BIT Circus 2018

Numerical Mathematics and Computational Science

Aalto University, August 20-22, 2018

Abstracts of presentations

Isogeometric analysis in structural mechanics and strain gradient elasticity

Viacehsalv Balobanov, Aalto University

The contribution considers the physico-mathematical models of structural mechanics within the theory of strain gradient elasticity. The problems are formulated in H^2 and H^3 Sobolev spaces, which leads to the requirement of higher continuity. The isogeometric conforming Galerkin method naturally provides C^{p-1}-continuity and therefore it is chosen as a basic method for the developed numerical tools. The main focus of the consideration is devoted to the implementation aspect and, particularly, user defined elements of commercial finite element software Abaqus. Issues such as the numerical shear locking phenomenon of the higher-order Timoshenko beam model or the static problem of the higher-order shell of arbitrary geometry are addressed. Error estimates for the corresponding conforming Galerkin discretizations are presented for verification of the method and its implementation.

Stress Reconstruction for mixed methods in Elasticity

Fleurianne Bertrand, Universität Duisburg Essen

We propose a new and simple way of reconstructing $H(\mathrm{div},\Omega)H(\mathrm{div},\Omega)$-conforming flux approximations for the $P2$ nonconforming finite element method of second order elliptic problems which fulfill the local mass conservation and optimal a priori error estimates. This reconstruction is crucially used in deriving an a posteriori error estimator which gives a guaranteed upper bound on the actual error. We also apply the same technique to the Stokes problem in order to reconstruct a $H(\mathrm{div},\Omega)H(\mathrm{div},\Omega)$-conforming pseudo-tensor approximation which are then used for a posteriori error estimation. Some numerical results are presented to illustrate the performance of the error estimators.

Best space of a fixed dimension

Andrea Bressan, University of Oslo

Consider the space $\mathbb{S}_{p,k,n}$ of piecewise polynomials $[0,1] \to \mathbb{R}$ of degree p on the uniform partitions

in n segments and having k continuous derivatives. Let $C_{p,k,n}$ be the best constant such that: $\forall f \in H^{p+1}(0,1)$

$$\|f - \Pi^{\perp} f\|_{L^2} \leq C_{p,k,n} \|\partial^{p+1} f\|_{L^2}.$$

Which pair of parameters (k,n) minimizes $C_{p,k,n}$ for a fixed degree and space dimension? We can not answer the question completely. However, we can compare the interesting cases $k=-1$ used in DG, $k=0$ used in FEM and $k=p-1$ used in IGA. The answer extends to broken Sobolev spaces and to tensor product spaces.

Approximation of Killing vector fields on the torus

Gaelle Brunet, University of Eastern Finland

The torus has always been an object with many curiosities. The torus has many fabulous properties which make it a part of many scientific projects, for instance, Stanford torus. NASA has designed Stanford torus, using the properties of the torus, for a space habitat capable of housing 10000 to 140000 permanent resident in case of a disaster on the earth. This project has not been realized but the idea was used in many fiction movies. However, this structure might not be able to withstand some force fields, and it can be interesting to know the vector fields which allow the sliding of this structure without tearing or wrinkling. These fields are called Killing vector fields. Therefore, we want to know if there exist some Killing vector fields on the torus. To find them, a system of PDEs must be solved, and exact solutions (if there exist) cannot be found systematically. Here, we want to approximate these Killing fields, and see if they persist if we distort the torus. We will see that the problem of this approximation is in fact a symmetric eigenvalue problem and it can be solved easily with the software Freefem++, developed by Frederic Hecht. In order to model the torus, it will be considered like a Riemannian submanifold of R^3 with a Riemannian metric associated at the parametrization. We will use a triangulation adapted with the Riemannian metric of a subset of R^2 to have a quasi-uniform triangulation of the torus, then we will solve the problem on this subset and represent the Killing vector fields. In another way, in fluid mechanic, the notion of Killing vector fields is important. In fact, these fields generate the group of continuous isometries of a manifold and are stationary solutions for the Navier Stokes and Euler equations.

Error analysis of a high-order numerical method on fitted meshes for a time-fractional diffusion problem

Hu Chen, Beijing Computational Science Research Center

In recent years, fractional derivatives are used widely for modelling physical processes. Time-fractional diffusion equations are used to model abnormal diffusion phenomena, where the mean square displacement is proportional to t^{α} with $0 < \alpha < 1$. There is much current interest in the construction and analysis of numerical methods for the solution of such problems, which typically exhibit a weak singularity at the initial time $t = 0$. In [1] a high-order scheme for Caputo fractional derivatives of order $\alpha \in (0,1)$ is proposed and analysed for time-fractional initial-value problems (IVPs) and initial-boundary value problems (IBVPs), on temporal meshes that are fitted

to the initial weak singularity. In the IBVP the spatial domain is the unit square, where a spectral method is used, but other domains (in $\mathbb{R}^d$ for $d \geq 1$) and other spatial discretisations (finite element, finite difference) could be handled by modifying our analysis.

It is proved in [1] that, when the fitted temporal mesh is chosen suitably, the scheme attains order $3 - \alpha$ convergence in the discrete L^∞ norm for the 1-dimensional IVP, and second-order convergence in $L^\infty(L^2)$ for the IBVP. Numerical results demonstrate the sharpness of these theoretical convergence estimates.

[1] Hu Chen and Martin Stynes, Error analysis of a second-order method on fitted meshes for a time-fractional diffusion problem, submitted for publication.

Electrical enclosures - Thermal design optimization

Ivo Dravins, Uppsala University

The electrical enclosure problem (EEP) is to find the thermally optimal placement of heat generating electrical components within an enclosed cooled domain. Basic examples of PDE-constrained optimization problems are given, with an overview of how these may be applied to the EEP. Challenges for its practical implementation are presented, and methods suggested for how to possibly address them.

On Bayesian inference of sparsely observed national scale epidemics

Robin Eriksson, Uppsala University

As epidemiological and demographic data increase in availability and resolution, realistic, first-principle based computational models of disease-spread become viable. We develop such models on top of detailed network data and set out to infer the parameters of them in a Bayesian setting. We approach the question of estimation uncertainty and model identifiability through a series of progressively realistic data-synthetic experiments.

The observed data includes two significant complications. First, by far, the most challenging issue is the sparsity of the observed disease data. Second, the actual information content of relatively costly measurements is low and only identifies the model weakly. Despite these challenges, we can show the feasibility of our parametrization strategy and perform a convergent parameter posterior exploration.

Fast integral equation methods for the isotropic heat equation

Fredrik Fryklund, KTH Royal Institute of Technology

The forced isotropic heat equation, with Dirichlet data in a two-dimensional multiply connected domain, is solved numerically with an efficient integral equation approach. First we discretise in time, which yields the inhomogeneous modified Helmholtz equation. At each time step, a particular solution is obtained by first applying the Partition of Unity Extension method to extend the resulting right-hand side to a function with compact support in a larger, geometrically simpler domain. Thereafter, the modified Helmholtz equation is solved with a spectral method. Adjusting

the boundary conditions accordingly, the homogeneous solution to be added to the particular solution is computed with a boundary integral solver, where only discretisation of the boundary is necessary, accelerated by the Fast Multipole Method. A special quadrature method removes errors associated with near singular kernels. With a suitable choice of parameters the error for solving the modified Helmholtz equation converges as a tenth order method down to 14 correct digits. For time-stepping we apply an adaptive implicit-explicit RungeKutta scheme.

In a previous paper we introduced the novel method Partition of Unity Extension for numerical function extension, but in the framework of solving the Poisson equation. Only minor modifications are required to adapt the solution method to the modified Helmholtz equation. The guidelines for setting parameters for the Poisson equation are sound for the modified Helmholtz equation as well. Our function extension algorithm is simple in implementation, but still general in terms of application. The most computationally demanding operations are precomputed and the the majority of the operations are trivially parallel. A stable and efficient method for function extension has been requested by the boundary integral equation community for quite some time. It offers the option to solve inhomogeneous linear elliptic partial differential equations without resorting to evaluating volume potentials.

In the Partition of Unity Extension, overlapping partitions are distributed along the boundaries, each associated with a weight function imposing compact support. On each partition a local extension is computed with smooth radial basis functions. The partition of unity blends the local extrapolations into a global one, with global regularity set by the weight functions.

A Posteriori Error Estimates for Elliptic Eigenvalue Problems Using Auxiliary Subspace Techniques

Harri Hakula, Aalto University

One feature of eigenvalue problems that complicates the estimation of error is the possibility of repeated or tightly-clustered eigenvalues, which arise very naturally in domains with symmetries or near-symmetries, and will heavily feature in our numerical experiments. When such eigenvalues are to be approximated in practice, it makes little sense to try to determine whether computed eigenvalue approximations that are very close to each other are all approximating the same (repeated) eigenvalue, or approximating eigenvalues that just happen to very close to each other. In this case, it is best to estimate eigenvalue error and associated invariant subspace error in a collective sense." We discuss dimension-independent theoretical results based on auxiliary subspaces in hp-setting and show numerical experiments in 2D.

Stability property of hyperbolic equations with damping and time delay

Jianghao Hao, Shanxi University

In this talk, we consider the stability property and energy decay property of hyperbolic equations with damping and time delay. Under suitable assumptions on the damping terms, time delay and initial data, we obtain that the decay estimates of the energy function is exponential decay, polynomial decay, or general decay which depends on the behavior of the damping.

Optimal $L^\infty(L^2)$ error analysis of a direct discontinuous Galerkin method for time-fractional reaction-diffusion problems

Chaobao Huang, Beijing Computational Science Research Center

In the last decade, fractional PDEs have been used to model many natural phenomena in physics, biology and chemistry. In this talk, time-fractional reaction-diffusion initial-boundary value problems in one space dimension are considered. Two types of boundary condition on the spatial domain Ω are examined: Dirichlet (see [1]) and Robin (see [2]). The solutions of such problems have in general a weak singularity near the initial time $t = 0$. Some new pointwise bounds on certain derivatives of this solution are derived. To solve these problem numerically, we use the well-known L1 discretisation in time on a graded mesh and a direct discontinuous Galerkin (DDG) finite element method in space on a uniform mesh. Discrete stability of the computed solution is proved. The error analysis is based on a non-trivial projection into the finite element space, which for the first time extends the analysis of the DDG method to non-periodic boundary conditions. The final convergence results imply how an optimal grading of the temporal mesh should be chosen. Numerical results show that our $L^\infty(L^2)$ error analysis for both types of boundary condition is sharp.

In the case of Robin boundary conditions [2], the coefficient of the zero-order reaction term is not required to be non-negative, which complicates the analysis. As well as an $L^\infty(L^2)$ error estimate, a $H^1(\Omega)$ error bound is proved at each discrete time level t_n; this $H^1(\Omega)$ bound is optimal for t_n not close to $t = 0$.

References:

[1] Chaobao Huang, Martin Stynes, and Na An, Optimal $L^\infty(L^2)$ error analysis of a direct discontinuous Galerkin method for a time-fractional reaction-diffusion problem, to appear in BIT Numerical Mathematics.

[2] Chaobao Huang and Martin Stynes, A direct discontinuous Galerkin method for a time-fractional diffusion equation with a Robin boundary condition, submitted for publication.

Solving eigenvalue Problems

Marko Huhtanen, University of Oulu

Solving eigenvalue problems are discussed, either in finite dimensions or for unbounded operators in infinite dimensions.

NEP-PACK: A julia package for nonlinear eigenvalue problems

Elias Jarlebring, KTH Royal Institute of Technology

We present an open-source library for nonlinear eigenvalue problems (NEPs), designed for scientists working on method development, high-performance computing, as well as specific NEP-applications. The package is constructed to provide easy access to may state-of-the-art methods, exploiting multiple dispatch and parametric types for efficiency. Moreover, the multiple dispatch allows us to incorporate problem specific structures in the methods, e.g. with the use of matrix functions applied to matrices with particular structure. This is joint work with E. Ringh, G. Mele

and P. Upadhyaya.

Computing canonical quantum observables using molecular dynamics

Aku Kammonen, KTH Royal Institute of Technology

Is it possible to efficiently compute the canonical quantum observables by using molecular dynamics and sampling all energy levels? In the limit when the temperature goes to zero only the ground state is occupied but as temperature increases so does the probability of higher energy levels being occupied.

The curse of dimensionality makes it practically impossible to compute the observables directly from the Schrödinger equation. Instead molecular dynamics is used. We present an algorithm that makes use of a Metropolis acceptance test when sampling both in position space and energy level space. Sampling in position space is done with the Langevin dynamics. In energy level space sampling is done by flipping Fock eigenvalues following a suitable dynamic. Numerical tests shows that sampling more energy levels does not increase the computational cost if the eigenvalues of the Fock matrix are known.

Symplectic integrators for the space- and time-dependent wave equation

Nikita Kopylov, Universitat Politècnica de València

The numerical time-integration of the non-stationary wave equation is considered. A class of time-averaged symplectic splitting methods with double commutators is analysed, and 4th - and 6th-order integrators are obtained. Using the structure of the problem and incorporating commutators, lets us circumvent the order barrier and build effective integrators. Such an approach allows to minimise the contribution of negative splitting coefficients and reduce the number of stages.

Optimal quotients and iterations for large generalized eigenvalue problems

Vesa Kotila, University of Oulu

Iterative methods are needed for the solution for eigenvalue problems, if the size or structure of the problem prohibits the use of direct methods. For standard Hermitian problems, the cubic asymptotic convergence rate of the Rayleigh quotient iterarion has been regarded invincible a judgement that we will show is erroneous. We will introduce an iteration that outperforms the Rayleigh quotient iteration in the standard Hermitian case, and is readily applicable to generalized eigenvalue problems (GEP) as well.

The iteration consist of two alternating processes. First, given an approximate eigenvector for GEP, the problem is projected to the one-dimensional vector space that is maximally aligned with the two (linearly independent) image vectors. An approximate eigenvalue is then obtained as a quotient; this gives rise to the notion of an optimal quotient and related structures. Second, with the new approximate eigenvalue, modified inverse iteration strategies are used to update the eigenvector.

Multiparametric shell eigenvalue problems

Mikael Laaksonen, Aalto University

We consider multiparametric shell eigenvalue problems that arise from introducing random material properties to the shell model. A notable feature of such problems is that, whereas the smallest eigenmode of a second order elliptic problem is always simple, for a shell eigenvalue problem this need not be the case. In fact the eigenmodes of shells of revolution appear to be clustered due to periodic nature of the angular components and in special cases also due to physical properties of the problem.

Sparse stochastic collocation [2] and spectral inverse iteration algorithms [1] have recently been proposed for resolving simple eigenmodes of multiparametric eigenvalue problems. If the material properties of the shell are constant in the angular direction, then eigenmodes may be computed by applying these algorithms to a reduced one-dimensional problem. In order to resolve the eigenmodes of the full two-dimensional problem, however, we extend the aforementioned algorithms in a way that subspaces associated to clustered eigenvalues may also be computed. Numerical experiments suggest that the proposed subspace algorithms are able to resolve the eigenclusters effectively.

Joint work with Harri Hakula.

References:
[1] H. Hakula and M. Laaksonen, Asymptotic convergence of spectral inverse iterations for stochastic eigenvalue problems, arXiv:1706.03558, 2017.
[2] R. Andreev and Ch. Schwab, Sparse tensor approximation of parametric eigenvalue problems, in Lect. Notes Comput. Sci. Eng., vol. 83, pp. 203-241, 2012.

Finite Element Discretization for a Total Variation Model

Andreas Langer, University of Stuttgart

We consider a newly introduced model which consists of a total variation regularization term and a combination of a quadratic L2-term and a non-smooth L1-term. This model has some nice advantages over usually used models in image reconstruction, as we will show by an analytic example. While mainly finite differences are used to solve respective image reconstruction problems, we present a finite element scheme. We demonstrate that for a particular finite element space the discrete model converges asymptotically to the continuous model. This is unfortunately not true for any finite element space, as a counterexample shows. Based on a primal-dual algorithm we demonstrate the applicability of a finite element method for the presented model.

Heterogeneous multiscale methods for applications in magnetization dynamics

Lena Leitenmaier, KTH Royal Institute of Technology

In certain magnetization dynamics problems, one is interested in the behavior on a rather big scale, but atomisic scale effects play an important role which makes it hard to get a sufficient solution using a model involving only the scale of interest. A possible way to deal with this is to use the framework of heterogeneous multiscale methods (HMM) in order to couple atomistic

spin dynamics (ASD), which is an ODE model, with a continuum level micromagnetics (MM) PDE model.

Symbols and exact regularity of symmetric pseudo-splines of any arity

Georg Muntingh, SINTEF Digital

Subdivision is a recursive method for generating curves, surfaces and other geometric objects. Rather than having a complete description of the object of interest at hand, subdivision generates the object by repeatedly refining its description starting from a coarse set of control points. Pseudo-splines form a family of subdivision schemes that provide a natural blend between interpolating schemes and approximating schemes, including the Dubuc-Deslauriers schemes and B-spline schemes.

Using a generating function approach, we derive expressions for the symbols of the symmetric m-ary pseudo-spline subdivision schemes. We show that their masks have positive Fourier transform, making it possible to compute the exact Hlder regularity algebraically as a logarithm of the spectral radius of a matrix. We apply this method to compute the regularity explicitly in some special cases, including the symmetric binary, ternary, and quarternary pseudo-spline schemes.

Continuum damage modelling within classical and strain gradient elasticity

Hoang Anh Tuan Nguyen, Aalto University

Continuum damage can be used to model the fracture, or material degradation process, in quasi-brittle media. The standard damage formulations suffer from the sensitivity to the spatial discretization, generating unphysically spurious damage zones at high levels of deformation. This research is devoted to an elasto-damage model based on strain gradient elasticity theory to remedy the aforementioned problem. The model can be considered as an extension to the damage model proposed in (Nguyen, 2018) built on the classical elasticity theory. By taking into account the strain gradient terms with corresponding internal length scale parameters, the nonlocality of materials is naturally expressed and size-dependent effects can be captured. The isotropic damage law is implemented through the higher order stress-strain relation. Numerical investigations of damage modeling for quasi-brittle materials is implemented by using the isogeometric analysis as an alternative to the conventional finite element method. Representative numerical examples considering different configurations, damage evolution laws, boundary and loading conditions are presented. Equilibrium stages of the materially nonlinear structures are traced by using the displacement control Newton-Raphson method. The accuracy and performance of the proposed approach is demonstrated by comparing the obtained responses with respect to reference solutions derived from experiments or other numerical approaches.

Perspectives on dynamic structural analysis of footbridges

Antti H. Niemi, University of Oulu

High strength of modern building materials allows to build pedestrian bridges with increased flexibility, lightness, and span length. This leads to smaller natural frequencies that may be close

to the walking and running frequencies of pedestrians crossing the bridge. As a consequence, excessive vibrations caused by resonance with dynamic loads may occur. For light bridges serviceability criteria for pedestrian induced vibrations can become the dominant design criterion and decision-making requires careful analysis of realistic structural models and dynamic load models. In this work, some aspects of mathematical and numerical modelling of dynamics of pedestrian bridges are discussed and different load models are compared.

Mean value interpolation for arbitrary polygons and polyhedra

Francesco Patrizi, University of Oslo (external partner SINTEF)

Mean value coordinates have been introduced as a way of expressing a point in the kernel of a star-shaped polygon as a convex combination of the vertices. It was shown that these coordinates can be successfully used to compute good parameterizations for surfaces represented as triangular meshes, based on convex combination maps. Such coordinates are particularly useful for interpolating data that are given at the vertices of the polygon. For this reason, they can be efficiently used in computer graphics and geometric modeling. Many other generalizations of barycentric coordinates to convex polygons have been introduced in the last decades. However, while such constructions break down when used in the non-convex setting, mean value coordinates were successfully extended for arbitrary planar polygons without self-intersections. Furthermore, Mean value coordinates were also addressed for the 3D case, for convex polyhedra or in the kernel of a star-shaped polyhedra. The Mean value coordinates can be seen as interpolant of a piecewise linear function defined on the boundary of the polygon (or polyhedra in the 3D case). In this talk we see the interpolation property for arbitrary given continuous function on the boundary of non-convex polygon and polyhedra. In particular, we will have interpolation for the Mean value coordinates on any non-convex polyhedra.

Iron loss estimation as an inverse problem

Lauri Perkkiö, Aalto University

Estimation of power loss inside an iron core of an electric machine is formulated as a Bayesian inverse problem. The unknown power loss acts as a volume heat source in the heat equation, and the source term is reconstructed using a boundary temperature measurement, augmented by a small number of point measurements inside the object. The sensor locations are optimized to minimize the posterior variance. The resulting 3D finite element-discretized problem requires some numerical tricks to be computable in practise.

Generalized approximate implicitization with prescribed conditions

Andrea Raffo, University of Oslo

Approximate implicitization is the process of determining an implicit form that matches a parametric representation as close as possible in some sense. In a discrete form, it has been numerically implemented by considering a least squares approach to a point cloud sampled from the original parametric variety. Examples of applications include approximating simple CAD geometries for

the purposes of visualization, segmentation and supporting intersection computations. However, naive approaches to approximate implicitization do not necessarily preserve properties inherent in the geometry such as translational and rotational symmetries.

In this talk we will show how approximate implicitization can be tailored to specific applications by imposing prior knowledge, such as known symmetries and interpolation conditions. The method will be illustrated by several examples and motivated by industrial applications.

Conformal invariants and numerical conformal mappings

Antti Rasila, Aalto University

We also consider numerical computation of certain conformal invariants such as conformal moduli, which can be used for finding the canonical conformal mapping by using the harmonic conjugate. We consider construction of conformal mappings between simply, doubly and multiply connected domains and their applications.

A second-order numerical method for a scalar monotonicity-preserving nonlocal nonlinear conservation law

Adrian Montgomery Ruf, University of Oslo

We consider a scalar equation called the 'nonlocal pair-interaction model' introduced by Du, Huan and LeFloch which is a nonlocal generalisation of scalar (local) conservation laws. The pair-interaction model enjoys a maximum principle and certain monotonicity properties and, consequently, the entropy inequalities are naturally satisfied. In this talk we will consider second-order numerical methods based on reconstruction and appropriate numerical integration which generalize certain second-order methods for local conservation laws.

Optimal spline spaces for $L2$ n-width problems

Espen Sande, University of Oslo

Recently there has been renewed interest in using splines of maximal smoothness, i.e. of smoothness C^{d1} for splines of degree d, in finite element methods for solving PDEs. This is one of the main ideas behind isogeometric analysis. This raises the issue of how good these splines are at approximating functions of a certain smoothness class, especially with respect to the L^2 norm. Building on previous work of Melkman and Micchelli, and Pinkus, we will in this talk study various function classes in $H^r(0,1)$ and show that they admit optimal spline spaces of all degrees $d \geq r1$. These results partially answer a conjecture of Evans, Bazilevs, Babuska and Hughes.

Flow-induced sound generation during voiced speech

Lukas Schickhofer, KTH Royal Institute of Technology

Voice production and the expression of sounds via speech is a crucial human trait and essential for our communication. Speech consists mainly of the source signal that is frequency-weighted by the acoustic filtering of the upper airways and vortex-induced sound through perturbation in

the flow field.

This study investigates the flow instabilities leading to vortex shedding and the importance of coherent structures in the supraglottal region downstream of the vocal folds for the far-field sound signal. Large eddy simulations of the compressible airflow through the glottal contriction are performed in realistic geometries obtained from three-dimensional magnetic resonance imaging data. Intermittent flow separation through the glottis is shown to introduce unsteady surface pressure through impingement of vortices. Additionally, dominant flow instabilities develop in the shear layer associated with the glottal jet. The relationship between hydrodynamic perturbations in the near field and the acoustic signal in the far field is examined by means of spatial and temporal Fourier analysis. Furthermore, the contribution of flow structures near the glottal jet to the sound output during voiced speech is assessed and the acoustic sources due to the unsteady supraglottal flow are identified with the aid of surface spectra.

A one-variable locking-free Reissner-Mindlin plate: variational formulations and isogeometric implementation

Loc Tran, Aalto University

We propose variational formulations of isotropic plates based on only one unknown. Herein, the in-plane displacements are the same as that of Kirchhoff-Love model while the transverse one can be expressed in term of bending deflection and its Laplace operator. It enables the present model to be free of shear-locking and also reduce two unknowns as compared to traditional Reissner-Mindlin model. However, it produces a fourth-order partial differential equation in strong form, resulting in the symmetrical third-order differential weak form. Based on these, we develop Isogeometric Galerkin formulations with B-Spline basic functions of order $p \geq 3$ to naturally fulfill the stringent C2-continuity. Convergence study and shear-locking test are presented to show the reliability and effective of the proposed formulations.

A density matrix approach to the convergence of the Self-Consistent Field iteration

Parikshit Upadhyaya, KTH Royal Institute of Technology

The Self-Consistent Field(SCF) iteration is an iterative algorithm used to solve a class of non-linear eigenvalue problems of the form $H(X)X = X\Lambda, X^TX = I$, where $H : C^{n\times k} \to C^{n\times n}, X \in C^{n\times k}$ and $\Lambda \in C^{k\times k}$ is a diagonal matrix. These problems arise in the context of quantum chemistry and electronic structure calculations as the discretized Kohn-Sham and Hartree-Fock equations, where we are interested in computing the k first eigenvalues. The Sufficient conditions for SCF exist in the current literature, e.g. in [1], [2] and [3]. In contrast to these results, we provide a convergence theory based on the analysis of SCF as a fixed point map where the density matrix is the state of the algorithm. This allows us to formulate an exact characterization of the convergence using the spectral radius of the fixed-point Jacobian. We then derive computable qualitative bounds for the convergence factor and make several interpretations with these bounds, in terms of the gaps between eigenvalues of the problem and the outer products of eigenvectors. Our numerical experiments with various problem sizes confirm our theoretical predictions for the convergence factor and also help us understand the utility of our upper bounds in providing more

insight into SCF convergence.

References:
[1] C. Yang, W. Gao, and J. C. Meza. On the convergence of the self-consistent field iteration for a class of nonlinear eigenvalue problems. SIAM J. Matrix Anal Appl., 30(4):1773-1788, 2009
[2] X. Liu, X. Wang, Z. Wen and Y. Yuan. On the convergence of the self-consistent field iteration in Kohn-Sham density functional theory. SIAM J. Matrix Anal Appl., 35(2):546-558, 2014
[3] E. Cances and C. Le Bris. On the convergence of SCF algorithms for the Hartree-Fock equations. M2AN, Math. Model. Numer. Anal., 2000

Local controllability for linear evolution equations with bilinear control

Cristina Urbani, Gran Sasso Science Institute, Université Pierre et Marie Curie

In control theory there are few results of controllability of equations via bilinear control with respect to boundary or localized controls. The reason is that, contrarily to boundary and additive control problems, the presence of a control that multiplies the state of the equation brings non linearity in the system. Therefore, there are no direct methods to approach these problems and usually the strategy consists in linearizing the equation around a given equilibrium or trajectory, studying the controllability of this simplified problem and then, if it is possible, deducing the desired property for the non linear system through an inverse mapping theorem.

I will present a result of bilinear controllability of evolution equations with an operator generating an analytic semigroup. Finally, I will apply the abstract result to some examples.

Joint work with F. Alabau, P. Cannarsa.

Lie-Poisson numerical schemes for isospectral flows

Milo Viviani, Chalmers University of Technology

The theory of isospectral flows encompasses a large class of dynamical systems, e.g., gradient flows, Lie-Poisson Hamiltonian systems, etc.. Their numerical resolution is a classical problem in geometric integration. The difficulty is due to the fact that the preservation of the spectra in the discrete flow requires the conservation of high order polynomials and, for example, no Runge-Kutta method can preserve arbitrary quadratic and cubic invariants at the same time. However, there exist high order numerical methods (e.g. RK-MK) which can do that, but in general they are not Lie-Poisson integrator. In this paper we present a general framework to set the isospectral flows and we provide a class of numerical methods of arbitrary order based on the Lie-Poisson reduction of Hamiltonian systems. Avoiding the use of any constraint, we provide a large class of geometric integrator for Hamiltonian and non-Hamiltonian isospectral flows. One of the advantage of these methods is that, together with the isospectrality, they have near conservation of the Hamiltonian and indeed they are Lie-Poisson integrators.

Continuous transportation as a material distribution topology optimization problem

Eddie Wadbro, Umeå University

Transportation problems have a long history in science. Already in 1781, Monge studied the problem of how to minimize the work required to move a commodity with a given initial mass distribution to a pre-specified target mass distribution. Monge's problem formulation considers the computation of transport paths, which distinguishes it from route planning problems that are restricted to an existing network. The seminal work by Monge has been generalized by many researchers. During the last few decades, there has been a renewed activity in studying these transportation problems. Currently, the problem is well understood from a theoretical perspective; however, the numerical treatment of the problem has this far received little, if any, attention.

Flow network problems are by far the most investigated domain of transportation theory, and have resulted in a row of now mature tools from linear, integer, and constraint programming. This should come as no surprise, since most transportation is undertaken on an existing infrastructure. However, from an economics perspective, it is on the other hand of interest to target not only transportation cost, but also the cost for road construction. Such considerations come into play also on a smaller scale, for instance in agriculture or forestry, when temporary or otherwise designated roads must be paved. Here, we consider a version of this problem aiming to minimize a combination of road construction and transportation cost by determining, at each point, the local direction of transportation. Here, we aim to solve numerically a continuous transportation problem using *material distribution* based topology optimization. The rationale for this is that road design is effectively a material distribution problem, and transportation is nothing but flow of matter.

Here, we consider a commodity that is produced or consumed at the space dependent rate q and transported with velocity $\boldsymbol{u}$, where $|\boldsymbol{u}| = v$, and $v : \mathbb{R}^2 \mapsto \mathbb{R}^+$ is a space dependent transportation speed. Moreover, we assume that the production, transport, and consumption of the product are all confined to be inside a region $\Omega \subset \mathbb{R}^2$. To model and solve the problem to minimize a combination of road construction and transportation cost, we use two design fields. The first of these, α is a material indicator function for the road layout, which in turn determines the transportation speed ($v = v_{\mathsf{max}}$ where $\alpha = 1$, and $v = v_{\mathsf{min}}$ where $\alpha = 0$). The second design field is determines at each point the local direction of transport.

This presentation covers the modeling of the problem, highlights how it can be formulated as a material distribution topology optimization problem, and shows optimized road designs for a few test cases where the supply and demand positions are concentrated around given points as well as distributed over given subdomains of Ω. By solving the optimization problem for a sequence of different weightings between road construction and transportation cost, we obtain a sequence of road designs corresponding to different tradeoffs between these costs. Such solutions and their corresponding relative road construction and transportation cost may provide guidance when making decisions regarding if and where to construct roads to increase transportation efficiency.

High order summation-by-parts finite difference operators for reentrant corners

Jonatan Werpers, Uppsala University

Finite difference methods are known to be simple and efficient for solving partial differential equations on simple domains. For somewhat complicated domains the summation by parts framework

together with weakly imposed boundary and interface conditions through the SAT technique provide tools for deriving provably stable high order schemes for a wide variety of equations, problems and boundary conditions. When the geometries get complicated enough it is often necessary to use some other method of discretisation. However, for large parts of the domain, a finite difference method might still be competitive.

In these cases, when the problem at hand demands adaptivity in mesh size or hybrid methods the traditional ways of using finite difference methods often come with certain costs. To decrease mesh size, or to change the method of discretisation in part of the domain, for stability reasons, one often has to introduce block interfaces in large parts of the domain even away from the particular area. Besides complicating the structure of the grid these interfaces also degrade accuracy in order to provide numerical stability of the scheme.

In this talk we will present summation by parts boundary closures around reentrant corners for a few different high order finite difference schemes. In combination with traditional summation by parts finite difference boundary closures for edges and regular interior corners this allows finite difference discretisations of non-rectangular domains without the introduction of block interfaces. Avoiding extra interfaces preserves the simplicity and efficiency of the method in the bulk of the domain while enabling provably stable couplings to other methods or finer grids. One example could be a large rectangular domain with a small square removed from its interior which is either not part of the problem domain or is discretised in a different way.

We will show that the new boundary closures yield provably stable interfaces in a similar way to traditional summation by parts operators and we will show that the schemes give higher order accuracy. We will also provide examples on how to do mesh refinement and hybrid schemes.

The analysis and application of Optimal Transport for Seismic Inversion

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Optimal transport has become a well-developed topic in the mathematical analysis. Due to their ability to incorporate differences in both signal intensity and spatial information, the related Wasserstein metrics have been adopted in a variety of applications, including seismic inversion. Full Waveform Inversion (FWI) is a PDE-constrained optimization in which the variable velocity in a forward wave equation is adjusted such that the solution matches measured data on the surface. L^2 norm is the conventional objective function measuring the difference between simulated and measured data, but it often results in the minimization trapped in local minima. One way to mitigate this is by selecting another misfit function with better convexity, and we proposed using the quadratic Wasserstein metric (W_2). The optimal map defining W_2 can be computed by quicksort (trace-by-trace comparison) or solving a Monge-Ampère equation (global comparison). Theorems pointing to the advantages of using optimal transport over L^2 norm will be discussed, and some large-scale computational examples will be presented. There is an interesting question about how to adapt datasets that are not naturally nonnegative and mass balanced into optimal transport theory.