

# Numerical Analysis and Scientific Computation with Applications

**NASCA' 13**

**Calais, June 24-25-26, 2013**

Celebrating the 20th Anniversary of "Université du Littoral Côte d'Opale" (ULCO)

## TOPICS

Large systems of equations  
Eigenvalue problems  
Control and model reduction  
Ill-posed problems  
Optimization  
Numerical Methods for PDEs  
Applications



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## Numerical Analysis and Scientific Computation with Applications (NASCA13)

The conference NASCA'13 is celebrating the 20<sup>th</sup> Anniversary of the "Université du Littoral Côte d'Opale" (ULCO) and is organized by the "Laboratoire de Mathématiques Pures et Appliquées" (LMPA) and the Engineering School EIL Côte d'Opale. This conference brings together diverse researches and practitioners from academia, research laboratories, and industries to present and discuss their recent works on numerical analysis and scientific computation with industrial applications. The main topics are

- Large Linear Systems and Eigenvalue Problems with Preconditioning,
- Linear Algebra and Control. Model Reduction,
- Ill-posed Problems, Regularisations,
- Numerical Methods for PDEs,
- Approximation Theory, Radial Basis Functions, Meshless Approximation,
- Optimization,
- Applications to Image and Signal Processing, Environnement, Energy Minimization, Internet Search Engines...

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# Abstracts of invited speakers



# Numerical Solution of Linear and Nonlinear Matrix Equations Arising in Stochastic and Bilinear Control Theory

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## Abstract

The reachability and observability Gramians of stable linear time-invariant systems are well-known to be the solutions of Lyapunov matrix equations. Considering the classes of linear stochastic or bilinear control systems, studying the concepts of reachability and observability again leads to the solutions of generalized Lyapunov equations, which we will call *Lyapunov-plus-positive equations*, since the generalization consists in adding a positive operator to the Lyapunov operator in the left-hand side of these equations. Model reduction methods analogous to balanced truncation for LTI systems can be based on solving these Lyapunov-plus-positive equations. Due to the large-scale nature of these equations in the context of model order reduction, we study possible low rank solution methods for them.

We show that under certain assumptions one can expect a strong singular value decay in the solution matrix allowing for low rank approximations. We further provide some reasonable extensions of some of the most frequently used linear low rank solution techniques such as the alternating directions implicit (ADI) iteration and the extended Krylov subspace method. These methods are compared to, or even serve as preconditioners for, tensor versions of standard Krylov subspace solvers for linear systems of equations that can also be applied efficiently in this context. By means of some standard numerical examples used in the area of bilinear and stochastic model order reduction, we will show the efficiency of the new methods. These results are mostly contained in [1].

Stochastic optimal control problems and generalizations of balanced truncation for stochastic and bilinear systems using, e.g., LQG balancing, lead to the need of numerically solving nonlinear matrix equations, where the linear part has exactly the form of a Lyapunov-plus-positive equation, while the quadratic term is as in the standard LTI case. We will briefly discuss variants of Newton's method employing any of the solvers for Lyapunov-plus-positive equations in the Newton step.

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# A tutorial on Bayesian Filtering

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## Abstract

In Bayesian filtering we are given two processes; one of them is hidden and the other one is observed, and the problem consists in restoring the hidden sequence from the available observations. This problem has a long history by now, and has found applications in such different fields as target tracking, statistical signal processing, digital communications, automatic speech recognition or bioinformatics.

Most often, it is assumed that the joint (hidden and observed) process is a so-called hidden Markov chain (HMC). Such statistical models have been used extensively because of their ability to model physical problems of interest, and because they enable the development of efficient filtering algorithms. The aim of this tutorial is to review the main Bayesian restoration techniques which have been proposed in HMCs or some of their recent extensions. We will start with the classical Kalman filter (KF) and some of its variants, such as extended or unscented KF. We will next address the rich class of sequential Monte Carlo algorithms, including particle filtering (PF) and auxiliary PF solutions. We will then review inference techniques in the presence of a third (the so called "jump") process, which models the different regimes of the HMC. Finally we will describe some recent extensions to multi-target filtering.

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# The localization of Arnoldi Ritz values for real normal matrices

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## Abstract

The Arnoldi algorithm is one of the most used method for computing eigenvalues of large non-symmetric matrices. In this talk we consider the problem of the localization of the Arnoldi Ritz values for real normal matrices. It is well known that they belong to the field of values which is the convex hull of the eigenvalues for a normal matrix. However, for real matrices the Ritz values are contained in smaller regions inside the field of values. We will derive characterizations of the Ritz values and we will use this to explain how to compute the boundaries of the region where they are located. We will show some numerical experiments for which this region has interesting shapes in the complex plane. This study is a step towards having a better understanding of Arnoldi Ritz values convergence.

# Network analysis via partial spectral factorization and Gauss quadrature

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## Abstract

Large-scale networks arise in many applications. It is often of interest to be able to identify the most important nodes of a network or to ascertain the ease of traveling between nodes. These and related quantities can be determined by evaluating expressions of the form  $u^T f(A)w$ , where  $A$  is the adjacency matrix that represents the graph of the network,  $f$  is a nonlinear function, such as the exponential function, and  $u$  and  $w$  are vectors, for instance, axis vectors. We discuss a novel technique for determining upper and lower bounds for expressions  $u^T f(A)w$  when  $A$  is symmetric and bounds for many vectors  $u$  and  $w$  are desired. The bounds are computed by first evaluating a low-rank approximation of  $A$ , which is used to determine rough bounds for the desired quantities for all nodes. These rough bounds indicate for which vectors  $u$  and  $w$  more accurate bounds should be computed with the aid of Gauss-type quadrature rules. This hybrid approach is cheaper than only using Gauss-type rules to determine accurate upper and lower bounds in the common situation when it is not known a priori for which vectors  $u$  and  $w$  accurate bounds for  $u^T f(A)w$  should be computed. Several computed examples, including an application to software engineering, illustrate the performance of the hybrid method.

# Multilevel low-rank approximation preconditioners

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## Abstract

A new class of methods based on low-rank approximations which has some appealing features will be introduced. The methods handle indefiniteness quite well and are more amenable to SIMD computations, which makes them attractive for GPUs. The method is easily defined for Symmetric Positive Definite model problems arising from Finite Difference discretizations of PDEs. We will show how to extend to general situations using domain decomposition concepts.

# Dynamical Models Explaining Social Balance and Evolution of Cooperation

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## Abstract

Social networks with positive and negative links often split into two antagonistic factions. Examples of such a split abound: revolutionaries versus an old regime, Republicans versus Democrats, Axis versus Allies during the second world war, or the Western versus the Eastern bloc during the Cold War. Although this structure, known as social balance, is well understood, it is not clear how such factions emerge. An earlier model could explain the formation of such factions if relationships were assumed to be symmetric initially. We show this is not the case for non-symmetric initial conditions. We propose an alternative model which (almost) always leads to social balance, thereby explaining the tendency of social networks to split into two factions. In addition, the alternative model may lead to cooperation when faced with defectors, contrary to the earlier model. The difference between the two models may be understood in terms of gossiping: whereas the earlier model assumed people talk about what they think of others, we assume people talk about what others did.

Why do we observe two antagonistic factions emerge so frequently? Already in the 1950s, social balance theorists showed that a network splits into two factions if only certain triads are present in the network [1, 2], and for long the focus was on finding such factions. More specifically, a network is socially balanced if its triads are socially balanced [3]. In balanced triads friends agree in their opinion of a third party, while foes disagree. Triads that are unbalanced are unstable: all three people have an incentive to adjust their relationships to reduce the stress such situations induce. In reality, we rarely observe a perfect split into factions, but only nearly so. In any case, it remains unclear how this translates into a dynamical model that would lead to social balance. Our goal here is to analyze two such dynamical models that could potentially explain the emergence of social balance.

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# Abstracts of participants



# A hysteresis two-phase flow relaxation system in porous media: Riemann solutions and a computational fractional step method

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## Abstract

In this work we report the development of an accurate computational method for solving a hysteresis model in porous medium with gravity via relaxation (e.g., [2]) by means of an operator splitting numerical strategy. A mathematical nonlinear model for hysteretic incompressible two-phase flow system in a porous medium is considered and a set of numerical experiments to this problem is presented along with analytical solutions of the one-dimensional hysteresis model at hand in order to validate our computations. The modeling of hysteresis in porous media flow is also scientific relevant for applications in CO<sub>2</sub> sequestration operations in large-scale heterogeneous formations, such as deep saline aquifers, and depleted oil and gas reservoirs [3]. The governing system is a set of highly nonlinear coupled time-dependent partial differential equations, of convection-dominated type with a degenerate parabolic nature [1], whose solutions lead to sharp gradients. Instead of the usual global pressure formulation, we adopt here a general phase formulation (e.g., [1]) jointly with an operator splitting procedure and a combined discretization of locally conservative finite volume and mixed finite element techniques to address this nonlinear problem which, in turn, also exhibit discontinuous fractional flow functions related to the both hyperbolic and parabolic operators in the differential equations. In addition, preliminary numerical experiments in 1D and 2D show that our methodology seems to be promising for simulating with efficiency nonlinear transport flow problems in porous media as such two-phase and three-phase flow problems [1, 2].

## References

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# A frequency domain approach for the acoustic wave equation using the tensorial spline Galerkin approximation

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## Abstract

In this work, we propose a numerical approximation of the non-stationary signal reconstruction based on the ocean tomography, also called the density of acoustic flow. Many numerical techniques are available and have been employed to solve numerically the acoustic equation. Here, in the first one, we use the Euler implicit scheme, and in the second we use the frequency domain method based on the Fourier transform, which leads to an intermediate elliptic differential equation in the frequency-domain. So, the above equation is solved by using the tensorial spline Galerkin method. Also, We give in after a comparison between the finite difference method based implicit Euler scheme and our proposed frequency domain method.

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# Expansion of the global error for symplectic schemes for stochastic Hamiltonian systems

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## Abstract

Consider the stochastic autonomous Hamiltonian system in the sense of Stratonovich

$$dP^i = -\frac{\partial H_0}{\partial Q^i} dt - \sum_{r=1}^d \frac{\partial H_r}{\partial Q^i} \circ dw_t^r, \quad dQ^i = \frac{\partial H_0}{\partial P^i} dt + \sum_{r=1}^d \frac{\partial H_r}{\partial P^i} \circ dw_t^r, \quad (1)$$

where  $P_0 = p$ ,  $Q_0 = q$ ,  $P, Q, p, q$  are  $n$ -dimensional column vectors, and  $w_t^r, r = 1, \dots, d$  are independent standard Wiener processes, for  $t \in [0, T]$ . The flow of (1) preserves the symplectic structure [1]. Moreover, the implicit scheme given by the following one step approximation

$$\begin{aligned} \bar{P}_{k+1}^i &= \bar{P}_k^i - h \frac{\partial H_0}{\partial Q^i} - \frac{h}{2} \sum_{r=1}^d \sum_{j=1}^n \frac{\partial}{\partial Q^i} \left( \frac{\partial H_r}{\partial Q_j} \frac{\partial H_r}{\partial P_j} \right) - h^{1/2} \sum_{r=1}^d \frac{\partial H_r}{\partial Q^i} \xi_{ki}, \quad \bar{P}_0 = p \\ \bar{Q}_{k+1}^i &= \bar{Q}_k^i + h \frac{\partial H_0}{\partial P^i} + \frac{h}{2} \sum_{r=1}^d \sum_{j=1}^n \frac{\partial}{\partial P^i} \left( \frac{\partial H_r}{\partial Q_j} \frac{\partial H_r}{\partial P_j} \right) + h^{1/2} \sum_{r=1}^d \frac{\partial H_r}{\partial P^i} \xi_{ki}, \quad \bar{Q}_0 = q. \end{aligned} \quad (2)$$

preserves the symplectic structure and is of first weak order [1, Theorem 4.2]. Here  $h = T/N$ , everywhere the arguments are  $(\bar{P}_{k+1}, \bar{Q}_k)$  and  $(\xi_{ki})$  are i.i.d. random variables with the law  $P(\xi = \pm 1) = 1/2$ .

Following a similar approach with the one used in [2] for the Euler scheme, we find a function  $\psi$  from  $[0, T] \times \mathbb{R}^{2n} \rightarrow \mathbb{R}$  such that, under certain conditions, for any smooth function  $f$  from  $\mathbb{R}^{2n} \rightarrow \mathbb{R}$ , for the global error  $Err(T, h) = Ef(P_T, Q_T) - Ef(\bar{P}_N, \bar{Q}_N)$  we have the expansion

$$Err(T, h) = -h \int_0^T E\psi(t, P_s, Q_s) ds + O(h^2). \quad (3)$$

We use (3) to explain the excellent long-term performance of the symplectic scheme (2) and to construct by extrapolation a second order symplectic scheme. The performance of the extrapolation method is illustrated on some numerical examples.

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# A block J-Lanczos method for Hamiltonian matrix

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## Abstract

The Lanczos method is an efficient tool for computing a few eigenvalues and associated eigenvectors of a large and sparse matrix. In this work we introduce a block structure preserving Lanczos method, namely block  $J$ -Lanczos algorithm. The Hamiltonian matrix is reduced to a Hamiltonian block  $J$ -tridiagonal (Hamiltonian block  $J$ -Hessenberg) form. Gerstner and Mehrmann [4] proposed the reduction of Hamiltonian matrices to Hamiltonian  $J$ -Hessenberg form and use it when solving the real algebraic Riccati equation via the symplectic  $QR$ -like algorithm. This form is also used by Benner and Fassbender in [1] to construct a family of implicitly restarted Lanczos methods for Hamiltonian and symplectic matrices (see also [2, 3]). It's also the based tools used by Ferng, Lin and Wang [5, 6] to construct a  $J$ -Lanczos algorithm for solving large sparse Hamiltonian eigenvalue problems. The main focus of this paper is to give new methods for computing Hamiltonian block  $J$ -tridiagonal form. Our approach is based on using  $\mathbb{R}^{2n \times 2s}$  as free module on  $(\mathbb{R}^{2s \times 2s}, +, \times)$ .

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# Projection Methods for Regularized Total Least Squares Approximation

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## Abstract

Regularized Total Least Squares is an appropriate approach when both the ill-posed data matrix and the observed data are contaminated by noise. However, direct Total Least Squares methods based upon computing the singular value decomposition are prohibitively expensive for large scale problems. Therefore, we consider projection-based Regularized Total Least Squares methods that project the problem onto the lower dimensional space. Specifically, two orthogonal projection methods are introduced to be combined with the Tikhonov regularization based Total Least Squares method developed by Lee et al. [1]. The first fixes the subspace dimension before the beginning of the iterations by using bidiagonal reduction. The second expands the subspace dynamically during the iterations by employing a generalized Krylov subspace expansion.

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# Boolean sum-based differential quadrature

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## Abstract

The Differential Quadrature Method (DQM) is a numerical discretization technique for the approximation of derivatives by means of weighted sums of function values. It was proposed by Bellman and coworkers in the early 1970's, and it has been extensively employed to approximate spatial partial derivatives (cf. e.g.[3]). The classical DQM is polynomial-based, and it is well known that the number of grid points involved is usually restricted to be below 30. Some spline based DQMs have been proposed to avoid this problem. Given a B-spline  $M$  centered at the origin, a cardinal lagrangian or hermitian spline with a compactly supported fundamental function is defined, from which the approximation of the derivatives are derived, but the construction of these spline interpolants depends strongly on the degree of the B-spline (see for instance [2] and [4]). In this work we present a general DQM based on interpolation and quasi-interpolation. First, we consider the construction of cardinal functions  $L$  with small compact supports such that  $L(j) = \delta_{j,0}$ ,  $j \in \mathbb{Z}$ ,  $\delta$  being the Kronecker sequence. They are linear combinations of translates of  $M$ . The cardinal spline  $L$  provides the interpolation operator  $\mathcal{L}$  given by  $\mathcal{L}f = \sum_{i \in \mathbb{Z}} f(i) L(\cdot - i)$ . Next, we revise some discrete quasi-interpolation operators  $\mathcal{Q}f = \sum_{i \in \mathbb{Z}} \lambda_i(f) M(\cdot - i)$  defined from the same B-spline (cf. e.g. [1]), whose coefficients  $\lambda_i(f)$  only use values of  $M$  in some neighbourhood of the support of  $M(\cdot - i)$ . Finally, the operators  $\mathcal{L}$  and  $\mathcal{Q}$  are properly combined to define new interpolation operators having compactly supported fundamental functions and achieving the maximal order of approximation.

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# On the computation of orthogonal rational functions

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## Abstract

Several techniques are known to compute a new orthogonal polynomial  $\varphi_{k+1}$  of degree  $k+1$  from  $\mathcal{L}_k := \text{span}\{\varphi_0, \dots, \varphi_k\}$  in case of (discrete) orthogonality on the real line. In the Arnoldi approach one chooses  $\Phi_k \in \mathcal{L}_k$  and makes  $x\Phi_k$  orthogonal against  $\varphi_0, \dots, \varphi_k$ . By taking as  $\Phi_k$  a linear combination of  $\varphi_k$  and the kernel (or GMRES) polynomial  $\psi_k(x) = \sum_{j=0}^k \varphi_j(0)\varphi_j(x)$ , one needs to orthogonalize only against  $\varphi_{k-2}, \varphi_{k-1}, \varphi_k$ , and obtains what in numerical linear algebra is called Orthores, Orthomin or SymLQ [1]. A construction of an orthogonal basis of rational Krylov subspaces for given prescribed poles  $z_j$  can be done via orthogonal rational functions (ORF) [2], and is required for instance in the approximate computation of matrix functions. Here, following [4], the choice of the continuation vector  $\Phi_k$  which is multiplied by  $x/(x - z_{k+1})$  becomes essential, for instance for preserving orthogonality in a numerical setting. By generalizing the techniques of [2, 3], we compare several approaches and find optimal ones.

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# Computing the inverse of a triangular Toeplitz matrix

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## Abstract

Using trigonometric polynomial interpolation, a fast and effective numerical algorithm for computing the inverse of a triangular Toeplitz matrix with real numbers has been proposed by Lin, Ching and Ng [1]. The complexity of the algorithm is two fast Fourier transforms (FFTs) and one fast cosine transform (DCT) of  $2n$ -vectors. In this paper, we present an algorithm with only two fast Fourier transforms (FFTs) of  $2n$ -vectors for calculating the inverse of a triangular Toeplitz matrix with real and/or complex numbers. A theoretical accuracy analysis is also considered. Numerical examples are given to illustrate the effectiveness of our method.

**Key words:** Trigonometric polynomial interpolation, Triangular Toeplitz matrix, Fast Fourier transforms

**AMSC (2010):** 65F05, 65F30

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# Penalization of Robin boundary conditions and application to tokamak plasmas

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## Abstract

We propose an original penalization method to take account of Neumann or Robin boundary conditions. The general principle of penalization is to extend a problem initially posed in a complex geometrical domain to a larger domain. The addition of forcing terms in the initial equations allows to recover the boundary conditions of the original problem. A theoretical study is presented for linear elliptic and parabolic problems. Numerical tests are then performed by discretizing the penalized problem using a finite difference method. Finally, the method is applied to a nonlinear advection-diffusion equation.

This work follows the results presented in [1], where a model for plasma/wall interaction in a tokamak has been developed by using a penalization method to enforce Dirichlet boundary conditions for ion density and momentum. The penalization method we propose allows to enhance the initial physical model by adding new variables, ionic and electronic temperatures. The evolution of these quantities is modeled by two advection-diffusion equations with Neumann or Robin boundary conditions on the wall of the tokamak. A numerical simulation of the 4 equations model is under development (SOLEGE-2D code).

This work is done in the framework of the Research Federation “Fusion par Confinement Magnétique - ITER” and the ANR “ESPOIR” project (ANR-09-BLAN-0035-01).

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# Blood flow modeling by wavelets in the presence of a stent

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## Abstract

We present in this paper, a new approach based on the Navier-Stokes equations and wavelets decomposition for modeling the blood-flow compartment in the artery with presence of the cardiovascular stent.

In fact, we propose a mathematical one-dimensional (1d) model obtained making simplifying assumptions on solutions and to define the profiles of velocity and pressure liquid (blood) through the variable geometry of the arteries interest of simulation in this context is to make a comparison between different geometries without varying other parameters (such as blood flow, the properties of elasticity of the aortic wall).

Our approach for solving optimization problems in complex geometry like the arteries, is to use first of methods and evolutionary algorithms, one-dimensional, based on a model that leads to equations of Navier-Stokes equations for estimating the velocity profile and blood pressure taking into account variations in the geometry pressure.

We made numerical simulations with Comsol.

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# On the Symplectic SVD-Like Decomposition

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## Abstract

The aim of this paper is to introduce a numerical methods to compute a symplectic SVD-like decomposition of a  $2n$ -by- $m$  rectangular real matrix and a  $J$ -SVD decomposition of  $2n$ -by- $2m$  rectangular real matrix, all of them based on symplectic reflectors. The first one used canonical Schur form of skew-symmetric matrix. The idea of the second one is to use symplectic reflectors to first reduce matrix in  $J$ -bidiagonal form and then transforming it to a diagonal one by using sequence of symplectic similarity transformations. It is given in parallel with the so called Golub-Kahan-Reinsch method. This methods allows us to compute eigenvalues of structured matrices (Hamiltonian matrix  $JAA^T$  and skew-Hamiltonian matrix  $A^JA$ ).

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# A time-splitting scheme for nonhydrostatic atmospheric model

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## Abstract

Continuously increasing power of computers has reached the point when real-time simulations based on the fully compressible equations of the atmosphere became possible. Although the hydrostatic assumption is proved to be a good approximation for synoptic and global scale processes, there is a strong current trend to return to the use of non-filtering governing equations in order to improve the forecasting skills for meso-scale phenomena where hydrostatic balance is not quite accurate [1,2,4]. Analysis of the linearized Euler equations reveals three principal types of atmospheric waves: acoustic, gravitational and inertial waves. The propagation speed of these waves is very different as well as their energy contribution. Opting to employ the full atmospheric equations for better description of the principal phenomena, one automatically involves the fastest acoustic and gravity waves and, therefore, should solve a stiff system [1,3,4].

In this research we construct a time-splitting finite difference scheme for the nonhydrostatic atmospheric model. Applying time-splitting, the fast acoustic and gravity waves are approximated implicitly, while relatively slow advective terms and Rossby modes are treated explicitly. Stability analysis of the scheme shows that the time step is not subjected to rigid limitation of the CFL condition with respect to fast modes and can be chosen according to physical considerations of accuracy. The performed numerical experiments show computational efficiency of the designed scheme and accuracy of the predicted atmospheric fields.

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# Homogenization of 3D photonic crystals and artificial magnetism.

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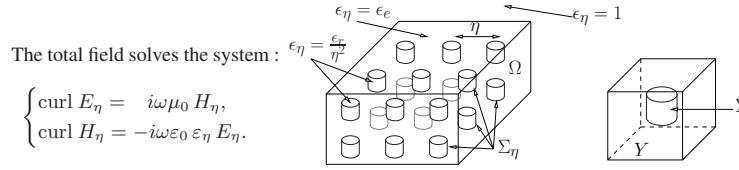
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## Abstract

In [1, 2, 3], a theory for artificial magnetism in two-dimensional photonic crystals has been developed for large wavelength (homogenization). Here we propose a full 3D generalization: the diffraction of a finite 3D-dielectric crystal is considered at a fixed wavelength and a limit analysis as the period tends to zero is performed.



Our goal is to describe the asymptotic behavior of  $(E_\eta, H_\eta)$  as  $\eta \rightarrow 0$  by determining their two-scale limit  $(E_0(x, y), H_0(x, y))$ . We evidence a new microscopic vector spectral problem which accounts the resonances of the crystal. The artificial magnetism is then described by a frequency dependent effective permeability tensor with possibly negative eigenvalues as it is the case for the metallic split-ring structure proposed by Pendry [4]. Numerical simulations will be presented.

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# A new model for shallow viscoelastic fluids

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## Abstract

We present a new reduced model [1] for gravity-driven free-surface flows of shallow viscoelastic fluids and its numerical simulation with an ad-hoc finite-volume technique.

The model is obtained by a formal asymptotic expansion of the upper-convected Maxwell model when the viscosity is small like the aspect ratio of the thin layer of fluid, while the relaxation time is kept finite. Additionally to the classical layer depth and velocity in shallow water models, the system describes also the evolution of two scalar stresses.

As mathematical properties, the model has an intrinsic energy equation, but the physically relevant energy is non-convex with respect to the conservative variables.

We thus propose a suitable well-balanced finite-volume discretization in the physically relevant pseudo-conservative variables, so that the physically relevant energy is convex. The energy-dissipating finite-volume scheme involves an approximate Riemann solver constructed with the relaxation technique.

We will illustrate the new model with numerical simulations.

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# Strong non-linear behavior of the effective thermal conductivity during heating of a wet porous medium

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## Abstract

We consider the great heating of the soil surface leading to the water phase change within the wet porous medium. Experimental temperature curves show that there is always a long plateau (up to one hour) at 100 degrees which is difficult to reproduce by numerical simulations, when using an ordinary continuous model for the heat transfer in the soil. We suspect that the global thermal conductivity changes a lot according to humidity present in the pores, then suitable models for this effective conductivity must be used.

In this work, we propose a simple approach to derive some effective conductivity laws via a 2D granular model of circular solid cylinders, packed in some regular ways, with the presence of a variable quantity of liquid water, which forms identical menisci in the gap around each point contact of the cylinder. The liquid contact angle is taken as a control parameter. The doubly periodic pattern is then reduced to a minimal computational domain using the symmetries of the system. The steady heat equation is numerically solved in this small domain, containing three different media (solid, liquid and air) using a Mixed Finite Element scheme. Some difficulties arise due to the high contrast between the conductivity of air and those of the solid part, so that extrapolation must be used to estimate accurately the heat flux through the domain.

Numerical results show that the effective conductivity has a strong non-linear behavior versus the volume percentage of liquid water in the porous granular medium. Even the 2D geometry is not directly applicable to the 3D real granular medium, we think that he can give some ideas to extend the results to our wet porous medium. The application of our work takes place in archaeology, where we study prehistoric fires in order to recover the hearths usage.

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# Efficient Deflation for Communication Avoiding Krylov Methods

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## Abstract

Krylov subspace methods (KSMs) are iterative algorithms commonly used to solve large, sparse, linear systems  $Ax = b$ . On modern computer systems, classical implementations of KSMs are communication-bound. Recent efforts have focused on *communication-avoiding* KSMs (CA-KSMs), which reorder classical Krylov methods to perform  $s$  computation steps of the algorithm for each communication step (see, e.g., the overview in [1]). This allows an  $O(s)$  reduction in total communication cost, which translates into significant speedups in practice [2].

However, reorganizing the algorithm to avoid communication can have undesirable numerical consequences. Floating point roundoff error in computing the  $s$ -step Krylov bases increases with  $s$  and the condition number of  $A$ , leading to ill-conditioned bases which can delay or even prevent convergence. We therefore seek to reduce the condition number of the system such that an acceptable rate of convergence can be maintained for the desired  $s$ .

In this work, we explore the use of explicit deflation in CA-KSMs. Explicit deflation is often used to increase the convergence rate in classical KSMs by removing eigenvector components associated with near-zero eigenvalues (see references in [4]). We derive the Deflated Communication-Avoiding Conjugate Gradient (CA-CG) algorithm, based on the Deflated CG algorithm of Saad [3]. Our analysis shows that the additional communication and computation costs of deflation are lower order terms in the context of CA-CG, maintaining the  $O(s)$  reduction in communication over  $s$  steps. Numerical results demonstrate that deflation significantly improves the convergence rate of CA-CG for minimal cost. We discuss practical implementation issues and heuristics for determining the number of approximate eigenvectors to use in deflation for CA-CG.

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# Condition and Error Estimates in Kalman Filter Design

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## Abstract

Kalman filters play a key role in the solution of the main linear optimal control and estimation problems. The Kalman filter design consists in finding the filter gain matrix determined by a matrix Riccati equation. As it is well known the numerical solution of this equation may face some difficulties. First, the equation may be ill conditioned, i.e. small perturbations in its coefficient matrices may lead to large variations in the solution. Therefore, it is necessary to have a quantitative characterization of the conditioning in order to estimate the accuracy of solution computed.

The second difficulty is connected with the stability of the numerical method and the reliability of its implementation. It is well known that the methods for solving the Riccati equations are generally unstable. This requires to have an estimate of the forward error in the solution.

The paper deals with the computation of condition numbers and residual-based forward error estimates pertaining to the numerical solution of Riccati equations arising in the continuous-time Kalman filter design. Efficient LAPACK-based condition and error estimators are proposed involving the solution of triangular Lyapunov equations along with one-norm computation.

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# Eigenvalue bounds for a preconditioned saddle point problem.

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## Abstract

Suppose the time-dependent or stationary Navier-Stokes system is discretized by a mixed finite element method and, in the evolutionary case, by an implicit or semi-implicit time-stepping. Further suppose the problem is linearized by a Picard iteration. In order to solve the corresponding algebraic system - which typically takes the form of a saddle point problem - it is crucial that an efficient preconditioner of the Schur complement is available. We consider a preconditioner involving a projection of the Neumann Laplacian and of the velocity operator onto the pressure space (Kay, Loghin, Wathen 2002). A variational method is used in order to obtain upper and lower bounds for the eigenvalues of the Schur complement. These bounds depend in an explicit way on the parameters involved.

# Preconditioning Chebyshev subspace iteration applied to sequences of dense eigenproblems in ab initio simulations

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## Abstract

Research in several branches of chemistry and materials science relies on large ab initio numerical simulations. The majority of these simulations are based on computational methods developed within the framework of Density Functional Theory (DFT) [?]. Among all the DFT-based methods the Full-potential Linearized Augmented Plane Wave (FLAPW) [?, ?] method constitutes the most precise computational framework to calculate ground state energy of periodic and crystalline materials. FLAPW provides the means to solve a high-dimensional quantum mechanical problem by representing it as a non-linear generalized eigenvalue problem which is solved self-consistently through a series of successive outer-iteration cycles. As a consequence each self-consistent simulation is made of dozens of sequences of **dense** generalized eigenproblems  $P : Ax = \lambda Bx$ . Each sequence,  $P_1, \dots, P_i \dots P_N$ , groups together eigenproblems with increasing outer-iteration index  $i$ .

Successive eigenproblems in a FLAPW-generated sequence possess a high degree of correlation. In particular it has been demonstrated that eigenvectors of adjacent eigenproblems become progressively more collinear to each other as the outer-iteration index increases [?]. This result suggests one could use eigenvectors, computed at a certain outer-iteration, as approximate solutions to improve the performance of the eigensolver at the next one. In order to maximally exploit the approximate solution, we developed a subspace iteration method augmented with an optimized Chebyshev polynomial accelerator together with an efficient locking mechanism (ChFSI).

The resulting eigensolver was implemented in C language and parallelized for both shared and distributed architectures. Numerical tests show that, when the eigensolver is preconditioned with approximate solutions instead of random vectors, it achieves up to a 5X speedup. Moreover ChFSI takes great advantage of computational resources by obtaining levels of efficiency up to 80 % of the theoretical peak performance. In particular, by making better use of massively parallel architectures, the distributed memory version will allow the FLAPW method users to simulate larger physical systems than are currently accessible.

Additionally, despite the eigenproblems in the sequence being relatively large and dense, the parallel ChFSI preconditioned with approximate solutions performs substantially better than the corresponding direct eigensolvers, even for a significant portion of the sought-after spectrum.

# Fast adaptive alternating linear schemes in higher dimensions. Part 1: linear systems

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## Abstract

We address an approximate solution of large-scale high-dimensional tensor-structured linear systems. The main area of applications is the solution of high-dimensional differential equations, which allow a low-parametric approximation of the multilevel matrix, right-hand side and solution in the tensor train format. We develop a method of Alternating Linear Scheme type, which performs a subsequent system reduction to each component of the tensor format. However, contrarily to the traditional ALS approaches, we make the method rank-adaptive, equipping it with the basis enrichment step using Krylov-type vectors. As a result, the theoretical convergence of the method is provided by the steepest descent (symmetric positive definite matrix) or FOM (general matrix) methods, while the practically observed one is significantly faster. We verify the technique on multidimensional probability equations, e.g. Fokker-Planck, chemical master equations, arising in biology and chemistry.

# Solving Vehicle Routing Problem with Soft Time Windows using A Hybrid Intelligent Algorithm

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## Abstract

Vehicle routing problems (VRPs) appear in many practically highly relevant areas of our daily life. In general, they are concerned with finding efficient routes, starting and ending at a central depot, for a fleet of vehicles to serve a number of customers with demands for certain commodity [1]. A common extension to the classical VRP known as vehicle routing problem with time windows (VRPTW), which has attracted much attention in the scientific community [2]. VRPTW includes vehicle routing problem with soft time windows (VRPSTW). For this problem, the deliveries remain possible outside the windows of time with some penalty costs. Koskosidis et al. transformed VRPSTW as a mixed integer problem, based on the treatment of the time window constraints as soft constraints [3]. Qureshi et al. gave a solution using an exact approach for VRPSTW, they solved elementary shortest path problem with resource constraints [4]. Ibaraki et al. analyzed acceleration techniques for local search algorithms in the multiple soft time windows [5]. In this paper, we present a hybrid algorithm for the vehicle routing problem with soft time windows, which tested on various data sets of VRPSTW benchmarks, the results reveal the high performance and efficiency of the proposed method.

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# Vector extrapolation and applications to partial differential equations

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## Abstract

In this talk, we study polynomial extrapolation methods. We discuss the design and implementation of these methods for computing solutions of fixed point methods. Extrapolation methods transform the original sequence into another sequence that converges to the same limit faster than the original one without having explicit knowledge of the sequence generator. One of the most popular vector extrapolation methods is the Reduced Rank Extrapolation (RRE) by Eddy [2] and Mesina [3].

Restarted methods permit to keep the storage requirement and the average of computational cost low. We apply these methods for solving problems arising from discretization of partial differential equations. Vector extrapolation methods are considered to be most effective when applied to nonlinear systems of equations, see [1, 4, 5].

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# Generation of traveling waves with the Petviashvili method

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## Abstract

The Petviashvili method is an iterative technique that originally appeared to generate lump solitary wave profiles of the Kadomtsev-Petviashvili I (KPI) equation [4]. The method has become popular in the community of researchers in water wave theory and nonlinear optics, because of its easy implementation, along with other alternatives, such as variants of Newton's method, squared operator methods, imaginary-time evolution methods (see [5] and references therein) or different variational procedures [1]. Some studies of convergence of the method have been made, concerning particular cases of its main application, which is the numerical approximation of traveling wave profiles in nonlinear dispersive systems [2, 3]. The purpose of this talk is analyzing the Petviashvili method as an iterative technique for the numerical resolution of a system of nonlinear equations in  $\mathbb{R}^m$ ,  $m > 1$ . Some general convergence results are derived and applied to the discretization of several systems for traveling wave generation. Acceleration techniques, with vector extrapolation methods, topological  $\epsilon$ -algorithms and Anderson mixing are also discussed.

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# Optimisation's method to find a common eigenvector of two matrices

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## Abstract

In [1] we have proved the sensitivity of computing the common eigenvector of two matrices, and we have designed a new approach to solve this problem based on the notion of the backward error.

In [2] we have proposed a solution based on the newton's method to find the common eigenvector of two matrices. In this paper we describe an approach to solve the problem, we implements two optimizations procedure to minimize directly the backward error. The first one is using the steepest descent method; the second is an implementation of the quasi-Newton method the BFGS, note that a recent optimization-based approach has been proposed for eigenvalue and generalized eigenvalue computations [5].

We mention that no assumptions are made on the matrices  $A$  and  $B$ .

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# Hybrid model for valuation of credit derivatives with stochastic parameters

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## Abstract

We introduce the intensity default barrier (IDB) model based on the conditional survival probability also called hazard function barrier, allowing an evaluation of credit derivatives under the risk-neutral probability with stochastic parameters. Moreover, the IDB is a hybrid and analytic model combining structural approach and reduced form methodology which discuss the impact of default intensity barrier and processes around the firm. Our model has succeeded to prove the Doob-Meyer decomposition of the default process associate to the random barrier. In this framework, we explain the default barrier process as a sum of its compensator which is a predictable process and a martingale relatively to the smallest filtration making the random barrier a stopping time. In addition, the IDB as the Shifted Square Root Diffusion (SSRD) Alfonsi's model is leaving the dependence between the stochastic default intensity and interest rate. The most interesting feature of this model is that it can be easily generalized to all credit derivatives products as Collateralized debt obligations (CDO) and credit default swaps (CDS).

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# RRE applied on nonsymmetric algebraic Riccati equations

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## Abstract

An important problem that arises in different areas of science and engineering is that of computing limits of sequences of vectors  $x_n$ , where the  $x_n$  are complex  $N$ -vectors with  $N$  very large. Such sequences may result from iterative methods or perturbation techniques and many of them may converge extremely slowly to their limits with a desired accuracy. Vector extrapolation methods are techniques which can be applied to such vector sequences. These methods transform a sequence of vectors generated by some process to a new one so that it converges faster than the initial sequence. Here, a suitable vector extrapolation method, namely the reduced rank RRE, may be applied to accelerate their convergence.

Our concern is a special kind of nonsymmetric algebraic Riccati equations (NARE) arising in transport theory of the general form

$$XCX - XD - AX + B = 0,$$

where  $A, B, C$ , and  $D \in \mathbb{R}^{n \times n}$  are given coefficient matrices. The computation of the minimal positive solution of this equation was shown in [1] to be done via computing the minimal positive solution of a vector equation. Many methods tried to compute this solution using specific iterative schemes but results showed that the convergence of vector sequences produced by such schemes tends to be very slow. Here, we will try to apply a vector extrapolation method, namely the RRE due to [4], to a vector sequence produced by an iterative method, namely the method of Y. Lin [2], and which succeeds to compute the minimal positive solution of NARE. Finally, we will compare our results with a fast Newton method of [3], a very efficient method.

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# A multiresolution trust region algorithm for optical flow computation

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## Abstract

Optical flow is a problem that has received considerable effort during the last years. In a variational setting, the problem is usually formulated as a minimization of an energy function which is a weighted sum of two terms: a data term and a regularization term. A classical strategy to minimize such functional is based on discretizing the corresponding Euler-Lagrange equations. Here we adopt a second strategy which has been less investigated in the context of optical flow, namely the minimization of the energy with a truncated Newton method involved in a multiresolution trust region approach. We demonstrate the competitiveness of this method for dense optical flow computation using four different models and three sequences of images.

# A global method for reactive transport in porous media.

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## Abstract

Underground media are endangered by anthropogenic as well as natural contaminations. The fate of contaminants in aquifers is controlled by hydrogeological conditions and chemical interactions. Risk assessment and resources management rely on numerical simulations, which must deal with sharp fronts evolving in time and space. Several reactive transport models have been designed to cope with these challenging difficulties [1].

In this talk, we discuss a global method which uses a chemistry model based on principal and secondary species and on total analytical concentrations. We show that, after space discretization, the model is a set of Algebraic Differential Equations (DAE) of large size. At each time step, we can reduce this size by eliminating unknowns and we can use the specific structure of the Jacobian to solve the linearized systems. We also discuss the use of logarithms to write the mass action laws and the impact on the condition number of the Jacobian. Numerical experiments with the Momas benchmark illustrate the efficiency of our global method, implemented in our software GRT3D.

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# Eigenvalue computations of normal matrices via complex symmetric form

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## Abstract

In this talk, relations between normal and complex symmetric matrices will be discussed. Constructive algorithms will be given for transforming normal matrices via unitary similarity to complex symmetric form. This reduction is only valid in its most general form for matrices with distinct singular values. If not, the resulting matrix exhibits a particular block structure related to the singular value distribution.

In both cases this reduction can be combined with some eigenvalue solvers for complex symmetric matrices, in order to obtain an eigenvalue decomposition of the original matrix. Numerical experiments will illustrate the speed and accuracy of this novel approach.

Though the framework proposed is theoretically reliable, the method may suffer from numerical pitfalls when multiple or close singular values are present. We will analyze the causes of such an issue and examine the overall behavior of the algorithm for some special distributions of singular values.

# On efficient estimation of matrix inverse

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## Abstract

Let  $A$  be a symmetric matrix. We use the extrapolation procedure developed in [1] in order to estimate useful quantities related with the matrix inverse. Using the spectral theorem for the matrix  $A$ , we can express its moments as a sum  $c_\nu(x) = (x, A^\nu x) = \sum_i \sigma_i^\nu \alpha_i^2(x)$ , where  $\alpha_i(x) = (x, u_i)$ , for  $\nu \in \mathbb{N}$ . We approximate  $c_{-1}(z)$  by extrapolating at the point  $-1$ , the  $c_\nu(x)$ 's for different values of the nonnegative integer index  $\nu$  by a conveniently chosen function obtained by keeping  $k$  terms in the preceding summations. The estimates of  $c_{-1}(z)$  lead to estimating the bilinear form  $u^T A^{-1} v$ . For appropriate chosen vectors  $u$  and  $v$ , we can obtain estimates of the elements of the matrix  $A^{-1}$ , its diagonal, the trace of  $A^{-1}$  [1] and other useful quantities arising in linear algebra problems. The above procedure can be extended to the nonsymmetric matrix case. The derived estimates will be compared with other existing methods [2] and statistical techniques will be proposed for improving them.

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# Simulation of thermal stabilization of soil around the wells in permafrost

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## Abstract

Permafrost takes place about 25% of the total land area of the globe (mainly in Alaska, the northern territories of Canada, Russia, China, highland areas) and is closely related with external influences. Extraction and transportation of oil and gas also has a significant effect on permafrost, as heat flux from the heated oil in wells and pipelines leading to permafrost thawing. This can lead to accidents and even to the destruction of wells. In order to reduce permafrost thawing near engineering structures there are used different methods of thermal stabilization of soils such as insulation materials and various devices to cool the soil, for example, seasonal cooling devices (SCDs), which operate without any external source of energy only by the laws of physics. To simulate the propagation of heat from wells in permafrost the mathematical model is suggested, which takes into account not only climatic and physical factors [1-2], but also thermophysical parameters of applied thermal insulations, as well as any devices (such as SCDs) used for thermal stabilization (cooling) of the soil. This leads to solution of three-dimensional quasilinear thermal diffusivity equation for a Stephan problem

$$\rho(c_v(T) + k\delta(T - T^*)) \frac{\partial T}{\partial t} = \operatorname{div}(\lambda(T)\operatorname{grad}T).$$

This equation is quasilinear due to dependence of the thermal parameters of the soil temperature. To solve this equation in a complex three-dimensional region, taking into account the location of wells and SCDs, with changing in time thermophysical properties of the medium, and with a nonlinear boundary condition on the surface of the soil associated with the solar radiation, there are developed a numerical algorithm and software packages Wellfrost for multiprocessor computational systems with “cloud technologies” approaches. A large series of numerical calculations were used in the design of several Russian oil and gas fields.

The study is supported by Program of UD RAS “Arktika”, project No 12–1–4–005.

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# High-order compact scheme for a fourth-order differential equation: spectral properties and convergence analysis

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## Abstract

In [1] we studied the convergence of a fourth-order compact scheme to the one-dimensional biharmonic problem is established in the case of general Dirichlet boundary conditions. This scheme invokes value of the unknown function as well as Pade approximations of its first-order derivative. The truncation error of the scheme is of fourth-order at interior points and of first order at near boundary points. Nonetheless, we prove that the scheme retains its fourth-order (optimal) accuracy. This is done by a careful inspection of the matrix elements of the discrete biharmonic operator. A number of numerical examples corroborate this effect.

We also present a proof for the convergence of the scheme for the time dependent problems  $u_t = u_{xxxx}$  and  $u_{xt} = u_{xxxx}$ . We show that the error is bounded by  $Ch^3$ .

In addition, we study of the eigenvalue problem  $u_{xxxx} = \nu u$ . We compute and display the eigenvalues and the eigenfunctions related to the continuous and the discrete problems. By the positivity of the eigenvalues, one can deduce the stability of of the related time-dependent problem  $u_t = -u_{xxxx}$ . We also study the eigenvalue problem  $u_{xxxx} = \nu u_{xx}$ . This is related to the stability of the linear time-dependent equation  $u_{xt} = \nu u_{xxxx}$ . Its continuous and discrete eigenvalues and eigenfunction (or eigenvectors) are computed and displayed graphically.

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# Dynamic estimation from distributed measurements using the RFS theory

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## Abstract

The aim of this work is to estimate dynamic parameters of an unknown and varying number of objects from distributed measurements. They are delivered by a scanning laser rangefinder in polar coordinates and they provide low-level information to the estimation process. The proposed framework is the Random Finite Set theory (RFS), considering as well cardinality and values of elements as random variables. The RFS theory is an elegant and natural way to model the target tracking problem as a birth and death process [1]. The RFS multi-object state model associated to this tracking problem integrates individual dynamics, uncertainties on evolution, target birth and target death process. It can be obtained under Markovian assumption:

$$\mathcal{X}_t = \left( \bigcup_{X_{t-1} \in \mathcal{X}_{t-1}} \Phi(X_{t-1}, W_{t-1}) \right) \bigcup (B(X_t))$$

where  $B(X_t)$  denotes the RFS associated to targets spawned from targets at time step  $t - 1$  and to spontaneous birth at time step  $t$  and  $\Phi$  represents the dynamics flow of the system and  $W$  is the evolution noise.

The RFS observation model includes measurement likelihood, target detection uncertainty at the sensor and clutter:

$$\mathcal{Z}_t = \left( \bigcup_{X_t \in \mathcal{X}_t} \tilde{Z}(X_t) \right) \bigcup (K_t)$$

where  $K_t$  is the RFS of clutter which is supposed to be Poisson distributed.

In this kind of problem, the knowledge of the posterior distribution  $p(\mathcal{X}_t | \mathcal{Z}_{1:t})$  is necessary. The Finite Set Statistics (FISST) provide tools to recursively calculate this distribution. For our tracking application, we adapt a computationnaly tractable approach (Probability Hypothesis Density: PHD) [2] which is a first-moment approximation.

The proposed approach consists in directly processing the measurements in polar coordinates while avoiding the classic detection step and using the Sequential Monte Carlo methods. It is augmented with a peak-to-track association using indexation techniques to obtain trajectories of each object. The obtained results on synthetic and real data show a significant benefit of this method compared to classic ones [3] in terms of estimation accuracy and tracks continuity.

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# An improved nonlinear model for image restoration

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## Abstract

The image denoising is a key step in image processing. This step can be treated by non-linear diffusive filters requiring solving evolving partial differential equations. In recent decades, several models have been proposed in the literature [1, 2, 3, 4, 5, 6]. Their computational efficiency has been proven and developed. In this work, a nonlinear diffusion equation based on the model proposed in [6, 7] is studied analytically and numerically tested for denoising image. Boundary conditions of Neumann are taken into account in this model and the existence, uniqueness and regularity of the solution are established in a Hilbert space. The discretization of the partial differential equation of the proposed model is performed using the finite element method. The efficiency of this model has been tested on many noisy images by a Gaussian, Poisson, Speckle or pepper and salt noise. Signal noise ratio (SNR) is used to estimate the quality of restored images.

## Acknowledgements

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# A moving asymptotes algorithm using new local convex approximations methods with explicit solutions

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## Abstract

A moving asymptotes algorithm using new local convex approximations methods of non-linear problem for unconstrained minimization is presented and analyzed. Convergence results under fairly mild assumptions are derived concerning the minimization algorithm. In particular, second order information are successfully employed for moving asymptotes location. In order to avoid the second derivatives evaluations we will propose to use a sequence of diagonal Hessian estimates, which use only first and zero order information accumulated during the previous iterations. As consequence, in each step of the iterative process, a strictly convex approximation sub-problem is generated and solved. All our subproblems will have *explicit* minimum, which reduce considerably the computational cost of our method and generate an iteration sequence, that is bounded and converges geometrically. In addition, an industrial application will be presented to illustrate the practical situations.

# A meshless method applied to Burger's type equations.

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## Abstract

In this talk we present a meshless method based on thin plate splines to solve Burger's type equations

$$\partial_t u + \mu(u \cdot \nabla)u - \nu \Delta u = f$$

on  $\Omega \times [t_0, T]$ , where  $\Omega$  is a bounded domain of  $\mathbb{R}^d$ ,  $d \geq 2$ ,  $\mu$  and  $\nu$  are two scalar parameters, with a Dirichlet boundary condition. The choice of using radial basis functions (RBF) is motivated by the fact that these methods do not depend upon the geometry of the domain, nor its dimension. We establish some theoretical results related to the existence of such interpolants using linear algebra techniques. The numerical approximation of the solution leads to a large-scale nonlinear differential matrix equation. We give a general framework for the application of an implicit Runge-Kutta scheme in the case of matrix differential equations. At each step of the time integration, a nonlinear matrix equation  $R(X) = 0$  has to be solved. At each iteration of the inexact-Newton algorithm used in this case, we have to solve a linear matrix equation of the form  $DR(X) = C$ , where  $DR(X)$  is the Fréchet derivative of  $R$ . As  $DR(X)$  cannot be easily identified to a matrix polynomial of the variable  $X$ , the global-GMRES algorithm shows to be particularly adequate. Numerical examples in dimension  $d = 2$  will be given to illustrate our method.

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# Abstraction-oriented optimal design: two example studies

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## Abstract

Optimal design process can be briefly said to be consisting of two parts: that is, the problem formulation and the solution search. It is clear that the type of formulation of the optimal design problem is significantly important since it affects not only the required computational power but also the solution to be obtained in various viewpoints. In the current study, we deal with optimal design problems to which we can introduce a kind of hierarchical structures. The problems can be then divided into subproblems referring to the introduced hierarchy, and the subproblems may also be subdivided into sub-subproblems and so on in some cases. We propose an approach to optimal design based on abstraction of such subproblems, where the subproblems are abstracted as their functions as well as their characteristics. On the basis of the abstraction, we can deal with such subproblems as a kind of objects that are independent of their actual formulation and design variables. Formulation of optimal design problems based on such an abstraction approach is expected to be computationally effective and also to give us a different viewpoint of the subproblems that they can be reused as building blocks in the case of dealing with another optimal design problems.

We introduce the general concept and formulation of the abstraction-oriented optimal design and discuss its capability and possibility through two types of example optimal design problems. One is a path design problem and the other is a structure design problem. As the path design problem, we deal with a kind of drawing order optimal design where the pattern to be drawn consists of a number of small pattern elements as well as combinations of such elements. A message written in alphabet character string is a typical example. As the structure design problem, we deal with a truss structure design. In this case, abstraction of subproblem is not as straightforward as the case of the path design problem; the manner of abstraction has to be evaluated and discussed in terms of various points of view. For both of the two example problems, we show a number of optimal design solutions and discuss the applicability and the feasibility of the abstraction-oriented optimal design.

We consider that this approach can be significantly promising especially in the case that the optimal design system is implemented with an adequate database. The database can be realized in a kind of self-similar manner[1] in which any objects can be dealt with in a practically same manner regardless of its hierarchical position. We discuss a general framework of the database. An example implementation of the database is also demonstrated.

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# Optimal Control of Linearized Navier-Stokes Equations via a Differential-Algebraic Riccati Decoupling

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## Abstract

We present an approach to solving optimal control problems for linearized Navier-Stokes equations that does not resort to divergence-free formulations. In particular we introduce a differential-algebraic Riccati decoupling of the optimality system and show well posedness. Also, we show how this new approach can be exploited for efficient numerical schemes and give application examples.

If formulated in the variables  $v$  and  $p$ , denoting velocity and pressure, the Navier-Stokes equations and its linearizations are *differential-algebraic equations* (DAEs). This means that the variables are subject to differential and to algebraic equations. In the case of Navier-Stokes, the velocity has to fulfill the (differential) momentum equation and the (algebraic) continuity equation, while the pressure is determined algebraically in terms of the velocity. This is true for abstract and for spatially semi-discretized formulations.

For theoretical considerations, one can formally eliminate the pressure and consider an ODE for the velocity formulated on a subspace of divergence-free functions. And thus, when it comes to optimal control, one can use well known results for ODEs to formulate necessary and sufficient optimality conditions. For applications, these reformulation as an ODE system is often not possible or inefficient.

We propose an approach that bases on the solution of the formal first order optimality conditions of a quadratic cost-functional, subject to linearized NSEs in the original variables  $v$  and  $p$ .

To solve the two-point boundary problem representing the optimality conditions, we introduce a differential-algebraic Riccati equation that leads to a decoupling of the primal and adjoint states. We investigate unique solvability of this Riccati equations and how it can be used for efficient numerical solution procedures for optimal control problems for flow equations.

The main advantage of a Riccati decoupling in general is the applicability of low-rank approximations to the Riccati solution that makes large scale problems accessible. A particular advantage of the presented formulation in the original variables is that it can be approached by common flow solvers. We will present application examples for distributed control of a driven cavity and a cylinder wake.

# Polynomial optimization and a Jacobi–Davidson type method for commuting matrices

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## Abstract

We introduce a new Jacobi–Davidson type eigenvalue solver for a set of commuting matrices, used for the global optimization of so-called Minkowski-norm dominated polynomials in several variables. The Stetter–Möller matrix method yields such a set of real non-symmetric commuting matrices since it reformulates the optimization problem as an eigenvalue problem. A drawback of this approach is that the matrix most relevant for computing the global optimum of the polynomial under investigation is usually large and only moderately sparse. However, the other matrices are generally much sparser and have the same eigenvectors because of the commutativity. This fact is used to design an efficient method for this problem: the most relevant matrix is used only in the outer loop and the sparser matrices are exploited in the solution of the correction equation in the inner loop to greatly improve the efficiency of the method. Some numerical examples demonstrate that the method proposed in this paper is more efficient than approaches that work on the main matrix, as well as conventional solvers for computing the global optimum, i.e., SOSTOOLS, GloptiPoly, and PHCpack.

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Polynomial optimization and a Jacobi–Davidson type method for commuting matrices  
Submitted.

# A generalized companion method to solve systems of polynomials

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## Abstract

A common method to compute the roots of a univariate polynomial is to solve for the eigenvalues of its companion matrix. If the polynomial is given in a Chebyshev basis, one refers to this matrix as the colleague matrix. By generalizing this procedure for multivariate polynomials, we are able to solve a system of  $n$ -variate polynomials by means of an eigenvalue problem. We obtain an efficient method that yields numerically accurate solutions for well-behaved polynomial systems. An advantage of the method is that it can work with any polynomial basis.

# Gradient observability and sensors: HUM approach

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## Abstract

The aim of this paper is to explore the concept of observability of the gradient for distributed hyperbolic systems and to reconstruct the gradient of state without the knowledge of the state, evolving in spatial domain  $\Omega$ . The method is based on an extension of the method HUM introduced by Lions [4], and does not take into account what may be the remaining part of the initial gradient of the region  $\Omega \setminus \omega$ .

We give definitions and characterizations and some properties of this kind of regional observability and we describe this approach to solve this problem.

The concept of gradient strategic sensors is characterized and applied to the wave equation. This emphasizes the spatial structure and location of the sensors in order that regional gradient observability can be achieved.

Finally we present numerical simulation and examples.

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# An Efficient Robust Solver for Optimal Control Problems for the Stokes Equations in the Time-Harmonic Case

Wolfgang Krendl, Valeria Simoncini, Walter Zuhlehnner

## Abstract

In this talk we will construct a robust solver for the optimal control problem for the Stokes equation, in the time-harmonic case. The discretization of the corresponding optimality system leads to a large and sparse  $8 \times 8$  block matrix in saddle point form. We use an iterative solver, more precisely, we apply the MINRES method. To guarantee efficiency, we constructed a preconditioner for the MINRES-method, which is robust with respect to the mesh size, the frequency  $\omega$  and the control parameter  $\alpha$ . Numerical examples are given which illustrate the theoretical results.

# Recent Numerical Improvements in Low-Rank ADI Methods

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## Abstract

Low-rank alternating directions implicit (LR-ADI) type methods have been proven to be efficient methods for the numerical approximation of solutions of large-scale linear matrix equations. Recently, we developed several efficiency improvements for the LR-ADI for Lyapunov equations [1]

$$AXE^T + EXA^T + GG^T = 0.$$

In particular these are, e.g.,

- the efficient computation of the Lyapunov residual and its norm [3],
- the handling of complex shift parameters [2],
- and the adaptive computation thereof.

After reviewing these ideas we show how these approaches can be carried over to the LR-ADI for large-scale Sylvester equations [4] of the form

$$AXC - EXB = FG^T.$$

If time permits special cases of the above Sylvester equation and the use of these methods in applications, e.g. in model order reduction [3], are also considered.

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# A two-layers shallow water Lattice Boltzmann model for sediment transport in free surface flows

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## Abstract

Sediments transport phenomena play a key role in the management of some irrigation canals since they can perturb their smooth running: sealing of gates, biased estimates of water volumes, levels and flows, threats for the safety of the canal structures and/or for the environment. In many real life situations, part of these phenomena and related problems may be managed with appropriate feedback control actions (mostly trough gates actuation). Effectiveness of this approach partly relies on a control model sufficiently representative of the global behaviour (and the main dynamical properties) of the real system but simple enough to allow real-time control and optimization.

In this context a commonly used model are the Saint-Venant-Exner's equations [3], a system of three couples equations including the mass and momentum balance equations for the water and a mass conservation law for the "fluidised" sedimental bed. Audusse and its co-workers showed in [1] the limitations of such an approach. Moreover they proposed an improved model based on two shallow water multi-layers approach, respectively for water and sediment transports which considers also the momentum balance equation for the sediment and the corresponding interaction terms. Although many numerical methods exist for the integration of these models, based on the coupled resolution of these equations, they reveal to be more suited for simulation than for the design of real time controller (or optimization) [2].

We propose therefore a 1D discrete Lattice Boltzmann model based on the aforementioned "two-layers" idea (denoted 2-swe 1D). Numerical results and performance obtained with this model in various simulation scenarii are compared with results obtained from the Audusse model (with a dedicated finite volume scheme) and from a complex bi-fluid 3D Lattice Boltzmann model. The proposed 2-swe 1D model indeed revealed to be faster for a given (1D) accuracy and besides allows the simulation of torrential/fluviat ("supercritical") transitions.

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# Constrained Non-negative Matrix Factorization with normalization steps.

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## Abstract

This contribution describes two slightly different iterative methods of Non negative Matrix Factorization (NMF). They all rely on the positivity constraint of each component of parts based factors. They also all aim at minimizing a specific cost function between the data matrix and the reconstructed one. Emphasize is made in this contribution on Frobenius based multiplicative NMF [3]. Particularly, a specific parametrization [1] is proposed in order to deal with some knowledge on part of the factorization, called the profile matrix. Moreover, weighted NMF appeared [2] to take into account drastically different uncertainties into the data matrix. The formalization of a weighted criterion together with the parametrization enables to provide a global update of the profile matrix. KKT conditions for this parametrization are detailed in order to provide necessary conditions to reach a stationary point.

However, each line of a profile matrix gathers in fact abundance coefficients which verify the sum to 1 constraint. As a result, a sequential algorithm which uses the previous update together with a normalization step is proposed within iterations. Two kinds of normalizations are investigated: the first one keeps the reconstructed matrix unchanged but loses the constraints within iterations. The other normalization propose to let the constraints verified but changes the reconstructed matrix during iterations.

For the first method, it is shown that its stationary points are obtained through normalization of the un-normalized stationary points. It is also verified that though constraints are lost within iterations, they are recovered asymptotically. The second method keeps the constraints verified within iteration but may prevent from moving toward the minimum of the criterion at a given iteration.

These two methods are experimented on a synthetic dataset and performances are discussed by using a Mixing Error Ratio [4].

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# An multi-step explicit polynomial method for the time integration of the heat conduction equation

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## Abstract

The paper discusses a method for solving boundary-value problems in the integration of the heat conduction equation. The method falls into the class of explicit iterative methods for parabolic equations [1]. Unlike the traditional explicit differencing schemes, the increase of the spatial template in our method squares the time step. The resulted difference schemes are robust and allow effective parallelization. The method is based on the construction of a difference time step operator in the form of Chebyshev and Lanczos polynomials. The polynomial is constructed in the space of Fourier transforms where the initial differential equation is approximated and the least polynomial order required for stability is calculated analytically. The algorithm of calculation each time step is implemented as recursive relations each of which is equivalent in labor to the explicit difference scheme. Therefore the method allows high parallelism and can be effectively used for the parallel computing of multidimensional problems.

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# Inverse Eigenvalue Problems Linked to Rational Arnoldi, and Rational (Non)Symmetric Lanczos

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## Abstract

In this talk we will discuss two inverse eigenvalue problems. First, given the eigenvalues and a weight vector a (extended) Hessenberg matrix is computed. This matrix represents the recurrences linked to a (rational) Arnoldi inverse problem. It is well known that the matrix capturing the recurrence coefficients is of Hessenberg form in the standard Arnoldi case. Considering, however, rational functions, admitting finite as well as infinite poles we will prove that the recurrence matrix is still of a highly structured form – the extended Hessenberg form. An efficient memory cheap representation is presented for the Hermitian case and used to reconstruct the matrix capturing the recurrence coefficients.

In the second inverse problem, the above setting is generalized to the biorthogonal case. Instead of unitary similarity transformations, we drop the unitarity. Given the eigenvalues and the two first columns of the matrices determining the similarity, we want to retrieve the matrix of recurrences, as well as the matrices governing the transformation.

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# Numerical methods for the simulation of a phase changing multi-components cryogenic fluid with heat transfer using the Lattice Boltzmann Method.

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## Abstract

Multi-component Fluids with phase change and heat transfer are often an issue for the physical modeling and for the numerical simulation stability, though they are of great interest for industrial and environmental understanding. The spreading of a cryogenic fluid has to be modeled with the consideration of at least two different fluid components which are indeed the fluid itself, which is supposed to experience liquid-gas phase change, and the surrounding air. The Lattice Boltzmann model allows us to incorporate additional physics in comparison to the traditional CFD method, which only describes the Navier-Stokes motion of a single-component flow, and which shows to be insufficient for our case. The Lattice Boltzmann model comes from the kinetic theory of gas and is derived from the non-equilibrium Boltzmann equation. It allows us to consider the mesoscopic behavior of the fluid, which corresponds to a scale between molecular dynamics and macroscopic dynamics. The phase change is modeled with a pseudo-potential model introduced by the authors Shan and Chen [1], which has known several improvements in terms of density ratio between condensed and non-condensed phases [4] [5], or for the surface tension between two different species [7]. The numerical stability of the model depends in great part of the stability of the force obtained from the pseudo-potential. We establish a discussion on the conditions that improves the numerical stability and therefore the obtainable density ratio.

First, we remind the Gauss-Hermite integral approximation for the discretisation of the Boltzmann equation[8]. We also expose numerical techniques for the simplification of the Maxwellian distribution of a fluid near equilibrium[8]. The Boltzmann Method uses a lattice which takes numerical weight and coefficient in order to recover the correct macroscopic properties. One of the necessary conditions of the used coefficients is to guaranty the isotropy of space. We will show the limit in stability of the single relaxation collision operator lattice Boltzmann model as an introduction.

We then will explain the main issues encountered when one is to derive equations for multiphase-multi-component fluid motion. The lattice implies extra care for the discretisation of the gradient operator, which is used for the derivation of the inter-particle interaction force obtained from the pseudo-potential [1] [6]. The way of incorporating this force term [2] in the Boltzmann equation is also of important matter, and deserves a discussion too. We will show the comparison of three ways of incorporation: the velocity shifting, which just adds an extra momentum to the non modified velocity field, the discrete force method, which takes into account the numerical weight from the Gaussian-Hermite approximation and the exact difference model which shows better numerical stability. We will also see that the use of different equation of states [3] improve the numerical stability of the model.

We will conclude with some visual results of a phase changing fluid superheated from above, the formation and rise of a bubble and the filming phase transition process. We also would like to notice that this work has been made possible by the INNOCOLD organization, that has established partnerships between the ULCO university and societies willing to accelerate their understanding of cryogenic fluids.

# On solving KKT linear systems arising in Model Predictive Control

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## Abstract

The approximate solution of Model Predictive Control problems [2, 3, 4] is often computed in an iterative fashion, requiring to compute, at each iteration, the solution of a quadratic optimization problem. The most expensive part of the latter problem is the solution of symmetric indefinite KKT systems, where the involved matrices are highly structured.

Recently, an algorithm for computing a block anti-triangular factorization of symmetric indefinite matrices, based on orthogonal transformations, has been proposed [1]. The aim of this talk is to show that such a factorization, implemented in a suitable way, can be efficiently used for solving the mentioned KKT linear systems.

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# Some results on the stability of Padé approximants

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## Abstract

In a recent paper, Trefethen and al. [1] have proposed a method to compute a robust Padé approximant based on the Singular Value Decomposition. They observe numerically that these approximants don't have neither Froissart doublets nor spurious poles. It is also known [2] that for these approximants, the application going from the Taylor coefficients  $(c_i)$  of the function to the vector of coefficients of the numerator and denominator of the Padé approximant is continuous.

In this talk we will study forward and backward conditioning of this application and will propose a mathematical analysis of these numerical phenomena.

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# Numerical Approximation of a Semilinear Obstacle Problem

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## Abstract

Let  $\Omega$  be an open bounded domain in  $\mathbb{R}^n$  with a smooth boundary  $\partial\Omega$ . Consider the following semilinear obstacle problem:

$$\begin{cases} \text{Find } u \in K = \{v \in H_0^1(\Omega); v \geq 0 \quad \forall v \in H_0^1(\Omega)\} \text{ such that} \\ \int_{\Omega} \nabla u \nabla (v - u) dx + \int_{\Omega} g(u)(v - u) dx + \int_{\Omega} f(v - u) dx \geq 0 \quad \forall v \in K, \end{cases} \quad (1)$$

where  $f$  is an element of  $L^2(\Omega)$  and  $g : L^2(\Omega) \rightarrow L^2(\Omega)$  is a non-negative contraction function satisfying some appropriate properties such that problem (1) admits a unique solution. In this paper we reformulate problem (1) as a nonlinear equation problem and we present its numerical approximation. First, we construct a continuous convex function  $\varphi : L^2(\Omega) \rightarrow \mathbb{R}$ , for which we can characterize its subdifferential  $\partial\varphi$ . Then we show that problem (1) is equivalent to the following problem: Find  $(u, \mu) \in H_0^1(\Omega) \times L^2(\Omega)$  such that

$$\Delta u + g(u) + \mu + h = 0 \quad \text{in } H_0^1(\Omega), \quad \text{and} \quad \mu \in \partial\varphi(u), \quad (2)$$

where  $h$  is a function of  $L^2(\Omega)$  depending only on the data of the problem. This formulation allows us to characterize the non-contact domain. To solve the reformulated problem, we apply a combination of an adequate projection method and a fixed point method. Then we consider a discretization of the problem based on finite element method. We prove the convergence of the approximate solutions to the exact one. This work is an extension of the ones presented in [1] and [2] in case of linear obstacle problem i.e.,  $g \equiv 0$ .

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# Multiple recurrences and the associated matrix structures stemming from normal matrices

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## Abstract

There are many classical results in which orthogonal vectors stemming from Krylov subspaces are linked to short recurrence relations, e.g., three-terms recurrences for Hermitian and short rational recurrences for unitary matrices. These recurrence coefficients can be captured in a Hessenberg matrix, whose structure reflects the relation between the spectrum of the original matrix and the recurrences. The easier the recurrences, the faster the orthogonal vectors can be computed possibly resulting in computational savings in the design of, e.g., iterative solvers.

In this talk we focus on multiple recursions, i.e., the  $(j + 1)$ th orthogonal vector satisfies

$$\mathbf{q}_{j+1} = \sum_{i=j-m}^j \rho_{j,i} A \mathbf{q}_i - \sum_{i=j-\ell}^j \gamma_{j,i} \mathbf{q}_i,$$

with  $\rho_{j,i}$ ,  $\gamma_{j,i}$  scalars, and  $A$  the matrix defining the Krylov space. Though many compelling results are around, the theoretical proof of the existence of this structure, and the associated construction of algorithms to efficiently retrieve the orthogonal vectors are rapidly becoming too cumbersome and technically involved.

In this talk we review classical results on short multiple recurrences for normal matrices and reformulate them in a matrix setting. We will present some powerful matrix building blocks allowing us to swiftly and elegantly predict the structure behind the recursions for a variety of settings. This results in a new manner to retrieve the orthogonal vectors.

# Finite difference schemes for a system of coupled Korteweg-de Vries equations

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## Abstract

In this talk, we construct new schemes for the system of coupled Korteweg-de Vries equations [1]

$$\begin{aligned}u_t + \mu_1 u u_x + \lambda_1 u_{xxx} + \gamma u_x + \kappa v_x &= 0, \\v_t + \mu_2 v v_x + \lambda_2 v_{xxx} + \gamma v_x + \kappa u_x &= 0, \\u(t, x) &= u(t, x + L), \quad v(t, x) = v(t, x + L) \\u(0, x) &= u_0, \quad v(0, x) = v_0,\end{aligned}\tag{1}$$

It is shown that the mass and momentum integrals as well as the Hamiltonian of the system are conserved by these schemes. Finally we show that the predictions of the theory are consistent with the numerical experiments.

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# A new analysis of block preconditioners for saddle point problems

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## Abstract

We consider linear systems

$$K \mathbf{u} = \mathbf{b}$$

of saddle point type; i.e.,  $K$  is of the form

$$K = \begin{pmatrix} A & B^T \\ B & -C \end{pmatrix},$$

where  $A$  is  $n \times n$  symmetric positive definite and  $C$  is  $m \times m$  and symmetric nonnegative definite with  $m \leq n$ .

For such systems, there is an abundance of works presenting or analyzing preconditioners in  $2 \times 2$  block form. This includes block diagonal, block triangular, (inexact) Uzawa and block incomplete factorization preconditioners. In this talk, we present a new, unified, analysis of these preconditioners, which yields sharper eigenvalue estimates while revealing the close connections that exist between the different variants.

# On computing maximum/minimum singular values of a generalized tensor sum

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## Abstract

We consider computing maximum/minimum (max/min hereafter) singular values of the following generalized tensor sum:

$$T := I_n \otimes I_m \otimes A + I_n \otimes B \otimes I_l + C \otimes I_m \otimes I_l \in \mathbb{R}^{lmn \times lmn}, \quad (1)$$

where  $A \in \mathbb{R}^{l \times l}$ ,  $B \in \mathbb{R}^{m \times m}$ ,  $C \in \mathbb{R}^{n \times n}$ ,  $I_m$  is the  $m \times m$  identity matrix, and the symbol “ $\otimes$ ” denotes the Kronecker product.

For computing max/min singular values of a large and sparse matrix  $M$ , max/min absolute eigenvalues of the normal matrix form or the augmented matrix form, i.e.,

$$M^T M @ @ @ @ @ \begin{pmatrix} O & M \\ M^T & O \end{pmatrix}$$

is widely used, and then standard eigensolvers are chosen such as the power method, the RQI method, the Lanczos bidiagonalization method, and the Jacobi–Davidson method. For the recent development, see, e.g., [1, 2].

We focus on the Lanczos bidiagonalization method for matrix  $T$  in (1). The method requires to compute matrix-vector multiplications:  $Tv$ ,  $T^T v$  that can be one of the most time consuming parts. In this talk, we present efficient computation of the max/min singular values based on two ideas below.

1. Efficient implementation of the mat-vecs using the tensor  $n$ -mode product [3];
2. How to choose a good initial guess from viewpoints of a tensor structure in  $T$ .

As a simple application, the following three-dimensional constant-coefficient PDE:

$$-\left(a_1 \frac{\partial^2 u}{\partial x^2} + a_2 \frac{\partial^2 u}{\partial y^2} + a_3 \frac{\partial^2 u}{\partial z^2}\right) + b_1 \frac{\partial u}{\partial x} + b_2 \frac{\partial u}{\partial y} + b_3 \frac{\partial u}{\partial z} + cu = g(x, y, z)$$

will be considered on the unit cube  $\Omega = [0, 1] \times [0, 1] \times [0, 1]$ , with Dirichlet boundary condition  $u(x, y, z) = 0$  on  $\partial\Omega$ .

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# Safe localization of eigenvalues \*

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## Abstract

Localizing some eigenvalues of a given large sparse matrix in a domain of the complex plane is a hard task when the matrix is non symmetric, especially when it is highly non normal. For taking into account, possible perturbations of the matrix, the notion of the  $\epsilon$ -spectrum or pseudospectrum of a matrix  $A \in \mathbb{R}^{n \times n}$  was separately defined by Godunov and Trefethen. Determining an  $\epsilon$ -spectrum consists of determining a level curve of the 2-norm of the resolvent  $R(z) = (zI - A)^{-1}$ . A dual approach can be considered: given some curve  $(\Gamma)$  in the complex plane, count the number of eigenvalues of the matrix  $A$  that are surrounded by  $(\Gamma)$ . The number of surrounded eigenvalues is determined by evaluating the integral  $\frac{1}{2i\pi} \int_{\Gamma} \frac{d}{dz} \log \det(zI - A) dz$ . This problem was considered in [1] where several procedures were proposed and more recently in [2] where the stepsize control in the quadrature is deeply studied. The present goal is to combine the two approaches: (i) consider the method PAT [4, 3] which is a path following method that determines a level curve of the function  $s(z) = \sigma_{\min}(zI - A)$ ; (ii) apply the method EIGENCNT of [2] for computing the number of eigenvalues included. The combined procedure will be based on a computing kernel which provides the two numbers  $(\sigma_{\min}(zI - A), \det(zI - A))$  for any complex number  $z \in \mathbb{C}$ . These two numbers are obtained through a common LU factorization of  $(zI - A)$ . In order to introduce a second level of parallelism, we consider a preprocessing transformation similar to the approach developed in SPIKE [5].

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# Accelerating strategies for the numerical approximation of functions of large matrices

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## Abstract

The evaluation of matrix functions is a common computational task, since several important applications involve  $f(A)$  or  $f(A)b$ , where  $A \in \mathbb{R}^{n \times n}$ ,  $b \in \mathbb{R}^n$  and  $f : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n}$  is a function for which  $f(A)$  is defined. In this talk we address both problems in the case of very large dimension  $n$  which requires *ad hoc* techniques; moreover, we consider the common case in which  $f$  can be approximated by a rational form and  $A$  is not necessarily symmetric.

We describe the acceleration techniques presented in [2]. They are inspired by an update framework for incomplete factorizations in inverse form proposed in the last decade started by the paper [1], and they are used both for approximating the rational matrix function and as preconditioners for the iterative Krylov linear system solvers.

For the  $f(A)b$  problem another approach is presented, as described in [3], which is a *restarted* version of the commonly employed Shift-and-Invert Krylov method, with new error estimates which can guide in the choice of an effective shift parameter and can perform as stopping criteria.

We discuss implementation issues of these methods (involving incomplete factorizations, restarts, preconditioning and much more) as well as their convergence behavior. Numerical tests complete the presentation.

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# Customized dictionaries for sparse approximation of PDEs with discontinuities in solution

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## Abstract

We propose the customization of hierarchical finite element bases with problem specific features to obtain a sparse representation of the solution within a dictionary of functions and to use  $l_1$  minimization as in [1] for the solution of the under-determined systems. In particular we use as enrichment tensor product B-splines and we modify them to incorporate problem specific features, like the shape of the domain (via weight functions [2]), or the nature of discontinuities (via special enrichment functions [3,4]) etc. A dictionary composed of a hierarchy of such customized functions is constructed and used in a multilevel finite element method.

Since a priori information about the domain geometry and singular features is present in the dictionary, extensive mesh refinement is avoided and the solution is nicely represented even at relatively coarser resolutions with few degrees of freedom. Compared with hierarchical FEM the resulting system size is small and hence it can efficiently solved by sparse recovery algorithms like orthogonal matching pursuit and its newer variants [5]. We present some numerical experiments to demonstrate that the method can be a viable alternative to classical adaptive finite element techniques.

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# On fast and effective algorithms for the TV Stokes for image processing

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## Abstract

Observing that the tangential vectors or the isophote directions of a 2D image correspond to an incompressible velocity field, it is then natural to impose that the tangential vector field is divergence free. Recent work show that Total Variation (TV) minimization of the tangential vector field under the above constraint, as a pre process, as opposed to minimizing only the TV of the image as it is normally done in the classical TV minimization model, is an essential step in recovering images with smooth details, cf. [1, 3]. The constrained minimization model, also known as the TV Stokes model, has already started to attract attention in the image processing community. A fast and effective algorithm based on a dual formulation of the constrained minimization has recently been proposed, cf. [2]. In this talk, we will provide an analysis of the dual algorithm and discuss its merits, as well as discuss its extension to image processing in the 3D.

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# A thick-restart Q-Lanczos method for quadratic eigenvalue problems

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## Abstract

We investigate how to adapt the Q-Arnoldi method [1] for the case of symmetric quadratic eigenvalue problems, that is, we are interested in computing a few eigenvalues  $\lambda$  and corresponding eigenvectors  $x$  of  $(\lambda^2 M + \lambda C + K)x = 0$ , where  $M, C, K \in \mathbb{R}^{n \times n}$  are all symmetric. This problem has no particular structure, in the sense that eigenvalues can be complex or even defective. Still, symmetry of the matrices can be exploited to some extent. For this, we perform a symmetric linearization  $Ay = \lambda By$ , where  $A, B \in \mathbb{R}^{2n \times 2n}$  are symmetric but the pair  $(A, B)$  is indefinite and hence standard Lanczos methods are not applicable. We implement a symmetric-indefinite Lanczos method [2] and enrich it with a thick restart technique [3]. This method requires using a shift-and-invert transformation,  $(A - \sigma B)^{-1}By = \theta y$ , combined with the use of pseudo inner products induced by matrix  $B$  for the orthogonalization of vectors (indefinite Gram-Schmidt). The projected problem is a pseudo-symmetric tridiagonal matrix. The next step is to write a specialized, memory-efficient version that exploits the block structure of  $A$  and  $B$ , referring only to the original problem matrices  $M, C, K$  as in the Q-Arnoldi method. This results in what we have called the Q-Lanczos method. We show results with a Matlab prototype as well as a parallel implementation in SLEPc [4].

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# Numerical behavior of stationary and two-step splitting iterative methods

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## Abstract

In this contribution we study numerical behavior of several stationary or two-step splitting iterative methods for solving large sparse systems of linear equations. We show that inexact solution of inner systems associated with the splitting matrix may considerably influence the accuracy of computed approximate solutions computed in finite precision arithmetic. We analyze several mathematically equivalent implementations and find the corresponding component-wise or norm-wise forward or backward stable implementations. The theory is then illustrated on the class of efficient two-step iteration methods such as Hermitian and skew-Hermitian splitting methods. We can show that some implementations lead ultimately to errors and residuals on the the roundoff unit level independently of the fact that the inner systems with the splitting matrix were solved inexactly on a much higher level (in practical situations this level corresponds to the uncertainty of input data or imperfection of underlying mathematical model). We give a theoretical explanation for this behavior which is intuitively clear and it is probably tacitly known. Indeed, our results confirm that implementations with simple updates for approximate solutions can solve the algebraic problem to the working accuracy. These implementations are actually those which are widely used and suggested in applications. Our results are examples of rather general fact that it is advantageous to use the update formulas in the form "new\_value = old\_value + small\_correction". Numerical methods are often naturally expressed in this form and in a sense this update strategy can be seen as variant of the iterative refinement for improving the accuracy of a computed approximate solution to various problems in numerical linear algebra.

# Intrinsic variational problems

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## Abstract

In this work, we investigate variational problems for many-bodies systems of which the lagrangian densities involve small sets of differential operators. We first define intrinsic densities with respect to a given system of differential operators. Next, we obtain Euler-Lagrange equations of motion for intrinsic densities, by using a curve straightening procedure. This framework encompasses, as a first example, constrained variational problems related to curvature and torsion. As a second example, we focus on the special case of actions depending on three quadratic forms with respect to positions and momenta. In that case, the reduction of order leads to an algebraic problem for the invariants of multivariate polynomials under permutation groups. We provide lastly some experiments for two examples of the previous kinds, that we numerically solve by three different methods.

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# A Minimal residual method for large scale Sylvester matrix equations

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## Abstract

In this talk, we present a new method for solving large scale Sylvester matrix equations of the form

$$AX + XB = EF^T$$

where  $A$  and  $B$  are square matrices of sizes  $n \times n$  and  $p \times p$  respectively and  $E, F$  are matrices of sizes  $n \times r$  and  $r \times n$  respectively.

The proposed method is an iterative method based on a projection onto extended block Krylov or block Krylov subspaces with a minimization, at each step, of the Frobenius norm of the residual. The obtained reduced order minimal residual problem is solved via different iterative solvers that exploit the structure of the matrix of the associated normal equation. Then, the low rank approximate solution is computed only when convergence is achieved and a stopping procedure based on an economical computation of the norm of the residual is proposed. Numerical tests are presented to show the effectiveness of the new method. These numerical examples compare the proposed minimal residual approach with the corresponding Galerkin-type procedures [1, 2, 3, 4, 5].

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# The Davison-Man method revisited and extended

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## Abstract

The Davison-Man method is an iterative technique for solving Lyapunov equations for which the approximate solution is updated through a matrix integral and a doubling procedure (see, e.g., [1]). In theory, the convergence is quadratic and, in practice, there are examples where the method stagnates and no further improvement is seen. In this work an implementation that avoids stagnation is proposed. The implementation is applicable to Lyapunov and Sylvester equations and has essentially optimal efficiency. Finally, an extension to large-scale case is presented and its convergence properties are analyzed.

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# Structured $QR$ algorithms for Hamiltonian symmetric matrices

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## Abstract

Efficient, backward-stable, doubly structure-preserving algorithms for the Hamiltonian symmetric and skew-symmetric eigenvalue problems are developed. Numerical experiments confirm the theoretical properties of the algorithms. Also developed are doubly structure-preserving Lanczos processes for Hamiltonian symmetric and skew-symmetric matrices.

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# Fast adaptive alternating linear schemes in higher dimensions. Part 2: eigenvalue problem

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## Abstract

We consider partial eigenvalue problems for large tensor-structured matrices arising from the discretization of high-dimensional operators. The matrix and solution are approximated in the tensor train format, and the eigenvalue problem is solved using the alternating directions approach. We propose a variant of the Alternating Linear Scheme which performs the rank adaptation, incorporating the Jacobi-Davidson step. This allows to justify the method using classical theory. The method is compared with the DMRG approach for certain examples from quantum chemistry. The convergence is similar to that of the DMRG approach, but the complexity can be substantially reduced, especially for a large number of degrees of freedom in each dimension.

# Stochastic simulation of discrete and continuous multifractal fields with zero values

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## Abstract

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Multifractal models have been developed in the beginning of the 1980s in the fields of turbulence and chaos theory, and since then, have been the subject of studies and papers in many fields of science, from mathematics, chaos theory, turbulence, particle physics, to more applied fields such as meteorology, oceanology, soil sciences, rainfall processes to name a few. The basic idea of multifractal fields or processes is to possess statistical scale invariance, and intermittency, resulting in huge fluctuations at all scales, and producing a stochastic field whose moment generating function is nonlinear and convex. Hence there is an infinite range of singularities, each having a specific fractal dimension, explaining the word “multifractal”. Since the beginning of the 2000s, several models have proposed to consider log-infinitely divisible (ID) stochastic processes to generate continuous (in scale) multifractal fields [1, 2]. The multifractal field is here the exponential of an ID stochastic integral on a cone. Such approach is quite general and can be used to generate stochastic fields [3] or time series [4].

However such approach, as the exponential of a quantity, cannot generate zeroes. For many applications, including rainfall [5] or soil processes, it is important to be able to generate zero values. Here we show how to generalize the previous approach, using a continuous stochastic product with some atoms at zero. We explain the construction of our new proposal, called “continuous  $\beta$ -multifractal model”; we show its multifractality and give its scaling exponents. We generate 1D and 2D simulations. We apply it to rainfall fields.

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# New Implementation of the Block GMRES method

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## Abstract

The Block GMRES is a block Krylov solver for solving nonsymmetric systems of linear equations with multiple right-hand sides. This method is classically implemented by first applying the Arnoldi iteration as a block orthogonalization process to create a basis of the block Krylov space generated by the matrix of the system from the initial residual. Next, the method is solving a block least-squares problem, which is equivalent to solving several least squares problems implying the same Hessenberg matrix. These later are usually solved by using a block updating procedure for the QR decomposition of the Hessenberg matrix based on Givens rotations. A more effective alternative was given in [2] which uses the Householder reflectors. In this paper we propose a new and simple implementation of the block GMRES algorithm, based on a generalization of Ayachour's method [1] given for the GMRES with a single right-hand side. Several numerical experiments are provided to illustrate the performance of the new implementation.

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# Exact Line and Plane Search for Tensor Optimization by Global Minimization of Bivariate Polynomials and Rational Functions

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## Abstract

Line search (LS) and plane search (PS) are an integral component of many optimization algorithms. We pose independent component analysis (ICA) as a data fusion problem in which a PS subproblem naturally arises. In tensor optimization problems LS and PS often amount to minimizing a polynomial. We introduce a scaled LS and PS and show they are equivalent to minimizing a rational function. Lastly, we show how to compute the global minimizer of both real and complex (scaled) LS and PS problems accurately and efficiently by means of a generalized eigenvalue decomposition.

# How to automatically ensure that a domain decomposition method will converge?

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## Abstract

Domain decomposition methods are a popular way to solve large linear systems. For problems arising from practical applications it is likely that the equations will have highly heterogeneous coefficients. For example a tire is made both of rubber and steel, which are two materials with very different elastic behaviour laws. Many domain decomposition methods do not perform well in this case, specially if the decomposition into subdomains does not accommodate the coefficient variations.

For three popular domain decomposition methods (Additive Schwarz, BDD and FETI) we propose a remedy to this problem based on local spectral decompositions. Numerical investigations for the linear elasticity equations will confirm robustness with respect to heterogeneous coefficients, automatic (non regular) partitions into subdomains and nearly incompressible behaviour. We will also present large scale computations (over a billion unknowns) conducted by Jolivet in Freefem++ which show that strong scalability is achieved.

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# Method of lines for nonlinear first order partial functional differential equations

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## Abstract

Classical solutions of initial problems for nonlinear functional differential equations of Hamilton Jacobi type

$$\partial_t z(t, x) = f(t, x, z_{(t, x)}, z_{\varphi(t, x)}, \partial_x z(t, x)), \quad (1)$$

are approximated by solutions of associated differential difference systems. A method of quasilinearization is adopted. Sufficient conditions for the convergence of the method of lines and error estimates for approximate solutions are given. Nonlinear estimates of the Perron type with respect to functional variables for given operators are assumed. The proof of the stability of differential difference problems is based on a comparison technique. The results obtained here can be applied to differential integral problems and differential equations with deviated variables.

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# Subspace Iteration with Approximate Spectral Projection

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## Abstract

The calculation of a segment of eigenvalues and their corresponding eigenvectors of a Hermitian matrix or matrix pencil has many applications. A new approach to this calculation based on a density matrix has been proposed recently [1] and a software package FEAST [2] has been developed. The density-matrix approach allows FEAST's implementation to exploit a key strength of modern computer architectures, namely, multiple levels of parallelism. Consequently, the software package has been well received. Nevertheless, theoretical analysis of FEAST has been lagging and that a convergence proof has yet to be established. In this talk, we offer a numerical analysis of FEAST. In particular, we show that the FEAST algorithm can be understood as the standard subspace iteration algorithm in conjunction with the Rayleigh-Ritz procedure. The novelty of FEAST is that it does not iterate directly with the original matrices, but instead iterates with an approximation to the spectral projector onto the eigenspace in question. Analysis of the numerical nature of this approximate spectral projector and the resulting subspaces generated in the FEAST algorithm not only establishes the algorithm's convergence, but also provides a number of other properties that can be leveraged to enhance FEAST's robustness.

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# Almost blind filtering of large signal sets

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## Abstract

In many applications associated with complex environments, *a priori* information on signals of interest can be obtained only at a few given times  $\{t_j\}_1^p \subset T = [a, b] \subset \mathbb{R}$  where  $a = t_1 < t_2 < \dots < t_{p-1} < t_p = b$  whereas it is required to estimate the signals at *any time*  $t \in T$ . For each  $t \in T$ , the signal is a stochastic vector. Typical examples are devices deployed in the stratosphere, underground or underwater. The choice of points  $t_j$  might be beyond our control (e.g. in geophysics and defence). In addition, the observations are *large* and noisy. Thus, all we can exploit is noisy observations and a *sparse* information on reference signals. A formalization of the problem is as follows.

Let  $\{\Omega, \Sigma, \mu\}$ ,  $\mathcal{K}_x = \{x_\omega \mid \omega \in \Omega\}$  and  $\mathcal{K}_y = \{y_\omega \mid \omega \in \Omega\}$  be a probability space, and sets of reference and observed stochastic signals, respectively. Theoretically,  $\mathcal{K}_x$  and  $\mathcal{K}_y$  are infinite signal sets. In practice, however, sets  $\mathcal{K}_x$  and  $\mathcal{K}_y$  are finite and *large*, each with, say,  $N$  signals. To each  $\omega \in \Omega$  we associate a unique signal pair  $(x_\omega, y_\omega)$  where  $x_\omega : T \rightarrow \mathcal{C}^{0,1}(T, \mathbb{R}^m)$  and  $y_\omega : T \rightarrow \mathcal{C}^{0,1}(T, \mathbb{R}^n)$ . Write

$$\mathcal{P} = \mathcal{K}_x \times \mathcal{K}_y = \{(x_\omega, y_\omega) \mid \omega \in \Omega\}$$

for the set of all such pairs. For each  $\omega \in \Omega$ , the components  $x_\omega = x_\omega(t)$ ,  $y_\omega = y_\omega(t)$  are Lipschitz continuous vector-valued functions on  $T$ .

We wish to construct a filter  $F^{(p-1)}$  that estimates *each* reference signal  $x_\omega(t)$  in  $\mathcal{P}$  from the corresponding observed input  $y_\omega(t)$  under the restriction that *a priori* information is available on only a few reference signals,  $\mathcal{K}_x^{(p)} = \{x_\omega(t_j)\}_1^p$ .

In practice,  $p \ll N$ . This restriction implies the following. Let us denote by  $\mathcal{K}_y^{(p)}$  a set of observed signals associated with  $\mathcal{K}_x^{(p)}$ . Then for all  $y_\omega(t)$  that do not belong to  $\mathcal{K}_y^{(p)}$ ,  $y_\omega(t) \notin \mathcal{K}_y^{(p)}$ , filter  $F^{(p-1)}$  is said to be a *blind* filter since no information on  $x_\omega(t) \notin \mathcal{K}_x^{(p)}$  is available. If  $y_\omega(t) \in \mathcal{K}_y^{(p)}$  then  $F^{(p-1)}$  becomes a *non-blind* filter since information on  $x_\omega(t) \in \mathcal{K}_x^{(p)}$  is available. Thus, depending on  $y_\omega(t)$ , the filter  $F^{(p-1)}$  is classified differently. Therefore, the proposed estimation procedure on  $\mathcal{K}_x$  is here called *almost blind* filtering.

The *almost blind* filtering is different from known non-blind, semi-blind and blind techniques [1, 2]. Indeed, for different  $y_\omega(t)$  we wish to keep the *same* filter  $F^{(p-1)}$ . In most known techniques, the number of filters should be equal to the number of signal pairs  $(x_\omega(t), y_\omega(t)) \in \mathcal{P}$ . It is not feasible since the number of signals in  $\mathcal{P}$  can be very large. On the other hand semi-blind techniques [1] require a knowledge of some ‘parts’ of *each* signal in  $\mathcal{K}_x$ . That is not the case here.

The proposed filter  $F^{(p-1)}$  is adaptive to a sparse set  $\mathcal{K}_x^{(p)}$ . The conceptual device behind the filter  $F^{(p-1)}$  is an extension of the least squares linear (LSL) filter (see, e.g., [2]) interpreted as a linear interpolation applied to random signal pairs in  $\mathcal{P}$  on each interval  $[t_j, t_{j+1}]$ . Therefore the proposed filter  $F^{(p-1)}$  is called the *adaptive interpolation* filter.

Write  $x(t, \omega) = x_\omega(t)$ ,  $\xi_j(t) = u(t - t_j) - u(t - t_{j+1})$  and  $u(t)$  for the unit step function. For all  $t \in [a, b]$  and  $\omega \in \Omega$ , the estimate of each reference signal is given by

$$\hat{x}(t, \omega) = F^{(p-1)}[y(t, \omega)] = \sum_{j=1}^{p-1} F_j[y(t, \omega)]\xi_j(t)$$

where  $F_j[y(t, \omega)] = \hat{x}(t_j, \omega) + B_j w_j(t, t_j, \omega)$ , and  $B_j$  is the optimal LSL sub-filter for increments  $v_j = x(t_{j+1}, \omega) - x(t_j, \omega)$ ,  $w_j(t_{j+1}, t_j, \omega) = w_j = y(t_{j+1}, \omega) - y(t_j, \omega)$  and is constructed in terms of covariance matrices associated with  $v_j$  and  $w_j$ .

Further, we justify the proposed filter by establishing an upper bound for the associated error and by showing that this upper bound is directly related to the expected error for an incremental application of the optimal LSL filter.

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# The existence and uniqueness of the weak solution of the Shallow Water Equations on a sphere

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## Abstract

The Shallow Water Equations (SWEs) are the coupled system of partial differential equations (PDEs) describing various atmospheric phenomena, namely motion of the water in low shell areas, river channels etc. Although the system of the SWEs is hyperbolic in nature [1], the existing numerical methods suffer from spurious oscillations introduced by used numerical procedures [2]. This problem is caused by the fact that the SWEs admit non smooth solutions that might contain blocks and contact discontinuities. A common approach to deal with this problem is to add diffusive terms to the momentum equation (semi-parabolic formulation) and also to the continuity equation (parabolic formulation) [2, 3]. When such terms are added, physical parameters vary rapidly, but continuously [3]. Hence we would rather do the analysis of the SWEs with diffusive terms. The existence and uniqueness theorem for classical and weak solutions of the SWEs on *planar* regions was proved by Ton [4], Kloeden [5], Cárdenas et al. [6] and other authors for various SWEs formulations (semi-parabolic and parabolic). When studying global atmospheric behavior one needs to solve systems of PDEs on spherical domains. To the best of our knowledge there is no existence and uniqueness theorem for the SWEs on a *sphere*. Therefore we extend Cárdenas result to a sphere for parabolic formulation of the SWEs.

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# Simulation of unsteady temperature fields in permafrost from two wells

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## Abstract

Permafrost areas are extremely important for Russian economy, as here there are produced about 93% of Russian natural gas and 75% of oil. Design and construction of work sites with producing wells in these areas have their own specifics. For example, according to Russian standards of construction it is assumed that two wells cannot be drilled at a distance from each other less than two thawing radius (the position of the zero isotherm from the well after of 25 years of operation). To simulate these processes a new mathematical model of heat distribution on several insulated wells in permafrost is constructed and investigated. On the base of this model numerical codes have been developed for simulation of temperature fields in the well-permafrost system, allowing to carry out computational experiments and make long-term forecasts for permafrost thawing in the presence of wells equipped with a number of insulating shells and support engineering design, taking into account the annual cycle of melting / freezing of the upper layers of the soil under the influence of seasonal changes of air temperature and solar radiation. This numerical method was laid an algorithm [1-2], approved for thermal fields computing around underground pipes, but with the specifics related to the possible phase transitions in the soil [3]. In the numerical calculations it were observed some patterns in increasing the speed of propagation of permafrost thawing between of the two wells, depending on various parameters. These results allow the standards in distance between wells to be corrected. The reliability of the numerical simulations was tested in 2012 for the "Russkoye" oil field, for which the numerical and experimental results differ by 5% after 3 years of wells operation starting. Developed software will be used for "cloud" technologies that will allow specialists to carry out remote numerical calculations on multiple-processor computers.

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# Approximating extended Krylov subspaces without explicit inversion

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## Abstract

It will be shown that extended Krylov subspaces –under some assumptions– can be retrieved without any explicit inversion or solution of linear systems. Instead we do the necessary computations of  $A^{-1}v$  in an implicit way using the information from an enlarged standard Krylov subspace.

It is known that both for classical and extended Krylov spaces, unitary similarity transformations exist providing us the matrix of recurrences [1]. In practice, however, for large dimensions computing time is saved by making use of iterative procedures to gradually gather the recurrences in a matrix. Unfortunately, for extended Krylov spaces one is required to frequently solve, in some way or another systems of equation. In this lecture we will integrate both techniques.

We start with an orthogonal basis of a standard Krylov subspace of dimension  $m + \overline{m} + p$ . Then we will apply a unitary similarity built by rotations compressing thereby the initial subspace and resulting in an orthogonal basis approximately spanning the extended Krylov subspace:

$$\mathcal{K}_{m,\overline{m}}(A, v) = \text{span} \left\{ A^{-\overline{m}+1}v, \dots, A^{-1}v, v, Av, A^2v, \dots, A^{m-1}v \right\}.$$

Numerical experiments support our claims that this approximation is very good if the large Krylov subspace contains  $\{A^{-\overline{m}+1}v, \dots, A^{-1}v\}$ , and can culminate in nonneglectable dimensionality reduction. We will extensively test our approach and compare with the results from [2]. Furthermore additional examinations of Ritz-value convergence plots are included revealing the interaction between Krylov, extended Krylov and the truncation procedure.

## References

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- [2] C. JAGELS AND L. REICHEL, *Recursion relations for the extended Krylov subspace method*, Linear Algebra and its Applications, 434 (2011), pp. 1716–1732.

# An implicit finite-volume TVD method for solving 2D hydrodynamics equations on unstructured meshes

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## Abstract

The paper presents a higher-order implicit finite-volume TVD scheme for solving 2D hydrodynamics equations on unstructured meshes. The equations are solved in cylindrical coordinates. The scheme is based on an approximation of integral conservation laws in cells. Basic quantities, density, temperature and velocity are stored in cell centers. The scheme can be considered as an extension of scheme [1]. In what they basically differ are relations between quantities in cell centers and quantities in mesh nodes (velocities and flows). In the proposed scheme, approximated solutions of the Riemann problem are used for coupling relations – the method proposed P. H. Maire and coauthors [2]. The Riemann problem is solved in Cartesian coordinates. With these relations the scheme gives more monotonic solutions by suppressing spurious oscillations. The scheme conserves mass and total energy. The nonlinear TVD scheme is used to attain to the second order of approximation for smooth solutions and for better monotony. Difference equations are reduced to linear equations for pressure and velocity in cell centers. They are solved with iterative methods which use Krylov subspaces, mainly the biconjugate gradient stabilized method.

The scheme was verified through numerous 1D and 2D tests. Their results demonstrate robustness and accuracy of the scheme. Some of them are presented in the paper.

## References

- [1] E. M. Vaziev, A. D. Gadzhiev, S. Y. Kuzmin. An implicit finite-volume method ROMB for numerical solving 2D hydrodynamics equations on unstructured meshes with triangular and quadrangular cells. VANT (Mathematical Modeling of Physical Processes), 4 (2006), 1528 (in Russian)
- [2] Abgrall R, Breil J, Maire P -H, Ovadia J. A cell-centered Lagrangian scheme for two-dimensional compressible flow problems. SIAM J. SCI. COMPUT. Vol. 29, No. 4, pp. 17811824, 2007

# Multi-GPU parallel uncertainty quantification for two-phase flow simulations

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## Abstract

One big problem in simulations for real-world engineering applications is the appropriate handling of small uncertainties in the involved quantities. These uncertainties include but are not limited to varying material parameters, physical constraints (e.g. temperature, gravitation) and shapes of geometrical objects. We are interested in introducing techniques for uncertainty quantification into the field of incompressible two-phase flows with the Navier-Stokes equations. There is a wide range of applications such as hydrotechnical construction design, coating processes, droplet formation and bubble flows which need two-phase flow simulations to get detailed behavior predictions.

To be able to consider uncertainties in our computer-based fluid experiments, we currently use non-intrusive stochastic collocation methods. Here, RBF kernel methods allow us to interpolate the response surface of the stochastic parameter space. Statistical moments are computed with appropriate quadrature methods on the interpolated function. We are also able to setup and analyze covariance functions of full fluid data fields for which we compute the eigenvalue decomposition. This gives us a starting point for an optimal reduced order representation with a Karhunen-Love decomposition.

Note, that we apply our in-house multi-GPU parallel fluid solver NaSt3DGPF to be able to perform hundreds of flow simulations. Also, all stochastic calculations are performed on GPU hardware to be able to overcome the large amount of data to be processed.

In our talk, we will briefly describe the applied fluid solver in its GPU-parallel version. Then the full stochastic framework is presented including some remarks on the GPU implementation. Finally a few model problem applications will be presented.

## *The Scientific Program*

	<b><i>Monday 24</i></b>	<b><i>Tuesday 25</i></b>	<b><i>Wednesday 26</i></b>
8h30-09h10	<b>Registration</b>	P. Talk <b>P. Benner</b> Room A	P. Talk <b>F. Desbouvries</b> Room A
09h10-10h10	<b>Opening</b> (9h10-9h30) Room A P. Talk <b>Y. Saad</b> (9h30-10h10)	Session A4  Session B4	Session A8  Session B8
10h10-10h40	Coffee Break	Coffee Break ( <b>Posters</b> )	Coffee Break
10h40-12h45	Session A1 Session B1 Session C1	Session A5 Session B5 Minisymposium 2	Session A9 Session B9
			P. Talk <b>L. Reichel</b> (12h20-13h) Room A
13h00	Lunch	Lunch	Lunch
14h30-15h10	P. Talk <b>G. Meurant</b> Room A	P. Talk <b>P. Van Dooren</b> Room A	
15h10-16h00	Session A2  Session B2	Session A6  Session B6	
16h-16h30	Coffee Break	Coffee Break ( <b>Posters</b> )	
16h30-18h10	Session A3  Session B3	Session A7  Session B7	
		<b>CONFERENCE DINNER</b> <b>20h00</b>	

## Liste of Participants

Name	Country	Name	Country
ABIDI Oussama	France	IAN Zwaan	Netherlands
ABUALNAJA Khadijah Mohammed	Saudi Arabia	JBILOU Khalide	France
ADDAM Mohamed	Morocco	KALMOUN El Mostafa	Saudi Arabia
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ANDA ONDO Diemer	France	KRENDL Wolfgang	Austria
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ASUKA Ohashi	Japan	LITVINOV Vladimir	Russia
BARLOW Jesse	USA	MACH Thomas	Belgium
BARRERA-ROSILLO Domingo	Spain	MAQUIGNON Nicolas	France
BECKERMANN Bernhard	France	MARION Philippe	France
BELHAJ Skander	Tunisia	MASTRONARDI Nicola	Italy
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BEN KAHLA Haithem	France	MERMRI El Bekkaye	Morocco
BENJELLOUN Mohammed	France	MERTENS Clara	Belgium
BENNER Peter	Germany	MEURANT Gérard	France
BENSIALI Bouchra	France	MITROULI Marinela	Greece
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BENTBIB Abdeslem Hafid	Morocco	NGUENANG Louis Bernard	France
BOUHAMIDI Abderrahman	France	NGUETCHUE Neossi	South Africa
BOUJENA Soumaya	Morocco	NICAISE Serge	France
BOURCHTEIN Andrei	Brazil	NICHOLAS Knight	USA
BOUREL Christophe	France	NOTAY Yvan	Belgium
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DESBOUVRIES François	France	REICHEL Lothar	USA
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HEILAND Jan	Germany	VAGANOVA Nataliia	Russia
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		ZASPEL Peter	Germany

