



# **ETNA25**

## **Recent Advances in Scientific Computation**

A Conference to celebrate the 25th birthday of ETNA

S. Margherita di Pula, Cagliari, Italy  
May 27–29, 2019





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A goal of this meeting is to spur interaction and collaboration between participants with different expertise. Such cross fertilization has served the scientific computing community well to reach the present state of knowledge.

The conference will be held at Santa Margherita di Pula outside Cagliari, Sardinia, Italy. A focus of the conference will be new developments in large-scale computation, with an emphasis on image restoration. However, many other topics also will be covered, including Krylov subspace iterative methods, preconditioning, matrix functions, solution of partial differential equations, network analysis, and the solution of ill-posed problems. The conference will have contributed and invited talks, as well as contributed and invited minisymposia.

In addition to providing a forum for researchers to exchange and develop new ideas, the conference also will celebrate the birthdays of ETNA (the 25th) and of Fiorella Sgallari.



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# Scientific Program

- **Plenary Speakers**

- **Michele Benzi**, Scuola Normale Superiore di Pisa, Italy
- **Dario Bini**, Università di Pisa, Italy
- **Franco Brezzi**, C.N.R., Italy
- **Marco Donatelli**, Università dell'Insubria, Italy
- **Andreas Frommer**, Bergische Universität Wuppertal, Germany
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- **Serena Morigi**, Università di Bologna, Italy
- **Fiorella Sgallari**, Università di Bologna, Italy
- **Daniel B. Szyld**, College of Science and Technology Temple University, USA
- **Raf Vanderbril**, KU Leuven, Belgium

- **Minisymposia**

1. **Matrix Equations: Analysis and Algorithms**  
Organized by Dario Bini and Silvia Noschese
2. **Matrix Functions**  
Organized by Claude Brezinski and Michael Eiermann
3. **Iterative Methods for Well and Ill Posed Problems**  
Organized by Alessandro Buccini and Kirk M. Soodhalter
4. **Orthogonal Polynomials and Their Applications in Krylov Space Methods, Interpolation, and Quadrature**  
Organized by Martin H. Gutknecht and Sotirios Notaris
5. **Modern Regularization of Inverse Problems: Theory and Application**  
Organized by Bernd Hofmann and Stefan Kindermann
6. **Krylov Subspace Methods and Their Applications**  
Organized by Thomas Mach and Marc Van Barel
7. **Gauss-type Quadrature Rules: Theory and Applications**  
Organized by Miroslav Pranić and Miograd Spalevic
8. **New Trends in Applied Mathematics: a Tribute to Sebastiano Seatzu**  
Organized by Giuseppe Rodriguez and Cornelis Van Der Mee

- **General Session**





# Abstracts

<b>Plenary Speakers</b>	<b>13</b>
1. M. Benzi, <i>Iterative solution techniques for the coupled Stokes–Darcy problem</i> . . .	15
2. D. A. Bini, <i>On matrix equations associated with random walks in the quarter plane</i>	16
3. F. Brezzi, <i>The virtual element methods. An overview</i> . . . . .	17
4. M. Donatelli, <i>Multigrid preconditioners for space-fractional diffusion equations</i> . . .	18
5. A. Frommer, <i>Analysis of block Krylov subspace methods relying on general block inner products</i> . . . . .	19
6. M. J. Gander, <i>Seven things I would have liked to know when starting to work on domain decomposition</i> . . . . .	20
7. S. Kindermann, <i>Heuristic parameter choice rules in inverse problems</i> . . . . .	21
8. V. Mehrmann, <i>Numerical analysis of finite element systems modeling elastic stents</i>	22
9. S. Morigi, <i>Sparsity-inducing non-convex non-separable regularization for convex image processing</i> . . . . .	23
10. F. Sgallari, <i>Space-variant regularization for image restoration problems</i> . . . . .	24
11. D. B. Szyld, <i>Asynchronous optimized Schwarz methods for the solution of PDEs on bounded domains</i> . . . . .	25
12. R. Vandebril, <i>QRylov</i> . . . . .	26
<b>1. Minisymposium on Matrix Equations: Analysis and Algorithms</b>	<b>27</b>
1. P. Benner, <i>On the solution of the nonsymmetric T-Riccati equation</i> . . . . .	29
2. F. De Terán, <i>Uniqueness of solution of generalized Sylvester-like equations with rectangular coefficients</i> . . . . .	30
3. B. Iannazzo, <i>Schur algorithms for matrix equations</i> . . . . .	31
4. D. Kressner, <i>Low-rank updates and divide-and-conquer methods for matrix equations</i>	32
5. M. Mazza, <i>Rank structure based solvers for 2D fractional diffusion equations</i> . . .	33
6. B. Meini, <i>Matrix equations in Markov modulated Brownian motion: theoretical properties and numerical solution</i> . . . . .	34
<b>2. Minisymposium on Matrix Functions</b>	<b>35</b>
1. B. Beckermann, <i>Low-rank updates of matrix functions</i> . . . . .	37
2. M. Helm, <i>The Fréchet derivative of rational approximations to the matrix exponential and its application on inverse parabolic problems</i> . . . . .	38
3. M. Popolizio, <i>On the numerical approximation of the matrix Mittag-Leffler function with applications to fractional calculus</i> . . . . .	39
4. M. Redivo-Zaglia, <i>Computation of matrix functions by Shanks’ transformations</i> . .	40

5. C. Schimmel, <i>Approximation of the trace of matrix functions based on decay bounds</i>	41
<b>3. Minisymposium on Iterative Methods for Well and Ill Posed Problems</b>	<b>43</b>
1. F. Benvenuto, <i>Predictive risk minimization for the expectation maximization algorithm with Poisson data</i>	45
2. E. de Sturler, <i>Truncation and recycling for iterative hybrid projection methods</i>	46
3. B. Morini, <i>Inexact restoration with subsampled trust-region methods for finite-sum minimization</i>	47
4. R. Ramlau, <i>Efficient minimization of Tikhonov functionals with a sparsity constraint</i>	48
5. M. Sabaté Landman, <i>Flexible GMRES for total variation regularization</i>	49
6. S. Serra-Capizzano, <i>The GLT class as a generalized Fourier analysis and applications</i>	50
<b>4. Minisymposium on Orthogonal Polynomials and Their Applications in Krylov Space Methods, Interpolation, and Quadrature</b>	<b>51</b>
1. A. Bultheel, <i>Orthogonal polynomials with a skew-Hermitian differentiation matrix</i>	53
2. W. Gautschi, <i>Gaussian quadrature rules – made accessible</i>	54
3. C. Glader, <i>Finite Blaschke products in Nevanlinna-Pick interpolation</i>	55
4. M. H. Gutknecht, <i>The Lanczos algorithms, CG, QD, and a whole circle of ideas</i>	56
5. S. E. Notaris, <i>Anti-Gaussian quadrature formulae based on the zeros of Stieltjes polynomials</i>	57
6. W. Van Assche, <i>Simultaneous Gauss quadrature</i>	58
<b>5. Minisymposium on Modern Regularization of Inverse Problems: Theory and Application</b>	<b>59</b>
1. S. Gazzola, <i>Adaptive regularization parameter choice rules for large-scale problems</i>	61
2. D. Gerth, <i>First steps towards the numerical quantification of source conditions</i>	62
3. T. Mach, <i>Adaptive cross approximation for ill-posed problems</i>	63
4. S. V. Pereverzyev, <i>Balancing principle in supervised learning for a general regularization scheme</i>	64
5. R. Plato, <i>Periodic autoconvolution: properties and regularization</i>	65
6. D. Wachsmuth, <i>Tikhonov and Bregman regularization of optimal control problems</i>	66
<b>6. Minisymposium on Krylov Subspace Methods and Their Applications</b>	<b>67</b>
1. D. Camps, <i>Approximate inverse-free rational Krylov methods and the link with FOM and GMRES</i>	69
2. H. Faßbender, <i>On the efficient solution of <math>T</math>-even polynomial eigenvalue problems</i>	70
3. L. Robol, <i>Solving quadratic matrix equations with infinite size coefficients</i>	71
4. V. Simoncini, <i>A GMRES convergence analysis for localized invariant subspace ill-conditioning</i>	72
5. N. Van Buggenhout, <i>Biorthogonal rational Krylov subspace methods</i>	73
<b>7. Minisymposium on Gauss-type Quadrature Rules: Theory and Applications</b>	<b>75</b>
1. M. C. De Bonis, <i>A quadrature method for Cauchy singular integral equations with additional fixed singularities of Mellin type</i>	77

2. K. Deckers, <i>Gauss-Kronrod quadrature formulae based on the zeros of Chebyshev orthogonal rational functions</i> . . . . .	78
3. C. Jagels, <i>Construction of Radau and Lobatto rules from orthogonal Laurent polynomials</i> . . . . .	79
4. R. Orive, <i>Cubature formulas for Gaussian weights. Old and new</i> . . . . .	80
5. S. Pozza, <i>Gauss quadrature for linear functionals and Lanczos algorithm</i> . . . . .	81
<b>8. Minisymposium on New Trends in Applied Mathematics: a Tribute to Sebastiano Seatzu</b>	<b>83</b>
1. C. Brezinski, <i>Our work on regularization</i> . . . . .	85
2. C. Estatico, <i>Regularization in Banach spaces for inverse scattering medical imaging</i>	86
3. L. Fermo, <i>Six years of research with Sebastiano</i> . . . . .	87
4. A. Quarteroni, <i>Numerical models for earthquake ground motion</i> . . . . .	88
5. L. Reichel, <i>Anti-Gauss-type quadrature rules</i> . . . . .	89
6. C. Seatzu, <i>Partial observation in discrete event systems</i> . . . . .	90
<b>Contributed Talks</b>	<b>91</b>
1. F. Arrigo, <i>Non-backtracking PageRank</i> . . . . .	93
2. H. B. Bingham, <i>Interpretation of transformed quantities of potential fields: the case of linear/nonlinear inversion</i> . . . . .	94
3. A. Buccini, <i>Parameter selection rules for <math>\ell^p - \ell^q</math> regularization</i> . . . . .	95
4. K. Burrage, <i>Generation of representative fibrotic patternings in the atria using Perlin noise</i> . . . . .	96
5. A. Concas, <i>On bipartization of networks</i> . . . . .	97
6. O. De la Cruz Cabrera, <i>Compact manifold regression with Sobolev regularization</i> .	98
7. P. Díaz de Alba, <i>A numerical method to solve integral equations by Gauss and anti-Gauss quadrature formulae</i> . . . . .	99
8. D. di Serafino, <i>Subspace accelerated split Bregman methods for constrained fused lasso problems with applications in portfolio optimization</i> . . . . .	100
9. J. Erhel, <i>Optimization problems in geochemistry</i> . . . . .	101
10. D. Fasino, <i>Ergodicity coefficients for second-order Markov chains</i> . . . . .	102
11. C. Fenu, <i>On the identification of the regularization parameter in ill-posed problems</i>	103
12. R. Jiwari, <i>A numerical algorithm for approximation and analysis of Burgers'-Fisher equation</i> . . . . .	104
13. M. Kuian, <i>Optimally conditioned Vandermonde-like matrices</i> . . . . .	105
14. D. Lera, <i>Solving global optimization problems by Peano space-filling curves</i> . . .	106
15. N. Mastronardi, <i>The computation of the Jordan structure of totally nonnegative matrices to high relative accuracy</i> . . . . .	107
16. M. Mitrouli, <i>On the estimation of the tuning parameter in regularized linear regression models</i> . . . . .	108
17. F. Pes, <i>A comparison of regularization methods for solving nonlinear problems</i> . .	109
18. G. Rodriguez, <i>Photometric stereo under unknown lights position</i> . . . . .	110
19. A. Salam, <i>Breakdowns and near breakdowns in symplectic reductions of a matrix to upper J-Hessenberg form</i> . . . . .	111
20. D. S. Watkins, <i>Core-chasing algorithms for the eigenvalue problem</i> . . . . .	112

21. J. R. Winkler, *Blind image deconvolution using a non-separable point spread function* . . . . . 113

**Index of speakers** . . . . . **121**

# **Plenary Speakers**



# ITERATIVE SOLUTION TECHNIQUES FOR THE COUPLED STOKES–DARCY PROBLEM

**M. Benzi**

Scuola Normale Superiore  
Piazza dei Cavalieri 7, 56126 Pisa, Italy  
`michele.benzi@sns.it`

The Stokes–Darcy problem is a coupled system of partial differential equations that arises in fluid mechanics. Discretization of the weak form of these equations by finite element methods leads to large, sparse linear systems with a double (or nested) saddle-point structure. In this talk I will discuss the iterative solution of these linear systems by preconditioned Krylov subspace methods. New block preconditioners will be introduced, analyzed, and compared with existing solvers. The effectiveness of the proposed preconditioners will be demonstrated both theoretically and numerically.

This is joint work with Fatemeh Panjeh Ali Beik (Valie-e-Asr University of Rafsanjan, Iran).

# ON MATRIX EQUATIONS ASSOCIATED WITH RANDOM WALKS IN THE QUARTER PLANE

**D. A. Bini**

Department of Mathematics, University of Pisa  
Largo Bruno Pontecorvo 5, Pisa, Italy  
dario.bini@unipi.it

The numerical solution of random walks in the quarter plane leads to solving matrix equations of the kind  $X = A_1 X^2 + A_0 X + A_{-1}$  where  $A_{-1}, A_0, A_1$  are semi-infinite tridiagonal matrices which share the Toeplitz structure everywhere except in the first row. Solving this kind of equations is an important task in the analysis of queuing networks encountered in the applications.

In this talk, we provide an introduction to the problem, present some models from the applications which motivate this analysis, and discuss some algorithmic approaches.

In particular, we provide conditions under which the solution can be written as the sum of a Toeplitz matrix and a compact correction, and present some algorithms which separately approximate the Toeplitz part and the correction part of the solution. The algorithms which we analyze include fixed point iterations, Newton's method, and the cyclic reduction iteration. Some computational issues are discussed, in particular, solving a Sylvester matrix equation having coefficients with infinite size, representing infinite matrices with a finite number of parameters, and implementing a matrix arithmetic for infinite matrices.



## THE VIRTUAL ELEMENT METHODS. AN OVERVIEW

**F. Brezzi**

Istituto di Matematica Applicata e Tecnologie Informatiche E. Magenes  
Consiglio Nazionale delle Ricerche  
Pavia, Italy  
`brezzi@imati.cnr.it`

The talk will recall the basic principles, the main features, and some more recent results of the Virtual Element Methods. The method is a member of the family of “Galerkin Methods” for dealing with the numerical solution of Partial Differential Equations, and is particularly aimed at the use of decompositions of the computational domain in polygons of polyhedral of very general shape, including elements with curved edges. Some applications to classical Engineering problems will also be outlined.

# MULTIGRID PRECONDITIONERS FOR SPACE-FRACTIONAL DIFFUSION EQUATIONS

**M. Donatelli**

Department of Science and High Technology, University of Insubria  
Via Valleggio, 11 – 22100 Como  
`marco.donatelli@uninsubria.it`

In the last decade Fractional Diffusion Equations (FDEs) have gained a lot of attention in wide range of applicative fields like finance, biology, turbulent flow, image processing, and cardiac electrophysiology. The reason essentially relies on the fact that the so-called *fractional derivative order* can be tuned in order to model enhanced diffusivity.

Even with local discretization methods like finite differences, the nonlocal nature of the fractional operators leads to dense linear systems to be solved. Fortunately, the resulting matrices have a *Toeplitz-like structure*, in the sense that they are expressed as a sum of products between diagonal and dense Toeplitz matrices.

Our contribution in this field is twofold. From one side, we exploit the aforementioned Toeplitz-like structure in order to perform a spectral analysis of the resulting coefficient matrices. On the other hand, we use the obtained spectral information for designing effective multigrid preconditioners for Krylov methods and for studying their convergence properties [1]. Moreover, we propose a robust multigrid preconditioner for the anisotropic problems with application to a space-fractional model for cardiac electrophysiology [2].

## References

- [1] M. Dehghan, M. Donatelli, M. Mazza, H. Moghaderi, *Multigrid methods for two-dimensional space-fractional diffusion equations*, J. Comput. Phys., 350 (2017) 992–1011.
- [2] M. Donatelli, R. Krause, M. Mazza, K. Trotti, *Multigrid preconditioned GMRES for anisotropic space-fractional diffusion equations*, submitted.

# ANALYSIS OF BLOCK KRYLOV SUBSPACE METHODS RELYING ON GENERAL BLOCK INNER PRODUCTS

**A. Frommer**, K. Lund and D.B. Szyld  
Fakultät für Mathematik und Naturwissenschaften  
Bergische Universität Wuppertal  
42097 Wuppertal, Germany  
frommer@math.uni-wuppertal.de

Block Krylov subspace methods for solving  $s$  simultaneous linear systems

$$A\mathbf{X} = \mathbf{B}, \text{ where } A \in \mathbb{C}^{n \times n}, \mathbf{B} = [\mathbf{b}_1 | \dots | \mathbf{b}_s] \in \mathbb{C}^{n \times s}$$

can be faster than methods that treat individually the systems  $A\mathbf{x}_i = \mathbf{b}_i$ ,  $i = 1, \dots, s$ , for two reasons: Since a block Krylov subspace is larger than any of the individual subspaces, one can extract more accurate approximations for the same total investment of matrix-vector multiplications. And since the multiplication of  $A$  with a block vector  $\mathbf{B}$  can be implemented more efficiently than  $s$  individual multiplications, they require less memory access and allow for batch communication.

Starting from the block FOM method, we develop a general concept of modified block FOM methods which includes block GMRES and a “Radau-Arnoldi” variant. We present results on variational characterizations, on properties of the underlying residual matrix polynomials and on comparisons between the iterates for different block inner products. Particular emphasis will then be put on shifted families of block linear systems of the form

$$(A + tI)\mathbf{X}_t = \mathbf{B}, \quad t \in T \subseteq \mathbb{C},$$

where we discuss a computational strategy to keep block residuals “co-spatial” for all  $t$  in the presence of restarts. This allows to build the block Krylov subspace only once for all shifts  $t$ , even after a restart. We show to which extent results from the non-block case do have a natural counterpart for the block case. Maintaining co-spatiality in restarts is mandatory for being able to express the error when approximating matrix functions via block Krylov subspaces, a topic which will be investigated in depth in Kathryn Lund’s contributed talk.

# SEVEN THINGS I WOULD HAVE LIKED TO KNOW WHEN STARTING TO WORK ON DOMAIN DECOMPOSITION

**M. J. Gander**

Section of Mathematics, University of Geneva  
2-4 Rue du Lievre, CP64, 1211 Geneva  
martin.gander@unige.ch

It is not easy to start working in a new field of research. I will give a personal overview over seven things I would have liked to know when I started working on domain decomposition (DD) methods:

1. Seminal contributions to DD not easy to start with
2. Seminal contributions to DD ideal to start with
3. DD solvers are obtained by discretizing 2.
4. There are better transmission conditions than Dirichlet or Neumann
5. "Optimal" in classical DD means scalable
6. Coarse space components can do more than provide scalability
7. DD methods should always be used as preconditioners

# HEURISTIC PARAMETER CHOICE RULES IN INVERSE PROBLEMS

**S. Kindermann**

Industrial Mathematics Institute, Johannes Kepler University of Linz

Linz, Austria

`kindermann@indmath.uni-linz.ac.at`

The choice of the regularization parameter is one of the most important part when computing a regularization for ill-posed problems. It strongly determines the quality of the reconstructed approximate solution and optimal convergence is only obtained by an appropriate selection of the regularization parameter.

One can distinguish between different types of parameter choice rules, namely those that use additional information on the exact solution or the noiselevel and those that only require the given data. The latter ones are called *heuristic* (or data-driven, noiselevel-free) parameter choice rules. Although they are the most practical ones from an application point of view, by a well-known result of Bakushinskii such methods cannot converge in the worst case. Nevertheless, a recent fruitful convergence theory for certain heuristic methods has been established by postulating additional properties of the noise in form of noise condition. In many situations, such noise conditions are satisfied both for random and also deterministic noise, such that the theory covers both deterministic and stochastic inverse problems.

In this talk we would like to give an overview on these rules and the philosophy behind and discuss the main convergence results for the most useful minimization-based heuristic rules, such as the heuristic discrepancy, the Hanke-Raus, and the quasioptimality rules for linear regularization theory. We end with an outlook on the extension of these results to convex Tikhonov regularization.

# NUMERICAL ANALYSIS OF FINITE ELEMENT SYSTEMS MODELING ELASTIC STENTS

L. Grubišić, M. Ljulj, **V. Mehrmann**, J. Tambača  
Institute for Mathematics, MA 4-5, TU Berlin  
Str. des 17 Juni 136, 10623 Berlin, Germany  
`mehrmann@math.tu-berlin.de`

A new model description for the numerical simulation of elastic stents is proposed. Based on the new formulation an  $\inf$ - $\sup$  inequality for the finite element discretization is proved and the proof of the  $\inf$ - $\sup$  inequality for the continuous problem is simplified. The new formulation also leads to faster simulation times despite an increased number of variables. The techniques also simplify the analysis and numerical solution of the evolution problem describing the movement of the stent under external forces. The results are illustrated via numerical examples, see [1].

## References

- [1] L. Grubišić, M. Ljulj, V. Mehrmann, and J. Tambača, Modeling and discretization methods for the numerical simulation of elastic stents, <https://arxiv.org/1812.10096>, Preprint 01-2019, Institute of Mathematics, TU Berlin, submitted for publication, 2019.

# SPARSITY-INDUCING NON-CONVEX NON-SEPARABLE REGULARIZATION FOR CONVEX IMAGE PROCESSING

**S. Morigi,**

Department of Mathematics, University of Bologna  
P.zza Porta San Donato 5, 40126 Bologna, Italy  
serena.morigi@unibo.it

A popular strategy for determining solutions to linear least-squares problems relies on using sparsity-promoting regularizers and is widely exploited in image processing applications such as, e.g., image denoising, deblurring and inpainting. It is well known that, in general, non-convex regularizers hold the potential for promoting sparsity more effectively than convex regularizers such as, e.g., those involving the  $\ell_1$  norm. To avoid the intrinsic difficulties related to non-convex optimization, the Convex Non-Convex (CNC) strategy has been proposed [2, 1], which allows the use of non-convex regularization while maintaining convexity of the total objective function. In this talk, a unified CNC variational model is proposed, based on a more general parametric non-convex non-separable regularizer. A primal-dual forward-backward splitting algorithm is proposed for solving the related saddle-point problem. Numerical experiments related to image deblurring, denoising and inpainting are presented which prove the effectiveness of the proposed approach.

## References

- [1] A. Lanza, S. Morigi, I. Selesnick, F. Sgallari, *Nonconvex nonsmooth optimization via convex-nonconvex majorization-minimization*, *Numerische Mathematik*, 136(2) (2017), pp. 343–381.
- [2] A. Lanza, S. Morigi, F. Sgallari, *Convex Image Denoising via Non-convex Regularization with Parameter Selection*, *Journal of Mathematical Imaging and Vision*, (56)2 (2016), pp.195–220.

## SPACE-VARIANT REGULARIZATION FOR IMAGE RESTORATION PROBLEMS

**F. Sgallari**

Department of Mathematics, University of Bologna  
Piazza di Porta San Donato 5, Bologna, Italy  
`fiorella.sgallari@unibo.it`

Ill-posed problems arise in many areas of science and engineering. Their solutions, if they exist, are very sensitive to perturbations in the data. Regularization aims to reduce this sensitivity. Typically, regularization methods replace the original problem by a minimization problem with a fidelity term and a regularization term. Image restoration is a typical ill-posed problem, which deals with the recovery of the original image from its degraded version by blur and noise. Regularizers for imaging problems can often be derived from a Bayesian framework and determined through a statistical point of view. In this talk we will discuss recent space-variant and directional variational regularization terms for image restoration problems based on explicit statistical assumptions on the gradients of the target image. In particular, starting from the classical TV regularizer, we will introduce several space-variant and also anisotropic generalizations based on sophisticated probabilistic assumptions. Compared to TV, the new regularizers are much more flexible and their several space-variant parameters are automatically computed. The numerical solution of the corresponding image restoration models will be presented and discussed.



# ASYNCHRONOUS OPTIMIZED SCHWARZ METHODS FOR THE SOLUTION OF PDES ON BOUNDED DOMAINS

M. El Haddad, J. C. Garay, F. Magoulés, and **D. B. Szyld**  
Department of Mathematics, Temple University  
Philadelphia, PA, USA  
szyld@temple.edu

Asynchronous methods refer to parallel iterative procedures where each process performs its task without waiting for other processes to be completed, i.e., with whatever information it has locally available and with no synchronizations with other processes. In this talk, an asynchronous version of the optimized Schwarz method is presented for the solution of differential equations on a large parallel computational environment. Convergence is proved under very mild conditions on the size of the subdomains, when optimal as well as approximate (non-optimal) interface conditions are utilized for Poisson's equation (and others) on the plane and on bounded rectangular domains. Numerical results are presented on large three-dimensional problems illustrating the efficiency of the proposed asynchronous parallel implementation of the method.

## QRYLOV

**R. Vandebril**

Department of Computer Science, KU Leuven  
Celestijnenlaan 200A, 3001 Leuven, Belgium.  
raf.vandebril@cs.kuleuven.be

In this lecture we will investigate the intimate connection between Krylov subspaces, structured matrices, and the QR algorithm.

We start by revisiting how Krylov subspaces are lurking behind the convergence and the implicit Q theorem in the classical QR algorithm. Both are essential in *understanding Francis's implicitly shifted QR algorithm*. From the QR algorithm, operating on a Hessenberg matrix, it is straightforward to deduce the QZ algorithm, operating on a Hessenberg – upper triangular pair. The implicit QZ algorithm is, like the QR algorithm, a bulge chasing algorithm, with the bulge hopping from one matrix to the other.

Next, we examine extended Krylov subspaces and see that the theory carries over neatly. Instead of a Hessenberg – upper triangular pair we end up with an *extended* Hessenberg – Hessenberg pair. The extended Hessenberg pair is highly structured: the  $i$ -th subdiagonal element must be zero in exactly one of the two Hessenbergs. The associated *extended QZ* algorithm is still a bulge chasing/hopping algorithm.

Finally, we discuss rational Krylov subspaces. Now we will have to deal with a Hessenberg – Hessenberg pair, where the poles determining the rational Krylov subspace are encoded in the subdiagonal elements of these Hessenberg matrices. Again we can deduce an implicit Q theorem and develop a *rational QZ* algorithm. We will, however, not be able to chase bulges anymore, instead we will have to manipulate the poles and end up with a pole swapping algorithm. The convergence will be governed by subspace iteration driven by rational functions. Some numerical experiments will reveal the advantages of using this rational QZ algorithm.

Many people contributed to this research. I especially like to thank Daan Camps, Karl Meerbergen, Paul Van Dooren, Nicola Mastronardi, David S. Watkins, and Thomas Mach.

# **1. Minisymposium on Matrix Equations: Analysis and Algorithms**

Organized by  
Dario Bini and Silvia Noschese



# ON THE SOLUTION OF THE NONSYMMETRIC T-RICCATI EQUATION

**P. Benner** and D. Palitta

Computational Methods in Systems and Control Theory (CSC)  
Max Planck Institute for Dynamics of Complex Technical Systems  
Magdeburg, Germany  
benner@mpi-magdeburg.mpg.de

We consider the nonsymmetric T-Riccati equation

$$0 = \mathcal{R}_T(X) := DX + X^T A - X^T B X + C, \quad (1)$$

where  $A, B, C, D \in \mathbb{R}^{n \times n}$  and sufficient conditions for the existence and uniqueness of a minimal (w.r.t. entry-wise comparison) solution  $X_{\min} \in \mathbb{R}^{n \times n}$  are provided. To date, the nonlinear matrix equation (1) is still an unexplored problem in numerical analysis and both theoretical results and computational methods are lacking in the literature. We provide some sufficient conditions for the existence and uniqueness of a nonnegative minimal solution and discuss its efficient computation. Both the small-scale and the large-scale settings are addressed and Newton-Kleinman-like methods are derived. The convergence of these procedures to the minimal solution is proved and several numerical results illustrate the computational efficiency of the proposed methods.

# UNIQUENESS OF SOLUTION OF GENERALIZED SYLVESTER-LIKE EQUATIONS WITH RECTANGULAR COEFFICIENTS

**F. De Terán**, B. Iannazzo, F. Poloni, and L. Robol  
Department of Mathematics, Universidad Carlos III de Madrid  
Avda. Universidad 30, 28911, Leganés, Spain  
fteran@math.uc3m.es

We provide necessary and sufficient conditions for the generalized  $\star$ -Sylvester matrix equation,  $AXB + CX^*D = E$ , to have exactly one solution for any right-hand side  $E$ . These conditions are given for arbitrary coefficient matrices  $A, B, C, D$  (either square or rectangular) and generalize existing results for the same equation with square coefficients [1]. We also review the known results regarding the existence and uniqueness of solution for generalized Sylvester and  $\star$ -Sylvester equations. The contents of this talk have been recently published in [2].

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## SCHUR ALGORITHMS FOR MATRIX EQUATIONS

M. Fasi and **B. Iannazzo**

Department of Mathematics and Computer Science,

University of Perugia, Italy

`bruno.iannazzo@unipg.it`

We consider matrix equations of the type  $r(X) = A$ , where  $r$  is a rational function and  $A$  and  $X$  are square matrices of the same size. We provide two algorithms for solving the matrix equation, deduced from two different evaluation schemes of the rational function  $r$  and more efficient, in term of computational cost, than existing algorithms for the same problem [1].

The algorithms are based on a reduction to (block) triangular matrices using the Schur form, followed by a substitution procedure. For triangular data and unknown, our algorithms for solving the equation have the same asymptotic cost as the evaluation schemes from which they are deduced.

The algorithms are then applied to the computation of primary matrix functions defined by an equation of the type  $f(X) = A$ , such as the matrix logarithm [2] and the Lambert  $W$  function (defined by the equation  $X \exp(X) = A$ ) [3].

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# LOW-RANK UPDATES AND DIVIDE-AND-CONQUER METHODS FOR MATRIX EQUATIONS

**D. Kressner**, P. Kürschner, S. Massei, and L. Robol  
Institute of Mathematics, EPFL  
Lausanne, Switzerland  
`daniel.kressner@epfl.ch`

Linear and quadratic matrix equations, such as the Sylvester and Riccati equations, play an important role in various applications, including the stability analysis and dimensionality reduction of linear dynamical control systems and the solution of partial differential equations. In this talk, we present algorithms for quickly updating the solution of such a matrix equation when its coefficients undergo low-rank changes. We demonstrate how our algorithm can be utilized, including the derivation of a new divide-and-conquer approach for matrix equations that feature hierarchical low-rank structure, such as HODLR, HSS, and banded matrices. Numerical experiments demonstrate the advantages of divide-and-conquer over existing approaches, in terms of computational time and memory consumption.

This talk is based on [1, 2].

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# RANK STRUCTURE BASED SOLVERS FOR 2D FRACTIONAL DIFFUSION EQUATIONS

S. Massei, **M. Mazza**, and L. Robol

Department of Science and High Technology, University of Insubria

Via Valleggio 11, 22100 Como Italy

`mariarosa.mazza@uninsubria.it`

In this work, we consider the discretization of time-space diffusion equations with fractional derivatives in space and either 1D or 2D spatial domains. The use of implicit Euler scheme in time and finite differences or finite elements in space leads to a sequence of dense large scale linear systems describing the behavior of the solution over a time interval. We prove that the coefficient matrices arising in the 1D context are rank structured and can be efficiently represented using hierarchical matrices (HODLR format). Qualitative and quantitative estimates for the rank of the off-diagonal blocks of these matrices are presented. Their rank structure is then leveraged to design fast solvers for problems with 2D spatial domains that can be reformulated as matrix equations. In detail, when the right-hand side of the fractional diffusion problem is regular or sparse, the known term of the matrix equation has low-rank properties. This enables the use of Krylov subspace methods which combined with the technology of hierarchically rank structured matrices yields a lower computational complexity in comparison with the current state of the art techniques.

# MATRIX EQUATIONS IN MARKOV MODULATED BROWNIAN MOTION: THEORETICAL PROPERTIES AND NUMERICAL SOLUTION

S. Ahn and **B. Meini**

Dipartimento di Matematica, Università di Pisa

Italy

`beatrice.meini@unipi.it`

The stationary analysis of a Markov modulated Brownian motion [2] becomes easy once the distribution of suitable first passage times is determined. However, this distribution cannot be obtained explicitly and its computation is ultimately reduced to solving a quadratic matrix equation (QME) in [2]. In relation to this, Ahn and Ramaswami [1] derived a nonsymmetric algebraic Riccati equation (NARE) and proved that the distribution can be obtained by using the minimal nonnegative solution of the equation.

In this talk we provide an algebraic connection between the QME and the NARE. More specifically we show that the NARE can be obtained by means of a linearization of a quadratic matrix polynomial associated with the QME. As a consequence, we explicitly relate the solutions of the QME with the solutions of the NARE. To conclude, we discuss some algorithms and accelerating techniques for computing the minimal nonnegative solution of the NARE.

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## **2. Minisymposium on Matrix Functions**

Organized by  
Claude Brezinski and Michael Eiermann



## LOW-RANK UPDATES OF MATRIX FUNCTIONS

**B. Beckermann**

Department of Mathematics, Université de Lille

59655 Villeneuve d'Ascq, France

Bernhard?Beckermann@univ-lille.fr

We consider the task of updating a matrix function  $f(A)$  when the matrix  $A$  of order  $n$  is subject to a low-rank modification. In other words, we aim at approximating  $f(A + D) - f(A)$  for a matrix  $D$  of rank  $k \ll n$ . The approach proposed in this paper attains efficiency by projecting onto tensorized Krylov subspaces produced by matrix-vector multiplications with  $A$  and  $A^*$ . We prove the approximations obtained from  $m$  steps of the proposed methods are exact if  $f$  is a polynomial of degree at most  $m$  and use this as a basis for proving a variety of convergence results, in particular for the matrix exponential and for Markov functions. We illustrate the performance of our method by considering various examples from network analysis, where our approach can be used to cheaply update centrality and communicability measures.

Joint work with D. Kressner & M. Schweitzer (EPFL).

# THE FRÉCHET DERIVATIVE OF RATIONAL APPROXIMATIONS TO THE MATRIX EXPONENTIAL AND ITS APPLICATION ON INVERSE PARABOLIC PROBLEMS

**M. Helm**

Institute for Numerical Mathematics and Optimization,  
TU Bergakademie Freiberg  
D-09596 Freiberg, Germany  
mario.helm@math.tu-freiberg.de

We consider an inverse problem, where a high dimensional parameter  $\mathbf{c}$  has to be identified from measurements of some components of the solution of the parametric initial value problem

$$\mathbf{u}'(t) = A(\mathbf{c})\mathbf{u}(t), \quad \mathbf{u}(0) = \mathbf{b}$$

at some given time points. Here  $A(\mathbf{c})$  is a large sparse symmetric negative definite matrix. Applying Gauß-Newton's method it is important to have information about the sensitivity of the forward solution with respect to the parameter  $\mathbf{c}$ . But due to the size of the problem, it is unfeasible to compute the dense and large Jacobian  $J$  directly. Therefore we will solve the linearized least square problems iteratively (e. g. by LSQR) which requires algorithms to compute products of the form  $J\mathbf{v}$  and  $J^T\mathbf{w}$

We present a new approach, where the forward solution is approximated using the rational best approximation of the exponential function. We will focus on the Fréchet derivatives of the corresponding rational matrix functions, their numerical evaluation and approximation errors with respect to the Fréchet derivative of the matrix exponential. We show how products with the Jacobian and its transpose can be implemented in an economic way, and present numerical examples.

# ON THE NUMERICAL APPROXIMATION OF THE MATRIX MITTAG-LEFFLER FUNCTION WITH APPLICATIONS TO FRACTIONAL CALCULUS

R. Garrappa and **M. Popolizio**

Department of Electrical and Information Engineering

Polytechnic University of Bari

Via E. Orabona 4, Bari, Italy

`marina.popolizio@poliba.it`

The important role played by the Mittag-Leffler (ML) function in fractional calculus is widely known. Furthermore, the ML function evaluated in matrix arguments has useful applications in studying theoretical properties of systems of fractional differential equations and in finding their solution.

In this talk we introduce the ML function with matrix arguments, we review some of its main applications and we discuss the problem of its computation with the challenges it raises.

Since the evaluation at matrix arguments may require the computation of derivatives of the ML function of possible high order we discuss in detail this topic and we show some new formulas for the ML function derivatives.

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# COMPUTATION OF MATRIX FUNCTIONS BY SHANKS' TRANSFORMATIONS

C. Brezinski\* and **M. Redivo-Zaglia**  
Dipartimento di Matematica "Tullio Levi-Civita"  
Università degli Studi di Padova, Italy  
`michela.redivozaglia@unipd.it`

Shanks' transformation is a well know sequence transformation for accelerating the convergence of scalar sequences. It can be recursively implemented by the scalar  $\varepsilon$ -algorithm of Wynn who also extended it to sequences of vectors and of square matrices satisfying a linear difference equation with scalar coefficients [4]. Another extension of the transformation to sequences of elements of a general vector space was proposed and studied by Brezinski in 1975, and can be implemented by the simplified topological  $\varepsilon$ -algorithm [1, 2]. Recently, a more general extension to the matrix case where the matrices can be rectangular and satisfy a difference equation with matrix coefficients, was proposed [3]. In the particular case of square matrices, this transformation can be recursively implemented by the matrix  $\varepsilon$ -algorithm of Wynn.

Numerical experiments on the computation of matrix functions will be presented.

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\*Laboratoire Paul Painlevé, Université de Lille, UMR CNRS 8524, UFR de Mathématiques, France, email: `claude.brezinski@univ-lille1.fr`



# APPROXIMATION OF THE TRACE OF MATRIX FUNCTIONS BASED ON DECAY BOUNDS

A. Frommer and **C. Schimmel**

Department of Mathematics, University of Wuppertal  
Gaußstraße 20, 42119 Wuppertal, Germany  
`schimmel@math.uni-wuppertal.de`

The computation of the trace of functions of sparse matrices is an important task in numerous applications. Since we assume  $A$  to be large and sparse, it is not possible to compute  $f(A)$  and extract the diagonal entries. Commonly, for sparse matrices  $A$ , the matrix  $f(A)$  exhibits a rapid decay away from the sparsity pattern of  $A$ , such that many entries of  $f(A)$  are very small in magnitude. Based on this observation, we present a method for approximating the trace of  $f(A)$ . The method requires decay bounds for the entries of  $f(A)$  and graph coloring algorithms and then computes just a few bilinear forms to determine an approximation of the trace of  $f(A)$ . The algorithm is compared to a stochastic trace estimator and the effectiveness of this approach is shown in numerical experiments.



# **3. Minisymposium on Iterative Methods for Well and Ill Posed Problems**

Organized by  
Alessandro Buccini and Kirk M. Soodhalter



PREDICTIVE RISK MINIMIZATION FOR THE EXPECTATION MAXIMIZATION  
ALGORITHM WITH POISSON DATA

**F. Benvenuto** and P. Massa  
Department of Mathematics, University of Genova  
Via Dodecaneso 35, 16146, Italy  
benvenuto@dima.unige.it

The Expectation Maximization algorithm is a reliable non-linear iterative method for approximating the solution of inverse problems when the forward model is linear, the emitting source is non-negative and data are Poisson variables. As the number of iterations plays the role of a regularization parameter, the main issue is to select it in order to regularize the solution. In this talk we present an estimator of the predictive risk and we propose to stop the algorithm when this estimator reaches its minimum value as a function of iterations. From the theoretical point of view, the estimator relies on a first order approximation of the non-linear iteration and the predictive risk is computed as the expectation of the Kullback-Leibler divergence. While the weakness of this method is the computational burden needed at each iteration, the strength is that it only depends on available data, and therefore it does not need any 'a priori' information. We also point out that this estimator can be thought of as a Poisson variant of the SURE (Stein's Unbiased Predictive Risk Estimator) which is defined for Gaussian noise. Finally, we show the performance of this method when applied to the count-based image reconstruction problem of the STIX (Spectrometer/Telescope for Imaging X-rays) instrument mounted onboard Solar Orbiter.

## TRUNCATION AND RECYCLING FOR ITERATIVE HYBRID PROJECTION METHODS

J. M. Chung, **E. de Sturler**, and J. Jiang  
Department of Mathematics, Virginia Tech  
Blacksburg, Virginia, USA  
sturler@vt.edu

Hybrid iterative algorithms can solve large linear discrete inverse problems very efficiently, as the regularization parameter can be determined dynamically during the iteration. This combines the efficiency of Krylov iterative methods with the opportunity of determining the optimal regularization parameter as the iteration proceeds. In this talk, we focus on methods based on Golub-Kahan Bidiagonalization (GKB). In contrast to the solution of standard least squares problems, where only a few vectors need to be stored in each iteration, hybrid algorithms must store all iteration vectors that span the Krylov space for the solution, since the regularization parameter is not known in advance. If the problem is very large, and convergence is not rapid, this may not be possible.

In this talk, we discuss truncation techniques that allow us to store only a modest number of vectors while using a hybrid projection approach and compute accurate solutions. In addition, this approach allows us to improve convergence by recycling selected subspaces for a sequence of linear inverse problems, from one problem to the next. We also provide convergence theory.

# INEXACT RESTORATION WITH SUBSAMPLED TRUST-REGION METHODS FOR FINITE-SUM MINIMIZATION

S. Bellavia, **B. Morini**, and N. Krejić  
Dipartimento di Ingegneria Industriale  
Università degli Studi di Firenze  
viale Morgagni 40, Firenze, Italia  
`benedetta.morini@unifi.it`

Convex and nonconvex finite-sum minimization arises in many scientific computing and machine learning applications. Recently, first-order and second-order methods where objective functions, gradients and Hessians are approximated by randomly sampling components of the sum have received great attention.

We propose a new trust-region method which employs suitable approximations of the objective function, gradient and Hessian built via random subsampling techniques. The choice of the sample size is deterministic and ruled by the inexact restoration approach. We discuss local and global properties for finding approximate first- and second-order optimal points and function evaluation complexity results. Numerical experience shows that the new procedure is more efficient, in terms of cost per iteration, than the standard trust-region scheme with subsampled Hessians.

# EFFICIENT MINIMIZATION OF TIKHONOV FUNCTIONALS WITH A SPARSITY CONSTRAINT

**R. Ramlau**

Industrial Mathematics Institute, Kepler University Linz

and

Johann Radon Institute for Computational and Applied Mathematics (RICAM)

Linz, Austria

ronny.ramlau@jku.at

In this talk we consider the stable solution of linear inverse problems  $Ax = y$  from noisy measurements  $y^\delta$  with  $\|y - y^\delta\| \leq \delta$ . A standard solution approach is Tikhonov regularization, where a solution is computed as the minimizer of the functional

$$J_\alpha(x) = \|y^\delta - Ax\|^2 + \alpha\Omega(x),$$

where  $\Omega(x)$  denotes a suitable penalty term. We specifically consider *sparsity penalties*  $\Omega(x) = \|x\|_{\ell_p}^p$ . The Tikhonov functional is usually minimized iteratively, but in particular if  $p < 2$ , then the methods converge slowly. In our approach, the Tikhonov functional is transformed to a quadratic functional that allows the use of fast minimization techniques. The numerical performance of the method is validated for examples from Tomography as well as from Single Molecule Microscopy.



## FLEXIBLE GMRES FOR TOTAL VARIATION REGULARIZATION

**M. Sabaté Landman**

Department of Mathematics, University of Bath  
United Kingdom

`m.sabate.landman@bath.ac.uk`

Krylov subspace methods are powerful iterative regularization tools for large-scale linear inverse problems, such as those arising in image deblurring and computed tomography. We exploit a flexible version of some Krylov subspace methods, which uses adaptive preconditioning to promote TV-like regularization in the solution. Numerical experiments and comparisons with other well-known methods for the computation of large-scale solutions are presented.

# THE GLT CLASS AS A GENERALIZED FOURIER ANALYSIS AND APPLICATIONS

**S. Serra-Capizzano**

Dept. of Humanities and Innovation, Insubria U.  
Como (Italy); Dept of Information Technology, Uppsala U. Uppsala (Sweden)  
stefano.serrac@uninsubria.it

Recently, the class of Generalized Locally Toeplitz (GLT) sequences has been introduced [1, 2] as a generalization both of classical Toeplitz sequences and of variable coefficient differential operators and, for every sequence of the class, it has been demonstrated that it is possible to give a rigorous description of the asymptotic spectrum in terms of a function (the symbol) that can be easily identified.

This generalizes the notion of a symbol for differential operators (discrete and continuous) or for Toeplitz sequences for which it is identified through the Fourier coefficients and is related to the classical Fourier Analysis.

The GLT class has nice algebraic properties and indeed it has been proven that it is stable under linear combinations, products, and inversion when the sequence which is inverted shows a sparsely vanishing symbol (sparsely vanishing symbol = a symbol which vanishes at most in a set of zero Lebesgue measure). Furthermore, the GLT class virtually includes any approximation of integro differential equations by local methods (Finite Difference, Finite Element, Isogeometric Analysis and, based on this, we demonstrate that our results on GLT sequences can be used in various directions.

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**4. Minisymposium on  
Orthogonal Polynomials and Their  
Applications in Krylov Space Methods,  
Interpolation, and Quadrature**

Organized by  
Martin H. Gutknecht and Sotirios Notaris



# ORTHOGONAL POLYNOMIALS WITH A SKEW-HERMITIAN DIFFERENTIATION MATRIX

**A. Bultheel**

Department of Computer Science, KU Leuven  
Celestijnenlaan 200A, 3001 Heverlee, Belgium  
adhemar.bultheel@cs.kuleuven.be

We are interested in solving a PDE of the form  $\partial_t u = \partial_x(a(x)\partial_x u)$ ,  $a(x) > 0$ . After discretization in the  $x$ -variable one arrives at a system  $\mathbf{u}'(t) = \mathcal{D}\mathcal{A}\mathcal{D}\mathbf{u}(t)$ ,  $\mathbf{u}(t) = [u(t, x_1), u(t, x_2), \dots]^T \in \ell^2$ ,  $\mathbf{u}(0) = \mathbf{u}_0$ ,  $\mathcal{D}$  is a finite difference approximation of the partial derivative  $\partial_x$  and  $\mathcal{A} = \text{diag}(a(x_1), a(x_2), \dots)$ . Stability requires the system to be dissipative:  $\frac{1}{2} \frac{d\|\mathbf{u}\|^2}{dt} = \mathbf{u}^T \mathbf{u}' = \mathbf{u}^T \mathcal{D}\mathcal{A}\mathcal{D}\mathbf{u} = (\mathcal{D}^T \mathbf{u})^T \mathcal{A}(\mathcal{D}\mathbf{u}) < 0$ . If  $\mathcal{D}$  is skew symmetric, then  $\mathcal{D}^T = -\mathcal{D}$  and stability is satisfied automatically. When using finite differences like  $\frac{f(x+\Delta/2) - f(x-\Delta/2)}{2\Delta}$ , then  $\mathcal{D}$  is skew symmetric, but that is a bit of an exception. However if we want to use spectral methods, then we assume  $u(t, \cdot) = \sum_n u_n(t) \varphi_n$  with  $\{\varphi_n\}_n$  an orthogonal basis for  $L^2(\mathbf{R})$ . If the Fourier basis  $\{\cos(n\xi), \sin(n\xi)\}_n$  on  $[-\pi, \pi]$  or the Hermite polynomials on  $\mathbf{R}$  are arranged in a column  $\hat{\Phi}$ , then they satisfy  $\xi \hat{\Phi}(\xi) = \mathcal{J} \hat{\Phi}(\xi)$  with a symmetric Jacobi matrix  $\mathcal{J}$ . Take the Fourier transform with the proper weight and the result is  $\Phi'(x) = i\mathcal{J}\Phi(x)$ , with  $\mathcal{D} = i\mathcal{J}$  skew Hermitian. A. Iserles and M. Webb recently used this idea and took the Fourier transforms of the Laguerre basis, which resulted in a rational basis that is essentially the rational basis found independently by F. Malmquist and S. Takenaka in 1926. A clever transformation to the unit circle allows to use the fast computation of the Fourier coefficients by FFT. In this lecture we shall explore the effect of free parameters that are still allowed in this approach.

## References

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## GAUSSIAN QUADRATURE RULES – MADE ACCESSIBLE

**W. Gautschi**

Department of Computer Science, Purdue University

West Lafayette, IN 47907-2107, USA

`wgautschi@purdue.edu`

A software repository for Gaussian quadrature is currently being prepared. It consists of a large number of datasets containing Matlab software that allows the user to generate Gaussian quadrature rules to arbitrary precision, for any number of quadrature points, and for a large variety of classical and nonclassical weight functions.

# FINITE BLASCHKE PRODUCTS IN NEVANLINNA-PICK INTERPOLATION

**C. Glader**

Department of Mathematics, Abo Akademi University  
Domkyrkotorget 1, Abo, 20500, Finland  
cglader@abo.fi

Finite Blaschke products play an important role in many problems of interpolation in the complex unit disk  $D$ , often referred to as Nevanlinna-Pick interpolation. Applications are found for example in systems theory in model-matching and design of digital filters. We focus on reviewing some constructive methods for classical Nevanlinna-Pick interpolation from the Schur class consisting of bounded analytic functions  $f$  in the Hardy space  $H^\infty$  on  $D$  such that  $\sup_{z \in D} |f(z)| \leq 1$ , minimal-norm interpolation in  $H^\infty$ , meromorphic interpolation by ratios of finite Blaschke products in  $D$ , and unimodular boundary interpolation by Blaschke products and ratios of such on the unit circle.

# THE LANCZOS ALGORITHMS, CG, QD, AND A WHOLE CIRCLE OF IDEAS

**M. H. Gutknecht**

Seminar for Applied Mathematics, ETH Zurich  
CH-8092 Zurich, Switzerland  
mhg@ethz.ch

In their seminal 1952 paper on the conjugate gradient (CG) method Hestenes and Stiefel pointed out that their method, which is applicable to linear systems of equations with symmetric positive definite matrix only, is closely related to certain orthogonal polynomials, the corresponding Gauss quadrature formulas, certain continued fractions, and their convergents (or 'partial sums'), which are Padé approximants.

Around the same time, in 1950 and 1952, Cornelius Lanczos published two related articles, of which the second one introduced a precursor of the biconjugate gradient (BiCG) method, which generalizes CG to the case of a nonsymmetric system. Here, the residual polynomials are formal orthogonal polynomials only, but the connections to continued fractions and Padé approximants persist. The latter are diagonal ones of the function

$$F(\zeta) := \mathbf{y}_0^H (\zeta \mathbf{I} - \mathbf{A})^{-1} \mathbf{x}_0 = \sum_{k=0}^{\infty} \frac{\mu_k}{\zeta^{k+1}}, \quad \text{where } \mu_k := \mathbf{y}_0^H \mathbf{A}^k \mathbf{x}_0,$$

that involves the resolvent of the matrix  $\mathbf{A}$  and its moments  $\mu_k$  with respect to the starting vectors  $\mathbf{x}_0$  and  $\mathbf{y}_0$ . Moreover, there is a relation to the qd algorithm of Rutishauser (1954). The understanding of all these connections became probably the key to Rutishauser's discovery of the LR algorithm (1955, 1958), which was later enhanced by John G. F. Francis to the ubiquitous QR algorithm (1961/62).

But this is not yet the full circle of ideas. E.g.,  $F$  can be viewed as transfer function of a single-input-single-output linear time-invariant system. Or the Lanczos process can be viewed as one operating on polynomials. It is then seen to be equivalent to the Stieltjes process and delivers an inverse symmetric LDU decomposition of the Hankel moment matrix  $\mathbf{M} := (\mu_{k+l})$ . So, essentially, the Lanczos process gives rise to a fast Hankel solver.



# ANTI-GAUSSIAN QUADRATURE FORMULAE BASED ON THE ZEROS OF STIELTJES POLYNOMIALS

**S. E. Notaris**

Department of Mathematics  
National and Kapodistrian University of Athens  
Panepistemiopolis, 15784 Athens, Greece  
notaris@math.uoa.gr

It is well known that a practical error estimator for the Gauss quadrature formula is by means of the corresponding Gauss-Kronrod quadrature formula developed by Kronrod in 1964. However, recent advances show that Gauss-Kronrod formulae fail to exist, with real and distinct nodes in the interval of integration and positive weights, for several of the classical measures (cf. [2]). An alternative to the Gauss-Kronrod formula, as error estimator for the Gauss formula, is the anti-Gaussian and the averaged Gaussian quadrature formulae presented by Laurie in 1996 (cf. [1]). These formulae always exist and enjoy the nice properties that, in several cases, Gauss-Kronrod formulae fail to satisfy. Now, it is quite remarkable that for a certain, fairly broad, class of measures, for which the Gauss-Kronrod formulae exist, the anti-Gaussian and averaged Gaussian formulae, based on the zeros of the corresponding Stieltjes polynomials, have elevated degree of exactness, and the estimates provided for the error term of the Gauss formula by either the Gauss-Kronrod or the averaged Gaussian formulae are exactly the same.

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# SIMULTANEOUS GAUSS QUADRATURE

**W. Van Assche**

Department of Mathematics, KU Leuven,  
Celestijnenlaan 200 B box 2400, BE-3001 Leuven, Belgium  
walter.vanassche@kuleuven.be

Suppose  $f : \mathbb{R} \rightarrow \mathbb{R}$  is a given function and  $\mu_1, \dots, \mu_r$  are positive measure on the real line. The goal is to approximate the  $r$  integrals  $\int f(x) d\mu_j(x)$ ,  $1 \leq j \leq r$ , by sums of the form  $\sum_{k=1}^N f(x_k) \lambda_k^{(j)}$ ,  $1 \leq j \leq r$ , using the same quadrature nodes  $\{x_j, 1 \leq j \leq N\}$  but with quadrature weights  $\{\lambda_k^{(j)}, 1 \leq k \leq N\}$  depending on the measure  $\mu_j$ . Similar to Gaussian quadrature, there is an optimal choice for the quadrature nodes that maximizes the degree of accuracy: one needs to take the zeros of a multiple orthogonal polynomial for the measures  $(\mu_1, \dots, \mu_r)$ . I will give properties of the quadrature nodes and the quadrature weights for two cases. First I will deal with  $r = 2$  and  $\mu_1$  and  $\mu_2$  positive measures with support on two disjoint intervals [1]; the second case is  $r = 3$  and the measures are normal weights with means  $-c, 0, c$  with  $c$  sufficiently large [2]. In these cases the quadrature nodes belong to  $r$  disjoint intervals  $\Delta_1, \dots, \Delta_r$  and the quadrature weights  $\lambda_k^{(j)}$  are positive for the nodes on  $\Delta_j$ , but alternate in sign for the other nodes. These nodes with alternating sign, however, are exponentially small and hence can be ignored in practice.

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**5. Minisymposium on  
Modern Regularization of Inverse:  
Problems Theory and Application**

Organized by  
Bernd Hofmann and Stefan Kindermann



# ADAPTIVE REGULARIZATION PARAMETER CHOICE RULES FOR LARGE-SCALE PROBLEMS

**S. Gazzola**

Department of Mathematical Sciences, University of Bath  
Bath BA2 7AY, United Kingdom  
S.Gazzola@bath.ac.uk

This talk introduces a new class of adaptive regularization parameter choice strategies that can be efficiently applied when regularizing large-scale linear inverse problems using a combination of projection onto Krylov subspaces and Tikhonov regularization, and that can be regarded as special instances of bilevel optimization methods. The links between Gauss quadrature and Golub-Kahan bidiagonalization are exploited to prove convergence results for some of the considered approaches, and numerical tests are shown to give insight.

# FIRST STEPS TOWARDS THE NUMERICAL QUANTIFICATION OF SOURCE CONDITIONS

**D. Gerth,**

Faculty of Mathematics, Chemnitz University of Technology  
09107 Chemnitz, Germany  
daniel.gerth@mathematik.tu-chemnitz.de

We consider linear ill-posed problems of the form  $Ax = y$  with possibly noisy data  $y$  and exact solution  $x^\dagger$ . A classical assumption in the theory of inverse problems are source conditions of the type  $x^\dagger \in \text{range}((A^*A)^\mu)$  for some  $\mu > 0$ . This allows to bound the worst-case error between approximate solutions and  $x^\dagger$  as the noise goes to zero, and it yields rules for an appropriate choice of the regularization parameter. In the real-world situation where a fixed operator  $A$  and a datum  $y$  are given, a good approximation to  $\mu$  is only available in specific cases, while in general  $\mu$  is unknown, rendering in particular a-priori parameter choice rules unfeasible. In this talk, we make a first attempt of breaking the disconnection between theory and practice. Based on the Kurdyka-Łojasiewicz inequality and the Landweber method, we develop an algorithm that allows to approximate  $\mu$  as long as the noise in the data is not too large. We show several numerical examples, including a controlled academical setup where all parameters are available, examples from the RegularizationTools toolbox, and the realistic case where no information about noise or smoothness is available at all.

We also show that there is a simple lower bound for the reconstruction error, which can be computed without any knowledge of a source condition. We again provide numerous numerical examples and explain how the lower bound allows us to better interpret the results of the approximation of  $\mu$ . It is notable that, if a source condition holds, the lower bound is of the same order as the upper bound.

## ADAPTIVE CROSS APPROXIMATION FOR ILL-POSED PROBLEMS

**T. Mach**, L. Reichel, M. Van Barel, and R. Vandebril  
Department of Mathematical Sciences, Kent State University, Ohio  
and Department of Computer Science, Leuven University, Belgium  
thomas.mach@gmail.com

Consider integral equations of the first kind with a smooth kernel and perturbed right-hand side, i.e. based on contaminated data. Discretization leads to linear systems of equations with singular values clustering near zero. The solution of these systems requires regularization damping or ignoring the small singular values.

Adaptive cross approximation (ACA) is an efficient way to use Gaussian elimination with rook pivoting to find low rank approximations to a given matrix. We will use ACA to approximate a small number of the largest singular values that are sufficient for an approximation of the solution.

Some of our results have been published in [1].

### References

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# BALANCING PRINCIPLE IN SUPERVISED LEARNING FOR A GENERAL REGULARIZATION SCHEME

**S. V. Pereverzyev**

RICAM, Austrian Academy of Sciences  
Altenberger Strasse 69, Linz, Austria  
`sergei.pereverzyev@oeaw.ac.at`

We discuss the parameter choice in learning algorithms generated by general regularization scheme. In contrast to classical deterministic regularization, the performance of regularized learning algorithms is influenced not only by the smoothness of a target function, but also by the capacity of a regularization space. In supervised learning both the smoothness and the capacity are intrinsically unknown. Therefore, we are interested in a posteriori regularization parameter choice rules and propose a new form of the balancing principle. We provide the analysis of the proposed rule and demonstrate its advantages in simulations.

Joint research with Peter Mathe (WIAS-Berlin) and Shuai Lu (Fudan University, Shanghai).



# PERIODIC AUTOCONVOLUTION: PROPERTIES AND REGULARIZATION

B. Hofmann and **R. Plato**

Department of Mathematics, University of Siegen  
Walter-Flex-Str. 3, 57072 Siegen, Germany  
plato@mathematik.uni-siegen.de

In the first part of this presentation, we consider some properties of the periodic autoconvolution operator. This includes monotonicity as well as mapping properties in Sobolev spaces of periodic functions. In addition, the optimality of regularization methods is investigated in a general framework. In a second part, recent results on a variational inequality formulation of Lavrentiev regularization for solving periodic autoconvolution equations are given. New convergence rates are presented which in fact is done in an abstract setting. Finally, the regularizing properties of a Galerkin scheme for solving periodic autoconvolution problems are considered.

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# TIKHONOV AND BREGMAN REGULARIZATION OF OPTIMAL CONTROL PROBLEMS

**D. Wachsmuth**

Institut für Mathematik,  
Universität Würzburg,  
97074 Würzburg, Germany,

`daniel.wachsmuth@mathematik.uni-wuerzburg.de`

In the talk, we review results on Tikhonov regularization of optimal control problems. A special feature of these problems are pointwise inequality constraints. Standard source conditions known from inverse problems theory are not applicable in the optimal control setting. We present conditions that give convergence rates for Tikhonov regularization. In addition, iterated Bregman regularization is introduced, where the indicator function of the feasible set enters. It turns out that classical results for iterated Tikhonov methods transfer to this new method. The talk ends with perspectives of open problems.

# **6. Minisymposium on Krylov Subspace Methods and Their Applications**

Organized by  
Thomas Mach and Marc Van Barel



# APPROXIMATE INVERSE-FREE RATIONAL KRYLOV METHODS AND THE LINK WITH FOM AND GMRES

**D. Camps**, S. Güttel, T. Mach, and R. Vandebril  
Department of Computer Science, KU Leuven  
Belgium  
daan.camps@cs.kuleuven.be

In this presentation we revisit the approximate rational Krylov method [1, 2, 3]. We present two alternative but mathematically equivalent formulations of the same algorithm. The first reformulation uses a *pole swapping* technique and is an implicit method, just like the original algorithm. The second reformulation explicitly solves shifted linear systems using the Arnoldi Hessenberg matrix. This reformulation leads us to a connection between the approximate rational Krylov method and the full orthogonalization method (FOM). Finally, we show how the approximate rational Krylov method can be modified to obtain a similar connection with GMRES.

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# ON THE EFFICIENT SOLUTION OF $T$ -EVEN POLYNOMIAL EIGENVALUE PROBLEMS

**H. Faßbender**, and Ph. Saltenberger  
ICM, AG Numerik, TU Braunschweig  
Universitätsplatz 2, 38106 Braunschweig, Germany  
h.fassbender@tu-braunschweig.de

The polynomial eigenvalue problem  $A(\lambda)u = 0$  for

$$A(\lambda) = \sum_{k=0}^d A_k \lambda^k, \quad A_k \in \mathbb{R}^{n \times n}$$

with  $A_k = A_k^T$  if  $k$  is even and  $A_k = -A_k^T$  otherwise is considered. Such matrix polynomials have been named alternating or  $T$ -even. The eigenvalues of such matrix polynomials  $A(\lambda)$  have a Hamiltonian eigenstructure; that is, the spectrum is symmetric with respect to both the real and the imaginary axis.

We discuss the numerical solution of  $T$ -even polynomial eigenvalue problems and show how a small part of the spectrum can be obtained using just  $\mathcal{O}(n^3)$  arithmetic operations. For that purpose, we apply the EVEN-IRA algorithm proposed in [2] to a special structure-preserving linearization proposed in [1]. In this particular situation, the Arnoldi iteration as a main part of the EVEN-IRA algorithm can be realized very efficiently.

## References

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# SOLVING QUADRATIC MATRIX EQUATIONS WITH INFINITE SIZE COEFFICIENTS

D. A. Bini, B. Meini, J. Meng, and **L. Robol**  
Department of Mathematics, University of Pisa  
Pisa, Italy  
leonardo.robol@unipi.it

When dealing with quadratic matrix equations  $A_{-1} + A_0X + A_1X^2 = 0$ , arising in the context of quasi-birth-death stochastic processes, one of the approaches is to rely on the Newton method; the latter is guaranteed to converge to the solution of interest in this context.

When the coefficients  $A_j$ , for  $j = -1, 0, 1$ , are infinite quasi-Toeplitz matrices, the same technique can be used. However, the computation of the Newton correction now requires the solution of Sylvester equations involving infinite matrices. We show that rational Krylov methods are applicable in this setting, with some adaptations needed to work in the infinite dimensional context. This is achieved exploiting the quasi-Toeplitz structure of the matrices under consideration. The numerical method has been implemented in the MATLAB toolbox `cqt-toolbox` [1].

## References

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# A GMRES CONVERGENCE ANALYSIS FOR LOCALIZED INVARIANT SUBSPACE ILL-CONDITIONING

G. Sacchi, and **V. Simoncini**  
Dipartimento di Matematica,  
Università di Bologna,  
Piazza di Porta S. Donato, 5,  
I-40127 Bologna, Italy  
valeria.simoncini@unibo.it

The Generalized Minimal RESidual (GMRES) method is a well established strategy for iteratively solving a large linear system  $Ax = b$ , where  $A \in \mathbb{R}^{n \times n}$  is a nonsymmetric and nonsingular coefficient matrix, and  $b \in \mathbb{R}^n$ . In the analysis of its convergence for  $A$  diagonalizable, a much used upper bound for the relative residual norm involves a min-max polynomial problem over the set of eigenvalues of  $A$ , magnified by the condition number of the eigenvector matrix of  $A$ . This latter factor may cause a huge overestimation of the residual norm, making the bound non-descriptive in practice. We show that when a large condition number is caused by the almost linear dependence of few of the eigenvectors, a more descriptive analysis of the method's behavior can be performed, irrespective of the location of the corresponding eigenvalues. The new analysis aims at capturing how the GMRES polynomial deals with the ill-conditioning; as a byproduct a new upper bound for the GMRES residual norm is obtained. A variety of numerical experiments illustrates our findings.

## References

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## BIORTHOGONAL RATIONAL KRYLOV SUBSPACE METHODS

**N. Van Buggenhout**, M. Van Barel, and R. Vandebril  
Department of Computer Science, KU Leuven  
Celestijnenlaan 200A, 3001 Leuven, Belgium  
`niel.vanbuggenhout@kuleuven.be`

Rational Krylov subspace methods use rational functions of a given matrix instead of polynomials to construct a Krylov subspace. The poles of these rational functions can be chosen and allow us to manipulate the convergence of the methods to an area of interest in the spectrum of the matrix.

An overview of known projections of matrices onto various Krylov subspaces is provided. Most notably orthogonal projection onto rational Krylov subspaces, which can be represented by an upper-Hessenberg or inverse upper-Hessenberg matrix pencil. Starting from these results we prove that a tridiagonal matrix pencil suffices to represent the oblique projection of a given matrix onto rational Krylov subspaces. This is the most sparse of several possible representations.

The tridiagonal matrix pencil relates to a six-term recurrence to construct a pair of biorthogonal bases for rational Krylov subspaces. This is a Lanczos-type iteration which elegantly generalizes the polynomial case, in which the recurrence consists of 4 terms. Furthermore this algorithm generalizes, besides Lanczos and biorthogonal Lanczos, several other known algorithms, e.g., AGR/CMV-factorization and more recent results concerning extended Krylov subspaces.

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# **7. Minisymposium on Gauss-type Quadrature Rules: Theory and Applications**

Organized by  
Miroslav Pranić and Miodrag Spalević



# A QUADRATURE METHOD FOR CAUCHY SINGULAR INTEGRAL EQUATIONS WITH ADDITIONAL FIXED SINGULARITIES OF MELLIN TYPE

**M. C. De Bonis** and C. Laurita

Department of Mathematics, Computer Science and Economics

University of Basilicata

Via dell'Ateneo Lucano 10, 85100 Potenza, ITALY

mariacarmela.debonis@unibas.it

This talk deals with a quadrature method for approximating the solutions of Cauchy singular integral equations with additional terms of Mellin convolution type defined as follows

$$a u(\tau) + \frac{b}{\pi} \int_{-1}^1 \frac{u(t)}{t-\tau} dt + \int_{-1}^1 k(t, \tau) u(t) dt + \int_{-1}^1 h(t, \tau) u(t) dt = g(\tau), \quad |\tau| < 1, \quad (2)$$

where  $u(\tau)$  is the unknown,  $h(t, \tau)$  and  $g(\tau)$  are sufficiently smooth functions,  $a$  and  $b$  are given real constants such that  $a^2 + b^2 = 1$ , and  $k(t, \tau)$  is a Mellin kernel. The first integral is understood in the Cauchy principal value sense.

Since several mathematical problems in physics and engineering can be reduced to the solution of integral equations of the form (2), the development of numerical methods for approximating their solution has been receiving an increasing interest in recent years. In particular, discretization schemes based on polynomial approximation have been considered in [1, 2, 3], mainly in the case where  $k(t, \tau)$  is a special Mellin kernel.

The unknown function  $u$  is approximated by a weighted polynomial that is the solution of a finite dimensional equation obtained by discretizing the integral operators by a Gauss-Jacobi quadrature rule. More precisely, in order to achieve stability and convergence results, the Gaussian formula is applied to the Mellin integral operator with a slight modification. The well conditioning of the involved linear systems is proved. The efficiency of the proposed method is shown through some numerical tests.

## References

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# GAUSS-KRONROD QUADRATURE FORMULAE BASED ON THE ZEROS OF CHEBYSHEV ORTHOGONAL RATIONAL FUNCTIONS

**K. Deckers**

Laboratoire de Mathématiques Paul Painlevé, Université de Lille  
Lille, France

karl.deckers@math.univ-lille1.fr

Consider the nested sequences of arbitrary complex or infinite poles  $\mathcal{A}_k := \{\alpha_j\}_{j=1}^k$ ,  $k = 1, 2, \dots$ , outside the interval  $I = [-1, 1]$ . Let  $\varphi_n$ ,  $n > 1$  denote the rational function with poles among  $\mathcal{A}_n$ , and orthogonal to the space of rational functions with poles among  $\mathcal{A}_{n-1}$  with respect to the Chebyshev weight function  $w(x) = (1-x)^a(1+x)^b$ , where  $a, b \in \{\pm 1/2\}$ . Whenever  $\alpha_n$  is real or infinite, the zeros  $\{x_{n,k}\}_{k=1}^n$  of  $\varphi_n$  are all real, distinct, and inside the interval  $I$ ; hence, they are the nodes in an  $n$ -point rational Gauss-Chebyshev quadrature formula that is exact in the space of rational functions  $\tilde{\mathcal{L}}_{2n-1}$  with poles among  $\tilde{\mathcal{A}}_{2n-1} := \{\alpha_k, \bar{\alpha}_k\}_{k=1}^{n-1} \cup \{\alpha_n\}$ .

In this talk we present  $(2n + 1)$ -point rational Gauss-Kronrod quadrature formulae of the form

$$\int_{-1}^1 f(x)w(x)dx = \sum_{k=1}^n \lambda_{2n+1,k} f(x_{n,k}) + \sum_{j=1}^{n+1} \lambda_{2n+1,n+j} f(y_{n+1,j}) + R_{2n+1}(f)$$

with positive weights  $\{\lambda_{2n+1,k}\}_{k=1}^{2n+1}$  and distinct nodes  $\{y_{n+1,j}\}_{j=1}^{n+1} \subset I$ , interlacing with the nodes  $\{x_{n,k}\}_{k=1}^n$ , that are exact (i.e.,  $R_{2n+1}(f) = 0$ ) in a space of rational functions  $\hat{\mathcal{L}}_m \supset \tilde{\mathcal{L}}_{2n-1}$  with  $m$  as large as possible.

# CONSTRUCTION OF RADAU AND LOBATTO RULES FROM ORTHOGONAL LAURENT POLYNOMIALS

**C. Jagels**

Hanover College

Hanover, IN, USA

`jagels@hanover.edu`

The construction of Gaussian rules can be viewed as a spectral decomposition of the tridiagonal Jacobi matrix generated by the Lanczos process. Radau and Lobatto rules follow from a modification of this matrix. Analogous rules exist for Laurent polynomials, polynomials that contain reciprocal powers. The analog of the tridiagonal recursion matrix is a pentadiagonal matrix. This talk discusses augmentations of the pentadiagonal matrix that yield a Radau and Lobatto rules that integrate exactly one or two more positive powers, negative powers, or a combination therein.

## CUBATURE FORMULAS FOR GAUSSIAN WEIGHTS. OLD AND NEW

**R. Orive**, and J. C. Santos–León  
Departamento de Análisis Matemático, Universidad de La Laguna  
The Canary Islands, Spain  
rorive@ull.es

In the first part of this talk some general features of Cubature formulas are recalled. As it is well known, despite what happens in the univariate case (Gaussian Quadrature rules), the problem of getting useful Cubature rules with a prescribed degree of algebraic precision and a reasonable number of nodes is far from being solved. In this sense, we focus on Cubature formulae for integrals with the Gaussian weight in  $\mathbf{R}^n$ , that is,

$$I(f) = \int_{\mathbf{R}^n} f(\mathbf{x}) e^{-\mathbf{x}^T \mathbf{x}} d\mathbf{x}.$$

Then, after reviewing some known rules for this kind of integrals, some new ones are introduced and their accuracy is checked by means of some numerical examples.



# GAUSS QUADRATURE FOR LINEAR FUNCTIONALS AND LANCZOS ALGORITHM

**S. Pozza**, M. Pranić, and Z. Strakoš  
Department of Numerical Mathematics, Charles University  
pozza@karlin.mff.cuni.cz

The Gauss quadrature can be naturally generalized to approximate quasi-definite linear functionals where the interconnections with (formal) orthogonal polynomials, (complex) Jacobi matrices and Lanczos algorithm are analogous to those in the positive definite case. In particular, the existence of the  $n$ -weight (complex) Gauss quadrature corresponds to successfully performing the first  $n$  steps of the Lanczos algorithm; see, e.g., [1, 2]. Such connections can also be extended to the case of (look-ahead) Lanczos algorithm.

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**8. Minisymposium on  
New Trends in Applied Mathematics:  
a Tribute to Sebastiano Seatzu**

Organized by  
Giuseppe Rodriguez and Cornelis Van Der Mee



## OUR WORK ON REGULARIZATION

S. Seatzu

with

**C. Brezinski**, M. Redivo-Zaglia, G. Rodriguez

Laboratoire Paul Painlevé, Université de Lille

Villeneuve d'Ascq, France

`claude.brezinski@univ-lille.fr`

In this talk, we give a short overview of the work on Tikhonov regularization done by the authors in Cagliari. Our main purpose was to present new procedures based on extrapolation and estimation of the error to find the best (or, at least a good) value of the regularization parameter(s).

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# REGULARIZATION IN BANACH SPACES FOR INVERSE SCATTERING MEDICAL IMAGING

**C. Estatico**

Department of Mathematics, University of Genoa  
Via Dodecaneso 35, I-16146 Genova, Italy  
estatico@dima.unige.it

In electromagnetic inverse scattering, the characterization of an (unknown) scattering object inside an investigation domain is based on retrieving the equivalent source from the scattered field outside the source region, due to the illumination by a known electromagnetic incident field. Inverse scattering imaging is very useful in biomedical applications where the dielectric properties of human tissues have to be restored by means of minimally-invasive techniques. The mathematical model of this inverse problem leads to the solution of an ill-posed, nonlinear and implicit 3D integral equation.

After a brief introduction about regularization theory in Banach spaces, in this talk we discuss a conjugate-gradient-based iterative regularization algorithm developed in  $L^p$  spaces, with  $1 < p < +\infty$ , for solving the inverse scattering problem which involves large-scale structured matrices. The proposed method can be useful for continuous monitoring of hemorrhagic brain strokes via microwaves. We will show numerical simulations with anatomically-realistic phantoms, as well as some preliminary experimental results.

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## SIX YEARS OF RESEARCH WITH SEBASTIANO

**L. Fermo**, C. van der Mee and S. Seatzu  
Department of Mathematics and Computer Science  
University of Cagliari, Italy  
fermo@unica.it

In the last ten years, Sebastiano Seatzu enjoyed studying nonlinear partial differential equations of integrable type (among the others [2, 3, 4, 5]). His interest laid in the applicative nature of these equations which are, for instance, used to describe electromagnetic waves in optical fibers and surface wave dynamics, and his intention was to solve them numerically following the whole path of the so-called Inverse Scattering Transform.

Such a research saw me as a co-author, along with Cornelis van der Mee, of his last eight works, of which six were published and two were incomplete.

In this talk we focus on the research which was in progress when he left us on February 13th, 2018, namely, the numerical treatment of the Korteweg-de Vries (KdV) equation which governs the propagation of surface water waves in long, narrow, shallow canals [1]

$$q_t - 6qq_x + q_{xxx} = 0, \quad x \in \mathbb{R}, \quad t > 0.$$

### References

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## NUMERICAL MODELS FOR EARTHQUAKE GROUND MOTION

**A. Quarteroni**

Politecnico di Milano and EPFL, Lausanne

`alfio.quarteroni@polimi.it`

Physics-based numerical simulations provide a powerful tool to study the ground motion induced by earthquakes in regions threatened by seismic hazards. They can be used to better understand the physics of earthquakes, improve the design of site-specific structures, and enhance seismic risk maps. The distinguishing features of a numerical method designed for seismic wave propagation are: accuracy, geometric flexibility and parallel scalability. High-order methods ensure low dissipation and dispersion errors. Geometric flexibility allows complicated geometries and sharp discontinuities of the mechanical properties to be addressed. Finally, since earthquake models are typically posed on domains that are very large compared to the wavelengths of interest, scalability allows to efficiently solve the resulting algebraic systems featuring several millions of unknowns. In this talk we present a spectral element discontinuous Galerkin method on hybrid (non-conforming) grids for the numerical solution of three-dimensional wave propagation problems in heterogeneous media.



## ANTI-GAUSS-TYPE QUADRATURE RULES

**L. Reichel**

Department of Mathematical Sciences, Kent State University  
Kent, OH 44242, USA  
reichel@math.kent.edu

Pairs of Gauss and anti-Gauss quadrature rules can be used to estimate the error in Gauss rules. Anti-Gauss rules were proposed by Laurie for nonnegative real measures on the real line. This talk reviews generalizations and simplifications of these rules, as well as extensions to matrix-values measures. Also anti-Gauss-type quadrature rules associated with multiple orthogonal polynomials will be described. Applications to network analysis will be discussed. This talk presents joint work with H. Alqahtani, C. Fenu, D. Martin, M. Pranić, and G. Rodriguez.

## PARTIAL OBSERVATION IN DISCRETE EVENT SYSTEMS

**C. Seatzu**

Dept. of Electrical and Electronic Eng., Univ. of Cagliari  
Piazza D'Armi, Cagliari, Italy  
seatzu@diee.unica.it

This talk focuses on a particular class of dynamic systems, namely *discrete event systems* (DESs), which provide the theoretical fundation for the study of dynamic artificial systems, namely man made systems [1]. A DES (or event-driven system), different from time-driven systems, is a dynamic system with a discrete state space, whose evolution depends entirely on the occurrence of asynchronous physical events that determine a state transition. DESs find application in several areas, such as computer science, telecommunication, manufacturing, transportation, logistics, etc. Several problems have been studied in this framework in the last decades, in particular supervisory control, reachability and deadlock analysis, and a series of problems related to the partial observation of the system evolution. In this talk we focus on the last class of problems: we introduce the fundamental problem of state state estimation under partial observation and a series of other problems that can be formulated in the same framework, such us fault diagnosis [2] and opacity analysis [3], two problems that are gaining a growing attention in the framework of cyber-physical systems.

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# **Contributed Talks**



# NON-BACKTRACKING PAGERANK

**F. Arrigo**, Desmond J. Higham, and V. Noferini

Department of Mathematics and Statistics, University of Strathclyde  
Glasgow, Scotland

`francesca.arrigo@strath.ac.uk`

The PageRank algorithm, which has been “bringing order to the web” for more than twenty years, computes the steady state of a classical random walk plus teleporting [3, 4]. Here we consider a variation of PageRank that uses a non-backtracking random walk. To do this, we first reformulate PageRank in terms of the associated line graph. A non-backtracking analog then emerges naturally [2, 5]. Comparing the resulting steady states, we find that, even for undirected graphs, non-backtracking generally leads to a different ranking of the nodes [6]. We then focus on computational issues, deriving an explicit representation of the new algorithm that can exploit structure and sparsity in the underlying network. Finally, we assess effectiveness and efficiency of this approach on some real-world networks.

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# INTERPRETATION OF TRANSFORMED QUANTITIES OF POTENTIAL FIELDS: THE CASE OF LINEAR/NONLINEAR INVERSION

V. Paoletti\*, **H. B. Bingham**, M. A. Abbas<sup>†</sup> and M. Fedi\*  
Department of Mechanical Engineering  
Technical University of Denmark  
Lyngby, Denmark  
hbb@mek.dtu.dk.

We propose an approach for the nonlinear constrained inversion of quantities derived from nonlinear transformations of potential field data. Among these quantities, the Normalized Source Strength (NSS, e.g., [1]) and the Total Gradient (TG, [2]) are always non-negative and minimally affected by the direction of the source's remanent magnetization. Our Generalized Singular Value Decomposition analysis on the NSS and TG problems shows that the inversion of quantities deriving from nonlinear transformations of potential field data by a linear algorithm introduces non-negligible errors, which make regularization necessary. Despite that, the linear inversion approach of NSS and TG is often used in the literature without investigating its theoretical and practical limits. We here employ a nonlinear iterative approach for constrained inversion of TG which leads to more reliable reconstructions of the subsurface density/magnetization distribution. The method has some similarities to the one developed by [3]. The linearization of the problem at each iteration allows monitoring the depth resolution of the inversion models and the influence of errors through monitoring tools normally used for linear problems, such as the Picard Plot.

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\*Department of Earth, Environment and Resources Science, University of Naples Federico II, Complesso di Monte S. Angelo, Naples, Italy, email: {fedi, paoletti}@unina.it

<sup>†</sup>Geology Department, South Valley University, Qena, Egypt, e-mail: mahmoud.ahmed1@sci.svu.edu.eg

## PARAMETER SELECTION RULES FOR $\ell^p - \ell^q$ REGULARIZATION

**A. Buccini** and L.Reichel

Department of Mathematical Sciences, Kent State University  
Kent, OH 44242, USA  
abuccini@kent.edu

Discrete ill-posed problems arise in many areas of science and engineering. Their solutions are very sensitive to perturbations. Regularization aims to reduce this sensitivity. Many regularization methods replace the original problem with a minimization one with a fidelity term and a regularization term. The use of a  $p$ -norm for the fidelity term and a  $q$ -norm for the regularization term, where  $0 < p, q \leq 2$ , has received considerable attention. The relative importance of these terms is determined by a regularization parameter.

The choice of a suitable regularization parameter is crucial. In this talk we discuss the various approaches for determining the regularization parameter automatically proposed in [1, 2, 3]. Computed examples of restoration of impulse noise and Gaussian noise contaminated images are presented.

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## GENERATION OF REPRESENTATIVE FIBROTIC PATTERNINGS IN THE ATRIA USING PERLIN NOISE

D. Jakes, **K. Burrage**, C. Drovandi, P. Burrage, A. Bueno-Orovio\*, and B. Lawson  
School of Mathematical Sciences, Queensland University of Technology  
Brisbane, Australia  
kevin.burrage@qut.edu.au

The extent of fibrotic burden in the atria consistently correlates with the occurrence, and reoccurrence after ablation, of atrial fibrillation. Given the complex and unique patterning of fibrotic regions for any afflicted atria, attention has grown towards recent imaging techniques that allow non-invasive mapping of these regions, and subsequently, to techniques that might allow for the identification of arrhythmic risk or targets for ablation. Specifically, computer simulation combined with late gadolinium-enhanced magnetic resonance imaging (LGE-MRI) data allows for patient-specific determination of if and where arrhythmia-sustaining rotors are predicted to form.

These approaches are limited by the spatial resolution and subjective interpretation of LGE-MRI data, and sample sizes are inherently small. In order to enable a mechanistic understanding of how different types of fibrotic patterning can promote arrhythmia, we instead propose an approach using Perlin noise that naturally generates such patterns, quantified by easily understood parameters that are estimated by Approximate Bayesian Computation.

Our method matches directly to the imaging data in terms of a set of metrics we propose, and thus generates patterns that are known to have a realistic distribution of fibrosis. We demonstrate the use of our generated patterns to explore the impacts of different micro-fibrotic structures on cardiac excitation, and discuss how our methods also apply to macroscopic patterns of fibrosis, or indeed to problems outside of cardiac electrophysiology altogether.

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\*Department of Computer Science, University of Oxford, Oxford, United Kingdom



## ON BIPARTIZATION OF NETWORKS

**A. Concas**, S. Noschese, L. Reichel and G. Rodriguez  
Department of Mathematics and Computer Science,  
University of Cagliari  
Viale Merello 92, 09123 Cagliari, Italy  
anna.concas@unica.it

Network analysis aims to identify important nodes in a network and to uncover structural properties of a network such as bipartivity. A network is said to be bipartite if its nodes can be subdivided into two nonempty sets such that there are no edges between nodes in the same set. It is a computationally difficult task to determine the closest bipartite network to a given network. The aim of this work is to describe how a given network can be approximated by a bipartite one by solving a sequence of simple optimization problems. Computed examples illustrate the performance of the described spectral bipartization method. We also show how this procedure can be applied to detect the presence of a large anti-community in a network and to identify it.

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# COMPACT MANIFOLD REGRESSION WITH SOBOLEV REGULARIZATION

**O. De la Cruz Cabrera**

Department of Mathematical Sciences, Kent State University

Kent, Ohio, U.S.A.

odelacru@kent.edu

Manifold regression generalizes the ideas of linear regression to include non-linear structures. Given  $n$  observations (points) in  $R^m$ , the goal is to construct a parameterized manifold embedded in  $R^m$  that “fits the data,” in some sense. Here we consider problems in which the topology of the manifold is known, and corresponds to some low dimensional compact manifold, like a closed loop, a torus, or a sphere. Sobolev regularization is used to control the overall curvature of the fitted manifold. We discuss some of the difficulties that arise, and some strategies to overcome them. For the simplest case, in which the manifold is a closed curve, we describe applications in single cell genomics and classification.

# A NUMERICAL METHOD TO SOLVE INTEGRAL EQUATIONS BY GAUSS AND ANTI-GAUSS QUADRATURE FORMULAE

**P. Díaz de Alba**, L. Fermo, and G. Rodriguez  
Department of Mathematics and Computer Science,  
University of Cagliari  
Viale Merello 92, 09123, Cagliari, Italy  
patricia.diazdealba@gmail.com

The aim of this talk is to present a global approximation method based on the Gauss and anti-Gauss quadrature rules [1, 2, 3] for the following integral equation

$$f(y) - \int_{-1}^1 k(x, y)f(x)w(x)dx = g(y), \quad y \in [-1, 1],$$

where  $f$  is the unknown function,  $k$  and  $g$  are two given functions and  $w(x) = (1-x)^\alpha(1+x)^\beta$  is a Jacobi weight with parameters  $\alpha, \beta > -1$ .

The convergence and the stability of the proposed method will be discussed in suitable weighted spaces and numerical tests will show the accuracy of the approach.

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# SUBSPACE ACCELERATED SPLIT BREGMAN METHODS FOR CONSTRAINED FUSED LASSO PROBLEMS WITH APPLICATIONS IN PORTFOLIO OPTIMIZATION

V. De Simone, **D. di Serafino**, and M. Viola\*  
Department of Mathematics and Physics,  
University of Campania “L. Vanvitelli”, Caserta, Italy  
daniela.diserafino@unicampania.it

Regularization by fused lasso has been successfully applied in minimization problems modelling a variety of applications, to promote sparsity and smoothness in the solution. In this talk, we focus on constrained fused lasso problems of the following form, which arise, e.g., in multi-period portfolio optimization:

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T C \mathbf{w} + \tau_1 \|\mathbf{w}\|_1 + \tau_2 \sum_{i=1}^{m-1} \|\mathbf{w}_{i+1} - \mathbf{w}_i\|_1, \\ & \text{s.t.} && A \mathbf{w} = \mathbf{b}, \end{aligned}$$

where  $\mathbf{w}_i \in \mathbb{R}^n$  for  $i = 1, \dots, m$ ,  $\mathbf{w} = (\mathbf{w}_1^T, \dots, \mathbf{w}_m^T)^T \in \mathbb{R}^{nm}$ ,  $C \in \mathbb{R}^{nm \times nm}$  is symmetric positive definite,  $A \in \mathbb{R}^{s \times nm}$  with  $s < nm$ ,  $\mathbf{b} \in \mathbb{R}^s$ ,  $\tau_1 > 0$  and  $\tau_2 > 0$ . We propose an acceleration technique for split Bergman methods, based on second-order subspace minimization steps, where the subspaces are orthant faces identified by the zero entries of the current iterate. A condition based on suitable measures of optimality is used to decide when the acceleration is needed. Numerical experiments on multi-period portfolio selection problems using real data sets show the effectiveness of the proposed method.

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\*Dept. of Computer, Control and Management Engineering, Sapienza University of Rome, Italy

## OPTIMIZATION PROBLEMS IN GEOCHEMISTRY

**J. Erhel**, and T. Migot

Inria

Rennes, France

`jocelyne.erhel@inria.fr`

Geochemistry involves aqueous reactions and mineral precipitation or dissolution. Quantities of solute species are assumed to be strictly positive, whereas those of minerals can vanish. The mathematical model is expressed as the minimization of Gibbs energy subject to positivity of mineral quantities and conservation of mass. Optimality conditions lead to a complementarity problem.

We show that, in the case of a dilute solution, this problem can also be considered as optimality conditions of another minimization problem, subject to inequality constraints. This new problem is easier to handle, both from a theoretical and a practical point of view.

Then we define a partition of the total quantities in the mass conservation equation. This partition builds a precipitation diagram such that a mineral is either precipitated or dissolved in each subset. We propose a symbolic algorithm to compute this diagram.

Simple numerical examples illustrate our methodology.

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## ERGODICITY COEFFICIENTS FOR SECOND-ORDER MARKOV CHAINS

**D. Fasino**, and F. Tudisco

Dept. of Mathematics, Computer Science and Physics  
University of Udine, Udine, Italy  
dario.fasino@uniud.it

We extend a class of ergodicity coefficients [1] from the matrix case to the higher-order setting of nonnegative stochastic tensors of order three, denoted hereafter with a bold letter  $\mathbf{P}$ . Similarly to the matrix case, the new higher-order ergodicity coefficients provide novel conditions that guarantee the existence and uniqueness of a positive  $\mathbf{Z}$ -eigenvector of  $\mathbf{P}$  corresponding to the eigenvalue one, i.e., a vector  $x$  such that  $\mathbf{P}xx = x$ . Moreover, they allow us to prove new conditions for the global convergence of the so-called higher-order and alternate higher-order power methods, defined by  $x_{k+1} = \mathbf{P}x_kx_k$  and  $x_{k+1} = \mathbf{P}x_kx_{k-1}$ , respectively. Example applications include the analysis of the behaviour of second-order Markov chains, such as the multilinear PageRank [2], and the convergence of the shifted higher-order power method [3].

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# ON THE IDENTIFICATION OF THE REGULARIZATION PARAMETER IN ILL-POSED PROBLEMS

**C. Fenu**, L. Reichel, G. Rodriguez, and H. Sadok  
Dept. of Mathematics and Computer Science,  
University of Cagliari, Italy  
kate.fenu@unica.it

We are concerned with the solution of discrete ill-posed problems of the form

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|, \quad (3)$$

where  $A \in \mathbb{R}^{m \times n}$  is a large matrix whose singular values decay gradually to zero without a significant gap.

A good approximation of the solution can often be computed by first replacing the least-squares problem (3) by a nearby problem, that is regularizing. Here we will discuss two of the most popular regularization methods, namely the Tikhonov regularization method and the Truncated Singular Value Decomposition (TSVD).

When an accurate bound for the norm of the error  $\|e\|$  is available, a suitable value of the regularization parameter can often be determined with the aid of the discrepancy principle. However, for many discrete ill-posed problems (3), such a bound is not known. Here we discuss the use of the Generalized Cross Validation (GCV) in the case of Tikhonov regularization. This method requires the minimization of the GCV function. We will present two fairly inexpensive ways to determine bounds for the GCV function for large matrices  $A$  [1, 2].

TSVD method allows one to replace the ill-conditioned matrix  $A$  by a well-conditioned low-rank matrix obtained by keeping the first  $k$  singular triplets of its Singular Value Decomposition. We will present a method to identify the regularization parameter  $k$  when the TSVD is used as a regularization method based on an extrapolation procedure.

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# A NUMERICAL ALGORITHM FOR APPROXIMATION AND ANALYSIS OF BURGERS'-FISHER EQUATION

**R. Jiwari**

Department of Mathematics, Indian Institute of Technology Roorkee  
Roorkee-247667, India  
ramlmaths@gmail.com

In this talk article, the authors proposed a numerical algorithm for approximation and analysis of Burgers'-Fisher equation  $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + au\frac{\partial u}{\partial x} + bu(1-u) = 0$ . Existence and uniqueness of weak solution, a priori error estimates of semi-discrete solution in  $L^\infty(0, T; L^2(\Omega))$  norm are proved. Nonlinearity of the problem is handled by lagging it to previous known level. The scheme is found to be convergent. Finally, numerical experiments are performed on some examples to demonstrate the effectiveness of the scheme. The proposed scheme found to be fast, easy and accurate.



## OPTIMALLY CONDITIONED VANDERMONDE-LIKE MATRICES

**M. Kuian**, L. Reichel, and S. Shiyanovskii\*

Department of Mathematical Sciences, Kent State University,  
Kent, OH 44242, USA.  
mkuian@kent.edu

Vandermonde matrices arise frequently in computational mathematics in problems that require polynomial approximation, differentiation, or integration. These matrices are defined by a set of  $n$  distinct nodes  $x_1, x_2, \dots, x_n$  and a monomial basis. A difficulty with Vandermonde matrices is that they typically are quite ill-conditioned when the nodes are real and  $n$  is not very small. The ill-conditioning often can be reduced significantly by using a basis of orthonormal polynomials  $p_0, p_1, \dots, p_{n-1}$ , with  $\deg(p_j) = j$ . This was first observed by Gautschi. The matrices so obtained are commonly referred to as Vandermonde-like and are of the form  $V_{n,n} = [p_{i-1}(x_j)]_{i,j=1}^n \in R^{n \times n}$ . Gautschi analyzed optimally conditioned and optimally scaled square Vandermonde and Vandermonde-like matrices with real nodes. We extend Gautschi's analysis to rectangular Vandermonde-like matrices with real nodes, as well as to Vandermonde-like matrices with nodes on the unit circle in the complex plane. Additionally, we investigate existence and uniqueness of optimally conditioned Vandermonde-like matrices. Finally, we discuss properties of rectangular Vandermonde and Vandermonde-like matrices  $V_{N,n}$  of order  $N \times n$ ,  $N \neq n$ , with Chebyshev nodes or with equidistant nodes on the unit circle in the complex plane, and show that the condition number of these matrices can be bounded independently of the number of nodes.

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\*Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA, e-mail: sshiyano@kent.edu

# SOLVING GLOBAL OPTIMIZATION PROBLEMS BY PEANO SPACE-FILLING CURVES

**D. Lera**, and Ya. D. Sergeyev\*

Dept. of Math. and Computer Sci., University of Cagliari

lera@unica.it

In this paper, the global optimization problem:  $\min_{y \in S} F(y)$  with  $S$  being a hyperinterval in  $R^N$  and  $F(y)$  satisfying the Lipschitz condition with an unknown Lipschitz constant is considered. It is supposed that the function  $F(y)$  can be multiextremal, non-differentiable, and given as a “black-box”. To attack the problem we consider the following two ideas. First, an approach that uses numerical approximations of space-filling curves to reduce the original Lipschitz multi-dimensional problem to a univariate one satisfying the Hölder condition [1]. Second, we propose different techniques for acquiring the Hölder information that can be distinguished with respect to the way the Hölder constant is estimated during the process of optimization. In particular, we consider techniques that use either a global estimate of the Hölder constant valid for the whole search region, or local estimates  $H_i$  valid only for some subregions of the domain [2, 3].

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\*DIMES, University of Calabria, and Lobachevsky State Univ. of Nizhni Novgorod, Russia

# THE COMPUTATION OF THE JORDAN STRUCTURE OF TOTALLY NONNEGATIVE MATRICES TO HIGH RELATIVE ACCURACY

T. Laudadio, **N. Mastronardi**, and P. Van Dooren  
Istituto per le Applicazioni del Calcolo "M.Picone"  
Consiglio Nazionale delle Ricerche  
via G. Amendola 122/D, 70126 Bari, Italy  
n.mastronardi@ba.iac.cnr.it

Given the the factorization of a singular totally nonnegative matrix [2, 3, 1]  $A$  of order  $n$  into the product

$$A = B_1 B_2 \cdots B_{n-2} B_{n-1} D C_{n-1} C_{n-2} \cdots C_2 C_1,$$

with  $B_i, C_i^T$  lower bidiagonal totally nonnegative matrices and  $D$  diagonal one, an algorithm for computing the size of the Jordan block associated to the zero eigenvalue was proposed in [3] with high relative accuracy in floating point arithmetic and  $O(n^4)$  computational complexity.

In this talk we propose a modification of the latter algorithm that computes the Jordan structure [4] of  $A$  with high relative accuracy in  $O(n^3)$  computational complexity.

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# ON THE ESTIMATION OF THE TUNING PARAMETER IN REGULARIZED LINEAR REGRESSION MODELS

**M. Mitrouli**

Department of Mathematics, University of Athens,  
Panepistimiopolis, 15784 Athens, Greece  
mmitroul@math.uoa.gr

In the regularized linear regression models the appropriate choice of the tuning parameter plays a dominant role in the selection of the correct model. Most statistical methods employ the tool of the generalized cross-validation (GCV) for the selection of values of this parameter. In this work, we are concerned with the estimation of this parameter rather than its direct computation. We study numerical methods based on extrapolation for estimating the GCV function. Error estimates developed from the solution of linear systems are also employed and tested. We apply simulations for different statistical designs and we report the Type I and Type II error rates in order to compare the behaviour of the proposed method with the corresponding estimates of the tuning parameter which are obtained by minimizing the exact GCV function.

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# A COMPARISON OF REGULARIZATION METHODS FOR SOLVING NONLINEAR PROBLEMS

**F. Pes** and G. Rodriguez

Department of Mathematics and Computer Science,

University of Cagliari, Italy

`federica.pes@unica.it`

Let us assume that  $F(\mathbf{x})$  is a nonlinear Fréchet differentiable function, with value in  $\mathbb{R}^m$  for any  $\mathbf{x} \in \mathbb{R}^n$ . For a given  $\mathbf{b} \in \mathbb{R}^m$ , we solve the least squares problem  $\min_{\mathbf{x}} \|\mathbf{r}(\mathbf{x})\|^2$ , where  $\mathbf{r}(\mathbf{x}) = F(\mathbf{x}) - \mathbf{b}$  is the residual vector function, by applying both Newton's and Gauss–Newton methods [1].

The nonlinear function  $F(\mathbf{x})$  is considered ill-conditioned in a domain  $\mathcal{D}$ , when the condition number  $\kappa(J)$  of the Jacobian  $J = J(\mathbf{x})$  of  $F(\mathbf{x})$  is large for any  $\mathbf{x} \in \mathcal{D}$ . It may also happen that, during the iteration of Gauss–Newton method, the matrix  $J$  becomes rank-deficient. Under this assumption, it is common to apply a regularization method to each step of the Gauss–Newton method. We compare this situation to applying the same regularization method to the initial nonlinear least squares problem. We apply these two approaches to a geophysical model used for electromagnetic data inversion [2, 3].

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## PHOTOMETRIC STEREO UNDER UNKNOWN LIGHTS POSITION

A. Concas, R. Dessì, C. Fenu, **G. Rodriguez**, and M. Vanzi  
Department of Mathematics and Computer Science, University of Cagliari  
Viale Merello 92, Cagliari, Italy  
rodriguez@unica.it

The *shape from shading* problem in Computer Vision consists of reconstructing the 3D shape of an object, starting from a set of images. This kind of procedures have important applications in many fields, among which rock art documentation in Archaeology [2]. The photometric stereo technique extracts shape and color information from pictures of an object, taken from the same point of view, but under different lighting conditions. While the classical shape restoration approach assumes the knowledge of the lights position, we will explore the situation where the position of the light sources is unknown. We will show that when at least 6 pictures of the observed object are available, the lights position can be estimated directly from the data [1]. Numerical experiments will illustrate the performance of the algorithm developed, on both computer generated and real-world data sets.

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# BREAKDOWNS AND NEAR BREAKDOWNS IN SYMPLECTIC REDUCTIONS OF A MATRIX TO UPPER $J$ -HESSENBERG FORM

**A. Salam**, and H. Ben Kahla  
LMPA, University Lille Nord de France  
BP 699, C.U. de la Mi-Voix, 62228 Calais, France  
salam@univ-littoral.fr

The algorithm JHESS, or the recent JHMSH algorithm and its variants, are based on symplectic similarity transformations for reducing a matrix to an upper  $J$ -Hessenberg form. This reduction is a crucial step in the  $SR$ -algorithm (which is a  $QR$ -like algorithm), structure-preserving, for computing eigenvalues and vectors, of a class of structured matrices.

Unlike its equivalent in the Euclidean case, these algorithms may meet fatal breakdowns, causing brutal stops of the computations or encounter near-breakdowns, which are source of serious numerical instability.

In this talk, we point out where such breakdowns or near-breakdowns occur and present efficient strategies for curing them. The effectiveness of such strategies are illustrated by numerical experiments.

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## CORE-CHASING ALGORITHMS FOR THE EIGENVALUE PROBLEM

**D. S. Watkins**

Department of Mathematics, Washington State University

Pullman, WA, USA

watkins@math.wsu.edu

Sixty years ago John Francis invented the winning general-purpose algorithm for computing eigenvalues of a matrix, the implicitly-shifted QR algorithm. This can also be applied to related problems, including the generalized eigenvalue problem. One might well think that after so many years everything that can be said about this algorithm has already been said, but this turns out not to be the case. Interesting variants and insights have been produced just in the past few years. Francis's algorithm is normally implemented as a bulge-chasing algorithm. Recently we have shown that there are some advantages to implementing it as a core-chasing algorithm instead. (Another interesting variant is the pole-swapping algorithm of Camps, Meerbergen, and Vandebriel.)

This talk will focus on the core-chasing approach. We will explain what it is and show that it is particularly advantageous in certain structured cases, e.g. unitary and unitary-plus-rank-one, including the problem of computing the roots of a polynomial.

This is joint work with Jared Aurentz, Thomas Mach, Leonardo Robol, and Raf Vandebriel. We have written a book [1] that summarizes our work.

### References

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# BLIND IMAGE DECONVOLUTION USING A NON-SEPARABLE POINT SPREAD FUNCTION

**J. R. Winkler**

Department of Computer Science, The University of Sheffield,  
Sheffield, United Kingdom

`j.r.winkler@sheffield.ac.uk`

This paper considers the problem of the removal of blur from an image that is degraded by a non-separable point spread function (PSF), when information on the PSF is not known. The non-separable nature of the PSF implies that two blurred images, taken by the same system such that the PSF can be assumed to be the same for both images, are required to determine the PSF. The most difficult part of the computation is the determination of the size of the PSF because this problem reduces to the determination of the rank of two matrices (one matrix for the horizontal component of the PSF and one matrix for the vertical component of the PSF). It is shown that this computation requires the determination of the greatest common divisor of two polynomials, after they have been transformed to the Fourier domain. The Sylvester resultant matrix and its subresultant matrices are used for this computation. A structure-preserving matrix method is used to perform each deconvolution, and thereby compute deblurred forms of the given blurred images because this method preserves the Toeplitz structure of the coefficient matrix in the linear algebraic equation.

The presentation includes examples that demonstrate the method.



## List of Participants

1. **Francesca Arrigo** (`francesca.arrigo@strath.ac.uk`)  
University of Strathclyde, UK.
2. **Bernhard Beckermann** (`bbecker@math.univ-lille1.fr`)  
Department of Mathematics, Laboratoire Painlevé, Université de Lille, Villeneuve d'Ascq, France.
3. **Peter Benner** (`benner@mpi-magdeburg.mpg.de`)  
Max Planck Institute for Dynamics or Complex Technical Systems, Magdeburg, Deutschland.
4. **Federico Benvenuto** (`benvenuto@dima.unige.it`)  
Università degli Studi di Genova, Genova, Italy.
5. **Michele Benzi** (`michele.benzi@sns.it`)  
Classe di Scienze, Scuola Normale Superiore, Pisa, Italy.
6. **Harry B. Bingham** (`hbb@mek.dtu.dk`)  
Department of Mechanical Engineering, Technical University of Denmark, Lyngby, DK.
7. **Dario Andrea Bini** (`dario.bini@unipi.it`)  
Dipartimento di Matematica, Università di Pisa, Pisa, Italy.
8. **Claude Brezinski** (`claudio.brezinski@univ-lille.fr`)  
University of Lille, France.
9. **Franco Brezzi** (`brezzi@imati.cnr.it`)  
Istituto di Matematica Applicata e Tecnologie Informatiche E. Magenes, Consiglio Nazionale delle Ricerche, Pavia, Italy.
10. **Alessandro Buccini** (`abuccini@kent.edu`)  
Kent State University, USA.
11. **Adhemar Bultheel** (`adhemar.bultheel@cs.kuleuven.be`)  
Department of Computer Science, KU Leuven, Heverlee, Belgium.
12. **Kevin Burrage** (`kevin.burrage@qut.edu.au`)  
Department of Mathematical Sciences, Queensland University of Technology, brisbane, Queensland, Australia.
13. **Pamela Burrage** (`pamela.burrage@qut.edu.au`)  
Queensland University of Technology, Brisbane, Australia.
14. **Daan Camps** (`daan.camps@cs.kuleuven.be`)  
Department of Computer Science, KU Leuven, Leuven, Belgium.
15. **Noe Angelo Caruso** (`ncaruso@sissa.it`)  
Department of Mathematics, SISSA, Italy.

16. **Anna Concas** ([anna.concas@unica.it](mailto:anna.concas@unica.it))  
Department of Mathematics and Computer Science, University of Cagliari, Cagliari, Italy.
17. **Patricia Díaz de Alba** ([patricia.diazdealba@gmail.com](mailto:patricia.diazdealba@gmail.com))  
Department of Mathematics and Computer Science, University of Cagliari, Cagliari, Italy.
18. **Maria Carmela De Bonis** ([mariacarmela.debonis@unibas.it](mailto:mariacarmela.debonis@unibas.it))  
Department of Mathematics, Computer Sciences and Economics, University of Basilicata, Potenza, Italy.
19. **Omar De la Cruz Cabrera** ([odelacru@kent.edu](mailto:odelacru@kent.edu))  
Department of Mathematical Sciences, Kent State University, Kent, USA.
20. **Eric de Sturler** ([sturler@vt.edu](mailto:sturler@vt.edu))  
Department of Mathematics, Virginia Tech, Blacksburg, Virginia, USA.
21. **Fernando De Terán** ([fteran@math.uc3m.es](mailto:fteran@math.uc3m.es))  
Department of Mathematics, Universidad Carlos III de Madrid, Leganés, Spain.
22. **Karl Deckers** ([Karl.Deckers@math.univ-lille1.fr](mailto:Karl.Deckers@math.univ-lille1.fr))  
Laboratoire de Mathématiques Paul Painlevé, Université de Lille, Villeneuve d'Ascq CEDEX, France.
23. **Daniela di Serafino** ([daniela.diserafino@unicampania.it](mailto:daniela.diserafino@unicampania.it))  
Dipartimento di Matematica e Fisica, Università della Campania, Caserta, Italy.
24. **Marco Donatelli** ([marco.donatelli@uninsubria.it](mailto:marco.donatelli@uninsubria.it))  
University of Insubria, Italy.
25. **Michael Eiermann** ([eiermann@math.tu-freiberg.de](mailto:eiermann@math.tu-freiberg.de))  
Institut fuer Numerische Mathematik und Optimierung, TU Bergakademie Freiberg, Freiberg, Germany.
26. **Jocelyne Erhel** ([jocelyne.erhel@inria.fr](mailto:jocelyne.erhel@inria.fr))  
INRIA, Rennes, France.
27. **Claudio Estatico** ([estatico@dima.unige.it](mailto:estatico@dima.unige.it))  
Department of Mathematics, University of Genoa, Genova, Italy.
28. **Mohamed Farhloul** ([mohamed.farhloul@umoncton.ca](mailto:mohamed.farhloul@umoncton.ca))  
Département de Mathématiques et Statistique, Université de Moncton, Moncton, Canada.
29. **Dario Fasino** ([dario.fasino@uniud.it](mailto:dario.fasino@uniud.it))  
Department of Mathematics, Comp. Science and Physics, University of Udine, Udine, Italia.
30. **Heike Fassbender** ([h.fassbender@tu-braunschweig.de](mailto:h.fassbender@tu-braunschweig.de))  
TU Braunschweig, Germany.

31. **Caterina Fenu** (`kate.fenu@unica.it`)  
Department of Mathematics and Computer Science, University of Cagliari, Italy.
32. **Luisa Fermo** (`fermo@unica.it`)  
Department of Mathematics and Computer Science, University of Cagliari, Cagliari, Italy.
33. **Andreas Frommer** (`frommer@math.uni-wuppertal.de`)  
Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Wuppertal, Wuppertal.
34. **Martin Jakob Gander** (`martin.gander@unige.ch`)  
Department of Mathematics, University of Geneva, Geneva, Switzerland.
35. **Walter Gautschi** (`wgautschi@purdue.edu`)  
Department of Computer Science, Purdue University, West Lafayette, USA.
36. **Silvia Gazzola** (`S.Gazzola@bath.ac.uk`)  
Mathematical Sciences, University of Bath, United Kingdom.
37. **Daniel Gerth** (`daniel.gerth@mathematik.tu-chemnitz.de`)  
TU Chemnitz, Germany.
38. **Christer Glader** (`cglader@abo.fi`)  
Department of Mathematics, Abo Akademi University, Finland.
39. **Martin Hermann Gutknecht** (`mhg@math.ethz.ch`)  
ETH Zurich, Langenthal, Switzerland.
40. **Mario Helm** (`mario.helm@math.tu-freiberg.de`)  
Institute for Numerical Mathematics and Optimization, TU Bergakademie Freiberg, Freiberg, Germany.
41. **Bernd Hofmann** (`hofmannb@mathematik.tu-chemnitz.de`)  
Faculty of Mathematics, Chemnitz University of Technology, Chemnitz, Germany.
42. **Bruno Iannazzo** (`bruno.iannazzo@unipg.it`)  
University of Perugia, Italy.
43. **Carl Jagels** (`jagels@hanover.edu`)  
Department of Mathematics, Hanover College, Hanover, USA.
44. **Ram Jiware** (`ram1maths@gmail.com`)  
Department of Mathematics, Indian Institute of Technology Roorkee, Roorkee, India.
45. **Stefan Kindermann** (`kindermann@indmath.uni-linz.ac.at`)  
Industrial Mathematics Institute, Johannes Kepler University Linz, Linz, Austria.
46. **Daniel Kressner** (`daniel.kressner@epfl.ch`)  
Institute of Mathematics, EPFL, Lausanne, Switzerland.

47. **Mykhailo Kuian** (mkuian@umn.edu)  
Mathematical Sciences, University of Minnesota, Minneapolis, USA.
48. **Daniela Lera** (lera@unica.it)  
Department of Mathematics and Computer Science, University of Cagliari, Italy.
49. **Bryan Wayne Lewis** (blewis@illposed.net)  
Kent State University, Richfield, USA.
50. **Thomas Mach** (thomas.mach@gmail.com)  
Department of Mathematical Sciences, Kent State University, Kent, United States.
51. **Nicola Mastronardi** (n.mastronardi62@gmail.com)  
Istituto per le Applicazioni del Calcolo, Consiglio Nazionale delle Ricerche, Bari, Italy.
52. **Mariarosa Mazza** (mariarosa.mazza@uninsubria.it)  
Department of Science and High Technology, University of Insubria, Como, Italy.
53. **Volker Mehrmann** (mehrmann@math.tu-berlin.de)  
Inst. f. Mathematics, TU Berlin, Berlin, Germany.
54. **Beatrice Meini** (beatrice.meini@unipi.it)  
Università di Pisa, Italy.
55. **Marilena Mitrouli** (mmitroul@math.uoa.gr)  
Department of Mathematics, National and Kapodistrian University of Athens, Athens, Greece.
56. **Boitumelo Moletsane** (boitumelo.moletsane@wits.ac.za)  
Department of Mathematics, University of the Witwatersrand, Johannesburg, South Africa.
57. **Serena Morigi** (serena.morigi@unibo.it)  
Department of Mathematics, University of Bologna, Bologna, Italy.
58. **Benedetta Morini** (benedetta.morini@unifi.it)  
Dipartimento di Ingegneria Industriale, Università degli Studi di Firenze, Firenze, Italia.
59. **Silvia Noschese** (noschese@mat.uniroma1.it)  
Dipartimento di Matematica "Guido Castelnuovo", SAPIENZA Università di Roma, Roma, Italy.
60. **Sotirios Notaris** (notaris@math.uoa.gr)  
Department of Mathematics, National and Kapodistrian University of Athens, Greece.
61. **Ramón Orive** (rorive@ull.es)  
Departamento de Análisis Matemático, Universidad de La Laguna, Santa Cruz de Tenerife, España.
62. **Valeria Paoletti** (paoletti@unina.it)  
Department of Earth, Environment and Resources Science, University of Naples Federico II, Italy.

63. **Sergei Pereverzyev** (`sergei.pereverzyev@oeaw.ac.at`)  
Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria.
64. **Federica Pes** (`federica.pes@unica.it`)  
Department of Mathematics and Computer Science, University of Cagliari, Italy.
65. **Robert Plato** (`plato@mathematik.uni-siegen.de`)  
Department of Mathematics, University of Siegen, Siegen, Germany.
66. **Marina Popolizio** (`marina.popolizio@poliba.it`)  
Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, Bari, Italy.
67. **Stefano Pozza** (`pozza@karlin.mff.cuni.cz`)  
Department of Numerical Mathematics, Charles University, Czech Republic.
68. **Miroslav Pranic** (`miroslav.pranic@pmf.unibl.org`)  
University of Banja Luka, Bosnia and Herzegovina.
69. **Alfio Quarteroni** (`alfio.quarteroni@polimi.it`)  
Department of Mathematics, Politecnico di Milano and EPFL, Lausanne, Milano, Italy.
70. **Ronny Ramlau** (`ronny.ramlau@ricam.oeaw.ac.at`)  
Industrial Mathematics Institute, Johannes Kepler University Linz, Linz, Austria.
71. **Michela Redivo-Zaglia** (`michela.redivozaglia@unipd.it`)  
Department of Mathematics, University of Padua, Padova, Italy.
72. **Lothar Reichel** (`reichel@math.kent.edu`)  
Department of Mathematical Sciences, Kent State University, Kent, OH, USA.
73. **Leonardo Robol** (`leonardo.robol@unipi.it`)  
Università di Pisa, Italy.
74. **Giuseppe Rodriguez** (`rodriguez@unica.it`)  
Department of Mathematics and Computer Science, University of Cagliari, Cagliari, Italy.
75. **Malena Sabaté Landman** (`M.Sabate.Landman@bath.ac.uk`)  
University of Bath, United Kingdom.
76. **Ahmed Salam** (`salam@univ-littoral.fr`)  
LMPA, University Lille Nord de France, Calais, France.
77. **Claudia Schimmel** (`schimmel@math.uni-wuppertal.de`)  
University of Wuppertal, Germany.
78. **Carla Seatzu** (`seatzu@diee.unica.it`)  
Department of Electrical and Electronic Engineering, University of Cagliari, Cagliari, Italy.
79. **Stefano Serra Capizzano** (`stefano.serrac@uninsubria.it`)  
Department of Humanities and Innovation, University "Insubria", Como, Italy.

80. **Fiorella Sgallari** (fiorella.sgallari@unibo.it)  
Department of Mathematics, University of Bologna, Bologna, Italy.
81. **Valeria Simoncini** (valeria.simoncini@unibo.it)  
Dipartimento di Matematica, Università di Bologna, Bologna, Italy.
82. **Kirk M. Soodhalter** (ksoodha@maths.tcd.ie)  
School of Mathematics, Trinity College Dublin, Dublin, Ireland.
83. **Miodrag M. Spalević** (mspalevic@mas.bg.ac.rs)  
Department of Mathematics, Faculty of Mechanical Engineering, University of Belgrade, Serbia.
84. **Daniel B. Szyld** (szyld@temple.edu)  
Department of Mathematics, Temple University, Philadelphia, USA.
85. **Gerardo Toraldo** (toraldo@unina.it)  
Dipartimento di Matematica e Applicazioni, Università di Napoli Federico II, Napoli, Italy.
86. **Walter Van Assche** (Walter.vanassche@kuleuven.be)  
Department of Mathematics, KU Leuven, Leuven, Belgium.
87. **Marc Van Barel** (marc.vanbarel@cs.kuleuven.be)  
Department of Computer Science, KU Leuven, Leuven (Heverlee), Belgium.
88. **Niel Van Buggenhout** (niel.vanbuggenhout@cs.kuleuven.be)  
Department of Computer Science, KU Leuven, Leuven, Belgium.
89. **Cornelis van der Mee** (cornelis@krein.unica.it)  
Department of Mathematics and Computer Science, University of Cagliari, Cagliari, Italy.
90. **Raf Vandebril** (Raf.Vandebril@cs.kuleuven.be)  
Department of Computer Science, KU Leuven, Leuven, Belgium.
91. **Daniel Wachsmuth** (daniel.wachsmuth@mathematik.uni-wuerzburg.de)  
Institute of Mathematics, University Wuerzburg, Wuerzburg, Germany.
92. **David S. Watkins** (watkins@math.wsu.edu)  
Department of Mathematics, Washington State University, Pullman, USA.
93. **Joab Winkler** (j.r.winkler@sheffield.ac.uk)  
Department of Computer Science, The University of Sheffield, Sheffield, United Kingdom.
94. **Abdelmalek Zine** (abdel-malek.zine@ec-lyon.fr)  
Department of Mathematics and Computer Sciences, Ecole Centrale de Lyon, Ecully, France.



# Index of speakers

Arrigo F., 93

Beckermann B., 37

Benner P., 29

Benvenuto F., 45

Benzi M., 15

Bingham H. B., 94

Bini D. A., 16

Brezinski C., 85

Brezzi F., 17

Buccini A., 95

Bultheel A., 53

Burrage K., 96

Camps D., 69

Concas A., 97

Díaz de Alba P., 99

De Bonis M. C., 77

De la Cruz Cabrera O., 98

de Sturler E., 46

De Terán F., 30

Deckers K., 78

di Serafino D., 100

Donatelli M., 18

Erhel J., 101

Estatico C., 86

Faßbender H., 70

Fasino D., 102

Fenu C., 103

Fermo L., 87

Frommer A., 19

Gander M. J., 20

Gautschi W., 54

Gazzola S., 61

Gerth D., 62

Glader C., 55

Gutknecht M. H., 56

Helm M., 38

Iannazzo B., 31

Jagels C., 79

Jiwari R., 104

Kindermann S., 21

Kressner D., 32

Kuian M., 105

Lera D., 106

Mach T., 63

Mastronardi N., 107

Mazza M., 33

Mehrmann V., 22

Meini B., 34

Mitrouli M., 108

Morigi S., 23

Morini B., 47

Notaris S. E., 57

Orive R., 80

Pereverzyev S. V., 64

Pes F., 109

Plato R., 65

Popolizio M., 39

Pozza S., 81

Quarteroni A., 88

Ramlau R., 48

Redivo-Zaglia M., 40

Reichel L., 89

Robol L., 71

Rodriguez G., 110

Sabaté Landman M., 49

Salam A., 111

Schimmel C., 41

Seatzu C., 90

Serra-Capizzano S., 50

Sgallari F., 24

Simoncini V., 72

Szyld D. B., 25

Van Assche W., 58

Van Buggenhout N., 73

Vandebril R., 26

Wachsmuth D., 66

Watkins D. S., 112

Winkler J. R., 113



