Numerical Linear Algebra: In honor of Maya Neytcheva

Satellite workshop to *The Swedish e-Science Academy*, 11–12 October 2023
`https://essenceofescience.se/swedish-e-science-academy-11-12-october-2023/`

Time and location

Time: 10 October 13:00–17:00 and 11 October 09:00-12:00
Location: Häggsalen (room: Å10132), (map)
Ångströmlaboratoriet
Lägerhyddsvägen 1
752 37 Uppsala
Transportation: Bus 4 goes from Central station to "Polacksbacken", and from there it is a short walk to Ångströmlaboratoriet. You can pay with creditcard or app on the bus (no cash). (`https://www.ul.se/` and timetable for Bus 4)

Registration of interest

Please fill in the following form if you plan to attend the workshop. The registration for the dinner on 10 October will close at 08:00 5 October.
`https://forms.gle/XqvKSeBg4XDdRDUJ6`

General description

In honor of Maya Neytcheva, Uppsala University, who is retiring in 2023 after a long and successful career, we hold this satellite workshop in the subject of numerical linear algebra. Hence, the purpose is the celebration of the scientific work of Maya Neytcheva, the sharing of current research, and fostering future research in the field.

The workshop consist of presentations and discussions related in a wide sense to the subject area of Maya Neytcheva's research.

Organizing committee

Sven-Erik Ekström, Uppsala University, `sven-erik.ekstrom@it.uu.se`, +46(0)18-471 2963
Gunilla Kreiss, Uppsala University, `gunilla.kreiss@it.uu.se`, +46(0)18-471 2968

Programme

Tuesday 10 Oct		Wednesday 11 Oct	
13:00–13:05	Introduction	09:15–10:00	Philipp Birken
13:05–14:00	Eddie Wadbro	10:00–10:15	*Coffee*
	Paolo Bientinesi	10:15–11:00	Stefano Serra-Capizzano
14:15–15:00	Svetozar Margenov	11:15–12:00	Michal Béreš
15:00–15:15	*Coffee*		Roman Iakymchuk
15:15–16:00	Petia Boyanova		
	Ivo Dravins		
16:15–17:00	Elias Jarlebring		
17:30	Dinner (Å106157, map)		

See affiliations, titles, and abstracts below.

Reduced Basis and Tensor-Train Techniques for Stochastic Galerkin Matrix Equations

Michal Béreš
Technical University of Ostrava, michal.beres@ugn.cas.cz

The topic of this talk is a computational framework tailored for the efficient solution of matrix equations derived from stochastic Galerkin discretization. Our approach begins with the construction of a reduced basis for the finite element part of the discretization using the Monte Carlo method. Employing a specialized sampling technique minimizes the required samples. Additionally, a deflation technique accelerates the iterative solution for a series of resulting linear systems. In the subsequent phase, the stochastic elements form a tensor polynomial basis. The final solution for the reduced problem is approximated through a tensor-train approximation.

Sequences of linear algebra problems

Paolo Bientinesi
Umeå University, pauldj@cs.umu.se

In this talk we reflect on the current state of high-performance linear algebra libraries. On the one hand, the BLAS and LAPACK libraries, both of which are more than 30 years old, remain the undisputed standard in terms of functionality and usage. Indeed, the importance of these libraries in science and engineering cannot be overstated. On the other hand, we observe that nowadays their rigid interface often represents an hindrance towards the optimization of scientific workflows. We argue that in many applications the following two facts hold true: 1) the computational bottleneck consists of not one, but a sequence, of linear algebra problems; 2) it is beneficial to tackle the sequence of problems as a whole, instead of one at the time (as one normally would). We showcase a few such cases, along with optimization opportunities and performance gains.

On Weather Prediction and Applications in Aviation

Petia Boyanova
Flightkeys GmbH, petia.boyanova@gmail.com

Accurate and timely weather forecasts are of great importance to society and various industries, with their significance heightened by the pressing need for climate change mitigation. This presentation aims to outline key aspects and challenges of weather prediction and to demonstrate its practical utilization in flight planning and efforts to decrease aviation's impact on global warming.

Iterative solvers vs linear and nonlinear invariants in compressible CFD

Philipp Birken
Lund University, philipp.birken@math.lu.se

We consider computational fluid dynamics for compressible flows. This plays an important role in the design of air planes and new renewable jet fuels, or in simulation of the atmosphere within weather and climate predictions. During the past decade, significant effort has been put into high order discontinuous Galerkin methods for these problems. A successful design principle has been to find methods that preserve properties of the differential equation, such as the underlying conservation law or the second law of thermodynamics in the form of an entropy inequality.

In this talk we focus on implicit discretizations in time, in particular space-time discretizations. To solve the arising nonlinear equation systems, iterative methods are needed. The question thus arises if these approximate solutions in turn preserve the properties of the discretization.

Firstly, we consider global and local conservation. As it turns out, many commonly used methods preserve the local conservation of an underlying implicit scheme. This includes pseudo-time iterations, Newton's method and Krylov subspace methods. However, there are prominent exceptions, in particular the Jacobi and Gauss-Seidel iterations. We present extensions of the Lax-Wendroff theorem for a fixed, finite number of iterations each time step. The iterative method defines a numerical flux that is inconsistent in general. We can describe the specific inconsistency as a form of slowed down time for pseudo-time iterations, Krylov methods, and thereby also Newton-Krylov methods. A simple technique based on the explicit Euler method can alleviate flux-inconsistency and can additionally be used to generate improved initial guesses for iterative methods.

Secondly, we look at entropy preservation of iterative methods, respectively of nonlinear invariants. As it turns, out, iterative methods do not preserve these. We present various ways that Newton's method can be adjusted to fix this problem. Numerical methods illustrate the advantages and disadvantages of the various fixes.

Stage-parallel preconditioning for implicit Runge–Kutta methods

Ivo Dravins
Ruhr Universität Bochum, ivo.dravins@rub.de

Fully implicit Runge–Kutta methods offer the possibility to use high-order-accurate time discretization with desirable stability properties. For general implicit Runge–Kutta methods all stages are coupled leading to a potentially costly and involved solution procedure which has been a major barrier to their widespread use. We present a stage-parallel block preconditioner for the class of L-stable Radau IIA Runge–Kutta methods. The preconditioner exploits a property of the coefficient matrices to construct a block lower-triangular preconditioner. During the application of the preconditioner, a basis change can be applied to obtain a block-diagonal form, in this way allowing us to decouple the stages when solving for the blocks. In the linear case this basis change can be applied directly – for non-linear equations further approximations are needed to achieve this decoupling. For the linear case, we discuss the analysis of the preconditioned matrices which are non-symmetric and in tensor form. We give eigenvalue bounds for the two- and three-stage methods under symmetric positive definite assumptions. We illustrate the performance by numerical examples, including also applications to non-linear problems.

Precision in linear algebra solvers and its impact on applications

Roman Iakymchuk
Uppsala University, roman.iakymchuk@it.uu.se

Until recent years, linear algebra solvers were predominantly operating with double precision or binary64. With the advent of AI, in particular deep learning, lower floating-point precisions formats were introduced to accommodate the need of these simulations; now the spectrum is shifted to fixed point and even integer arithmetic, promoting block floating point arithmetic. This change has also impacted the linear algebra algorithm development where the concept of mixed-precision was introduced for faster and energy-efficient but still reliable solvers. In this talk, I will provide a brief overview on mixed-precision, introduce to the strategy of mixing precisions in a controllable way, and provide preliminary results with applications.

Computational graphs for matrix functions

Elias Jarlebring
Royal Institute of Technology, eliasj@kth.se

Many numerical methods for evaluating matrix functions can be naturally viewed as computational graphs. In this work we rephrase these methods as directed acyclic graphs (DAGs) and show how that can be used to study existing techniques, improve them, and derive new ones. Improvements are achieved by using that the accuracy of these matrix techniques can be characterized by the accuracy of their scalar counterparts, thus designing algorithms for matrix functions can be regarded as a scalar-valued optimization problem. The derivatives needed during the optimization can be calculated automatically by exploiting the structure of the DAG, in a fashion analogous to backpropagation. The approach is incorporated in the GraphMatFun.jl, a Julia package that offers the means to generate and manipulate computational graphs, optimize their coefficients, and generate Julia, MATLAB, and C code to evaluate them efficiently at a matrix argument. The software also provides tools to estimate the accuracy of a graph-based algorithm and thus obtain numerically reliable methods. For the exponential, for example, using a particular form (degree-optimal) of polynomials produces implementations that in many cases are cheaper, in terms of computational cost, than the Padé-based techniques typically used in mathematical software. The optimized graphs and the corresponding generated code are available online.

Large-Scale Scientific Computing and Optimal Preconditioning Solution Methods

Svetozar Margenov

Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, margenov@parallel.bas.bg

The talk is on robust preconditioning solution methods for large-scale linear systems arising after discretization of boundary value problems by the finite difference or finite element method. The goal is to obtain a uniformly bounded relative condition number of the preconditioned matrix, where the computational complexity of each iteration is $\mathcal{O}(N)$, N beeing the number of unknowns. The first part of the presentation discusses some earlier joint results with Maya Neicheva on Algebraic Multilevel Iteration (AMLI) methods for non-conforming finite element systems. A pioneering result here is the uniform estimate of the CBS constant in the case of non-nested Crouzeix-Raviart finite element spaces, independent of the coefficient and/or mesh anisotropy. Then, some recent results on non-overlapping domain decomposition (DD) preconditioning are presented. At the operator level, a key property is that the energy norm associated with the Steklov-Poincaré operator is spectrally equivalent to the Sobolev norm of index 1/2. The new multiplicative non-overlapping DD preconditioner is defined by approximating the Schur complement using the best uniform rational approximation (BURA) of $L_\gamma^{1/2}$. Here, L_γ denotes the discrete Laplacian over the interface γ. Some numerical tests are included to build on the understanding of theoretical estimates. Brief concluding remarks are given at the end.

Material distribution topology optimization for boundary dominated physics

Eddie Wadbro

Karlstad University, eddie.wadbro@kau.se

In the classical design optimization by the material distribution method (density-based topology optimization), a so-called material indicator function represents the presence/absence of material inside the domain. To use this approach for boundary-effect-dominated problems, we need to identify the boundaries of the design at each iteration and compute the contribution of the boundary terms to the governing equations. To this end, we introduce a new approach by defining a boundary indicator function on the mesh faces (edges in 2D and facets in 3D).

We present a density-based topology optimization formulation to design acoustic liners with maximal sound absorption. We model the wave propagation using the Helmholtz equation with a Wentzell boundary condition to account for the visco-thermal losses at the design's boundaries. Svanberg's method of moving asymptotes (MMA) solves the optimization problem. The numerical experiments produce highly efficient acoustic liners working in the targeted frequency range. The frequency response for the optimized designs has been validated using a linearized Navier–Stokes model.

GLT theory: analysis and numerical applications

Stefano Serra-Capizzano[1,2]

[1] *Department of Science and High Technology, Insubria University - Como, Italy; s.serracapizzano@uninsubria.it*

[2] *Department of Information Technology - Uppsala University - Uppsala; serra@it.uu.se*

Keywords: Approximated PDEs, FDEs, IDEs, eigenvalues, singular values, Weyl distributions, Krylov methods, multigrid, multi-iterative solvers

Abstract

Recently, the class of Generalized Locally Toeplitz (GLT) sequences has been introduced [40, 41] as a generalization both of classical Toeplitz sequences and of variable coefficient differential operators and, for every sequence of the class, it has been demonstrated that it is possible to give a rigorous description of the asymptotic spectrum [12, 44] in terms of a function (the symbol) that can be easily identified; see also [43].

This generalizes the notion of a symbol for differential operators (discrete and continuous) or for Toeplitz sequences, where for the latter it is identified through the Fourier coefficients and is related to the classical Fourier Analysis (see [13]).

The GLT class has nice algebraic properties and indeed it has been proven that it is stable under linear combinations, products, and inversion when the sequence which is inverted shows a sparsely vanishing symbol (sparsely vanishing symbol = a symbol which vanishes at most in a set of zero Lebesgue measure). Furthermore, the GLT class virtually includes any approximation of partial differential equations (PDEs), fractional differential equations (FDEs), integro-differential equations (IDEs) by local methods (Finite Difference, Finite Element, Isogeometric Analysis etc) and, based on this, we demonstrate that our results on GLT sequences can be used in a PDE/FDE/IDE setting in various directions, including preconditioning, multigrid, spectral detection of branches, fast 'matrix-less' computation of eigenvalues, stability issues, symmetrized problems.

The seminal papers on the considered spectral theory are [13, 44, 43, 40, 41].

The GLT theory is organized in books and revue papers [28, 29, 30, 4, 5, 6].

The other references contain applications and theoretical results, where the GLT machinery has been used.

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