results.

Numerical solution of the coupled reaction-diffusion system by quintic b-spline collocation method

A. Rashid

The mathematical model of Reaction-diffusion equations represents a wide variety of physical, chemical, and biological processes. Tumor growth can be modeled by reaction-diffusion systems. The reaction diffusion equations have been used to model tissue development through the spatial and temporal distribution of morphogenesis. The process of Protein trafficking in cells involves can be modeled by reaction-diffusion equations. The development of efficient numerical methods for reaction-diffusion equations and particularly for coupled Reaction Diffusion system has been an active area of research. The collocation method using quintic B-spline is derived for solving the coupled Reaction Diffusion system. The method is based on CrankNicolson formulation for time integration and quintic B-spline functions for space integration. The von Neumann stability is used to prove that the scheme is unconditionally stable. Newtons method is used to solve the nonlinear block pentadiagonal system obtained. Numerical tests for single, two, and three solitons are used to assess the performance of the proposed scheme.

Finite differences method for the first order 2-D partial equation

M. Rasulov, E. Sahin and M. Soguksu

In this study a method for finding the exact and numerical solution of the Cauchy problem for the two dimensional scalar equation

$$\frac{\partial u(x, y, t)}{\partial t} + \frac{\partial F_1(u(x, y, t))}{\partial x} + \frac{\partial F_2(u(x, y, t))}{\partial y} = 0, \quad (1)$$

$$u(x, y, 0) = u_0(x, y) \quad (2)$$

is suggested. Here, the given functions $F_i(u)$, ($i = 1, 2$) satisfy some conditions that show the nature of these functions.

It is known that the classical solution of the problem (1), (2) does not exist. In order to find the weak solution of the problem (1), (2) the following special auxiliary problem

$$\frac{\partial v(x, y, t)}{\partial t} + \int_b^y F_1(u(x, \eta, t)) d\eta + \int_a^x F_2(u(\xi, y, t)) d\xi = 0, \quad (3)$$

$$v(x, y, 0) = v_0(x, y). \quad (4)$$

Here the function $v_0(x, y)$ is any smoother solution of the equation $\frac{\partial^2 v_0(x, y)}{\partial x \partial y} = u_0(x, y)$.

Theorem *If the function $v(x, y, t)$ is solution of the auxiliary problem (3), (4), then the function $u(x, y, t)$ expressed by $u(x, y, t) = \frac{\partial^2 v(x, y)}{\partial x \partial y}$ is a weak solution of the main problem (1) and (2).*

The special auxiliary problem whose solution is more smoother than the solution of the main problem is introduced, which makes possible to develop efficient and sensitive algorithms that describe all physical properties of the investigated problem accurately.

Hybrid functions for nonlinear differential equations with applications to physical problems

M. Razzaghi

Orthogonal functions have been used when dealing with various problems of the dynamical systems. The main advantage of using orthogonal functions is that they reduce the dynamical system problems to those of solving a system of algebraic equations. The approach is based on converting the underlying differential equation into an integral equation through integration, approximating various signals involved in the equation by truncated orthogonal functions, and using the operational matrix of integration to eliminate the integral operations. This matrix can be uniquely determined based on the particular orthogonal functions. The Bernoulli polynomials and Taylor series are not based on orthogonal functions, nevertheless, they possess the operational matrix of integration. In the present work, we first solve the nonlinear ordinary differential equations. We then solve a variety of physical problems which fall into this category. This method consists of reducing the solution of nonlinear differential equations to a set of algebraic equations by first expanding the candidate function in terms of hybrid functions with unknown coefficients. These hybrid functions which consist of block-pulse functions and Bernoulli polynomials, are presented. The operational matrix of integration is introduced. This matrix together with the properties of hybrid functions, are then utilized to evaluate the unknown coefficients for the solution of nonlinear differential equations. The numerical solutions are compared with available exact or approximate solutions in order to assess the accuracy of the proposed method.

Modelling of a fed-batch culture applying simulated annealing

Ol. Roeva and T. Trenkova

Mathematical forms and their parameters used to describe cell behaviors constitute the key problem of bioprocess modelling, in practical, in parameter estimation. The model building leads to information deficiency and to non unique parameter identification. While searching for new, more adequate modeling metaphors and concepts, methods which draw their initial inspiration from nature have received the early attention. In this paper a Simulated Annealing (SA) algorithm is proposed to identify the unknown parameters in a non-linear mathematical model of a fed-batch cultivation process. SA as an optimization technique was first introduced to solve problems in discrete optimization, mainly combinatorial optimization. Subsequently, this technique has been successfully applied to solve optimization problems over the space of continuous decision variables. This meta-heuristic algorithm is a stochastic relaxation technique, using the Metropolis algorithm based on the Boltzmann distribution in statistical mechanics, for solving nonconvex optimization problems. SA can deal with arbitrary systems and cost functions; statistically guarantees finding an optimal solution (SA has the ability to avoid getting stuck at local minima); guarantees a convergence upon running sufficiently large (infinite) number of iterations; is relatively easy to code, even for complex problems. This makes annealing an attractive option for optimization problems.

A set of unstructured models is suggested to model biomass growth, glucose utilization, acetate formation and oxygen consumption of a *E. coli* cultivation process. The non-linear model contains

5 state variables and 7 parameters. The model identification is carried out using experimental data from the *E. coli* MC4110 fed-batch cultivation process. In order to increase the performance of the SA algorithm the adjustments of its parameters depending on the considered problem is provided. With the appropriate choice of the SA parameters the accuracy of the estimates and the computing time could be optimized to a not inconsiderable degree.

The resulting non-linear model predicts adequate and with a high degree the variation of the considered state variables. Simulation results reveal that accurate and consistent estimates can be obtained using SA algorithm.

Qualocation for a singularly perturbed boundary value problem

H-G. Roos and Z. Uzelac

We consider the singularly perturbed boundary value problem

$$Lu := -\varepsilon u'' - bu' + cu = f \quad \text{in } (0, 1) \quad \text{with } u(0) = u(1) = 0,$$

where the parameter ε is small and positive, and b, c, f are smooth functions with $b(x) > \beta > 0$, and $c(x) > \gamma > 0$ in $[0, 1]$,

While the theory of finite element methods for solving the problem is well developed, there is not so much known concerning collocation based on splines of higher degree. It seems that the C^1 collocation method is not the optimal method for solving the problem because it requires non-optimal smoothness on the solution. Therefore we combine Galerkin and collocation in generating collocation method by Galerkin with an adapted quadrature rule. For solving boundary integral equations, this qualocation technique is well known. Using splines of degree r , we prove on a Shishkin mesh for the qualocation method

$$\|\tilde{u}_N - u\|_\varepsilon \leq C(N^{-1} \ln N)^r,$$

i.e., the same error estimate as for the Galerkin technique. We report the results of numerical experiments that support the theoretical findings.

Error estimates for finite element methods applied to singular perturbation problems

H-G Roos

First we consider the reaction-diffusion problem

$$\begin{aligned} \mathcal{L}u &:= -\varepsilon^2 \Delta u + cu = f \quad \text{in } \Omega \subset \mathbb{R}^2, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

where Ω is polygonal and convex, $0 < \varepsilon \ll 1$ and $f \in L_2(\Omega)$, $c \in C(\overline{\Omega})$ with $c \geq c_0 > 0$. We discretize with linear or bilinear elements on a shape-regular mesh. Then one can prove assuming some more regularity of f the uniform in ε estimate in the ε -weighted H^1 norm

$$\|u - u_h\|_\varepsilon \leq Ch^{1/2}.$$

Next we consider

$$-\varepsilon\Delta u - bu_x + cu = f \quad \text{in } \Omega = (0, 1)^2,$$

$$\frac{\partial u}{\partial x}\Big|_{x=0} = 0, \quad u|_{x=1} = 0 \quad \text{and} \quad u|_{y=0} = u|_{y=1} = 0.$$

We assume $b \in W^{1,\infty}(\Omega)$, $c \in L_\infty(\Omega)$, $b \geq \beta > 0$ with some constant β , $0 < \varepsilon \ll 1$ and

$$c + \frac{1}{2}b_x \geq \gamma > 0.$$

The problem is characterized by characteristic (or parabolic) boundary layers at $y = 0$ and $y = 1$, moreover due to the Neumann condition on the outflow boundary there exists a weak exponential layer. For that problem we obtain on a shape-regular mesh

$$\|u - u_h\|_\varepsilon \leq Ch^{1/3}.$$

Finally we study the same problem but with Dirichlet boundary conditions at the outflow boundary. We use a Shishkin mesh close to the exponential layer but do nothing for the characteristic layers. Then one can prove

$$\|u - u^N\|_\varepsilon \leq C \left(N^{-1/2} + (\varepsilon N)^{1/2} + N^{-1} \ln N \right).$$

Parallel program systems for problems of the dynamics of elastic-plastic and granular media

O. Sadovskaya

Parallel program systems for numerical solution of 2D and 3D dynamic problems on the basis of universal mathematical model describing small strains of elastic, elastic-plastic and granular media are worked out. In the case of elastic material the model is reduced to the system of equations, hyperbolic by Friedrichs, written in terms of velocities and stresses in a symmetric form. In the case of elastic-plastic material the model is a special formulation of the Prandtl–Reuss theory in the form of variational inequality with one-sided constraints on stresses. Generalization of the model to describe the deformation of a granular material is obtained by means of the rheological approach, taking into account different resistance of a material to tension and compression. Computational domain may have a block structure, composed of an arbitrary number of layers, strips in a layer and blocks in a strip from different materials with self-consistent curvilinear interfaces. At the external boundaries of computational domain the main types of dissipative boundary conditions in terms of velocities, stresses or mixed boundary conditions can be given. Shock-capturing algorithm is proposed for implementation of the model on multiprocessor computer systems. It is based on the two-cyclic splitting method with respect to spatial variables and the special procedure of the stresses correction. 1D systems of equations in spatial directions are solved by means of the explicit monotone ENO scheme. The parallelizing of computations is carried out using the MPI library and the SPMD technology. The data exchange between processors occurs at step “predictor” of the finite-difference scheme. Numerical computations were performed on clusters of ICM SB RAS (Krasnoyarsk) and JSCC RAS (Moscow).

This work was supported by the Russian Foundation for Basic Research (grant no. 11-01-00053).

On thermodynamically self-consistent formulations of dynamic models of deformable media and their numerical implementation

V. Sadovskii

Mathematical models of the dynamics of elastic-plastic and granular media are formulated as variational inequalities for hyperbolic operators with one-sided constraints describing the transition of a material in plastic state. On this basis a priori integral estimates are constructed in characteristic cones of operators, from which follows the uniqueness and continuous dependence on initial data of solutions of the Cauchy problem and of the boundary-value problems with dissipative boundary conditions.

Original shock-capturing algorithms are developed which can be considered as a realization of the splitting method with respect to physical processes. Such algorithms automatically satisfy the properties of monotonicity and dissipativity on discrete level. They are applicable for computation of the solutions with singularities of the type of strong discontinuities (elastic-plastic shock waves) and of discontinuities of displacements. The two-cyclic splitting method with respect to spatial variables is applied for numerical solution of two-dimensional and three-dimensional problems.

Earlier thermodynamically self-consistent systems of conservation laws were considered by S.K. Godunov and his colleagues in relation to the models of reversible thermodynamics (elasticity theory, gas dynamics and electrodynamics). The present report addresses a generalization of this approach for the analysis of thermodynamically irreversible models taking into account plastic deformation of a medium.

This work was supported by the Russian Foundation for Basic Research (grant no. 11-01-00053).

About equivalence between integrating of set of equilibrium equations and solving of a variational problem in hydrodynamics

L. Savin and A. Kornaev

In this paper we show, that the classic approach which, that is direct integration of differential equations, and also another, alternative approach connected with finding minimum of objective functional are equal in some problems of hydrodynamics. The modified objective functional is presented. It is shown, for example, that the numerical solving process is easier with alternative approach.

Applications of RFBs to the stabilization of the convection-diffusion-reaction problems in two space dimensions. PART 1: Convection-dominated flows

A. Sendur, A. Nesliturk and A. Kaya

The residual-free bubbles (RFB) can assure stabilized methods, but they are usually difficult to compute, unless in special limit cases. Therefore it is important to devise numerical algorithms that provide cheap approximations to the RFB functions, contributing a good stabilizing effect to the numerical method in any flow regime. Here we propose a stabilization technique, based on the RFB method and particularly designed to treat the interesting case in which the convection dominates. We replace the RFB functions by their cheap, yet efficient approximations which retain the same qualitative behavior. The approximate bubbles are computed by adding suitable internal points inside each element, the choice of whose nodes are critical and determined by minimizing the residual of a local problem with respect to L_1 norm. The resulting numerical method has similar stability features with the RFB method. This fact is also confirmed by numerical experiments.

Applications of RFBs to the stabilization of the convection-diffusion-reaction problems in two space dimensions. PART 2: Reaction-dominated flows

A. Sendur, A. Nesliturk and A. Kaya

The residual-free bubbles (RFB) can assure stabilized methods, but they are usually difficult to compute, unless in special limit cases. Therefore it is important to devise numerical algorithms that provide cheap approximations to the RFB functions, contributing a good stabilizing effect to the numerical method in any flow regime. Here we propose a stabilization technique, based on the RFB method and particularly designed to treat the interesting case in which the reaction dominates. We replace the RFB functions by their cheap, yet efficient approximations which retain the same qualitative behavior. The approximate bubbles are computed by adding suitable internal points inside each element, the choice of whose nodes are critical and determined by minimizing the residual of a local problem with respect to L_1 norm. The resulting numerical method has similar stability features with the RFB method. This fact is also confirmed by numerical experiments.

An effective method of electromagnetic field calculation

A. Shamaev and D. Knyazkov

There are several problems at holographic lithography which need considerable calculation resources: synthesis of a hologram for a given topology, simulation of an aerial image reconstruction, hologram optimization problem. The most time-consuming part of these problems is electromagnetic field calculation, which leads to integrals having the following convolution type:

$$f(x, y) = \int \int K(x, y, \xi, \eta) \varphi(\xi, \eta) d\xi d\eta. \quad (1)$$

Number of topology elements could be equal to 10^{10} and more. This leads to necessity to use HPC-computers. A method allowing to calculate (??) on these systems in an appropriate time should also be developed.

It was designed an algorithm for finding the convolution (1) at far-field zone allowing to perform (on up-to-date computing systems) the mentioned above calculations for topologies having the size comparable with real IC layer topologies. The main idea of the algorithm is to use analytical solution for diffraction problem on an elementary square (so-called "big pixel") at far-field zone and to reduce (1) to the following convolution:

$$f(i, j) = \sum_{k, l=1}^N S(i - k, j - l) \varphi(k, l),$$

which could be calculated using two-dimensional fast Fourier transform (FFT). The algorithm was implemented in C++ programming language as a part of BigPixel software package. The program was designed to be used on a usual cluster supercomputer.

The report contains detailed algorithm description, effectiveness and scalability analysis and calculation examples performed on MVS-100K JSCC RAS and MIIT T4700 clusters (having 100 TFLOPS and 4.7 TFLOPS peak performance correspondingly) for some test topologies.

Some new approaches for solving Navier-stokes equations for viscous heat-conducting gas

V. Shaydurov, G. Shchepanovskaya, A. Vyatkin and M. Yakubovich

In this talk, we deal with two-dimensional Navier-Stokes equations for viscous heat-conducting gas:

$$\begin{aligned} \frac{D\rho}{Dt} &\equiv \frac{\partial\rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0, \\ \frac{1}{2u} \frac{D(\rho u^2)}{Dt} + \frac{\partial}{\partial x} (P - \tau_{xx}) - \frac{\partial\tau_{xy}}{\partial y} &= 0, \\ \frac{1}{2v} \frac{D(\rho v^2)}{Dt} - \frac{\partial\tau_{xy}}{\partial x} + \frac{\partial}{\partial y} (P - \tau_{yy}) &= 0, \end{aligned}$$

$$\frac{D(\rho e)}{Dt} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = -P \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \Phi.$$

Transport operator D/Dt is approximated by some modification of trajectories method that gives explicit difference expressions in each equation. Other terms in equations are approximated by finite element method. This approach gives numerical scheme that has no limitation between temporal and spatial steps for high Reynolds number. Other advantage consists in preservation of mass and full energy of flow at discrete level.

Theoretical investigations are illustrated by numerical examples for supersonic flow in channels with obstacles.

Construction of robust schemes stable to perturbation in the data, for singularly perturbed parabolic convection-diffusion equations

G. Shishkin

Standard upwind difference schemes on *uniform meshes* (as well as the finite element method schemes) used to solve singularly perturbed problems do not converge ε -uniformly in the maximum norm. Moreover, with values of the parameter ε and mesh step-size h for which the schemes converge, difficulties arise when constructing monotone schemes which are ε -uniformly stable to perturbations in the data of the discrete problem.

Note that the regular component of the discrete solution is ε -uniformly well conditioned. The singular component is ε -uniformly well conditioned only under the condition when the interval, on which the problem is considered, is a value of order $\mathcal{O}(\varepsilon \psi(N))$, $\psi(N) = o(N)$. Such a behaviour of the discrete regular and singular components motivates the construction of a numerical method for singularly perturbed problems based on the special *decomposition of the discrete solution*.

In this talk, for a Dirichlet problem to a singularly perturbed parabolic convection-diffusion equation, a difference scheme of the solution decomposition method is constructed. This method uses decomposition of the discrete solution into the regular and singular components which are solutions of *discrete subproblems* solving on *uniform meshes*. The constructed difference scheme is ε -uniformly well conditioned, it converges ε -uniformly in the maximum norm, and also it is ε -uniformly stable to perturbations in the data of the discrete problem.

This research was supported by the Russian Foundation for Basic Research under grant No.10-01-00726.

Experimental technique for studying ε -uniformly convergent schemes for parabolic convection-diffusion equations

L. Shishkina, G. Shishkin and P. Hemker

Quite often, difference schemes constructed for singularly perturbed problems are sufficiently complicated that gives rise to difficulties in their analysis and efficiency study; for example, among them are schemes of improved and high-order accuracy for partial differential equations. The reason is that orders of the convergence rate for such schemes with respect to different variables may be different; in this case, it is difficult to analyze the contribution to the error of the grid solution from the approximation errors in each variable.

The technique developed for analysis of discrete solutions for singularly perturbed problems for ordinary differential equations, for elliptic equations are well-known. The technique of studying singularly perturbed problems for parabolic equations is intensively developed at present.

This presentation describes the technique of research of an ε -uniformly convergent scheme based on the defect correction method for a parabolic convection-diffusion equation with the Neumann boundary condition on that part of the boundary through which the characteristics of the reduced equation leave the domain. We analyze the error components generated by the approximation of the problem in both spatial and time variables. An algorithm is discussed for constructing an "optimal scheme", i.e., a finite difference scheme for which the orders of errors in space and time are close (namely, these errors are of the same order up to a logarithmic factor).

This research was supported by the Russian Foundation for Basic Research under grant No.10-01-00726.

Characterization of a cubic interpolation scheme dependent on two parameters

D. Simian and C. Simian

The aim of the paper is to introduce a cubic interpolation scheme using Bézier curves. Classical methods consider that the interpolation points correspond to the values $t \in \{0, 1/3, 2/3, 1\}$ in the parametric representation of the Bézier interpolation curve. We renounce to this condition and introduce two parameters $t_1, t_2 \in (0, 1)$ which values determine the position of the interpolation points on the Bézier curve. These parameters have a big influence on the curve shape. In fact we obtain a family of Bézier interpolation curves depending on two parameters. We make a geometric characterization of the interpolation curves and compare the results with the geometric characterization made by Stone and DeRose. The difference is that our characterization take into account the position of the interpolation points and not the position of the Bézier control points. We realized a partition of the domain $T = [0, 1] \times [0, 1]$ where the parameters lie according to the geometric characterization of the interpolation Bézier curve: with one or two inflexion points, with loop, with cusp, a convex or concave arch.

The analysis of the possibility of integration of our cubic interpolation curves in a spline curve and a comparison with Catmull - Rom splines are presented in the end.

Computation and graphic representations are made using MATLAB.

Finite differences method for one dimensional nonlinear parabolic equation with double nonlinearity

B. Sinsoysal and T. Coruhlu

In this paper we will investigate the initial-boundary problem

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} K \left(\frac{\partial \sigma(u)}{\partial x} \right) - \frac{\partial Q(u)}{\partial x}, \quad (1)$$

$$u(x, 0) = u_0(x), \quad (2)$$

$$u(0, t) = u_1(t), \quad u(\ell, t) = u_2(t) \quad (3)$$

in $D_T = \{(x, t) \mid 0 \leq x \leq \ell, 0 < t < T\} \subset R^2$. Here, $u_0(x)$, $u_1(t)$ and $u_2(t)$ are given functions, $u(x, t)$ is an unknown function, $K(s)$, $\sigma(u)$ and $Q(u)$ are known functions with respect to s , u , respectively which satisfy some conditions.

Since the equation (1) is nonlinear the classical solution of the problem (1)-(3) does not exist. In order to find the weak solution of the problem (1)-(3), the following auxiliary problem

$$\frac{\partial v(x, t)}{\partial t} = K \left(\frac{\partial \sigma(u(x, t))}{\partial x} \right) - Q(u),$$

$$v(x, 0) = v_0(x),$$

$$u(0, t) = u_1(t), \quad u(\ell, 0) = u_2(t)$$

is introduced. Here $v_0(x)$ is any differentiable solution of the equation $\frac{dv_0(x)}{dx} = u_0(x)$.

Using the advantages of the suggested auxiliary problem, at first the higher resolution numerical scheme for the solution of the main problem is developed, then the convergence of the numerical solution to the weak exact solution in sense of mean is proven.

Numerical solution of functional differential equations in partial derivatives on a remote server through a web interface

S. Solodushkin

The goal this work is presentation of information and computing server that provides an interface to a MATLAB solver of functional differential equations in partial derivatives(PFDE).

The class of solvable equations contains parabolic and hyperbolic equations with appropriate initial and border conditions.

The front-end of the elaborated system is a web server IIS and the back-end is a MATLAB Run Time Server. Remote user should have a modern web browser only; it is not necessary to setup any plugins.

Numerical algorithms were realized as a MATLAB .m-files (see V. G. Pimenov and A. B. Lozhnikov. Difference schemes for the numerical solution of the heat conduction equation with aftereffect. // Proceedings of the Steklov Institute of Mathematics. Volume 275, Supplement 1,

2011, p. 137-148). At the development stage appropriate .m-files were compiled into dynamic linking libraries (DLL) by means of the `deploytool` — built-in tool of MATLAB. The front-end — web interface — was elaborated with ASP.NET4 /C#.

Remote user fills a web form, he types the parameters of the equation and grids characteristics. These data are sent to the C#-handler which call an appropriate DLL. Numerical solution and 3D plot are embedded in a web page that is sent to the user. 3D plot is interactive, i.e it allows rotation by means of the mouse in order to better review. The processing of these user manipulations performed on the server side; AJAX is used for the organization of client-server interaction without refreshing the web page.

Efficient on-line generation of the correlation of the fGn process

M. Sousa, A. Suarez, J. Lopez and C. Lopez

Several traffic measurement studies have revealed singular statistical properties, such as self-similarity and long-range dependence, that cannot be overlooked in modeling Internet traffic. Self-similarity refers to the preservation of a common stochastic law describing the burstiness of traffic across different time scales, from seconds to days. Long-range dependence (LRD) means the existence of substantial correlations between the volume of traffic generated in widely separated time intervals, that is, a correlation structure decaying slowly in time. Both properties were discovered for variable-bit-rate (VBR) video traffic, for traffic in wide area networks, for Ethernet networks and for Web traffic. The finding of self-similarity and LRD, in turn, spurred the research on queueing models with fractal input traffic and the assessment of their impact on network performance as well. As these works demonstrate, the effect of LRD on packet loss and delay may be drastic, leading to subexponential decay of the buffer overflow probability and, consequently, buffer sizes much larger than those predicted by memoryless or short-memory (i.e., Markov) processes. Aside from the specific application in communications networks, self similar processes are ubiquitous across many other fields in science and engineering. Prevalent examples appear in statistical physics, chemistry and biology. They are also of interest as underlying models in time series analysis, like meteorological and hydrological data, stock markets data, rare events in finance and insurance, or biometric signals. Several stochastic processes consistent with self-similarity and LRD have been proposed to model the behavior of traffic, or any other physical magnitude exhibiting fractal variability, in a tractable way, such as fractional Gaussian noise (fGn), fractional ARIMA (fARIMA), the superposition of on-off sources with heavy-tailed distributions and the M/G/ ∞ occupancy process. More recently, the multi-scale nature of network traffic has also been successfully modeled with wavelet functions. In the realm of simulation, the introduction of self-similar models poses one fundamental problem related to the efficient generation of synthetic traces, because the intrinsic invariance of the statistical properties of self-similar processes results in a high complexity for computing its trajectories. Moreover, since simulations must produce long samples, preferably with indefinite length, long traces must be synthesized on demand. In this sense, the main drawback of fGn and fARIMA processes is that only off-line methods for synthesizing traces are efficient enough to be of practical use. To overcome this drawback, we focus on the M/G/ ∞ process as the base stochastic object for fast simulation of self-similar and LRD processes. This is the occupancy process of a M/G/ ∞ queueing system, and has several outstanding advantages. First, the process is theoretically simple and amenable to analysis. As such, there exists a substantial body of research results about the systems behavior. Second, by varying the service time distribution, many different forms of the autocorrelation function can be obtained, either shortrange or long-range dependent. Finally, the

process can be trivially simulated in discrete time so as to obtain traces with linear complexity, in an incremental and on-line method. In a previous work we proposed an on-line generator of the correlation structure of the fGn process based on the M/G/ ∞ process. Some lack of precision in the generation of samples of the distribution of the service time of the queueing system was observed in the case of heavy-tailed distributions. So, in this paper we propose an improvement of the accuracy and efficiency of the generator taking advantage of the properties of heavy-tailed distributions. The generator is also modified to be able to deal with discrete random variables with long tails in the left side.

A compact fourth-order iterative solver for singular Poisson equations

A. Stephane, C. Xavier and Z. Belkacem

This work presents a simple and efficient compact fourth-order solver for the singular-Poisson equation. This solver is based on a mixed formulation. The Poisson equation is split into a system of partial differential equations of first-order, and then discretized using a fourth-order compact scheme. This way leads to a sparse linear system, but introduces new variables related to the gradient of the main variable. By means of the Schur factorization, this linear system to be solved retrieves its initial size. The factorized system is solved using a conjugated-gradient preconditioned by an aggregation-based algebraic multigrid method. Experimental results, including comparisons with second-order solver, show that this proposed Poisson solver is fourth-order accurate while remaining competitive in comparisons with standard second-order solver.

Simulation of severe pollution events by bulgarian emergency response system

D. Syrakov and M. Prodanova

Last years several severe pollution events took place. The eruption of Iceland volcano in April 2010 caused enormously big troubles for air transport over Europe for a long period of time. The losses and inconveniences for air companies, common business and usual passengers are difficult to be estimated but in any case are rather considerable. The severe accident in Fukushima Nuclear power plants in 2011, due to quite intensive earthquake causing tsunami, also caused serious anxiety among the population not only in the neighbourhood, but even in countries quite far from the accident location.

Bulgarian ERS (BERS) was upgraded as to be able to simulate the dispersion of volcanic ash released by Iceland volcano as well nuclear materials from Fukushima Daiichi NPP. The results of simulating the latest event are presented in the specialised web-site of the system. In addition, in both cases BERS took part in the respective ENSEMBLE exercises. Short description of BERS as well as its results and comparisons with other model results are the object of this work.

Verified numerical computations for solutions to semilinear elliptic boundary value problems on arbitrary polygonal domains

A. Takayasu, X. Liu and Sh. Oishi

Let Ω be a bounded polygonal domain on \mathbf{R}^2 with arbitrary shape. This study is devoted to the Dirichlet boundary value problem of a semilinear elliptic equation of the form:

$$\begin{cases} -\Delta u = f(\nabla u, u, x), & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, \end{cases} \quad (1)$$

where $f : H_0^1(\Omega) \rightarrow L^2(\Omega)$ is assumed to be Fréchet differentiable. Generally, verified numerical computations for differential equations try to prove the existence of solution with guaranteed error bounds. Our verified computation approach will explore the existence and local uniqueness of the solution for (1). Namely, if an approximate solution \hat{u} is given by a certain numerical method, we will try to validate the existence of exact solution u in the neighborhood of its approximation:

$$\|u - \hat{u}\|_{H_0^1} \leq \rho.$$

We will explain how to evaluate ρ with verification in the talk.

Especially, on non-convex domains, it is well-known that the exact solution may have a lack of H^2 -regularity. In that case, a priori error estimate for FEM, needed in our approach, is very difficult to obtain. Using the Hyper-circle equation, we have a proposed method to give the concrete value of a priori error estimate on non-convex domains.

Adaptive artificial boundary conditions for 2D Schrödinger equation

V. Trofimov and A. Denisov

As it is well-known, many physical processes, including the laser pulse or beam propagation, are described by nonlinear or linear Schrodinger equation. Frequently, one requires the solution of this equation in big domain or in unbounded domain. Hence, developing of artificial boundary conditions is of great interest, especially for the case of multidimensional domain. This is why the different types of such conditions have been proposed early and are developed continuously. However, there are many problems with both accuracy and realization in computer codes such boundary conditions.

In this report we develop adaptive artificial boundary conditions for 1D and 2D linear and non-linear (Kerr nonlinearity) Schrodinger equation. Let us notice that the adaptive artificial boundary conditions mean their adaptability to the solution of the problem near the artificial boundary of considered domain. This approach allows us to increase many times the efficiency of application of the artificial boundary conditions.

Obviously, additional difficulties appear at realization of such kind of boundary conditions in finite-difference scheme constructed for nonlinear Schrodinger equation in multidimensional case. First of them relates to inversion of 2D finite-difference operator, corresponding to Schrodinger equation with complicated boundary conditions. We developed two-step iterative method for possibility to write the conservative finite-difference scheme.

Second of them refers to a computation of phase of the laser beam near the artificial boundaries. In this connection we discuss an influence of both round-off error and small value of intensity on accuracy of computation of the beam phase. The right choosing of the corresponding parameters allows to avoid the appearance of reflected wave.

Third problem consists in approximation of artificial boundary conditions at angular points of considered rectangular domain on the accuracy of computer simulation results. In this report we give big attention to solution of this problem.

It is necessary to stress that one of the main feature of artificial boundary conditions developed by us is their simplicity and universality of their applications for various types of Schrodinger equation. This feature is illustrated by various examples.

This report was supported partly by Russian Foundation for Basic Research.

Comparative analysis of decomposition schemes for a singularly perturbed reaction-diffusion equation with third-kind boundary conditions

I. Tselishcheva

We consider approximations for a singularly perturbed reaction-diffusion equation; the second-order derivatives are multiplied by the perturbation parameter ε^2 , where ε takes any values in the interval $(0,1]$. On the boundary of the domain, the third-kind condition admitting both Dirichlet and Neumann conditions is given. With an example of ODE, we construct and study continual and difference (on piecewise uniform meshes condensing in the boundary layers) schemes based on an overlapping domain decomposition method in the case of sequential and parallel computations. We give conditions that ensure the ε -uniform convergence of solutions of the decomposition schemes with increasing the number of iterations.

A comparative analysis of the efficiency of the decomposition schemes for sequential and parallel computations is made. It is shown (in contrast to the parabolic convection-diffusion case considered earlier) that the increase in the number of solvers in parallel schemes leads to the solution acceleration, as compared to the sequential method, without loss in the accuracy of the solution of the decomposed scheme. Lower and upper bounds for the error of the decomposition method and for the number of iterations are obtained. Conditions are found under which the parallel scheme solves the problem faster than the sequential one; moreover, the error in the solution of the parallel scheme does not exceed the error of the sequential scheme. Namely, the time required for the solution of the problem reduces practically P times, where P is the number of parallel processors; and computational costs for solving the sequential and parallel versions of schemes are close. The results of this study can be generalized to the case of a singularly perturbed elliptic reaction-diffusion equation on a rectangle.

I am indebted to Prof. G.I. Shishkin for his help and problem formulation. This work was supported by the RFBR grant No. 10-01-00726.

Flux-splitting schemes for parabolic problems

P. Vabishchevich

To solve boundary value problems for parabolic equations of second order, schemes of splitting with respect to spatial variables are in common use: classical methods of alternating directions, locally one-dimensional schemes etc. In problems with highly varying coefficients it is convenient to treat fluxes (directional derivatives) as unknowns. The original equation can be written as a system of equations, where the unknown quantities include not only the solution itself but also its derivatives in particular directions (fluxes). For a parabolic equation of second order we consider additive schemes (splitting schemes) based on splitting with respect to spatial directions. Two-level locally one-dimensional schemes are constructed using a reduction of the original equation to a formulation in flux variables. Unconditional stability is established for flux-based locally one-dimensional schemes of the first- and second-order approximation in time.

Numerical solution of dynamic problems in block media with thin interlayers on supercomputers with GPUs

M. Varygina

Several nature materials such as rock have distinct structurally inhomogeneous block-hierarchical structure. Block structure appears on different scale levels from the size of crystal grains to the blocks of rock. Blocks are connected to each other with thin interlayers of rock with significantly weaker mechanical properties.

Parallel computation algorithm for the numerical modeling of dynamic interactions of elastic blocks through thin viscoelastic interlayers in structurally inhomogeneous medium such as rock is developed. Monotonous grid-characteristic scheme with the balanced number of time steps in blocks and interlayers is used for the numerical solution. The algorithm is implemented by the CUDA technology (Compute Unified Device Architecture) on supercomputer with graphics processing units.

The computations of planar wave propagation induced by short and long Λ -impulses on a boundary of the domain composed from blocks of rock with microfractured viscoelastic interlayers were performed. These computations performed on supercomputer for the large number of layers allowed to analyze specific "pendulum" waves related to the structural inhomogeneity. The results of numerical analysis to demonstrate peculiar quality of planar wave propagation in materials with layered microstructure are shown.

This work was supported by the RFBR grant no. 11-01-00053.

Computational algorithms for some convolution equations

A. Vasilyev and V. Vasilyev

For approximate solution of multi-dimensional singular integral equation

$$au(x) + v.p. \int_{\mathbf{R}^m} K(x-y)u(y)dy = v(x), \quad (1)$$

one suggests a certain computational scheme to explain mathematically the transfer to finite dimensional approximation and convergence of approximate solution to exact ones.

Given kernel $K(x)$ of the equation (1) we construct discrete kernel $K_d(\tilde{x})$, $\tilde{x} \in \mathbf{Z}^m$, where \mathbf{Z}^m is integer point lattice in m -dimensional space. Define the functions of discrete variable $u_d(\tilde{x})$ on \mathbf{Z}^m , and consider the equation

$$au_d(\tilde{x}) + \sum_{\tilde{y} \in \mathbf{Z}^m} K_d(\tilde{x} - \tilde{y})u_d(\tilde{y}) = v_d(\tilde{x}) \quad (2)$$

instead of (1) (by definition $K_d(0) = 0$). It is treated as discrete analogue of the equation (1); $v_d(\tilde{x})$ is restriction of the right hand side $v(x)$ onto lattice \mathbf{Z}^m .

We take the cube Q_N in \mathbf{R}^m of size $N \in \mathbf{Z}$,

$$Q_N = \{\tilde{x} \in \mathbf{Z}^m : |\tilde{x}| = \max|x_j| \leq N, j = 1, 2, \dots, m\},$$

and then given discrete kernel K_d and right hand side v_d one constructs their periodical Q_N -approximations K_{dN}, v_{dN} by restriction of K_d, v_d on Q_N and periodic continuation on whole \mathbf{Z}^m . Further we consider the equation

$$au_{dN}(\tilde{x}) + \sum_{\tilde{y} \in \mathbf{Z}^m} K_{dN}(\tilde{x} - \tilde{y})u_{dN}(\tilde{y}), \quad \tilde{x} \in \mathbf{Z}^m,$$

instead of the equation (2). Really the last system of linear algebraic equations consists of finite number of different equations.

New family of iterative methods with high order of convergence for solving nonlinear systems

M. Vassileva, Al. Corderoy and J. Torregrosaz

In this paper we develop a family of predictor-corrector iterative methods for solving nonlinear systems of equations. We are seeking a high order of convergence and few Jacobian and/or functional evaluations. The order of convergence of the developed methods, called M4A, M6A and M8A, is four, six and eight, respectively. By applying the pseudocomposition technique on each previous method we get to increase the order of convergence of these schemes, obtaining new methods denoted by M5GA, M10GA and M14GA, with orders of convergence five, ten and fourteen, respectively. The pseudocomposition technique consists of the following: we consider a method which order of convergence p as a predictor, whose penultimate step is of order q , and then we use a corrector step based on the Gauss quadrature. So, we obtain a family of iterative schemes whose order of convergence is $\min\{q + p, 3q\}$. This is a general technique to improve the order of convergence of known methods. To analyze and compare the efficiency of the methods we use two indexes: the classic index of efficiency $I = p^{1/d}$ and the computational index of efficiency $CI = p^{1/(d+op)}$, where p is the order of convergence, d is the number of functional evaluations at each iteration and op is the number of operations, products and quotients, per iteration. Numerical examples allow us to compare the different iterative schemes and to confirm the theoretical results.

One specification of Mann-Ishikawa iterations

V. Verzhbitskii and I. Yumanova

The problem of improving computational efficiency of applied methods is always relevant due to high demand for iterative methods for solving finite-dimensional nonlinear equations. One way to achieve this goal is building a concrete iterative processes such as Mann-Ishikawa iterations (that is the processes of the Fejer type) that improve the convergence and extend the scope of applicability of the simple iterations method as a basis. The specification for equation of the form

$$x = \varphi(x) \tag{1}$$

consists in creating a method of fixing the parameter of these processes of the specified type. There is the ratio in which the line segment joining the points x_k (the point of the (k) th approximation of this method) and $\tilde{x}_{k+1} = \varphi(x_k)$ (the result of one step of simple iterations method) is divided. It is possible divide the line segment externally.

In the previous works the authors suggested to find a parameter as a ratio of residuals of the equation $x - \varphi(x) = 0$ in these points and demonstrated the advantages of the received modifications for one-dimensional case.

Investigation of scalar equations have provided a clue to building effective methods for solving systems of nonlinear equations of the form (1), that is the case with mapping $\varphi : \mathbf{R}^n \rightarrow \mathbf{R}^n$. We study two approaches to obtaining approximations such as the Mann-Ishikawa iterations to solutions of systems. One way is the vector approach, this method uses the ratio of the norms of residuals for finding parameters of the method. The other way is the componentwise approach that shift tracking of approximations in each coordinate more subtle. The results of the testing of the new methods for a large number of nonlinear systems characterize methods as quite successful.

Comparison of surface subdivision algorithms for triangular polyhedral meshes

K. Vlachkova and T. Halacheva

We present a new program package for interactive implementation and 3D visualization of three fundamental algorithms for surface subdivision based on triangular polyhedral meshes. Namely, these are Loop algorithm, Modified Butterfly algorithm, and $\sqrt{3}$ -subdivision algorithm. Our work and contributions are in the field of experimental algorithmics and algorithm engineering.

We have chosen Java 3D and Java applet application as our main implementation and visualization tools. This choice ensures platform independency of our package and its direct use by the clients, without any restrictions. The applet is prepared to work with the client's file system and hence it can be used for experiments using the client's data sets. The latter allows the clients to test and compare the results from implementation of the three algorithms on arbitrary triangular polyhedral meshes.

We have performed extensive experimentation with our package. We have compared the performance of the three algorithms based on different criteria and using meshes of increasing complexity. The experimental results are presented and analyzed.

On asymptotic-numerical investigation of generation and motion of fronts in phase transition models

V. Volkov and N. Nefedov

We consider the singularly perturbed parabolic differential equation of reaction-diffusion-advection type

$$\varepsilon^2 \left(\Delta u + \vec{v}(x, y, u) \vec{\nabla} u - u_t \right) = f(u, x, y, \varepsilon), \quad (x, y) \in D \in R^2, \quad t > 0,$$

where $\varepsilon > 0$ is a small parameter and functions f and \vec{v} are sufficiently smooth. We look for solutions satisfying some initial conditions and the boundary conditions and containing the internal layers (solutions of contrast structures type).

Problems for reaction-diffusion-advection equations are often used to describe wide classes of practical applications in chemical kinetics, synergetics, astrophysics, biology, etc. In many important cases the solutions of these problems feature boundary and internal layers.

The main results of the work are:

1. We study the generation of contrast structure problem and we have proved, that in times of order $\varepsilon^2 \ln \varepsilon$ the solution with moving internal layers develops from the smooth initial function of quite general type.
 2. We have received the equations, which allow to find localization of moving fronts and describe their form and properties.
 3. We use this information for numerically-analytic investigation of such type problems, modelling the oil extraction. We have carried out a number of numerical experiments which show that the combination of the asymptotic and the numerical methods allows considerably decrease the time of the numerical calculations.
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Finite element methods for fourth order singularly perturbed problems

C. Xenophontos, M. Melenk, N. Madden, L. Oberbroeckling, A. Zouwani and P. Panaseti

We consider fourth order singularly perturbed boundary value problems (BVPs) in one-dimension and the approximation of their solution by the hp version of the Finite Element Method (FEM). If the given problem's boundary conditions are suitable for writing the BVP as a system, then we prove that the hp FEM on the Spectral Boundary Layer Mesh can give a robust approximation that converges exponentially, provided the data of the problem is analytic. We also consider the case when the approximation belongs to a finite dimensional subspace of H^2 and we construct suitable hierarchical basis functions for the approximation. We show again that the Spectral Boundary Layer Mesh yields a robust approximation that converges exponentially. Numerical examples will be presented that agree with the analysis.

Fast verified division algorithm for double-double arithmetic

N. Yamanaka and Sh. Oishi

In a numerical calculation sometimes we need higher-than double-precision floating-point arithmetic to allow us to be confident a result. An alternative approach is to store numbers in a multiple-component format, where a number is expressed as unevaluated sums of ordinary floating-point words, each with its own significand and exponent. Sometimes merely doubling the number of bits in a double-floating-point fraction is enough, in which case arithmetic on double-double operands would suffice. A double-double number is an unevaluated sum of two double precision numbers, capable of representing at least 106 bits of significand. It consisted in representing a number x as the unevaluated sum of two basic precision floating-point numbers:

$$x = x_h + x_l \tag{1}$$

such that the significands of x_h and x_l do not overlap, which means here that

$$|x_l| \leq \varepsilon |x_h|, \tag{2}$$

where ε denote the machine epsilon; in double precision $\varepsilon = 2^{-53}$.

In this talk we will discuss about a fast verified division algorithm for double-double arithmetic. Yamanaka and Oishi have already developed a division algorithm for double-double arithmetic. The algorithm is designed to achieve the results as if computed in 2-fold working precision only using the floating point operations of double arithmetic and it is superior than Hida *et. al.*'s division algorithms in QD/DD in terms of the number of floating operations and the execution time. To construct a verified algorithm, we've analyzed the maximum error of the algorithm carefully and we propose fast verified division algorithm for double-double arithmetic. By numerical experiments it is shown that the proposed algorithm is faster than conventional method based on Hida *et. al.*'s division algorithms.

An automation of the recursive formulation of the tau method for numerical solution of initial value problems in ordinary differential equations

B. Yisa and R. Adeniyi

The Canonical Polynomials forms the basis function in approximating the solution to Ordinary Differential Equations(ODEs) by the recursive formulation of the tau method which was originally proposed by Lanczos in 1956 and which was later developed by Ortiz in 1969. However, the construction of the so-called canonical polynomials for the general m-th order ODE is very difficult but desirable. In this paper, we shall address this problem with the ultimate aim of automating this variant of the tau method while at the same time incorporate its error estimate.

A new discontinuous Galerkin method for parabolic equations with discontinuous coefficients

X. Yu, R. Zhang, G. Zhao and T. Feng

The parabolic equations with discontinuous coefficients play a great role in many physical applications. For example, in the numerical simulation of radiation hydrodynamics, since energy is usually transported in a variety of media, the conductivity coefficients are discontinuous on the media interface and are of several quantity differences in sometimes. Therefore, it is of great theoretical significance and practical value to study the numerical methods with high order accuracy.

There have been many works for solving parabolic problems with discontinuous coefficients by finite difference methods, finite volume methods and finite element methods. In here we give a new discontinuous Galerkin method for the parabolic equation with discontinuous coefficients. Theoretical analysis shows that this method is L^2 stable. When the finite element space use interpolative polynomials of degrees k , the convergent rate of the semi-discrete discontinuous Galerkin scheme has an order of $O(h^k)$. Numerical examples for both one dimensional and two dimensional problems demonstrate the validity of our method.

Quadrature formula with five nodes for functions with a boundary layer component

A. Zadorin and N. Zadorin

We construct the quadrature formula for an integral:

$$I(u) = \int_a^b u(x) dx, \tag{1}$$

where a function $u(x)$ has a form:

$$u(x) = p(x) + \gamma\Phi(x), \tag{2}$$

$p(x)$ is a regular component and $\Phi(x)$ is known boundary layer component, constant γ is not given. For a solution of a singularly perturbed boundary value problem the representation (2) has a place.

Newton-Cotes formulas, based on the approximation of the integrand by a Lagrange polynomial, lead to large errors, if a function $u(x)$ includes a boundary layer component.

We construct quadrature formula with five nodes, using nonpolynomial interpolation of the integrand, exact for a boundary layer component. We prove that constructed formula has the order of accuracy $O((b-a)^5)$, uniformly on a boundary layer component $\Phi(x)$ and its derivatives. On a base of constructed formula we obtain the composite quadrature formula of the accuracy $O(h^4)$, uniformly on the boundary layer component, h is mesh step.

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Spline solution for fourth-order fractional integro-differential equations

W. Zahra and S. Elkholy

In this paper, we introduce a new approach based on spline function for approximating the solution of fourth-order fractional integro-differential equations. Quintic polynomial spline is used for deriving consistency relations which can be used for finding an approximate solution for this class of boundary value problems. Convergence analysis of the method is discussed. Some numerical illustrative examples are included to demonstrate the practical usefulness of the proposed method.

Numerical Study of Travelling Multi-Soliton Complexes in the Driven NLS Equation

E. Zemlyanaya and N. Alexeeva

The externally driven nonlinear Schrödinger equation (NLS) has a wide range of applications in the models of condensed matter physics. We study uniformly travelling multi-soliton solutions of the NLS equation within the frame of the following numerical approach. Instead of the initial partial differential equation we consider the ordinary differential equation where the uniform velocity plays a role of additional parameter. Stability and bifurcations are classified, numerically, on the basis of the corresponding linearized eigenvalue problem. The above analysis has been completed by direct numerical simulations of the partial differential NLS equation. Details of numerical approach are presented. Existence of stably travelling two-soliton complexes is demonstrated. Comparison with the case of parametrically driven NLS equation has been done.

Asynchronous differential evolution with restart

E. Zhabitskaya and M. Zhabitsky

Asynchronous Differential Evolution (ADE) [1] is an effective method for solving derivative-free global optimization problems. It provides effective parallel realization.

In this work we derive ADE with restart. Improvement in the probability of convergence is demonstrated on a set of benchmark functions. Applications of ADE method to real optimization problems in physics are discussed.

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Uniform grid approximation of nonsmooth solutions to singularly perturbed convection-diffusion equation with characteristic layers

U. Zhemukhov

A mixed boundary problem for a singularly perturbed convection-diffusion equation is considered in the square $\Omega = (0, 1)^2$ with the boundary $\partial\Omega$:

$$\begin{aligned} Lu \equiv -\varepsilon\Delta u + a\frac{\partial u}{\partial x} + qu &= f(x, y), & (x, y) \in \Omega, \\ \frac{\partial u}{\partial \mathbf{n}} &= \varphi(x, y), & (x, y) \in \partial\Omega_N, \\ u &= g(x, y), & (x, y) \in \partial\Omega_D, \end{aligned}$$

where $a = \text{const} > 0$, $q = \text{const} > 0$, \mathbf{n} is the unit vector of an outer normal to $\partial\Omega_N$, and $\varepsilon \in (0, 1]$ is a small parameter. The domain boundary consists of the parts $\partial\Omega_D = \Gamma_1 \cup \Gamma_3$ and $\partial\Omega_N = \Gamma_2 \cup \Gamma_4$, where Γ_k are the sides of the square Ω , ordered in the counterclockwise direction starting from $\Gamma_1 = \{(x, y) \in \partial\Omega \mid x = 0\}$, whereas $a_k = (x_k, y_k)$ are its vertices, ordered in the similar way being $a_1 = (0, 0)$.

Sufficient smoothness of the right-hand side and the boundary functions is assumed, which ensures the required smoothness of the solution in the domain under consideration, with exception of the neighborhoods of the corner points. In the corner points themselves the following conditions only are assumed to hold true

$$\left. \frac{dg_1}{dy} \right|_{y=0} = -\varphi_1(0), \quad \left. \frac{dg_1}{dy} \right|_{y=1} = \varphi_2(0), \quad \left. \frac{dg_2}{dy} \right|_{y=0} = -\varphi_1(1), \quad \left. \frac{dg_2}{dy} \right|_{y=1} = \varphi_2(1),$$

which are named zero-order compatibility conditions, where $g_1(y) = g(0, y)$, $g_2(y) = g(1, y)$ and $\varphi_1(x) = \varphi(x, 0)$, $\varphi_2(x) = \varphi(x, 1)$. Numerous researches show that the solution of the original problem has a compound structure, which includes a regular boundary layer near the right-hand

boundary Γ_3 , two characteristic layers near the lower and upper boundaries Γ_2 and Γ_4 , corner layers with corner singularities in neighborhoods of the vertices a_2, a_3 and corner singularities in neighborhoods of the incoming vertices a_1, a_4 . All these present certain difficulties when dealing with a numerical solution of the problem posed.

For a numerical solution of the given problem a *nonuniform* monotone difference scheme on a rectangular piecewise uniform Shishkin grid is used. Nonuniformity of the scheme means that firstly the form of the difference equations, used for the approximation, is different in different grid points, secondly it depends on the value of the small perturbation parameter.

Under the assumptions made, convergence of the numerical solution to the exact solution, uniformly in parameter ε is proved in a discrete uniform metric, at convergence rate $O(N^{-3/2} \ln^2 N)$, where N is the number of the grid points in each coordinate direction.

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