# *Two Days of*
# *Numerical Linear Algebra and Applications*

## (*Due Giorni di*
## *Algebra Lineare Numerica e Applicazioni*)

# Program and Abstracts

Università degli Studi di Napoli Federico II, Italy

February 14-15, 2022

# Contents

# Welcome and Information

# Welcome Address

Dear friends and colleagues,

we are pleased to welcome you to the 17th edition of the workshop *Two Days of Numerical Linear Algebra and Applications*, which aims at gathering the Italian Numerical Linear Algebra scientific community to discuss recent advances in this area and to promote the exchange of novel ideas and the collaboration among researchers. The workshop themes concern theoretical and computational issues as well as applications. The topics of interest include large-scale linear systems, linear least squares problems, preconditioning, eigenvalues and eigenvectors, SVD, structured matrices, tensors, matrix functions, rational Krylov methods, and randomized linear algebra algorithms. The applications include optimization and control, signal/image processing and inverse problems, networks and graphs, machine learning, finance, contact mechanics and fluid flow problems, to name just a few. The scientific program consists of 2 keynote talks by internationally renowned speakers and 35 contributed talks by young and senior scholars, from institutions in Italy and other European countries.

The organization of the workshop is the result of the efforts of the Scientific Committee and the Local Organizing Committee. We also acknowledge the support of several sponsors, including the Università di Napoli Federico II and its Dipartimento di Matematica e Applicazioni "R. Caccioppoli", the V:ALERE Program of the Università della Campania "L. Vanvitelli", and the Istituto Nazionale di Alta Matematica - Gruppo Nazionale per il Calcolo Scientifico (INdAM-GNCS).

We hope you enjoy the workshop and your stay in Naples.

The Scientific Committee and the Local Organizing Committee
*Dario Bini, Fabio Di Benedetto, Daniela di Serafino,*
*Valentina De Simone, Giuseppe Izzo, Marco Viola*

# Scientific Committee

- **Dario Bini**
  Università di Pisa

- **Fabio Di Benedetto**
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- **Daniela di Serafino**
  Università degli Studi di Napoli Federico II

# Local Organizing Committee

- **Daniela di Serafino - Chair**
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- **Valentina De Simone**
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- **Giuseppe Izzo**
  Università degli Studi di Napoli Federico II

- **Marco Viola**
  Università degli Studi della Campania "L. Vanvitelli"

# Venue and Travel Information

## Venue

The workshop will be held at the Federico II Conference Center in via Partenope 36, 80121 Naples, Italy.

The Conference Center is located on the beautiful seaside of the city, just in front of Castel dell'Ovo. It is not far from the historic center of the city, which has earned the UNESCO World Heritage Site denomination. By walking through the streets of Naples, one can see the traces of its millennial history, with a wealth of historical buildings and monuments, from medieval castles to classical ruins, and 448 historical churches (the largest number in the World for a single city).

## Wi-Fi Connection

'Eduroam' and 'Wi-Fi_UniNa' are available on site to the authorized users. As an alternative, the participants can use the *dedicated Wi-Fi network* 'ALGEBRA' whose password is 'arvadelt'.

## Getting to Naples

You can reach Naples in different ways:

- by plane, landing at Naples Capodichino Airport (Aeroporto di Capodichino - NAP) and using the Alibus public transportation or the taxi service;

- by train (both regional and high-speed trains), stopping at Naples Central Train Station (Stazione Napoli Centrale);

- by car, via the E45 motorway (A1 coming from North, A3 coming from South);

- by ferry, arriving at Naples Port (Porto di Napoli).

The Unico Alibus ticket allows only one journey on the Alibus shuttle, on the route Capodichino Airport / Central Train Station / Port or vice

versa, and the use of all means of transport of the companies participating in the UNICOCAMPANIA consortium in Naples urban area. A ticket costs € 5.00 at authorized retailers and on board. The maximum journey time is 90 minutes after stamping.

Alibus shuttles make the following stops:

- from Capodichino Airport: Piazza Garibaldi (Central Train Station), Immacolatella / Porta di Massa, and Molo Angioino/Beverello (Stazione Marittima);

- from Naples Port: Molo Angioino/Beverello (Stazione Marittima), Immacolatella / Porta di Massa (Naples Port), Varco Pisacane (in front of Port Authority), Piazza Garibaldi (Central Train Station) and Capodichino Airport.

The taxi lane in the airport is located in front of 'Arrivals'. Taxi lanes are also outside the main entrance of the Central Train Station and inside the Port of Naples.

Flat rates are in use for predetermined urban and suburban routes (City Center, Molo Beverello, Mergellina, Capodichino Airport, etc.). Those rates include any extra charge (to/from airport, night ride, holiday, luggage, animals) but motorway tolls and radio-taxi calls. Please, note that the flat fares must be requested before the trip starts and are per cab, not per passenger. Fares are available at https://www.aeroportodinapoli.it/ (click/tap on 'PARKING & BUS' and then on 'Taxi' in the rightmost column).

A shared taxi service connecting Capodichino Airport, Central Train Station and Molo Angioino/Beverello (Stazione Marittima) is also available. At the airport, the shared taxi area is near the roundabout of Viale Ruffo di Calabria, opposite the Local Police station. The sign 'TAXI COLLETTIVO' is shown on the front windshield of shared taxi cars, along with the Naples City Council logo, the route and the price per person. The cost per passenger is € 6.00 including luggage.

# Workshop Schedule

| Monday, February 14, 2022 – Morning | | |
|---|---|---|
| 8.30 - 8.50 | | *Registration & Opening* |
| | *Chair:* | F. Di Benedetto |
| 8.50 - 9.10 | I. Simunec | Computation of generalized matrix functions with rational Krylov methods |
| 9.10 - 9.30 | M. Rinelli | Refined decay bounds on the entries of spectral projectors associated with sparse Hermitian matrices |
| 9.30 - 9.50 | M. Gnazzo | Distance to singularity for quadratic matrix polynomials |
| 9.50 - 10.10 | L. Robol | Mixed precision recursive block diagonalization for bivariate functions of matrices |
| 10.10 - 10.30 | M. Popolizio | Numerical approximation of the Mittag–Leffler function for large sparse low rank matrices |
| 10.30 - 11.00 | | *Coffee break* |
| | *Chair:* | D. Bini |
| 11.00 - 11.40 | M. Benzi | Solving linear systems of the form $(A + \gamma UU^T)\mathbf{x} = \mathbf{b}$ |
| | *Chair:* | V. Simoncini |
| 11.40 - 12.00 | M. Viola | On linear algebra in interior point methods for solving $\ell_1$-regularized optimization problems |
| 12.00 - 12.20 | S. Leveque | Parameter-Robust Preconditioning for Oseen Iteration Applied to Navier–Stokes Control Problems |
| 12.20 - 12.40 | A. Franceschini | A Reverse Constrained Preconditioner for saddle-point matrices in contact mechanics |
| 12.40 - 14.10 | | *Light lunch* |

| Monday, February 14, 2022 – Afternoon | | |
|---|---|---|
| | *Chair:* | N. Guglielmi |
| 14.10 - 14.30 | D. Palitta | On ParaDiag for BDFs |
| 14.30 - 14.50 | S. Maset | Relative error propagation in linear ordinary differential equations: long-time behavior of condition numbers |
| 14.50 - 15.10 | M. Viviani | Solving cubic matrix equations arising in conservative dynamics |
| 15.10 - 15.30 | A. Farooq | How perturbations propagate along the solutions of linear ordinary differential equations: a relative error analysis |
| 15.30 - 15.50 | M. Manucci | Some challenging issues in the linear algebra of contour integral methods for PDEs |
| 15.50 - 16.20 | | *Coffee break* |
| | *Chair:* | S. Noschese |
| 16.20 - 16.40 | S. Gazzola | Regularization by inexact Krylov methods |
| 16.40 - 17.00 | A. Falini | A novel matrix-factorization algorithm for the analysis of Hyperspectral Images |
| 17.00 - 17.20 | A. Cicone | Inverse problems in signal processing: a Numerical Linear Algebra prospective |
| 17.20 - 17.40 | C. Scalone | On the approximation of low-rank rightmost eigenpairs of a class of matrix linear operators |
| 17.40 - 18.00 | T. Bevilacqua | BDDC preconditioners for virtual element discretizations of the Stokes equations |

| Tuesday, February 15, 2022 – Morning | | |
|---|---|---|
| | *Chair:* | D. Fasino |
| 8.50 - 9.10 | N. Segala | Numerical solution of the graph $p$-Laplacian partial eigen-problem |
| 9.10 - 9.30 | P. Deidda | Geometrical properties of the graph $p$-Laplacian spectrum |
| 9.30 - 9.50 | A. Savostianov | Graph Topological Stability via Matrix Differential Equations |
| 9.50 - 10.10 | C. Faccio | Density forms of liquid water revealed by the Total Communicability of the corresponding graph |
| 10.10 - 10.30 | G. Ceruti | Time integration of Tree Tensor Networks |
| 10.30 - 11.00 | | *Coffee break* |
| | *Chair:* | D. di Serafino |
| 11.00 - 11.40 | M. Tůma | Solving sparse-dense least squares |
| | *Chair:* | B. Iannazzo |
| 11.40 - 12.00 | D. Fasino | Remember where you came from: Hitting times for second-order random walks |
| 12.00 - 12.20 | K. Prokopchik | Nonlinear Label Spreading on Hypergraphs |
| 12.20 - 12.40 | A. Cortinovis | Randomized algorithms for trace estimation |
| 12.40 - 14.10 | | *Light lunch* |

| Tuesday, February 15, 2022 – Afternoon | | |
|---|---|---|
| | *Chair:* | S. Serra Capizzano |
| 14.10 - 14.30 | L. Gazzola | An efficient preconditioner for the coupled contact mechanics and fluid flow in fracture network |
| 14.30 - 14.50 | K. Trotti | Matrices associated to two conservative discretizations of Riesz fractional operators and related multigrid solvers |
| 14.50 - 15.10 | C. Janna | Improving AMG interpolation through energy minimization |
| 15.10 - 15.30 | F. Durastante | AMG Preconditioners based on parallel hybrid coarsening exploiting multi-objective graph matching |
| 15.30 - 15.50 | F. Marcuzzi | The minimal realization problem in physical coordinates |
| 15.50 - 16.20 | | *Coffee break* |
| | *Chair:* | M. Redivo-Zaglia |
| 16.20 - 16.40 | F. Marchetti | The extended Rippa's algorithm in RBF interpolation |
| 16.40 - 17.00 | J. Giacomini | Preconditioning in collocation and interpolation with radial basis functions |
| 17.00 - 17.20 | R. Campagna | Linear algebra of HP-splines |
| 17.20 - 17.40 | M. Dessole | Deviation maximization for rank-deficient problems |
| 17.40 - 18.00 | | *Closing* |

# Keynote Talks

# Solving linear systems of the form $(A + \gamma UU^T)\mathbf{x} = \mathbf{b}$

Michele Benzi

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We consider the solution of large linear systems of the form

$$(A + \gamma UU^T)\mathbf{x} = \mathbf{b}$$

with $A$ of size $n \times n$, $\gamma > 0$ a parameter and $U$ of size $n \times k$, by preconditioned Krylov subspace methods. We make the following assumptions:

- $A$ is possibly singular, but $A + \gamma UU^T$ is nonsingular;

- forming $A + \gamma UU^T$ explicitly is undesirable, for example due to loss of structure or sparsity in $A$;

- the dimension $k$ is much smaller than $n$, but not small.

Linear systems of this form arise in several areas of scientific computing, including the solution of the Stokes and Navier-Stokes problems with augmented Lagrangian methods, the solution of reduced KKT systems in constrained optimization, the discretization of certain integro-differential equations, the solution of PDEs with non-local boundary conditions, and elsewhere. Solving such linear systems can be challenging, especially for large values of the parameter $\gamma$. We will present and investigate different variants of a preconditioning technique based on a suitable splitting of the coefficient matrix. The performance of these preconditioners will be illustrated by means of numerical experiments on a variety of test problems.

*Joint work with* C. Faccio

## Solving sparse-dense least squares

Miroslav Tůma

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Our focus is on efficient solution of the unconstrained linear least squares (LS) problems that can be provided in the form

$$\min_x \|Ax - b\|_2, \tag{1}$$

where $A \in \mathcal{R}^{m \times n}$ ($m \geq n$) is a large sparse matrix and $b \in \mathcal{R}^m$ is given. Solving the LS problems numerically is often significantly harder than solving large and sparse systems of linear equations. One important obstacle to get efficient solvers is internal sparsity structure of the normal equations. This structure does not need to be visible when applying black-box direct methods. But the structure may visibly influence solving large problems when using preconditioned iterations. Our presentation will discuss the LS problems in which the system matrix contains rows with very different densities.

There are several classical contributions to solving the LS problem that focus on the problem, and one can find them summarized in the monograph by Åke Björck and some later surveys. In this presentation, we discuss a number of solution approaches. For example, we consider direct sparse-dense preconditioning, Schur complement reductions, combination of the QR factorization with stretching [1] as well as the null-space approach [2]. Experimental problems demonstrate not only strengths but also limitations of various approaches to solve these sparse-dense LS problems.

*Joint work with* J. Scott

## References

[1] J. A. Scott and M. Tůma, *A computational study of using black-box QR solvers for large-scale sparse-dense linear least squares problems*, ACM Transactions on Mathematical Software, 2021, to appear.

[2] J. A. Scott and M. Tůma, *A null-space approach for symmetric saddle point systems with a non zero (2,2) block*, preprint, 2021.

# Contributed Talks

# BDDC preconditioners for virtual element discretizations of the Stokes equations

Tommaso Bevilacqua

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The balancing domain decomposition by constraints (BDDC) preconditioners are domain decomposition methods based on the subdivision of the computational domain of partial differential equations (PDEs) into non-overlapping subdomains. BDDC methods represent an evolution of balancing Neumann-Neumann methods, that have been used extensively in the past to solve large scale finite element problems. In our work, we apply BDDC to solve PDEs where the space discretization is performed by virtual element methods (VEM), a new family of methods introduced in 2013, which could be considered as a generalization of finite element methods to arbitrary element-geometry. The advantage of these methods is that we can apply them on a wide choice of general polygonal meshes without integrating complex non-polinomial functions on the elements, keeping a high degree of accuracy. Here we present a BDDC algorithm to solve the Schur complement system obtained from a recent divergence free VEM discretization of the two-dimensional Stokes equations. Firstly, we briefly present the VEM mathematical framework, then we analyze theoretically the convergence of the proposed BDDC preconditioners and finally we report some computational results that validate the theoretical estimates.

# Linear algebra of HP-splines

Rosanna Campagna

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*Exponential-polynomial splines* are a natural generalization of polynomial splines important in several applications ranging from geometric modeling to image analysis passing through isogeometric analysis and system theory. They are piecewise-defined functions consisting of segments belonging to the null space of a differential operator $L_\ell = (\mathcal{D} + \alpha\mathcal{I})^\ell$, where $\alpha \in \mathbb{C}$, $\mathcal{D}$ is the first derivative operator, $\mathcal{I}$ is the identity operator and $\ell \in \mathbb{N}$. In case $\alpha \in \mathbb{R}$, they are called *hyperbolic-polynomial splines.*

In this talk, we discuss the properties of the family of hyperbolic-polynomial penalized splines, named HP-splines, proposed in [1] obtained through the solution of a linear system that strongly depends on $\alpha$. The parameter $\alpha$ plays an important role also on the conditioning affecting the constructive method. A theoretical bound for the condition number of the matrix defining the linear system is given, based on classical results of generalized singular values decomposition. Reproduction of the exponential space $\mathbb{E}_{2,\alpha} = \{e^{-\alpha x}, \; xe^{-\alpha x}\}$ is also proved, together with the first and second moments, which find an interesting counterpart in statistics, generalizing the inspiring results valid for the analog polynomial P-splines [2].

*Joint work with* C. Conti

## References

[1] R. Campagna and C. Conti, *Penalized hyperbolic-polynomial splines*, Applied Mathematics Letters, Volume 118 (2021).

[2] P. H. C. Eilers and B. D. Marx, *Flexible smoothing with B-splines and penalties*, Statistical Science, Volume 11(2) (1996).

# Time integration of Tree Tensor Networks

Gianluca Ceruti

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Time integration of high-dimensional problems, arising from the discretization of PDEs such as the Vlasov-Poisson equation of plasma physics and Schoedinger equation in many-body quantum mechanics, is a challenging numerical task: the total amount of information required to be stored and computed exceeds standard computational capacity. Time dependent model order reduction techniques are desirable.

In the present talk, dynamical low-rank approximation for matrices together with the matrix and the Tucker projector splitting integrator is introduced. Two remarkable properties of these integrators are presented, namely: the exactness property and the robustness with respect to small singular values. Then, the memory storage requirements for tensors in Tucker format are discussed and Tree Tensor Networks are introduced. Based upon a new compact formulation of the Tucker projector splitting integrator, the Recursive Tree Tensor Network integrator is presented.

*Joint work with* Ch. Lubich *and* H. Walach

# Inverse problems in signal processing:
# a Numerical Linear Algebra prospective

Antonio Cicone

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In signal processing the time-frequency analysis of nonlinear and non-stationary processes, as well as the determination of the unknown number of active sub-signals of a blind-source composite signal are, in general, challenging inverse problem tasks. Standard techniques, like short-time Fourier transform, and wavelet transform are limited in addressing the problem. An alternative approach, proposed in 1998 in the Hilbert Huang Transform (HHT), is to first decompose the signal into simpler components and then analyze them separately. HHT is having a big impact in many filed of research (15300 citations in Scopus). HHT is made of two stages: the signal decomposition into simple oscillatory components via the Empirical Mode Decomposition (EMD) method, and their time-frequency representation via the Hilbert Transform. However, the mathematical properties of EMD and its generalizations, like the Ensemble EMD, are still under investigation. For this reason, an alternative technique, called Iterative Filtering (IF), was recently proposed. In this talk, we review IF mathematical properties, and the ones of its recently developed generalization, which is called Risampled Iterative Filtering (RIF) [1]. Furthermore, we show how Numerical Linear Algebra allows to guarantee a priori convergence of these methods and to speed up calculations, producing what is called the Fast Iterative Filtering (FIF) and Fast Risampled Iterative Filtering (FRIF) techniques [1]. Some applications will be presented, as well as open problems that are waiting to be tackled.

*Joint work with* G. Barbarino *and* H. Zhou

## References

[1] G. Barbarino and A. Cicone, *Stabilization and Variations to the Adaptive Local Iterative Filtering Algorithm: the Fast Resampled Iterative Filtering Method*, submitted (2021), ArXiv:2111.02764

# Randomized algorithms for trace estimation

Alice Cortinovis

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Computing or estimating the trace of a large symmetric matrix $A$ is a problem that arises in a wide variety of applications, such as Frobenius norm estimation, log determinant computations, triangle counting in graphs, and lattice quantum chromodynamics.

The Hutchinson's trace estimator is a popular technique to approximate the trace of a large-scale matrix $A$ by computing the average of quadratic forms $X^T A X$ for many samples of a random vector $X$. In this talk, we present new tail bounds that apply to symmetric indefinite matrices $A$ for Rademacher and Gaussian random vectors [1].

The Hutch++ algorithm [2] is a more efficient trace estimation algorithm that reduces the variance of the Hutchinson's trace estimator by combining it with the randomized singular value decomposition, which obtains a low-rank approximation of $A$ by multiplying the matrix with some random vectors. In this talk, we present an improved version of Hutch++ which aims at minimizing the computational cost – that is, the number of matrix-vector multiplications with $A$ – needed to achieve a trace estimate with a target accuracy [3].

*Joint work with* D. Kressner *and* D. Persson.

## References

[1] A. Cortinovis and D. Kressner, *On randomized trace estimates for indefinite matrices with an application to determinants*, Foundations of Computational Mathematics, (2021).

[2] R. A. Meyer, C. Musco, C. Musco, and D. P. Woodruff, *Hutch++: Optimal stochastic trace estimation*, In Symposium on Simplicity in Algorithms (SOSA), pages 142–55. SIAM (2021).

[3] D. Persson, A. Cortinovis, and D. Kressner, *Improved variants of the Hutch++ algorithm for trace estimation*, arXiv preprint arXiv:2109.10659, (2021).

# Geometrical properties of the graph $p$-Laplacian spectrum

Piero Deidda

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The spectrum of the graph $p$-Laplacian operator, including the limit cases $p = 1$ and $p = \infty$, has tight relations with different geometrical properties of the graph itself. The spectrum of the 1-Laplacian has been proved to provide approximations of the Cheeger cuts of the graph. Similarly, the spectrum of the discrete $\infty$-Laplacian is related to the maximal radius that allows to inscribe a fixed number of disjoint balls in the graph. Particulary significative in these approximations is the number of nodal domains induced by the corresponding eigenfunctions. In this work we present new upper and lower bounds for this number. Moreover, we provide a characterization of the graph $\infty$-Laplacian eigenvalues and properties of its eigenfunctions in terms of extremal points of a class of functionals involving only weighted linear Laplacians. We compare our results with the analogous counterparts in the continuum case and use them to define efficient numerical methods to compute the partial eigenspectrum of the graph $p$-Laplacian, including the limit cases.

*Joint work with* M. Putti, F. Tudisco, M. Burger, N. Segala

## References

[1] T. Bĥuler, M. Hein, *Spectral clustering based on the graph p-Laplacian*, Proceedings of the 26th Int. Conf. on Machine Learning (2009).

[2] F. Tudisco, M. Hein, *A nodal domain theorem and a higher-order Cheeger inequality for the graph p-Laplacian*, Journal of Spectral Theory, 8 (2018).

[3] P. Juutinen and P. Lindqvist, *On the higher eigenvalues for the $\infty$-eigenvalue problem*, Calc. of Variations and Part. Diff. Eq., 23 (2005).

[4] L. Bungert, Y. Korolev, *Eigenvalue Problems in $L^\infty$: Optimality Conditions, Duality, and Relations with Optimal Transport*, arXiv (2021).

[5] P. Deidda, M. Putti and F. Tudisco, *Nodal domain count for the generalized graph p-Laplacian*, in preparation.

# Deviation maximization for rank-deficient problems

Monica Dessole

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The problem of finding a rank-revealing QR (RRQR) decomposition of a matrix $A$ is nowadays a classic problem in numerical linear algebra. RRQR factorization has been introduced [2] for least squares problems where the matrix has not full column rank: in such a case, a plain QR computation may lead to an $R$ factor in which the number of nonzeros on the diagonal does not equal the rank and the matrix $Q$ does not reveal the range nor the null space of the original matrix. Since the QR factorization is essentially unique once the column ordering is fixed, these techniques all amount to finding an appropriate column permutation. In this talk we introduce a recent block pivoting technique we called "Deviation Maximization" [1] that is based on correlation analysis, and apply it to compute RRQR as an alternative to the well known block version of the QR factorization with the column pivoting method [3], currently implemented in the `xgeqp3` subroutine of LAPACK. We show that the resulting algorithm, named QRDM, has similar rank-revealing properties of QP3 and shorter execution times. We present numerical results on a wide data set of numerically singular matrices.

*Joint work with* F. Marcuzzi

## References

[1] M. Dessole and F. Marcuzzi, *Deviation Maximization for Rank-Revealing QR Factorizations*, submitted to Numerical Algorithms (2021).

[2] G. Golub and V. Klema and G.W. Stewart, *Rank degeneracy and least squares problems*, Technical report STAN-CS-76-559, Department of Computer Science, Stanford University (1976).

[3] G. Quintana-Ortì and X. Sun and H. Bischof, *A BLAS-3 Version of the QR Factorization with Column Pivoting*, SIAM Journal on Scientific Computing, 19, n.5 (1998), pp. 1486–1494.

# AMG Preconditioners based on parallel hybrid coarsening exploiting multi-objective graph matching

Fabio Durastante

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In this talk, we describe preliminary results from a multi-objective graph matching algorithm, in the coarsening step of an aggregation-based Algebraic MultiGrid (AMG) preconditioner, for solving large and sparse linear systems of equations on high-end parallel computers. On one hand, we focus on the task of improving the convergence behavior of the AMG method when applied to highly anisotropic problems. On the other hand, we describe the first step towards the extension of the parallel package `AMG4PSBLAS` [1] to exploit multi-threaded parallelism at the node level on multi-core processors. The proposed matching approach balances the need to simultaneously compute high weights and large cardinalities in the matching by a new formulation of the weighted matching problem that combines both these objectives using a parameter $\lambda$. The matching is computed by a parallel $2/3-\varepsilon$-approximation algorithm for maximum weighted matchings [2,3]. The results show that the new matching algorithm with a suitable choice of the parameter $\lambda$ computes effective preconditioners in the presence of anisotropy.

*Joint work with* P. D'Ambra, S. M. Ferdous, S. Filippone, M. Halappanavar*, and* A. Pothen

## References

[1] P. D'Ambra, F. Durastante and S. Filippone, *AMG Preconditioners for Linear Solvers towards Extreme Scale*, SIAM J. Sci. Comput. **43**, 2021, no. 5, pp. S679–S703.

[2] S M Ferdous, Algorithms for degree-constrained sub-graphs and applications, Ph.D. thesis, Purdue University, West Lafayette, IN, USA, 2021.

[3] F. Manne and M. Halappanavar, *New Effective Multithreaded Matching Algorithms*, Proceedings of IEEE 28th IPDPS, 2014, pp. 519–528.

# Density forms of liquid water revealed by the Total Communicability of the corresponding graph

Chiara Faccio

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In various parts of chemistry, graph theory has long been applied to create simple mathematical models of molecules and their links. Typically, the atoms (or the molecules) correspond to the graph nodes, and their chemical bonds correspond to the edges. In this talk, based on [2], we propose a new order parameter based on the Total Communicability to identify the low-density liquid (LDL) and high-density liquid (HDL) phases of liquid water. Although network-based approaches have been applied to the investigation of other water-related processes, the problem of determining the LDL and HDL phases using centrality measures has not been considered before. The Total Communicability [1] of a node $v_i$ is defined as: $TC(v_i) = [e^{\beta A}\mathbf{1}]_{\mathbf{i}}$, where $\mathbf{1}$ is the vector of ones, $A$ is the adjacency matrix of the network, and $\beta > 0$ is a parameter. This quantity has an interpretation in terms of walks on the graph, it takes into account the global properties of the network, and it can be computed efficiently using algorithms for computing the action of a matrix function on a vector, that is, for computing the vector $f(A)v$ for a matrix $A$ (usually large and sparse), a vector $v$, and function $f$.

*Joint work with* M. Benzi, I. Daidone*, and* L. Zanetti-Polzi

## References

[1] M. Benzi and C. Klymko, *Total communicability as a centrality measure*, Journal of Complex Networks, Volume 1, Issue 2, (2013), pp. 124–149.

[2] C. Faccio, M. Benzi, L. Zanetti-Polzi and I. Daidone, *Low, high and very-high density forms of liquid water revealed by a medium-range order descriptor*, arXiv preprint arXiv:2110.13747 (2021).

# A novel matrix-factorization algorithm for the analysis of Hyperspectral Images

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The extraction of information from Hyperspectral Images (HSI) is a field of research important in many applications. In the aerospace sector, for example, it is useful to monitor changes of the Earth surface, or to find salient information from urban geo-spatial data. HSI can be thought as a 3-way tensor where the abundant information present on the third-mode should be carefully analized in order to neglect unnecessary redundancies. Therefore, dimensionality reduction techniques play a fundamental role. We propose a matrix factorization algorithm based on the iterative Stewart's QLP decomposition, see [1]-[2] that can be applied to HSI after vectorization is performed. In particular, provided a given threshold, only an automatically selected subspace will be used to approximate the original HSI. The algorithm is validated on saliency and change detection tasks and some comparisons are made with standard techniques based on non-negative-matrix factorizations, see [3].

*Joint work with* F. Mazzia

## References

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# How perturbations propagate along the solutions of linear ordinary differential equations: a relative error analysis

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In this talk, we are going to present how perturbations in the coefficient matrix $A$ propagate along the solutions of n-dimensional linear ordinary differential equations

$$\begin{cases} y'(t) = Ay(t), \ t \geq 0, \\ y(0) = y_0. \end{cases}$$

In other words we are considering the conditioning of the problem

$$(y_0, A) \mapsto e^{tA} y_0$$

and an asymptotic analysis of condition numbers, as $t \to +\infty$, will be given. The analysis is accomplished for the case where $A$ is normal matrix.

We remark that conditioning of such problems attained less attention in literature. At the best of our knowledge there are only two papers [1] and [2] on this topic. These papers present computational aspects of the condition number. On the other hand our study is more on theoretical aspects of the condition number. It studies how this condition number depends on the time $t$ and the initial data $y_0$. Also the asymptotic behavior of condition number as $t \mapsto +\infty$ is part of our study.

*Joint work with* S. Maset

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# Remember where you came from: Hitting times for second-order random walks

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Effective mathematical models for navigation and diffusion processes in complex networks are often based on random walks, i.e., Markov chains $\{X_n\}$ with a stochastic matrix $P$ describing edge transition probabilities,

$$\mathbf{P}(X_{n+1} = j | X_n = i) = p_{ij}.$$

This idea has recently been extended by accounting for an earlier step using, e.g., non-backtracking random walks or other network navigation strategies encountered in machine learning algorithms. The transitions of the resulting stochastic processes are described by formulas such as the following:

$$\mathbf{P}(X_{n+1} = k | X_n = j, X_{n-1} = i) = p_{ijk}.$$

Such processes can be naturally recast as Markov chains on the edges of the original network. Following this approach, non only stationary densities but also mean hitting times and return times can be defined for these second-order random walks.

In the present work, we investigate the problem of computing these second-order mean hitting and return times and analyze their relations with the stationary density of the process. One of our guiding questions is the following: To what extent do known facts in Markov chain theory (e.g., Kac's lemma and Kemeny's constant) carry over to second-order random walks?

*Joint work with* A. Tonetto *and* F. Tudisco

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# A Reverse Constrained Preconditioner for saddle-point matrices in contact mechanics

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The accurate simulation of fault and fracture behavior is of great importance in the context of geomechanics. While several phenomena need to be captured, such as micro-seismicity and fracture propagation, their physical description is quite complex, due to the strong coupling between fractures and mechanical deformation. The frictional contact problem is the main challenge of this effort, producing a stiff non-linear problem associated with linearized Jacobian matrices that are difficult to solve efficiently. We enforce the constraint using Lagrange multipliers and deal with two different discretizations, one intrinsically stable and the other requiring a stabilization correction [1]. The focus of this presentation is on preconditioning strategies for the arising saddle-point Jacobian matrices. We propose a constraint preconditioner based on the elimination of the Lagrange multipliers unknowns. In such a way, the primal Schur complement is similar to a stiffness matrix and state-of-the-art multigrid techniques for structural matrices [2] are very effective. Suitable augmentation for the intrinsically stable case is presented. We provide numerical evidences of the robustness and efficiency by solving large size problems from various applications.

*Joint work with* M. Frigo, C. Janna *and* M. Ferronato.

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# An efficient preconditioner for the coupled contact mechanics and fluid flow in fracture network

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For many subsurface application, such as geothermal energy production and $CO_2$ sequestration, a major role is played by the coupled simulation of frictional contact mechanics and fluid flow in fractured porous medium. In addition, large domains with high resolution representations of the geological structures and their heterogeneous properties are usually required to achieve the desired accuracy. These aspects naturally reflect on the growing demand for better performance of sophisticated and computationally expensive models. In this talk, the focus is on the linear solver, that is the most time consuming component of a simulation, and in particular on the design of a scalable and efficient preconditioning framework for the coupled contact mechanics and fluid flow problem. The model relies on the explicit discretization of the fractures, with the Lagrange multipliers method used to impose the contact constraints. Low order finite elements are used for the mechanics, while a cell-centered finite volume scheme has been adopted for the fluid flow. The arising system of equations has been properly stabilized to satisfy the inf-sup condition.

We design a scalable preconditioning framework for the 3x3 block matrix exploiting the natural unknown subdivision and a state-of-the-art aggregation-based multigrid solver. Two different approaches have been derived with the identification of theoretical bounds for the eigenvalue distributions of the preconditioned matrices. The two methods are tested on real world cases to prove the algorithmic scalability, the influence of the relative weight of fracture-based unknowns and the performance on a real-world problem.

*Joint work with* M. Ferronato, A. Franceschini

# Regularization by inexact Krylov methods

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This talk will present theoretical and algorithmic aspects of regularization methods based on inexact Krylov methods for the solution of large-scale discrete inverse problems. Specifically, we will introduce two new inexact Krylov methods that can be efficiently applied to unregularized or Tikhonov-regularized least squares problems, and we present their theoretical properties, including links with their exact counterparts and strategies to monitor the amount of inexactness. We then describe how the new methods can be applied to solve separable nonlinear inverse problems arising in blind deblurring, where both the sharp image and the parameters defining the blur are unknown. We show that the new inexact solvers (which can naturally handle varying inexact blurring parameters while solving the linear deblurring subproblems within a variable projection method) allow for a much reduced number of total iterations and substantial computational savings with respect to their exact counterparts. This talk is based on the work described in [1].

*Joint work with* M. Sabatè Landman.

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# Preconditioning in collocation and interpolation with radial basis functions

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The collocation method and the interpolation problem with radial basis functions usually produce large and dense linear systems with bad conditioned coefficients matrices. We consider the solution of these linear systems by iterative methods. A translation technique based on Rokhlin's fast multipole method [1] has been used to speed up the action of the coefficients matrix on a given vector.

In order to improve the efficiency of these iterative methods a preconditioning matrix is necessary [2]. We study preconditioning techniques that can be efficiently used to solve this kind of linear systems.

*Joint work with* N. Egidi, P. Maponi, A. Perticarini

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# Distance to singularity for quadratic matrix polynomials

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Given a regular matrix polynomial, an interesting problem consists in the computation of the nearest singular matrix polynomial, which determines its distance to singularity. When this distance is small, the conditioning of the eigenvalues is affected by small perturbations.

In this talk we focus - for simplicity - on the case of a regular quadratic matrix polynomial $\lambda^2 A + \lambda B + C$ with $A, B, C \in \mathbb{C}^{n \times n}$ and look for the nearest (with respect to the Frobenius norm) singular quadratic matrix polynomial $\lambda^2(A + \Delta A) + \lambda(B + \Delta B) + (C + \Delta C)$. To do this we generalize the idea presented in [1] for pencils, by imposing that the determinant of the perturbed matrix polynomial nihilates on a set of complex points $\{\mu_i\}_{i=1}^{N}$ with $N > 2n$, which implies that the determinant vanishes identically. We proceed by successively minimizing, with respect to perturbations of fixed norm $\|[\Delta A, \Delta B, \Delta C]\|_F = \varepsilon$, the functional

$$F_\varepsilon\left(\Delta A, \Delta B, \Delta C\right) = \frac{1}{2} \sum_{i=1}^{N} \sigma_{\min}^2\left(\mu_i^2(A + \Delta A) + \mu_i(B + \Delta B) + (C + \Delta C)\right)$$

where $\sigma_{\min}$ denotes the smallest singular value. We do the minimization by integrating the gradient system associated with the functional. In addition, to drive the functional to zero, we tune the norm value $\varepsilon$ by an iterative method. Our technique also applies to structured problems, for example to palindromic polynomials, by projecting the gradient onto the structure. Illustrative examples will be shown during the talk.

*Joint work with* N. Guglielmi

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# Improving AMG interpolation through energy minimization

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Algebraic Multigrid (AMG) is a very popular iterative method in several applications due to its effectiveness in solving linear systems arising from the discretization of PDEs. The key feature of AMG is its optimality that is its ability to guarantee, at least in some problems, a convergence rate that is independent of the mesh size. This feature is obtained through a good interplay between the smoother and the interpolation. Unfortunately, for difficult problems such as those arising from linear elasticity or diffusion problems with strong contrasts in the coefficients, standard smoothers and interpolation techniques are not enough to ensure fast convergence. In these cases, improving the prolongation operator by minimizing its energy may greatly enhance AMG convergence [1,2]. In this talk, we show how energy minimization can be seen as a constrained minimization problem, where the constraint is twofold: the prolongation must be sparse, and its range must contain the operator near-kernel. To solve this problem, we propose an iterative algorithm based on the null-space method and preconditioning to speed-up the set-up time. Finally, thanks to some numerical experiments we demonstrate how the convergence rate can be significantly increased at a reasonable set-up cost.

*Joint work with* A. Franceschini *and* G. Isotton

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# Parameter-Robust Preconditioning for Oseen Iteration Applied to Navier–Stokes Control Problems

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In this talk I will present novel, fast, and parameter-robust precon-
ditioned iterative methods for distributed time-dependent Navier–Stokes
control problems with Crank–Nicolson discretization in time. The key in-
gredients of the solver are a saddle-point type approximation for the linear
systems, an inner iteration for the $(1, 1)$-block accelerated by a generaliza-
tion of the preconditioner for convection–diffusion control derived in [2],
and an approximation to the Schur complement based on a potent com-
mutator argument applied to an appropriate block matrix. The flexibility
of the commutator argument, which is a generalization of the technique
derived in [1], allows one to alternatively apply a backward Euler scheme
in time, as well as to solve the stationary Navier–Stokes control problem.
A range of numerical experiments validate the effectiveness of our new
approach.

*Joint work with* J. W. Pearson*, based on the paper [3].*

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trol*, submitted, arXiv preprint arXiv:2108.00282.

# Some challenging issues in the linear algebra of contour integral methods for PDEs

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We generalize ideas in the recent literature [1] and develop new ones [2] in order to propose a general class of contour integral methods for linear convection–diffusion PDEs and in particular for those arising in finance. These methods aim to provide a numerical approximation of the solution by computing its inverse Laplace transform. The choice of the integration contour is determined by the computation of a few suitably weighted pseudo-spectral level sets of the leading operator of the equation, defined as:

$$\sigma_{\epsilon,t}(A) = \left\{ z \in \mathbb{C} \ : \ e^{-\Re(z)t} \sigma_{\min}(A - zI) \leq \epsilon \right\}. \tag{2}$$

A fast and reliable approximation of these weighted pseudo-spectral level sets is fundamental for the use of contour integral methods. We propose a new fast pseudospectral roaming method and we show results of its application in some illustrative parabolic problems.

*Joint work with* N. Guglielmi *and* M. López Fernández

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# The extended Rippa's algorithm in RBF interpolation

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In the context of RBF interpolation, Rippa's algorithm is a well known Leave-One-Out Cross Validation (LOOCV) method for the tuning of the shape parameter. In this talk, we present and discuss the extension of Rippa's scheme to a more general $k$-fold CV setting, which has been provided in [1]. Letting $n$ be the number of data sites, the so-constructed Extended Rippa's Algorithm (ERA) is advantageous if $k \approx n$, since in this case the costly resolution of many *large* linear systems is avoided.

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# The minimal realization problem in physical coordinates

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The *minimal (state-space) realization problem* can be formulated as follows: "Given some input-output data $u(k), y(k)$ , $k = 0, \ldots, N$, find a state-space description of minimal size $n_x$ that is capable of reproducing the given data". The first algorithm for this problem has been developed by Ho and Kalman [1] in 1966, for single-input-single-output (SISO) state-space models. Nowadays, the solution algorithms for general multi-input-multi-output (MIMO) state-space models are the so-called "subspace methods" [2]. The minimal realization is not unique: given an invertible basis-change matrix $T$, the system transformed in the new coordinates $\tilde{x} = T^{-1}x$ maintains the same input-output behavior.

In this talk we deal with the minimal realization problem of systems described by physical-mathematical models; in these systems the state variables have a physical meaning. Then, we try to solve a harder problem: to find a minimal realization whose state vector is expressed in the *physical base*, that is true when each of its state variables has a twin variable in the physical-mathematical model describing the real system. We present the results from a novel approach [3].

*Joint work with* C. Faccio

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# Relative error propagation in linear ordinary differential equations: long-time behavior of condition numbers

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We consider the propagation, along the solution of a linear ordinary differential equation $y'(t) = Ay(t)$, of perturbations in the initial value $y(0) = y_0$. Of course, this propagation is well understood when the perturbations are measured by absolute errors. In this talk, we analyze the propagation when the perturbations are measured by relative errors, rather than absolute errors. In other words, we are interested in the relative conditioning of the linear problem $y_0 \mapsto e^{tA}y_0$, i.e. the conditioning of the action of the matrix exponential $e^{tA}$ on a vector. Our analysis is a qualitative study of the long-time behavior of this conditioning. We introduce three condition numbers: the first is relevant to a fixed direction of perturbation, the second considers the worst case for the direction of perturbation and the third considers the worst case for the direction of perturbation and the initial value. The long-time behavior of these three condition numbers is studied. We discuss in which manner a strong nonnormality of the matrix $A$ can affect this long-time behavior and its onset. This study extends the previous work [1], where only normal matrices $A$ were considered.

*Joint work with* A. Farooq

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# On ParaDiag for BDFs

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Many parallel-in-time (PinT) paradigms have been developed in the last decades to efficiently solve time-dependent partial differential equations (PDEs). In this talk we focus on the ParaDiag scheme whose most peculiar feature consists in the explicit diagonalization of the matrix stemming from the adopted time-stepping method [1]. However, certain classes of time integrators lead to a discrete operator which is not diagonalizable. This is the case of Backward Differentiation Formulas (BDFs) like the backward Euler scheme. With the aim of overcoming such a drawback, different approaches have been developed in the literature [2]. In this talk, we illustrate a novel technique. In particular, we show how to exploit the circulant-plus-low-rank structure of the discrete BDF operators to design a new, successful implementation of the ParaDiag paradigm. The efficiency of our original scheme is displayed by several numerical examples.

*Joint work with* M. J. Gander

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# Numerical approximation of the Mittag–Leffler function for large sparse low rank matrices

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The evaluation of matrix functions and, in particular, the numerical computation of the Mittag-Leffler (ML) functions, is a current topic at the moment. Here we discuss relevant issues related to this topic, with a special focus on large sparse low rank matrices. The conditioning of the ML function, which is an essential tool to assess the quality of the approximation, is also addressed. We illustrate our findings with some numerical tests which support our results.

*Joint work with* R. Garrappa *and* T. Politi

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# Nonlinear Label Spreading on Hypergraphs

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Semi-supervised learning is the problem of finding clusters in a graph or a point-clould dataset where we are given "few" initial input labels. Label Spreading (LS) is a standard technique for this problem, which can be interpreted as a random walk diffusion process of the labels on the graph [1]. Recent work in network science has shown that in many graph algorithms a great advantage can be obtained when accounting directly for higher-order interactions modeled as hypergraphs, where, for example, a hyperedge directly connects all the authors of a paper in a co-authorship network [2]. In this work we propose a variation of LS for hypergraphs where the standard random walk Laplacian matrix is replaced by a nonlinear Laplacian-inspired map which is defined in terms of the hypergraph incidence matrix [3]. We show the convergence of the new nonlinear diffusion process to the global minimum of a regularized objective function that aims at reducing the variance across the hyperedge nodes and we demonstrate the efficiency of our approach on a variety of point cloud and network datasets.

*Joint work with* A. Benson *and* F. Tudisco

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# Refined decay bounds on the entries of spectral projectors associated with sparse Hermitian matrices

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Spectral projectors of Hermitian matrices play a key role in many applications, and especially in electronic structure computations. Linear scaling methods for gapped systems are based on the fact that these special matrix functions are localized, which means that the entries decay exponentially away from the main diagonal or with respect to more general sparsity patterns. The relation with the sign function together with an integral representation is used to obtain new decay bounds, which turn out to be optimal in an asymptotic sense. The influence of isolated eigenvalues in the spectrum on the decay properties is also investigated and a superexponential behaviour is predicted.

*Joint work with* M. Benzi

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# Mixed precision recursive block diagonalization for bivariate functions of matrices

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Various numerical linear algebra problems can be formulated as evaluating bivariate function of matrices [1]. The most notable examples are the Fréchet derivative along a direction, the evaluation of (univariate) functions of Kronecker-sum-structured matrices and the solution of Sylvester matrix equations.

We propose a recursive block diagonalization algorithm for computing bivariate functions of matrices of small to medium size, for which dense liner algebra is appropriate. The algorithm combines a blocking strategy, as in the Schur-Parlett scheme, and an evaluation procedure for the diagonal blocks. We discuss two implementations of the latter. The first is a natural choice based on Taylor expansions, whereas the second is derivative-free and relies on a multiprecision perturb-and-diagonalize approach. In particular, the appropriate use of multiprecision guarantees backward stability without affecting the efficiency in the generic case. This makes the second approach more robust.

The method has cubic complexity and it is closely related to the well-known Bartels-Stewart algorithm for Sylvester matrix equations when applied to $\frac{1}{x+y}$. We validate the performances of the proposed numerical method on several problems with different conditioning properties.

*Joint work with* S. Massei

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# Graph Topological Stability via Matrix Differential Equations

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Understanding the underlying topology of data requires representing more than dyadic relationships between agents and poses the question of graph's generalizations that exploit higher-order interactions, [1]. Among the direct applications one can find neurology, chemistry, regulatory networks, PageRank, etc. One possible approach is the use of simplicial complexes, with simplices related through the boundary operators. Such operators satisfy the Hodge theory [2], and, thus, comprise higher-order Hodge Laplacians whose kernels correspond to different topological features in the graph. For example, 0-order Laplacians describe the connected components and 1-order Hodge Laplacians the 1-dimensional holes.

In the current work we discuss the topological stability of the graph through a spectral matrix nearness problem for the 1-order Hodge Laplacian. Specifically, the objective is to find the "smallest" perturbation of the graph's weights such that the number of 1-dimensional holes is increased at least by 1. Firstly, the work formulates the proper weighted generalization of the Hodge Laplacian and, then, suitably extends the constrained gradient flow method [3]. Method's performance is illustrated on synthetic quasi-triangulation datasets and transportation networks.

*Joint work with* N. Guglielmi *and* F. Tudisco

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# On the approximation of low-rank rightmost eigenpairs of a class of matrix linear operators

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We are interested in computing the rightmost eigenpairs of a linear matrix valued operator. We make a priori the hypothesis (as this is a common property of several applications) for which the corresponding eigenmatrix has quickly decaying singular values. This allows us to constrain to a low-rank manifold the search of approximate eigensolutions. Thanks to the solution of an appropriate ordinary differential equation, we are able to approximate the rightmost eigenpair of the linear operator. From the analysis of the behaviour of such ODE on the whole space, we conclude that, under generic assumptions, the solution converges globally to its leading eigenmatrix, when the rightmost eigenvalue is simple and real. After that, we project the differential equation on a low-rank manifold of prescribed rank. The projected operator is nonlinear and this makes the analysis more subtle. Finally, we propose two explicit numerical methods. The numerical experiments show that the approach is effective and competitive.

*Joint work with* N. Guglielmi *and* D. Kressner.

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# Numerical solution of the graph $p$-Laplacian partial eigen-problem

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In the last years the graph $p$-Laplacian eigenvalue problem has become central in applications related to machine learning, such as for example spectral clustering and classification. Several numerical approaches have been proposed to compute the variational eigenpairs as critical points of the $p$-Rayleigh quotient. However, the approximation of the partial $p$ eigen-spectrum is still an open issue.

We propose a new approach at the numerical approximation of the eigenpairs of the graph $p$-Laplacian. The approach originates from the Dynamic Monge-Kantorovich reformulation of the $L^1$ optimal transport problem developed in [1] and makes use of the convergence results presented in [2]. We introduce a family of Transport Energy functionals and define corresponding gradient flows (along descending and ascending direction) forming a sequence of generalized weighted linear graph-Laplacians whose eigenpairs converge in some sense to the graph $p$-Laplacian eigenpairs. Numerical experiments on realistic test cases show the ability of the developed numerical schemes to identify eigenpairs of the graph $p$-Laplacian for general values of the parameter $p$, including the limit cases $p = 1$ and $p = \infty$. We highlight the geometrical properties of the numerical eigenpairs and compare them to available and new theoretical findings.

*Joint work with* P. Deidda, M. Putti

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# Computation of generalized matrix functions with rational Krylov methods

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Generalized matrix functions [4] are an extension of the notion of standard matrix functions to rectangular matrices, defined using the SVD instead of an eigenvalue decomposition. In this talk, we consider the computation of the action of a generalized matrix function on a vector and we present a class of algorithms based on rational Krylov methods [3]. These algorithms incorporate as a special case previous methods based on the Golub-Kahan bidiagonalization [1]. By exploiting the quasiseparable structure of the projected matrices, we show that the basis vectors can be updated using a short recurrence, which can be seen as a generalization to the rational case of the Golub-Kahan bidiagonalization. We also prove error bounds that relate the error of these methods to uniform rational approximation on an interval containing the singular values of the matrix. The effectiveness of the algorithms and the accuracy of the bounds is illustrated with numerical experiments.

*Joint work with* A.A. Casulli.

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# Matrices associated to two conservative discretizations of Riesz fractional operators and related multigrid solvers

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Due to the non-local behavior of fractional differential operators, Fractional Diffusion Equations (FDEs) have been proven useful to model anomalous diffusion phenomena appearing in several applicative fields, like plasma physics or imaging. In this talk, we focus on a two-dimensional conservative steady-state Riesz fractional diffusion problem. As is typical for problems in conservative form, we adopt a Finite Volume (FV) discretization approach. Precisely, we use both classical FVs and the so-called Finite Volume Elements (FVEs). In the FV method we use fractionally-shifted Grünwald formulas to discretize the Riemann-Liouville fractional derivatives at control volume faces in terms of function values at the nodes. In the FVE case, the solution is approximated in the space of $C^0$ finite elements and then fractionally derived using exact formulas for fractional derivatives of a polynomial. While FVEs have already been applied in the context of FDEs, classical FVs have only been applied in first order discretizations. By exploiting the Toeplitz-like structure of the resulting coefficient matrices, we perform a qualitative study of their spectrum and conditioning through their symbol, leading to the design of a second order FV discretization. This same information is leveraged to discuss parameter-free symbol-based multigrid methods for both discretizations. Tests on the approximation error and the performances of the considered solvers are given as well.

*Joint work with* M. Donatelli, R. Krause, M. Mazza*, and* M. Semplice.

# On linear algebra in interior point methods for solving $\ell_1$-regularized optimization problems

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The efficiency and robustness of interior point methods depend on the availability of effective linear algebra solvers, able to take into account the features of the optimization problem to be solved [1]. Here we consider nonsmooth convex problems of the form

$$\min_{\mathbf{x}} f(\mathbf{x}) + \tau_1 \|\mathbf{x}\|_1 + \tau_2 \|L\mathbf{x}\|_1, \quad \text{s.t. } A\mathbf{x} = \mathbf{b},$$

where $f : \mathbb{R}^n \mapsto \mathbb{R}$ is twice continuously differentiable and convex, $L \in \mathbb{R}^{l \times n}$, $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$, $m \leq n$, and $\tau_1, \tau_2 > 0$. Problems of this form arise in several real-life applications, e.g. portfolio optimization, signal and image processing, machine learning, compressed sensing, and are usually solved by specialized versions of first-order methods. For these problems we develop variants of an Interior Point-Proximal Method of Multipliers that use proper linear algebra solvers and take advantage of the expected sparsity in the optimal solution. We show the effectiveness of our approach versus state-of-the-art first-order methods by focusing on the problem of restoring images corrupted by Poisson noise. Further details and applications are given in [2].

*Joint work with* V. De Simone, D. di Serafino, J. Gondzio, *and* S. Pougkakiotis

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# Solving cubic matrix equations arising in conservative dynamics

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In this paper we consider the spatial semi-discretization of conservative PDEs. Such finite dimensional approximations of infinite dimensional dynamical systems can be described as flows in suitable matrix spaces, which in turn leads to the need to solve polynomial matrix equations, a classical and important topic both in theoretical and in applied mathematics. Solving numerically these equations is challenging due to the presence of several conservation laws which our finite models incorporate and which must be retained while integrating the equations of motion. In the last thirty years, the theory of geometric integration has provided a variety of techniques to tackle this problem. These numerical methods require to solve both direct and inverse problems in matrix spaces. We present two algorithms to solve a cubic matrix equation arising in the geometric integration of isospectral flows. This type of ODEs includes finite models of ideal hydrodynamics, plasma dynamics, and spin particles, which we use as test problems for our algorithms.

*Joint work with* M. Benzi

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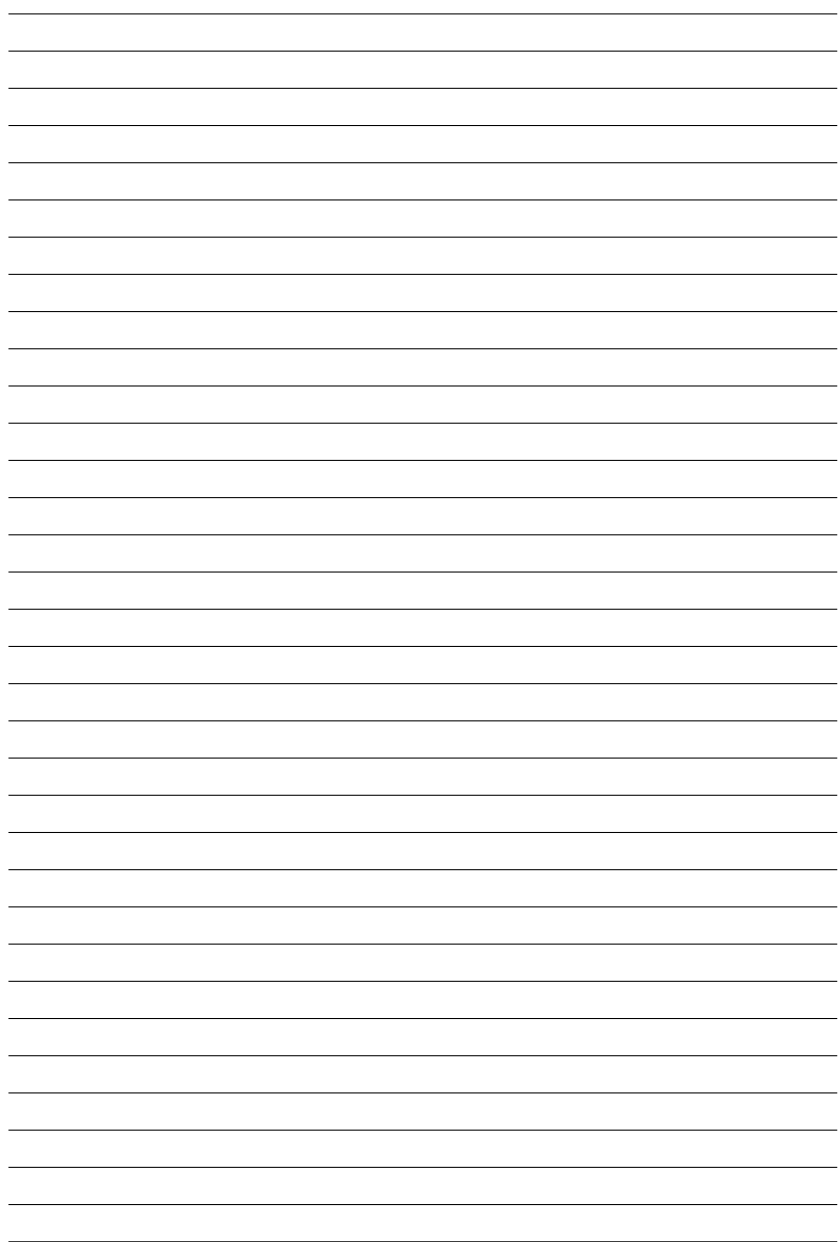**Francesco Tudisco**, Gran Sasso Science Institute
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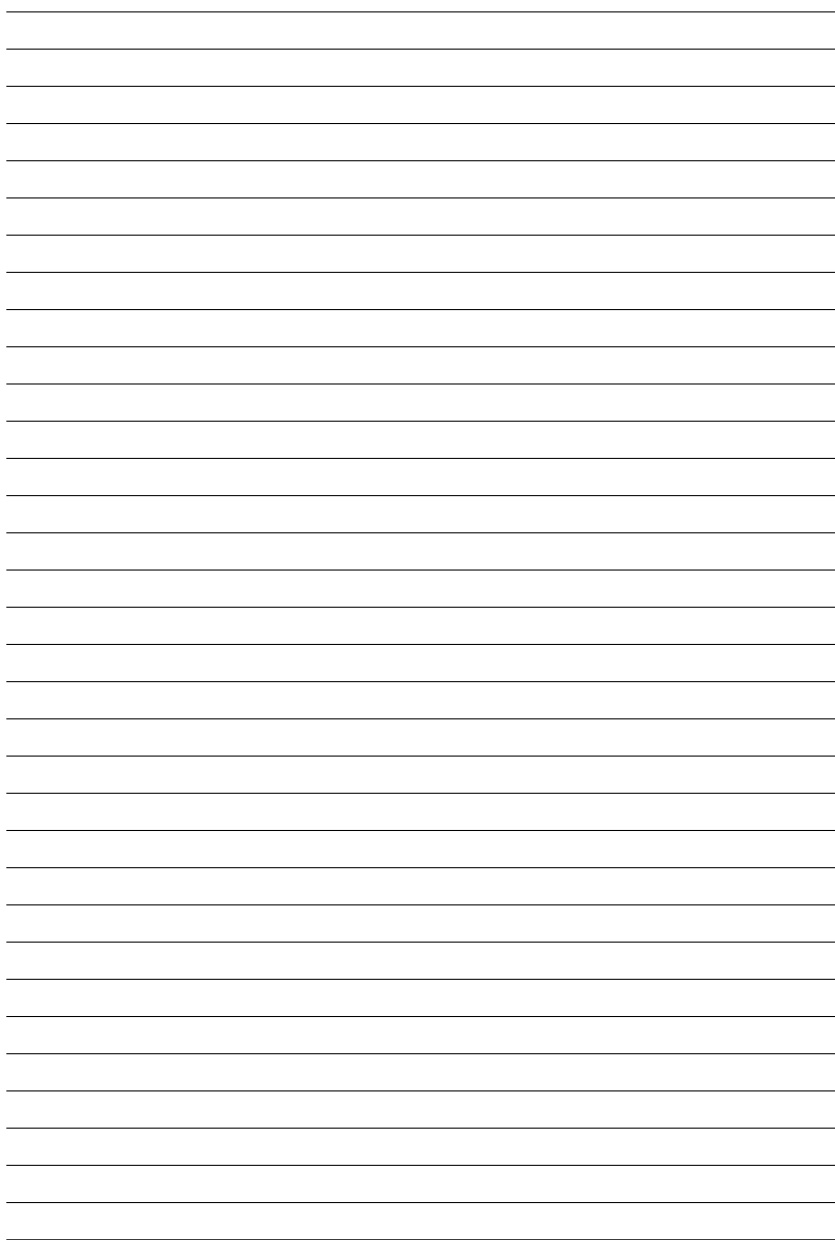kl.trotti@uninsubria.it

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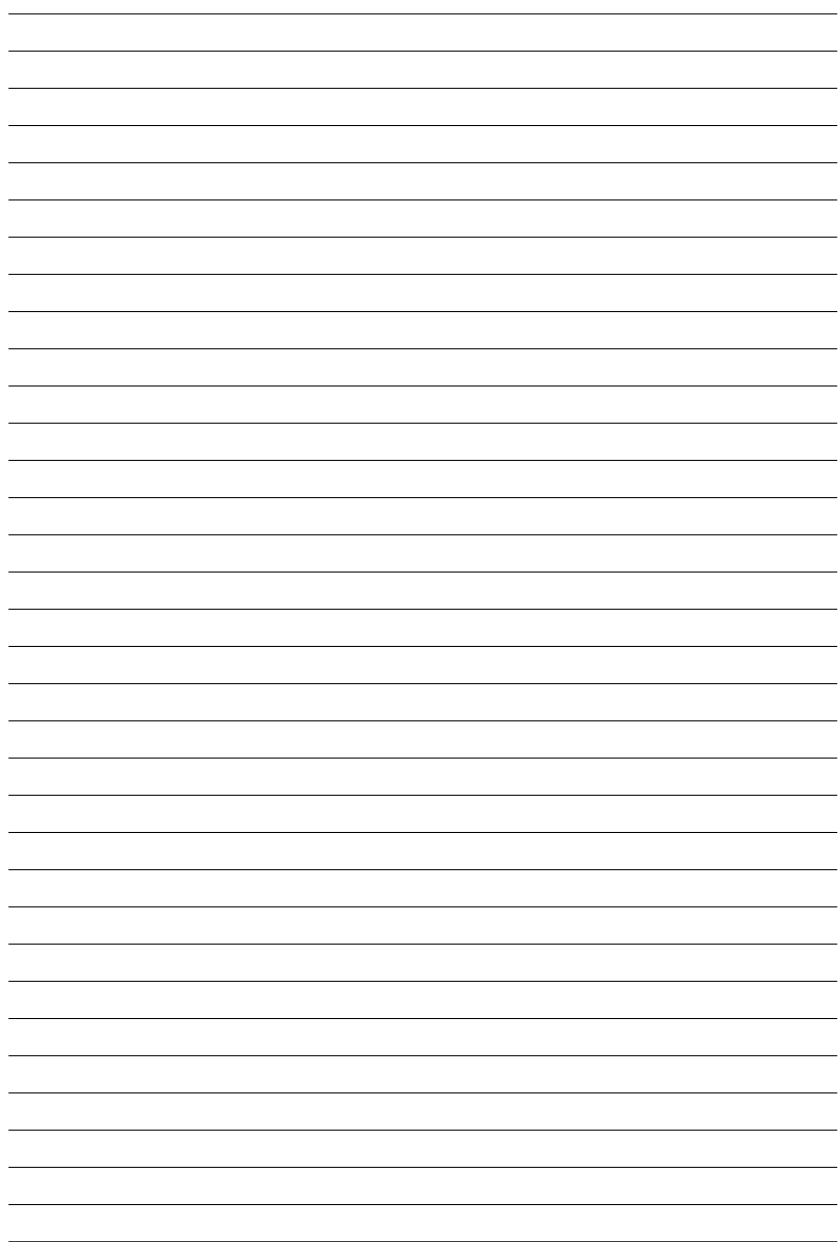mirektuma@karlin.mff.cuni.cz

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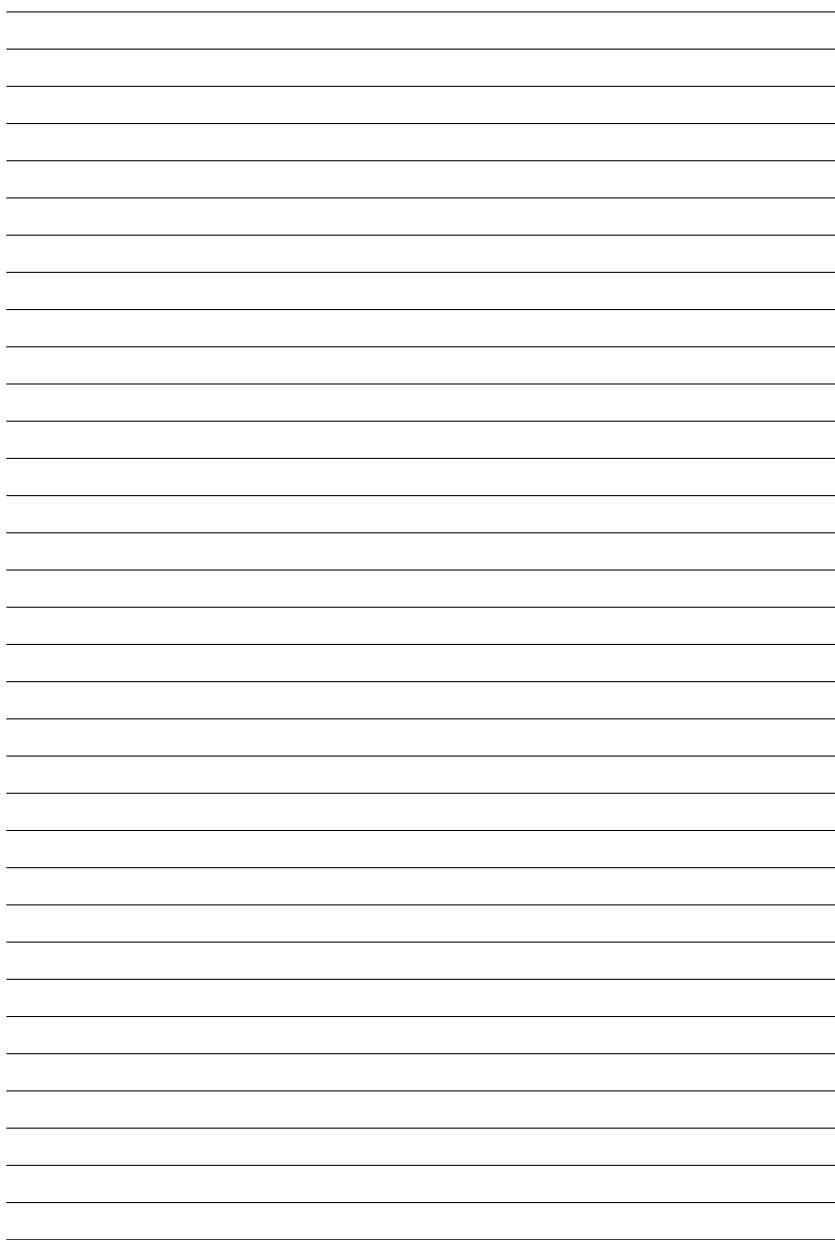
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