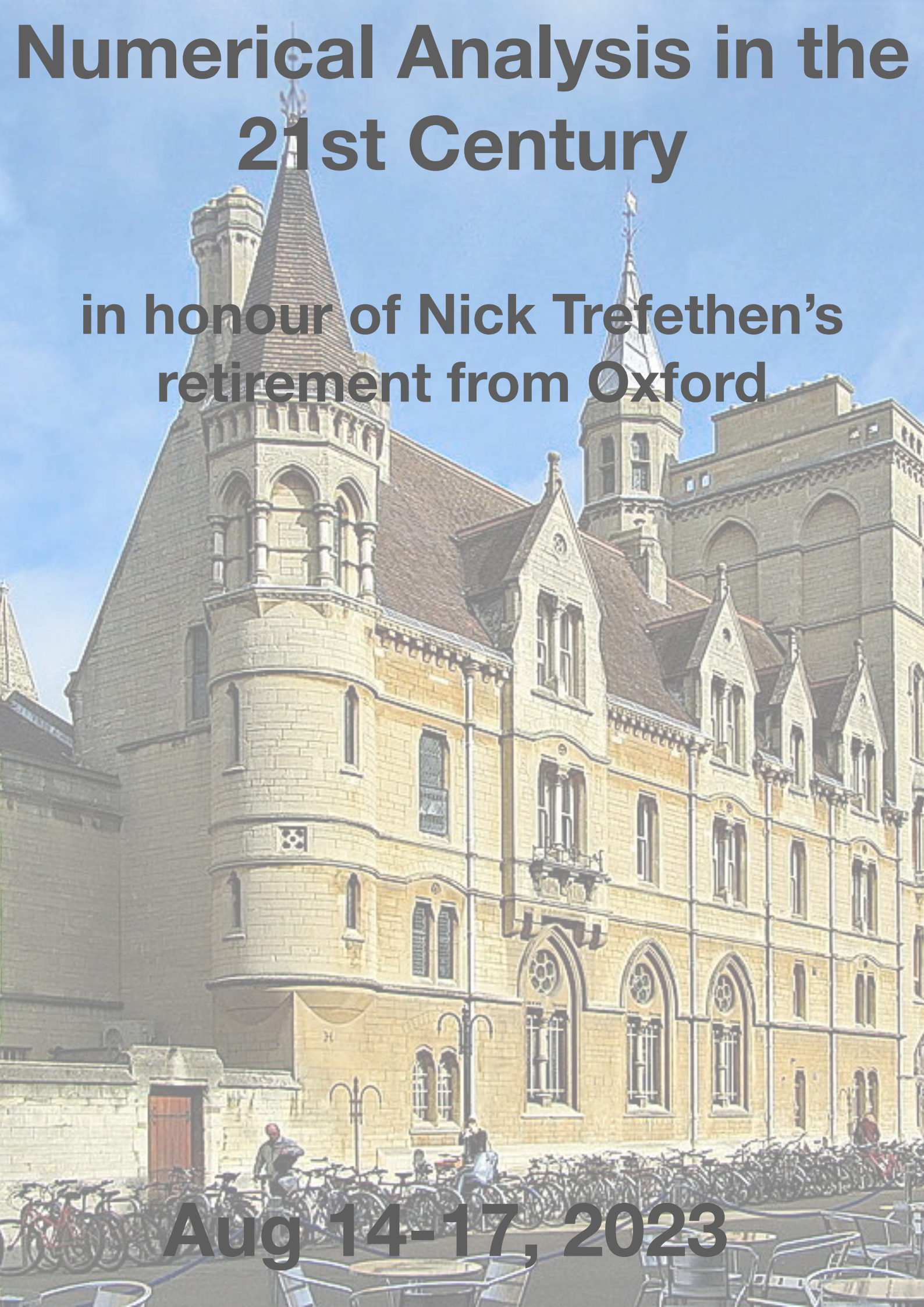
Numerical Analysis in the 21st Century

in honour of Nick Trefethen's retirement from Oxford



Aug 14-17, 2023

For more information:
https://21stcenturyna.github.io/

The open-source LaTeX template, AMCOS_booklet, used to generate this booklet is available at `https://github.com/maximelucas/AMCOS_booklet`

Contents

About

Numerical Analysis in the 21st Century

We are excited to organise the conference Numerical Analysis in the 21st Century in honour of Nick Trefethen's retirement from Oxford. The conference will take place at the Blavatnik School of Government and Balliol College, Oxford, UK from August 14-17, 2023. Nick Trefethen is a well-respected professor at the University of Oxford's Mathematical Institute, and this conference is a great opportunity to celebrate his contributions to the field of numerical analysis.

Organising committee

Patrick Farrell	patrick.farrell@maths.ox.ac.uk
Yuji Nakatsukasa	nakatsukasa@maths.ox.ac.uk
Alex Townsend	townsend@cornell.edu

Timetable

Monday, 14th August

8:00-9	Welcome reception and remarks at Blavatnik School
9:00-9:45	Plenary 1: Mark Embree
	Contour Integral Eigensolvers, Rational Interpolation, and System Identification
9:45-10:30	Plenary 2: Anna-Karin Tornberg
	TBD
10:30-11	Coffee break
11-11:45	Plenary 3: André Weideman
	Beyond Blow-up
11:45-12:30	Plenary 4: Toby Driscoll
	AAA rational approximation on a continuum
12:30-1:45	Lunch
1:45-2:30	Plenary 5: Randy LeVeque
	Rapid tsunami forecasting using fake quakes and ML
2:30-3:15	Plenary 6: Coralia Cartis
	To randomise or not to randomise? (That is the question...)
3:15-3:45	Coffee break
3:45-5:50	Minisymposium sessions 1-6

Monday's Minisymposium sessions

Mini 1: Interpolation and Approximation Methods
Mini 2: Spectral and Polynomial Methods
Mini 3: Techniques related to Numerical Linear Algebra
Mini 4: Numerical Optimization and Analysis
Mini 5: Numerical Methods for Differential Equations
Mini 6: Early-career researchers I

Monday	Mini 1	Mini 2	Mini 3	Mini 4	Mini 5	Mini 6
3:45	Berrut	Olver	Moufawad	Toh	Hansen	Leveque
4:10	Fortunato	Papadopoulos	Burke	Hall	Engström	Heinzelreiter
4:35	Salazar Celis	Slevinsky	Baglama	Chok	Toro	Drysdale
5:00	Goodrich	Burns	Hashemi	Ang	Rufai	Buggenhout
5:25	Austin	Vasil	MacDonald	Shustin	Xue	Cisneros

Tuesday, 15th August

9:00-9:45	Plenary 7: Steven Strogatz
	Nick Trefethen as a writer of mathematics and about mathematics
9:45-10:30	Plenary 8: Folkmar Bornemann
	A Müntz Surprise
10:30-11	Coffee break
11-11:45	Plenary 9: Nick Hale
	The barycentric resampling matrix revisited
11:45-12:30	Plenary 10: Kathryn Gillow
	Computing Linear Functionals of Solutions to PDEs
12:30-1:45	Lunch
1:45-2:30	Plenary 11: Laurette Tuckerman
	Order-of-magnitude speedup for computing steady states and traveling waves
2:30-3:15	Plenary 12: Abinand Gopal
	A new solver for PDEs in exteriors of open arcs
3:15-3:45	Coffee break
3:45-5:25	Minisymposium sessions 7-12
6:30-10:00	Banquet at Balliol College. Jazz Band: the Park Town Strutters.
	Gentlemen are requested to wear ties.

Tuesday's Minisymposium sessions

Mini 7: Least Squares Problems
Mini 8: Numerical Methods for Quantum and Molecular Systems
Mini 9: Algorithmic Approaches in Numerical Analysis
Mini 10: Tools in Numerical Linear Algebra
Mini 11: Numerical Geometry and Shape Optimization
Mini 12: Early-career researchers II

Tuesday	Mini 7	Mini 8	Mini 9	Mini 10	Mini 11	Mini 12
3:45	Scott	Hassan	Derevianko	Damle	Paganini	Yu
4:10	Widdershoven	Ukena	Serkh	Montanelli	Zavalani	Trujillo
4:35	Meier	Mikkelsen	Zerbinati	Stoll	Baier-Reinio	Daužickaitė
5:00	Costa	Bellotti	Singh	Fink Shustin	Linß	-

Wednesday, 16th August

9:00-9:45	Plenary 13: Cleve Moler
	Exploring Matrices
9:45-10:30	Plenary 14: Alan Edelman
	Some new results on the maximum growth factor in GE
10:30-11	Coffee break
11-11:45	Plenary 15: Martin Gander
	Time Parallel Time Integration
11:45-12:30	Plenary 16: Heather Wilber
	What can the square root approximation problem teach us?
12:30-1:45	Lunch
1:45-2:30	Plenary 17: Daan Huybrechs
	Numerical methods in a rectangular world
2:30-3:15	Plenary 18: Cécile Piret
	Computation of fractional derivatives of analytic functions
3:15-3:45	Coffee break
3:45-4:30	Plenary 19: Gunnar Martinsson
	Pivoting and randomization in numerical linear algebra
4:30-5:15	Plenary 20: Anne Greenbaum
	Optimal polynomial approximation to rational matrix functions

Thursday, 17th August

9:00-10:40	Minisymposium sessions 13-17
10:40-11:15	Coffee break
11:15-12	Plenary 21: Nick Higham
	The Power of Bidiagonal Matrices
12-12:20	Closing Remarks: Nick Trefethen
	Memos

Thursday's Minisymposium sessions

Mini 13: Numerical Linear Algebra
Mini 14: Innovative Approaches in Numerical Methods
Mini 15: Applications of Numerical Analysis
Mini 16: Advances in Numerical Analysis and novel applications
Mini 17: Computational Approaches in Biological Systems and Data Analysis

Thursday	Mini 13	Mini 14	Mini 15	Mini 16	Mini 17
9:00	Szyld	Betcke	de Melo Virissimo	Herremans	Mahapatra
9:25	Colbrook	Zhao	Treinen	Horning	Benkova
9:50	Xu	Al Daas	Chama	Corless	Pasha
10:15	Hecht	Bergamaschi	Osborne	Mastronardi	Zhu

List of Abstracts – Plenary Speakers

A Müntz Surprise

Folkmar Bornemann

Technische Universität München

In a recent paper, quantifying the exponential growth of coefficients in the expansion, Nick wrote that “typical sets of powers deemed useful by Müntz’s theorem would in fact be useless in any actual [computation]". Well, this is one of the few rare occasions of saying: “Objection, Your Honour". To make my point, I show that the concrete 10-digit problem

What is the error of $L^2(0,1)$-best-approximation of the function $\sin(\pi x)$ in the linear span of $1, x^2, x^3, x^5, x^7, \ldots, x^{541}$, where the exponents are the first 100 primes?

can actually be solved to machine precision in a few lines of Chebfun code — notwithstanding that the coefficients of the expansion get as large as 3.3×10^{64}.

To randomise or not to randomise? (That is the question...)

Coralia Cartis

Mathematical Institute, University of Oxford

We discuss random and deterministic subspace methods for nonconvex optimization problems. We are interested in the global optimisation of functions with low effective dimensionality, that vary only along certain important directions or components. We show that the effective subspace of variation can be efficiently learned in advance of the optimization process; we contrast this with random embedding techniques that focus directly on optimization rather than learning. For local optimization, we will also address efficient choices of subspaces that blend randomisation techniques with expert deterministic choices.

AAA for rational interpolation on continuua and conformal maps

Toby Driscoll

University of Delaware

The AAA algorithm of Nakatsukasa, Sète, and Trefethen has rapidly risen to prominence as a fast and powerful way to approximate functions in the complex plane. As originally presented, AAA incrementally constructs an approximation based on a fixed initial discretization, which is not ideal in some cases where a good initial distribution of nodes may be difficult to discern. By also incrementally adding nodes from the domain based on the latest residual, the algorithm can be adapted to work well automatically even when singularities are very close to or on the interval. In addition, Trefethen and Costa have shown how to use AAA to approximate conformal maps. By incorporating known fractional-power singularities into the computation of the boundary correspondence, this idea can be used to obtain high accuracy on simply- and doubly-connected domains with boundary corners.

Some new results on the maximum growth factor in Gaussian elimination

Alan Edelman

MIT

We combine modern numerical computation with theoretical results to improve our understanding of the growth factor problem for Gaussian elimination. On the computational side we obtain lower bounds for the maximum growth for complete pivoting for $n = 1 : 75$ and $n = 100$ using the Julia JuMP optimization package. At $n = 100$ we obtain a growth factor bigger than $3n$. The numerical evidence suggests that the maximum growth factor is bigger than n if and only if $n \geq 11$.

We also present a number of theoretical results. We show that the maximum growth factor over matrices with entries restricted to a subset of the reals is nearly equal to the maximum growth factor over all real matrices. We also show that the growth factors under floating point arithmetic and exact arithmetic are nearly identical. Finally, through numerical search, and stability and extrapolation results, we provide improved lower bounds for the maximum growth factor. Specifically, we find that the largest growth factor is bigger than $1.0045n$, and the lim sup of the ratio with n is greater than or equal to 3.317. In contrast to the old conjecture that growth might never be bigger than n, it seems likely that the maximum growth divided by n goes to infinity as $n \to \infty$.

(Joint Work with John Urschel)

Contour Integral Eigensolvers, Rational Interpolation, and System Identification

Mark Embree

Virginia Tech

Contour integral techniques form a rich class of algorithms for computing eigenvalues within a target region of the complex plane. With this region we can associate a low-order dynamical system that has the sought-after eigenvalues as its poles. Using contour integrals we can sample the transfer function of this low-order system in various ways: computing eigenvalues amounts to data-driven system identification. We will present a general framework that casts contour integral eigensolvers (for linear and nonlinear problems) as system identification algorithms. This perspective provides a natural way to incorporate sketched samples, as well as modern Loewner-based system identification techniques. We will demonstrate the merits of this Loewner methods for computing eigenvalues of networks of vibrating strings, such as spider webs. (This talk describes work with Jonathan Baker, Michael Brennan, Dan Folescu, Jennifer Green, and Serkan Gugercin.)

Time Parallel Time Integration

Martin Gander

University of Geneva

I will present an up to date overview on the emerging research area of time parallel time integration, more recently also referred to as PinT (Parallel in Time) methods. I will explain the four main classes of such methods: multiple shooting type methods for initial value problems, waveform relaxation methods based on domain decomposition, space-time multigrid methods, and also direct space-time parallel methods.

Computing Linear Functionals of Solutions to PDEs: From Finite Elements to Machine Learning

Kathryn Gillow

University of Oxford

In many areas of application the quantity of interest is not the solution of a partial

differential equation, but a linear functional of that solution. We begin by revisiting adjoint based methods for finite element computations of such functionals, and discuss the advantages of these methods in both the continuous and discontinuous finite element framework. We then explore how the lessons learnt in the finite element setting can be used when approximating linear functionals of solutions to PDEs computed using machine learning techniques.

A new solver for PDEs in exteriors of open arcs

Abinand Gopal

Yale University

When numerically solving a constant-coefficient elliptic PDE, it is often advantageous to first reformulate the problem as a boundary integral equation. Typically, this is done by expressing the solution as the integral of an unknown density function multiplied by a kernel given by the free space fundamental solution of the PDE or its normal derivative. The unknown density function is then obtained by solving a second kind Fredholm integral equation where the right-hand side is given by the boundary data.

However, when the domain consists of the exterior of an open arc in 2D or an open surface in 3D, these standard integral representations encounter challenges. In this talk, we introduce a new representation which involves the composition of the standard single layer operator with a certain hypersingular integral operator. We show that the kernel of the composite operator can be efficiently evaluated numerically and that the resulting discretization can be rapidly inverted using a fast direct solver.

This is joint work with Shidong Jiang (Flatiron Institute) and Vladimir Rokhlin (Yale University).

Optimal Polynomial Approximation to Rational Matrix Functions Using the Lanczos and Arnoldi Algorithms

Anne Greenbaum

University of Washington

Given an n by n matrix A and an n-vector b, along with a rational function $R(z) := D(z)^{-1}N(z)$, we show how to find the optimal approximation to $R(A)b$ from the Krylov space, $\text{span}(b, Ab, \ldots, A^{k-1}b)$, using the basis vectors produced by the Lanczos or Arnoldi algorithm. Here *optimal* is taken to mean optimal in the $D(A)^*D(A)$-norm or, possibly, a different norm for Hermitian problems. Similar to the case for linear systems, we show

that for non-Hermitian problems, eigenvalues alone cannot provide information about the convergence behavior of this algorithm and we discuss other possible error bounds for highly nonnormal matrices.

The barycentric resampling matrix revisited: An application to delay/functional differential equations

Nick Hale

Stellenbosch University

The barycentric interpolation formula is a fundamental tool in function approximation and spectral collocation methods. When the interpolation and evaluation points are fixed, the interpolation can be represented as a matrix-vector product. In previous work [Driscoll & H, IMAJNA 2016] this *barycentric resampling matrix* was used as the basis of a technique for incorporating boundary conditions in spectral collocation by downsampling the discretised differential operators to smaller grids and using the additional constraints to 'square up' the system.

In this talk we show how barycentric resampling matrices can be used to implement spectral collocation methods for delay- and, more generally, functional differential equations. We introduce the approach by means of a few illustrative examples (including state-dependent delay), demonstrate the convenience of its use in the form of a Chebfun implementation, and investigate an example application in solving the α-Riccati equation, $u'(t) = -u(t) + u^2(\alpha t)$, with $\alpha > 1$..

The Power of Bidiagonal Matrices

Nicholas Higham

Manchester University

Bidiagonal matrices are one of the simplest types of matrices, with just a diagonal and a subdiagonal or superdiagonal. We show that they are nevertheless powerful tools in a variety of settings, especially when they are combined by multiplying them together. In particular, we use properties of bidiagonal matrices to show that it is possible to compute with tiny relative error the ∞-norm condition number of any $n \times n$ nonsingular totally nonnegative matrix (such as a Vandermonde matrix with real points in increasing order) in $O(n^2)$ flops, given a special form of the LU factorization of the matrix. One of Nick Trefethen's most highly cited papers is *Pseudospectra of Matrices* in the proceedings of the 1992 Dundee Conference on Numerical Analysis, which discusses and illustrates pseudospectra for 13 example matrices. We explain how the spectra of several of these

matrices can be understood with the aid of bidiagonal matrices.

Numerical methods in a rectangular world

Daan Huybrechs

KU Leuven

One of the recent papers of Nick Trefethen is called "Rectangular eigenvalue problems". The topic of that paper is part of a theme, and that theme is the topic of this talk: numerical methods in a rectangular world. In an ideal world all linear systems are square and well-conditioned, solutions are unique and computable to machine precision. There are many reasons why that is rarely the case in practice and we will review some of them. They are all too familiar. As it happens, rectangular systems enjoy several benefits over square systems even when things look bleak. We will review some of those too. But the best reason is: simpler methods! There are many variants of rectangular systems, and the most extreme perspective is a continuous one that lies at the heart of a software package called Chebfun.

Rapid Tsunami Forecasting Using Fake Quakes and Machine Learning

Randall LeVeque

University of Washington

Producing rapid real-time forecasts for tsunamis in the first few minutes of an earthquake is a challenging problem. Accurate forecasts often rely on direct measurements of the tsunami, which are only available at sparse locations, and only after the tsunami has passed the sensors. Real-time numerical modeling of the tsunami is also time consuming. We attempt to bypass these restrictions by training a convolutional neural network (CNN) that can forecast tsunami wave heights based only on Global Navigation Satellite System (GNSS) data, which is available within minutes at many existing stations in earthquake-prone regions. Training the model requires a large set of hypothetical earthquakes that are drawn from a geophysically reasonable probability distribution. These are generated using a Karhunen-Loeve expansion, as implemented in the FakeQuakes software. Tsunami simulations are performed for each using the GeoClaw software. Studying adversarial examples designed to fool the model leads to some new insights on the robustness and stability of CNNs.

Pivoting and randomization in numerical linear algebra

Gunnar Martinsson

UT Austin

The talk will survey a set of randomized algorithms for selecting a subset of the columns of a matrix whose spanning volume is close to maximal. This task is the core challenge when designing pivoting strategies for efficiently computing rank revealing QR and LU decompositions. It also arises in the context of computing low rank approximations to matrices (in particular when a CUR or interpolatory decomposition is desired), and in selecting "matrix skeletons" in fast algorithms for handling large dense matrices that arise in numerical methods for elliptic PDEs.

The main takeaway of the talk is that the column selection problem becomes computationally tractable if we first extract a random "sketch" of the row space of the matrix. To be precise, the sketch we need is a collection of random linear combinations of the rows of the original matrix. We will describe how to efficiently extract such a sketch, and then how to best use it to find a set of good spanning columns. Interestingly, in this environment, it turns out that LU with partial pivoting (LUPP) does as well as column pivoted QR (CPQR) in building a rank-revealing factorization. The is important since LUPP executes much faster on modern hardware than CPQR.

Exploring Matrices

Cleve Moler

Mathworks

I will describe a evolving collection of experiments that supplement courses in linear algebra and computational science. Topics include matrix multiplication, rotation matrices, Rubik's cube, computer graphics, SVD, and Simulink models of vehicle dynamics. The materials include short videos and interactive MATLAB software.

Computation of fractional derivatives of analytic functions

Cécile Piret

Michigan Technological University

A fractional derivative refers to a derivative of order generalized to real and imaginary numbers. Fractional calculus has a long and fascinating history, thought to be first documented in a 1695 letter by Leibnitz responding to L'Hôpital's inquiry about a half derivative. It remained somewhat of a theoretical curiosity for about 300 years before

finally gaining steam in the last couple of decades, and being found relevant in a vast and still expanding number of applications that include diffusion, potential theory, rheology, transport theory, or ecology. Yet, few high order numerical schemes exist, especially on an equispaced lattice.

In collaboration with Bengt Fornberg, we propose a new high order numerical method, based on the trapezoidal rule with end correction, to compute and explore fractional derivatives of analytic functions in the complex plane, including along their Riemann sheets, using only function values on an equispaced grid. This new method applied to an old problem opens doors to a better computational framework not only in the realm of fractional calculus, but also in the accurate evaluation of special functions, such as hypergeometric functions of various orders.

Nick Trefethen as a writer of mathematics and about mathematics

Steven Strogatz

Cornell University

We all know that Nick is a brilliant and innovative mathematician. But he's also an extraordinary writer, stylist, and expositor. In this talk, I'll highlight some of Nick's signature moves as a writer of mathematics — and commentator on the mathematical enterprise — using examples from his textbooks, articles, essays, index cards, and apologies.

Quadrature error estimates for layer potentials

Anne-Karin Tornberg

KTH

When numerically solving PDEs reformulated as integral equations, so called layer potentials must be evaluated. The quadrature error associated with a regular quadrature rule for evaluation of such integrals increases rapidly when the evaluation point approaches the surface and the integrand becomes sharply peaked. Error estimates are needed to determine when the accuracy becomes insufficient and a more costly special quadrature method should be utilized.

In this talk, we start by considering simple integrals in one dimension, and build up to layer potentials over smooth surfaces in three dimensions. We consider surfaces topologically equivalent to both a sphere and a torus, and discretizations based on Gauss-Legendre quadrature and/or the trapezoidal rule. The analysis involves contour integrals, residue

calculus and branch cuts, and a complexification of the parameter plane is used to generalize results from planar curves.

Numerical examples are given to illustrate the performance of the quadrature error estimates. The estimates for integration over curves are in many cases remarkably precise, and the estimates for curved surfaces in 3D are also sufficiently precise, with sufficiently low computational cost, to be practically useful.

Memos

Nick Trefethen

University of Oxford/Harvard

It seems I typed my first research memo as an undergraduate, in November 1976. Quite a few memos later, I'll tell some stories.

Order-of-magnitude speedup for computing steady states and traveling waves via Stokes preconditioning

Laurette Tuckerman

PMMH-CNRS-ESPCI-Sorbonne

Steady states and traveling waves play a fundamental role in understanding hydrodynamic problems. Even when unstable, these states provide the bifurcation-theoretic explanation for the origin of the observed states. In turbulent wall-bounded shear flows, these states have been hypothesized to be nodes organizing the trajectories within a chaotic attractor. Numerical computation of these flows must performed with Newton's method, or one of its generalizations, since time-integration cannot converge to unstable equilibria. The bottleneck is the solution of linear systems involving the Jacobian of the Navier-Stokes or Boussinesq equations. Originally such computations were carried out by constructing and directly inverting the Jacobian, but this is unfeasible for the matrices arising from three-dimensional hydrodynamic configurations in large domains.

A popular method is to seek states that are invariant under numerical time integration. However, equilibria may also be found by seeking flows that are invariant under a single very large Backwards-Euler Forwards-Euler timestep, much larger than those which can be used for time-integration. We show that this method, called Stokes preconditioning, is 10 to 50 times faster than the multiple timestep method at computing steady states in plane Couette flow and traveling waves in pipe flow. Moreover, it can be carried out without any changes to previously existing time-integration codes. We explain the convergence

rate as a function of the integration period and Reynolds number by computing the full spectra of the operators corresponding to the Jacobians of both methods and we propose extensions that may be used for flows in which the Coriolis force or the advective terms dominate.

Beyond Blow-up

André Weideman

Stellenbosch University

Finite time blow-up is a common occurrence in nonlinear differential equations. This presentation is a survey of numerical techniques for dealing with this, and in particular the computation of post-blow-up solutions. Two standard tricks are transformations (that is, converting the problem into one with bounded solutions), and deformation of the path of integration into the complex plane in order to bypass the singularity. Model problems include members of the Painlevé family and a nonlinear heat equation with quadratic forcing term.

What can the square root approximation problem teach us?

Heather Wilber

UT Austin

In the last few decades, there has been a surge of new developments in computational rational approximation. We explore some of these exciting new ideas by focusing on a single famous problem, the rational approximation of the square root function. This problem goes back to at least ancient Babylon, and yet it still has plenty to teach us about central questions in computational mathematics. The problem serves as a useful springboard for investigating what is possible with effective tools for constructing and computing with rational approximations to functions, and it also arises naturally in several fundamental tasks related to the evaluation of functions of matrices and operators. We highlight new results related to these tasks, including a new method for solving certain partial differential equations that combines rational approximation at the operator level with powerful, high-accuracy direct solvers (such as the hierarchical Poincaré Steklov method).

List of Abstracts – Contributed Speakers

Monday, 14th August

A multigrid proximal gradient method for nonsmooth convex optimisation

Andersen Ang

University of Southampton

We study the combination of proximal gradient descent with multigrid for solving a class of possibly nonsmooth strongly convex optimization problems. We propose a multigrid proximal gradient method called MGProx, which accelerates the proximal gradient method by multigrid, based on utilizing hierarchical information of the optimization problem. MGProx applies a newly introduced adaptive restriction operator to simplify the Minkowski sum of subdifferentials of the nondifferentiable objective function across different levels. We provide a theoretical characterization of MGProx. First we show that variables at all levels exhibit a fixed-point property at convergence. Next, we show that the coarse correction is a descent direction for the fine variable in the general nonsmooth case. Lastly, under some mild assumptions we provide the convergence rate for the algorithm. In the numerical experiments, we show that MGProx has a significantly faster convergence speed than proximal gradient descent and proximal gradient descent with Nesterov's acceleration on nonsmooth convex optimization problems such as the Elastic Obstacle Problem.

On Trigonometric Interpolation in an Even Number of Points

Anthony Austin

Naval Postgraduate School

In contrast to odd-length trigonometric interpolants, even-length trigonometric interpolants need not be unique; this is apparent from the representation of the interpolant in the (real or complex) Fourier basis, which possesses an extra degree of freedom in the choice of the highest-order basis function in the even case. One can eliminate this

degree of freedom by imposing a constraint, but then the interpolant may cease to exist for certain choices of the interpolation points. On the other hand, the Lagrange representation developed by Gauss always produces an interpolant despite having no free parameters. We discuss the choice Gauss's formula makes for the extra degree of freedom and show that, when the points are equispaced, its choice is optimal in the sense that it minimizes both the standard and 2-norm Lebesgue constants for the interpolation problem. For non-equispaced points, we give numerical evidence that Gauss's formula is no longer optimal and consider interpolants of minimal 2-norm instead. We show how to modify Gauss's formula to produce a minimal-norm interpolant and that if the points are equispaced, no modification is necessary.

Golub-Kahan-Lanczos Bidiagonalization (GKLB) Methods for Computing Singular Triplets for Very Large Sparse Matrices and Applications

James Baglama

University of Rhode Island

There are numerous GKLB based methods for finding a few of the largest (smallest) singular triplets for very large sparse matrices, and one of the most popular being the efficient thick-restarted GKLB algorithm often referred to as IRLBA (Baglama and Reichel, 2005). The ubiquitousness of the IRLBA method has lead to numerous implementations in programming languages R, Python, MATLAB syntax, and C++. Moreover, starting in 2016, the MATLAB internal function svds.m references (based) on IRLBA. In this presentation, we will provide a review of IRLBA, along with recently developed updates, a hybrid version, and a unique option to explicitly deflate in the GKLB (and IRLBA) process to compute the next set of largest singular triplets of a matrix from an already computed partial singular value decomposition (Baglama and Perovic, 2023). The hybrid version leverages a new idea, iterative refined Ritz vectors, where we replace the approximate singular values in the original refined scheme with the latest computed refined Ritz value until convergence. Several criteria are used to determine which restarted process is to be used. We will also present several numerical examples and an application to singular value thresholding.

Rational sinc interpolants and point shifts

Jean-Paul Berrut

Université de Fribourg

The interpolation of functions with steep gradients is greatly improved by putting more points in the vicinity of these gradients. In pseudospectral methods, a conformal map of

the domain is used for that purpose and usually introduced into the polynomials replacing the functions appearing in the differential equation. The exponential convergence is conserved. However, because of the use of the chain rule, this leads to complicated differentiation matrices. To avoid this, the first two authors have suggested in 2001 to use a linear rational barycentric interpolant instead of the usual polynomial one when solving a differential equations on an interval. Differentiation formulas as simple as those of the interpolating polynomial lead to systems that are themselves as simple as those of the classical polynomial pseudospectral method. The first author has adapted the method to the (Fourier) periodic case. Here we treat the case of the infinite line, replacing the sinc interpolant with a linear rational sinc one, and we show that here as well the exponential convergence is conserved with the conformal map. We also demonstrate through numerical examples how point shifts greatly improve the interpolant's accuracy when approximating functions with steep gradients.

A new Legendre polynomial-based approach for non-autonomous linear ODEs

Niel Van Buggenhout

Charles University

In nuclear magnetic resonance spectroscopy a sample is placed into a time-varying magnetic field, the behavior of the nuclear spins inside this sample can be described by an ODE. For a smooth matrix valued function $H(t)$, the Hamiltonian of the system, and the identity matrix I, this ODE is

$$\frac{d}{dt}U(t) = H(t)U(t), \qquad U(-1) = I, \qquad t \in [-1, 1]\,.$$

Using a convolution-like product between bivariate functions, a new analytical expression for the solution $U(t)$ can be formulated. The bivariate functions arise from the fact that in this framework the matrix valued function must be cast into the form $H(t)\Theta(t-s)$, where $\Theta(t-s)$ is the Heaviside step function. Whereas other expressions, e.g., the Magnus expansion, do not perform well for large-to-huge matrices $H(t)$, this new expression might be suitable to tackle these challenging problems.

Computing the solution analytically is complicated, therefore we propose a numerical method based on discretizing the convolution-like product. The discretization uses Legendre polynomials as a basis, the bivariate functions can then be represented by an infinite matrix of expansion coefficients.

In this talk we discuss the scalar case, i.e., where $H(t)$ is a function, understanding this case is paramount to developing a method for the matrix case. We show that the expression for $U(t)$ corresponds to solving an infinite system of equations. Thanks to the

off-diagonal decay structure in the coefficient matrices, the system can be truncated to a finite system of equations, which can be solved using standard linear algebra techniques. We show numerical experiments which illustrate the spectral accuracy of our method and by looking at pseudospectra of the coefficient matrix we try to explain its numerical behavior.

Krylov Subspace Recycling For Matrix Functions

Liam Burke

Trinity College Dublin

We discuss a new augmented Krylov subspace method which allows for the efficient evaluation of a sequence of matrix function applications on a set of vectors using Krylov subspace recycling. If selected appropriately, the recycling subspace can be used to accelerate the convergence of each problem in the sequence, leading to an overall reduction in the computational overhead required to evaluate the full sequence of function applications, in comparison to standard Krylov subspace methods. We present results of numerical experiments demonstrating the effectiveness of the method using examples from practical applications such as Quantum Chromodynamics.

Corner cases of the generalized tau method

Keaton Burns

MIT

It is now well understood how to produce banded spectral discretizations of many PDEs using Petrov-Galerkin methods with orthogonal polynomials. One of the primary remaining challenges to building fully automatic fast spectral solvers is incorporating arbitrary boundary conditions. For domains with a single bounded dimension (e.g. an annulus or spherical shell), this can be reliably achieved with rectangular collocation or the ultraspherical method, among others. For domains with multiple bounded dimensions (e.g. closed squares and cubes), consistency conditions at the corners and shared edges pose a challenge, particularly with mixed boundary conditions. Here we will discuss a generalized tau scheme where analytic perturbations are added to the PDEs and boundary conditions that result in consistent and exactly solvable discrete systems. In particular, we will examine the Poisson equation with generic mixed boundary conditions on the square and cube, but the results extend to general elliptic equations on hypercubes. These tau-perturbed systems can be easily modified to use different test, trial, and tau spaces and satisfy the full (hyper)octahedral symmetries of the domain, making them particularly favorable for incorporation into spectral element schemes.

Rational Function Approximation as Constrained Optimization

James Chok

University of Edinburgh

Function approximation traditionally writes the target function as a linear combination of a set of basis functions $\{P_n(x)\}$. However, when written as a rational function with an n-degree polynomial divided by an m-degree polynomial, it gives an approximation as good as using $n + m$ basis functions. Rational functions have the added benefit of providing better approximations to non-smooth functions. We propose a new method for rational function approximation. Using Bernstein Polynomials, we pose the problem as a constrained optimization problem, which is solved approximately using a computationally cheap iteration scheme. We also present preliminary approximation bounds.

Split-step methods with finite difference schemes and analytic continuation formulas

Jorge Cisneros

UT Austin

Finite difference schemes provide a popular and intuitive approach to numerically solve nonlinear initial-boundary value problems (IBVPs). Often, this leads to the introduction of ghost points, where the numerical method depends on grid points outside of the working domain. The usual heuristics of doing this for second-order problems do not generalize to higher order, and incorporating boundary conditions and addressing ghost points is a serious numerical issue. Our approach tackles this problem by the implementation of split-step methods to separately solve the linear and nonlinear problems. In this talk, I will present the Unified Transform Method (UTM), introduced by A. S. Fokas, and how it is used to solve initial-boundary value problems for linear IBVPs. The UTM solution representations are then treated to give analytic continuation formulas that can be applied at ghost points in the split-step method. We present our developments via the application to the nonlinear Schrödinger equation on the finite interval. We discuss the continuum limit of the solutions and numerical results. This is joint work with Bernard Deconinck.

Computation and Certification of the Pseudospectral Boundary

Catherine Drysdale

University of Birmingham

The pseudospectrum is a well-established tool for the analysis of linear operators often demonstrating important factors such as the sensitivity to perturbation of the eigenvalues [1]. Efficient calculation of the pseudospectrum for unbounded operators in infinite dimensional spaces is a relatively unexplored territory. Often finite-dimensional subspaces are used in place of the infinite dimensional space. However, the use of finite dimensional subspaces changes the qualitative nature of pseudospectral contours from unbounded curves with asymptotic behaviour at infinity to closed loops. The overlap between these curves forms the well-resolved of the pseudospectrum, meaning parts of the spectrum with no spectral pollution. Therefore, it is useful to have a certification process for these calculated points. Especially, when computations on finite domains are used to support asymptotic results. In this talk, we demonstrate an adaptive method to reliably follow the boundary points of the pseudospectrum of the operator. We test this method on a simple, yet challenging model that has been used to explore the dynamics of thin film of viscous fluid on the interior surface of a rotating cylinder [2] where the pseudospectra contours are expected to be parabolic with respect to the imaginary axis.

This joint work with Lyonell Boulton.

[1] L. N. Trefethen and M. Embree, Spectra and Pseudospectra, Princeton University Press, Princeton and Oxford, 2005.

[2] Journal of Fluid Mechanics, Volume 497, 25 December 2003, pp. 201 - 224.

Time-dependent Steklov–Poincaré operators and space-time Robin–Robin decomposition for the heat equation

Emil Engström

Lund University

Domain decomposition methods are a set of widely used tools for parallelization of PDE solvers. The elliptic case is well studied, but there are few convergence results for parabolic equations, especially in the weak space-time setting. The aim of this work is to construct a framework for analyzing domain decomposition methods for parabolic equations in a weak space-time formulation, inspired by recent studies in space-time discretization methods. The framework is based on the same principles as the elliptic case, namely studying the properties of the corresponding Steklov–Poincaré operators. Important properties of these operators are derived and used to show that three common domain decomposition methods are well defined. Finally we prove convergence of the Robin–Robin method in this new framework. This is a joint work with Eskil Hansen.

Interpolating through resonances with rational functions

Daniel Fortunato

Flatiron Institute

Reduced-order modeling is a powerful technique for amortizing the cost of solving many parameter-dependent PDEs across a range of parameter values. However, when the parameter space contains values that put the PDE at or near resonance, polynomial interpolation between solutions can catastrophically fail. In this talk, we explore how rational approximations and the AAA algorithm may be used to efficiently interpolate between solutions of parameter-dependent PDEs in the presence of resonances.

Interpolating Continuous Functions on the Unit Hypercube

Ben Goodrich

Columbia University

Let y be a real-valued continuous function of a vector of $n \geq 2$ variables, $\mathbf{x} \in [0,1]^n$. Kolmogorov's (1963) Superposition Theorem (KST) claims that every such y can be expressed exactly using a finite number of additions of compositions of univariate functions, but researchers have only be able to explicitly construct Hölder continuous versions of the unknown functions. Fridman (1967) and Sprecher (1970) prove that the KST can be satisfied with unknown functions that are Lipschitz continuous but lack a first derivative at some points. Actor (2018) came close to making Fridman and Sprecher's vision of a Lipschitz continuous KST a reality in floating-point software but was unable to achieve a computationally practical implementation using a sequence of piecewise linear functions. Our approach differs in that we define the unknown Lipschitz continuous function in Sprecher's (1970) variant of the KST via its Chebyshev expansion and attempt to choose a generating function for the coefficients that satisfies the jointly sufficient conditions for a KST. Our construction is numerically sound because it uses the same principles as Chebfun, but it remains to be shown analytically that it allows the KST to be satisfied. One of Trefethen's former students claimed in Montanelli and Yang (2020, p.6) that "If we were able to construct a Lipschitz continuous inner function [in the KST], we would be able to obtain estimates" of y whose upper bound to the approximation error does not depend on n. We conjecture that the unknown univariate inner function in the KST has a Chebyshev interpolant of the form

$$\frac{3 + 4/8^{k+1}}{7} + \sum_{j=0}^{k} \frac{1}{2^{3(j+1)-2}} T_{2^j}(x)$$

which is admissible for any finite k and we intend to show it can satisfy the KST as $k \uparrow \infty$.

Direct solution of equations in large-scale linear optimization

Julian Hall

University of Edinburgh

The performance of simplex and interior point method implementations when solving linear programming and quadratic programming problems is largely dependent on the efficiency with which linear systems of equations can be solved. This talk will discuss modern techniques for solving unsymmetric systems for simplex implementations, plus symmetric positive definite and quasidefinite systems generated by interior point method implementations. There will be a particular emphasis on the scope for exploiting parallel computing. The setting for the work is the world's leading open-source linear optimization software, HiGHS.

Rectangular eigenvalue methods

Behnam Hashemi

University of Leicester

We consider ODE and PDE eigenvalue problems and discuss latest developments on the numerical methods that involve quasimatricres and rectangular matrices. Assuming eigenfunctions are well-approximated by the column space of a quasimatrix or a rectangular matrix, we use a least-squares framework to compute expansion coefficients of the eigenfunctions. The focus is on the flexibility and strength of the methods proposed in a joint work with Nakatsukasa (SISC 2022), and with Nakatsukasa and Trefethen (ACOM, 2022). We present numerical results for solving several ODE and PDE eigenvalue problems on different domains.

Convergence analysis of the nonoverlapping Robin–Robin method for nonlinear elliptic equations

Eskil Hansen

Lund University

The nonoverlapping Robin–Robin method is commonly encountered when discretizing elliptic equations, as it enables the usage of parallel and distributed hardware. Convergence has been derived in various linear contexts, but little has been proven for nonlinear equations. In this talk we present a convergence analysis for the Robin–Robin method applied to nonlinear elliptic equations with a p-structure, including degenerate diffusion

equations governed by the p-Laplacian. The analysis relies on a new theory for nonlinear Steklov–Poincaré operators based on the p-structure and the L^p-generalization of the Lions–Magenes spaces. This framework allows the reformulation of the Robin–Robin method into a Peaceman–Rachford splitting on the interfaces of the subdomains, and the convergence analysis then follows by employing elements of the abstract theory for monotone operators. This is joint work with Emil Engström (Lund university)

Efficient numerical linear algebra for large-scale PDE-constrained optimization problems

Bernhard Heinzelreiter

Maxwell Institute in Edinburgh

PDE-constrained optimization problems arise in various applications in industry and can also be useful in other mathematical fields. Applications can be found in physics, e.g. flow control, chemistry, e.g. control of reaction-diffusion processes, biology, medical imaging, optimal transport, and many others. Due to the lack of analytical solutions to these problems in general, the fast and robust numerical solution is of utmost importance. However, their discretization often results in huge-scale systems of linear or possibly also non-linear equations. Black-box solvers, such as direct solvers for linear systems, often fail when applied to these systems. In order to make them feasible, information about the systems themselves and the structure of the PDEs has to be taken into account. During the previous years, preconditioned iterative methods have already been successfully applied to PDE-constrained optimization problems (see for example [4, 3, 2]).

In this talk, we will discuss some recent developments to mitigate the issues associated with solving the huge-scale systems for obtaining accurate solutions. These include a sequential homotopy method, based on that derived in [5] for general nonlinear constrained optimization problems, which we apply to the optimization of distributed PDE systems, making use of a preconditioning strategy to enable real-time optimization of the controller. Further, in the linear quadratic case of time-dependent control problems, we consider a method for solving the integro-differential Riccati equation for obtaining feedback controls, which combines a reformulation of the equation, the approach of [1], and an efficient numerical method in order to achieve fast converging solutions.

[1] Helmut Harbrecht and Ilja Kalmykov. “Sparse Grid Approximation of the Riccati Operator for Closed Loop Parabolic Control Problems with Dirichlet Boundary Control”. SIAM Journal on Control and Optimization 59.6 (Jan. 2021), pp. 4538–4562. issn: 0363-0129. doi: 10.1137/20M1370604.

[2] John W. Pearson and Martin Stoll. “Fast iterative solution of reaction-diffusion control

problems arising from chemical processes". SIAM Journal on Scientific Computing 35.5 (2013). issn: 10648275. doi: 10.1137/120892003.

[3] John W. Pearson and Andrew J. Wathen. "A new approximation of the Schur complement in preconditioners for PDE-constrained optimization". Numerical Linear Algebra with Applications 19.5 (2012). issn: 10705325. doi: 10.1002/nla.814.

[4] John W. Pearson and Andrew J. Wathen. "Fast iterative solvers for convection-diffusion control problems". Electronic Transactions on Numerical Analysis 40 (2013). issn: 10689613.

[5] Andreas Potschka and Hans Georg Bock. "A sequential homotopy method for mathematical programming problems". Mathematical Programming 187.1-2 (2021). issn: 14364646. doi: 10.1007/s10107-020-01488-z.

Parallel-in-time solvers for the all-at-once Runge–Kutta discretization

Santolo Leveque

Scuola Normale Superiore

Time-dependent PDEs arise very often in many scientific areas, such as mechanics, biology, economics, or chemistry, just to name a few. Of late, many researchers have devoted their effort in devising parallel-in-time methods for the numerical solution of time-dependent PDEs. As opposed to the classical approach, in which an approximation of the solution at a time t is computed by a sequential time-stepping, parallel-in-time methods approximate the solution of the problem for all times concurrently. This in turns adds a new dimension of parallelism and allows to speed-up the numerical solution on modern supercomputers.

In this talk, we present a fully parallelizable preconditioner for the all-at-once linear system obtained when employing a Runge–Kutta method in time. The resulting system is solved iteratively for the numerical solution and for the stages of the method. By employing classical theory of block matrices, one is able to derive an optimal preconditioner for the system considered. This results in a block-diagonal solve for all the stages at all the time-steps, and a Schur complement obtained by solving again systems for the stages of the method. Since at each linear iteration one has to solve for the latter system, we introduce a new block-preconditioner based on the SVD of the (real) Runge–Kutta coefficient matrix $A_{\mathrm{RK}} = U\Sigma V^{\top}$.

A range of numerical experiments validate the robustness of the preconditioner with respect to the discretization parameters and to the number of stages, as well as very

promising scalability and parallel efficiency indices.

Joint work with Luca Bergamaschi (University of Padua), Ángeles Martínez (University of Trieste), and John W. Pearson (University of Edinburgh).

Nearest Neighbor Sampling of Point Sets using Random Rays

Colin Macdonald

University of British Columbia

We propose a framework for the sampling, compression, and analysis of distributions of point sets and other geometric objects embedded in Euclidean spaces. Nearest neighbours of points on a set of randomly-selected "rays" (line segments) are recorded, forming a "signature" of the data. From this signature, statistical information about the data set, as well as certain geometrical information, can be extracted. We present some illustrating examples of the proposed sampling strategy, including registration and point-cloud classification. This is joint work with Lewis Liu, Louis Ly, and Richard Tsai. This project is also related to the numerical solution of PDEs using the closest point methods, developed during my time at Oxford.

S-Step and Flexible Enlarged Conjugate Gradient Methods

Sophie Moufawad

American University of Beirut

In [2], a new approach for reducing communication in Krylov subspace methods was introduced. It consists of enlarging the Krylov subspace by a maximum of t vectors per iteration, based on a domain decomposition of the graph of A. Therefore, the approximate solutions of the system $Ax = b$ are sought from the enlarged Krylov subspace, which is a superset of the Krylov subspace. Several enlarged conjugate gradient versions that converge faster than CG in terms of iterations were introduced, such as MSDO-CG and SRE-CG. To further speedup the parallel runtime, the s-step enlarged CG versions [1] are presented, whereby s iterations of the enlarged CG methods are merged into one iteration, by performing denser operations that require less communications when parallelized. The s-step enlarged CG methods, similarly to the enlarged CG methods, converge faster than classical CG in terms of iterations, but require much more memory per iteration. Thus, we explore different options for reducing the memory requirements of these enlarged CG methods, without affecting much their convergence. This leads to the flexible enlarged CG versions, where at some iteration the maximum number of introduced basis vectors is halved. Convergence results are presented.

[1] *S-Step Enlarged Krylov Subspace Conjugate Gradient methods*, SIAM Journal on Scientific Computing, 42:1, pp. A187-A219, 2020.

[2] L. Grigori and S. Moufawad and F. Nataf. *Enlarged Krylov Subspace Conjugate Gradient methods for Reducing Communication.* SIAM Journal on Matrix Analysis and Applications, 37:2, pp. 744-773, 2016.

Sparse hp-FEM with p up to a billion

Sheehan Olver

Imperial College London

A longstanding open problem is hp methods where the complexity is optimal in both h and p, even in the deceptively simple 1D case. Beuchler & Schoeberl (2006) introduced a p-FEM method in 2D/3D for triangular/tetrahedral meshes, based on orthogonal polynomials in simplices, which results in very sparse discretisations. By reducing their construction back to 1D an amazing thing happens: the Cholesky decomposition of the resulting discretisations almost completely decouples across elements, in a way that is both ridiculously parallelisable and also achieves optimal complexity with h and p, allowing us to scale up to extremely high orders (as high as a billion!). This can be adapted to higher dimensions on ball-annuli elements using semiclassical orthogonal polynomials and tensor products using ADI a la Fortunato & Townsend (2020), albeit with p not quite a billion (perhaps 10k in 2D and 1k in 3D).

Sparse hp-FEM and spectral methods for the Helmholtz equation posed on disks and annuli via generalized Zernike annular polynomials

Ioannis Papadopoulos

Imperial College London

Recently, factorization techniques were introduced for computing with hierarchies of semiclassical Jacobi polynomials with (quasi) optimal complexity. Such hierarchies allow one to quickly build generalized families of multivariate orthogonal polynomials (in Cartesian coordinates) for higher dimensions: namely Zernike polynomials for the disk and Zernike annular polynomials for the annulus. With these generalized families at hand, one may construct sparse and very high order hp-FEM and spectral element methods for both the strong and weak forms of the Helmholtz equation. The cells are an innermost disk (omitted if the domain is an annulus) and concentric annuli. With both methods, the Fourier modes decouple and may be solved in parallel. In the case of the hp-FEM method,

the discretization matrix is symmetric positive-definite (for the positive-definite Helmholtz equation) and the solve scales with linear complexity. We demonstrate the effectiveness of these methods on various problems including PDEs with variable coefficients and data with discontinuities in the radial direction.

An adaptive one-step block method for integrating reaction-diffusion Brusselator system

Mufutau Ajani Rufai

Free University of Bozen-Bolzano

In this talk, a variable stepsize formulation of a new one-step block method will be proposed and efficiently used for solving reaction-diffusion Brusselator differential systems using large integration intervals. The basic properties of the new method will be theoretically analyzed. The proposed method will be implemented in an adaptive mode by adapting the number and position of the nodes utilized in the approximation to ensure that the truncation error is kept within a specified bound. The reliable and accurate performance of the introduced method will be observed based on reasonable error estimation and adaptive strategy presented in this talk. Some of the reaction-diffusion Brusselator real-life model problems will be numerically solved to evaluate the performance and efficiency of the proposed method.

Greedy rational interpolation and continued fractions

Oliver Salazar Celis

ING Belgium

One of the features of the AAA algorithm is the greedy selection of the interpolation points. We give an interpretation of this greedy selection for rational interpolation in terms of the table of rational interpolants. It turns out that the obtained ordering from such a selection necessarily implies (as implicitly intended) that two successive rational interpolants on a diagonal staircase path in that table are different. The tool used to show this are Thiele continued fractions. An additional consequence of this result is that the recursive construction of these continued fractions will not break down when combined with the greedy selection. We illustrate the remarkable accuracy of these continued fractions when constructed in this way, including best approximations and the calculation of poles and zeros.

Manifold-Free Riemannian Optimization

Boris Shustin

Tel Aviv University

Optimization problems constrained on smooth manifolds can be solved via the framework of Riemannian optimization. To that end, a geometrical description of the constraining manifold, e.g., tangent spaces, retractions, and cost function gradients, is required. In this talk, we present a novel approach that allows performing approximate Riemannian optimization based on a manifold learning technique, in cases where only a noiseless sample set of the cost function and the manifold's intrinsic dimension are available.

Polynomial and rational measure modifications of orthogonal polynomials via infinite-dimensional banded matrix factorizations

Richard Mikael Slevinsky

University of Manitoba

We describe fast algorithms for approximating the connection coefficients between a family of orthogonal polynomials and another family with a polynomially or rationally modified measure. The connection coefficients are computed via infinite-dimensional banded matrix factorizations and may be used to compute the modified Jacobi matrices all in linear complexity with respect to the truncation degree. A family of orthogonal polynomials with modified classical weights is constructed that support banded differentiation matrices, enabling sparse spectral methods with modified classical orthogonal polynomials.

A Feasible method for linearly constrained convex SDP problems

Kim-Chuan Toh

National University of Singapore

In this work, we consider the low rank decomposition (SDPR) of general convex semidefinite programming problems (SDP) that contain both a positive semidefinite matrix and a nonnegative vector as variables. We develop a rank-support-adaptive feasible method to solve (SDPR). The method is able to escape from a saddle point to ensure its convergence to a global optimal solution for generic constraint vectors. We prove its global convergence and local linear convergence without assuming that the objective function is twice differentiable. The iteration complexity of our algorithm is better than previous results in the literature. In order to overcome the degeneracy issues of SDP problems, we develop two strategies based on random perturbation and dual refinement. These techniques enable us to solve some primal degenerate SDP problems efficiently,

for example, Lovasz theta SDPs. Our work has extended the Riemannian optimization approach for solving SDP problems. Numerical experiments are conducted to verify the efficiency and robustness of our method.

The ADER approach for constructing very-high order schemes for approximating hyperbolic equations

Eleuterio Toro

University of Trento, Italy

Sixty years ago, the Russian mathematician Sergei Godunov introduced his method to solve the Euler equations of gas dynamics, thus creating the Godunov school of thought for the numerical approximation of hyperbolic conservation laws. The building block of the original first-order Godunov upwind method is the conventional piece-wise constant data Riemann problem. ADER is a fully discrete approach to construct high-order extensions of the Godunov first-order method, in which the conventional Riemann problem is replaced by the generalised Riemann problem GRPk, a piece-wise smooth data Cauchy problem in which the equations may include stiff source terms and k is the degree of the polynomials to represent the data. The ADER methodology operates in both the finite volume and the discontinuous Galerkin finite element frameworks. The schemes extend to systems with stiff or non-stiff source terms, in multiple space dimensions, on structured or unstructured meshes. The resulting schemes are of arbitrary order accuracy k+1 in both space and time; there is no theoretical accuracy barrier. There are by now several methods for solving the generalized Riemann problem, thus giving rise to several classes of ADER schemes. In numerous applications performed over the years it has been established that these schemes are orders-of-magnitude cheaper than low-order methods for attaining a prescribed, small error and are therefore mandatory for ambitious scientific and technological applications. Here I review some key aspects of the ADER methodology and discuss its strengths, shortcomings and issues of current research interest. Sample applications will be shown.

Generalising the classical tau method for fun and profit

Geoff Vasil

University of Edinburgh

The classical tau method for differential equations refers to solving an approximate system exactly over polynomials, instead of finding approximate solutions to exact ODEs & PDEs. While very similar, this distinction has practical consequences for the analysis and acquisition of solutions. Classical methods set the residual as the span of the highest

numerical basis elements. However, once an appropriate residual space is proscribed, a finite polynomial solution exists independent of any algorithm to obtain it. Chebyshev polynomials are excellent numerically, but even lowly monomials (however poorly conditioned in a computer) are fantastic for analysing solutions on paper. This talk will present some data on using a wider range of tau polynomials. We will show the dependence of eigenvalues on the choice of residual space, including the appearance of spurious spectrum and the accuracy of resolved modes. Finally, we will discuss systematic efforts to optimise performance by considering tau-corrections as oscillatory low-rank updates to differential operators.

Computation of 2D Stokes flows via lightning and AAA rational approximation

Yidan Xue

University of Oxford

Fluid flow at low Reynolds numbers is governed by the Stokes equations. In a recent study, Brubeck and Trefethen (2022) introduced a 'lightning' method to approximate Stokes flows using rational functions with poles exponentially clustered near corner singularities. In this work, we present a solver for computing 2D Stokes flows in smooth boundary and multiply-connected domains using lightning and AAA rational approximation. For smooth boundary problems, we show that the solver performance can be greatly improved by placing poles outside smooth boundaries using the AAA rational approximation (Nakatsukasa, Sète and Trefethen, 2018). In addition, we broaden the application of the solver to multiply-connected problems using a series method. We compute Stokes flows in several engineering-driven problems and validate our results against corresponding analytical solutions. Solutions to most problems are computed to at least 8-digit in a second. In conclusion, we present a solver suitable for computing most 2D Stokes flow problems. The speed and accuracy of this solver to several engineering problems have been shown. As a 'ten digit algorithm' (Trefethen, 2005), one can adapt it to their Stokes flow problems and obtain high-accuracy solutions easily. We believe this work will have a broad impact in both numerical analysis and fluid mechanics.

Tuesday, 15th August

Finite Difference formulation of any lattice Boltzmann scheme: consistency, stability and convergence

Thomas Bellotti

CMAP, Ecole polytechnique, France

Lattice Boltzmann schemes rely on the enlargement of the size of the target problem to approximate the solution of PDEs in a highly parallelizable and efficient kinetic-like fashion, split into collision and stream phases. This structure, despite the well-known advantages from a computational standpoint, is not suitable to construct a rigorous notion of consistency with respect to the target equations and to provide a precise notion of stability. Partly due to this reason, lattice Boltzmann schemes have historically been largely overlooked by numerical analysts, though they are a source of many interesting theoretical questions. To alleviate these shortages and introduce a rigorous framework, we demonstrate that any lattice Boltzmann scheme can be rewritten as a corresponding multi-step Finite Difference scheme on the conserved variables at the fully discrete level. This is achieved by devising a suitable formalism based on operators, commutative algebra and polynomials. Therefore, the notion of consistency of the corresponding Finite Difference scheme allows to invoke the Lax-Richtmyer theorem in the case of linear lattice Boltzmann schemes. Moreover, we show that the frequently-used von Neumann-like stability analysis for lattice Boltzmann schemes entirely corresponds to the von Neumann stability analysis of their Finite Difference counterpart. More generally, the usual tools for the analysis of Finite Difference schemes are now readily available to study lattice Boltzmann schemes. Their relevance is verified through numerical illustrations. Overall, this contribution shows that lattice Boltzmann schemes are indeed objects germane to the framework of Numerical Analysis. Bellotti T., Graille B., Massot M. - Finite Difference formulation of any lattice Boltzmann scheme – Numer. Math. – 152, 1-40 (2022) Bellotti T. - Truncation errors and modified equations for the lattice Boltzmann method via the corresponding Finite Difference schemes - ESAIM: M2AN, In Press (https://doi.org/10.1051/m2an/2023008) Bellotti T. - Initialisation from lattice Boltzmann to multi-step Finite Difference methods: modified equations and discrete observability – Submitted (https://arxiv.org/abs/2302.07558)

The continuum AAA-LS algorithm and applications

Stefano Costa

The IEEE

The AAA-LS algorithm has a continuous counterpart, which allows for greater computational efficiency and speed, as well as domains bounded with generic parametric arcs. Some examples are presented that illustrate how it can be implemented, with applications ranging from conformal maps to physical electric and magnetic models.

Fine-grained Theory and Hybrid Algorithms for Randomized Numerical Linear Algebra

Anil Damle

Cornell University

Randomized algorithms have gained increased prominence within numerical linear algebra and they play a key role in an ever-expanding range of problems driven by a breadth of scientific applications. In this talk we will explore two aspects of randomized algorithms by (1) providing experiments and accompanying theoretical analysis that demonstrate how their performance depends on matrix structures beyond singular values (such as coherence of singular subspaces), and (2) showing how to leverage those insights to build hybrid algorithms that blend favorable aspects of deterministic and randomized methods. A broad range of randomized algorithms will be considered, relevant motivating applications will be discussed, and numerical experiments will illuminate directions for further research.

Ieva Daužickaitė

Charles University

We consider the solution of a least-squares problem $\min_x \|bAx\|_2$ via GMRES based iterative refinement with randomized preconditioning. Randomized techniques can give effective preconditioners for dense least-square problems and require randomly sketching the coefficient matrix to obtain a smaller representation and then computing its deterministic factorisation. The process can be made more efficient by using a mixed precision framework, where different steps of the algorithm are performed in different precisions. Caution is needed when choosing the precisions so that we acquire a final solution of a required accuracy. In this work, we consider a preconditioner coming from a QR factorization of the sketched coefficient matrix. We theoretically analyse how the preconditioner and the convergence of iterative refinement is affected by performing expensive computations in low precisions and illustrate it numerically linear optimization software, HiGHS.

ESPIRA for recovery of exponential sums and its application

Nadiia Derevianko

University of Göttingen

We introduce a new method – ESPIRA (Estimation of Signal Parameters by Iterative

Rational Approximation) – for the recovery of complex exponential sums (see *Derevianko, Plonka, and Petz, (2022) IMA Journal of Numerical Analysis*). Our new recovery procedure is based on the observation that Fourier coefficients of exponential sums have a special rational structure. To reconstruct this structure in a stable way we use the AAA algorithm for rational approximation (see *Nakatsukasa, Sète, and Trefethen, (2018) SIAM J. Sci. Comput.*). During the talk we will present results regarding application of the AAA algorithm to this special recovery problem. We need at least $2M + 1$ Fourier coefficients for the recovery of an exponential sum of order M. We show that the Fourier coefficients can be also replaced by DFT coefficients which makes the algorithm more suitable for applications. Furthermore we show that ESPIRA can be interpreted as a matrix pencil method applied to Loewner matrices, special construction of which via an adaptive selection of index sets stabilizes the matrix pencil method (MPM). During the talk we will demonstrate that ESPIRA strongly outperforms Prony-type methods such as ESPRIT and MPM for noisy data and for signal approximation by short exponential sums.

Semi-Infinite Linear Regression and Its Applications

Paz Fink Shustin

Tel-Aviv University

Finite linear least squares is one of the core problems of numerical linear algebra, with countless applications across science and engineering. Consequently, there is a rich and ongoing literature on algorithms for solving linear least squares problems. In this talk, we explore a variant in which the system's matrix has one infinite dimension (i.e., it is a quasimatrix). We call such problems semi-infinite linear regression problems. As we show, the semi-infinite case arises in several applications, such as supervised learning and function approximation, and allows for novel interpretations of existing algorithms. We explore semi-infinite linear regression rigorously and algorithmically. To that end, we give a formal framework for working with quasimatrices, and generalize several algorithms designed for the finite problem to the infinite case. Finally, we suggest the use of various sampling methods for obtaining an approximate solution.

On the Numerical Analysis of the Coupled Cluster Method in Quantum Computational Chemistry

Muhammad Hassan

Laboratoire Jacques-Louis Lions, Sorbonne Université

A central problem in quantum chemistry is the computation of the eigenvalues of the

electronic Hamiltonian– an unbounded, self-adjoint operator acting on a Hilbert space of antisymmetric functions. The main difficulty in the resolution of this problem is the extremely high dimensionality of the eigenfunctions, being functions of at least 3N variables where N denotes the number of electrons in the system. A popular approach to deal with this complexity is to use a non-linear ansatz to represent the sought-after eigenfunction. This has led to the development of the density matrix renormalization group (DMRG), in which the ansatz consists of a tensor train, and the coupled cluster methodology, in which the ansatz consists of a so-called exponential cluster operator acting on a judiciously chosen reference state. The latter methods are regarded as the 'gold standard' in quantum chemistry for certain molecular systems. Surprisingly, however, despite the huge representation of computational chemistry in high performance and supercomputing resource usage, there is a dearth of rigorous numerical analysis for these methodologies. The goal of this talk is to present a new a priori analysis for the standard version of the coupled cluster approach, namely, the single-reference coupled cluster method. Under the minimal assumption that the sought-after eigenvalue is non-degenerate and the associated eigenfunction is not orthogonal to a chosen reference, we prove that the continuous coupled cluster equations are always locally well-posed. Under the same minimal assumption and provided that the discretisation is fine enough, we prove that certain classes of discrete coupled cluster equations are also locally well-posed, and we derive residual-based error estimates with guaranteed positive constants. This is joint work with Yvon Maday and Yipeng Wang (Sorbonne Université).

Accuracy and stability in molecular dynamics with constraints

Carl Christian Kjelgaard Mikkelsen

Umeå University

In molecular dynamics with constraints the main task is to integrate a system of differential algebraic equations of the form

$$\dot{q} = v, \tag{0.1}$$
$$Mv = f(q) - G(q)^T \lambda, \tag{0.2}$$
$$g(q) = 0, \tag{0.3}$$

where (q, v) represents the position and velocity of all atoms, M is a diagonal and nonsingular mass matrix, g is the constraint function, G is Jacobian of g. The standard algorithm for this problem is the SHAKE algorithm:

$$v_{k+\frac{1}{2}} = hM^{-1}(f(q_k) - G(q_k)^T \lambda_k), \tag{0.4}$$
$$q_{k+1} = q_k + hv_{k+\frac{1}{2}}, \tag{0.5}$$
$$g(q_{k+1}) = 0. \tag{0.6}$$

Here $q_k \approx q(t_k)$ and $v_{k+\frac{1}{2}} \approx v(t_{k+\frac{1}{2}})$, where $t_k = kh$ and $t_{k+\frac{1}{2}} = (k+1/2)h$. In general, equation (0.6) is a nonlinear equation for the Lagrange multiplier, i.e.,

$$g(\phi_k(\lambda)) = 0, \quad \phi_k(\lambda) = q_k + h(v_{k-\frac{1}{2}} + hM^{-1}(f(q_k - G(q_k)^T\lambda))). \qquad (0.7)$$

We explain the need for high accuracy when solving this equation. The state-of-the-art software is dominated by solvers that converge locally and linearly. We demonstrate that high accuracy and good hardware utilization can be achieved using a class of specialized sparse solvers that exploit the context. We discuss open questions and highlight the potential for accelerating in silico drug development and discovery in the future. This is joint work with Barcelona Supercomputing Center and Zaragoza University.

Uniform convergence of an arbitrary order balanced FEM applied to a singularly perturbed shell problem

Torsten Linß

FernUniversität in Hagen

Let y be a real-valued continuous function of a vector of $n \geq 2$ variables, $\mathbf{x} \in [0,1]^n$. Kolmogorov's (1963) Superposition Theorem (KST) claims that every such y can be expressed exactly using a finite number of additions of compositions of univariate functions, but researchers have only be able to explicitly construct H¨older continuous versions of the unknown functions. Fridman (1967) and Sprecher (1970) prove that the KST can be satisfied with unknown functions that are Lipschitz continuous but lack a first derivative at some points. Actor (2018) came close to making Fridman and Sprecher's vision of a Lipschitz continuous KST a reality in floating-point software but was unable to achieve a computationally practical implementation using a sequence of piecewise linear functions.

Our approach differs in that we define the unknown Lipschitz continuous function in Sprecher's (1970) variant of the KST via its Chebyshev expansion and attempt to choose a generating function for the coefficients that satisfies the jointly sufficient conditions for a KST. Our construction is numerically sound because it uses the same principles as Chebfun, but it remains to be shown analytically that it allows the KST to be satisfied.

One of Trefethen's former students claimed in Montanelli and Yang (2020, p.6) that "If we were able to construct a Lipschitz continuous inner function [in the KST], we would be able to obtain estimates" of y whose upper bound to the approximation error does not depend on n. We conjecture that the unknown univariate inner function in the KST has a Chebyshev interpolant of the form

$$\frac{3 + 4/8^{k+1}}{7} + \sum_{j=0}^{k} \frac{1}{2^{3(j+1)-2}} T_{2^j}(x)$$

which is admissible for any finite k and we intend to show it can satisfy the KST as $k \uparrow \infty$.

We study a boundary value problem that describes the bending of an axisymmetrically loaded thin shell. The thickness of the shell appears in the differential equation as a singular perturbation parameter. As a consequence layers form and must be resolved by the numerical scheme.

We show that the energy norm naturally associated with the standard weak formulation fails to capture the layers. Using an idea by Lin and Stynes [1], we devise an alternative variational formulation whos induced norm (a so called "balanced norm") is stronger. This is then discretised using arbitrary order conforming FEM. We proof convergence on a layer-adapted mesh that is robust with respect to the perturbation parameter.

This is joint work with Norbert Heuer, Pontificia Universidad Católica de Chile.

[1] R. Lin and M. Stynes. A balanced finite element method for singularly perturbed reaction-diffusion problems. *SIAM J. Numer. Anal.*, 50(5):2729–2743, 2012.

Are sketch-and-precondition least squares solvers numerically stable?

Maike Meier

University of Oxford

Sketch-and-precondition techniques are popular for solving large least squares (LS) problems of the form $Ax = b$ with $A \in \mathbb{R}^{m \times n}$ and $m \gg n$. This is where A is "sketched" to a smaller matrix SA with $S \in \mathbb{R}^{\lceil cn \rceil \times m}$ for some constant $c > 1$ before an iterative LS solver computes the solution to $Ax = b$ with a right preconditioner P, where P is constructed from SA. Popular sketch-and-precondition LS solvers are Blendenpik and LSRN. We show that the sketch-and-precondition technique is not numerically stable for ill-conditioned LS problems. Instead, we propose using an unpreconditioned iterative LS solver on $(AP)y = b$ with $x = Py$ when accuracy is a concern. Provided the condition number of A is smaller than the reciprocal of the unit round-off, we show that this modification ensures that the computed solution has a comparable backward error to the iterative LS solver applied to a well-conditioned matrix. Using smoothed analysis, we model floating-point rounding errors to provide a convincing argument that our modification is expected to compute a backward stable solution even for arbitrarily ill-conditioned LS problems. Joint work with Yuji Nakatsukasa, Alex Townsend, and Marcus Webb

The linear sampling method for random sources

Hadrien Montanelli

Inria & IP Paris

We present in this talk an extension of the linear sampling method for solving the sound-soft inverse acoustic scattering problem with randomly distributed point sources. The theoretical justification of our method is based on the Helmholtz–Kirchhoff identity, the cross-correlation between measurements, and the volume and imaginary near-field operators. Implementations in MATLAB using boundary elements, the SVD, Tikhonov regularization, and Morozov's discrepancy principle will also be discussed.

Numerical Shape Optimization with B-Spline Wavelets

Alberto Paganini

University of Leicester

The term shape optimization refers to searching for a domain that minimizes a given shape function, that is, a function that maps domain shapes to real numbers. Shape optimization problems can be tackled numerically by constructing a diffeomorphism that maps an initial guess to an approximately optimal solution. In this presentation, we discuss the pros and cons of constructing such diffeomorphisms using B-Spline wavelets. This is joint work with Prof. Ralf Hiptmair and Ren Ning.

Solving large linear least squares problems with equality constraints

Jennifer Scott

Rutherford Appleton Laboratory and University of Reading

Our interest is in solving large sparse linear least squares problems that are subject to one or more linear constraints that must be satisfied exactly. While some classical approaches are theoretically well founded, they can face difficulties when the matrix of constraints contains dense rows or if an algorithmic transformation used in the solution process results in a modified problem that is much denser than the original one. We propose a number of possible approaches with an emphasis on requiring that the constraints be satisfied with a small residual. Numerical experiments on problems coming from practical applications are used to demonstrate the effectiveness of the different ideas. This is joint work with Miroslav Tuma, Charles University, Prague.

An algorithm for the efficient evaluation of the Epstein zeta function on finite lattices

Kirill Serkh

University of Toronto

In this talk, we present an algorithm for rapidly evaluating a generalization of the Epstein zeta function, that describes oscillating multidimensional singular lattice sums, where summation is restricted to geometries with nontrivial boundaries. This function has wide reaching applications in condensed matter physics, describing boundary and finite size effects in the computation of long-range crystal forces and energies. The runtime of our algorithm is independent of the number of lattice points involved in the calculation. We illustrate the performance of our algorithm with several numerical experiments.

Uniform and unitary rational approximations of the matrix exponential

Pranav Singh

University of Bath

The exponential function maps the imaginary axis to the unit circle and for many applications this unitarity property is also desirable from its approximations. We show that this property is conserved not only by the (k,k)-rational interpolant of the exponential on the imaginary axis, but also by (k,k)-rational barycentric approximants that minimize a linearized approximation error. These results are a consequence of certain properties of singular vectors of Loewner-type matrices associated to linearized approximation errors. Prominent representatives of this class are rational approximants computed by the adaptive Antoulas–Anderson (AAA) method and the AAA–Lawson method. Our results also lead to a modified procedure with improved numerical stability of the unitarity property and reduced computational cost. Rational approximants generated by these approaches lead to an improved method for computing the matrix exponential of skew-Hermitian matrices, which has applications in the solutions of dispersive PDEs such as the Schrödinger equation. In particular, when the 'relevant' spectrum is small or split into smaller components, matrix exponential methods based on AAA and AAA–Lawson methods substantially outperform Padé approximants and global approximation methods such as Chebyshev based methods.

Efficient numerical linear algebra for Gaussian processes

Martin Stoll

TU Chemnitz

In this talk I will present some basic formulation that arise in the training of Gaussian processes. For large scale data sets this requires the solution of large linear systems. Additionally, we also need to estimate the trace of a function of a matrix, which is numerically challenging. Additionally, for efficient optimization methods to be efficient we accurately need to compute the gradients of the objective function, which again require the evaluation of matrix functions times a vector.

Parameter identification for the SIRD model using PDE-constrained optimisation

Andrés Miniguano Trujillo

Maxwell Institute for Mathematical Sciences

The standard Susceptible, Infected, Recovered, and Deceased model (SIRD) is a system of three compartments whose evolution is governed by a set of nonlinear ordinary differential equations. There are three parameters that capture the dynamics of the disease, namely the effective transmission rate β, the recovery rate , and the death rate m. The latter can often be estimated from clinical data, however the other two parameters represent a challenge for decision makers to understand the behaviour of a disease that can rapidly evolve. In this work, we present a PDE-constrained optimisation approach for learning the pair of parameters (β, γ) recovered from data. We present a first order optimality system and a numerical solution technique that allows a user to quickly recover the contact and recovery rates from a given set of observations. We will also present an extension of this work when spatial data is available.

Pseudospectra of generalized Schrödinger operators

Riko Ukena

TU Hamburg

Let A be a bounded linear operator on $\ell^p(\mathbb{Z})$. The minimum of

$$\nu(A) := \inf\{\|Ax\| : \|x\| = 1\} \tag{0.8}$$

and $\nu(A^*)$ is the inverse of the norm, $\|A^{-1}\|$, of the inverse of A. We approximate $\nu(A)$ by restricting the infimum (0.8) to elements $x \in \ell^p(\mathbb{Z})$ with support of diameter D, and we quantify the approximation error in terms of D. For the simple case of one-sided as

well as bi-infinite matrices,

$$H(b) \;=\; \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & * & \bullet & & & \\ \ddots & b_{-1} & * & \bullet & & \\ & + & b_0 & * & \bullet & \\ & & + & b_1 & * & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix},$$

with one varying diagonal (no matter which one) and finitely many constant diagonals (here simplified as $+$, $*$ and $\bullet$), considered as acting on $\ell^p(\mathbb{N})$, resp. $\ell^p(\mathbb{Z})$, we derive pseudospectral inclusions and Hausdorff-approximations, avoiding spectral pollution, purely by looking at the set of finite subwords of the potential b.

Tensor-based methods for the solution of overdetermined systems of polynomial equations

Raphaël Widdershoven

KU Leuven

Solving (overdetermined) systems of linear equations is an essential practice in many scientific disciplines, with well-established solution tools from numerical linear algebra. Extending these tools for systems of polynomial equations enables the solution of more complex problems. Current methods for these polynomial systems were typically not designed for engineering applications, where noise is present but additional equations are provided to compensate. Instead, these methods focus on square systems, which have a fixed number of roots (equal to the Bézout number), typically more than expected from the physical interpretation of the problem. We contribute to the development of tensor-based tools to handle the polynomial case, specifically for engineering applications. The method involves computing the nullspace of the so-called Macaulay matrix, from which it recovers the roots through a low-rank decomposition of a third-order tensor. In many practical cases, this method is guaranteed to retrieve all roots. Different algorithms for the low-rank decomposition are presented, especially useful in the case of noise. As a result, the method can take advantage of additional noisy equations to improve the estimates of roots. The practical utility is shown for a blind multi-source localisation problem where the position of two transmitters is estimated solely on the power received at an arbitrary configuration of antennas in their vicinity. Computing the nullspace of the Macaulay matrix is currently the bottleneck in the proposed method. We therefore additionally introduce an algorithm that reduces the asymptotic computational complexity from $O(d^6)$ to $O(d^5)$ and the memory complexity from $O(d^4)$ to $O(d^3)$, specifically for bivariate systems. It uses low displacement rank to transform the Toeplitz-block-(block-

)Toeplitz-structured Macaulay matrix into a Cauchy-like matrix, which is then decomposed in a rank-revealing LU-factorisation through the Schur algorithm.

Leveraging the AAA algorithm and the Hankel norm approximation in reduced-order modeling

Annan Yu

Cornell University

Large-scale linear, time-invariant (LTI) dynamical systems are widely used to characterize complicated physical phenomena. We propose a two-stage algorithm to reduce the order of a large-scale LTI system given samples of its transfer function for a target degree k of the reduced system. In the first stage, the adaptive Antoulas—Anderson (AAA) algorithm is used to construct a degree d rational approximation of the transfer function that corresponds to an intermediate system, which is then further reduced in the second stage using ideas from the theory on Hankel norm approximation (HNA). We study the numerical issues of a canonical HNA algorithm by Glover and provide a remedy for the numerical instabilities of the systems generated by HNA. We show that a carefully selected rational approximation of degree d gives us a numerically stable algorithm that is more efficient than SVD-based algorithms and more accurate than moment-matching algorithms.

High-Order-Integration for Regular Closed Surfaces

Gentian Zavalani

TU Dresden & Center for Advanced Systems Understanding (CASUS)

In this talk, we present high-order surface quadratures (HOSQ) approximating regular surface integrals on closed surfaces. HOSQ rests on curved surface triangulations realised due to k^{th}-order interpolation of the closest point projection $\pi : \mathcal{M}_h \longrightarrow \mathcal{M}$, extending initial linear surface approximations $\mathcal{M}_h$ of mesh size $h > 0$. The surface quadratures rest on a novel diffeomorphic square-triangle transformation yielding an alternative to Duffy's transformation, termed square-squeezing. Square-Squeezing enables to pull-back interpolation and integration tasks to the standard square, suppressing Runge's phenomenon when choosing Chebyshev–Lobatto interpolation nodes. For regular initial linear surface approximations $\mathcal{M}_h$, we provide algebraic approximation rates scaling purely with the interpolation degree, $\deg = k$, and not, as most common, with the mesh size $h > 0$. Consequently, instead of mesh-refinements, high-accurate surface integral approximations for coarse meshes can be reached by choosing high interpolation degrees. We will present numerical results for a wide variety of regular surface integrals,

demonstrating the approximation power of the HOSQ method and its applicability to numerical differential geometry.

When rational function meets virtual elements: "The lightning Virtual Element Method"

Umberto Zerbinati

University of Oxford

Since its introduction the Virtual Element Method (VEM) has been recognised by the numerical analysis community as a valuable tool for the solution of partial differential equations (PDEs). The mathematical infrastructure is what makes the VEM shine and reveals all its advantages, the (not so) downsides of the VEM are the practical aspects of its implementation. The true brilliance behind the VEM is the use of the so-called projection operators that allow you to assemble the stiffness and mass matrices without the necessity of actually computing the virtual component of the basis functions. Following the "no free lunch" principle resorting to projection operators for assembling local matrices results in a lack of coercivity that requires the use of an additional stabilisation term in the weak formulation of the problem. The lightning Virtual Element Method here proposed aims to get rid of the stabilisation term by actually computing, in an extremely efficient manner, the virtual component of the local VEM basis functions. In particular, the lightning VEM approximates the virtual part of the basis functions using rational functions with poles clustered exponentially close to the corners of each element of the polynomial tessellation. This results in two great advantages, first the mathematical analysis of a priori error estimates is much easier and essentially identical to the one for any other non-conforming Galerkin discretisation. Furthermore, the fact that the lightning VEM truly computes the basis functions allows the user to access the pointwise value of the numerical solution without needing any reconstruction techniques. The cost of the local construction of the VEM basis is the implementation price that one has to pay for the advantages of the lightning VEM method, but as we will see the embarrassingly parallelizable nature of this operation will ultimately result in a cost-efficient scheme compared to standard VEM and FEM.

Thursday, 17th August

Parallel Memory-Independent Communication Bounds for SYRK

Hussam Al Daas

STFC, Rutherford Appleton Laboratory

This talk focuses on the parallel communication cost of multiplying a matrix with its transpose, known as a symmetric rank-k update (SYRK). SYRK requires half the computation of general matrix multiplication because of the symmetry of the output matrix. Recent work has demonstrated that the sequential I/O complexity of SYRK is also a constant factor smaller than that of general matrix multiplication. Inspired by this progress, we establish memory-independent parallel communication lower bounds for SYRK with smaller constants than general matrix multiplication, and we show that these constants are tight by presenting communication-optimal algorithms. The crux of the lower bound proof relies on extending a key geometric inequality to symmetric computations and analytically solving a constrained nonlinear optimisation problem. The optimal algorithms use a triangular blocking scheme for parallel distribution of the symmetric output matrix and corresponding computation.

Parallel Matrix-free polynomial preconditioners for discrete fracture network models

Luca Bergamaschi

Department of Civil Environmental and Architectural Engineering, Unviersity of Padua

A robust matrix-free, communication avoiding parallel, high-degree polynomial preconditioner for the Conjugate Gradient method is proposed, for large and sparse symmetric positive definite linear systems. We use this preconditioned framework to solve a 3×3 block system arising in the simulation of fluid flow in large-size discrete fractured networks. We apply our polynomial preconditioner to a suitable Schur complement related with this system, which can not be explicitly computed because of its size and density. Numerical results [1] confirm the excellent properties of the proposed preconditioner up to very high polynomial degrees. The parallel implementation achieves satisfactory scalability by taking advantage from the reduced number of scalar products and hence of global communications. References [1] L. Bergamaschi and A. Martinez, Parallel Newton-Chebyshev polynomial preconditioners for the conjugate gradient method, Computational and Mathematical Methods, 3 (2021), e1153. [2] L.Bergamaschi, M.Ferronato, G.Isotton, C.Janna, and A. Martinez, Parallel Matrix-free polynomial preconditioners with application to flow simulations in discrete fracture networks, Computer & Mathematics with Applications, to appear, 2023.

Fast numerical solvers for pattern formation problems in mathematical biology

Karolina Benkova

Maxwell Institute for Mathematical Sciences, Heriot Watt University

Many of the mechanisms governing pattern formation in embryonic development have been identified and described by systems of PDEs. As some of the parameters or functions in these PDEs may be impossible to measure in laboratory conditions, we can use optimal control theory, in particular PDE-constrained optimization, to identify them. Given experimental data as the desired states, we can pose a minimisation problem so that the equations in the constraints evolve the state as close as possible to the desired state while also minimising the amount of control (or external biological mechanism) applied. In this talk, we will present a numerical solver for a problem with reaction-diffusion PDEs as constraints, by making use of a preconditioner for the large-scale saddle-point problems that arise. Moreover, we will discuss how to solve the numerical problems that arise when the PDEs are chemotaxis equations, present the flux-corrected transport technique and outline how this could be applied within the optimization setting.

Scientific Computing in Rust - Why it is time for yet another language

Timo Betcke

University College London

Rust is a relatively new low-level systems programming language that combines high performance and guaranteed memory safety with a clear and modern language design, and excellent tooling support. Since version 1.0, released in 2015, Rust has quickly become popular in industry as a modern alternative to C/C++. Moreover, over the last few years a number of projects have come up to develop a native Scientific Computing ecosystem in Rust. In this talk we want to take the opportunity to demonstrate the journey in our own group from mainly Python driven development to Rust as foundation of our scientific computing activities. We discuss the maturity of the ecosystem, advantages of Rust (and challenges to overcome), and show off some of our current Rust based projects.

Stable and Convergent Finite Element Discretizations for Mixed Formulations of Elasticity, in the incompressible limit.

Abdoulkadri Chama

University Abdou Moumouni

This work concerns the development of finite element approximations for small-strain two-dimensional linear elasticity problems, utilizing the three-field mixed elasticity method with displacement, stress, and strain as independent variables. Our goal is to construct

and analyze finite element spaces that exhibit uniform stability in the incompressible limit for the mixed formulations. We will present numerical examples to demonstrate the convergence behavior of the theory we have developed. If our findings are promising, we aim to extend the methodology to three-dimensional incompressible hyperelasticity problems, with potential applications in bifurcation analysis of wrinkling. Moreover, we aspire to contribute to the field of magnetohydrodynamics by employing our expertise in numerical approximations of partial differential equations.

Infinite-dimensional eigenvalue problems: Five cautioning examples

Matthew Colbrook

University of Cambridge

To quote the opening sentence of a much-loved book by Nick Trefethen and Mark Embree, "Eigenvalues are among the most successful tools of applied mathematics." However, many finite-dimensional eigenvalue problems arise from an underlying infinite-dimensional problem. Several, often quite subtle, phenomena may appear when dealing with such problems. This talk presents five examples, all in MATLAB! We discuss how to overcome these issues using "solve-then-discretise" methods and how to figure out which problems can be solved. This talk is based on joint work with Alex Townsend.

Blendstrings: An environment for computing with smooth functions

Rob Corless

Maple Transactions

A "blendstring" is a piecewise polynomial interpolant formed of high-degree two-point Hermite interpolational polynomials on each piece, something like a higher-order cubic spline but more like a chebfun. Blendstrings can be used for accurate representation of smooth functions on a line segment, or more generally a polygonal path, in the complex plane. This paper discusses some properties of these objects including how to evaluate, differentiate, and integrate them efficiently, and describes a prototype Maple implementation. Blendstrings can be differentiated exactly and integrated exactly. Compatible blendstrings can be combined algebraically. Applications to the solution of differential equations and the computation of Mathieu functions and generalized Mathieu eigenfunctions are shown.

Climate prediction and numerical analysis: questions of practical importance

Francisco de Melo Virissimo

London School of Economics

Modern research in climate change relies on Earth System Models (ESMs), which are highly complex and nonlinear mathematical representations of the planet Earth. Since ESMs are too complicated to be tractable analytically, we must rely on computers to extract useful information from them. Numerically solving these models is a highly complex task, with two key practical consequences. First, being complex and nonlinear, ESMs require the use of several numerical schemes and involves different computational strategies to accommodate for the multiplicity of scales and components present. These numerical choices vary from model and is also dependent on the user needs, as well as the computational resources available to them. Secondly, being chaotic means that its initial value problem is sensitive to small changes in e.g. initial condition, so its state (or climate) can only be characterised as a distribution, requiring an ensemble of simulations instead of a single one. Hence, different numerical approximations could lead to differences in the resulting distributions, particularly in shape and extreme values. This is important as it can cause ambiguity in our interpretation of future climate. Despite that, this issue has been largely neglected in both climate and mathematical literature. In this talk, we will review and discuss the use of numerical schemes in ESMs and individual components. Using a conceptual but low-dimensional representation of the climate system, we will also present a systematic study of how different numerical methods might change the resulting climate distribution. In addition to the uncertainties from initial condition, parameter and model formulation, this study suggests a fourth level of "structural" uncertainty in climate modelling – in the numerical formulation. This has implications to the design and interpretation of climate ensembles, which brings climate change research to the core of 21st century applied numerical analysis research. *Join work with Dave Stainforth.

Fast Approximations of Trefethen Functions due to Euclidean Degree Interpolation

Michael Hecht

Center for Advanced Systems Understanding / Helmholtz-Zentrum Dresden-Rossendorf

We follow Nick Trefethen's suggestion, stating that total or maximum degree choices for multivariate polynomial interpolation and regression for a class of analytic functions, we term Trefethen functions, might be sub-optimal compared to the choice of Euclidean degree. We have realised a generalisation of Newton's divided difference scheme (DDS) that is capable for interpolating multivariate functions for any choice of downward closed index sets efficiently and numerically stable, including the total, maximum, and Euclidean degree choices. We demonstrate that the optimal geometric approximation rate for the

Runge function is reached by DDS (up to dimension 5), suggesting this optimality to extend to other Trefethen funtions. Consequently, while scaling sub-exponentially with dimension in runtime and storage complexity Euclidean-degree-interpolation resists the curse of dimensionality. Extensions to regression tasks show again the Euclidean degree to be superior to the other degree choices, especially when it comes to regression tasks of equispaced data. Though for all degree choices regression maintains limited due to the results of Platte et al., we give some examples of how the extended stability range of Euclidean-degree-regression might impact computational tasks in numerical differential geometry and beyond.

Numerical approximation with clustered poles

Astrid Herremans

KU Leuven

Recent research by Trefethen et al. shows that rational functions with clustered poles form an excellent approximation set for functions with branch point singularities at known locations. These types of approximation problems arise when solving PDEs on domains with corners, leading to the development of lightning solvers. On the one hand, the approximation set is interesting from a numerical point of view. The obtained systems are highly ill-conditioned, yet accurate results can still be obtained when switching to a rectangular method. This is a familiar phenomenon with enriched approximation sets, and raises numerical questions such as the existence of approximations with bounded coefficients. On the other hand, it turns out that the lightning method also answers more purely mathematical questions of historical importance. When using optimal parameters, the lightning approximation to x^α matches the convergence rate of the best nonlinear rational approximation, as determined by Stahl in 1996. In a broader context, recent research indicates that pole clustering fits in a surprisingly general scope, being intimately related to activation functions in neural networks as well as mesh refinement in hp methods. Questions arise whether the idea of pole clustering can be extended, potentially leading to multivariate approximations.

Fast contour integral methods for bounded semigroups with explicit error bounds

Andrew Horning

MIT

Contour integral methods provide a powerful class of time-dependent PDE solvers associated with analytic semigroups. They combine exponentially convergent quadrature,

embarrassing parallelizability, and global-in-time representations for rapid solution and evaluation on a finite-time horizon. In this talk, we propose new rapidly convergent contour integral schemes for more general semigroups, where traditional methods based on analyticity and contour deformation fail. The schemes are accompanied by explicit error bounds and automated near-optimal parameter selection, so the user need only provide the semigroup generator and error tolerance for a finite time horizon. Our approach is based on a regularized Laplace transform that couples the exponentially convergent trapezoidal rule with acceleration techniques for slowly converging Fourier series. We illustrate the algorithm and bounds with examples from Koopman theory, uncertainty quantification, and control theory.

Numerical simulation of calcium cycling in urinary bladder smooth muscle

Chitaranjan Mahapatra

Indian Institute of Technology Bombay, India

In the last decades, mathematical and numerical modelling of the physiological system is a research topic that has attracted remarkable interest to understand various pathological conditions in a better way for exploring new pharmacological targets. Urinary incontinence, which is also known as involuntary leakage of urine is usually the result of overactivity of the urinary bladder smooth muscles (UBSM), which control the bladder. The intracellular calcium (Ca2+) dynamics plays an essential role in the contraction and relaxation of the UBSM cell. This study establishes a whole cell Ca2+ model based on the numerical modelling of the UBSM cell with respect to experimental data. Simulation of electrophysiology and intracellular Ca2+ dynamics in UBSM comprises fast stochastic dynamics in tiny sub-compartments, partial differential equations (PDEs) with stochastic source terms for concentration fields, and the globally coupling membrane potential. We use highly unstructured meshes appropriate for the spatial heterogeneity of intracellular Ca2+ release, and adaptive time-stepping algorithms appropriate for the simulation of stochastic channel opening and closing in sub-compartments like the Ca2+ release units (CRUs). A set of reaction-diffusion equations describes the behavior of the intracellular concentration fields on length scales from tens of nano meters to cell size (tens of micro meters) and milliseconds to tens of seconds. Detailed highly stochastic CRU models drive source functions in the PDE model. The time scale separation between fast stochastic CRU dynamics and slower PDE dynamics limits efficiency with traditional approaches. We present new methods to circumvent that problem. Membrane potential introduces a global spatial coupling across the whole cell due to its large coupling length. We developed an efficient adaptive finite element simulator interface for the numerical simulation of this multi-physics and multiscale problem. In this work we have presented an efficient and novel computational approach for the simulation of intracellular Ca2+ dynamics in UBSM

tissues.

On the stability of recurrence relations

Nicola Mastronardi

Istituto per le Applicazioni del Calcolo, CNR

In this talk we consider recurrence relations arising in different contexts and analyze their stability properties. In particular, we focus on recurrence relations for: classical orthogonal; polynomials of a discrete variable, such as Krawtchouk, Meixner, and Hahn polynomials; computation of modified moments for Pollaczek and half-range Hermite weights; evaluation of Bessel functions; computation of the Hilbert transform of Jacobi weights. Two techniques are usually considered to evaluate recurrence relations: the recurrence relation computed in a forward fashion, given the initial condition(s); the recurrence relation computed in a backward fashion, starting from dummy condition(s). These techniques have been extensively studied. Nevertheless, such approaches turn out to be unstable in some cases. Here, we propose a new algorithm, based on linear algebra tools, able to evaluate, in most cases, the considered recurrence relation in a reliable way. As applications, we consider the computation of two different kinds of integrals with the Hermite and Pollaczek-type weights, via product quadrature rules. To this aim, the modified moments respect to a system of orthogonal polynomials need to be computed. Some approaches to compute the aforementioned modified moments are proposed in the literature, but they turn out to be unstable. We show that such moments can be accurately computed by the proposed algorithm. ’

Analysis and Numerical Approximation of Stationary Second-order Mean Field Game Partial Differential Inclusions

Yohance Osborne

University College London

Mean Field Games (MFG) are models for Nash equilibria of large population stochastic differential games. Under simplifying assumptions, these equilibria are described by nonlinear systems in which a Hamilton—Jacobi—Bellman (HJB) equation and a Kolmogorov—Fokker—Planck (KFP) equation are coupled. The advective term of the KFP equation is often built under the hypothesis that the Hamiltonian of the HJB equation is continuously differentiable. However, in many cases of practical interest, the underlying optimal control problem may give rise to bang-bang controls, which typically lead to nondifferentiable Hamiltonians. In this talk we will present results on the analysis and numerical approximation of stationary second-order MFG systems for the general case

of convex, Lipschitz, but possibly nondifferentiable Hamiltonians. In particular, we will propose a generalization of the MFG system as a Partial Differential Inclusion (PDI) based on interpreting the partial derivative of the Hamiltonian in terms of subdifferentials of convex functions. We present results that guarantee the existence of unique weak solutions to the stationary MFG PDI under a monotonicity condition similar to one that has been considered previously by Lasry & Lions. Moreover, we will propose a monotone finite element discretization of the weak formulation of the MFG PDI, and present results that confirm the strong H^1-norm convergence of the approximations to the value function and strong L^q-norm convergence of the approximations to the density function.

Recycling MMGKs for Large-scale dynamic and streaming data

Mirjeta Pasha

Tufts University

The ubiquity of inverse problems in many fields of science is associated with emerging challenges on obtaining relevant solutions to large-scale and data-intensive inverse problems such as ill-posedness, large dimensionality of the parameters, and the complexity of the model constraints. Edge-preserving constraint has received considerable attention due to the need for reconstructing high-quality and sharp images. The use of the ℓ_q-norm in the gradient of the image in the regularization term has shown potential. One typically replaces the ℓ_q-norm term with a sequence of ℓ_2-norm weighted gradient with weights determined from the current solution estimate. To overcome the large dimensionality, (hybrid) Krylov subspace methods can be employed to solve the two-norm regularized problems. One of the disadvantages of such approaches is the need to generate a new Krylov subspace from scratch for every new two-norm regularized problem. The majorization minimization Krylov subspace method (MMGKS) combines norm reweighting with generalized Krylov subspace to solve the reweighted problem and defines the regularization parameter in a relatively small subspace that expands at each iteration. The basis expansion is repeated until a sufficiently accurate solution is found. Nevertheless, for massive data problems that require many expansion steps to converge, storage and the cost of repeated orthogonalization may present overwhelming memory and computational requirements. In this talk we discuss a new method (RMMGKS) that keeps the memory requirements bounded through recycling the solution subspace by alternating between enlarging and compressing the GKS subspace. Numerical examples from dynamic photoacoustic tomography and streaming X-ray CT are used to illustrate the effectiveness of the described methods. This is joint work with Misha Kilmer (Tufts University) and Eric de Sturler (Virginia Tech).

Convergence of randomized and greedy relaxation schemes for solving nonsingular linear systems of equations

Daniel Szyld

Temple University, Philadelphia

We extend results known for the randomized Gauss-Seidel and the Gauss-Southwell methods for the case of a Hermitian and positive definite matrix to certain classes of non-Hermitian matrices. We obtain convergence results for a whole range of parameters describing the probabilities in the randomized method or the greedy choice strategy in the Gauss-Southwell-type methods. We identify those choices which make our convergence bounds best possible. Our main tool is to use weighted ℓ_1-norms to measure the residuals. A major result is that the best convergence bounds that we obtain for the expected values in the randomized algorithm are as good as the best for the deterministic, but more costly algorithms of Gauss-Southwell type. (Joint work with Andreas Frommer, Wuppertal)

Spectral Methods for Capillary Surfaces

Ray Treinen

Texas State University

Capillary surfaces satisfy the equation that the mean curvature of the surface is proportional to the height of the surface at each point. These surfaces model the equilibrium shapes of liquid interfaces and the usual boundary conditions encode the wetting properties of that fluid with the container with the nonlinear natural boundary conditions. We present spectral methods for computing capillary surfaces. We consider radially symmetric configurations as well as the general PDE problem. In the course of developing these methods for the full PDE problem we will also present spectral methods for the Plateau problem for minimal surfaces as well as problems for constant mean curvature surfaces.

Computing the pseudospectra of linear operators

Kuan Xu

University of Science and Technology of China

In his 1999 Acta Numerica paper *Computation of pseudospectra*, Nick Trefethen wrote, "This field will also participate in a broader trend in the scientific computing of the future, the gradual breaking down of the walls between the two steps of discretization (operator -> matrix) and solution (matrix -> spectrum or pseudospectra)." The truth of this prophecy is partly demonstrated by the recent developments in the representation/approximation of linear operators. In this talk, we identify the classes of linear operators for which

the pseudospectra can be calculated with a numerical functional analysis approach using these representations, highlighting the advantages of the proposed method in speed and accuracy.

Barycentric rational interpolation of exponential clustered poles

Kelong Zhao

Central South University, China

In this talk, I will present a rational interpolation method that can effectively handle analytic functions with branch point singularities on the boundary. The accuracy of this method is not only in line with theoretical expectations, but can also approach machine accuracy, making it a valuable tool for solving complex problems. The key to its effectiveness is the identification of interpolation nodes that match the equilibrium potential. The derivation of these nodes is based on a method we developed in our previous work, which involves solving Symm's integral equation to obtain a constant element approximation of the continuous density function that satisfies the equilibrium potential. Based on this approximate density function, we can then obtain the interpolation nodes. One interesting observation is that when the number of poles is close to the number of nodes, the rational interpolation method loses its effectiveness and no longer meets the expected level of accuracy. From the perspective of the potential, I will illustrate this phenomenon with a concrete example and demonstrate the root exponential convergence of the method. This rational interpolation method can be applied to sector regions and polygonal regions, and can effectively handle analytic functions with multiple branch point singularities.

Chebfun for AI

Shengxin (Jude) Zhu

Beijing Normal University

We shall discuss how Chebfun can be employed in a couple of popular machine learning and AI scenarios, such as language models, hyper-spectral image processing, approximating algorithms design and so on.

List of Participants

Andersen Ang	andersen.ang@soton.ac.uk
Anthony Austin	apacom@meromorphic.net
James Baglama	jbaglama@uri.edu
Aaron Baier-Reinio	aaron.baier-reinio@hertford.ox.ac.uk
Kim Batselier	k.batselier@tudelft.nl
Thomas Bellotti	thomas.bellotti@polytechnique.edu
Karolina Benkova	k.benkova@ed.ac.uk
Luca Bergamaschi	luca.bergamaschi@unipd.it
Jean-Paul Berrut	jean-paul.berrut@unifr.ch
Timo Betcke	t.betcke@ucl.ac.uk
Folkmar Bornemann	bornemann@tum.de
Niel Van Buggenhout	buggenhout@karlin.mff.cuni.cz
Liam Burke	burkel8@tcd.ie
Keaton Burns	kjburns@mit.edu
Coralia Cartis	cartis@maths.ox.ac.uk
Oliver Salazar Celis	oliver_salazar@yahoo.com
Abdoulkadri Chama	chamabdoul@gmail.com
Jon Chapman	chapman@maths.ox.ac.uk
Ivan Cheltsov	ic488@bath.ac.uk
James Chok	james.chok@outlook.com
Matthew Colbrook	mjc249@cam.ac.uk
Stefano Costa	stefano.costa@ieee.org
Robert Corless	rob.corless@gmail.com
Hussam Al Daas	hussam.al-daas@stfc.ac.uk
Anil Damle	damle@cornell.edu
Ieva Dauzickaite	dauzickaite@karlin.mff.cuni.cz
Nadiia Derevianko	n.derevianko@math.uni-goettingen.de
Toby Driscoll	driscoll@udel.edu
Catherine Drysdale	c.n.d.drysdale@bham.ac.uk
Alan Edelman	edelman@mit.edu
Mark Embree	embree@vt.edu
Emil Engström	emil.engstrom@math.lth.se
Oliver Ernst	oernst@math.tu-chemnitz.de
Jessica Farmer	jessica.farmer@stfc.ac.uk
Patrick Farrell	patrick.farrell@maths.ox.ac.uk

Silviu Filip	silviu.filip@inria.fr
Daniel Fortunato	dan.fortunato@gmail.com
Jaroslav Fowkes	jaroslav.fowkes@maths.ox.ac.uk
Martin Gander	martin.gander@unige.ch
Kathryn Gillow	kathryn.gillow@maths.ox.ac.uk
Ben Goodrich	bg2382@columbia.edu
Abinand Gopal	abinand.gopal@yale.edu
Nick Gould	nick.gould@stfc.ac.uk
Anne Greenbaum	greenbau@uw.edu
Nick Hale	nickhale@sun.ac.za
Julian Hall	jajhall@ed.ac.uk
Eskil Hansen	eskil.hansen@math.lth.se
Behnam Hashemi	bh241@leicester.ac.uk
Muhammad Hassan	muhammad.hassan@sorbonne-universite.fr
Michael Hecht	m.hecht@hzdr.de
Bernhard Heinzelreiter	b.heinzelreiter@sms.ed.ac.uk
Astrid Herremans	astrid.herremans@kuleuven.be
Nicholas Higham	nick.higham@manchester.ac.uk
Andrew Horning	horninga@mit.edu
Daan Huybrechs	daan.huybrechs@cs.kuleuven.be
David Keyes	david.keyes@kaust.edu.sa
Teresa Laudadio	teresa.laudadio@cnr.it
Piers Lawrence	piers.lawrence@eigenpoly.com
Randall LeVeque	rjl@uw.edu
Santolo Leveque	santolo.leveque@sns.it
Torsten Linß	torsten.linss@fernuni-hagen.de
Colin Macdonald	cbm@math.ubc.ca
Chitaranjan Mahapatra	cmahapatra97@gmail.com
Maike Meier	maike.meier@balliol.ox.ac.uk
India Marsden	indiamarsden@yahoo.co.uk
Gunnar Martinsson	pgm@oden.utexas.edu
Nicola Mastronardi	nicola.mastronardi@cnr.it
Carl C. Kjelgaard Mikkelsen	spock@cs.umu.se
Maike Meier	maike.meier@maths.ox.ac.uk
Andrés Miniguano-Trujillo	Andres.Miniguano-Trujillo@ed.ac.uk
Cleve Moler	moler@mathworks.com
Hadrien Montanelli	hadrien.montanelli@polytechnique.edu
Sophie Moufawad	sm101@aub.edu.lb
Yuji Nakatsukasa	nakatsukasa@maths.ox.ac.uk
Jitse Niesen	j.niesen@leeds.ac.uk

Yohance Osborne	yohance.osborne.16@ucl.ac.uk
Alberto Paganini	admp1@leicester.ac.uk
Ioannis Papadopoulos	ioannis.papadopoulos13@imperial.ac.uk
Mirjeta Pasha	mirjeta.pasha@tufts.edu
Taejun Park	taejun.park@worc.ox.ac.uk
Jorge Cisneros Paz	jorge.cisneros@utexas.edu
Cécile Piret	cmpiret@mtu.edu
John Reid	john.reid9@talktalk.net
Mufutau Ajani Rufai	mufutauajani.rufai@unibz.it
Jennifer Scott	jennifer.scott@reading.ac.uk
Kirill Serkh	kserkh@math.toronto.edu
Paz Fink Shustin	pfink22@gmail.com
Boris Shustin	borisshy@gmail.com
Pranav Singh	ps2106@bath.ac.uk
Mikael Slevinsky	Richard.slevinsky@umanitoba.ca
Martin Stoll	martin.stoll@mathematik.tu-chemnitz.de
Steven Strogatz	shs7@cornell.edu
Daniel Szyld	szyld@temple.edu
Jemima Tabeart	tabeart@maths.ox.ac.uk
Kim-Chuan Toh	mattohkc@nus.edu.sg
Anna-Karin Tornberg	akto@kth.se
Alex Townsend	townsend@cornell.edu
Nick Trefethen	trefethen@maths.ox.ac.uk
Ray Treinen	rt30@txstate.edu
Laurette Tuckerman	laurette@pmmh.espci.fr
Riko Ukena	riko.ukena@tuhh.de
Geoffrey Vasil	gvasil@ed.ac.uk
Francisco de Melo Virissimo	f.de-melo-virissimo@lse.ac.uk
André Weideman	weideman@sun.ac.za
Raphaël Widdershoven	raphael.widdershoven@kuleuven.be
Heather Wilber	heather.wilber@oden.utexas.edu
Kuan Xu	xukuan2011@gmail.com
Yidan Xue	xue@maths.ox.ac.uk
Annan Yu	ay262@cornell.edu
Gentian Zavalani	g.zavalani@hzdr.de
Umberto Zerbinati	umberto.zerbinati@maths.ox.ac.uk
Kelong Zhao	clonezhao.1994@csu.edu.cn
Zhengbo Zhou	zhengbo.zhou@outlook.com
Shengxin (Jude) Zhu	Shengxin.Zhu@bnu.edu.cn

Sponsors

The conference is extremely grateful for funding from many organisations.

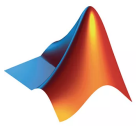
Sponsors

Engineering and Physical Sciences Research Council

Heilbronn Institute for Mathematical Research

Institute of mathematics & its applications

LONDON MATHEMATICAL SOCIETY EST. 1865



MathWorks®

QJMAM

siam®

Society for Industrial and Applied Mathematics