SIAM Student Chapter

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Prague SIAM Student Chapter Workshop

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Noise Revealing in Golub–Kahan Bidiagonalization and Regularization in Discrete Inverse Problems

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Joint work with Iveta Hnětynková.

We consider a linear inverse problem $Ax \approx b$, where A is a linear operator with smoothing property and b represents an observation vector polluted by noise. Typically these problems are *ill-posed*, meaning that noise in the the data, especially its high-frequency components, may give rise to significant errors in computed approximations of x. It was shown in [Hnětynková, Plešinger, Strakoš -2009] that high-frequency noise reveals during the Golub–Kahan iterative bidiagonalization in the left bidiagonalization vectors. In the talk we will present a way of determining the iteration with optimal noise revealing property and suggest reduction of the high-frequency part of the noise by subtracting the corresponding (properly scaled) left bidiagonalization vector from the data vector b.

CG Methods in Non-standard Inner Product for Saddle-point Algebraic Linear Systems with Indefinite Preconditioning

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Developing a good solver for saddle-point algebraic linear systems is often a challenging task, due to indefiniteness and poor spectral properties of the coefficient matrix. In the past few years, the employment of indefinite preconditioners leading to systems which are symmetric (and sometimes even positive definite) in a non-standard inner product has drawn significant attention.

In its basics, the method works as follows: given the linear system $\mathcal{A}x = b$, let $\mathcal{P}$ be a preconditioner and $\mathcal{D}$ be a symmetric and positive definite matrix such that the preconditioned system is symmetric in the inner product defined by $\mathcal{D}$, that is, $\mathcal{D}\mathcal{P}^{-1}\mathcal{A} = (\mathcal{P}^{-1}\mathcal{A})^T\mathcal{D}$. If, in addition, $\mathcal{D}\mathcal{P}^{-1}\mathcal{A}$ is positive definite, then the Conjugate Gradients method in the $\mathcal{D}$-inner product can be employed on the preconditioned system, and the rate of convergence of the method, measured in the error $\mathcal{D}\mathcal{P}^{-1}\mathcal{A}$-norm, only depends on the (all) *real* eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$.

The aim of the seminar is twofold. Firstly, we briefly review the theory behind this strategy and discuss some of its applications in literature, also reporting on some advances in the spectral estimates of one of the preconditioned matrix.

Secondly, we explore the sometimes overlooked relation between the non-standard minimized norm of the error and the Euclidean one. Particular emphasis is given to the case when $\mathcal{D}$ is close to singular.

On the Numerical Solution of Large-scale Linear Matrix Equations Using Python

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The M.E.S.S. software suite for solving large scale matrix equations and related problems is the successor of the obsolete LyaPack MATLAB toolbox. The software suite consists of a new MATLAB toolbox and a separate C library C-M.E.S.S. which works independent from MATLAB. Due to the fact that many scientists use Python with NumPy and SciPy for their implementations we want to provide the key algorithms of M.E.S.S. there as well. We describe and compare two possible approaches for the implementation with special focus on their multicore performance.

MOR of Quadratic-Bilinear Differential Algebraic Equations

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We consider model order reduction of bilinear descriptor systems using interpolatory projection framework. Such nonlinear descriptor systems can be represented by a series of generalized linear descriptor systems by utilizing the Volterra–Weiner approach [1]. Each of the linear subsystem can be decomposed further into strictly proper and polynomial parts. Standard projection for bilinear systems can construct an interpolating approximation but does not match the polynomial part. This may result in an unbounded error in terms of H_2 or H_∞ norm. Assuming that the polynomial part of each subsystem is constant, we proposed a model reduction approach that not only achieves interpolation but also retains the constant polynomial part of each subsystem. Also, we show that by Carlaman Bilinearization we can approximate quadratic-bilinear (DAE) differential algebraic equations to bilinear DAE and the transformation can preserve a special structure of the pencil.

[1] Wilson J. Rugh. Nonlinear system theory. Johns Hopkins University Press Baltimore, 1981

Fréchet Derivatives of Matrix Functions and their Applications

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For a matrix function $f : \mathbb{C}^{n\times n} \mapsto \mathbb{C}^{n\times n}$ we can define its Fréchet derivative as the unique linear function satisfying $f(A + E) = f(A) + L_f(A, E) + o(\|E\|)$ for any E. This derivative is used to define the condition number of a matrix function, but is also used in many application areas including matrix optimization, nuclear safety, model reduction, and image registration.

This talk summarizes our recent research into higher order derivatives of matrix functions and further explains some of their interesting applications. In particular we look at how changes in each element of A affect $f(A)$ and how we can calculate the most sensitive elements quickly. One area in which this problem is particularly useful is in the sensitivity analysis of differential equations describing nuclear activation—the process of inducing radioactivity in materials—which is an important safety issue.

Microbial Enhanced Oil Recovery and Efficient Parameter Estimation

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Microbial Enhanced Oil Recovery (MEOR) is a so called tertiary oil extraction technology allowing the partial recovery of oil entrapped in porous media, thus increasing the life of mature oil reservoirs. When certain types of microbes are stimulated, i.e. supplied with nutrient, in core samples of reservoir sandstone in the laboratory, they improve oil production by mobilizing residual oil trapped in the pore space. The bacterial growth at an oil water interface causes a substantial reduction in interfacial tension and influences other parameters as porosity and permeability. Modeling this process is a challenging task. The model equations are of convection-diffusion type with source terms and have nonlinear dependencies on a set of parameter. Additionally we have to consider continuity equations. We have implemented a first version of a 2D-PDAE model and have run parameter estimation for a partial model. Furthermore we present an efficient parameter estimation algorithm based on a reduced approach to solve large scale problems. It allows multiple shooting structure exploitation with the effort of single shooting.

Reactive Transport Modeling in Unsaturated Porous Media

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Motivated by a flow-through laboratory experiments performed within the project "Dynamic Capillary Fringes – A Multidisciplinary Approach", we developed a numerical simulator for multiphase multicomponent reactive flow in porous media (macroscopic approach) which is able to consider simultaneously multiphase flow, solute transport and diffusion, exchange between the liquid phase and the gas phase, absorption, geochemical reactions and microbiological processes.

In a flow-through laboratory experiment performed at the Karlsruhe Institute of Technology, Germany, the oxygen phase transfer, the growth and the transport of a bacteria (green fluorescent *Escherichia coli*) were investigated. The results of numerical simulations of bacterial growth and transport in the capillary fringe, with nutrient supply under steady-state and transient flow conditions are finally compared to the experimental data.

Imaging, Modeling and Computations of Hemodynamics in Cerebral Aneurysms

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The aneurysm is a local expansion of a vessel. This disease is dangerous only in the case of rupture. With increasing popularity of imaging methods an aneurysm is often discovered on the brain artery. The need of accurate computation of the velocity and pressure fields in patient specific geometries is motivated exactly by the question which aneurysm has tendency to rupture.

Even if we consider incompressible newtonian fluid, the problem is quite challenging. We will start with the question of correct boundary conditions on the vessel walls, which can have significant influence on the usual measures. We will then discuss the appropriate hemodynamic parameters which affects the growth or rupture of the aneurysm. Finally, we will mention the possibility of involvement of interaction with elastic wall to the model.

Numerical Issues in Mathematical Modeling of Float Glass Forming Process

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The float glass process (Pilkington process) is the standard industrial scale process for manufacturing flat glass. The first phase of the process is the flow of the glass melt down an inclined plane (spout), and its impact on the tin bath, which makes the process a practical example of a multicomponent physical system. Our objective is to develop a mathematical model for the process, and implement a numerical scheme that would allow us to perform computer simulations of the process.

For the computer simulation of the process we use a Cahn–Hilliard–Navier–Stokes type model which conceptually belongs to the class of so-called diffuse interface models. These models treat the interface between the components as a thin layer across which the components can mix, and that, among others, automatically take into account the surface tension effects. This allows one to avoid highly specialized and difficult to implement interface tracking methods. The cost to pay is the need to use a very fine spatial resolution in particular at the interface between the components. Another difficulty arises when the numerical simulation is being run with material parameters corresponding to the real setting, in particular when there is a high viscosity and density contrast between the components of the system. We will discuss the numerical challenges that must be addressed in order to make the numerical simulation based on the Cahn–Hilliad–Navier–Stokes type model applicable in the modeling of Pilkington process.

An Implicit Midpoint Spectral Approximation of Nonlocal Cahn–Hilliard Equations

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The talk is concerned with the convergence analysis of a numerical method for nonlocal Cahn–Hilliard equations. The temporal discretization is based on the implicit midpoint rule and a Fourier spectral discretization is used with respect to the spatial variables. The sequence of numerical approximations is shown to be bounded in various norms, uniformly with respect to the discretization parameters, and optimal order bounds on the global error of the scheme are derived. The uniform bounds on the sequence of numerical solutions as well as the error bounds hold unconditionally, in the sense that no restriction on the size of the time step in terms of the spatial discretization parameter needs to be assumed.

This is joint work Christof Melcher (Aachen) and Endre Süli (Oxford).