CANA23

Challenges and Advances in Numerical Analysis

A Conference in honor of Prof. Giuseppe Rodriguez on his 60th birthday

Cagliari, Italy
June 5–9, 2023

Fondazione di Sardegna

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The conference will be held at the University of Cagliari, Sardinia, Italy. A goal of this meeting is to spur interaction and collaboration between participants with different expertise.

The talks will cover several topics including numerical linear algebra techniques, iterative methods, preconditioning, matrix functions, solution of differential problems, solution of integral equations, numerical quadrature, network analysis, and the solution of ill-posed problems.

The conference will also be a special occasion for celebrating the birthday of Giuseppe Rodriguez.

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The conference is organized with the patronage of University of Cagliari.
Financial support is acknowledged from:

- Department of Mathematics and Computer Science, University of Cagliari
- Research project "Computational Methods and Networks in Civil Engineering (COMANCHE)", 2021, Fondazione di Sardegna, Italy

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Abstracts

List of Abstracts

A STRUCTURE-PRESERVING UPWIND DG SCHEME FOR A DEGENERATE PHASE-FIELD TUMOR MODEL

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The purpose of this talk is to present an upwind DG approximation of a degenerate phase-field tumor model that preserves the physical properties of the continuous model.

The tumor model that we consider is based on the one presented in [3], which consists of a Cahn-Hilliard equation for the tumor variable and a diffusion equation for the nutrient variable, coupled by proliferation and cross-diffusion terms. In this sense, we propose several modifications to this model that impose important physically meaningful bounds on the phase-field variable.

Then, we extend the work in [2, 1] to develop a nonlinear discrete scheme based on a convex-splitting time discretization and an upwind discontinuous Galerkin (DG) spatial scheme that approximates the solution of the continuous model preserving its physical properties (mass conservation, pointwise bounds and energy stability).

Finally, we use FEniCSx and its built-in Newton's method to approximate the nonlinear scheme and carry out several numerical experiments. These tests compare our DG scheme with a continuous finite element spatial discretization, which presents numerical spurious oscillations due to the cross-diffusion terms. In addition, they show the behavior of the model under different choices of parameters, mobility and proliferation functions.

References

[1] D. Acosta-Soba, F. Guillén-González, and J. R. Rodríguez-Galván, *An unconditionally energy stable and positive upwind DG scheme for the Keller–Segel model*, Submitted, arXiv preprint 10.48550/arxiv.2209.10508 (2022).

[2] D. Acosta-Soba, F. Guillén-González, and J. R. Rodríguez-Galván, *An upwind DG scheme preserving the maximum principle for the convective Cahn–Hilliard model*, Numerical Algorithms, 92 (2022), pp. 1589–1619.

[3] A. Hawkins-Daarud, K. G. van der Zee, and J. T. Oden, *Numerical simulation of a thermodynamically consistent four-species tumor growth model*, International Journal for Numerical Methods in Biomedical Engineering, 28 (2012), pp. 3–24.

A SMOOTHING ANALYSIS FOR MULTIGRID METHODS APPLIED TO TEMPERED FRACTIONAL PROBLEMS

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We consider the numerical solution of time-dependent space-tempered fractional diffusion equations. The use of Crank-Nicolson in time and of second-order accurate tempered weighted and shifted Grünwald difference in space leads to dense (multilevel) Toeplitz-like linear systems. By exploiting the related structure, we design an ad-hoc multigrid solver and multigrid-based preconditioners, all with weighted Jacobi as smoother. A new smoothing analysis is provided, which refines state-of-the-art results expanding the set of suitable Jacobi weights. Furthermore, we prove that if a multigrid method is effective in the non-tempered case, then the same multigrid method is effective also in the tempered one. The numerical results confirm the theoretical analysis, showing that the resulting multigrid-based solvers are computationally effective for tempered fractional diffusion equations.

ENERGETIC BEM FOR THE NUMERICAL SOLUTION OF ELASTODYNAMICS CONTACT PROBLEMS

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We investigate the numerical solution of unilateral contact problems, which consider the elastodynamic stresses of a body in contact with a rigid obstacle. Such problems arise in numerous mechanical applications, from fracture dynamics and crash tests to rolling car tires. Mathematically, the nonlinear boundary condition corresponding to the contact interaction translates into a variational inequality for the linear elastodynamic equations. In spite of a wide computational literature on the topic, a rigorous theoretical analysis is difficult and results about the existence of solutions are only known for simplified model problems. Nevertheless, the importance of this study for practical purposes, above all in the time-domain framework, is clear and treatment by BEMs represents a natural choice [2], given that the contact is confined to the boundary while the interior dynamics is linear. For this reason, we propose the Energetic BEM (see e.g. [1]), that provides an efficient and stable numerical strategy for linear elastodynamics, here adapted for the solution of contact problems. This translates in the assembly of E-BEM matrices, that allow an accurate discretization of the involved Poincaré-Steklov operator, then followed by an Uzawa method, employed as an iterative solver for the nonlinear problem. Stability, convergence and implementation aspects of the E-BEM are discussed and numerical results are presented for a range of 2D geometries, with unilateral contact conditions imposed on part of the boundary (without friction).

References

[1] A. Aimi, G. Di Credico, M. Diligenti, C. Guardasoni, *Highly accurate quadrature schemes for singular integrals in energetic BEM applied to elastodynamics*, JCAM, 410 (2022), 114186.

[2] H. Gimperlein, F. Meyer, C. Ozdemir, E. P. Stephan, *Time domain boundary elements for dynamic contact problems*, CMAME, 333 (2018), pp. 147–175.

FRACTIONAL GRAPH LAPLACIAN FOR IMAGE RECONSTRUCTION

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Image reconstruction problems, like image deblurring and computer tomography, are usually ill-posed and require regularization. A popular approach to regularization is to substitute the original problem with an optimization problem that minimizes the sum of two terms, an ℓ^2 term and an ℓ^q term with $0 < q \leq 1$.

In this work, we propose to use the fractional Laplacian of a properly constructed graph in the ℓ^q term to compute extremely accurate reconstructions of the desired images. A simple model with a fully plug-and-play method is used to construct the graph and enhanced diffusion on the graph is achieved with the use of a fractional exponent in the Laplacian operator. Since this is a global operator, we propose to replace it with an approximation in an appropriate Krylov subspace. Some selected numerical examples in image deblurring and computer tomography show the performances of our proposal.

References

[1] S. Aleotti, A. Buccini, M. Donatelli, *Fractional Graph Laplacian for image reconstruction*, in progress.

[2] D. Bianchi, A. Buccini, M. Donatelli, E. Randazzo, *Graph Laplacian for image deblurring*, Electronic Transactions on Numerical Analysis, 2021, 55, pp. 169–186

[3] A. Buccini, M. Donatelli, *Graph Laplacian in $\ell^2 - \ell^q$ regularization for image reconstruction*, Proceedings - 2021 21st International Conference on Computational Science and Its Applications, ICCSA 2021, 2021, pp. 29–38

COMPUTING THE ROOTS OF MANDELBROT POLYNOMIALS: AN EXPERIMENTAL ANALYSIS

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The celebrated Mandelbrot set is formed by the complex numbers c such that the sequence $x_0 = 0$, $x_{i+1} = x_i^2 + c$, does not diverge to infinity. Relevant points of this set are the numbers c for which the sequence $\{x_i\}$ provides a cycle of finite length k. These values are the roots of the polynomial $p_k(z)$ of degree $n = 2^k - 1$ defined by the recurrence $p_1(z) = z + 1$, $p_{i+1} = zp_i(z)^2 + 1$, $i = 1, \ldots, k-1$. Efforts to compute these roots have been done by several authors [2], [4]. In this talk we provide an algorithm based on the Ehrlich-Aberth iterations [1] complemented by the Fast Multipole Method of [3], and by the fast search of near neighbors of a set of complex numbers, that have a cost of roughly $O(n)$ arithmetic operations per step. In our experiments, the number of iterations needed to arrive at numerical convergence is practically constant. This allows to compute the roots of $p_k(x)$ up to degree $n = 2^{24} - 1$ in a few minutes on a laptop with 16 GB RAM and an Intel I3 processor. Larger degrees can be treated on platforms with a higher amount of RAM.

References

[1] O. Aberth. *Iteration methods for finding all zeros of a polynomial simultaneously*. Math. Comp., 27 (1973), pp. 339–344.

[2] N. J. Calkin, E. Y. S. Chan, and R. M. Corless. *Some facts and conjectures about Mandelbrot polynomials*. Maple Trans., 1, (2021).

[3] L. Greengard and V. Rokhlin. *A fast algorithm for particle simulations*. J. Comput. Phys., 73 (1987), pp. 325–348.

[4] D. Schleicher. *On the efficient global dynamics of Newton's method for complex polynomials*. Nonlinearity, 36 (2023).

ON THE ROAD... TO THE TREATMENT OF NEAR-BREAKDOWN IN THE CONJUGATE GRADIENT ALGORITHM

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The conjugate gradient algorithm for solving systems of linear equations with a symmetric positive definite matrix was obtained in 1952 by Magnus Rudolph Hestenes (1906-1991) and Eduard Stiefel (1909-1978).

It is a direct method since, for a system of dimension N, it converges in N iterations at most. When N is large, it is used as an iterative method.

The conjugate gradient algorithm makes use of two recurrence relations each of them depending on a rational coefficient changing at each step. It cannot suffer from a breakdown due to a division by zero in the computation of the coefficients of the recurrence relations.

However, the algorithm can suffer from a near-breakdown when the denominator of one of these coefficients (or when the coefficient itself) is close to zero, thus leading to rounding errors and non-convergence.

First, we will give some academic examples showing that a near-breakdown really arises. Then, we will derive the recurrence relations for jumping over it.

This work is unfinished since we have not yet programmed it, and we have no numerical results to present.

A VARIATIONAL NON-LINEAR CONSTRAINED MODEL FOR THE INVERSION OF FDEM DATA

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In this talk we consider the reconstruction of the electrical conductivity of the ground using Frequency Domain Electromagnetic (FDEM) induction devices. This nonlinear ill-posed inverse problem is of the form

$$\boldsymbol{\Sigma} = \arg\min_{\boldsymbol{\Sigma}} \sum_{j=1}^{N} \left\| M(\boldsymbol{\sigma}_j) - \boldsymbol{b}_j \right\|_2^2, \tag{1}$$

where $\boldsymbol{\Sigma} = [\boldsymbol{\sigma}_1, \dots, \boldsymbol{\sigma}_N]$ collects the electrical conductivity at certain depths, $\boldsymbol{B} = [\boldsymbol{b}_1, \dots, \boldsymbol{b}_N]$ are the measured data, and the vector function $\boldsymbol{M}(\boldsymbol{\Sigma})$ returns the readings predicted by the model.

Even though the model is separable, treating each $\boldsymbol{\sigma}_j$ separately creates artifacts in the reconstructions. To remove them we consider the following variational problem

$$\arg\min_{\boldsymbol{\Sigma} \geq 0} \frac{1}{2} \left\| \boldsymbol{M}(\boldsymbol{\Sigma}) - \boldsymbol{B} \right\|_F^2 + \frac{\gamma}{q} \left\| \boldsymbol{D}(\boldsymbol{\Sigma}) \right\|_q^q, \tag{2}$$

where $\gamma > 0$, $0 < q < 1$, and $\boldsymbol{D}(\boldsymbol{\Sigma})$ is the two-dimensional Laplacian of $\boldsymbol{\Sigma}$.

In this talk we present the results obtained in [1]. Firstly, we describe a new variational model for (1). Secondly, we prove the regularization properties of $\ell^2 - \ell^q$ in the nonlinear case. Finally, we show the advantages of the proposed approach on both synthetic and real data.

References

[1] A. Buccini and P. Díaz de Alba. *A variational non-linear constrained model for the inversion of FDEM data*. Inverse Problems 38 (2022), p. 014001.

GRAPH SIGNAL PROCESSING AND WAVELET PACKETS

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Nowadays graphs became of significant importance given their use to describe complex system dynamics, with important applications to real world problems, e.g. graph representation of the brain, social networks, biological networks, spreading of a disease, etc.. In this work we introduce a novel graph wavelet packets construction, to our knowledge different from the ones known in literature. We get inspired by the Spectral Graph Wavelet Transform defined by Hammond et all. in [1], based on a spectral graph wavelet at scale $s > 0$, centered on vertex n, and a spectral graph scaling function, respectively. Moreover after defining the wavelet packet spaces, and the associated tree, we obtain a dictionary of frames for $\mathbb{R}^N$, with known lower and upper bounds. We will give some concrete examples on how the wavelet packets can be used for compressing, denoising and reconstruction by considering a signal, given by the fRMI (functional magnetic resonance imaging) data, on the nodes of voxel-wise brain graph $\mathcal{G}$ with 900.760 nodes (representing the brain voxels) defined in [2]-[3].

References

[1] D. K. Hammond, P. Vandergheynst , and R. Gribonval, *Wavelets on graphs via spectral graph theory*, Appl. Comput. Harmon. Anal. **30** (2011) 129–150.

[2] A. Tarun, D. Abramian, M. Larsson, H. Behjat, and D. Van De Ville, *Voxel-Wise Brain Graphs from Diffusion-Weighted MRI: Spectral Analysis and Application to Functional MRI*, preprint (2021).

[3] A. Tarun, H. Behjat, T. Bolton, D. Abramian, D. Van De Ville, *Structural mediation of human brain activity revealed by white-matter interpolation of fMRI*, NeuroImage 213 (2020) 116718.

INVERSE PROBLEMS IN SIGNAL PROCESSING. NEW RESULTS FROM THE NUMERICAL ANALYSIS

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In many applied fields of research, like Geophysics, Medicine, Engineering, and Finance, to name a few, a classical problem is the identification of hidden quasi-periodicities and frequency patterns, and their extraction from a given signal, like, for instance, chirps.

Standard methods based on Fourier and Wavelet Transform, historically used in Signal Processing, proved to be limited when nonlinear and non-stationary phenomena are present. For this reason in the last two decades, several new nonlinear methods have been developed by many research groups around the world, and they have been used extensively in many applications.

In this talk, we will briefly review the Hilbert-Huang Transform (a.k.a. Empirical Mode Decomposition method) and discuss its known limitations. Then, we will introduce the Fast Iterative Filtering technique [2] and its generalizations to handle multidimensional, multivariate, or highly non-stationary signals, as well as the newly developed time-frequency representation called IMFogram [1]. We will discuss the theoretical and numerical properties of these methods and show their applications to real-life data. We will conclude the talk by reviewing the main open problems in this research field.

References

[1] P. Barbe, A. Cicone, W. S. Li, H. Zhou. Time-frequency representation of nonstationary signals: the IMFogram. Pure and Applied Functional Analysis, Volume 7, Number 1, 27-39, 2022.

[2] A. Cicone, H. Zhou. Numerical Analysis for Iterative Filtering with New Efficient Implementations Based on FFT. Numerische Mathematik, 147 (1), pages 1-28, 2021

TWO FORMULATIONS FOR THE CAPACITATED STEINER TREE PROBLEM

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We face a variant of the Steiner tree problem in which some commodities must be sent from the root node to terminal nodes through transshipment nodes with limited capacity. We present two formulations for this problem. The second one uses the notion of cardinality of terminals assigned to a transshipment node as in [1]. An immediate benefit of the second formulation is that it is stronger than the first one. Moreover, we present two classes of inequalities which exploit the cardinality effect of the second formulation and use separation heuristics to identify and sequentially add valid inequalities to further improve the lower bound. This approach is embedded in a branch-and-bound to obtain the optimal solution and results in a branch-and-cut algorithm. We test our solution approach on a large set of random generated instances. The experimentation clearly shows that this approach is able to identify the optimal solution at the root node in most of the problem instances with limited capacity. For problem instances with larger capacity, the proposed cuts are shown to be useful, even if the first formulation is sometimes easier to solve.

References

[1] M. Di Francesco, M. Gaudioso, E. Gorgone, I. Murthy *A new extended formulation with valid inequalities for the Capacitated Concentrator Location Problem*, European Journal of Operational Research, 289 (2021), pp. 975–986.

A NEW FAST NYSTRÖM METHOD FOR SOLVING LINEAR VOLTERRA INTEGRAL EQUATIONS ON INFINITE INTERVALS

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Recently in [1, 2, 3] a numerical method has been introduced for the numerical solution of the following linear Volterra integral equations of the second kind on the half line

$$f(t) - \int_0^t k(s,t) f(s)\, ds = g(t), \quad t \geq 0,$$

where the kernel $k(s,t)$ is a given function defined on $\Delta = \{(s,t) \,|\, 0 \leq s \leq t\}$, $g(t)$ is a known function on $\mathbb{R}^+$ and $f(t)$ is the unknown solution. This method is of Nyström type and consists in discretizing the integral operator by a product quadrature rule based on a truncated Lagrange interpolation process. The involved modified moments, depending on the kernel function, are approximated by a truncated gaussian quadrature formula.

The aim of this talk is to propose a new efficient Nyström method that is much faster than the previous one. It is also based on a product type quadrature rule, but it has the advantage of requiring the computation of modified moments that are independent of the kernel function and can be computed exactly a priori. This produces a great saving of the computational cost.

Such kind of integral equations are of interest because they play an important role in many areas of sciences and, in particular, arise from the reformulation of differential models describing metastatic tumor growth whose unknown solutions represent biological observables as the metastatic mass or the number of metastases [4].

We give sufficient conditions under which the method is convergent in suitable weighted spaces of continuous functions and lead to solve well conditioned linear systems. Numerical examples showing its reliability as well as comparisons with the results obtained with the previous method are presented.

References

[1] M. C. De Bonis, C. Laurita, V. Sagaria, *A numerical method for linear Volterra integral equations on infinite intervals and its application to the resolution of metastatic tumor growth models*, Appl. Num. Math., 172 (2022), pp. 475–496.

[2] I. M. Bulai, M. C. De Bonis, C. Laurita, V. Sagaria, *Modeling metastatic tumor evolution, numerical resolution and growth prediction, Mathematics and Computers in Simulation*, 203 (2023), pp. 721–740.

[3] I. M. Bulai, M. C. De Bonis, C. Laurita, V. Sagaria, *Matlab toolbox for the numerical solution of linear Volterra integral equations arising in metastatic tumor growth models*, Dolomites Research Notes on Approximation 15(2) (2022), pp. 13–24.

[4] N. Hartung, *Efficient resolution of metastatic tumor growth models by reformulation into integral equations*. Discrete and Continuous Dynamical Systems - Series B 20(2), (2015), pp. 445–467.

[5] I. M. Bulai, M. C. De Bonis, C. Laurita, *Numerical solution of metastatic tumor growth models with treatment via Volterra integral equations approach*, in progress.

IMPROVING THE GRAPH BASIS FUNCTION PARTITION OF UNITY METHOD

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Partion of Unity Methods (PUMs) are mesh-free interpolation techniques that enable us to reduce cost-intensive computations, when the number of scattered data is very large. PUM interpolants are given by a sum of local radial kernel approximants and weight functions, where the entire domain is decomposed into several smaller sub-domains of variable radius. Very recently PUMs were combined with a local graph basis function (GBF) approximation method in order to obtain low-cost global interpolation in an efficient way on graphs [1, 2]. However, further developments are needed in order to provide more adaptive techniques for the selection of the partitions on the graph. Here we investigate how to tailor the PUM best possibly to the underlying topology of the graph providing an efficient decomposition with overlapping communities.

References

[1] R. Cavoretto, A. De Rossi, W. Erb, *Partition of Unity Methods for Signal Processing on Graphs*, Journal of Fourier Analysis and Applications, 27 (2021), Article number 66.

[2] R. Cavoretto, A. De Rossi, W. Erb, *GBFPUM-A MATLAB Package for Partition of Unity Based Signal Interpolation and Approximation on Graphs*, Dolomites Res. Notes Approx., 15 (2022), pp. 25–34.

ENERGETIC BOUNDARY ELEMENT METHOD FOR 3D ELASTODYNAMICS

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We consider a boundary integral reformulation of 3D time-domain elastodynamic (vector) wave problems, defined in unbounded domains external to an open polyhedral screen, endowed with a Dirichlet type boundary and null initial conditions. For the resolution of the corresponding Boundary Integral Equation, we use the space-time energetic Galerkin Boundary Element Method (introduced for the first time in [1]) with double analytical integration in time variable. The resulting weakly singular double integrals in space variables are then evaluated by inner analytical and outer numerical integrations [2]. In the presented numerical examples, graded meshes are used to recover the quasi-optimal approximation convergence rates known for screens and for polygonal domains in 3D [3] and the singular behaviour of the solutions from corners and edges.

References

[1] A. Aimi, M. Diligenti, *A new space-time energetic formulation for wave propagation analysis in layered media by BEMs*, Int. J. Numer. Meth. Engng., 75(9) (2008), pp. 1102–1240.

[2] A. Aimi, L. Desiderio, S. Dallospedale, C. Guardasoni, *A space-time Energetic BIE method for 3D Elastodynamics. The Dirichlet case.*, Comput. Mech., (2023), to appear.

[3] A. Aimi, G. Di Credico, H. Gimperlein, E.P. Stephan, *Higher-order time domain boundary elements for elastodynamics - graded meshes and hp versions.*, Numer. Math., (2023), under review.

ON THE NUMERICAL TREATMENT OF LINEAR AND NONLINEAR INVERSE PROBLEMS IN APPLIED GEOPHYSICS

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This talk is concerned with numerical methods for linear and nonlinear inverse problems that arise in applied Geophysics. The main purpose is to reconstruct the electrical conductivity and the magnetic permeability profiles of the soil by using Electromagnetic induction (EMI) techniques. In particular, we solve the following problem

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

where $\mathbf{A} \in \mathbb{R}^{m\times n}$ is a linear/nonlinear operator related to the mathematical model, $\mathbf{b} \in \mathbb{R}^m$ is the measured data, and $\mathbf{x} \in \mathbb{R}^n$ is the unknown, i.e. the electrical conductivity and/or magnetic permeability soil profiles.

A MATLAB software including all the numerical procedures have been developed.

This research line is in collaboration with Cagliari Numerical Analysis Group.

References

[1] G.P. Deidda, P. Díaz de Alba, F. Pes, and G. Rodriguez. *Forward electromagnetic induction modelling in a multilayered half-space: An open-source software tool*. Remote Sens., 15(7):1772, 2023.

[2] A. Buccini and P. Díaz de Alba. *A variational non-linear constrained model for the inversion of FDEM data.* Inverse Problems, 38(1): 014001, 2022.

[3] G.P. Deidda, P. Díaz de Alba, G. Rodriguez, and G. Vignoli. *Inversion of Multiconfiguration Complex EMI Data with Minimum Gradient Support Regularization: A Case Study.* Math. Geosci., 52(7): 945–970, 2020.

[4] G.P Deidda, P. Díaz de Alba, C. Fenu, G. Lovicu, and Rodriguez. *FDEMtools: a MATLAB package for FDEM data inversion.* Numer. Algorithms, 84(4): 1313–1327, 2020.

[5] P. Díaz de Alba, L. Fermo, C. Van der Mee, and G. Rodriguez. *Recovering the electrical conductivity of the soil via a linear integral model.* J. Comput. App. Math., 352:132–145, 2019.

[6] G.P. Deidda, P. Díaz de Alba and G. Rodriguez. *Identifying the magnetic permeability in multi-frequency EM data inversion*. Electron. Trans. Numer. Anal., 47:1–17, 2017.

CONICCURV: A CURVATURE ESTIMATION ALGORITHM FOR PLANAR POLYGONS

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This work presents a derivative free algorithm (*ConicCurv*) to estimate the curvature of a plane curve from a sample of data points. It is based on a known method to estimate tangents that is grounded on classic results of Projective Geometry and Bézier rational conic curves [1]. The curvature values estimated by ConicCurv are invariant to Euclidean changes of coordinates and reproduce the exact curvature values if the data are sampled from a conic. It is shown that ConicCurv has convergence order 3 and if the sample points are uniformly arc-length distributed, the convergence order is 4. The performance of ConicCurv is compared with some of the most frequently used algorithms to estimate curvatures [2] and its effectiveness is illustrated in the calculation of L-curves corners [3].

References

[1] G. Albrecht, J. P. Bécar, G. Farin, D. Hansford, *On the approximation order of tangent estimators*, Computer Aided Geometric Design 25 (2008), pp. 80–95.

[2] A. Belyaev, *Plane and space curves. Curvature. Curvature-based features.* Max-Planck-Institut für Informatik, (2004).

[3] P. C. Hansen, T. K. Jensen, G. Rodriguez, *An adaptive pruning algorithm for the discrete L-curve criterion*, Journal of Computational and Applied Mathematics, 198(2), (2007), pp. 483–492.

SYMMETRIZATION TECHNIQUES IN IMAGE DEBLURRING

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We present a couple of preconditioning techniques that can be used to enhance the performance of iterative regularization methods applied to image deblurring problems with a variety of point spread functions (PSFs) and boundary conditions. More precisely, we first consider the anti-identity preconditioner, which symmetrizes the coefficient matrix associated to problems with zero boundary conditions, allowing the use of MINRES as a regularization method. When considering more sophisticated boundary conditions and strongly nonsymmetric PSFs, the anti-identity preconditioner improves the performance of GMRES. We then consider both stationary and iteration-dependent regularizing circulant preconditioners that, applied in connection with the anti-identity matrix and both standard and flexible Krylov subspaces, speed up the iterations. A theoretical result about the clustering of the eigenvalues of the preconditioned matrices is proved in a special case. The results of many numerical experiments are reported to show the effectiveness of the new preconditiong techniques, including when considering the deblurring of sparse images.

ITERATIVE REGULARIZATION IN BANACH SPACES

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It is well-known that one-step iterative gradient methods to minimize the residual functional $\Phi(x) = \frac{1}{p}\|Ax - y\|_Y^p$, with $p > 1$, act as implicit regularization algorithms for solving the functional equation $Ax = y$ characterized by an ill-posed linear operator $A : X \longrightarrow Y$ between two Banach spaces X and Y, when combined with an early-stopping criterion to prevent over-fitting of the noise on the data y.

We show that gradient-based minimization of the residual, involving both the dual spaces X^* and Y^*, can be fully understood in the context of proximal operator theory, with suitable Bregman distances as proximity measure [1, 3]. Moreover, some relationships with classical projection algorithms of numerical linear algebra, such us Cimmino and Kaczmarz ones, are discussed [2]. After reviewing the key concepts of modular and duality map, we apply Banach spaces iterative regularization to deblurring and subsurface prospecting ima-ging problems.

References

[1] B. Bonino, C. Estatico, M. Lazzaretti, *Dual descent regularization algorithms in variable exponent Lebesgue spaces for imaging*, Numer. Algorithms, 92 (2023), pp. 149–182.

[2] P. Brianzi, F. Di Benedetto, C. Estatico, *Preconditioned iterative re-gularization in Banach spaces*, Comp. Optim. Appl., vol. 54 (2013), pp. 263–282.

[3] M. Lazzaretti, L. Calatroni, C. Estatico, *Modular-proximal gradient algorithms in variable exponent Lebesgue spaces* , SIAM J. Sci. Compu., 44 (2022), pp. 1–23.

ROLE EXTRACTION BY MATRIX EQUATIONS

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The nodes in a network may be grouped into equivalence classes according to the role they play. The grouping is based upon their connections with nodes in either the same role or different roles [1]. Browet and Van Dooren introduced a node similarity matrix for solving this role extraction problem in directed graphs [2]. The sought matrix is the solution of the matrix equation

$$X - \beta^2(AXA^T + A^TXA) = AA^T + A^TA,$$

where A is the adjacency matrix of the network. In a later step, the similarity matrix allows grouping together nodes assigned to the same role. However, this procedure tacitly relies on the assumption that connections inside and between the different roles are fairly uniform, a condition rarely fulfilled in real-world networks. In this talk, I propose a variant of the Browet-Van Dooren method that operates on a suitable diagonal scaling of the adjacency matrix to compensate for the inhomogeneity of node connections.

References

[1] J. Reichardt and D. White, *Role models for complex networks*, Eur. Phys. J. B 60 (2007), pp. 217–224.

[2] A. Browet and P. Van Dooren, *Low-rank similarity measure for role model extraction*, in Proceedings of the 21st MTNS Symposium, 2014, pp. 1412–1418.

CHAINED STRUCTURE OF DIRECTED GRAPHS

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The need to determine the structure of a graph arises in many applications.

Recently, in [1, 2] the notions of chained undirected and chained directed graphs has been introduced. For an undirected graph, the notion of chained graph generalizes bipartivity and allows the determination of *central nodes* of the graph; see [1]. The analysis is based on the use of spanning trees for the graph. A generalization to directed graphs is described in [2]. Under suitable conditions, the chained structure can be uncovered by using spanning trees for directed graphs. When applicable, this analysis allows the definition of central nodes, and has been used to shed light on the structure of graphs that arise in a variety of applications [2]. However, some directed graphs do not have a directed spanning tree, and then the approach to define central nodes of an undirected graph proposed in [2] cannot be applied.

In this talk, we present the notion of chained structure for directed graphs presented in [2] and discuss its extension based on spanning forests instead of on spanning trees. This allows us to identify a chained structure, if present, for a general directed graph. Moreover, we allow edge weights different from one. This generalizes results both in [1, 2] and allows us to define weighted chained structures both for undirected and directed graphs.

References

[1] A. Concas, L. Reichel, G. Rodriguez, and Y. Zhang, *Chained graphs and some applications*, Appl. Netw. Sci., 6:39 (2021).

[2] A. Concas, C. Fenu, L. Reichel, G. Rodriguez, and Y. Zhang, *Chained structure of directed graphs with applications to social and transportation networks*, Appl. Netw. Sci., 7:64 (2022).

ON ANTI-GAUSSIAN SCHEMES APPLIED TO INTEGRAL EQUATIONS

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This talk deals with the application of anti-Gaussian schemes to second-kind Fredholm integral equations of the type

$$f(y) + \int_{\mathcal{D}} k(x,y) f(x) d\mu(x) = g(y), \quad y \in \mathcal{D}.$$

Here, the kernel k and right-hand side g are given, the function f is to be determined, and $d\mu(x)$ is a nonnegative measure supported on a bounded or unbounded domain $\mathcal{D} \subset \mathbb{R}$.

Old and new results will be presented, including extensions to the bivariate case.

This work has been developed with Giuseppe Rodriguez and other collaborators of the Cagliari Numerical Analysis Group.

References

[1] P. Díaz de Alba, L. Fermo, G. Rodriguez. Solution of second kind Fredholm integral equations by means of Gauss and anti-Gauss quadrature rules. Numerische Mathematik 146:699–728, 2020.

[2] P. Díaz de Alba, L. Fermo, G. Rodriguez. Anti-Gauss cubature rules with applications to Fredholm integral equations on the square. In progress.

[3] D. L. Djukić, L. Fermo, R. Mutavdžić Djukić. Averaged cubature schemes on the real positive semiaxis. Numerical Algorithms, 92: 545–569, 2023.

[4] D. L. Djukić, L. Fermo, R. Mutavdžić Djukić. On the numerical solution of bivariate Fredholm integral equations on unbounded domains. In progress.

[5] L. Fermo, L. Reichel, G. Rodriguez, and M. M. Spalević. Averaged Nyström interpolants for the solution of Fredholm integral equations of the second kind. Submitted.

STOCHASTIC GRADIENT DESCENT FOR LINEAR INVERSE PROBLEMS IN VARIABLE EXPONENT LEBESGUE SPACES

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Variable exponent Lebesgue spaces $\ell^{(p_n)}$ have been recently proved to be the appropriate functional framework to enforce pixel-adaptive regularisation in signal and image processing applications, combined with gradient descent (GD) or proximal GD strategies. Compared to Hilbert settings, however, the application of these algorithms in the Banach setting of $\ell^{(p_n)}$ is not straightforward due to the lack of a closed-form expression and the non-separability property of the underlying norm. We propose the use of the associated separable modular function, instead of the norm, to define algorithms based on GD in $\ell^{(p_n)}$ and consider a stochastic GD to reduce the per-iteration cost of iterative schemes, used to solve linear inverse real-world image reconstruction problems.

References

[1] Z. Kereta, and B. Jin, *On the convergence of stochastic gradient descent for linear inverse problems in Banach spaces*, SIAM J. Imaging Sci. (in press), 2023.

[2] M. Lazzaretti, L. Calatroni, and C. Estatico, *Modular-proximal gradient algo- rithms in variable exponent Lebesgue spaces* , SIAM J. Sci. Compu., 44(6), 2022.

[3] B. Bonino, C. Estatico, and M. Lazzaretti, *Dual descent regularization algorithms in variable exponent Lebesgue spaces for imaging*, Numer. Algorithms, 92(6), 2023.

GRASSMANN EXTRAPOLATION AS A TOOL TO ACCELERATE BORN-OPPENHEIMER MOLECULAR DYNAMICS

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Born-Oppenheimer molecular dynamics (BOMD), is a powerful, yet expensive computational tool, where the system's nuclei are propagated classically on a potential energy surface generated on the fly with Density Functional Theory (DFT). The iterative solution to the DFT non-linear equations is the most computationally demanding step in BOMD: to speed up such calculations, various extrapolation strategies have been developed to use information available at previous simulation steps as a guess for the iterative procedure.

In this contribution, we present an approach to extrapolate density matrices, rank n projectors that codify the quantum mechanical information, by using computable maps between the Grassmann manifold where they are defined to its tangent space and back [1]. After comparing the new approach to the state of the art, we discuss its current limitations, with particular focus on energy conservation problems. We introduce a time-reversible extrapolation and an approximately reversible one, that exhibits optimal performance and good numerical stability.

References

[1] É Polack et al., *Grassmann Extrapolation of Density Matrices for Born–Oppenheimer Molecular Dynamics*, J. Chem. Theory Comput. 17 (2021), pp. 6965–6973.

A DEFECT-CORRECTION ALGORITHM FOR QUADRATIC MATRIX EQUATIONS, WITH APPLICATIONS TO QUASI-TOEPLITZ MATRICES

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A defect correction formula for the quadratic matrix equation $A_1X^2 + A_0X + A_{-1} = 0$ is presented. More specifically, assume that $\widetilde{G}$ is an approximation of the sought solution G. Then, by following the ideas of [2] and [3], we derive an equation for the defect $H = G - \widetilde{G}$ and express H in terms of an invariant subspace of a suitable pencil. This equation allows us to introduce a modification of the Structure-preserving Doubling Algorithm (SDA), that enables refining an initial approximation to the sought solution.

Finally, we show an application to the analysis of random walks in the quarter plane, where the matrix coefficients A_i, $i = -1, 0, 1$, as well as the sought solution G, are infinite matrices endowed of the quasi-Toeplitz structure (QT matrices). Numerical experiments confirm the effectiveness of the proposed method. More details can be found in [1].

References

[1] D. A. Bini, B. Meini, *A defect-correction algorithm for quadratic matrix equations, with applications to quasi-Toeplitz matrices*, 2022; arXiv:2212.09491.

[2] A. Bunse-Gerstner, V. Mehrmann, *A symplectic QR like algorithm for the solution of the real algebraic Riccati equation*. IEEE Trans Automat Control. (1986) 31(12):1104–1113.

[3] V. Mehrmann, E. Tan, *Defect correction methods for the solution of algebraic Riccati equations*. IEEE Trans Automat Control. (1988) 33(7):695–698.

A NON-STANDARD NUMERICAL METHOD PRESERVING GLOBAL PROPERTIES OF INTEGRO-DIFFERENTIAL SYSTEMS

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We propose a numerical method for a general integro-differential system of equations which includes a number of age-of-infection epidemic models in the literature [1, 2]. The numerical solution is obtained by a non-standard discretization of the nonlinear terms in the system, and agrees with the analytical solution in many important qualitative aspects. Both the behaviour at finite time and the asymptotic properties of the solution are preserved for any value of the discretization parameter. These properties, together with the fact that the method is linearly implicit, actually make it a computationally attractive tool and, at the same time, a stand-alone discrete model describing the evolution of an epidemic [3, 4].

References

[1] F. Brauer. *Age of infection in epidemiology models*, Electronic Journal of Differential Equations, 2005.

[2] D. Breda, O. Diekmann, W. F. de Graaf, A. Pugliese and R. Vermiglio, *On the formulation of epidemic models (an appraisal of Kermack and McKendrick)*, J. of Biological Dynamics, 6:sup2, 103–117, 2012.

[3] E. Messina, M. Pezzella and A. Vecchio, *A non-standard numerical scheme for an age-of-infection epidemic model*, J. Comput. Dyn., 9 (2), 239–252, 2022.

[4] E. Messina, C. Panico and A. Vecchio, *Global stability properties of non-standard discretization for renewal epidemic models*, in preparation.

SIMULTANEOUS APPROXIMATION OF HILBERT AND HADAMARD TRANSFORMS ON BOUNDED INTERVALS

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In this talk we propose a method to approximate the weighted Hilbert and Hadamard transforms of a given function f

$$\mathcal{H}_0(fw,t) = \int\!\!\!\!\!\!-_{-1}^{1} \frac{f(x)}{x-t} w(x)dx \qquad \mathcal{H}_1(fw,t) = \int\!\!\!\!\!\!=_{-1}^{1} \frac{f(x)}{(x-t)^2} w(x)dx \tag{3}$$

where $t \in (-1,1)$ and $w(x) = (1-x)^\alpha(1+x)^\beta$, $\alpha, \beta > -1$ is a Jacobi weight.
The proposed method is obtained by means of a simultaneous approximation technique involving the extended Lagrange interpolation process (cf. [1]) based on the zeros of the polynomial $p_{m+1}(w)p_m(w)$, where $\{p_n(w)\}_n$ denotes the orthonormal sequence w.r.t the weight w. Moreover, we introduce a scheme that combines the product formula based on the zeros of $p_m(w)$ and the above introduced extended product rule. Such scheme allows a significant reduction in the number of evaluations of the function f. The numerical stability and convergence of this combined scheme are proved in suitable weighted uniform spaces. Finally, some numerical tests are presented in order to highlight the efficiency of the combined scheme and to confirm the theoretical estimates.

References

[1] G. Criscuolo, G. Mastroianni, D. Occorsio. *Convergence of Extended Lagrange Interpolation*, Mathematics of Computation, 55(191) (1990), pp. 197–212.

S-STEP AND FLEXIBLE ENLARGED CONJUGATE GRADIENT METHODS

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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.

References

[1] S. Moufawad. *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.

DIRECT AND INVERSE PROBLEM FOR GAS DIFFUSION IN POLAR FIRN

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Simultaneous use of partial differential equations in conjunction with data analysis has proven to be an efficient way to obtain the main parameters of various phenomena in different areas, particularly in the study of climate change (including global warming) over the past centuries. This requires estimating different gas concentrations in the atmosphere, mainly CO2. In this context, Antarctic and Greenland Polar snow and ice constitute a unique archive of past climates and atmospheres.

The mathematical model of gas trapping in deep polar ice (FIRN) has been derived in [1], consisting of a parabolic partial differential equation that is almost degenerate at one boundary extreme. In this talk, we present the theoretical aspects of existence, uniqueness and simulation for such direct problem ([2]) and consequently formulate the inverse problem that attempts at recovering the diffusion coefficients using given generated data ([3]).

References

[1] E. , P. Martinerie, C. Hogan, et al. (2012). *A new multi-gas constrained model of trace gas non-homogeneous transport in Firn*, Atmos. Chem. Phys., 12, 11465–11483.

[2] S. Moufawad, N. Nassif, and F. Triki, *Direct Problem of Gas Diffusion in Polar Firn*, Arxiv preprint arxiv:2207.07352, 2022.

[3] S. Maad. *Identification of Gas Diffusion Coefficients in Polar Firn*. 2022. American University of Beirut, Master thesis.

NETWORK ANALYSIS WITH THE AID OF THE PATH LENGTH MATRIX

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Let a network be represented by a simple graph $\mathcal{G}$ with n vertices. A common approach to investigate properties of a network is to use the adjacency matrix $A = [a_{ij}]_{i,j=1}^{n} \in \mathbb{R}^{n\times n}$ associated with the graph $\mathcal{G}$, where $a_{ij} > 0$ if there is an edge pointing from vertex v_i to vertex v_j, and $a_{ij} = 0$ otherwise. Both A and its positive integer powers reveal important properties of the graph. This talk proposes to study properties of a graph $\mathcal{G}$ by also using the path length matrix for $\mathcal{G}$. The $(ij)^{th}$ entry of the path length matrix is the length of the shortest path from vertex v_i to vertex v_j; if there is no path between these vertices, then the value of the entry is ∞. Powers of the path length matrix are formed by using min-plus matrix multiplication and are important for exhibiting properties of $\mathcal{G}$. We show how several known measures of communication such as closeness centrality, harmonic centrality, and eccentricity are related to the path length matrix, and we introduce new measures of communication, such as the harmonic K-centrality and global K-efficiency, where only (short) paths made up of at most K edges are taken into account. The sensitivity of the global K-efficiency to changes of the entries of the adjacency matrix also is considered.

WEIGHTED POLYNOMIAL APPROXIMATION ON $(0, +\infty)$ BY DE LA VALLÉE POUSSIN MEANS

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The talk deals with the construction of certain de la Vallèe Poussin type means on $(0, +\infty)$, obtained as the discretization of delayed arithmetic means of Fourier partial sums. We prove that in suitable weighted spaces of functions the norms of such operators are bounded. A comparison with Lagrange interpolating polynomial sequence is shown. Some numerical tests are proposed to confirm the theoretical results.

AN ARNOLDI-BASED PRECONDITIONER FOR ITERATED TIKHONOV REGULARIZATION

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Many problems in science and engineering give rise to linear systems of equations that are commonly referred to as large-scale linear discrete ill-posed problems. These problems arise for instance, from the discretization of Fredholm integral equations of the first kind. The matrices that define these problems are typically severely ill-conditioned and may be rank deficient. Because of this, the solution of linear discrete ill-posed problems may not exist or be extremely sensitive to perturbations caused by error in the available data. These difficulties can be reduced by applying Tikhonov regularization. We describe a novel "approximate Tikhonov regularization method" based on constructing a low-rank approximation to the matrix in the linear discrete ill-posed problem by carrying out a few steps of the Arnoldi process. The iterative method so defined is transpose-free. Our work is inspired by Donatelli and Hanke whose approximate Tikhonov regularization method seeks to approximate a severely ill-conditioned block-Toeplitz matrix with Toeplitz-blocks by a block-circulant matrix with circulant-blocks.

A SIMPLE YET EFFECTIVE TENSOR-BASED ODE MODEL FOR DEEP LEARNING

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In the past few years, applied mathematicians started looking at the forward propagation step of deep learning techniques in terms of discretization methods, e.g., forward Euler, applied to an unknown, underlying differential operator. Each layer of the network is seen as a time step of the discretization method [1, 2]. This point of view paved the way for so-called neural ordinary differential equations (ODE) [3]. In the latter framework, the deep learning process is modeled by an ODE: Inputs are translated into initial values whereas outputs are viewed as the ODE solution evaluated at the final time step. Information propagates along the ODE flow in place of the net so that the extremely problem-dependent design of the latter is no longer needed. The training phase is now employed to learn the parameters definining the neural ODE. In this talk we present a novel tensor-based neural ODE, namely an ODE defined by tensors, to model a deep learning process. Preliminary results on classification problems show the potential of such new tool.

References

[1] L. Ruthotto, E. Haber, *Deep Neural Networks Motivated by Partial Differential Equations*, J Math Imaging Vis, 62 (2020), pp. 352–364.

[2] E. Haber, L. Ruthotto, *Stable architectures for deep neural networks*, Inverse Problems, 34 (2017).

[3] R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. K. Duvenaud, *Neural Ordinary Differential Equations*, Advances in Neural Information Processing Systems, 31 (2018).

A PROJECTION METHOD FOR UNDERDETERMINED LINEAR LEAST-SQUARES PROBLEMS

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In this talk, we describe a projection method for the computation of the minimal-L-norm solution of underdetermined linear least-squares problems. The method consists of an initial projection of the problem which takes into account the null space of L. A solution method that expresses the solution subspace as the direct sum of the null space of L and its orthogonal complement has been introduced in [1] for the solution of large linear discrete ill-posed problems. It has been applied in [2] coupled to the truncated SVD, and it has been employed in [3, 4] in iterative methods for solving large scale Tikhonov minimization problems with a linear regularization operator in general form. We show the reason why the method cannot be applied in conjunction with the GSVD and we propose an approach to overcome this issue. Numerical experiments demonstrate the performance of the method.

References

[1] J. Baglama, L. Reichel, *Decomposition methods for large linear discrete ill-posed problems*, J. Comput. Appl. Math., 198 (2007), pp. 332–343.

[2] S. Morigi, L. Reichel, F. Sgallari, *A truncated projected SVD method for linear discrete ill-posed problems*, Numer. Algorithms, 43 (2006), pp. 197–213.

[3] M. E. Hochstenbach, L. Reichel, *An iterative method for Tikhonov regularization with a general linear regularization operator*, J. Integral Equ. Appl., 22 (2010), pp. 465–482.

[4] Y. Park, L. Reichel, G. Rodriguez, X. Yu, *Parameter determination for Tikhonov regularization problems in general form* , J. Comput. Appl. Math., 343 (2018), pp. 12–25.

MATHEMATICAL MODELLING AND RECONSTRUCTION FOR TERAHERTZ TOMOGRAPHY DATA

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Terahertz imaging is a promising technique in particular in non-destructive testing consider the imaging problem of terahertz (THz). In contrast to X-ray scanners, Terahertz scanners are usually cheaper and can be safely operated in an idustrial invironment. Since typical polymers exhibit low absorption in a range of frequencies up to several THz, this type of radiation is a highly suitable candidate for performing non-destructive testing in a safe way. In the talk we present a nonlinear mathematical model describing a full THz tomography experiment, and consider linear approximations connecting THz tomography with standard computerized tomography and the Radon transform. Based on the derived models we propose different reconstruction approaches for solving the THz tomography problem, which we then compare on experimental data obtained from THz measurements of a plastic sample.

SHANKS' TRANSFORMATIONS, ANDERSON ACCELERATION, AND APPLICATIONS TO SYSTEMS OF EQUATIONS

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In computational sciences it is often necessary to obtain the limit of a sequence of objects of a vector space that converges slowly to its limit or even diverges. It is possible, in some situations, to modify the method that produces the original sequence. However, in many instances, the process by which the sequence is produced is hidden into a black box or too cumbersome for this approach to be practical.

Thus, a solution is to transform this sequence, by means of a sequence transformation, into a new sequence which, under some assumptions, converges faster. Among these techniques Shanks' transformation is arguably the best all-purpose method for accelerating convergence of sequences.

The aim of this talk is to present a general framework for Shanks' transformation(s) of sequences, which. includes the Minimal Polynomial Extrapolation (MPE), the Reduced Rank Extrapolation (RRE), the Modified Minimal Polynomial Extrapolation (MMPE), the Topological Shanks transformation (TEA and STEA algorithm), and also Anderson Acceleration (AA).

Applications to the solution of systems of equations will be discussed.

References

[1] C. Brezinski, M. Redivo-Zaglia, Y. Saad, *Shanks sequence transformations and Anderson acceleration*, SIAM Rev., 60 (2018) 646–669

[2] C. Brezinski, S. Cipolla, M. Redivo-Zaglia, Y. Saad, *Shanks and Anderson-type acceleration techniques for systems of nonlinear equations*, IMA J. Numer. Anal., 42 (2022) 3058–3093.

ON SOLVING SOME CAUCHY SINGULAR INTEGRAL EQUATIONS BY DE LA VALLÉE POUSSIN FILTERED APPROXIMATION

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A numerical solution of Cauchy Singular Integral Equations with constant coefficients based on some non standard polynomial quasi-projection of de la Vallée Poussin type is proposed.

Such kind of approximation presents several advantages over classical Lagrange interpolation such as the uniform boundedness of the Lebesgue constants, the near best order of uniform convergence to any continuous function, and a strong reduction of Gibbs phenomenon [1].

These features are inherited by the proposed numerical method which is stable and convergent, and provides a near best polynomial approximation of the sought solution by solving a well conditioned linear system. The numerical tests confirm the theoretical error estimates and, in case of functions subject to Gibbs phenomenon, they show a better local approximation compared with analogous Lagrange projection methods [2].

References

[1] W. Themistoclakis. *Uniform approximation on* $[-1,1]$ *via discrete de la Vallée Poussin means*, Numer. Algorithms, 60(4)(2012), pp. 593–612.

[2] M. C. De Bonis and G. Mastroianni., *Direct methods for CSIE in weighted Zygmund spaces with uniform norm*, Riv. Mat. Univ. Parma, 2 (2011), pp. 29–55.

ON KRYLOV METHODS FOR LARGE SCALE CBCT RECONSTRUCTION

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Krylov methods are a powerful family of iterative solvers for linear systems, which are commonly used for inverse problems due to their intrinsic regularization properties. Moreover, these methods are naturally suited to large-scale problems, as they only require matrix-vector products with the system matrix (and its adjoint) to compute approximate solutions, and they display a very fast convergence. Even if this class of methods has been widely studied, its use in applied medical physics and applied engineering is still very limited, e.g. in realistic large-scale Computed Tomography (CT) problems, and more specifically in Cone Beam CT (CBCT).

In this talk I will present our attempt to breach this gap by providing a general framework for the most relevant Krylov methods applied to 3D CT problems within an open source framework: the Tomographic Iterative GPU-based Reconstruction (TIGRE) toolbox [1].

I will show different examples in synthetic and real-world 3D CT applications (medical CBCT and μ-CT datasets), and show how Krylov subspace methods perform in this setting, including the most well-known Krylov solvers for non-square systems (CGLS, LSQR, LSMR), possibly in combination with Tikhonov regularization, and methods that incorporate total variation (TV) regularization.

References

[1] M. Sabaté Landman, A. Biguri, S. Hatamikia, R. Boardman, J. Aston and C-B. Schönlieb, *On Krylov Methods for Large Scale CBCT Reconstruction*, preprint (2022).

REVIEW OF THE CONVERGENCE OF THE CONJUGATE GRADIENT METHOD

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Krylov subspace methods [1, 2, 3] are widely used to iteratively solve a variety of linear systems of equations with one or several right-hand sides, or for solving nonsymmetric eigenvalue problems.

The Conjugate Gradient (CG) method is known as one of the best iterative methods for solving symmetric positive definite linear systems. It generates a symmetric triangular matrix with a specific structure that can be very helpful in understanding the convergence behavior of the conjugate gradient method. Its study also provides an interesting alternative to Chebyshev polynomials.

We will also provide a sample formula based on a rational function for the A-norms of the error and residual norms, based on the eigenvalue decomposition of the matrix and the right-hand side. By minimizing this rational function over a convex subset, we can obtain sharp bounds. We use techniques from constrained optimization rather than solving the classical min-max problem.

References

[1] J. Liesen, Z. Strakos, *Krylov subspace methods: principles and analysis*, Numer. Math. and Scientific Comput., Oxford University Press, first edition (2013).

[2] G. Meurant and J. Tabbens, *Krylov methods for non-symmetric linear systems: From theory to computations,* Springer Series in Computational Mathematics, 57 (2020).

[3] Y. Saad, *Iterative Methods for Sparse Linear Systems*. The PWS Publishing Company, Boston, 1996. second edition, SIAM, Philadelphia, (2003).

ON THE KERNEL OF THE VECTOR EPSILON-ALGORITHM

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The vector Epsilon-algorithm introduced by P. Wynn is a powerful method for accelarating the convergence of vector sequences. The algorithm is an extension of the scalar Epsilon algorithm, obtained by replacing the inverse of a real number in the scalar case, by the psoeudo-inverse of a vector in the vector case. The kernel of the vector Epsilon is the set of sequences transformed by the algorithm to stationnary sequences (the constant is a limit or anti-limit of the sequence). It is well-known that the kernel contains sequences satisfying some difference equations.

In this talk, we show that this condition is only sufficient and that the kernel contains other kind of sequnces. We show also how the use of Clifford algebra, can be very helpful for understanding and deriving new results of the algorithm. In particular, we give necessary and sufficient condition for caracterizing the kernel. Examples for illustrations as well as geometrical interpretations are given.

References

[1] C. Brezinski, A. Salam, *Matrix and vector sequence transformations revisited*, Proc. Edinburgh Math. Soc., 38 (1995) 495-510.

[2] A. Salam, *An algebraic approach to the vector ε-algorithm*, Numer. Algorithms, 11 (1996) 327–337.

[3] P. Wynn, *Acceleration techniques for iterated vector and matrix problems*, Math. Comp., 16 (1962) 301–322.

GAUSS-TYPE QUADRATURE RULES FOR VARIABLE-SIGN WEIGHT FUNCTIONS

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When the Gauss quadrature formula G_n is applied, it is usually assumed that the weight function (or the measure) is non-negative on the integration interval $[a, b]$. In the present paper, we introduce a Gauss-type quadrature formula Q_n for weight functions that change the sign in the interior of $[a, b]$. It proves that all nodes of Q_n are pairwise distinct and contained in the interior of $[a, b]$. Moreover, G_n (with a non-negative weight function) turns out to be a special case of Q_n. Obtained results on the remainder term of Q_n suggest that the application of Q_n makes sense both when the points from the interior of $[a, b]$ at which the weight function changes sign are known exactly, as well as when those points are known approximately. The accuracy of Q_n is confirmed by numerical examples.

Keywords: Gauss quadrature rule, variable-sign weight function, modifier function, Vandermonde matrix, maximum norm

PERFECT SHIFTS FOR HESSENBERG-HESSENBERG PENCILS

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In this talk we analyze the stability of the problem of performing a rational QZ step with a shift that is an eigenvalue of a given regular pencil $H - \lambda K$ in unreduced Hessenberg–Hessenberg form. This problem appears when downdating orthogonal rational functions with prescribed poles, i.e., remove a node from the corresponding discrete inner product. In exact arithmetic, the backward rational QZ step moves the eigenvalue to the top of the pencil, while the rest of the pencil is maintained in Hessenberg–Hessenberg form, which then yields a deflation of the given shift. But in finite-precision the rational QZ step gets "blurred" and precludes the deflation of the given shift at the top of the pencil. In this talk we show that when we first compute the corresponding eigenvector to sufficient accuracy, then the rational QZ step can be constructed using this eigenvector, so that the exact deflation is also obtained in finite-precision.

If time permits, we show how the residual can be improved using a scaling procedure and how the method can be applied to general rank structured pencils.

AN APPLICATION OF DYNAMIC PROGRAMMING FOR THE CONTAINMENT OF PESTS AND ALIEN SPECIES INVASIONS IN AGRICULTURE.

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Exotic populations are becoming a nuisance in natural ecosystems while pests in agriculture have always represented problems in view of the damage that they induce to crops. Mathematical models for ecosystems evolution can be formulated via suitable dynamical systems, in which these damaging agents are represented by time dependent variables. In several cases it it possible to assess the ultimate system's behavior and further, to link the various outcomes via bifurcations. Here we consider a few specific ecological situations for which the analytic determination of the steady states and the transcritical bifurcations among them is available. In this setting it is possible to force the system to move from an undesired equilibrium to a more convenient one, by acting on the system parameters. As these actions entail human effort of some kind and therefore a related cost, it is desirable to determine a strategy for which the sought outcome is attained at the minimum cost. Dynamic programming provides the means to tackle this problem, allowing the detection of the cheapest path bringing the system from the current configuration to the expected goal. We propose and describe an algorithm for this purpose.

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