ABSTRAKTY

Matematický model chování nože bubnové sekačky

Stanislav Bartoň

Nůž bubnové sekačky je volně otočný okolo upevňovacího čepu. Odstředivá síla, která vzniká při rotaci bubnu ho napřímí v radiálním směru. Síly které vznikají při sečení se nůž snaží zaklopit zpět. Předložený článek studuje vliv působících sil na chování nože, zejména jeho oscilace okolo ustálené polohy a vliv těchto oscilací na chování sekačky.

Finite element approximation of an elliptic problem with a nonlinear boundary condition

Ondřej Bartoš, Miloslav Feistauer, Filip Roskovec

Many engineering problems can be described using elliptic partial differential equations equipped with nonlinear Newton boundary conditions, e.g. electrolysis of aluminium or radiation heat transfer problem. We look at a problem with (possibly non-integer) powers in its boundary condition in a two-dimensional polygonal domain. The exact solution loses regularity near boundary vertices and to some extent also near boundary edges. When this problem is discretized and solved using a finite element method (FEM) or a discontinuous Galerkin (DG) method, the order of convergence is expected to be divided by the power appearing in the nonlinear boundary condition. In practise, FEM and DG often converge with such a rate as if there was no nonlinearity on the boundary. We attempt to explain this behaviour, how it changes if the error is measured in different norms of Sobolev spaces or if the exact solution is zero on a large part of the boundary.

Několik poznámek ke stabilizačním technikám pro konvekčně-difuzní problémy

Marek Brandner, Petr Knobloch

V příspěvku velmi stručně shrneme různé numerické přístupy pro řešení konvekčně-difuzních problémů založených na metodě konečných diferencí, konečných objemů a konečných prvků. Pokusíme se vystihnout společné vlastnosti a rozdíly jednotlivých přístupů. Na závěr uvedeme některé zkušenosti získané při implementaci stabilizačních technik.

Multilevel Monte Carlo Method for Safety Analysis of Radioactive Waste Repositories

Jan Březina

We shall apply principles of the Multilevel Monte-Carlo method to realistic 2D transport problems in a fractured porous media. In particular we use models with continuum-fracture coupling and explicit description of fracture network. We consider random permeability of the matrix and the fractures and randomly generated fracture network. We shall provide comparison of different approaches to the approximation of distribution functions and quantiles of selected random quantities using efficient MLMC calculations.

Simple Finite Elements in Python – Development Notes and Applications

Robert Cimrman

SfePy (http://sfepy.org) is a software for solving systems of coupled partial differential equations (PDEs) by the finite element method in 1D, 2D and 3D. It can be viewed both as black-box PDE solver, and as a Python package which can be used for building custom applications. The talk will briefly introduce both the software and the related Open-Source project management lessons learned so far by the author. Then two applications of the software will be presented, namely an approach to multiscale modelling based on the theory of homogenization, and a recently proposed method/solver for ab-initio electronic structure calculations based on the FEM and the density functional theory.

Bayesian approach to the solution of identification problems using surrogate models

Simona Domesová, Michal Béreš

By the solution of identification problems we understand the estimation of e.g. material parameters of boundary value problems. An observation that corresponds to unknown input parameters is given and the aim is to determine these parameters. The Bayesian approach expects that the observed data are corrupted by noise; the vector of input parameters is treated as a random vector and the aim is to describe its joint probability distribution.

Samples from the posterior distribution can be provided using Markov Chain Monte Carlo methods, but they typically require a high number of evaluations of the related forward problem. To reduce the number of evaluations, we use methods based on the delayed acceptance Metropolis–Hastings algorithm. Proposed procedures work with surrogate models constructed using two different approaches – the stochastic collocation method and radial basis functions.

Gradient-free and gradient-based methods for shape optimization of water turbine blade

Jiří Egermaier

The purpose of our work is the shape optimization of the runner wheel geometry in water turbine. The fluid flow is computed by own developed IgA-based incompressible flow solver containing turbulence model. The shape optimization is implemented by gradient-free and gradient-based methods. Combination of these methods is also possible. Gradient-free methods generally find global minimum of the objective function, need no gradient evaluation, but they are CPU consuming. Gradient-based methods find local minimum of the objective function and need gradient evaluation. Complexity of this evaluation requires automatic differentiation. We use Particle Swarm Optimization (PSO) method as gradient-free method, Interior Point OPTimizer (IPOPT) package based on Interior point line search filter method as gradient-based method and Code Differentiation Package (CoDiPack) for automatic differentiation.

On the DGM for the solution of an elliptic equation with a nonlinear Newton boundary condition

Miloslav Feistauer

The contribution will be devoted to the analysis of the discontinuous Galerkin method (DGM) for the numerical solution of an elliptic boundary value problem with a nonlinear Newton boundary condition in a two-dimensional polygonal domain. Problems of this type appear in the modeling of electrolysis of aluminium, radiation heat transfer problems or in nonlinear elasticity. Using the monotone operator theory, it is possible to prove the existence and uniqueness of the exact weak solution and the approximate DG solution. The main attention is paid to the study of error estimates. To this end, the regularity of the weak solution is investigated and it is shown that due to the singular boundary points, the solution looses regularity in a vicinity of these points. It comes out that the error estimation depends essentially on the opening angle of the corner points and the nonlinearity in the boundary term. It also depends on the parameter defining the nonlinear behaviour of the Newton boundary condition. Theoretical results are accompanied by numerical experiments showing nonstandard behaviour of the error in the L^2-norm and the H^1-seminorm.
The results were obtained in cooperation with Filip Roskovec, Ondřej Bartoš and Anna-Margarete Sändig.

Strategies for computation of Lyapunov exponents estimates

Cyril Fischer

The Lyapunov exponents (LE) provide a simple numerical measure of the sensitive dependence of the dynamical system on initial conditions. The positive LE in dissipative systems is often regarded as an indicator of the occurrence of deterministic chaos. However, their usage is not limited to the chaotic processes. The values of LE can help to assess stability of particular solution branches of dynamical systems.
The contribution exploits an occasion to compare experimental data and fairly accurate analytical models of simple mechanical systems: spherical pendulum and ball in a spherical cavity. The measured and computed data cover various regimes of movement: stable and unstable, periodic or chaotic. This way we can assess several methods for enumeration of LE for experimental data and corresponding analytical models.

Modelování přechodu mezní vrstvy z laminárního do turbulentního režimu

Jiří Fürst

Přednáška podává přehled postupů používaných pro matematické modelování přechodu mezní vrstvy z laminárního do turbulentního režimu. Pozornost bude přitom zaměřena především na metody založené na řešení Reynoldsově středovaných Navierových-Stokesových rovnic. Ve stručnosti bude popsán proces přechodu do turbulence a jeho rozdělení na jednotlivé kategorie. Dále budou popsány základní rysy a omezení e^n modelu založeného na analýze Orrovy-Sommerfeldovy rovnice. Poté bude v základních rysech popsána skupina modelů založených na konceptu intermitence a na empirických vztazích pro začátek a délku přechodu. Nakonec bude zmíněn model vybudovaný na konceptu tzv. laminární kinetické energie. Pro tento model bude provedena podrobnější analýza a bude ukázána modifikace modelu pro případy proudění s nepříznivým tlakovým gradientem.

Numerical verification of systems of linear and nonlinear equations

Milan Hladík

Verification is a technique to a posteriori determine rigorous bounds of numerically computed solutions. More formally, let x^* be a numerically computed solution of a system of linear (or nonlinear) equations. The aim is to determine bounds $l \leq x^* \leq u$ such that the true solution provably lies in $[l, u]$.

To this end, we utilize interval computation. Notice that direct application of interval arithmetic leads to unnecessarily (and sometimes hugely) overestimated bounds. Therefore, more convenient approach is to compute an approximate solution x^* by a standard method first, and to compute safe bounds after then. For this second step we present a method based on the Krawczyk operator, utilizing not only interval computation, but also the fixed-point theory, among others. The method also employs preconditioning by the approximate inverse matrix, which is however the main limiting factor in the usage in higher dimensions.

Notice that verification of solutions of systems of equations is a first step to verify also eigenvalues of matrices or optimal solutions of optimization problems (such as linear programming or semidefinite programming).

Inverse modeling of coupled groundwater flow and heat transport: choice of parameters and measured data

Milan Hokr

The solved problem is a thermal effect of tunnel on surrounding rock, with contribution of groundwater advective heat transport. Both temperature and flow rate measurements are available, as several years long series. All the hydraulic and thermal parameters of the rock are considered unknown or uncertain (laboratory sample analyses are not necessarily valid for the field scale). A set of inverse problems is solved, differring by selection of the solved processes (individual water flow or heat transport, or the two coupled), selection of unknown parameters, balancing weight of residuals of field data and a-priori laboratory data, or different formulation of problem boundaries. Public available software with a gradient-based optimization method is used for calculation, linked through standard input and output files of the process simulation code. We also demonstrate how the more constrained models, where the surface temperature of individual places is used as the model input, provide better fit, but less knowledge of the processes and its parameters. Using the global tunnel air temperature for all places as the input, we get worse fit, but a more realistic model and more understanding of the process.

DG method for pricing European options under Merton jump-diffusion model

<u>Jiří Hozman</u>, Tomáš Tichý

We present the discontinuous Galerkin method applied to European option pricing under Merton jump- diffusion model, i.e., when the evolution of the asset prices is driven by a Lévy process with a finite activity. The valuation of options under such model with Gaussian jumps requires solving a degenerate parabolic partial integro-differential equation (PIDE), i.e., a functional equation which involves both integrals and derivatives of an unknown pricing function. The integral term related to jumps leads to new theoretical and numerical issues regarding solving of pricing PIDE in comparison with the standard approach for pricing PDEs. For practical purposes of numerical pricing of options in such models we propose an explicit-implicit scheme arising from the discontinuous piecewise polynomial approximation. Finally, the preliminary numerical results are presented on reference benchmarks.

Funkce příslušnosti fuzzy množiny definovaná odezvou modelu

Jan Chleboun, Judita Runcziková

Funkce příslušnosti fuzzy množiny je běžně definována způsobem, který lze nazvat apriorním. Příkladem může být trojúhelníkové nebo lichoběžníkové fuzzy číslo vzniklé fuzzifikací dané známé hodnoty, přičemž parametry k fuzzifikaci použité funkce příslušnosti volí uživatel dle svého uvážení. Vzniklé fuzzy množiny pak mohou vstupovat do modelu, jehož odezva na nejistá vstupní data je předmětem zkoumání. V některých případech je však situace odlišná, neboť je třeba pracovat se dvěma modely závislými na týchž vstupních parametrech, přičemž odezva O modelu A je přibližně známa například z měření a cílem je vyšetřit šíření nejistoty modelem B. V příspěvku se navrhuje ze změřené odezvy O identifikovat hodnoty vstupních parametrů – data D, která pak budou tvořit jádro fuzzy množiny. Hodnota fuzzifikační funkce příslušnosti pro perturbovaná data D je poté odvozena z rozdílu mezi již známou odezvou O a vypočtenou odezvou modelu A při perturbovaných vstupních datech D. Takto vytvořená fuzzy množina je použita při analýze fuzzy odezvy modelu B na vstupní fuzzy parametry vzniklé fuzzifikací dat D.

Optimal control of parallel system of two continuously degrading components

Čeněk Jirsák

Maintenance optimization is a common topic in mathematical reliability theory. Motivation for our model are continuously deteriorating systems consisting of components working in parallel with a redundancy. An example of such a system might be a group of coal mills in a power plant, where 7 out of 8 mills must be operating for an efficient coal burning. Such systems are usually modeled as multistate stochastic systems using standard tools (mainly Markov chains and processes). Our focus is to apply continuous deterioration to the model. So far we can find an optimal policy only for a simple deterministic models. For more complex models we use numerical approximation such as simulated annealing.

Numerical simulation of generalized Newtonian fluids in bypass geometry

Radka Keslerová, Tomáš Padělek, Hynek Řezníček

The aim of this work is to describe and discuss the results of numerical study of Newtonian fluids in the bypass tube. The different radius of stenosed vessel were tested. A Newtonian mathematical model was used for an investigation of bypass flow. The fundamental system of equations is the system of generalized Navier-Stokes eqautions for incompressible laminar flow. Newtonian fluids flow in the bypass is numerically simulated by using open source CFD tool, OpenFOAM with a SIMPLE algorithm and by central finite volume method using explicit Runge-Kutta time integration. Considered geometry is based on 3D hexahedral structured mesh in bypass tube with different radius of stenosis (a narrowing of blood vessel). Numerical results are compared for two different type of fluids (Newtonian and non-Newtonian) and for two way of numerical modelling (OpenFOAM and homemade software).

Modeling of Galfenol and Terfenol-D

Ielizaveta Kholmetska

The contribution concentrates on modeling magnetostrictive materials. Magnetostrictive materials form a subclass of materials with memory that is characterized by the interplay between mechanical stress and magnetic field. They are used, for example, for vibration sensors and devices for converting mechanical energy into electrical energy. Their memory is represented by hysteresis operators.
The work focuses on the mathematical modeling and identification of the model parameters based on the measured data of such materials as Galfenol and Terfenol-D. The parameters identification is performed by minimizing the squared error between experimental and simulated magnetic and magnetostrictive curves. There are three models proposed and compared with measured data: non-hysteretic, non-hysteretic with feedback and hysteretic models.

Numerická stabilita řešení rovnic nelineárního nosníku

Jan Klesa

Příspěvek se zabývá stabilitou numerického řešení deformace nosníku v závislosti na čase. Popis chování nosníku je založen na formulaci podle D. H. Hodgese, tj. nosník z lineárního elastického materiálu s velkými deformacemi. Praktické použití tohoto matematického modelu je např. pro modelování chování listů nosného rotoru vrtulníku. Rovnice představují soustavu nelineárních parciálních diferenciálních rovnic. Pro jejich numerické řešení byla použita metoda konečných diferencí. Byly vyzkoušena různá schémata pro numerickou náhradu prostorových derivací, tj. výpočet z hodnot v časové vrstvě N, N+1 a N+1/2. Všechna tato schémata jsou nestabilní a nepoužitelná. Pro numericky stabilní řešení je nutné provést náhradu derivací v časové úrovni v rozmezí cca od N+0,6 do N+0,8.

An Adaptive Recursive Multilevel Approximate Inverse Preconditioning: How to Compute the Schur Complement

Jiří Kopal

System of linear algebraic equations in the form Ax = b, where A is a square, large and sparse matrix, represents a commonly solved problem in science and engineering. Iterative methods based on Krylov subspaces, in particular the conjugate gradient method for SPD case, offers a very efficient choice for solving such problems. In practice, iterative methods are most often used in their preconditioned form. We deal with a particular strategy to obtain preconditioner which is based on the incomplete version of the generalized Gram–Schmidt process employed in a multilevel framework. It delivers direct and inverse factorization (incomplete) at the same time and on every level. Both types of incomplete factorizations can be used as a preconditioner. We point out some interesting relations between direct and inverse factors and some connection among variants of the algorithm.

Mathematical modeling of coupled transport processes in porous media

Lukáš Krupička

This contribution deals with mathematical modeling of coupled heat transport and water flow in unsaturated porous media. The model is based on conservation equations, e.g. mass conservation equation and energy conservation equation. The complete model consists of two nonlinear partial differential equations with unknown total pressure head and temperature and prescribed boundary and initial conditions. The contribution deals with the existence of a weak solution and an illustrative numerical example.

Noise in residuals of LSQR, LSMR, and CRAIG regularization

Marie Kubínová

We consider a linear inverse problem $Ax \approx b$, where A is a linear operator with smoothing property and b represents an observation vector polluted with noise. Due to the smoothing property of A, these problems are typically *ill-posed*, meaning that noise in the the data, especially its high-frequency components, may give rise to significant errors in computed approximations of x. Golub–Kahan iterative bidiagonalization represents the core algorithm in several regularization methods for solving this type of problems. Using existing results on noise propagation in this process, we study the match between the noise vector and residuals of three bidiagonalization-based regularization methods – LSQR, LSMR, and CRAIG. We derive explicit relations between the residuals and noise contaminated bidiagonalization vectors. We consider a general noise setting.
Joint work with Iveta Hnětynková and Martin Plešinger.

From local to global theories of iteration

Václav Kučera

Iteration is a key concept in numerical mathematics. The theoretical analysis of numerical algorithms then tries to answer such questions as when do the iterates converge, how fast, what do they converge to, etc. For nonlinear problems, such results are usually local, based essentially on Banach's fixed point theorem and variations thereof in some neighborhood of the exact solution. But the question is what happens globally, for example in Newton's method. Global theories of iteration do exist but use different tools than the numerical community. In this talk, we give an overview of the field of holomorphic dynamics dealing with global aspects of iteration of complex functions. We give an overview of classic and modern results, as well as open problems, and their implications for Newton's method.

Preconditioning Method for Homogenization of Anisotropic Materials

Martin Ladecký

Within the problem of homogenization of anisotropic materials, we use spectral Fourier bases to obtain homogenized material properties on rectangular domains. Discretization leads to large systems of linear equations, which we have to solve. These large systems can be preconditioned by matrices arising from discretization of certain homogeneous problems. We present its theoretical justification and relevant numerical experiments.

Multi-objective Reliability-based Design Optimization with Meta-models

Matěj Lepš

Reliability-based design optimization (RBDO) searches for a trade-off between costs and safety under assumption of uncertainties. We concentrate on the double-looped reliability-based design optimization, in which the system reliability is assessed within the inner loop and a designing process is performed in the outer loop. A common approach expressed as a single-objective optimization is transformed into a multi-objective case providing results as an approximation of the Pareto front composed of the compromising solutions between cost and reliability. The double-loop formulation of RBDO provides the most accurate approximation of the Pareto front but is computationally demanding even if advanced simulation techniques are used for rare failure events. Several of these techniques will be presented and their advantages and disadvantages will be discussed. Despite the reduction in evaluation time using advanced simulation techniques compared to a crude Monte Carlo method, the computational effort is still high with a complex model as a performance function, e.g. a finite element model. The computational model can be replaced by its surrogate in order to reduce the computational costs. This meta-model fits the responses evaluated by the original model for the predetermined data, so called a Design of Experiment (DoE). Since the design variables change with every iteration and a meta-model is utilized for a reliability assessment, the meta-model is trained only in the vicinity of the relevant design variable which makes the meta-model computationally faster and more precise. The DoE can be then updated by selected points from advanced simulation techniques' samples with respect to two criteria: first, beneficial samples are located in the vicinity of the limit state, which divides the space into a safe region and a failure domain, and second, these samples should be also placed in the sparsest position of the DoE. The described method is illustrated on a classical RBDO benchmark with two objective functions; the first objective is a cost function to be minimized, the second objective is a structural reliability expressed by a reliability index to be maximized.

Parallel TDNNS-FEM for elastodynamics of thin-walled structures

Dalibor Lukáš, Lukáš Malý, Erika Straková, Joachim Schoeberl

We recall a mixed finite element method for the Hellinger-Reissner formulation of elasticity that relies on a stable ansatz with tangential-continuous displacements and normal-normal continuous stresses (TDNNS). It turns out that recently proposed hexahedral geometrically anisotropic elements are robust with respect to the thickness, i.e., they are free of the shear-locking effect. This is confirmed up to ultrasonic frequencies by solution to a quasi-periodic eigenvalue problem on a single element. At the end novel results on parallel acceleration by means of domain decomposition methods or spectral finite elements are presented.

Kombinace Gaussovy–Newtonovy metody s kvazinewtonovskými metodami

Ladislav Lukšan, Jan Vlček

Gaussovu-Newtonovu metodu pro minimalizaci součtu čtverců nelineárních funkcí lze zefektivnit použitím kvazinewtonovských aktualizací. Obvykle se používá matice normální soustavy rovnic, která se koriguje pomocí kvazinewtonovských aktualizací Broydenova typu, nebo se obě metody kombinují. V tomto příspěvku se zaměříme na metody používající aktualizace v součinovém tvaru používající aproximaci Jacobiovy matice. V této souvislosti uvedeme novou metodu vhodnou pro použití QR rozkladu nebo iterací metody LSQR.

Structured fluids

Josef Málek

Most fluid-like substances, such as geomaterials, biofluids and polymeric liquids, are complex fluids exhibiting intricate nonlinear rheological response and structures. The aim of the talk is to present unified novel viewpoints how to describe the responses of such materials. A particular attention will be devoted to the mechanical and thermodynamical underpinnings of the considered models and their consequences towards the long-time and large-data existence of generalised (weak) solutions of relevant initial and boundary value problems. Finally, we present several results concerning the computation of experimentally relevant problems regarding flows of such complex fluids. The lecture will be based on several joint papers and discussions with Jan Blechta, Miroslav Bulíček, Vít Průša, K. R. Rajagopal, Endré Süli and Karel Tůma.

Mathematical modeling in pharmacotherapy: Parameter estimation problem

Ctirad Matonoha

The model we are dealing with is a 1D mixed PDE/ODE model that is spatially discretized using a finite difference scheme. Some part of input experimental or testing data is not available, so it must be somehow optimized or fitted. The main goal is an estimation of diffusion parameters of different compounds.

Simulation of Dislocation Pileup Using Quasicontinuum Method

Karel Mikeš

In this contribution, the molecular statics is used to model dislocations. In order to decrease the excessive computational cost, the quasicontinuum (QC) method is used. In QC method, only the relevant subset of atoms, so-called repatoms, is selected to represent the entire system. Consequently, two types of solving domain is considered. The dislocation mechanism can be exactly captured in region of high interest where the atomistic structure is exactly represented. An adaptive QC algorithm has been introduced. The adaptive extension of the area of high interest is based on three different error estimators, namely deformation gradients, local lattice disregistry, and change of local energy. The QC method is studied for the case of dislocation pileup in two-dimensional hexagonal lattices with next-to-nearest interactions described by the Lennard-Jones potential. Its accuracy and efficiency is compared against the full atomistic model.

Optimalizace trajektorie průmyslového robota při výrobě rámového kompozitu

Jaroslav Mlýnek

Příspěvek je zaměřen na problematiku optimalizace trajektorie průmyslového robota. V článku je popsán matematický model postupného průchodu 3D polyuretanového rámu navíjecí hlavou při provádění tří návinů uhlíkových vláken. Rám je připevněn ke koncovému efektoru robota. Za účelem dodržení požadovaných úhlů návinů a zajištění rovnoměrné hustoty jednotlivých vrstev návinů je potřebné stanovit optimalizovanou trajektorii end-efektoru robota. Při optimalizaci trajektorie je využito prostředků lineární algebry a diferenciální evoluční algoritmus. Matematický model a sestavený optimalizační algoritmus umožňují určit diskrétní množinu parametrů „tool-centre-point", která definuje optimalizovanou trajektorii robota.

Mathematical modeling in pharmacotherapy: Compartmental vs. PDE/ODE based approach

Štěpán Papáček, Jurjen Duintjer Tebbens

Our work aims to formulate and test a novel modeling approach in pharmacotherapy. Although the multi-compartmental approach has been used for decades, only the PDE/ODE based approach allows to calculate the spatial distribution of drug inside a compartment. This is particularly important knowing that too high levels of drug concentration can be harmful or even mortal. Both the compartmental and PDE/ODE based model will be calibrated with experimental in vitro data from liver cells, and the subsequent comparison of a drug rifampicin concetration will be evaluated for each of two models.

On the extreme eigenvalues of certain matrices of non-standard inner products of Hermite polynomials

Martin Plešinger, Ivana Pultarová

In this contribution, we focus on Hermite orthogonal polynomials and in particular on Gram matrices of such polynomials in non-standard (shifted) inner products. The weight function of the non-standard inner product is obtained from the Gauss probability density function by its horizontal shift by a real parameter. We are interested in the spectral properties, in particular the extreme eigenvalues of these matrices and some of their modifications. We show how the eigenvalues depend on the parameter.
https://www.sciencedirect.com/science/article/pii/S0024379518300582

Explicitní integrace pohybových rovnic řešená na počítačovém clusteru

Václav Rek

Díky aktuálním výpočetním možnostem současné výpočetní techniky řada firem zabývajících se vývojem analytického software založeném na MKP, investuje do vývoje explicitních numerických metod. To se týká například programu RFEM, který obsahuje řešič založený na numerické metodě dynamické relaxace. Paralalizace pak umožňuje získání výsledků z velkých úloh v rozumném čase. Mezi významné typy uvažovaných nelinearit, při explicitním řešení, patří velká deformační kinematika a nelineární okrajové podmínky. Pro účely numerického řešení nelineární dynamiky stavebních a strojních konstrukcí byl navržen hyperparalelní numerický řešič, který bude dále představen. Řešič distribuuje numerický výpočet na heterogenním počítačovém clusteru složeném z počítačů obsahujících vícejádrové procesory. Řešené numerické modely uvažují velkou rotační kinematiku při malých přetvořeních ve spojení s Kurush-Kuhn-Tuckerovými okrajovými podmínkami.

Estimate of vegetation efficiency on reducing dust concentration produced by a surface coal mine

Hynek Řezníček, Luděk Beneš

The study try to answer a question: How can vegetation help to reduce dust concentration in a village near a surface coal mine. The flow field and the concentrations are computed on 2D cuts with a real geometry for Bilina coal mine. An in-house CFD solver, based on finite volume method AUSM+up scheme, is used to compute the flow field. System of the RANS equations for viscous incompressible flow with variable density is used for description of the flows. The two equations turbulence model is used for the closure of this set of equations. The transport equation for concentration of passive contaminant is solved. Petroff's model of the dust deposition on vegetation is employed. It reflect four main processes leading to particles deposition on the leaves: Brownian diffusion, interception, impaction and gravitational settling. Three different configuration of vegetation were computed: Two heights of the trees are consid- ered, 15 m for fully grown forest and 3 m for planted trees. Results for these two configurations were compared to situation without any vegetation.

Stavová úloha pro časoprostorovou tvarovou optimalizaci dutiny razníku při lisování skla

Petr Salač, Jan Stebel

V příspěvku je představena časoprostorová stavová úloha tvarové optimalizace dutiny razníku pro lisování skleněné produkce. Systém forma, skleněný výlisek, razník a dutina razníku je zde uvažován ve čtyřech po sobě jdoucích časových intervalech. V prvním je razník v dolní poloze obklopen novou sklovinou, ve druhém je razník již v horní poloze a výlisek dále chladne ve formě, v třetím razník lisuje další výlisek v dolní poloze se sklovinou v následující formě karuselového lisu a výlisek je stále ve formě a ve čtvrtém intervalu je uvažována samotná forma bez výlisku do okamžiku dalšího plnění pro její další cyklus. Stavová úloha ve tvaru smíšeného problému pro rovnici energie je nejprve formulována v diferenciálním tvaru a následně převedena do slabé formulace v Bochnerově prostoru. Účelový funkcionál je ve tvaru druhé mocniny rozdílu teploty v časovém okamžiku před separací razníku a skleněného výlisku od předem zvolené konstanty ve váhovém prostoru v povrchové vrstvě razníku.

Multivariate smooth interpolation that employs polyharmonic functions

Karel Segeth

We follow the variational way of constructing splines called smooth interpolation for multivariate interpolation employing polyharmonic functions.

To this end, we choose the system of functions $exp(-ikx)$ for the basis of the space where we minimize functionals and measure the smoothness of the result. The general form of the interpolation formula is then the linear combination of the values of some radial basis functions (polyharmonic splines) and low-order polynomials.

We also present a simple numerical example. Computer aided geometric design or geographic information systems are the fields where the smooth approximation in 2D and 3D is often used.

Computer implementation of nonlinear system of hypoplastic model of granular material

Lenka Siváková

Here presented model of hypoplasticity of granular material is based on the work of Kolymbas and Bauer. A general rate-independentequation describing stress when compressing the granular material was applied to different types of loading: isotropic, anisotropic, anisotropic volume preserving, unilateral deformation. The computer implementation of this constitutive equation showed types of loading mentioned above and that it is possible to model "ratchetting"- the hysteresis behavior of granular materials at alternating loading. The program in Matlab of this model is presented here.

Různé typy řešení reakčně-difúzní rovnice na mřížkách a grafech

Petr Stehlík

Představíme si motivaci pro studium reakčně difúzních rovnic na mřížkách a grafech, která je jednak teoretická (diskretizace) i praktická (zejména ekologické aplikace). Dále se budeme zabývat zajímavými typy řešení pro tyto rovnice a budeme zkoumat zejména vlastnosti, které se liší mezi standardní úlohou na spojité oblasti a na oblasti diskrétní. Půjde zejména o dva typy řešení. V první části prozkoumáme prostorově heterogenní řešení a jejich stabilitu. V druhé části budeme zkoumat tzv. dvoubarevné cestující vlny. Jak uvidíme, obě úlohy spolu úzce souvisí a jsou spojeny i se zajímavým algebraickým problémem týkajícím se perturbace semidefinitních matic.

Operator preconditioning, discretization and decomposition into subspaces

Zdeněk Strakoš

Coupling infinite dimensional formulations of difficult problems (e.g., in numerical PDEs) with efficient finite dimensional computations represents, in general, a challenge. It can rarely be resolved while considering the individual steps of the solution process separately and then approaching them within isolated disciplines. This contribution will concentrate on transformation of the original problem to the form that allows fast computation, which is commonly called preconditioning, and on its relationship with discretization.

Algebraically constructed preconditioners are based on an approximate solution of (a part of) the dicretized problem. One may ask in which way they provide a global exchange of information in function spaces associated with the underlying mathematical infinite dimensional model. This question can be addressed within the framework of the so called operator preconditioning.

We will consider linear equations in the abstract infinite-dimensional Hilbert space setting with bounded, coercive and self-adjoint operators. It is shown that preconditioning can be interpreted as transformation of the discretization basis and that any algebraic preconditioning of a symmetric positive definite algebraic problem (arising from discretization) can be equivalently seen as transformation of the discretization basis as well as of the associated inner product.

Motivated, in particular, by the works of Faber, Manteuffel, Parter, Oswald, Dahmen, Kunoth and Rude published in the early 90's, we will also present an abstract formulation of operator preconditioning based on the idea of decomposition of a Hilbert space into a finite number of (infinite-dimensional) subspaces. Results will be formulated using the concepts of norm equivalence and spectral equivalence of infinite-dimensional operators. Using infinite-dimensional function spaces, this can help in describing, in a concise way, some common principles behind various computational techniques.

This contribution will present results of a joint work with Jakub Hrnčíř, Tomáš Gergelits, Josef P. Málek, Jan Papež and Ivana Pultarová.

Local Eigenvalue Analysis using Contour Integral Method

Erika Straková

The generalized eigenvalue problem is an essential problem in many areas of engineering such as analysis of mechanical vibrations, electrical networks, optical waveguides, or in quantum chemistry. The traditional algorithms often locate all eigenvalues and use costly diagonalization. The presented method computes eigenvalues of a matrix pencil only in a given domain of interest. The method relies on complex integrals of the resolvent operator.

Numerical approximation of a mathematical model of float glass forming process

Petr Sváček

In this paper the modelling of glass flow as viscous liquid is considered during the float glass production. The simplified mathematical model is described, which takes into account the free surface of the flow, the temperature distributrion and the flow over the tin bath. The numerical approximation with the aid of the finite element method is described. The numerical results are shown.

Limit analysis in perfect plasticity and inf-sup conditions on convex cones

Stanislav Sysala

The contribution is devoted to a limit analysis problem related to perfect plasticity. This problem describes a plastic collapse and enables to find a limit value of a load parameter. No solution exists beyond the limit value. The limit analysis problem can be defined either in terms of stresses (the static principle) or in terms of displacements (the kinematic principle). The kinematic principle leads to a convex optimization subject to constraints generating a convex cone. This cone depends on a prescribed plastic (yield) criterion. Using the polar cone, a specific inf-sup condition between stress and displacement fields is introduced. We analyze whether this condition holds or not depending on a plastic criterion, boundary conditions or material parameters. If the inf-sup condition is satisfied then it is possible to prove the equivalence between the static and kinematic principles of limit analysis or derive computable majorants of the limit load parameters. A particular attention is paid to the von Mises yield criterion where the inf-sup condition coincides with the one for incompressible flow media. In this case, we illustrate the computable majorants on numerical examples. This contribution is a joint work with J. Haslinger (Prague) and S. Repin (Jyväskylä, St. Petersburg).

QR factorization in the PLASMA library

<u>Jakub Šístek</u>, Jack Dongarra, Jakub Kurzak, and Julien Langou

We describe recent developments of the QR factorization functions in PLASMA, a numerical linear algebra library for dense matrices aiming at multicore and manycore systems. Parallel execution relies on the data-dependent tasks of the OpenMP runtime. An emphasis is given on rectangular matrices with more rows than columns, for which a new version of the tree-based hierarchical QR has been implemented. It is shown that an optimal algorithm needs to adapt the amount of parallelism to the available hardware.

Industry 4.0 and the Future of Mathematics Education

Pavel Šolín

In this presentation we will give a concise overview of the fourth industrial revolution, and describe its anticipated impact on workforce and education. We will comment on the changing needs of employers, and how they are changing the paradigm in K-12 higher education in the U.S. We will describe various types of online courses, with an emphasis on self-paced gamified courses. Students take these courses on their own, with only occasional interaction with a teacher. The teacher serves as a coach rather than being the primary source of knowledge. Also, these courses do not require exams. We will show a live demonstration of how such as a mathematics course may look in the future.

On improving accuracy of the error estimates in CG

Petr Tichý

In practical conjugate gradient (CG) computations it is very important to monitor the quality of an approximate solution to $Ax = b$. A natural quantity for measuring the quality of an approximate solution is the A-norm (energy norm) of the error. This quantity is unknown during the CG computations, but it can be estimated using quadrature-based bounds. One can further improve the accuracy of these estimates based on the assumed decrease of the energy norm in d consecutive iterations. In this presentation we suggest some heuristic techniques how to choose d adaptively in order to reach the required accuracy of the estimates.

O některých složených implicitních schématech časové integrace ve stavební dynamice

Jiří Vala

Značné výzkumné úsilí je v posledních letech věnováno hledání co nejefektivnějšího výpočtového schématu pro časovou integraci problémů stavební dynamiky. Z původních evolučních problémů, reprezentovaných zpravidla počátečními problémy pro soustavy parciálních diferenciálních rovnic 2. řádu hyperbolického typu, vznikají prostorovou diskretizací počáteční problémy pro rozsáhlé soustavy obyčejných diferenciálních rovnic. Ty se následně numericky řeší jako diferenční buď klasickou Newmarkovou metodou (1952), nebo různými jejími vylepšeními, např. dvoukrokovým algoritmem podle Batheho a Baiga (2005), případně tříkrokovým podle Wena a kol. (2017). Platnost tradovaných výsledků o konvergenci a stabilitě pro lineární úlohy přitom nelze přebírat v případě nutnosti iteračních postupů pro nelineární problémy. Příspěvek se pokusí o shrnutí současného stavu problematiky včetně některých původních výsledků a konkrétních stavebních aplikací.

The investigation of penalization approach for inlet boundary condition in flow driven vibrations of vocal folds

Jan Valášek

The contribution presents the simulation of the human vocal folds vibration excited by the fluid flow. The special attention is paid to the inlet boundary conditions. The classical Dirichlet boundary condition in the form of prescribed velocity has the drawback of unphysical pressure increase during channel closing phase of vocal folds vibration cycle. The another often chosen possibility is the do-nothing type of boundary condition with given pressure drop between inlet and outlet. It usually leads to quite high oscillation of inlet velocity. In order to overcome these disadvantages, the penalization approach is investigated, where beside the given pressure drop the inlet velocity is weakly enforced with the aid of the penalization term. Numerical results will be presented.

Dynamický útlum – srovnání různých koncepcí z hlediska fyzikální podstaty a účinků na stavební konstrukce

Adéla Vaněčková, Miroslav Trcala, Ivan Němec

Zdroje dynamického útlumu mohou být různorodé. Nejčastěji je útlum zaváděn do výpočtů ve formě zavedení tlumicích sil, jako součinu vektoru rychlosti a matice tlumení do pohybové rovnice. V praxi se matice tlumení většinou předpokládá jako lineární kombinace matice hmotnosti a matice tuhosti (tzv. Rayleighův útlum). Tento útlum primárně předpokládá jako zdroj útlumu viskozitu vnějšího prostředí, i když člen Rayleighova útlumu s maticí tuhosti implikuje i vnitřní útlum materiálu. Explicitně je vnitřní viskosita materiálu respektována při použití příslušných materiálových modelů. K dynamickému tlumení dochází i v případě použití nepružných materiálů, kdy odtěžování probíhá po jiné dráze, než zatěžování a dochází tak k disipaci při zatěžovacích cyklech. Příspěvek se věnuje srovnání různých druhů útlumu na kmitání stavební konstrukce.

Flux reconstructions for lower bounds on eigenvalues

Tomáš Vejchodský

Flux reconstruction techniques are well known to provide guaranteed a posteriori error bounds for linear elliptic partial differential boundary value problems. This talk will show that exactly the same techniques can be used for the corresponding eigenvalue problem to compute lower bounds of eigenvalues. In particular, the talk will explain the straightforward usage of the standard flux reconstructions in the classical methods for lower bounds on eigenvalues such as the Weinstein, Kato, and Lehmann–Goerisch methods.

Stability for some ALE higher order discretizations

Monika Balázsová, Miloslav Feistauer, <u>Miloslav Vlasák</u>

We assume a parabolic problem in a time-dependent domain, where the time-dependence of the domain is described by the prescribed ALE (Arbitrary Lagrangian-Eulerian) mapping. So far, these problems were typically analyzed for methods up to the order two in time, e.g. Euler method, Crank-Nicolson method or discontinuous Galerkin method with piecewise linear elements. We will present a stability analysis for the higher order methods based on the continuous and discontinuous Galerkin method of arbitrary order and their Runge-Kutta equivalents.

Užití nekonečněkrát opakované aktualizace BNS a myšlenky sdružených směrů u minimalizačních metod s omezenou pamětí

<u>Jan Vlček</u>, Ladislav Lukšan

Pro zlepšení efektivity metody L-BFGS s omezenou pamětí bylo v literatuře navrženo opakování některých aktualizací BFGS. Vhodné aktualizace je však třeba vybírat, protože mohou prodloužit dobu výpočtu. Je ukázáno, že v rámci podobné metody BNS lze (za jistých podmínek) aktualizace BFGS opakovat nekonečně krát bez patrného zvýšení počtu aritmetických operací. Limitní aktualizaci získáme řešením Ljapunovovy maticové rovnice, jejíž řád lze snížit kombinací s metodami používající vektorové korekce na konjugovanost. Navržený algoritmus je globálně konvergentní pro konvexní dostatečně hladké funkce a numerické výsledky naznačují jeho efektivitu.

Numerical Simulation of Flow Induced Airfoil Vibrations with Large Amplitudes

Ondřej Winter

The subject of this contribution is the numerical simulation of the interaction of two-dimensional incompressible viscous flow and a vibrating airfoil. A solid airfoil with two degrees of freedom, which can rotate around the elastic axis and oscillate in the vertical direction, is considered. The numerical simulation consists of the finite volume solution of the Navier-Stokes equations, coupled with the system of ordinary differential equations describing the airfoil motion. The time-dependent computational domain and a moving grid are taken into account with the aid of the arbitrary Lagrangian–Eulerian (ALE) formulation of the Navier–Stokes equations. Special attention is paid to the time discretization and the solution of the non-linear discrete problem on each time level is performed. Numerical solutions are obtained with free accessible open-source code OpenFOAM. The computational results are compared with known aerodynamical data and with results of aeroelastic calculations obtained by a linear approximation.