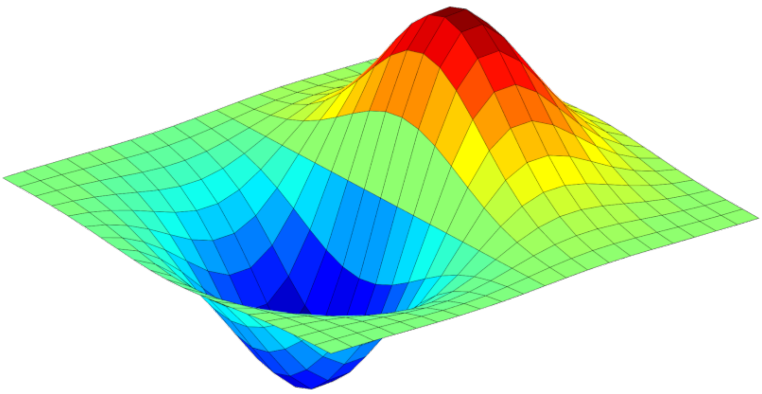
Institute of Geonics of the CAS, Ostrava

SNA'23

Seminar on Numerical Analysis

Modelling and Simulation
of Challenging Engineering Problems



Winter School

Methods of Numerical Mathematics and Modelling,
High-Performance Computing, Numerical Linear Algebra

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Short Abstracts

Contents

Some consideration on the use of spectral projectors for large scale eigenvalue computations

P. Arbenz

In this talk we remind of two methods to compute eigenvalues (and the corresponding vectors) of large sparse symmetric eigenvalue problems in an interval: (1) subspace iteration applied to polynomials approximating the characteristic function of intervals and (2) subspace iteration with projectors based on contour integration. Contour integration originates in the Cauchy integral formula and thus requires complex computation. We discuss techniques to avoid complex computations and their efficiencies w.r.t. the unmodified approaches.

On solution of shape optimization for Stokes problem with stick-slip condition

V. Arzt, P. Beremlijski

The shape optimization for the Stokes problem with the stick-slip boundary condition can be modelled as the minimization of the composite function generated by the objective and the control-state mapping. It can be shown that this composite function is generally non-differentiable (nonsmooth). For this nonsmooth problem, we have to use methods that work with the calculus of Clarke. We use the bundle trust method proposed by Schramm and Zowe. In each step of the iteration process, we must be able to find the solution of the state problem (Stokes problem with the stick-slip condition) solved by semi-smooth newton method with BiCGstab as inner solver and compute one arbitrary Clarke subgradient. Finite differences are used for the approximation of this subgradient.

On preconditioning of some fully implicit Runge-Kutta methods

O. Axelsson, I. Dravins, M. Neytcheva

In this presentation we discuss preconditioners for the fully implicit Runge-Kutta (IRK) methods of arbitrary order of accuracy. IRK offer the possibility to use high order accurate time discretization to match space discretization accuracy, an issue of significant importance for many large scale problems of current interest with (many) millions of spatial degrees of freedom and long time intervals. We consider one particular formulation of the IRK methods, namely, based on Radau quadratures, which is strongly A-stable. For the arising large algebraic systems we introduce efficient preconditioners, that (1) use only real arithmetic, (2) demonstrate robustness with respect to problem and discretization parameters and (3) allow for fully stage-parallel solution. The preconditioners are based on the observation that the lower-triangular part of the IRK matrices has larger in magnitude values, compared to their strictly upper-triangular part. We analyze the spectrum of the corresponding preconditioned systems and illustrate their performance of the corresponding iterative solution methods with numerical experiments. We also comment on some specific properties of the Radau-quadrature based Runge-Kutta matrices, which facilitate the attractive properties of the suggested preconditioners.

A new approach to solving quasilinear boundary value problems with p-Laplacian using optimization

M. Bailová

The talk focuses on finding weak solutions of a specific type of quasilinear boundary value problem with p-Laplacian. The classical approach is based on the fact that such solutions are related to critical points of the corresponding functional with a certain geometry. Therefore, a mountain pass theorem can be used to prove the existence of its nontrivial critical points. We present a novel approach that can be considered an alternative to the classic mountain pass-based method. A new way of proving the existence of nontrivial weak solutions is introduced. We show that the nontrivial solutions of the problem are related to critical points of a functional different from the energy functional, and some solutions correspond to its minimum. This idea is new even for $p = 2$. We also present two algorithms based on the introduced theory.

Solution of PDEs with uncertainties in parameters by the stochastic Galerkin method with geotechnical applications

M. Béreš

An efficient solution of a partial differential equation with parameters or uncertainties in input data can be a difficult task. The stochastic Galerkin method solves a PDE with uncertainties via the discretization of both the physical and the stochastic space. The resulting basis is assumed as a product of the two bases: finite elements (FE) for the discretization of physical space, and polynomials for the discretization of stochastic space. This approach leads to an enormous system of equations with a number of degrees of freedom surpassing the capabilities of any standard method for the solution of linear systems. The solution of such a system requires specialized tools for a feasible solution. A very efficient tool for the solution is the reduced basis (RB) approach. The RB approach aims at a compression of the FE basis. The compressed FE basis has orders of magnitude smaller size and the resulting reduced system is much easier to solve. In this talk, we will discuss a Monte Carlo based approach to the construction of RB. We examine measures of error for stopping criteria and adaptive polynomial basis selection. Additionally, we briefly discuss an efficient solution for reduced systems using the Tensor Train approximation. We will use problems inspired by geotechnical applications for the demonstration of the discussed methods.

Multilevel Monte Carlo contaminant transport in service of the safety assessment of deep geological repository

J. Březina, J. Stebel, M. Špetlík, P. Exner

Excavation disturbed zone (EDZ) in the vicinity of the galleries of the repository of radioactive waste can be a substantial part of the preferential path for contaminant transport. The excavation-induced stress field changes modify the micro-fracture network leading to disturbed macroscopic transport properties: permeability, porosity, and dispersivity. The safety of individual storage positions of the repository can vary depending on the local properties of EDZ and its interaction with surrounding fractures. We will characterize the safety of a single storage position in terms of a certain quantity based on a simulation of contaminant transport. In order to deal with intrinsic uncertainties in the transport model parameters, we shall apply the multilevel Monte Carlo method.

Interactive multiobjective optimization of hydraulic pump design

J. Burkotová, P.A. Pour, T. Krátký, K. Miettinen

In this contribution, we present a hydraulic pump design optimization problem. The considered pump model involves computationally expensive CFD simulations that bring several challenges into the solution process. The aim of the optimization is to find a pump design with maximal efficiencies at three different flow rates. We solve this multiobjective optimization problem with an interactive surrogate-assisted reference-vector guided evolutionary algorithm, and we demonstrate the potential of the interactive approach to solve real-world problems. In the interactive solution process, the preference information provided by a decision maker is utilized to guide the search into the region of interest. In this way, we reduce the computational time compared to the non-interactive approach.

Direct construction of reciprocal mass matrix and higher order finite element method

R. Cimrman, R. Kolman, J.A. González, K.C. Park

When solving dynamical problems of computational mechanics, such as contact-impact problems or cases involving complex structures under fast loading conditions, explicit time-stepping algorithms are usually preferred over implicit ones. The explicit schemes are normally combined with the lumped (diagonal) mass matrix so that the calculations are efficient and moreover dispersion errors in wave propagation are partially eliminated. As an alternative to lumping with advantageous properties, the reciprocal mass matrix is an inverse mass matrix that has the same sparsity structure as the original consistent mass matrix, preserves the total mass, captures well the desired frequency spectrum and leads thus to efficient and accurate calculations. In the contribution we comment on the usability of the reciprocal mass matrix in connection with higher order FEM.

On an ODE decomposition for biochemical networks due to Erich Bohl and Ivo Marek and its usage for preconditioning in PDE's

J. Duintjer Tebbens, M. Lanzendörfer, C. Matonoha, Š. Papáček

The talk presents a technique proposed by Erich Bohl and Ivo Marek in 2005 to transform systems of nonlinear ODE's arising in biochemical networks into a set of smaller, quasi-linear subsystems. The precise meaning of quasi-linearity for this context will be explained and it will be shown that the subproblems can be expressed as linear ODE's with matrices that are negative M-matrices. The technique was used to prove existence and uniqueness results, but may as well have computational advantages when compared with solving the original system of nonlinear ODE's. When the ODE's are inflated to PDE's through the addition of spatial resolution, the technique can be used as a basis for matrix-free preconditioning. The talk will present an example from modeling intra-cellular gene regulation.

Block preconditioning with approximate inner solvers for incompressible flow problems based on IgA discretization

J. Egermaier, H. Horníková

We deal with efficient numerical solution of the incompressible Navier-Stokes equations discretized using isogeometric analysis (IgA) approach resulting in large sparse linear systems of saddle-point type. Therefore an efficient iterative method for these systems is necessary. Based on our previous works a Krylov subspace method GMRES with a suitable block preconditioning meets this requirement. Within the framework of the preconditioner, it is also necessary to solve inner systems. In this work, we will discuss the use and properties of approximate inner solvers based mainly on multigrid techniques for solving these systems.

Guaranteed lower bounds to effective PDE parameters

L. Gaynutdinova, M. Ladecký, I. Pultarová, J. Zeman

We are interested in computing guaranteed lower bounds to effective (homogenized) coefficients of heat and elasticity 2D and 3D operators. We compare some approximation spaces to the dual heat problem and show that Lagrange finite elements yield a more efficient method that the usually used Nedelec elements. We show a discretization of the dual solution space of the elasticity equation based on Bogner-Fox-Schmit elements.

Quality assessment of volume reconstructions in Single Particle Analysis

E. Havelková, I. Hnětynková

In this contribution, we focus on discrete inverse problems arising in volume reconstruction in Cryo-electron microscopy single-particle analysis (SPA). Such problems represent a very large-scale well-structured overdetermined approximation problem $Ax \sim b$. The large dimensionality of the problem combined with missing information and the presence of extreme amounts of noise in the data make the solution a challenging task. Computationally efficient methods and regularization techniques need to be applied to obtain reliable solution approximation. Evaluation of the quality of the obtained approximates is however complicated. Despite strong regularization the computed approximates are polluted by noise that propagates from the input data. Residual an error norms are typically non-descriptive here. Alternative quality assesement techniques thus need to be used in SPA. We present an overview of some of these techniques, discuss their advantages and disadvantages and illustrate them on computations with realistic data.

Development, validation, and application of a solver for non-isothermal non-adiabatic packed bed reactors

T. Hlavatý, M. Isoz, M. Khýr

Packed bed reactors are the most frequently used devices to perform heterogeneously catalyzed reactions on industrial scales. The main contribution of our work is the development of a numerical model applicable to simulations of such reactors. The developed model is based on the finite volume method, couples the momentum, mass and energy balances, and is free of any empirical closures. As such, the solver falls into the domain of the direct numerical simulation. In the talk, we will (i) present the new solver fundamental working principles, (ii) report on the verification of each of the solver components against existing literature data and (iii) demonstrate an application of the solver on an industrially relevant case of ethylene oxichlorination performed in a tubular reactor packed with Raschig rings coated by CuCl2 catalyst.

Recent development of the core problem theory in the context of the Total Least Squares minimization

I. Hnětynková, M. Plešinger, J. Žáková

In various areas, there is a need to solve multi-observation linear data-fitting problems $AX \approx B$ contaminated by errors, and also irrelevant or redundant data. In that case, Total Least Squares (TLS) is the method of choice for approximating the unknown solution X. However, here we deal with a principal difficulty that already the simplest single observation TLS problem may not have a solution. This can be resolved by the prior orthogonal core reduction of the data, extracting the necessary and sufficient information for solving the original problem into a core problem of smaller dimensions. In the single observation case, a core problem is then uniquely TLS solvable. Core reduction was recently generalized to multi-observation problems (including general formulations with a tensor model and/or a tensor observation) and solvability of the resulting core problems has been analyzed. In this contribution, we present our recent results in this direction.

New variant of the SMALSE algorithm

D. Horák, Z. Dostál, J. Kružík, M. Pecha, D. Hrbáč

SMALSE-rho and SMALSE-M algorithms are efficient tools for solution of the quadratic programming problems with equality constraint and simple bound. These algorithms consists of an outer loop for update of parameters rho or M, approximation of the Lagrange multipliers for equality contraint and MPRGP algorithm used as an inner solver for problems with penalized equality constraint and simple bound. SMALSE terminates if norms of the equality constraint violation and norm of the projected gradient are sufficiently small compared to the norm of the righ hand side multiplied by the relative tolerance. MPRGP in general terminates, if norm of the projected gradient is less than norm of the violation of the equality constraint multiplied by SMALSE M-parameter decreasing depending on the augmented Lagrangian increase. We avoid the accurate solution of inner problems in this way. The presentation deals with the new SMALSE-rhoM variant updating both, M and rho parameters and modifications of this MPRGP criterium reducing numbers of iterations.

Numerical valuation of the investment project flexibility: a comparison of European, Bermudan and American option styles

J. Hozman, T. Tichý

The real options approach interprets a flexibility value, embedded in a project, as an option premium. The essential impact on the true real option value has a perspective of dates on which the option may be exercised, namely only at the maturity (European style) or at any time up to expiration (American style) or at one of a finite discrete set of times up to expiration (Bermudan style). The object of interest is to valuate and compare the selected real put options with respect to various option styles. The problem we face is described by PDEs of the Black-Scholes type, equipped with the terminal condition enforced at time instants resulting from the specific option style considered. Since the early exercise is allowed (not only at expiration date), closed-form pricing formulae are not available in general. Therefore, as a numerical approach, the discontinuous Galerkin method is applied together with an implicit Euler scheme. Finally, the presented valuation scheme is employed for reference experiments.

Node renumbering strategies for efficient direct methods in selected problems of soil mechanics

D. Hrbáč, J. Kružík, D. Horák, J. Kruis

This paper gives an experimental evidence of the computational and memory efficiency of standard reordering techniques available in PETSc library and their effect on the PETSc Cholesky solver performance. The sparse matrices chosen for numerical testing come from domain decomposition of the FETI type of the slope stability problem and the best QMD reordering was able to reduce the factorization time by factor up to 1000, the solve by factor up to 40, number of nonzero entries in factorized matrix by factor 30 and memory requirements by factor 25.

Ratcheting and the propagation of uncertainy in a hypoplasticity model

J. Chleboun, J. Runczíková

The behavior of granular materials such as soil, sand, or gravel under an external load does not fit to common elasticity models. Instead, various hypoplastic models have been designed. In the contribution, the model proposed by Pavel Krejčí and his co-workers is used. In the model, input parameters are considered uncertain and the effect of uncertain data on model outputs is investigated. Namely, the result of periodic loading and unloading is studied. The hypoplastic material is made more compact and more solid under cyclic mechanical stress and tends to a limit state. This accumulation of deformation is called ratcheting. Since the inputs are uncertain, the set of limit states is not a one-point set. This is why the range of limit ratcheting states is investigated.

A note on Clifford algebras

D. Janovská

Many research fields, such as physics, robotics, machine vision and computer graphics, rely on geometric models of external world. In these applications geometric objects and their transformations are traditionally formalized using linear algebra, i.e. all geometric concepts have to be represented by vectors and matrices. Compared with traditional linear algebra, geometric algebra (also known as Clifford algebra) is a powerful mathematical tool that offers a natural and direct way to model geometric objects and their transformations. Geometric entities, such as lines, planes and volumes, become basic elements of the algebra and can be manipulated by a rich set of algebraic operators that have a direct geometric significance. We would like to study the algebra R^8 as ordinary normed vector space with an additional multiplication derived from the Clifford algebra C^4.

Quasi-Newton iterative methods for some elliptic PDEs with power order nonlinearities

J. Karátson

In this talk we consider nonlinear elliptic problems arising in various physical and other applications, where the model describes a stationary state of the given process, such as heat flow, elastic beam or rod models, glaciology etc. A standard way to solve such problems is a finite element discretization coupled with some Newton-like iteration. This talk gives a brief summary on various results in an operator approach where quasi-Newton methods are constructed via spectral equivalence, also interpreted as variable preconditioning. The considered problem classes depend on the structural conditions of the nonlinearity. The robustness of the method is illustrated by numerical tests for some real-life models.

Effect of parallelization on the calculation of internal forces for nonlinear material models

T. Koudelka, J. Kruis

Most materials used in civil engineering exhibit nonlinear responses on the loading, e.g. concrete or soils. The stress-strain relation of the material model may thus represent a very complex calculation needed to carry out at every integration point of the model. The stresses at integration points are used in the calculation of the internal force vector, which is evaluated repeatedly during the iterative procedure. Thus the parallelization of this process may increase computation performance significantly. The contribution will compare different parallelization approaches on the selected material models.

Model order reduction of transport-dominated systemsusing shifted proper orthogonal decomposition and artificial neural networks

A. Kovárnová, M. Isoz

Transport-dominated systems pose a great challenge for common mode-based techniques of model order reduction. In our work, we utilize the shifted proper orthogonal decomposition, an a-posteriori method for model order reduction of systems with transport, and combine it with interpolation via artificial neural networks to produce a time-continuous reduced order model. The resulting framework is purely data driven, i. e. no information about the structure of the full order model is needed. In the talk, we will (i) present the main principle of the method and (ii) demonstrate its applicability on several examples from computational fluid mechanics, with the emphasis on particle-laden flows.

Coupled thermo-hygro-mechanical modeling of bentonite in engineered barrier of nuclear waste repository

T. Krejčí, J. Kruis, T. Koudelka, D. Mašín

Compacted expansive clays and mainly bentonite are widely used in sealing geological structures because of their high swelling capacity, low permeability, and favorable retardation properties. The bentonites are tested as a part of engineered barriers in high-level radioactive waste storage and disposal in many countries, including the Czech Republic. Nuclear waste repositories are planned as complex structures with high safety and reliability demands. The bentonite backfill is subjected to hydration from the surrounding rock, the nuclear waste's heating up, and various mechanical effects that interact in a complex coupled thermo-hygro-mechanical (THM) phenomena. Recent research proved the need to perform large-scale or medium-scale heating tests simulating repository conditions in underground laboratories. This contribution presents a coupled thermo-hygro-mechanical model of bentonite in a heated mockup test, which is the auxiliary analysis accompanying this test. The analysis follows the staggered coupling algorithm combining a hypoplastic mechanical model for expansive clays with an extended micromechanical-based model for heat and moisture transfer in deforming medium. The numerical results are compared with measured data, and the model is subsequently validated.

Multi-time step methods for lattice discrete particle models

J. Kruis, J. Vorel

Lattice discrete particle models are used in many areas of research. For example, they can be used in analysis of concrete, polymers and other materials. The number of particles is usually very high and efficient method for time integration has to be used. In connection with the lattice discrete particle models, explicit methods prevails. With respect to localization of nonlinear effects into relatively small area, different time steps in domain solved are strongly required. Such numerical approach is called sub-cycling or multi-time step methods. This contribution concerns with sub-cycling algorithm with two time steps. The shorter time step is used in the area where nonlinear behaviour is concentrated while longer time step is used in the remaining part of the domain. First numerical examples are promissing. Different time steps lead to shorter computational time.

Implementation of wall functions into a hybrid fictitious domain-immersed boundary method

L. Kubíčková, M. Isoz

Hybrid fictitious domain-immersed boundary method (HFDIB), as a specific variant of standard immersed boundary methods, is a simulation approach used in computational fluid dynamics. The approach avoids usage of complex geometry-conforming computational domains. Instead, a simple domain is used and the geometry is projected onto it by a scalar field and an adjustment of governing equations. Hence, the time spent on mesh generation is substantially reduced, which is advantageous in geometry optimizations where it allows for a massive optimization speed-up. Nevertheless, there is a problem with simulation of the fluid behavior in the boundary layer in the vicinity of the immersed walls. Especially, in simulation of highly turbulent flows, where the boundary layer is very thin and the usage of sufficiently fine mesh is unaffordable. We aim to solve this problem by implementing Reynolds averaged turbulence models in our custom HFDIB variant. In particular, we implemented the k-ω turbulence model complemented by blended wall functions for closure variables and velocity.

Low-Mach consistency of a class of linearly implicit schemes for the compressible Euler equations

V. Kučera, M. Lukáčová-Medviďová, S. Noelle, J. Schütz

We give an overview of our analysis of the asymptotic consistency of a class of linearly implicit schemes for the compressible Euler equations. This class is based on a linearization of the nonlinear fluxes at a reference state and includes the scheme of Feistauer and Kučera (J. Comput. Phys., 2007) as well as the class of RS-IMEX schemes as special cases. We prove that the linearization gives an asymptotically consistent solution in the low-Mach limit under the assumption of a discrete Hilbert expansion. The existence of the Hilbert expansion is shown under simplifying assumptions.

Discrete Green's operator preconditioning: Theory and applications

M. Ladecký

The discretisation of elliptic problems on fine grids leads to systems of linear equations with millions to billions of unknowns, which favour iterative solvers over direct solvers. However, the number of iterations of iterative solvers can grow with increasing system size. This issue may be overcome by the discrete Green's operator (DGO) preconditioning, which makes iteration count independent of the system/grid size. This approach uses the inverse of a linear system matrix of a reference elliptic problem discretised on the same grid as the preconditioner.

We studied the DGO preconditioning from a linear algebra viewpoint and showed that all individual eigenvalues of such preconditioned systems can be bounded purely from the knowledge of the material data of the problems, both original and reference. We developed a simple algorithm to compute these bounds. In this lecture, we will discuss the theoretical aspects of these results and practical applications of the DGO preconditioning to periodic homogenisation problems discretised on regular grids.

On thermodynamically consistent coupling of the Barcelona Basic Model with a hydraulic model for unsaturated soils

T. Ligurský

The Barcelona Basic Model (BBM) is a constitutive model describing elastoplastic behaviour of unsaturated soils. It was proposed originally as a mechanical model, without taking into account hydraulic processes in the soils. Recently, this model has been exploited widely in some engineering applications where hydraulic effects have been captured as well, for instance, in modelling of clay-based barriers for nuclear waste disposal. However, surprisingly little work has been done in verification of basic thermodynamical principles of coupled hydro-mechanical models incorporating BBM to the best knowledge of the author. In this lecture, a formulation of BBM will be described, and a theoretical analysis of its thermodynamically consistent coupling with a hydraulic model will be presented. It will be shown in particular that the resulting restrictions on the hydraulic model do not seem to be completely physically consistent and other poromechanical models should be used.

Guaranteed L2 error bounds for finite element approximations of Laplace eigenfunctions

X. Liu, T. Vejchodský

For conforming finite element approximations of the Laplacian eigenfunctions, a fully computable guaranteed error bound in the L2 norm sense is proposed. The bound is based on the a priori error estimate for the Galerkin projection of the conforming finite element method, and has an optimal speed of convergence for the eigenfunctions with the worst regularity. The resulting error estimate bounds the distance of spaces of exact and approximate eigenfunctions and, hence, is robust even in the case of multiple and tightly clustered eigenvalues. The accuracy of the proposed bound is illustrated by numerical examples.

Comparison of preconditioners for poroelasticity

T. Luber

Poroelastic models describe a coupled system of a fluid flow through porous media interacting 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. We will focus on the time-step problem that arises after discretization in time by implicit Euler method in in three field formulation in displacement, flux and pressure. This leads to a linear coupled 3 by 3 block system. We will present and compare different block preconditioners that are naturally constructed using straightforward functional and algebraic arguments and use to them to solve the system using preconditioned Krylov method(s).

Professor Radim Blaheta - The Teacher

D. Lukáš

This is a memorial contribution to Professor Radim Blaheta, whom I was honoured to assist in his classes. To my best knowledge Radim was the first at our university to introduce teaching functional analysis and weak formulations of partial differential equations, yet explaining the main ideas from an engineering point of view. This turned into a unique course Mathematical Modelling and FEM. Another course on Iterative Methods accessed his broad expertise on the subject to master students of applied mathematics.

Determination of the initial stress by analysis of convergences on the tunnel walls

J. Malík, A. Kolcun

Reliable determination of the initial stress tensor has a decisive influence on the solution of a number of geomechanical tasks. Knowledge of the original stress tensor allows you to enter boundary conditions and reliably model stress states in the vicinity of a mine work such as a tunnel. The lecture will present a new method of determining the initial stress tensor based on measuring the distances between selected pairs of points on the tunnel walls during excavation, which we call convergences. The method is based on the application of linear algebra, especially on the conditional number of the matrix and the Tikhonov regularization method, which allows us to eliminate errors arising in the measurement of convergences.

Building a fuel moisture model for the coupled fire-atmosphere model WRF-SFIRE from data: From Kalman filters to recurrent neural networks

J. Mandel, J. Hirschi, A.K. Kochanski, A. Farguell, J. Haley
D.V. Mallia, B. Shaddy, A.A. Oberai, K.A. Hilburn

The WRF-SFIRE modeling system couples a high-resolution multi-scale atmospheric model with a wildfire spread model by the level set method and with a fuel moisture model. The fuel moisture model uses atmospheric variables (temperature, relative humidity, rain) to estimate the equilibrium fuel moisture contents and then runs a time-lag differential equation model of the time evolution of the moisture content in a dead wood stick. In a learning mode, the model state and parameters are corrected by assimilating data from fuel moisture sensors using an augmented extended Kalman filter. However, the nature of the model remains the same, which limits its accuracy. In a forecast mode, the model runs from the atmospheric state provided by a weather forecast without the Kalman filter, since the sensor data are still in future and not known.

The principal observation here is that the modeling and filtering process is a nonlinear operator which acts on a representation of the probability distribution of the model state, and it can be learned from data. So, we replace the differential equation model and the Kalman filter by a recurrent neural network. We pre-train the network by choosing the initial weights to implement an approximate solver of the differential equation of the model, and then learn the network weights by using the sensor data. In the forecast mode, the trained model then provides fuel moisture forecast from a weather forecast alone.

Optimal preconditioning methods and algorithms

S. Margenov

The talk is in the field of development and analysis of preconditioning solution methods for large-scale linear systems arising after discretization of boundary value problems by the finite element method. The goal is to obtain a uniformly bounded relative number of the condition of the preconditioned matrix, where the computational complexity of each iteration is $O(N)$. In the first part of the talk, joint results with Prof. Radim Blaheta will be discussed. Then, some recent results on domain decomposition methods and preconditioning of multiscale and multiphysics problems will be presented.

Simulation of solids and binary fluid interface interactions considering wetting effects

K. Miranda

In this work a computational tool has been developed to study multiphase interactions, more precisely ternary phase systems where a solid and a drop phase interact in a common incompressible Newtonian carrier fluid, considering the immersed solid phase properties (including wetting effects), the type of drops and the characteristics of the carrier fluid as controlling parameters. We use an Eulerian-Lagrangian methodology where the continuity and the Navier-Stokes equations are solved numerically by using a pseudo-spectral method for the carrier fluid. The drop phase is modelled by the Phase Field Method (PFM) and the solid phase is described using the Direct Forcing approach (DF) and inserted to the carrier fluid in the form of a virtual force. The approaches taken in this work consider the solid-fluid and fluid-drop interface as a smooth transition layer represented by a continuous hyperbolic function. In order to have a ternary phase system, the solid phase is coupled to the binary fluid phase by introducing a single well potential in the free-energy density functional, which can also control the solid surface wetting property. The implemented tool is proven to give reliable results in the studied applications.

Post-buckling solution for nonlinear beam developed by D.Y. Gao

H. Netuka, J. Machalová

This paper analyzes buckling problem for the nonlinear beam model which was published by D.Y. Gao in 1996. Using mathematical methods, new results regarding the post-buckling solution are presented. But only pure buckling problems are considered, i.e. the vertical load is omitted here. Some computational results are introduced for fixed axial loading, and finally we discuss the effect of input parameters on the results, which leads to interesting observations.

Computational costs related to Bohl-Marek decomposition applied to a class of biochemical networks

Š. Papáček, C. Matonoha, J. Duintjer Tebbens

This study presents an application of one relatively unknown technique, previously proposed in Bohl and Marek (2005), related to the mathematical modeling of biochemical networks with mass conservation properties. We continue in direction of papers devoted to inverse parameter estimation problems for mathematical models describing drug-induced enzyme production networks. Aware of the complexity of general PBPK models, we focus on the case of enzyme-catalyzed reactions with a substrate transport chain only. Although our ultimate goal is to propose an efficient and reliable procedure for fitting model parameters to experimental data, i.e., to solve an inverse problem, here, we study specific numerical issues within the framework of the forward initial value problem for ODEs. More precisely, for the two model formulations, (i) the classical formulation and (ii) the 'quasi-linear' Bohl-Marek formulation, we determine and compare the computational costs related to both.

Remarks on the paper *Adaptive error control for multigrid finite element methods*

J. Papež

By their 1995 paper, Becker, Johnson, and Rannacher have significantly contributed to the field of a posteriori error estimation. In particular, the results derived therein allow for estimating the error of a non-Galerkin solution, i.e., the exact algebraic solution is not assumed. Moreover, the paper proposes stopping criteria for the algebraic (multigrid) solver aiming at balancing the two components of the error estimator, which are related to the algebraic and discretization errors, respectively. These ideas became a basis for many later developments. Nevertheless, the issue of deriving guaranteed (i.e. unknown-factors-free) upper bounds on the errors and mathematically fully justified stopping criteria for (arbitrary) iterative algebraic solver is not resolved in the paper. The results are based on the assumption on the coarsest-level Galerkin orthogonality, involve unknown mesh-dependent multiplicative factors stemming from the use of inverse inequalities, and the relationship of the error indicators to the related components of the error is not known. We will recall the results of Becker, Johnson, and Rannacher, present a generalization for inexact coarse grid solve and a variant of the estimate that is robust with respect to the number of levels in multilevel hierarchy.

Matrix decay phenomenon and its applications

S. Pozza

In matrix computation, it is common to divide matrices into dense and sparse categories. Even though such categories are not precisely defined, we can think of a sparse matrix as one whose number of zero elements is large enough to be conveniently exploitable and a dense one as a matrix that is not sparse. It is important to note that the notion of sparsity does not consider the magnitude of the nonzero elements. This can be an issue since, in many applications, one has to deal with dense matrices in which most elements are so close to zero to being negligible. These matrices are close to being sparse in the sense that they are sparse upon truncation. Moreover, the nonnegligible elements are usually localized in some part of the matrix, and the magnitude of the other elements tends to decay to zero as we move away from them. As a simple example, consider the inverse of a tridiagonal matrix. Such an inverse is usually dense; however, under some conditions, the magnitude of its elements quickly decays to zero as we move away from the diagonal. Therefore, the inverse can be considered banded upon truncation.

In this lecture, we will introduce the basics of the decay phenomenon in the matrix function case. Then we will show how to predict the decay phenomenon and exploit it in matrix computation. In particular, we will present the results obtained with Valeria Simoncini on a-priori bounds for the approximation of matrix function by Krylov subspace methods, a relaxed strategy for the inexact Arnoldi method, and their extension to the rational case. We will also show how the decay phenomenon is fundamental for a new strategy for non-autonomous systems of linear ODEs that we have developed with Pierre-Louis Giscard and Niel Van Buggenhout.

$\star$-procedure to solve non-autonomous ODEs

S. Pozza, N. Van Buggenhout

The time ordered exponential (TOE) is the solution to a linear non-autonomous ordinary differential equation. Its computation remains a challenging problem. Recently a symbolical method was developed to express the TOE in terms of the so-called $\star$-product. The $\star$-product is defined as the integral over the product of bivariate discontinuous generalized functions. We present a discretization of the $\star$-product based on an expansion of these functions in a basis of Legendre polynomials. The computation of their expansion coefficients can be obtained up to high accuracy thanks to an analytical formula for the integral over the product of three Legendre polynomials and can be computed efficiently by exploiting their formulation as the Hadamard product of a Hankel and Toeplitz matrix. Thanks to this expansion the symbolical expression for the TOE can be approximated by a linear system of equations which can be solved efficiently. Numerical experiments show the effectiveness of the proposed procedure.

Nonlinear acceleration, inexact Newton, and nonlinear generalized conjugate residual approaches

Y. Saad

There has been a surge of interest in recent years in general-purpose *acceleration* methods that take a sequence of vectors converging to the limit of a fixed point iteration, and produce from it a faster converging sequence. A prototype of these methods, one that attracted much attention recently, is the Anderson Acceleration (AA) procedure. This talk will begin with a discussion of these general acceleration methods, focusing on Anderson acceleration, and highlighting the link between AA and secant-type methods. This link will enable us to adapt to the nonlinear context a class of methods rooted in Krylov subspace techniques for solving linear systems.

Inexact and primal multilevel FETI-DP methods

B. Sousedík

We study a framework that allows to solve the coarse problem in the FETI-DP method approximately. It is based on the saddle-point formulation of the FETI-DP system with a block-triangular preconditioner. One of the blocks approximates the coarse problem, for which we use the multilevel BDDC method as the main tool. This strategy then naturally leads to a version of multilevel FETI-DP method, and we show that the spectra of the multilevel FETI-DP and BDDC preconditioned operators are essentially the same. The theory is illustrated by a set of numerical experiments, and we also present a few experiments when the coarse solve is approximated by algebraic multigrid.

Improving computational efficiency of contact solution in fully resolved CFD-DEM simulations with arbitrarily-shaped solids

O. Studeník, M. Kotouč Šourek, M. Isoz

The abundance of industrial processes containing both solid and liquid phases generate demand for fully resolved models allowing for detailed analysis and optimization of these processes. An established approach providing such models is based using a variant of an immersed boundary method to couple the computational fluid dynamics (CFD) and discrete element method (DEM). In the talk, we will present our custom and monolithic implementation of a fully-resolved CFD-DEM solver and concentrate on the intricacies of solving contact between two arbitrarily-shaped solids. We shall propose an efficient contact treatment based on the concept of a virtual mesh, which provides the mesh resolution required by DEM through dividing the space around the contact point in a finite volume fashion without any changes to the CFD mesh itself. A substantial part of the talk will devoted to the parallelization of the contact solution, especially in the context of the domain decomposition method imposed by the CFD solver.

Preconditioning in solution of electron-molecule scattering problems

M. Šarmanová

In this work, we study low-energy electron-molecule collisions. The collision of an electron with a molecule can be mathematically formulated in the language of partial integro-differential equations derived from stationary Schrödinger equation. The discretization converts the problem into many systems of linear algebraic equations with complex symmetric matrices. In this work we deal with (iterative) methods for solving complex and symmetric systems of linear algebraic equations. In particular, we focus on finding a preconditioning technique for Krylov subspace methods that takes into account the special structure of the system of equations arising from the mathematical model of electron-molecule collision.

The block Lanczos algorithm

D. Šimonová

The Lanczos algorithm is a widely spread algorithm which generates an orthogonal basis of the corresponding Krylov subspace. In many cases the block Lanczos algorithm is used. In the case of the nonblock Lanczos algorithm, its theoretical properties are well known and a few significant results of its numerical analysis were presented, but we don't know much about the block Lanczos. In the poster, we summarize the theoretical properties of the block Lanczos and provide numerical experiments to better understand the behavior of the block Lanczos in finite precision.

Domain decomposition solver for immersed boundary finite element method

J. Šístek

Immersed boundary finite element method (FEM) presents an attractive approach to simulations avoiding the generation of large body-fitted meshes, which can be tedious and challenging for complex geometries. However, the price to pay are more complicated methods for the weak enforcement of Dirichlet boundary conditions, poor conditioning of stiffness matrices, and non-standard numerical integration at the vicinity of the boundary. We develop multilevel balancing domain decomposition by constraints (BDDC) method tailored to the solution of the linear systems arising in the context of the immersed boundary FEM with adaptive grid refinement. We present these concepts, our implementation, and numerical results for the Poisson problem on complex engineering geometries. This is a joint work with Fehmi Cirak, Eky Febrianto, Matija Kecman, and Pavel Kůs.

Poroelasticity: Mathematical modelling, numerical solution and applications

J. Stebel

The lecture deals with the modelling of flow and mechanics in porous media based on the Biot consolidation theory. In the first part, I will introduce the classical Biot system. I will give an overview of results on well-posedness and finite element approximation and present some solution techniques based on monolithic or splitting schemes and suitable preconditionings.

The second part will be devoted to applications in rock hydro-mechanics, which involves treating inhomogeneities and fractures. A brief survey of modelling approaches will be given. I will then focus on the so-called discrete fracture-matrix (DFM) approach which couples the rock matrix and discrete fracture network. Here, some nonlinear effects have to be taken into account such as non-penetration contact conditions and stress-permeability relations. I will explain the derivation of DFM models and their suitable discretizations and show examples of their use in geotechnical applications.

Numerical approximation of the spectrum of self-adjoint operators, operator preconditioning and an unfinished talk with Radim Blaheta

Z. Strakoš

This contribution will present several results relating eigenvalues of matrices and spectra of self-adjoint operators, with connection to operator preconditioning. They were obtained jointly with Tomáś Gergelits, Kent-André Mardal and, in particular, Bjørn Fredrik Nielsen. But they are much in line with many discussions that we had together with Radim Blaheta over several decades and that were for me always enlightening and very pleasant. Due to involvement in many other projects and duties we have not transformed them into a real joint project that would end up in a joint paper. Our intention to change this will remain unfinished. But our interactions have definitely been for me very rewarding, professionally and even more personally.

Behaviour of the Gauss-Radau upper bound

P. Tichý, G. Meurant

Consider the problem of solving systems of linear algebraic equations $Ax = b$ with a real symmetric positive definite matrix A using the conjugate gradient (CG) method. In this talk we discuss and analyze the behaviour of the Gauss-Radau upper bound on the A-norm of the error, based on viewing CG as a procedure for approximating a certain Riemann-Stieltjes integral. This upper bound depends on a prescribed underestimate μ to the smallest eigenvalue of A. We concentrate on explaining a phenomenon observed during computations showing that, in later CG iterations, the upper bound loses its accuracy, and it is almost independent of μ. We construct a model problem that is used to demonstrate and study the behaviour of the upper bound in dependence of μ, and developed formulas that are helpful in understanding this behavior.

L^2 stability of macroscopic traffic flow models on networks using numerical fluxes at junctions

L. Vacek, V. Kučera, C.-W. Shu

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. The scheme also requires limiters which prevent spurious oscillations in the numerical solution and keep the numerical traffic density in an admissible interval. 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. We present numerical experiments, including a junction with complicated traffic light patterns with multiple phases.

Comparison of different approaches to determination of resonant frequencies of coupled vibro-acoustic systems

J. Valášek, J. Hubálek

The contribution deals with the 2D vibro-acoustic model of human phonation. Its aim is to determine first few acoustic resonant frequencies for the setup motivated by the phonation into tubes or straws. The first acoustic resonance during this therapeutic technique is significantly changed in comparison to common phonation without tubes. This change can be explained by considerable interaction of acoustics with mechanically compliant vocal folds and vice versa, see [Horáček et al. 2017]. Here, the vocal folds vibrations are described using linear elasticity theory and the acoustics is modelled with the help of acoustic potential. The both subproblems are numerically approximated by the finite element method and the monolithic coupling strategy is chosen. Two approaches of resonant frequencies determination is applied - the modal analysis and the tranfer function approach. In the end the numerical results of the both approaches are compared.

Discrete element method for the analysis of concrete structures

R. Varga

The Discrete Element Method (DEM) is a numerical method based on the motion and contacts of individual elements. It is mainly used in partial masses, but its possibilities of use for continuous problems are overshadowed by other methods, such as the Finite Element Method (FEM). However, its application for the analysis of building structures can be found, for example, in the problem of the size and propagation of cracks in concrete and reinforced concrete structures. These problems combine problems of continuum and particulate behavior, which causes problems in the calculations and optimization of commonly used FEM due to frequent changes in the mesh or the need for parameters that are difficult to detect in common practice. By using DEM, these problems are eliminated, but there is a need to properly define the properties of the solid bonded contacts, which are not found in the conventional DEM. This can be achieved using a variety of methods. This work is concerned with the possibility of replacing the contacts using rod elements (Euler-Bernoulli beam). However, to exploit this possibility, the properties of the member elements, such as cross-section and elastic modulus corresponding to the joint, need to be determined.