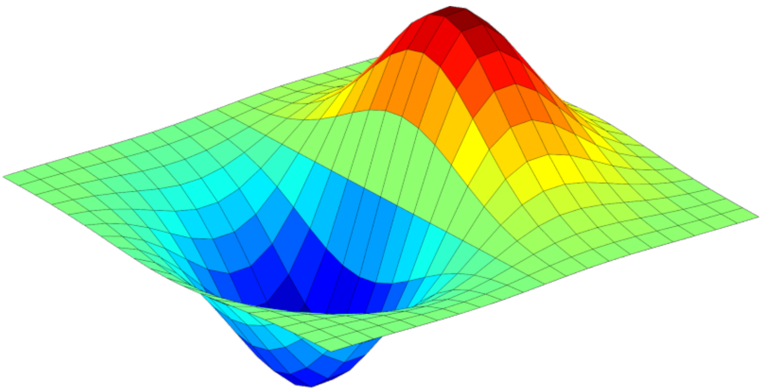
VŠB – Technical University of Ostrava
Institute of Geonics of the CAS, Ostrava

SNA'25

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

Ostrava, January 27 – 31, 2025

Short Abstracts

Contents

Solving Stokes problem with stick-slip boundary conditions by semi-smooth* Newton method

V. Arzt

The contribution will present Stokes's problem with nonlinear stick-slip boundary conditions and its solution solved by the semismooth* Newton method. This method was initially developed by J. Outrata, H. Gfrerer and J. Valdman and used for solving contact problems involving Coulomb friction. Additionally, we will compare the efficiency of this method with the implementation of the semismooth Newton method developed by R. Kučera.

Bayesian inversion with neural network surrogates for TSX parameters estimation

M. Béreš

This poster presents a Bayesian inversion framework for estimating poroelastic parameters on subdomains in Tunnel Sealing Experiment (TSX). The model, implemented in FEniCSx, is based on linear poroelasticity and incorporates uncertainties inherent in geotechnical applications. The inversion process utilizes the Delayed Acceptance Metropolis-Hastings (DAMH) algorithm with subchains, accelerated by dynamically refined deep neural network (MLP) surrogates. These surrogates significantly reduce computational costs while preserving the asymptotic exactness of the sampling process.

Shape optimization of water turbines

M. Brandner

The tool for optimization of Francis turbine runner wheel blades shape will be presented. The unsteady flow is modelled by the Navier-Stokes equations. The numerical model is based on isogeometric analysis and the optimization procedure is based on the formulation of the continuous adjoint problem using Cea's formal derivation technique.

Predicting deep water infiltration using Kalman filtering and Richards equation

J. Březina

The drop in the water table over the last decade remains despite rainfall levels being consistent with previous averages. Increased evapotranspiration due to elevated temperatures and rising water consumption could be contributing factors. To address these questions, deep infiltration unaffected by evapotranspiration must be monitored. Direct measurement is challenging, motivating an indirect approach through soil moisture profile measurements combined with suitable inversion modeling. This approach also circumvents the need for extensive fine-tuning of moisture sensors.

This work couples the Richards equation, a nonlinear model describing water movement in unsaturated soils, with the Unscented Kalman Filter (UKF) to achieve two key objectives: assimilation of soil moisture profile measurements and weather data (interpolated from external models), and calibration of soil and measurement parameters over long time series. We demonstrate the limitations of the approach using synthetic data and present partial results from laboratory datasets.

Towards efficient numerical solution of flexoelectric problems

R. Cimrman

The growing attention to flexoelectricity (FX), i.e. the bidirectional coupling between strain gradients and electric polarization, has been driven by advances in miniaturization, as the FX effect is much stronger than piezoelectricity (PZ) at small scales. Our interest in achieving macroscale FX by designing and 3D printing electroactive PZ-based metamaterials requires accurate numerical models of both the PZ microstructure and the resulting FX or PZ metamaterial. However, FX presents significant challenges for numerical modeling due to the large differences in magnitudes of the resulting linear system matrix blocks (similar to PZ) and the continuity requirements due to the second-order spatial derivatives involved. The standard FEM can be used when a mixed formulation is employed, but then the matrix is larger and its block structure is even more complicated. We present our ongoing experimental and numerical approaches and first results on electroactive PZ and FX structures obtained using a custom 3D printer with in-situ poling developed by our team members.

Tests of neural network diabatization method on 1D models of avoided crossing

M. Ćosićová

This work is focused on mathematical modeling of non-adiabatic processes. The essence of this task is to find the solution of the time-dependent Schrödinger equation. Using the well-known Born-Oppenheimer separation, this problem can be converted into a system of partial differential equations describing the motions of the nuclei of atoms. The particular form of the system is determined by the choice of the so-called electronic basis, which serves to "discretize" the equation with respect to the electronic space variables. By choosing a special, so-called diabatic, basis, we are able to cancel out some of the terms of this system and therefore also significantly improve the numerical behavior of it. Construction of the diabatic representation of a potential energy matrix is, however, a complicated task that very often requires a detailed knowledge of different physical properties of the considered system. In this work we study an alternative approach based on the use of neural networks, that have proved themselves to be very useful in numerous applications within computational chemistry. We investigate the impact of setting various internal parameters of the neural network diabatization method, introduced in [J. Chem. Theory Comput. 2020, 16, 6456-6464]. In particular, we study the effect of the choice of activation functions, definition of the loss function, or numbers of hidden layers and neurons. To compare individual results, we present several statistical quantities illustrating the performance of the method on a simple one-dimensional artificial model of the avoided crossing.

Coupled simulation of flow and deformation in fractured porous media: Discretizations, solvers and applications

M. Ferronato

The simultaneous simulation of frictional contact mechanics and fluid flow in fractured geological media is a tightly coupled physical processes and a key component in the design of sustainable technologies for several subsurface applications, such as geothermal energy production, CO_2 sequestration and underground gas storage. Typically, the aperture and slippage between the contact surfaces drive the fluid flow in the fractures, while the pressure variation perturbs the stress state in the surrounding medium and influences the contact mechanics itself. This usually produces a stiff non-linear problem associated with a series of generalized saddle-point linear systems, whose solution is often hard to obtain efficiently.

In these lectures, we focus on a blended finite element/finite volume method, where the porous medium is discretized by low-order continuous finite elements with nodal unknowns, cell-centered Lagrange multipliers with a stabilization are used to prescribe the contact constraints, and the fluid flow in the fractures is described by a classical two-point flux approximation scheme. The numerical solution scheme is built by using an active-set strategy coupled with an inner Newton method. The resulting Jacobian matrix gives rise to a block generalized saddle-point problem that requires a special treatment for an efficient solution. To this aim, we discuss the basic algebraic properties of the linearized discrete equations and develop a class of scalable preconditioning strategies based on the physically-informed block partitioning of the unknowns and state-of-the-art multigrid techniques. Finally, a set of numerical results concerning fractured porous media applications illustrate the robustness of the proposed approach, its algorithmic scalability, and the computational performance in large-size realistic problems. In particular, we will present two real-world engineering applications dealing with: (i) the development of ground fissures due to aquifer over-exploitation, and (ii) the potential inception of fault slip in underground gas storage sites.

Hybrid Schwarz preconditioners for linear systems arising from discontinuous Galerkin method

T. Hammerbauer

We present the analysis and numerical study of two-level hybrid Schwarz method used as a preconditioner for system of algebraic equations arising from discontinuous Galerkin (DG) discretization. The coarse mesh is obtained by the agglomeration of the elements of the fine mesh, which is another advantage of DG method. We present theoretical results concerning condition number bounds of the preconditioned system. Moreover we show the numerical results concerning the computation of those bounds to demonstrate its accuracy. Finally, we present results showing the advantage of this method.

Discrete and continuum models of robust biological transportation networks

J. Haškovec

Motivated by recent results on formation and adaptation of biological transport networks, we study a discrete model consisting of an energy consumption function constrained by a linear system on a graph. We discuss how structural properties of the optimal network patterns, like sparsity and (non)existence of loops, depend on the convexity/concavity of the metabolic part of the energy functional. We then introduce robustness of the network in terms of algebraic connectivity of the graph and explain its impact on the network structure. Passing to the continuum limit as the number of edges and nodes of the graph tends to infinity, we recover a nonlinear system of PDEs. This elliptic-parabolic system consists of a Darcy's type equation for the pressure field and a reaction-diffusion equation for the network conductance. We explain how the robustness property is reflected on the level of the PDE description. We give both analytical results and systematic numerical simulations for the PDE system, providing interesting insights into the mechanisms of network formation and adaption in biological context.

Unified approach to data extraction from multilinear approximation problems

I. Hnětynková

Error contaminated linear approximation problems appear in a large variety of applications. The presence of redundant or irrelevant data complicates their solution. Such data can be removed by the core reduction yielding a minimally dimensioned subproblem called the core problem. Direct core reduction has been introduced previously for problems with matrix models and vector, or matrix, or tensor observations. For the cases of vector and matrix observations an iterative Krylov subspace method, the generalized Golub-Kahan bidiagonalization, can also be used. In this talk we unify previously studied variants of linear approximation problems under the general framework of a multilinear approximation problem. We show how to extend the generalized Golub-Kahan bidiagonalization such that it yields the core problem for any multilinear approximation problem. We discuss various properties of this iterative process.

Improving performance of augmented Lagrangians

D. Horák

SMALE is an efficient algorithm for solving quadratic programming problems with simple bounds and linear equality constraints. There are two variants of this method: one updates the parameter for precision control of an inner solver by a factor less than one (the preferable variant, as it does not change the Hessian via penalty update), and the other updates the penalty by a factor greater than one (resulting in a lower number of outer iterations and fewer Hessian multiplications in the inner solver). We use the MPRGP algorithm as an inner solver for solving bound-constrained quadratic programming problems.

We introduce a new theoretically supported variant that updates both these parameters: multiplying the penalty by a factor greater than one and multiplying the parameter for precision control for the MPRGP stopping criterion by the square root of this factor. The larger penalty accelerates the outer loop, while the larger parameter for precision control accelerates the inner solver. Numerical experiments with the Total-FETI method demonstrate the effectiveness of this new variant.

What is a reasonable level of agreement between POD analyses of simulated and measured flow fields?

M. Isoz

Proper orthogonal decomposition (POD) is a go-to method in several fields of physics and mathematics, including flow-field analysis, model order reduction, or statistics, where POD is known as the principal component analysis. Still, it is hard to find best-practice approaches for POD application in all these fields. In this contribution, we focus on applications of POD in the first mentioned area, but with implications towards the second. In particular, we try to establish what is an achievable level of agreement between POD analyses of the simulation and experimental data. To do so, we simulate and measure the flow behind a circular cylinder at the Reynolds number of ≈ 5000. The measured and simulated flow fields are first compared with the aid of standard validation measures such as the mean-field analysis or comparison of turbulence spectra. Next, we discuss the data intensity of POD with respect to its convergence for higher modes and how the convergence is affected by the enforcement of symmetry in the data. Finally, attempts to draw conclusions are made with respect to requirements on POD as a method for a reduced basis construction in model order reduction.

The authors acknowledge the financial support provided by the Ministry of Education, Youth, and Sports of the Czech Republic via the project No. CZ.02.01.01/00/23_020/0008501 (METEX), co-funded by the European Union.

Signorini problem

L. Kapera

The Signorini problem is an elastostatics problem in linear elasticity. It consists in finding the elastic equilibrium configuration of an elastic body, which is by a part of its boundary in possible contact with a rigid frictionless obstacle. At points of this part of boundary it is not a priori known, which boundary condition applies - Dirichlet or homogenous Neumann, but at each point exactly one of them applies, what is crucial for the subsequent solution of the task. The statement of the problem so involves not only equalities but also inequalities, therefore constrained optimization methods or fixed point method need to be used to solve the problem.

Estimating mean and variance of random coefficients in stochastic variational problems

A. Khan

We address the challenge of identifying both deterministic and stochastic coefficients in stochastic partial differential equations through an abstract inversion framework. This approach formulates the inverse problem within a stochastic optimization setting, deriving essential solution map properties to ensure solvability and establish optimality conditions. A robust regularization framework, including total-variation regularization, is designed to capture rapidly varying coefficients. For finite-dimensional noise, the problem is parameterized and solved via the stochastic Galerkin framework. Leveraging Hessian-based optimization methods ensures rapid convergence. Numerical results confirm the feasibility and effectiveness of the proposed methodology.

Accelerating parameter identification in bread baking simulations via model order reduction

A. Kovárnová, M. Isoz, T. Hlavatý, M. Sluková, T. Moucha

Bread has been one of the cornerstones of people's diets for thousands of years, and its recipes and baking procedures are being improved to this day. However, mathematical modeling of bread baking is still a complicated task, as bread is a multiphase system and models need to cover heat transfer, mass transfer, and deformation. Furthermore, the literature often lacks specific values of some of the coefficients used in the models, such as thermal conductivity, providing relatively wide ranges of possible values. In this contribution, we operate on a preliminary model of rigid dough baking and compare the temperature values computed by the model with an experiment. We then strive to determine the optimal values of the thermal conductivity of the solid phase and the coefficient of evaporation. The computational costs are reduced by employing model order reduction. We utilize a posteriori methods, i. e. temperature fields for several pairs of parameters are used to construct the reduced order model, which then cheaply predicts temperature fields for any pair of parameters in between. In particular, we combine proper orthogonal decomposition for the reduced basis construction with interpolation via artificial neural networks.

The authors acknowledge the financial support provided by the Ministry of Education, Youth, and Sports of the Czech Republic via the project No. CZ.02.01.01/00/23_020/0008501 (METEX), co-funded by the European Union.

Fixed-stress method for a class of nonlinear poroelasticity problems

J. Kraus

In this talk we consider a nonlinear model commonly used in the field of poroelasticity for the study of the quasi-static mechanical behaviour of a fluid-saturated porous medium whose permeability depends on the divergence of the displacement. This model has many practical applications, e.g., in medicine to mathematically describe biological structures like tissues, organs, cartilage and bones, which are known for a nonlinear dependence of their permeability/hydraulic conductivity on solid dilation.

We first formulate the fixed-stress split method to iteratively solve the coupled poroelasticity problem under investigation and then prove its linear convergence for sufficiently small time steps under the assumption that the hydraulic conductivity is a strictly positive, bounded and Lipschitz-continuous function.

The talk is concluded with the presentation of some numerical tests illustrating the efficient and stable performance of the proposed fixed-stress split scheme.

Differential forms and Whitney elements in numerical electromagnetics

D. Krpelík

Differential forms provide a powerful foundation for representing electromagnetic fields, and their discrete counterparts-Whitney elements-revolutionize numerical methods for solving Maxwell's equations. We examine the theoretical underpinnings of Whitney elements, focusing on their ability to preserve the geometric structure of fields and their integral properties on discrete meshes. Attention will also be given to the intriguing interplay between geometry, topology, and numerical accuracy, including the implications of the discrete Hodge star operator and gauge invariance. By exploring these features, this presentation aims to bridge mathematical theory and practical simulation challenges.

A regularization strategy for discontinuity when modeling coupled water and heat flow in freezing unsaturated soil

M. Kuráž

Freezing tightly couples the water and heat flow. In most porous media, the interface between liquid and frozen water is not sharp and a slushy zone is present. There are two distinct approaches for mathematical modeling of freezing. It is the equilibrium approach which allows an instant freezing under given conditions and non-equilibrium approach where a specific timing in the freezing process is considered. In this contribution, we specifically target the equilibrium approach.

The key mathematical model for the equilibrium approach is the Clausius-Clapeyron equation, which allows the derivation of a soil freezing curve relating temperature to pressure head. Implementing freezing soil accurately is not a straight-forward. Using the Clausius-Clapeyron equation creates a discontinuity in the freezing rate and latent heat at the freezing point. Little attention has been paid to the adequate description of the numerical treatment of this phenomenon and to the computational challenges that it poses. Numerical approximation of this discontinuous system is prone to spurious oscillations. In this contribution, we show the application of regularization of the discontinuous term. This treatment successfully stabilizes the computation and can remove oscillations. To avoid over-regularization, we present here a minimax strategy to determine optimal regularization parameters. We further compare an over-regulized setup with the non-equilibrium approach, where we show that a succesfull regulalization is equivalent to incorporating a minimal timing to the freezing process. Finally - for validating our implementation and computational approach - experimental laboratory data of the volumetric water content and temperature profiles from previously published soil freezing experiments were represented here with the optimally regulized equilibrium approach.

Non-newtonian fluids in characterizing porous media

M. Lanzendörfer

The talk will shortly review some conceptual models of the porous media flow and transport in relation to non-newtonian fluids, namely the simple shear-thinning and yield-stress fluids. We will revisit the standard generalized Darcy law approach as well as two relatively recent methods utilizing flow of aqueous polymer solutions in order to characterize the functional pore size distribution of rocks or soils. We will discuss the promises as well as issues of the approach.

A thermodynamically consistent full hydro-mechanical coupling

T. Ligurský

Swelling clays can be very useful as sealing and buffer materials, for instance in nuclear waste engineering barriers. To simulate their possible behaviour reliably, one needs a thermodynamically consistent poromechanical model with a two-directional hydro-mechanical coupling using convenient state variables. Unfortunately none completely satisfactory has been found yet. In this talk, a simple thermodynamical fully coupled poroelastoplastic framework will be introduced, and a consistent hydro-mechanical model with swelling developed according to it will be presented. The stress is affected by the water content via the suction and the water content is affected by the volumetric strain in the model. The water mass content is expressed directly, not by means of the degree of saturation. Promising results of a numerical simulation of coupled hydro-mechanical processes in bentonite during hydration will be shown.

Biot's poroelasticity in numerical experiments

T. Luber

Poroelasticity encompasses hydromechanical models that describe the coupled interaction between the mechanical deformation of a solid matrix and fluid flow through its porous structure. This presentation focuses on Biot's model, which couples linear elasticity for solid deformations with Darcy's law for saturated fluid flow.

This model was originaly devised for modelling soils but found wide applications from rock mechanics to modeling flow in biological tissues.

We explore selected benchmark problems inspired by geomechanical applications and test the behaviour of preconditioned Krylov methods and splitting schemes for this system.

These solver strategies are implemented using a standard finite element discretization for space and an implicit Euler scheme for time. Their performance is compared in terms of total iteration counts and error reduction behavior.

PU based operator preconditioning in Boundary Element Methods

D. Lukáš, Z. Machaczek

In operator preconditioning we utilize the opposite-order mapping properties of the single-layer and hyper-singular boundary integral operators. However, in 3 spatial dimensions the lowest-order discretizations of the operators by discontinous piecewise constant and continuous piecewise linear functions, respectively, do not match in terms of degrees of freedom. Therefore, a dual mesh is often introduced to discretize the single-layer operator. Unfortunately, the assembly of the preconditioner is significantly more expensive than the operator itself. In this paper we propose and analyze a novel construction of continuous piecewise polynomial basis functions to discretize the hyper-singular operator, both in 2 and 3 dimensions. We prove that it forms an optimal preconditioner to the original single-layer operator discretized by the piecewise constants. We avoid the dual mesh. The efficiency of our approach is documented by numerical experiments performed on GPUs.

Identification of material parameters in the nonlinear Gao beam model

J. Machalová

This research focuses on identifying material parameters in contact problems through the nonlinear beam model developed by D.Y. Gao in 1996. The model is governed by a nonlinear fourth-order ordinary differential equation and represents a beam resting unilaterally on a perfectly rigid or elastic foundation. Determining the beam's material properties and the elastic foundation's modulus is formulated as an optimal control problem using a least squares cost functional. The study delves into the theoretical aspects of the problem, particularly addressing the existence of solutions and their finite element approximations. Furthermore, practical applications of the approach will be illustrated with several numerical examples.

Mathematical model for energy storage and release in the form of compressed air

J. Malík, A. Kolcun

According to recent analyses, compressed air is the most efficient way to store large volumes of energy. At present, for energy release, compressed air is discharged from underground spaces to a gas turbine which is connected to a power generator. The disadvantage of this method is that due to adiabatic expansion, the air must be heated.

In 2024, a completely new method of storing and releasing energy in the form of compressed air using a water turbine was patented. The talk will describe a mathematical model describing the processes involved in the release of energy. Numerical simulations show that compressed air does not need to be heated. It is therefore a completely new green technology. The mathematical model allows to set appropriate parameters depending on the magnitude of the stored energy and power. This method of energy storage has been verified on a small scale model, which confirmed the validity of the mathematical model.

Optimization system UFO - version 2024

C. Matonoha, L. Lukšan

We will describe the last version of the software system for universal functional optimization UFO. This systems can solve a broad class of continuous optimization problems with various types of objective function and constraints. The UFO system contains more than 40 classes of optimization methods. This system uses a special input language, which describes optimization problems and chooses optimization methods. The optimization control program is then generated by the UFO macroeditor and computation is started. The problem description can be very general and is realized by the input language.

Calculating the non-linear baryonic density using the Zeldovich approximation

T. Ondro, D. Horák

The absorption lines in the spectra of high redshift sources are being revealed as an extremely powerful tool in observational cosmology. We have investigated an approach for recovering the thermal parameters and Jeans length based on the Zeldovich approximation, with appropriate smoothing, to compute the density and peculiar velocity fields. We show, that this approach is suitable for generating large number of synthetic spectra with various input data and parameters, and thus ideal for interpreting the high-quality data obtained from quasar absorption spectra surveys.

Error estimate for least-squares problems solved by LSQR and CGLS

J. Papež

In [Meurant, Papež, Tichý; Numerical Algorithms 88, 2021], we introduced an adaptive estimate for the energy norm of the error in the conjugate gradient (CG) method. This estimate is computationally inexpensive and numerically reliable in finite-precision computations.

In this talk, we present the results from [Papež, Tichý; Numerical Algorithms 97, 2024] where we have extended the estimate to the LSQR and CGLS algorithms for solving least-squares problems involving general rectangular matrices. The estimate is applicable for preconditioned variants of these algorithms and can be seamlessly integrated into existing codes.

We emphasize the applicability of the estimates in finite-precision arithmetic, noting that their derivation relies exclusively on local orthogonality, a property generally well-preserved in computations. Additionally, the evaluation of the estimates remains inexpensive. Finally, we explore their use in stopping criteria.

Recent development of the core problem theory in the context of the total least squares minimization

M. Plešinger

This contribution focuses on solving (multi)linear approximation problems with the method of the total least squares and on the reduction of such problems to the so-called core problem within. Although the core problem concept brought important results on solvability of the vector right-hand side problem, it is not completely true for the problem with matrix right-hand side as the core problem within may not have a TLS solution. Our goal is to examine the 'internal structure' of the matrix right-hand side core problems as well as to 'look around' these problems in order to find possible generalizations.

2D elastoplastic contact problems in MATLAB: Mortar methods and quadratic optimization

L. Pospíšil, T. Světlík, R. Varga, M. Čermák

This poster presents the latest advancements in our MATLAB library for solving 2D contact problems in elastoplasticity using the finite element method. Contact detection is handled using mortar methods, ensuring high accuracy and robustness. Our approach involves dualization, which transforms the problem into a quadratic programming problem with linear equality and inequality constraints. To efficiently solve the resulting dual problem, we employ state-of-the-art quadratic optimization algorithms, specifically the SMALE and MPRGP methods. Benchmark tests in 2D demonstrate the effectiveness of our implementation, showcasing its capability to address complex contact problems in computational mechanics.

Preconditioning of PDEs with guaranteed spectral bounds

I. Pultarová

We present preconditioning of PDEs with possibly time derivatives or convective terms. The preconditioners are based on Laplacian and diagonal scaling. We show three methods which can provide guaranteed spectral bounds of resulting preconditioned matrices. Some illustrative examples are shown.

On the symplectic LL^T factorization

M. Rozložník

In this contribution we analyze the numerical stability of two algorithms that are frequently used for computing the symplectic LL^T factorization of a symmetric positive definite matrix that is near symplectic.

Solvers for extreme scale computing

U. Rüde

This talk presents research on massively parallel solution algorithms for elliptic PDE. An old 1982 publication reminds us that multigrid methods can solve the Poisson equation with only 30 N FLOPS on a grid with N unknowns. They can thus produce the solution not only with asymptotically optimal complexity, but also with a surprisingly low absolute work count. With this motivation, we present the HyTeG multigrid framework that implements the multigrid method on hybrid tetrahedral grids. We demonstrate that it is possible to achieve scalability on up to several hundred thousand processors and then solve linear systems with up to 10 sup 13 (10 trillion) unknowns in a solution time of a few minutes.

Convergence improvement of 2D linear elasticity solvers using preconditioning and deflation

A. Růžička

We present the results from the numerical experiments performed on a simple 2D model problem of linear elasticity solved by variants of the FETI method, specifically by FETI-1 and TFETI-1, and (T)FETI-2. For each of these methods, cases both with and without dualization of the decomposed problem were tested. For FETI-1 and TFETI-1, cases with no, lumped, and Dirichlet FETI preconditioning of the dualized problem were compared. (T)FETI-2 is regarded here as (T)FETI-1 with deflation applied on the CG method. Various methods of deflation are tested and compared, specifically those enforcing the equality of displacements of the corresponding corner nodes of adjacent subdomains, enforcing an equality of means of the nodes' displacements on opposite sides of the adjacent subdomains' interfaces and the moment equilibrium of the internal forces between the corresponding nodes on opposite sides of these interfaces, by eigenvectors of the system matrix, and by a discrete wavelet, Fourier and cosine transform. An effect of the preconditioning/deflation is analyzed considering numbers of PCG/DCG iterations, solution times, and spectral properties of particular operators.

The numerical linear algebra of deep neural networks

Y. Saad

As the sudden ascent of Artificial Intelligence (AI) has caught the world off guard, it is becoming critical to members of the Numerical Linear Algebra (NLA) community to react to this trend, to understand it, and to contribute to the advancement of machine learning. What is fascinating and rather encouraging is that NLA is at the core of machine learning and AI. In this talk we will give a quick overview of Deep Learning with an emphasis on Deep Neural Networks, and Large Language Models (LLMs). The very first step of LLMs is to convert the problem into one that can be exploited by numerical methods, or to be more accurate, by optimization techniques. All AI methods rely almost entirely on essentially 4 ingredients: data, optimization methods, statistical intuition, and linear algebra. Thus, the first task is to map words or sentences into tokens which are then embedded into Euclidean spaces. From there on, the models refer to vectors and matrices.

We will show a few examples of important developments in ML that were heavily based on linear algebra ideas. Among these, we will briefly discuss LoRa, a technique in which low-rank approximation was used to reduce computational cost in some models, leading to gains of a few orders of magnitude. Another contribution that used purely algebraic arguments and that had a major impact on LLMs is the discovery that the nonlinear "self-attention" in LLMs can be approximated in a way that leads to huge savings in computations, decreasing computational complexity from quadratic in the number of variables to linear.

The talk will be mostly a survey of known recent methods in AI with the primary goal of unraveling the mathematics of transformers. A secondary goal is to initiate a discussion on the issue of how NLA specialists can participate in research in machine learning.

Poroelastic model of fractured rock with anisotropy

J. Stebel

We present a mathematical model of coupled flow and mechanics in a fractured rock with generally anisotropic conductivity and elasticity tensors both in the rock and fractures. The response of fractures includes nonlinearities due to impermeability and due to variable cross-section.

Numerical modeling of coupled water, vapour and heat transport in beech forest soil

V. Steinbach

The interaction between water, vapour and heat transport in soils is often an overlooked phenomena. Many works on numerical modeling treat these components through means of separate models thus missing their inter-dependent dynamics. Such an approach can be viable in some cases but in the case of the beech forest ecosystem it is crucial to take interactions into account. The purpose of this presentation is to give an extensive description of the Saito-Sakai model which simulates coupled water, vapour and heat transport in vadose zone. The boundary conditions are assumed to be surface energy balance for heat component and evaporation/rainfall intensity for water component.

Using extensive monitoring data from pilot site AMALIA we'll perform calibration and validation of Saito-Sakai model implementation in DRUtES numerical solver. Once validated we'll gain a mid-term model for beech forest location of AMALIA pilot site which can be then loaded by climatic scenarios and can help us understand the changes in hydrologic qualities over the upcoming years caused by climate change.

Towards high-fidelity non-spherical CFD-DEM: Advancing DEM contact models

O. Studeník

Non-spherical granular matter dispersed in a fluid appears in both natural and industrial settings. These include, among others, fluidization, suspension flows, or hydraulic transport. Such systems may be, with a high level of fidelity, simulated through the coupling of the computational fluid dynamics (CFD) with the discrete element method (DEM). However, the achievable fidelity of CFD-DEM solvers is commonly limited by the fact that the majority of available DEM solvers are designed to consider only spheres. Furthermore, all the available CFD-DEM solvers are based on coupling two standalone solvers through an interface. In this contribution, we present a monolithic CFD-DEM solver implemented solely in the OpenFOAM C++ library capable of treating arbitrarily shaped particles. In fact, out of the available approaches to non-spherical DEM, we have selected the most geometrically accurate one allowing for arbitrary polyhedral shapes. The biggest emphasis in the talk will be given to the internal workings of a newly designed DEM solver. Its connection with the standard Hertz model will be discussed and verifications against state-of-the-art DEM solver LIGGGHTS will be presented.

The authors acknowledge the financial support provided by the Ministry of Education, Youth, and Sports of the Czech Republic via the project No. CZ.02.01.01/00/23_020/0008501 (METEX), co-funded by the European Union.

Advanced continuation and iterative methods for slope stability analysis in 3D

S. Sysala, M. Béreš, S. Bérešová, T. Luber

This contribution deals with solution of slope stability problems in 3D by the finite element method and incremental procedures like the shear strength reduction or limit load methods. A complex solution concept enabling to overcome spurious numerical oscillations, reduce overestimation of safety factors, and solve ill-conditioned systems of linearized equations is proposed and supported by recent mathematical results. In particular, we build on Mohr-Coulomb plasticity, Davis' modifications of the nonassociated plastic flow rule and related optimization approaches, indirect continuation techniques, mesh adaptivity, Newton-like and deflated Krylov's methods with preconditioners. The suggested solution concept is implemented using in-house codes in Matlab and illustrated with numerical benchmarks on slope stability.

Improved handling of nonlinear constraints in 2D steel frame optimization

T. Světlík, M. Čermák

Poster addresses methods for handling nonlinear constraints in the optimization of 2D steel frame structures under ultimate limit state (ULS) and serviceability limit state (SLS) conditions. Constraints are expressed in two distinct formulations, linearized using first-order Taylor expansions, and aggregated into a unified representation. This approach enhances constraint robustness and avoids issues associated with individual linearizations, reducing the overal number of iteration cycles.

Speeding up an unsteady flow simulation by the adaptive BDDC and Krylov subspace recycling

J. Šístek, M. Hanek, J. Papež

Means of acceleration of iterative methods for sequences of linear systems have been extensively studied in literature. A widely used approach is recycling the subspace within a Krylov method combined with deflation. Another natural approach is based on improving the preconditioner. In domain decomposition methods, adaptive selection of coarse space is the state of the art leading to powerful preconditioners. We compare these two approaches and study their combination for unsteady incompressible flow problems governed by the Navier-Stokes equations. These are solved by the pressure-correction scheme in connection with the finite element method. This approach leads to sequences of linear systems over the time steps.

Our particular interest is the Poisson problem of pressure. Results for the problem of flow behind the sphere for Reynolds numbers 100 and 300 are presented. We demonstrate that by using these approaches we are able to save about one half of the computational time.

Solving large sparse linear systems and least squares

M. Tůma

The lecture will deal with solving the systems of linear algebraic equations and the least squares problems by the approaches generally known as direct methods. Such methods are traditionally based on two concepts that have been developed and modified over time. First of these concepts is the use of the Gaussian elimination. It is generally considered as the basic transformation that enables seamless application of the inverse of the matrix by its conversion into a factorized form. Second underlying concept is the heavy use of the matrix structure. Taking into account the pointwise or blockwise matrix sparsity structure and its changes throughout the solution process, capturing sparsity plays a key role to get a useful solution of the considered problems efficiently.

Steady development of computer architectures and more advanced study of underlying applications are significantly enhancing the contemporary solution methods by additional tools like replacement of matrix blocks by their approximate low-rank substitutes or by intentional less accurate processing that may save memory or may lead to higher computational speed. Another basic implication of this development is the need to combine direct methods with iterative ones to get useful approximate solutions of very large problems. But, despite all of this, the importance of sparsity considerations in contemporary solution approaches does not seem to be decreased. This is a motivation for this, relatively low level oriented, explanation of basic concepts in this field of numerical linear algebra.

Parameter fitting of DEM-BBM models using the Newmark method

R. Varga

This poster investigates how individual parameters influence the behavior of a Discrete Element Method-Beam Bound Model (DEM-BBM) under the Newmark integration scheme. The focus is on examining the effects of varying the time step, Newmark method parameters, and Rayleigh damping parameters on quasi-static crack propagation modeling.

Selected inequalities in the analysis of domain decomposition methods

P. Vodstrčil

In this talk, we will illustrate different types of inequalities that play an important role in the convergence analysis of FETI methods. In particular, we will show how these inequalities provide some estimates on the spectrum of the Schur complement of the stiffness matrix.

Lattice discrete particle model for 3D-printed alloy structures

J. Vorel, A. Jíra, J. Kruis

This paper presents advancements in the Lattice Discrete Particle Model (LDPM) tailored for simulating 3D-printed titanium alloy structures. The study highlights the model's ability to incorporate material mesostructure, including particle size distribution and inherent porosity, which are characteristics of 3D printing techniques. A novel approach integrating a volumetric-deviatoric split extends the model's applicability to metals. The elastoplastic model is further enhanced by incorporating isotropic damage. Simulation results demonstrate the significant impact of porosity on yield strength and overall structural performance, particularly for thin specimens approaching the printing resolution limits.

Mathematics of neural networks

J. Vybíral

We define the mathematical concept of Artificial Neural Networks (ANN) and discuss its basic properties. We study the properties of ANNs from the point of view of approximation theory - i.e., which functions can be reconstructed effectively by neural networks with small number of layers and small width. We show in which sense they outperform linear methods of recovery and how they can be used to avoid the curse of dimensionality. We provide also lower bounds, showing the limits of recovery by ANNs.