

HA-LU 2019

International conference in honor of Ernst Hairer
and Christian Lubich

Gran Sasso Science Institute, L'Aquila

17–21 June 2019

Program at a glance

	June 17	June 18	June 19	June 20	June 21
9.15	<i>Opening</i>	Sanz-Serna	Overton	Hochbruck	Zennaro
10.00	Wanner	Gander	Yserentant	Chartier	Vilmart
10.45	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>
11.15	Ascher	Quarteroni	Vandereycken	Jahnke	Cohen
12.00	Deuffhard	Banjai	Palencia	Li	Lasser
12.45	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>
14.30	Ostermann	Akrivis	<i>Group photo</i>	Hairer	
15.15	Gonzalez-Pinto	Calvo			
16.00	<i>Coffee break</i>	<i>Coffee break</i>			
16.30	<i>Photo exhibition</i>				

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Monday, 17 June 2019

Zigzags with Bürgi, Bernoulli, Euler and the Seidel-Entringer-Arnol'd triangle

Gerhard Wanner
University of Geneva

17 Jun
10:00

We explain nice connections between

- a recently discovered work by Jost Bürgi (1584) on the oldest iteration method;
- a somehow forgotten work of Joh. Bernoulli (1742) on iterated involutes;
- a somehow forgotten work of Désiré André (1879) on alternating permutations and their elegant treatment by R.C. Entringer (1966) as well as their generalizations (the Seidel-Entringer-Arnol'd triangle and the Boustrophedon Theorem).

We meet the Sinus function, the Euler-Bernoulli numbers and the series for $\tan x$ and $\sec x$ several times.

This is a joint work with Ph. Henry.

Different faces of stiffness

Uri Ascher
University of British Columbia

17 Jun
11:15

The words “stiff”, “stiffness”, “stiffening”, etc., arise often in applications when simulating, calibrating and controlling dynamics. But these words often have different meanings in different contexts. A subset on which we will concentrate includes: (1) decaying numerical ODE stiffness; (2) highly oscillatory stiffness; (3) stiffness matrix; and (4) numerical stiffening. Some of these terms are popular in scientific computing, while others come from mechanical engineering. A potential confusion may arise in this way, and it gets serious when more than one meaning is encountered in the context of one application. Such is the case with the simulation of deformable objects in visual computing, where all of the above appear in one way or another under one roof.

In this talk I will describe the various meanings of stiffness, how they arise in the above context and how they are related, what practical challenges they bring up, and how these challenges are handled. The concepts and their evolution will be demonstrated. It is about meshes, their resolution and spectral properties.

Convergence results for collocation methods different from the Bible

17 Jun
12:00

Peter Deuffhard
Zuse Institute Berlin

The talk presents convergence results based on a nonlinear convergence theory for collocation methods, both for boundary value problems and initial value problems. For boundary value problems, the existence of so-called "ghost solutions" arises, which are non-consistent discrete solutions. For initial value problems, the special usefulness for stiff ODEs comes up naturally in terms of the condition numbers.

Low-rank splitting integrators for stiff differential equations

17 Jun
14:30

Alexander Ostermann
University of Innsbruck

The efficient numerical integration of large-scale matrix differential equations is an important and extensively studied problem in numerical analysis. Large-scale matrix differential equations typically arise from the space discretization of semi-linear partial differential equations. Examples include evolution equations in two space dimensions and differential Lyapunov and Riccati equations. The problems are usually stiff and standard numerical methods require a large amount of computing time and memory.

In the first part of the talk we propose a numerical low-rank approximation that is based on splitting methods. In particular, we split the stiff linear part of the vector field from the non-stiff non-linear one. The linear part is integrated exactly by employing the action of the matrix exponential function. This action is approximated numerically by an interpolation at Leja points. The non-stiff non-linear part, however, is integrated by a projector-splitting method. This provides a dynamic low-rank approximation that does not suffer from possible small singular values. We carry out a rigorous stiff error analysis of the proposed method and illustrate its benefits by numerical examples.

In the second part of the talk, we propose a dynamic low-rank integrator for the Vlasov-Maxwell system. This system of partial differential equations describes a collisionless plasma interacting with an electro-magnetic field. The key idea is to constrain the dynamics of the system to a low-rank manifold by means of a projection on the tangent space. The dynamics of the system is then represented by the low-rank factors, which are determined by solving lower-dimensional partial differential equations. The divergence of the electric field resulting from Maxwell's equations, however, is not consistent with the charge density computed from the Vlasov equation. To remedy this problem we propose a correction based on Lagrange multipliers which enforces Gauss' law up to machine precision.

On the convergence in ℓ_p norms of a MoL approach based on AMF-W-methods for m -dimensional linear parabolic problems of diffusion-reaction type

17 Jun
15:15

Severiano Gonzalez-Pinto
University of La Laguna

Results of convergence in ℓ_p -norms for a MoL (Method of Lines) approach applied to m -dimensional ($m \geq 2$) linear parabolic problems of diffusion-reaction type on rectangular domains, are supplied. The space semi-discretization is based on central differences and the time integration is carried out with AMF-W-methods, which reduce the algebra computational costs to the level of one-dimensional problems on each spatial direction, in a similar way as methods of Alternating Direction Implicit-type (ADI) do.

Most of known results on convergence (PDE convergence) are restricted to the ℓ_2 -norm and currently depend on the number of spatial dimensions m . Here, we present results of convergence (PDE convergence) of order two in time (and in space) in both norms (ℓ_2 and ℓ_∞), independently of the number of space dimensions m and of the spatial grid, when time-independent boundary conditions are considered. In case of time-dependent boundary conditions, the PDE order of convergence is *almost* two in the ℓ_2 -norm when $m \geq 2$ and order one in the uniform norm for $m \geq 3$. Besides for $m = 2$, a slight modification of the AMF-W method allows to get convergence of order *almost* two in the uniform norm. Some ideas about the proofs are presented and some numerical examples to illustrate the theory are also given. This is a joint work with Ernst Hairer and Domingo Hernandez-Abreu.

[1] S. Gonzalez-Pinto, E. Hairer, D. Hernandez-Abreu, Convergence in ℓ_2 and ℓ_∞ norm of one-stage AMF-W methods for parabolic problems, submitted.

[2] W. Hundsdorfer, J.G. Verwer, Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations, Springer 2003, in Springer Series in Computational Mathematics.

[3] G. I. Marchuk, Splitting and alternating direction methods. In: Handbook of Numerical Analysis I, Eds. P.G. Ciarlet, J. L. Lions, North-Holland 1990, Amsterdam, pp. 197-462.

Tuesday, 18 June 2019

Numerical integrators for the Hamiltonian Monte Carlo method

Jesus Maria Sanz Serna
University Charles III of Madrid

18 Jun
9:15

The Hamiltonian Monte Carlo method is a widely popular technique for obtaining samples from arbitrary probability distributions. The method is based on integrating a system of Hamiltonian differential equations and its computational cost depends almost exclusively on the efficiency of the numerical integrator used to simulate the Hamiltonian dynamics. In the talk I'll describe the specific features of the required numerical integration and the construction of algorithms tailored to the task.

The Method of Reflections

Martin Gander
University of Geneva

18 Jun
10:00

The method of reflections was invented to obtain approximate solutions of the motion of more than one particle in a given environment, provided that one can represent the solution for one particle rather easily. This motivation is quite similar to the motivation of the Schwarz domain decomposition method, which was invented to prove existence and uniqueness of solutions of the Laplace equation on complicated domains, which are composed of simpler ones, for which existence and uniqueness of solutions was known. Like for Schwarz methods, there is also an alternating and a parallel method of reflections, but interestingly, the parallel method is not always convergent. I will carefully trace the historical development of the method of reflections, give several precise mathematical formulations, an equivalence result with the alternating Schwarz method for two particles, and also an analysis for a one dimensional model problem with three particles of the alternating, parallel, and a more recent averaged parallel method of reflections. This will reveal that the method of reflections for more than two particles is fundamentally different from the Schwarz method.

18 Jun
11:15

Modeling the heart function

Alfio Quarteroni
Politecnico di Milano

In this presentation I will highlight the interplay between data science and computational science to efficiently solve real life large scale problems. The leading application that I will address is the numerical simulation of the heart function. Mathematical models based on first principles allow the description of the blood motion in the human circulatory system, as well as the interaction between electrical, mechanical and fluid-dynamical processes occurring in the heart. This is a classical environment where multi-physics processes have to be addressed. Appropriate numerical strategies can be devised to allow an effective description of the fluid in large and medium size arteries, the analysis of physiological and pathological conditions, and the simulation, control and shape optimization of assisted devices or surgical prostheses. This presentation will address some of these issues and a few representative applications of clinical interest.

18 Jun
12:00

Fast and oblivious quadrature for the Schrödinger equation

Lehel Banjai
Heriot-Watt University of Edinburgh

Fast and oblivious quadrature was introduced by López-Fernández, Lubich and Schädle for convolutions with a kernel whose Laplace transform is a sectorial operator. The algorithm can compute N steps of a convolution quadrature approximation of the convolution while using only $\mathcal{O}(\log N)$ active memory and with $\mathcal{O}(N \log N)$ computational complexity. In this talk we describe how oblivious quadrature can be extended to some non-sectorial operators. In particular we present an application to a non-linear Schrödinger equation describing the suppression of quantum beating.

18 Jun
14:30

Energy-decaying Runge-Kutta methods for phase field equations

Georgios Akrivis
University of Ioannina

We use the scalar auxiliary variable formulation to construct and analyze a class of energy-decaying, extrapolated and linearized Runge-Kutta methods for the Allen-Cahn and Cahn-Hilliard phase field equations. This is a joint work with Buyang Li and Dongfang Li.

High-order stroboscopic averaging methods for highly oscillatory delay problems

18 Jun
15:15

Mari Paz Calvo
University of Valladolid

In this talk we introduce and analyze heterogeneous multiscale methods for the numerical integration of highly oscillatory systems of delay differential equations with constant delays. The methodology suggested provides algorithms of arbitrarily high order, which are based on the idea of the stroboscopic averaging method for highly oscillatory ordinary differential equations. Numerical experiments illustrating the performance of the methods are also reported. This is a joint work with Jesus Maria Sanz Serna and Beibei Zhu.

Wednesday, 19 June 2019

Crouzeix's Conjecture

19 Jun
9:15

Michael Overton

Courant Institute of Mathematical Sciences, New York University

Crouzeix's conjecture is among the most intriguing developments in matrix theory in recent years. Made in 2004 by Michel Crouzeix, it postulates that, for any polynomial p and any matrix A , $\|p(A)\| \leq 2 \max(|p(z)| : z \in W(A))$, where the norm is the 2-norm and $W(A)$ is the field of values (numerical range) of A , that is the set of points attained by v^*Av for some vector v of unit length. Crouzeix proved in 2007 that the inequality above holds if 2 is replaced by 11.08, and recently this was greatly improved by Palencia, replacing 2 by $1 + \sqrt{2}$. Furthermore, it is known that the conjecture holds in a number of special cases, including $n = 2$. We use nonsmooth optimization to investigate the conjecture numerically by locally minimizing the "Crouzeix ratio", defined as the quotient with numerator the right-hand side and denominator the left-hand side of the conjectured inequality. We also present local nonsmooth variational analysis of the Crouzeix ratio at conjectured global minimizers. All our results strongly support the truth of Crouzeix's conjecture.

This is joint work with Anne Greenbaum and Adrian Lewis.

Multigrid methods and numerical homogenization

19 Jun
10:00

Harry Yserentant

Technical University of Berlin

Numerical homogenization tries to approximate solutions of elliptic partial differential equations with strongly oscillating coefficients by the solution of localized problems over small subregions. I will present in this talk two classes of such methods that can both be analyzed by means of the now classical theory of iterative methods developed in the early nineties of the last century. One is itself a rapidly convergent iterative method and the other one is based on the construction of modified, problem adapted discrete solution spaces.

19 Jun 11:15 **Critical points of quadratic low-rank optimization problems**

Bart Vandereycken
University of Geneva

The absence of spurious local minima in certain non-convex minimization problems, e.g. in the context of recovery problems in compressed sensing, has recently triggered much interest due to its important implications on the global convergence of non-convex optimization algorithms. One example is low-rank matrix sensing under rank restricted isometry properties. It can be formulated as a minimization problem for a quadratic cost function constrained to a low-rank matrix manifold, with a positive semidefinite Hessian acting like a perturbation of identity on cones of low-rank matrices. We present an approach to show strict saddle point properties and absence of spurious local minima for such problems under improved conditions on the restricted isometry constants. This is joint work with André Uschmajew (MPI Leipzig).

19 Jun 12:00

Estimates for functions of self-adjoints operators in non euclidean norms

Cesar Palencia de Lara
University of Valladolid

Given a closed, densely defined linear operator $A : D(A) \subset X \rightarrow X$ on a Banach space X , there are natural ways to define $f(A)$ as a bounded and linear operator on X , f being a suitable holomorphic mapping on some neighbourhood of the spectrum of A . On the other hand, in case A is a normal operator on a Hilbert space, it makes sense to consider $f(A)$ even for measurable mappings on the spectrum of A .

In the talk, hybrid situations of Banach spaces X and linear operators A which admits coherent versions as non-negative, self-adjoints operators in some linked Hilbert spaces are considered. Then, the possibility of defining $f(A)$ as a bounded operator on X , for real differentiable mappings $f : [0, +\infty) \rightarrow \mathbb{C}$, is explored. Finally, some resolvent estimates in maximum-norm for the space discretizations of elliptic operators are presented.

Thursday, 20 June 2019

Leapfrog Chebyshev methods

20 Jun
9:15

Marlis Hochbruck

Karlsruhe Institute of Technology

In this talk we consider variants of the leapfrog method for second order differential equations. In numerous situations the strict CFL condition of the standard leapfrog method is the main bottleneck that thwarts its performance. Based on Chebyshev polynomials new methods have been constructed that exhibit a much weaker CFL condition than the leapfrog method.

We will analyze the stability and the long-time behavior of leapfrog-Chebyshev methods in two-step formulation. This analysis indicates that one should modify the schemes proposed in the literature in two ways to improve their qualitative behavior.

For linear problems, we propose to use special starting values required for a two-step method instead of the standard choice obtained from Taylor approximation. For semilinear problems, we propose to introduce a stabilization parameter as it has been done for Runge-Kutta-Chebyshev methods before. For the stabilized methods we prove that they guarantee stability for a large class of problems.

While these results hold for quite general polynomials, we show that the polynomials used in the stabilized leapfrog Chebyshev methods satisfy all the necessary conditions. In fact, all constants in the error analysis can be given explicitly.

The talk concludes with numerical examples illustrating our theoretical findings. This is joint work with Constantin Carle and Andreas Sturm.

Averaging techniques for Vlasov and Vlasov-Poisson equations

20 Jun
10:00

Philippe Chartier

INRIA Rennes

In this talk, I will present some recent work on the use of averaging techniques to derive asymptotic models of Vlasov and Vlasov-Poisson equations. I will in particular discuss to what extent they can help to design uniformly accurate numerical methods. This is a joint work with N. Crouseilles, M. Lemou, F. Méhats and X. Zhao.

A splitting method for partial differential equations with random parameters and random initial data

20 Jun
11:15

Tobias Jahnke

Karlsruhe Institute of Technology

Partial differential equations provide well-established models for many processes and phenomena in science and technology. In many real-life applications, however, some part of the information that is required to solve the mathematical problem is not available or cannot be measured with the desired accuracy. In this talk, we present a splitting method for time-dependent, semilinear partial differential equations with a number of random parameters and with random initial data. The main idea is to switch between two different discretizations of the stochastic variable, namely a stochastic Galerkin method on sparse grids for the linear parts of the right-hand side, and a stochastic collocation method for the nonlinear part. With this strategy each subproblem can be propagated very efficiently. The new method is computationally much cheaper than standard stochastic Galerkin methods, and numerical tests show that it outperforms standard stochastic collocation methods, too.

This is joint work with Benny Stein.

Averaged Dynamics

20 Jun
12:00

Xue-Mei Li

Imperial College of London

Perturbation and Approximation underly almost all applications of physical mathematical models. The averaging method, first introduced for approximate periodic motions, is now widely used for a large class of problems in both pure and applied mathematics. We will focus on averaged dynamics for two scale differential equations with randomness and report on new advancements in Stochastic Averaging.

The purpose of averaging is easy to describe. Suppose that we have a system of variables interacting with each other and moving at different scales of speed (of order 1 and of order $\frac{1}{\epsilon}$) with the fast variables “fast oscillatory”. Both slow and fast variables evolve in time according to some rules, for example solving a family of differential or stochastic differential equations. The aim is to determine whether the slow variables can be approximated by an autonomous systems of equations, called the effective dynamic, as ϵ is taken to 0 and the speed of the fast variables tends to infinity.

We will discuss recent work with M. Hairer on averaged dynamics with memory, tackling equations driven by fractional noise. This leads to very different behaviour from the white noise case and requires new techniques recently developed in the context of rough path theory.

Random loops

20 Jun
14:30

Martin Hairer

Imperial College of London

A “rubber band” constrained to remain on a manifold evolves by trying to shorten its length, eventually settling on a closed geodesic, or collapsing entirely. It is natural to try to consider a noisy version of such a model where each segment of the band gets pulled in random directions. Trying to build such a model turns out to be surprisingly difficult and generates a number of nice geometric insights, as well as some beautiful algebraic and analytical objects. We will survey some of the main results obtained on the way to this construction.

Friday, 21 June 2019

Searching for the most stable switching laws of linear switched systems via antinorms

21 Jun
9:15

Marino Zennaro
University of Trieste

We deal with discrete-time *linear switched systems* of the form

$$x(n+1) = A_{\sigma(n)} x(n), \quad \sigma : \mathbf{N} \longrightarrow \{1, 2, \dots, m\},$$

where $x(0) \in \mathbf{R}^k$, the matrix $A_{\sigma(n)} \in \mathbf{R}^{k \times k}$ belongs to a finite family

$$\mathcal{F} = \{A_i\}_{1 \leq i \leq m}$$

associated to the system and σ denotes the *switching law*.

It is known that the *most stable switching laws* are associated to the so-called *spectrum-minimizing products* of the family \mathcal{F} . Moreover, for a family \mathcal{F} of matrices that share an invariant cone K and is normalized (i.e., its *lower spectral radius* $\check{\rho}(\mathcal{F})$ is equal to 1), for any initial value $x(0)$ in the interior of K the *most stable trajectories* lie on the boundary of the *unit antiball* of a so-called *invariant Barabanov antinorm*. Under suitable conditions, a canonical constructive procedure for Barabanov antinorms of polytope type has been recently proposed by Guglielmi and Z. (2015).

Still for families sharing an invariant cone K , in this talk we first show how to provide lower bounds to $\check{\rho}(\mathcal{F})$ by a suitable adaptation of the Gelfand limit to the setting of antinorms, which could be of some practical interest when the above mentioned constructive procedure fails.

Then we consider a family of matrices \mathcal{F} that share an *invariant multicone* K_{mul} (see the recent papers by Brundu and Z. (2018, 2019)) and show how to generalize some of the known results on antinorms from the case of families sharing an invariant cone. These generalizations are of interest because invariant multicones may well exist when invariant cones do not.

This is a joint work with Nicola Guglielmi, Gran Sasso Science Institute.

Long time integration of stochastic differential equations: the interplay of geometric integration and stochastic integration

21 Jun
10:00

Gilles Vilmart
University of Geneva

The preservation of geometric structures, such as the symplecticity of the flow for deterministic Hamiltonian systems, often reveals essential for an accurate numerical integration, and this is the aim of geometric integration. In this talk we highlight the role that some geometric integration tools, that were originally introduced in the deterministic setting, play in the design of new accurate integrators to sample the invariant distribution of ergodic systems of stochastic ordinary and partial differential equations. In particular, we show how the ideas of modified differential equations, Butcher trees, and processing techniques permit to increase at a negligible overcost the order of accuracy of stiff integrators.

This talk is based on joint works with Assyr Abdulle (EPF Lausanne), Ibrahim Almuslimani (Univ. Geneva), Charles-Edouard Béhier (Univ. Lyon), David Cohen (Univ. Umeå), Adrien Laurent (Univ. Geneva), Gregorios A. Pavliotis (Imperial College London), Konstantinos C. Zygalakis (Univ. Edinburgh).

Exponential integrators for stochastic partial differential equations

21 Jun
11:15

David Cohen
University of Umeå

The aim of the presentation is to give a brief, and hopefully not too technical, overview on the numerical discretisation of various stochastic partial differential equations (SPDEs) by exponential-type integrators. We begin by introducing SPDEs and the main ideas behind exponential integrators. We next present recent results on the use of such numerical schemes for the time integration of stochastic wave equations, stochastic Schrödinger equations, and stochastic heat equations.

Semiclassical molecular dynamics according to the blue book

21 Jun
12:00

Caroline Lasser
Technical University of Munich

The talk aims at numerical methods for time-dependent Schrödinger equations in high dimensions with highly oscillatory solutions. We discuss established and new convergence results for Gaussian wave packet methods in various flavours.

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