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http://panm21.math.cas.cz

panm@math.cas.cz

ABSTRAKTY

Discontinuous Galerkin method for problems in time-depend domains – theory and applications

Monika Balázsová

Most of the theoretical mathematical results on the solvability and numerical analysis of nonstationary partial differential equations are obtained under the assumption that a space domain is independent of time. However, problems in time-dependent domains are important in a number of areas of science and technology. This is particularly the case of fluid-structure interaction problems, when the flow is solved in a domain deformed due to the coupling with an elastic structure. There are various approaches to the solution of problems in time-dependent domains, very popular technique is the arbitrary Lagrangian-Eulerian (ALE) method. In this talk we present an ALE version of the space-time discontinuous Galerkin method, which is based on piecewise polynomial approximations over finite element meshes, in general discontinuous on interfaces between neighbouring elements. We show that the proposed method is numerically unconditionally stable and demonstrate its robustness on a numerical solution of the nonlinear elasticity benchmark problem. The developed method is also applied to the numerical simulation of air flow in a simplified model of human vocal tract and flow induced vocal folds vibrations.

Visualization of vector fields

Stanislav Bartoň

Modern computer algebra software can be used to visualize vector fields. One of the most used is the Maple program. This program is used to visualize two and three-dimensional vector fields. The possibilities of plotting direction vectors, lines of force, equipotential curves and the method of colouring the surface area for two-dimensional cases are shown step by step. For three-dimensional arrays, these methods are applied to various slices of three-dimensional space, such as a plane or a cylindrical surface. Finally, the temporal evolution of the vector fields is illustrated by animations based on the above methods.

A posteriori goal-oriented error estimates for elliptic problems discretized by the discontinuous Galerkin method

Ondřej Bartoš

We deal with the numerical solution of linear elliptic problems using the discontinuous Galerkin method with focus on the goal-oriented a posteriori error estimates. Our aim is to estimate the error of the quantity of interest represented by a linear functional. The abstract error estimate is based on the knowledge of the (exact) solution z of the dual problem corresponding to the primal one. In order to define a computable estimate, the dual solution z has to be replaced by its approximation z_h and the remaining term represented by difference $z - z_h$ is usually neglected. In this presentation we propose an approach which estimates the neglected term. Consequently, we are able to derive an uppper error estimate. These types of estimates are known for the conforming finite element approximation but are new in the framework of discontinuous Galerkin method. Moreover, we introduce an efficient implementation approach allowing a simultaneous solution of the primal and dual problems. Finally, numerical examples will be presented.

Reduced basis solver for stochastic Galerkin formulation of Darcy flow with uncertain material parameters

Michal Béreš

In this contribution, we present a solution of the stochastic Galerkin (SG) matrix equations coming from the Darcy flow problem with uncertain material coefficients in the separable form. The SG system of equations is kept in the compressed tensor form and its solution is a very challenging task. Here, we present the reduced basis (RB) method as an iterative solver which looks for a low-rank representation of the solution. The construction of the RB consists of iterative expanding of the basis using Monte Carlo sampling. This approach requires multiple solutions of systems of equations. We aim to introduce an efficient computation framework for the solution. This includes: speeding up the solution within Monte Carlo samples using the deflated conjugate gradients (DCG), adaptive precision for the solution of reduced systems, cheap residual estimate and sampling strategy within the Monte Carlo sampling. We test the method on a set of problems with a varying random behaviour of the material on subdomains as well as different geometries of subdomains.

Numerical realization of the Bayesian inversion accelerated using surrogate models

Simona Bérešová

A natural approach to the solution of inverse problems based on uncertain observed data is the Bayesian inversion. The result of such an inverse problem is the posterior distribution of unknown parameters. This contribution focuses on the numerical realization of the Bayesian inversion focusing on problems governed by computationally expensive forward models such as numerical solutions of partial differential equations. Samples from the posterior distribution are generated by the Markov chain Monte Carlo (MCMC) methods accelerated using surrogate models. A surrogate model is understood as an approximation of the forward model which should be computationally much cheaper. However, the target distribution is not modified, i.e. samples from the exact posterior distribution are provided. In addition, non-intrusive surrogate models can be updated during the sampling process resulting in an adaptive MCMC method. The use of the surrogate models significantly reduces the number of evaluations of the forward model needed for a reliable description of the posterior distribution. Described sampling procedures are implemented in the form of a Python package.

Coupling of boundary and finite element methods in the framework of Netgen/NgSolve

Adam Bílek, Dalibor Lukáš

The main goal of this work is to implement the higher-order boundary element method for solving 2D and 3D problems in the NGSolve software and then use it in combination with the finite element method to solve engineering problems. NGSolve is a high-performance multiphysics finite element software. Main task is to determine the coefficients of the matrices of a single layer and a double layer potentials. To do this, it is necessary to solve multidimensional integrals, which are often singular. These integrals have different types of singularities depending on the mutual position of the element couples. Specifically, in 3D, these integrals are four-dimensional and four cases of the mutual positions can occur, where in each we remove singularity and reduce the dimensionality of the integral by using Sauter and Schwab technique to achieve maximum efficiency. With these matrices, we are then able to calculate the missing data at the boundary and subsequently using a representation formula anywhere in the solution domain.

Numerické řešení turbulentního nestlačitelného proudění pomocí isogeometrické analýzy

Marek Brandner

Příspěvek bude zaměřen na numerické řešení problému turbulentního nestlačitelného vazkého proudění oblastí ve tvaru zpětného schodu. Bude prezentován matematický model založený na Reynoldsových středovaných Navierových-Stokesových rovnicích a dvourovnicovém k-ω modelu turbulence. Dále bude stručně popsáno využití isogeometrické analýzy, numerická schémata pro prostorovou a časovou diskretizaci, metody lineární a nelineární stabilizace a postup řešení získaných soustav lineárních rovnic. Na závěr budou prezentovány výsledky numerických experimentů a krátce zhodnoceny klady a zápory zvoleného přístupu.

Bayesovská inverze pro transportní vlastnosti zóny porušení v důsledku ražby

Jan Březina

Zóna porušení (EDZ) v okolí chodeb úložiště radioaktivního odpadu je potencionální transportní cestou kontaminace do významných poruchových zón což by mělo vliv na celkovou bezpečnost úložiště. Parametry transportního modelu (zejména porozita a permeabilita) jsou významně ovlivněny změnami napětí při ražbě a následně při zatopení chodeb úložiště. Představíme nelineární poroelastický model vzniku a dalšího vývoje EDZ. Pro experimentální data z kontinuálního měření pórových tlaků během ražby určíme pomocí Bayesovské inverze aposteriorní rozdělení pro parametry poroelastického modelu. Zejména získáme rozdělení pro permeabilitu a porozitu, která použijeme pro sestavení stochastického modelu transportu kontaminace podél EDZ. Nakonec aplikujeme víceúrovňovou metodu Monte Carlo pro aproximaci hustoty pravděpodobnosti indikátoru bezpečnosti odvozeného od hodnot koncentrace kontaminantu.

Multiobjective computationally expensive optimization problem of pump design

Jana Burkotová

The contribution aims to present a multiobjective optimization problem in the pump industry. Pump shape optimization is based on computationally expensive CFD simulations, limiting the maximum number of objective function evaluations. To reduce computational cost and solve the problem in a reasonable time, surrogate models have been successfully used. The presented method is based on Kriging assisted evolutionary multiobjective method K-RVEA using uncertainty information to access the quality of the approximations and confidence intervals. The next challenge in real-world optimization is to cope with a situation when evaluations of samples fail for different reasons, such as geometry or mesh creation error. The classification model is incorporated into the proposed algorithm to predict the failure region to save computational resources.

Valuation of two-factor options under Merton jump-diffusion model using orthogonal spline wavelets

Dana Černá

Two-asset Merton jump-diffusion model for valuation of European-type options is represented by a nonstationary integro-differential equation with two state variables. The drawback of most classical methods is that due to the integral term matrices arising from discretization are full and, moreover, badly conditioned. In this talk, we present a construction of a new orthogonal spline-wavelet basis and show that the Galerkin method with the constructed basis combined with the Crank-Nicholson scheme leads to sparse matrices, which are well-conditioned even without any preconditioning. Furthermore, the method is high-order convergent. Numerical experiments are presented for a European-type option on the maximum of two assets to illustrate the efficiency and applicability of the proposed scheme.

Regime-based non-stationary autoregressive models in evaporation estimation

Dagmar Dlouhá, Lukáš Pospíšil, Viktor Dubovský

Our interest in free water surface evaporation is given by the ongoing and planned hydric recultivation of the former Ležáky–Most quarry region. The most complex model for evaporation estimation is Penman-Monteith Equation, which requires several input quantities, such as air temperature, wind speed, heat storage in water, net radiation, etc. However, sometimes all of these values are not available or measurable, therefore in our studies, we are looking for simplified models. In this contribution, we consider autoregressive models, where we assume that the output variable (in our case prediction of evaporation) depends linearly on its previous values. We present a generalization of these models to non-stationary settings. Here, we assume that coefficients of linear dependency are changing in time switching between the finite number of regimes. The analysis aims to simultaneously identify optimal regimes and optimal autoregressive coefficients.

Goal-oriented error estimates for nonlinear partial differential equations and adaptivity

Vít Dolejší

Solving numerically partial differential equations (PDEs), we are frequently not interested in the approximate solution itself but we need to approximate the value of a certain solution-dependent functional. The necessity to estimate the error of this target quantity gives rise to the goal-oriented error estimates. They are based on the formulation and solution of adjoint problem which is well-established for linear PDEs but for nonlinear ones, a formulation based on the Jacobian of the primal problem is usually used. We develop this approach but the adjoint problem employs a suitable linearization which guarantees the adjoint consistency of the numerical scheme. Furthermore, we propose stopping criteria for iterative solvers which balances the discretization and algebraic errors. Furthermore, the derived estimates are combined with anisotropic *hp*-mesh adaptation method. Several numerical examples demonstrate the efficiency of this algorithm.

The comparison of selected meta-heuristic algorithms for solving regression causality problems in data classification

Vojtěch Dorňák, Lukáš Pospíšil, Martin Čermák

One of the most common problems in data analysis is classification - a pre-trained algorithm aims to assign a label to an observation. While neural networks are nowadays a popular choice for this task, the conventional deterministic approaches provide some advantages, for instance, more straightforward interpretation of the optimal fitting decision model parameters or the smaller demand on the amount of training data. Recently, we developed a new method based on causality, i.e., conditional probabilities. The key component of this approach is the optimization regression problem with an objective function consisting of the Kullback-Leibler divergence, with the feasible set consisting of separable simplexes. However, this problem is analytically unsolvable. In the contribution, we present the method and compare the performance of two meta-heuristic approaches: simulated annealing, a single-solution search; and particle swarm optimization, a population-based search.

Extension of time-profiles for nuclear receptor-induced enzyme production with spatial resolution

Jurjen Duintjer Tebbens

The subject of the talk is efficient modelling of the intracellular action of a drugs binding to the nuclear receptors. The binded complex enters the cell nucleus and acts on DNA, resulting in enhanced production of an enzyme supposed to metabolize, among others, the substances responsible for the disease. We will present an extension of an ODE based model for the action of the drug Rifampicin. The extension consists of a first attempt to add spatial resolution for substances that are active in the cytoplasm, which can be beneficial to analyze important issues like local exceeding of toxic drug levels or delay of transport. For the resulting mixed systems of PDEs coupled with ODEs, we are particularly interested in efficient solution of the arising sparse linear systems.

Identification and analysis of cyclostationary random processes

Cyril Fischer

The strong quasi-periodic response emerging in nonlinear dynamical systems is characterized in certain regimes by a beating effect that combines self-excited and forced vibrations. The presence of symmetric or asymmetric beatings indicates an exchange of energy between individual degrees of freedom of the model. In the stochastic case, the response acquires statistical properties that vary cyclically with time. A cyclostationary process emerges. The analysis of detailed properties of such a response is feasible using methods developed for such cyclostationary processes.

On the properties of hybrid methods for the solution of large scale discrete inverse problems

Eva Havelková

Discrete inverse problems of the form $Ax \approx b$ arise in many practical applications. The ill-conditioning of the large-scale matrix A in combination with the presence of noise in the vector b make their solution a challenging task. Hybrid methods represent a combination of iterative projection methods with direct regularization applied on the projected problem. Such a combination has shown to be efficient in prevention of semi-convergence and thus over-fitting of the solution while maintaining the computational cost feasible. In this presentation we concentrate on iterative hybrid LSQR method with inner Tikhonov regularization. We describe the algorithm, its key properties and connections. Further, we focus on the properties of the solution of the projected problem and its residual vector. Suitable stopping criteria and their dependence on the choice of the regularization parameter will be discussed. Numerical experiments performed on problems arising in cryo-electron microscopy single particle analysis will be used for demonstration.

DG method for real options valuation in natural resources industry

Jiří Hozman, **Tomáš Tichý**

The real options approach plays an important role in the decision-making process, because it provides a solution to the optimal investment decision that captures the flexibility value embedded in a project. Since this methodology interprets the flexibility value as the option premium, various option pricing techniques are widely used to value flexibility. We present here the discontinuous Galerkin method applied to real options valuation arising in natural resources industry, especially options to change operating scale. Assuming values of both the project and the embedded option are determined in terms of time and underlying output commodity price (e.g., iron ore, gold, slate, etc.), which follows a relevant stochastic process, one can describe evolution of the project/option prices by the partial differential equations of the Black-Scholes type, linked through a payoff function given the type of the flexibility provided. The governing equations are discretized by the discontinuous Galerkin method over a finite element mesh and they are integrated in temporal variable by a semi-implicit Euler scheme. The special attention is paid to the treatment of early-exercise feature (i.e., American constraint) that is handled by additional penalty term incorporated to the governing equation and its discrete version to the numerical scheme. The capabilities of the approach presented are documented on the selected individual real options (i.e., flexibility types) from the reference experiments as well as using real market data from case studies.

Inverse analysis of a piano recording

Barbora Chlebišová, **Dalibor Lukáš**

The paper aims towards an automatic generation of music sheets from a piano recording. In this preliminary study we sample all the tones of a piano. These samples are processed by FFT and we arrive at nonnegative vectors of amplitudes, which serve as a basis for the subsequent analysis of a recording. The recording is split into beats, each of which is also processed by FFT. The inverse analysis now rely on the least-square fitting of the recording amplitude vector onto the space of sampled amplitude vectors. The resulting linear combination must be nonnegative. We show that polyphonic recordings can be well analyzed.

Úloha hypoplasticity s nejistými daty

Jan Chleboun

Hypoplastické chování vykazují například sypké materiály jako písek nebo zemina. Matematicky lze hypoplasticitu modelovat soustavou nelineárních obyčejných diferenciálních rovnic, přičemž cílem modelování je sledovat chování materiálu při střídavém zatěžování a odtěžování. Tímto procesem se sypký materiál postupně zhutňuje a jeho chování se blíží jistému limitnímu stavu. V matematickém modelu vystupují parametry, jež jsou obtížně měřitelné a jejich číselná hodnota je značně nejistá. Záměrem příspěvku je posoudit, jak se rozsah nejistoty ve vstupních parametrech promítne do rozsahu hodnot sledovaných výstupních veličin modelu. K tomu je využit aparát fuzzy množin, kde cílem je popsat fuzzy množinu výstupní veličiny v závislosti na fuzzy množinách vstupních parametrů.

Optimal control of the parallel system with continuous wear

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 linear deterministic models. For more general settings we use numerical approximation. The numerical approach for finding an optimal policy will be the focus of the poster.

Validation of numerical simulations of a simple immersed boundary solver for fluid flow in branched channels

Radka Keslerová, Anna Lancmanová

This work deals with the flow of incompressible viscous fluids in a two-dimensional branched channel. Using the immersed boundary method, a new finite difference solver was developed to interpret the channel geometry. The numerical results obtained by this new solver are compared with the numerical simulations of the older finite volume method code, which use a structured multiblock mesh, and with the results obtained with OpenFOAM, where an unstructured grid (quadrilaterals or triangles) is used. The aim of this work is to verify whether the immersed boundary method is suitable for fluid flow in channels with more complex geometry with difficult grid generation.

Správnost zkrácených lineárních detekčních kódů

Štěpán Klapka, Adam Rychtář

Příspěvek se věnuje problematice detekčních vlastností lineárních a cyklických kódů, které se potřebují pro kvantifikaci rizika při kontrole integrity dat, a to jak při jejich přenosu, tak při jejich dlouhodobém ukládání.

Determination of the initial stress tensor from deformation of underground opening 2: applications

Alexej Kolcun, Josef Malík

In this paper the implementation of the method for initial stress detection is described. Benchmark tasks and real models are analysed. A comparison with alternative methods is given.

Computational damage modelling of fiber building composites

Vladislav Kozák

Fiber cement composites belong to the class of promising concretes with higher mechanical resistance to cracking. This allows for a finer and more economical design; therefore, a new perspective on the creation of building structures or the replacement of steel structures is necessary. These load-bearing structures can result in stresses in the body exceeding the strength of the material, leading to gradual failure. Such failures are often initiated by surface or near surface cracks, which reduces the strength of the material. The XFEM application is able to overcome the disadvantages of simulating the propagation of cohesive cracks; however, it must handle the absence of a sharp singularity at the crack tip with a more complex derivation of the required stresses from the displacements. The complete computational model includes the formation and propagation of cracks, their bridging by fibers, loss of cohesion between the fibers and the matrix, their mutual sliding by friction and destruction of the fibers; viscoelastic behavior is preferred.

Alternatives to the FETI natural coarse space

David Horák, Jakub Kružík, Marek Pecha, Zdeněk Dostál, Václav Hapla, David Hrbáč

The presentation deals with the modification of the FETI-1 and TFETI methods eliminating projector onto kernel of natural coarse space matrix as the same effect can be achieved by using the Moore-Penrose pseudoinverse of the local stiffness matrices. This modification is reachable by means of projecting a suitable pseudoinverse onto the range of the local stiffness matrix, i.e. onto kernel of the transpose of the stiffness matrix kernel. This operation is purely local and very cheap. The coarse problem solution contained in the penalized term of the Hessian of the QP problem ensuring the homogenized equality constraint satisfaction could be omitted as well. Numerical experiments demonstrating efficiency of this approach projecting interface forces onto stiffness matrix range instead of ensuring their orthogonality to the stiffness matrix kernel resulting in equality constraint with natural coarse space matrix and associated coarse problem solution will be presented.

Numerical optimization of parameters in systems of differential equations

Václav Kučera

We present results on the estimation of unknown parameters in systems of ordinary differential equations in order to fit the output of models to real data. The numerical method is based on the nonlinear least squares problem along with the solution of sensitivity equations corresponding to the differential equations. We will present the performance of the method on the problem of fitting the output of basic compartmental epidemic models to data from the Covid-19 epidemic. This allows us to draw several conclusion on the natural limitations of these models and their validity.

Mathematical modeling of hydrodynamical processes in porous medium under phase changes due evaporation and freezing/melting

Michal Kuráž

Mathematical modeling in soil system sciences typically covers three distinct fields: hydrodynamics, thermodynamics and transport of solutes. A very typical property of all hydrodynamical processes in soils is an extremely low velocity of the liquid motion, flow regime is typically laminar. Due to low kinetic forces the flow field is significantly affected by osmotic and temperature gradient. Further, the flow area is scattered into microscopic pore paths, where phase changes such as evapotranspiration and ice crystallization can significantly affect local porous medium hydraulic properties. Setting up boundary conditions representing meteorological conditions is again nontrivial. In this talk it will be explained how to adapt the governing flow equation for describing flow processes together with liquid phase changes due freezing/melting and evapotranspiration. A special attention will be given to real-world application of smart farming system developed and installed on vineyards Finca Ecohumus, San Juan, Argentina.

Finding vertex-disjoint cycle cover of undirected graph using the least-squares method

Jan Lamač

Finding a vertex-disjoint cycle cover (called a 2-factor) of a given undirected graph G consists in finding a set of disjoint cycles which are subgraphs of G and contain all vertices of G. It is well known that a 2-factor of an undirected 2-factorable graph can be found in polynomial time by transforming the problem into a problem of finding a perfect matching in a larger graph. When we prescribe further conditions on this cycle cover (e.g. number of components, minimal cycle length) the problem of finding a 2-factor becomes NP-hard. In this contribution we investigate the properties of the least-squares solution of the system of equations with a matrix being the incidence matrix of the given undirected graph G and we propose an algorithm that uses this solution for finding a 2-factor of the graph G.

Shear-thinning fluids in porous media: an inverse problem of estimating the pore size distribution

Martin Lanzendörfer

The linear Darcy law for the flow of water through porous media can be viewed (among many other idealizations) as a macroscopic sum of Hagen-Poiseuille-type flows through many microscopic capillaries. From this point of view, the permeability of the media is determined by the distribution of the capillaries, in particular by their radii - the pore size distribution. Considering non-Newtonian fluids, this capillary bundle concept offers an interesting nonlinear relation between the pore size distribution and the apparent permeability with respect to, e.g., shear-thinning fluids. In fact, it appears that the flow rates observed for various fluid rheologies and/or under varying hydraulic gradients can be used to obtain a reasonable estimate of the pore size distribution, leading to an interesting alternative to costly porosimetry techniques.
There are many aspects, both practical and theoretical, to be discussed. We will focus on three of them: the radially symmetric flow around the injected/pumped borehole, the open question of the optimal choice of experiments, and the "one to rule them all": the sensitivity of the numerical inversion with respect to the measurement error.

Preconditioners for poroelasticity with geotechnical applications

Tomáš Luber

Poroelastic models describe a coupled system of a fluid flow through porous media coupled with deformation of the porous matrix. For the poster we will consider a Biot's model that couples a fully saturated Darcy's flow with deformation described by linear elasticity. More precisely, we will consider the time-step problem that arises from discretization of the model by implicit Euler method in three field formulation in displacement, flux and pressure. This problem has a natural block structure given by distinct physical fields which will be exploited to analyze the problem and to propose several block preconditioners. Finally, these preconditioners will be tested in geotechnical setting and their performance will be compared in terms of numbers of iterations and computational demands.

Hierarchical real-time optimal planning of collision-free trajectories of collaborative robots

Dalibor Lukáš

In collaborative robotics the manipulator trajectory has to be planned to avoid collisions, yet in real-time. In this paper we pose the problem as minimization of a quadratic functional among piecewise linear trajectories in the angular (joint) space. The minimization is subjected to nonlinear inequality constraints that are cheap to evaluate. The very first and most critical step of the computation is to find an initial trajectory that is free of collisions. To that we minimize a weighted sum of the violated constraints until they become feasible. Sometimes an incremental growing of the obstacle helps. The initial trajectory is then optimized while preserving feasibility at each step. We solve a sequence of simple-bound constrained quadratic programming problems formulated in the dual space of Lagrange multipliers, which are related to the original linearized inequality constraints that are active or close-to-active. Finally, we refine the trajectory parameterization and repeat the optimization within a hierarchical approach until an overall prescribed time limit, being well below a second, is reached.

Detection of the generalized synchronization of chaotic systems: auxiliary system approach with delayed communication

Volodymyr Lynnyk, Branislav Rehák

The generalized synchronization is one of several kinds of synchronization of chaotic systems in the master-slave synchronization. This synchronization is established if a functional relation exists between states of both systems. However, finding this relationship is a difficult task; hence other means to detect the generalized synchronization were proposed, the auxiliary system approach is one of them. This approach is based on adding a copy of the slave system with different initial conditions and simultaneously observing the outputs of the slave and auxiliary systems. The indication of the established general synchronization is the existence of a relation between outputs of the auxiliary and slave systems that is easier to detect than any relation between states of two chaotic systems (as the definition of the generalized synchronization requires). We focus on applying the auxiliary system approach to detect the generalized synchronization under delayed communication between the master and slave systems. Attention will also be paid to the robustness of the proposed scheme against numerical errors.

Determination of the initial stress tensor from deformation of underground opening 1: theoretical background

Josef Malík, Alexej Kolcun

In this paper a method for the detection of the initial stress tensor is proposed. The method is based on measuring distances between some pairs of points located on the wall of underground opening in the excavation process. The methods is based on the solution of twelve auxiliary problems in the theory of elasticity with force boundary conditions. The positions of the pairs of points on the wall of underground openings are studied. The pairs must be located so that the condition number of the least square matrix has the minimal value, which guarantees a reliable estimation of initial stress tensor. In the paper the theoretical aspects of the method is studied.

Mathematical models and computational algorithms for 3D and 4D image processing in developmental biology and medicine

Karol Mikula

We present mathematical models and numerical algorithms based on nonlinear advection-diffusion equations used for image filtering, segmentation and tracking in a large-scale 3D+time laser scanning microscopy images leading to automated reconstruction of the cell lineage tree during the first hours of embryogenesis. To achieve that goal, we discretize the nonlinear partial differential equations by the finite volume method, natural to image processing applications, and develop efficient and stable numerical schemes suitable for massively parallel computer architecture. This is a common work with colleagues from Institute of Developmental Biology CNRS and Ecole Polytechnique, Paris, France and University of Bologna, Italy.

New methods in collision of bodies analysis

Ivan Němec, Jiří Vala, Hynek Stekbauer, Michal Jedlička, Daniel Burkart

The widely used method for solution of impacts of bodies, called the penalty method, is based on the contact force proportional to the length of the interpenetration of bodies. This method is regarded as unsatisfactory by the authors of this contribution, because of a inaccurate fulfillment of the energy conservation law and violation of the natural demand of impenetrability of bodies. Two new methods for the solution of impacts of bodies, suggested by the authors, fulfill these demands exactly, or approximately, but much better than the penalty method. The energy method exactly fulfills the conservation of energy law and the kinematic method exactly fulfills the condition of impenetrability of bodies. Both of these methods are superior in comparison with the penalty method, which is demonstrated by the results of several numerical examples.

Mixed precision GMRES-based iterative refinement with recycling

Eda Oktay

Krylov subspace recycling is a well-known technique for reusing information across sequential invocations of a Krylov subspace method on systems with the same or a slowly changing coefficient matrix. In this talk, we present a mixed precision GMRES-based iterative refinement solver incorporated with Krylov subspace recycling approach. The insight in this algorithm is that in each refinement step, we call preconditioned GMRES on a linear system with the same coefficient matrix, with only the right-hand side changing. In this way, the GMRES solves in subsequent refinement steps can be accelerated by recycling information obtained from the first step. After giving a background on GMRES-based iterative refinement and Krylov subspace recycling, we present numerical experiments that show the advantage of combining this approach.

An enhanced model parameter estimation by a slow-fast decomposition based on the first order two time-scale expansion

Štěpán Papáček, Ctirad Matonoha

Some dynamical systems, e.g. biochemical networks, are characterized by more than one time scale. On the paradigmatic example of a drug-induced enzyme production we show how the slow-fast decomposition can serve for an enhanced parameter estimation when the slowly changing features are rigorously incorporated. The method has been developed to reduce confidence intervals for the estimated parameters. Our approach, based on the first order two time-scale expansion, is demonstrated on an in vivo model of xenobiotic metabolizing enzyme induction containing 8 reactions, 6 state variables and 15 parameters, as a case study.

Distributed approaches into machine learning

David Horák, Jakub Kružík, Zachary Langford, Marek Pecha, Richard Tran Mills

Popular machine learning frameworks provide only multi-threading parallelism on shared memory and are designed as off-the-shelf packages. They are convenient and efficient for building high-level software solutions; however, they typically lack monitoring convergence related to underlying solvers and the development of model scores during the training phases of predictors. Currently used machine learning applications perform parallelism on a task level or orchestration based on multiple container instances of an application running in Kubernetes or Microsoft Azure. In our poster, we present novelty approaches to distributed machine learning involving native data parallelism on clusters. We point out the impact of scalable solvers adaptation on ML problem structure and low-precision computation. The results will be presented on real-world datasets.

A Lanczos-like method for non-autonomous linear ordinary differential equations

Stefano Pozza

The time-ordered exponential (TOE) is the solution of a system of first-order linear differential equations with generally non-constant coefficients. Its approximation is crucial in many applications, for instance, in nuclear magnetic resonance (NMR), where it appears as the solution of the Schrödinger equation. In NMR applications, simulating particle dynamics is of great importance. Unfortunately, modeling a large number of particles leads to huge ODE systems whose numerical solution is still a challenge. Two new approaches for TOE approximation have been introduced in recent years: the path-sum and the *-Lanczos methods. They both rely on a convolution-like product, the so-called *-product. We will show an accurate approximation of such a product and why this may be the key to the efficient numerical computation of TOEs.

Guaranteed two-sided bounds to homogenized coefficients

Ivana Pultarová

We deal with a classical homogenization problem of getting effective coefficients of a second order elliptic partial differential equation. We suggest a numerical procedure which yields guaranteed arbitrarily close two-sided bounds to the effective coefficients. While the upper bounds naturally follow from any finite element approximation of the variational form of the problem, to obtain the lower bounds we must employ a dual variational problem. We introduce a simple divergence free approximation function spaces based on a finite element discretization. We consider a 3D setting, which is rarely dealt with in this context so far. Moreover, we simplify the theoretical background of building the dual formulation, and thus all parts of the procedure are theoretically justified. Some illustrative examples are presented.

Contact problem for nonlinear Gao beam model – parameter identification

Jana Radová

Identification problem is a framework of mathematical problems dealing with the identification of unknown coefficients of a given differential equation. The identification of parameters consists of using experimentally measured data to determine coefficients of the given differential equation. This contribution focuses on the identification of the coefficients representing the material properties or modulus of foundation of a nonlinear beam model that is known as the Gao beam. A solution of the identification problem is obtained by minimization of the given quadratic cost functional which depends on the material parameters or modulus of foundation and the solution of the state problem which is represented by the contact problem for Gao beam model. Numerical solution is based on using finite element method and some optimization techniques. The presented theory is illustrated by several numerical examples.

Small gain theorem for systems described by quasilinear parabolic equations

Branislav Rehák, **Volodymyr Lynnyk**

Stability of interconnection of two or several dynamical systems is a crucial property that needs to be satisfied. The small gain theorem has been recognized as an effective tool for guaranteeing stability of interconnection of dynamical systems, even for systems with time delays.
In this contribution, the small gain theorem for connection of systems described by quasilinear parabolic equations is investigated. Conditions guaranteeing Lyapunov stability for the interconnenction of two such systems are derived. This is achieved by introducing a Lyapunov function defined on a suitable Sobolev space. Attention is also paid to time-delay systems. Here, the stability of the interconnection of systems is demonstrated using a generalization of the Lyapunov-Krasovskii od Lyapunov-Razumikhin fucntionals to systems, again defined on a Sobolev space. The results are illustrated by numerical simulations.

Numerical stability of block classical Gram–Schmidt

Miroslav Rozložník

The block version of the classical Gram–Schmidt (BCGS) method is often employed to efficiently compute orthogonal bases for Krylov subspace methods and eigenvalue solvers, but a rigorous proof of its stability behavior has not yet been established. It is shown that the usual implementation of BCGS can lose orthogonality at a rate worse than $O(\epsilon)\kappa^2(X)$, where $\kappa(X)$ is the condition number of the input matrix X and ϵ is the unit roundoff. A useful intermediate quantity denoted as the Cholesky residual is given special attention and, along with a block generalization of the Pythagorean theorem, this quantity is used to develop more stable variants of BCGS. These variants are proven to have $O(\epsilon)\kappa^2(X)$ loss of orthogonality with relatively relaxed conditions on the intrablock orthogonalization routine satisfied by the most commonly used algorithms. A variety of numerical examples illustrate the theoretical bounds.

Comparison of LES model (PALM v 6.0) results to the wind-tunnel measurements for neutrally stratified Urban boundary layer

Hynek Řezníček, Jan Geletič, Martin Bureš, Pavel Krč, Jaroslav Resler, Kateřina Vrbová, Arsenii Trush, Petr Michálek, Matthias Sühring

The capability of PALM core to simulate the complex air-flow within the urban canopy has been studied and a realistic buildings layout from the Prague-Dejvice quarter has been chosen as a testing domain. The model of the urban area has been 3D-printed* and placed in the Climatic wind tunnel (see Kuznetsov S. et al.: Flow and turbulence control in a boundary layer wind tunnel using passive hardware devices. Experimental Techniques 41(6) 2017). Beside the general agreement of the observed and simulated air-flow, the influence of the passageways leading through some buildings in the domain and their affect on the air-flow in the courtyard has been studied.

PALM is an urban climate model which is capable to simulate turbulent air-flow within the urban canopy. It consists of a dynamic solver for the Navier-Stokes equations. By default, the model uses the LES approach in which the bulk of the turbulent motions is explicitly resolved. Following the paper (Gronemeier et al.: Evaluation of the dynamic core of the palm model system 6.0 in a neutrally stratified urban environment: comparison between les and wind-tunnel experiments. Geoscientific Model Development 14(6) 2021) the simulation is conducted as a blind test (no tunnel-model tuning) and the domain contains all the roughness passive hardware devices in the wind-tunnel in the front of the simulated section to create a realistic urban canopy turbulence (see Kuznetsov et al.: Flow and turbulence control in a boundary layer wind tunnel using passive hardware devices. Experimental Techniques 41(6) 20172017).

A spherical basis function interpolation with particular trend functions

Karel Segeth

When measuring some physical fields, we may know the expected results quite well and only the difference between the measured values and the model described by a known formula is worth interpolating. Our contribution is concerned with such a situation. As the data is measured on the surface of a sphere in 3D, we employ a spherical interpolation with a simple spherical radial basis function of the quadric type complemented with a trend function corresponding to the theoretical model, in particular a polynomial of degree 2 considered in Cartesian coordinates. We prove the existence of the interpolation formula of the type considered and discuss the variational formulation of this interpolation problem. We present a simple computational example.

Two-dimensional nonlinear elastic plate

Radek Svačina

This paper deals with a nonlinear static plate model based on Berger theory, which shall be understood as a specific case of a generalization of the Woinowsky-Krieger mathematical model of a beam bending. It is considered a plate bending with forces acting in the middle plane of the plate and contact problem with an elastic foundation, where the normal compliance condition is employed. A variational equation of the problem and a functional of the total potential energy corresponding to the variational equation are derived. Under additional assumptions on data (e.g. clamped plate), existence and uniqueness of the solution is proven. A numerical solution is based on using Galerkin method and Courant approximation. The theory is illustrated by several numerical examples.

Převod dat ze softwaru ANSYS do prostředí MATLAB pro efektivní analýzu konstrukcí

Tadeáš Světlík

Metoda konečných prvků (MKP) je nejrozšířenější metoda pro diskretizaci a numerické řešení parciálních diferenciálních rovnic a nerovnic využívaná pro numerické řešení úloh stavební mechaniky a navrhování konstrukcí. Metoda je založena na nahrazení spojitého prostoru řešení a okrajových podmínek aproximací prostorem s konečnou dimenzí, přičemž s komplexností úlohy výrazně roste i časová náročnost výpočtu. Připravovaná nová generace evropských norem předpokládá významné zapojení numerického modelování do procesu návrhu konstrukcí a staveb. Základním požadavkem bude tedy nejenom přesnost daného řešení ale především efektivita numerických algoritmů využívajících MKP. Cílem tohoto příspěvku je představit způsob exportu dat nutných pro MKP model převzatý ze softwaru ANSYS a jejich import do programovacího prostředí MATLAB, ve kterém je úloha řešena s využitím efektivního vektorizovaného kódu. Tento skript využívá nových optimalizačních algoritmů vhodných pro budoucí paralelizaci s cílem řešit rozsáhlé úlohy přesahující aktuální možnosti softwaru ANSYS.

Užití pružně-plastických modelů při odhadování zón poškození způsobených ražbou hlubinných tunelů

Stanislav Sysala

Náš výzkum je motivován problematikou hlubinného ukládání vyhořelého jaderného paliva v krystalických horninách. V okolí stěn ražených tunelů a úložných vrtů jsou pozorovány zvýšené koncentrace napětí, tvorba a spojování trhlin různých rozměrů nebo výlomy ve tvaru V-zářezů. Predikce různých typů zón poškození jsou potřebné nejen pro stabilitu podzemních děl, ale také pro analýzu trasportních procesů radioaktivních látek. V příspěvku prezentujeme prvotní výsledky týkající se predikce zón poškození pomocí různých pružně-plastických modelů (Drucker-Prager, Mohr-Coulomb, Hoek-Brown). Studujeme závislost výsledků na volbě konečných prvků, hustotě sítě, počátečním napětí nebo na materiálových parametrech. Cílem práce je také popis veřejně dostupných a vektorizovaných kódů v Matlabu a Pythonu obsahující inovativní konstrukci implicitních konstitutivních operátorů a jejich zobecněných derivací. Příspěvek vychází ze spolupráce se Zdeňkem Michalcem, Martinem Besedou a dalšími kolegy.

Homogenization of the transport equation describing convection-diffusion processes in a material with fine periodic structure

David Šilhánek

In the present contribution we discuss mathematical homogenization and numerical solution of the elliptic problem describing convection-diffusion processes in a material with fine periodic structure. Transport processes such as heat conduction or transport of contaminants through porous media are typically associated with convection-diffusion equations. It is well known that the application of the classical Galerkin finite element method is inappropriate in this case since the discrete solution is usually globally affected by spurious oscillations. Therefore, great care should be taken in developing stable numerical formulations. We describe a variational principle for the convection-diffusion problem with rapidly oscillating coefficients and formulate the corresponding homogenization theorems. Further, based on the variational principle, we derive a stable numerical scheme for the corresponding homogenized problem. Several numerical examples will be solved to illustrate the overall performance of the proposed method.

Lanczos algorithm in finite precision

Dorota Šimonová

In 1989, Greenbaum developed a mathematical model of the finite precision CG computations. In particular, it has been shown that the finite precision CG computations can be seen (up to some small inaccuracy) as the exact CG computations for a matrix having many eigenvalues distributed throughout tiny intervals about the eigenvalues of the original matrix. In the current paper [Greenbaum, Liu and Chen, SIAM J. Sci. Comput., 43 (2021)], the authors consider several CG variants that became popular because of the possibility of a better parallelization and study properties of the corresponding mathematical models. In our presentation, we will study mathematical models of other CG variants and provide the corresponding numerical experiments. We will try to explain in more detail some phenomenons observed in the above mentioned paper.

A parallel domain decomposition solver for immersed boundary finite element method

Jakub Šístek

Immersed boundary finite element method (FEM) presents an attractive approach to simulations. It avoids the generation of body-fitted meshes, which can be tedious and challenging for complex geometries and large-scale parallel simulations. However, the price to pay are more complicated methods for the weak enforcement of Dirichlet boundary conditions, poor conditioning of the stiffness matrices, and nonstandard numerical integration at the vicinity of the boundary. We are interested in combining the method with adaptive mesh refinement, which is nontrivial in parallel setting, but still advantageous for many problems that need a fine resolution at the boundary. Our primary aim is to develop a scalable iterative method for the arising large systems of algebraic equations. This method is obtained by adjusting the multilevel Balancing Domain Decomposition by Constraints (BDDC) to fragmented subdomains. This is a joint work with Fehmi Cirak, Eky Febrianto, Matija Kecman, and Pavel Kůs.

On error estimation in the conjugate gradient method

Petr Tichý

The (preconditioned) conjugate gradient (P)CG method is the iterative method of choice for solving linear algebraic systems $Ax = b$ with a real symmetric positive definite matrix A. To solve the underlying practical problems efficiently, it is important to know when to stop the CG iterations. Stopping criteria are application dependent. The relevant quantities for monitoring the quality of the approximate solution x_k are, e.g., the A-norm of the error, the Euclidean norm of the error, the normwise backward error, or the residual norm. Some of the above mentioned quantities cannot be easily evaluated, however, they can be estimated. In this presentation, we recall known results and then concentrate on estimating the A-norm of the error. Our aim is to improve the accuracy of the estimates using information from d forthcoming CG iterations. We suggest a heuristic strategy for the adaptive choice of d such that the relative accuracy of the resulting estimates is within a prescribed tolerance. Numerical experiments demonstrate that the suggested strategy is efficient and robust.

Comparison of different finite element method on fluid structure interaction

Karel Vacek

This paper focuses on mathematical modelling and finite element simulation of a problem of fluid-structure interaction problems. A simplified problem of two-dimensional incompressible fluid flow interacting with structure, whose motion is described with one or two degrees of free- dom, is considered. The problem is mathematically described and numerically approximated using the finite element method. For numerical treatment two approaches are discussed - the first one is based on coupled velocity-pressure unknowns, whereas for the second approach a decoupling strategy is used, usually known as the projection method. For the first case the finite element spaces that satisfy Babuška-Brezzi inf-sup condition are used. Two possibilities (Taylor Hood and Scott-Vogelius elements) are used and their application is discussed. For the decoupled approach also the equal order (P_1/P_1) element is used except the previously mentioned ones. The practical realisation of these approaches is discussed and its applicability is tested on several numerical examples as for the flow around the cylinder. The numerical results are shown and compared to reference data.

Godunov-like numerical fluxes for conservation laws on networks and L^2 stability

Lukáš Vacek

Godunov-like numerical fluxes for conservation laws on networks and L^2 stability Abstrakt: We describe a numerical technique for the solution of macroscopic traffic flow models on networks of roads. On individual roads, we consider the standard Lighthill-Whitham-Richards model which is discretized using the discontinuous Galerkin method along with suitable limiters. In order to solve traffic flows on networks, we construct suitable numerical fluxes at junctions based on preferences of the drivers. We prove that our semi-discrete DG solution is L^2 stable on several types of networks. We present numerical experiments, including a junction with complicated traffic light patterns with multiple phases.

On a computational approach to multiple contacts/impacts of elastic bodies

Jiří Vala, **Václav Rek**

Most problems of engineering dynamics are analysed computationally using some finite element technique together with the method of discretization in time. Whereas relevant physical processes admit some intuitive kind of mathematical linearization and related computational simplification of corresponding systems of partial differential equations of evolution of hyperbolic type, supplied by a priori known Dirichlet, Neumann, etc. boundary conditions and some initial Cauchy ones, the presence of contact-impact problems for multiple elastic bodies brings numerous difficulties with interface phenomena, implemented at least in form of some variational inequalities containing unknown abstract functions, typically displacements related to appropriate geometrical configurations from Bochner-Sobolev spaces. Consequently most computational tricks with the aim of generation of sparse linear algebraic systems are not available at all, or do not result in effective computational tools because of the duty of utilization of very short time steps in (only conditionally stable) explicit algorithms, to cover all possible mutual collisions of particular bodies properly. A distributed computing platform, suggested in this paper, opens a possibility of a robust and effective approach to such class of problems. An illustrative example shows an impact of structures assembled from a finite number of shells.

Interpolation between finite element meshes respecting mass and energy conservation for flow problems

Jan Valášek, Petr Sváček

The contribution deals with the remeshing procedure between two computational finite element meshes. The remeshing represented by the solution interpolation onto a new mesh is needed in many applications like e.g. in aeroacoustics, here we are particularly interested in the numerical flow simulation of a gradual channel collapse connected with a severe deterioration of the computational flow mesh quality. Since the classical Lagrangian projection from one mesh to another is a dissipative method not respecting conservation laws, a conservative interpolation method introducing constraints is described. The constraints have form of Lagrange multipliers enforcing conservation of the desired flow quantities, like e.g. total fluid mass, flow kinetic energy or flow potential energy. Then the interpolation problem turns into an error minimization problem, such that the resulting quantities of proposed interpolation satisfy these physical properties while staying as close as possible to the results of Lagrangian interpolation in the L^2 norm. The proposed interpolation scheme does not impose any restrictions on mesh generation process and it has a relatively low computational cost. The implementation details are discussed and test case is shown.

Discrete Element Method ve stavebnictví

Radek Varga

Discrete Element Method (DEM) je numerická metoda založena na pohybech a interakcích částic, která je využívána především v oblasti dynamiky sypkých hmot. Ačkoliv metoda ve své základní podobě není vhodná pro modelování spojitých úloh, s jistými úpravami ji lze využít například pro modelování šíření trhlin v betonu.
Cílem příspěvku je rešerše dosavadního výzkumu v oblasti modelování spojitých hmot, a možnosti aplikace v oblasti stavebního inženýrství, zejména pak konstrukce staveb. Práce se zaměřuje na několik možností aplikace DEM pro spojité úlohy, například kombinaci s metodou konečných prvků FDEM (Finite-Discrete Element Method), primárně však na využití DDEM (Deformable Discrete Element Method). Tato modifikace umožňuje deformaci částic v závislosti na napětí. Výstupy rešerše budou následně použity pro budoucí výzkum v této oblasti.

Residual error bounds for eigenfunctions

Tomáš Vejchodský, Xuefeng Liu

We propose fully computable a posteriori error bounds for approximate eigenfunctions of compact self-adjoint operators in Hilbert spaces. Special attention is paid to the case of tight clusters and multiple eigenvalues because corresponding eigenfunctions are then sensitive to small changes of the problem. These bounds are motivated by the Davis–Kahan $\sin\theta$ theorem, which estimates the error by a norm of the residual. We generalize this approach to weakly formulated eigenvalue problems and bound the suitable (usually dual and hence not computable) norm of the residual by the Prager–Synge technique using $H(\mathrm{div})$ conforming flux reconstructions of gradients of approximate eigenfunctions. Numerical examples indicate the higher accuracy of resulting bounds.

A posteriori error estimate for incomplete discontinuous Galerkin method

Miloslav Vlasák

The aim of the talk is the presentation of an accurate a posteriori error estimate for the incomplete variant of the interior penalty discontinuous Galerkin method (IIPG). Since the method is nonconforming, the design of a suitable error norm is crucial. We will present the error norm as a dual norm of residual of the extended formulation and derive a guaranteed upper bound to this error with the aid of the equilibrated flux reconstruction technique. Possible extension to other variants of discontinuous Galerkin method will be discussed as well as the efficiency estimates.