Titles and Abstracts

Elena Celledoni (Norges teknisk-naturvitenskapelige universitet)

Title: An introduction to shape analysis and deep learning for optimal reparametrizations of shapes: Part I & Part II

Abstract:

Shape analysis is a mathematical approach to problems of pattern and object recognition and has developed considerably in the last decade. The use of shapes is natural in applications where it is interesting to compare curves or surfaces independently of their parametrisation. Considering a smooth setting where the parametrized curves or surfaces belong to an infinite dimensional Riemannian manifold, one defines the corresponding shapes to be equivalence classes of curves differing only by their parametrization. Under appropriate assumptions, the Riemannian metric can be used to obtain a meaningful measure of distance on the space of shapes.

One computationally efficient approach to shape analysis is based on the Square Root Velocity Transform, and we have proposed a generalisation of this approach to shapes on Lie groups and homogeneous manifolds.

A computationally demanding task for approximating shape distances is finding the optimal reparametrization. The problem can be phrased as an optimisation problem on the infinite dimensional group of orientation preserving diffeomorphisms $\mathrm{Diff}^{+}(\Omega)$, where Ω is the domain where the curves or surfaces are defined. In the case of curves, one robust approach to compute optimal reparametrizations is based on dynamic programming, but this method seems difficult to generalize to surfaces.

We consider here alternative approaches, one is based on signatures and another method is inspired by a "Riemannian" gradient descent approach obtained by representing the gradient gradE in terms of an othonormal basis of TidDiff+(Ω) and projecting gradE on a finite dimensional subspace. The approximations are obtained composing in succession a number of elementary diffeomorphism equal to the number of iterations, and optimizing on few parameters at the time. This method can be improved by optimizing simultaneously over a larger number of parameters in an approach reminiscent of deep learning.

The two lectures are built on material taken from [1-5].

References:

[1] E. Celledoni, M. Eslitzbichler, and A. Schmeding, (2016) Shape analysis on Lie groups with applications in computer animation. J. Geom. Mech.,8(3):273-304, 2016.

[2] E. Celledoni, S. Eidnes, A. Schmeding, (2018) Shape analysis on homogeneous spaces: a generalised SRVT framework. Abel Symposia. vol.13.

[3] E. Celledoni, H. Gl¨ockner, J. Riseth, A. Schmeding, (2022) Deep neural networks on diffeomorphism groups for optimal shape reparameterization, arXiv:2207.11141.

[4] E. Celledoni, P. E. Lystad, N. Tapia, (2019) Signatures in Shape analysis: An efficient approach

to motion identification. Lecture Notes in Computer Science (LNCS). vol. 11712 LNCS.
[5] J. N. Riseth, (2021) Gradient-based algorithms in shape analysis for reparametrization of parametric curves and surfaces, Feb. 2021, Master thesis, NTNU.

Elena Celledoni (Norges teknisk-naturvitenskapelige universitet)

Title: Deep learning from the point of view of numerical analysis: Part I & Part II

Abstract:

Deep learning neural networks have recently been interpreted as discretisations of an optimal control problem subject to an ordinary differential equation constraint. A large amount of progress made in deep learning has been based on heuristic explorations, but there is a growing effort to mathematically understand the structure in existing deep learning methods and to design new approaches preserving (geometric) structure in neural networks. The (discrete) optimal control point of view to neural networks offers an interpretation of deep learning from a numerical analysis perspective and opens the way to mathematical insight [1,6,7].

We discuss a number of interesting directions of current and future research in structure preserving deep learning. Some deep neural networks can be designed to have desirable properties such as invertibility and group equivariance or can be adapted to problems of manifold value data. Neural networks can be designed so to guarantee stability and contractivity and that can be used to solve inverse problems in imaging.

The two lectures are built on material taken from [1-5,8,9].

References:

[1] M. Benning, E. Celledoni, M. J. Ehrhardt, B. Owren, and C. B. Sch¨onlieb, (2019) Deep learning as optimal control problems: models and numericalmethods. Journal of Computational Dynamics, 6(2):171-198, 2019.

[2] E. Celledoni, M. J. Ehrhardt, C. Etmann, R. I. McLachlan, B. Owren, C. B. Sch¨onlieb, F. Sherry, (2021) Structure preserving deep learning. European journal of applied mathematics.

[3] E. Celledoni, M. J. Ehrhardt, C. Etmann, B. Owren, C. B. Sch¨onlieb, F. Sherry, (2021) Equivariant neural networks for inverse problems. Inverse Problems.

[4] E. Celledoni, A. Leone, D. Murari, and B. Owren, (2023) Learning Hamiltonians of constrained mechanical systems, J. Comput. Appl. Math. 417, Paper No. 114608, 12 pp.

[5] E. Celledoni, D. Murari, B. Owren, C.-B. Sch¨onlieb, and F. Sherry,(2022) Dynamical systems' based neural networks, arXiv preprint arXiv:2210.02373.

[6] W. E, (2017) A Proposal on Machine Learning via Dynamical Systems, Commun. Math. Stat. 5, 1-11.

[7] E. Haber and L. Ruthotto, (2017) Stable architectures for Deep Neural Networks , Inverse Problems 34 (1).

[8] H. Noren, S. Eidnes, E. Celledoni, (2023) Learning Dynamical Systems from Noisy Data with Inverse-Explicit Integrators, arXiv:2306.03548.

[9] F. Sherry, (2023) E. Celledoni, M. J. Ehrhardt, D. Murari, B. Owren,and C.-B. Sch¨onlieb,

Designing Stable Neural Networks using Convex Analysis and ODEs, arXiv preprint: 2306.17332.

Jing Gao (Xi'an Jiaotong University)

Title: Asymptotic computation for the multivariate highly oscillatory integral over a simplex

Abstract:

We construct the extended Filon type method for the multivariate oscillatory integral on a regular simplex. First, the multivariate Hermite and Lagrange interpolations are constructed over the simplex. Based on the multivariate interpolating configuration, the underlying extended Filon methods are presented to reduce the integration error for the whole regime of the oscillatory parameter. In particular, the exact computations of the moments are also provided. Numerical results illustrate that the error decreases with increasing oscillatory parameter and more interpolating nodes.

Chengming Huang (Huazhong University of Science and Technology)

Title: Fractional polynomial collocation for third-kind Volterra integral equations with singularities

Abstract:

In this talk, we develop a collocation method for solving third-kind Volterra integral equations. In order to achieve high order convergence for problems with nonsmooth solutions, we construct a collocation scheme on a modified graded mesh using a basis of fractional polynomials, depending on a certain parameter λ. For the proposed method, we derive an error estimate in the L^∞-norm, which shows that the optimal order of global convergence can be obtained by choosing appropriate parameter λ and modified mesh, even when the exact solution has low regularity. Numerical experiments confirm the theoretical results and illustrate the performance of the method. This talk is based on a joint work with Dr. Zheng Ma.

Lun Ji (AMSS, CAS)

Title: Low regularity time integration of NLS via discrete Bourgain spaces

Abstract:

We study a filtered Lie splitting scheme for the cubic periodic nonlinear Schrodinger equation on the torus T^d with $d\geq 1$. This scheme overcomes the standard stability restriction in Sobolev spaces $H^s(T^d)$ for which $s>\frac{d}{2}$ is required. In particular, our analysis now allows us to handle initial data in $H^s(T^d)$ for $s>\max\{\left(0,\frac{d}{2}-1\right)\}$. Moreover, we establish low regularity error estimates in discrete (in time) Bourgain spaces, and prove convergence of order $\tau^{s/2}$ in $L^2(T^d)$, where τ denotes the time step size of the scheme.

References:

[1] L. Ji, A. Ostermann, F. Rousset, K. Schratz, Low regularity error estimates for the time integration of 2D NLS, arXiv:2301.10639

[2] A. Ostermann, F. Rousset, K. Schratz, Fourier integrator for periodic NLS: low regularity estimates via Bourgain spaces, to appear in J. Eur. Math. Soc.

[3] A. Ostermann, F. Rousset, K. Schratz, Error estimates at low regularity of splitting schemes for NLS, Math. Comp. 91, 169-182 (2022).

Jian Liu (University of Science and Technology of China)

Title: Dynamics and Numerical Methods for Energetic particles in Fusion Devices

Abstract:

Various energetic particles exist in plasmas, such as runaway electrons in tokamaks, alpha particles as fusion products, and energetic electrons in earth space as the cause of aurora. However, it is hard to model and calculate the dynamics of energetic particles in plasmas due to its multi-scale and nonlinear nature. Structure-preserving algorithms are crucial to accurately simulate energetic particle dynamics in different problems. We will introduce the modeling, algorithms, and physical results of energetic particles in fusion devices. The requirement of advanced numerical methods for this topic is also discussed.

Alexander Ostermann (University of Innsbruck, Austria)

Title: Splitting methods for PDEs: analysis and applications

Abstract:

Splitting methods are a well-established tool for the numerical integration of time-dependent partial differential equations (PDEs). The basic idea behind these methods is to split the vector field into disjoint parts, integrate them separately with an appropriate time step, and combine the single flows in the right way to obtain the sought after numerical approximation. Splitting methods also play a fundamental role in dynamic low-rank integrators.

The application of splitting methods to various time-dependent PDEs will be discussed. These include reaction-diffusion equations, the Vlasov-Poisson equations (a kinetic model in plasma physics), the Korteweg-de Vries (KdV) and the Kadomtsev–Petviashvili (KP) equation. It is shown that splitting methods can have superior geometric properties (such as preservation of positivity and favourable long term behaviour) as compared to standard time integration schemes. Moreover, it is often possible to overcome a CFL condition that occurs in standard discretizations. Another benefit of splitting methods is the fact that they can be implemented by relying on existing methods and codes for simpler problems, and they often allow parallelism in a straightforward way.

Alexander Ostermann (University of Innsbruck, Austria)

Title: Boundary corrected Strang splitting

Abstract:

Strang splitting is a well-established method for the numerical integration of evolution equations. It allows parts of the vector field to be integrated using specially tailored methods and the numerical approximation to be represented as a composition of these (often simpler) flows. Such a splitting approach can lead to high computational efficiency. However, if the original problem is subject to non-periodic boundary conditions, a simple splitting of the vector field can also lead to problems:

the accuracy of the numerical solution suffers, and the observed order of convergence is reduced. The reason for this behavior is some incompatibility of the intermediate steps in the splitting with the prescribed boundary conditions. One remedy is to modify the boundary conditions for the intermediate steps to avoid these incompatibilities. However, the exact form of this modification requires careful analysis of the problem under consideration. In this talk, I will explain some strategies that have been developed in recent years to address this problem.

Alexander Ostermann (University of Innsbruck, Austria)

Title: Integration of NLS with low regularity initial data

Abstract:

Standard numerical integrators such as splitting schemes or exponential integrators suffer from order reduction when applied to semi-linear dispersive problems with non-smooth initial data. In my lecture, I will focus on the cubic nonlinear Schrödinger equation with periodic boundary conditions.

To begin, we will discuss the convergence of smooth solutions in Sobolev norms. The basic techniques for this come from the work of Lubich. To show first-order convergence for the standard Lie splitting in H^s, one needs initial data in H^{s+2}; to obtain second order for Strang splitting one needs initial data in H^{s+4}, i.e. four additional derivatives. Numerical experiments show that these regularity requirements are sharp.

To reduce these strong assumptions, new classes of integrators has been developed recently. These integrators, called low-regularity integrators, are based on the variation-of-constants formula and make use of certain resonance based approximations in Fourier space. They exhibit superior convergence rates at low regularity.

Alexander Ostermann (University of Innsbruck, Austria)

Title: Bourgain techniques for error estimates at low regularity

Abstract:

Standard numerical integrators such as splitting methods or exponential integrators suffer from order reduction when applied to semi-linear dispersive problems with non-smooth initial data. In this talk, we focus on the cubic nonlinear Schrödinger equation with periodic boundary conditions. For such problems, we present filtered integrators that exhibit superior convergence rates at low regularity. Furthermore, due to the nonexistence of suitable embedding results, the error analysis at very low regularity cannot be carried out in the usual framework of Sobolev spaces. Instead, completely new techniques are required. They are based on Bourgain's seminal work and will be sketched in the talk. Numerical examples illustrating the analytic results will be given.

Brynjulf Owren (Norges teknisk-naturvitenskapelige universitet)

Title: Nonlinear stability of numerical methods on Riemannian manifolds: Part I & Part II

Abstract:

Stability is a fundamental property of numerical methods for stiff nonlinear ordinary differential equations. It is important for controlling the growth of error in the numerical approximation and is used in combination with local error estimates to obtain bounds for the global error. Stability bounds can also in some situations be used to ensure the existence and uniqueness of a solution to the algebraic equations arising from implicit integrators.

In the literature, one can find a large variety of stability definitions for numerical integrators with various different aims. Some of them apply to linear test equations, others are of a more general nature and apply to nonlinear problems with certain prescribed properties. Most of the stability definitions found in the literature are developed for problems modelled on linear spaces. In particular, there is a well-established nonlinear stability theory, where an inner product norm is used to measure the distance between two solutions and the corresponding numerical approximations. The overall idea of B-stability is that whenever the norm of the difference between two solutions of the ODE is monotonically non-increasing, the numerical method should exhibit a similar behaviour, that is, the difference in norm between the two corresponding numerical solutions should not increase over a time step. We shall here consider systems of ODEs whose solutions evolve on a smooth manifold. We are primarily interested in numerical integrators which are intrinsic, that are not developed for a particular choice of local coordinates, or based on a specific embedding of the manifold into an ambient space. There are several such numerical methods available in the literature. In these lectures we start by giving a brief introduction to Riemannian manifolds, presenting the most important ingredients we shall use and give some basic results.

We then generalise B-stability to Riemannian manifolds, replacing the inner product norm with the Riemannian distance function. We define what we mean by a nonexpansive system on a Riemannian manifold, and we state the definition of Bstability of a general numerical method in this setting. As examples of numerical methods, we shall use geodesic versions of the implicit Euler method (GIE) and the implicit midpoint rule (GIMP). Then we prove a B-stability result for the GIE method in the case that the manifold has non-positive sectional curvature. We also demonstrate numerical experiments for a particular vector field on the two-sphere, S2, showing that neither the GIE nor the GIMP method is B-stable on this manifold which has positive sectional curvature. We briefly discuss also for this example a non-uniqueness issue with the GIE method which is different from what is known from the Euclidean setting. Finally, we present a bound for the global error of numerical methods, based on the monotonicity condition.

References:

[1] M. Arnold, E. Celledoni, E. Çokaj, B. Owren, D. Tumiotto, B-stability of numerical integrators on Riemannian manifolds, arXiv preprint arXiv:2308.08261

[2] J. C. Butcher, A stability property of implicit Runge-Kutta methods, BIT 15 (1975), 358-361.

[3] E. Celledoni, S. Eidnes, B. Owren, and T. Ringholm, Energy-preserving methods on Riemannian

manifolds, Mathematics of Computation 89 (2020), no. 322, 699-716.
[4] M. Kunzinger, H. Schichl, R. Steinbauer, and J. A. Vickers, Global Gronwall estimates for integral curves on Riemannian manifolds, Revista Matematica Complutense 19 (2006), no. 1, 133-137
[5] J. M. Lee, Introduction to Riemannian manifolds, Graduate Texts in Mathematics, vol. 176, Springer, Cham, 2018.
[6] J. W. Simpson-Porco and F. Bullo, Contraction theory on Riemannian manifolds, Systems & Control Letters 65 (2014), 74-80.

Brynjulf Owren (Norges teknisk-naturvitenskapelige universitet)

Title: An introduction to deep learning techniques via a dynamical systems approach: Part I & Part II

Abstract:

The impact of neural networks and deep learning in recent years has been profound and unprecedented. The number and variety of applications of the methods have skyrocketed over just a few years, and this technology has become an almost indispensable ingredient in a steadily increasing number of products that are important in intelligent industrial automation and in the everyday life of people. But in the wake of the vast progress in this area, several questions and concerns have been raised about the robustness, reliability, accuracy, reproducibility and feasibility of neural networks. For example, in classification problems it is well-known that small perturbations to an image can result in dramatic changes to the output with hazardous consequences for the user of the system. Similarly, if a neural network has been trained to classify objects with a given fixed orientation, it may generalize poorly when executed on objects which have been rotated compared to the training data. Such types of problems have recently been addressed successfully by using principles from numerical analysis and geometry. The first example can be studied as a problem of stability, an important insight is that a neural network can be understood and analysed by means of an associated dynamical system. The second example has been tackled by means of equivariant neural networks, where the key is to design the network in such a way that its behaviour is not influenced by certain transformations to the data. Improvements to robustness and reliability of neural networks usually come at a price, such as reduced expressivity, accuracy or efficiency. Thus, the use of advanced mathematical methods for the design and analysis of neural networks is still in its infancy.

In these lectures we shall present a class of neural network algorithms from the perspective of dynamical systems. Casting the models into the form of differential equations enables us to make use of known methodology from numerical methods for ODEs to analyse robustness properties disguised as stability of numerical schemes. Training of neural networks can be studied as optimal control problems. We shall also present ways to account for symmetries in data by means of equivariant transformations. Finally, we may consider deep neural networks as a means to approximate the solution to dynamical systems, in particular with applications to structure

preserving models.

References:

[1] M. Benning, E. Celledoni, M. J. Ehrhardt, B. Owren, and C-B Schönlieb, Deep learning as optimal control problems: models and numerical methods J. Comput. Dyn. 6 (2019), no. 2, 171-198.

[2] E. Celledoni, M. J. Ehrhardt, C. Etmann, R. I. McLachlan, B. Owren, C.-B. Schönlieb, and F. Sherry, Structure-preserving deep learning, European J. Appl. Math. 32 (2021), no. 5, 888-936.

[3] E. Celledoni, M. J. Ehrhardt, C. Etmann, B. Owren, C. B. Schönlieb, and F. Sherry, Equivariant neural networks for inverse problems, Inverse Problems, 37 (2021), no. 8, Paper No. 085006, 26

[4] E. Celledoni, A. Leone, D. Murari, and B. Owren, Learning Hamiltonians of constrained mechanical systems, J. Comput. Appl. Math. 417 (2023), Paper No. 114608, 12 pp.

[5] E. Celledoni, D. Murari, B. Owren, C.-B. Schönlieb, and Ferdia Sherry, Dynamical systems' based neural networks, arXiv preprint arXiv:2210.02373.

[6] T. Cohen, M. Geiger, and M. Weiler, A general theory of equivariant CNNs on homogeneous spaces. In: Advances in Neural Information Processing Systems 32, pp. 9145–9156 (2019)

[7] F. Sherry, E. Celledoni, M. J. Ehrhardt, D. Murari, B. Owren, and C.-B. Schönlieb, Designing Stable Neural Networks using Convex Analysis and ODEs, arXiv preprint arXiv:2306.17332.

Chunmei Su (Tsinghua University)

Title: A convexity-preserving and perimeter-decreasing parametric finite element method for the area-preserving curve shortening flow

Abstract:

We propose and analyze a semi-discrete parametric finite element scheme for solving the area-preserving curve shortening flow. The scheme is based on Dziuk's approach (SIAM J. Numer. Anal. 36(6): 1808-1830, 1999) for the anisotropic curve shortening flow. We prove that the scheme preserves two fundamental geometric structures of the flow with an initially convex curve: (i) the convexity-preserving property, and (ii) the perimeter-decreasing property. To the best of our knowledge, the convexity-preserving property of numerical schemes which approximate the flow is rigorously proved for the first time. Furthermore, the error estimate of the semi-discrete scheme is established, and numerical results are provided to demonstrate the structure-preserving properties as well as the accuracy of the scheme. This talk is based on the joint work with Wei Jiang and Ganghui Zhang.

Bin Wang (Xi'an Jiaotong University)

Title: Geometric two-scale integrators for highly oscillatory system

Abstract:

In this talk, we consider a class of highly oscillatory Hamiltonian systems which involve a scaling parameter. We apply the two-scale formulation approach to the problem and propose two new time-symmetric numerical integrators. The methods are proved to have the uniform second order accuracy at finite times and some near-conservation laws in long times. Numerical experiments illustrate the performance of the proposed methods over the existing ones.

Dongling Wang (Xiangtan University)

Title: Completely monotonicity-preserving schemes for convolutional integrals and their applications

Abstract:

The kernel function of the Riemann-Liouville integral is a completely monotonic function, so from the perspective of the structure preserving algorithm, we introduce completely monotonicity-preserving (CM-preserving) schemes. As an application, we will prove that the (CM-preserving) schemes can accurately preserving the optimal long-term algebraic decay rate of a class of power nonlinear fractional order models. Then we discuss the long-term behavior of numerical solutions for a class of nonlinear sub-diffusion models, including time fractional order porous media models and p-Laplace equations.

Wansheng Wang (Shanghai Normal University)

Title: Efficient stability-preserving numerical methods for nonlinear coercive problems in vector space

Abstract:

Strong stability (or monotonicity)-preserving time discretization schemes preserve the stability properties of the exact solution and have proved very useful in scientific and engineering computation, especially in solving hyperbolic partial differential equations. The main aim of this work is to further extend this to exponential stability-preserving numerical methods for general coercive system whose solution is exponentially growing or decaying and the rate of growth or decay can be quantified by a (\omega,\tau^\ast) function in general vector space with a convex functional. Under the same stepsize condition as for strong stability, sharper exponential stability results are derived for explicit and diagonally implicit Runge-Kutta methods and variable coefficients linear multistep methods for nonlinear problems. The new developments in this paper also include their applications to various linear and nonlinear evolution problems.

Xinyuan Wu (Nanjing University)

Title: Structure-preserving exponential-type Runge-Kutta integrators

Abstract:

This talk presents structure-preserving exponential Runge-Kutta integrators, including energy-preserving exponential Runge–Kutta integrators, simplectic exponential Runge-Kutta integrators for first-order semilinear Hamiltonian systems. This talk also concerns structure-preserving extended Runge-Kutta-Nystr¨om (ERKN) methods for second-order semilinear Hamiltonian systems, including simplectic ERKN methods and energy-preserving ERKN methods.

Ruili Zhang (Beijing Jiaotong University)

Title: Symplectic methods for the guiding center dynamics of charged particle

Abstract:

The guiding center is a potent model that is frequently used in astrophysics, space physics, fusion research, and arc plasmas to solve the multiscale dynamics of magnetized plasmas, whose canonical Hamiltonian formulation has always been pursued. In this talk, we give the non-canonical Hamiltonian form and canonical Hamiltonian form of the guiding center. For the non-canonical Hamiltonian form of guiding center, we provide a general procedure of the guiding center canonicalization. With the canonicalization schemes, the canonical symplectic simulation of guiding center dynamics is realized. Moreover, we express the dynamics of the guiding center as a constrained Hamiltonian system with two constraints, whose solution flow of the guiding center is on a canonical symplectic submanifold. In this canonical Hamiltonian form, the dynamics frame of the guiding center can be established, where traditional symplectic methods can be applied directly.

Xiaofei Zhao (Wuhan University)

Title: Numerical methods for disordered NLS

Abstract:

In this talk, I will consider the numerical solution for the disordered nonlinear Schrodinger equation (NLS). The model is a standard cubic NLS with a spatial random potential. The roughness and/or randomness of the potential brings some numerical difficulties. The performance of some classical time integrators will reviewed, and the low-regularity integrator will be applied to tackle the possible roughness. Then, a quasi-Monte Carlo time-splitting method will be considered to tackle the randomness and improve the sampling accuracy. The full error bound will be presented and numerically verified.