Special Session 80: Advances in the Numerical Solution of nonlinear evolution equations

Mechthild Thalhammer, University of Innsbruck, Austria

The intention of this special session on "Advances in the numerical solution of nonlinear evolution equations" is to gather mathematicians and theoretical physicists, interconnected through their field of application, the analytical tools, or the numerical methods used. The scope of topics includes but is not limited to Schrödinger type equations, highly oscillatory equations, parabolic problems, and adaptive integration methods for partial differential equations.

Defect and local error of exponential splitting schemes

Winfried Auzinger
Vienna University of Technology, Austria
w.auzinger@tuwien.ac.at
Othmar Koch, Mechthild Thalhammer

Linear or nonlinear evolution equations with a right-hand side split up into two parts can often be solved in an efficient way by splitting up the problem in each integration step. We discuss an approach for analyzing the error of exponential splitting schemes. The scheme is associated with an approximate flow, which can be characterized in detail. The defect of the scheme with respect to the given problem is now a well-defined quantity. The (local) order of the scheme can be characterized by the asymptotic behavior of the defect, and local defect integration is the theoretical basis for a posteriori error estimation. Several aspects of this approach are discussed. As an example, Schrödinger type equations are considered.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Some mathematical results on time-dependent density functional theory

Eric Cances
Ecole des Ponts and INRIA, France
cances@cermics.enpc.fr
Gabriel Stoltz

Time-dependent Density Functional Theory (TDDFT) is a widely used method in chemistry and materials science to model electronic excited states and non-adiabatic electron dynamics. In the case of a finite molecular system containing N electrons, TDDFT models read as coupled systems of N nonlinear Schrödinger equations. In a perfect crystal, the number of electrons is infinite, and the electronic state of the system must be described by a density matrix, that is a self-adjoint operator on L2(R3). After recalling the basics of TDDFT, I will present a TDDFT model for crystals with local defects and show how it can be used to compute the macroscopic time-dependent polarizability of a crystal.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Projected explicit Lawson methods for the integration of Schrödinger equation

Begona Cano
Universidad de Valladolid, Spain
bego@mac.uva.es

We will prove that explicit Lawson methods, when projected onto one of the invariants of nonlinear Schrödinger equation (norm) are also automatically projected onto another invariant (momentum) for many solutions. As this procedure is very cheap and geometric because two invariants are conserved, it offers an efficient tool to integrate many regular solutions of this equation till long times. Numerical comparisons with splitting methods will also be shown.

$\longrightarrow \infty \diamond \infty \longleftarrow$

A simple moving mesh method for blow-up problems

Shaohua Chen
Cape Breton University, Canada
george_chen@cbu.ca
Lauren DeDieu

We introduce a simple moving mesh method in which the mesh is generated directly from the physical domain and add higher order difference terms to make the mesh moves more smoothly and orthogonally. Then, we apply this method to heat equations with both single blow-up point and blow-up at space infinity.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Exponential integrators for nonlinear Schrödinger equations over long times

David Cohen
Karlsruhe Institute of Technology, Germany
david.cohen@unibas.ch
Ludwig Gauckler

Near-conservation over long times of the actions, of the energy, of the mass and of the momentum along the numerical solution of the cubic Schrödinger equation with small initial data is shown. Spectral discretisation in space and one-stage exponential integrators in time are used. The proofs use modulated Fourier expansions.

$\longrightarrow \infty \diamond \infty \longleftarrow$

High-order numerical methods for the stationary Gross-Pitaevskii equation

Ionut Danaila
LMRS, University of Rouen, France
ionut.danaila@univ-rouen.fr

We compute vortex states of a rotating Bose-Einstein condensate by numerically solving the stationary Gross-Pitaevskii (GP) equation in 2D and 3D. Different types of methods are used: (i) direct minimization of the GP energy functional using Newton methods or steepest descent methods based on Sobolev gradients and (ii) imaginary time propagation of the wave function. Advantages and drawbacks of each method are summarized and convergence properties are presented. We also show that a high spatial accuracy scheme is compulsory to accurately capture configurations with quantized vortices. We present numerical setups using 6th order finite difference schemes and finite elements with mesh adaptivity that were successfully used to compute a rich variety of difficult cases with quantized vortices.

⟶ ∞ ◇ ∞ ⟵

High-order accurate Runge-Kutta discontinuous Galerkin methods for a two-dimensional nonlinear Dirac model

Xia Ji
Chinese Academy of Sciences, Peoples Rep of China
jixia@lsec.cc.ac.cn

The aim of this paper is to develop high-order accurate Runge-Kutta local discontinuous Galerkin methods approximations of two dimensional nonlinear Dirac equation. The DG methods discussed here are a class of the finite element methods, which adopt completely discontinuous piecewise polynomial space for the numerical solutions and the test functions in the spatial variables, coupled with explicit and nonlinearly stable high order Runge-Kutta time discretization. The propogation of single dromion and the interaction of two dromions are studied. We also prove three continuum conservation laws of the 2D NLD model and an entropy inequality, i.e. the total charge non-increasing of the semi-discrete RKDG methods, which are demonstrated by various numerical examples.

⟶ ∞ ◇ ∞ ⟵

Efficient time integration in nonlinear acoustics

Barbara Kaltenbacher
Alps-Adriatic University of Klagenfurt, Austria
barbara.kaltenbacher@aau.at
Mechthild Thalhammer

The propagation of high intensity ultrasound as used in a large number of applications ranging from cleaning or welding to medical therapy is described by nonlinear wave equations. Among these models are the classical Westervelt and Kuznetsov equation but also more recent modified and/or generalized models. A particular challenge due to nonlinearity and the presence of different wave lengths is efficient and robust time integration. For this purpose, a promising approach are operator splitting techniques exploiting the intrinsic structure of the equations. In this talk we will discuss possible additive or exponential splitting approaches, address their convergence, and show the results of first numerical tests.

⟶ ∞ ◇ ∞ ⟵

On the causality of real-valued semigroups and diffusion

Richard Kowar
University of Innsbruck, Austria
richard.kowar@uibk.ac.at

We show that a process modeled by a strongly continuous real-valued semigroup (that has a space convolution operator as infinitesimal generator) cannot satisfy causality. We present and analyze a causal model of diffusion that satisfies the semigroup property at a discrete set of time points $M := \{\tau_m \,|\, m \in \mathbb{N}_0\}$ and that is in contrast to the classical diffusion model not smooth. More precisely, if v denotes the concentration of a substance diffusing with constant speed, then v is continuous but its time derivative is discontinuous at the discrete set M of time points. It is this property of diffusion that forbids the classical limit procedure that leads to the noncausal diffusion model in Stochastics. Furthermore, we show that diffusion with constant speed satisfies an inhomogeneous wave equation with a time dependent coefficient.

⟶ ∞ ◇ ∞ ⟵

A micro-macro parareal algorithm with application to singularly perturbed ordinary differential equations

Frederic Legoll
Ecole Nationale des Ponts et Chaussees, France
legoll@lami.enpc.fr

We introduce a parareal algorithm for the time-parallel integration of micro-macro systems. We apply this algorithm to a prototypical example of such a micro-macro model, namely singularly perturbed ordinary differential equations. The system we consider includes some fast and some slow variables, the limiting dynamics of which (in the limit of infinite time scale separation) is known. The algorithm first computes a cheap but inaccurate macroscopic solution using a coarse propagator (by only evolving the slow variables according to their limiting dynamics). This solution is iteratively corrected by using a fine-scale propagator (simulating the full microscopic dynamics on both slow and fast variables), in the parareal algorithm spirit. We provide a numerical analysis of the convergence of the algorithm, the efficiency of which is illustrated by representative numerical experiments. Joint work with T. Lelievre and G. Samaey.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Some recent mathematical contributions to multiscale modelling for polymeric fluids

Tony Lelievre
Ecole des Ponts ParisTech, France
lelievre@cermics.enpc.fr

In this talk, I will present two recent works concerning multiscale models for polymeric fluids.

First, I will present a numerical closure procedure that we recently proposed in [1] to get, from a microscopic model, a closed macroscopic model. This procedure is related to the so-called quasi-equilibrium approximation method, and can be seen as a justification of this approach.

Second, I will discuss the longtime behaviour of some models for rigid polymers (liquid crystals models). Such models are interesting since their longtime behaviour may be quite complicated, including convergence to periodic in time solutions. I will explain how such convergence can be proven using entropy techniques, see [2].

References: [1] V. Legat, T. Lelievre and G. Samaey, A numerical closure approach for kinetic models of polymeric fluids: exploring closure relations for FENE dumbbells, Computers and Fluids, 43, 119-133, (2011). [2] L. He, C. Le Bris and T. Lelievre, Periodic long-time behaviour for an approximate model of nematic polymers, http://arxiv.org/abs/1107.3592 .

$\longrightarrow \infty \diamond \infty \longleftarrow$

Optimal bilinear control of Gross-Pitaevskii equations

Daniel Marahrens
DAMTP, University of Cambridge, England
D.O.J.Marahrens@damtp.cam.ac.uk
Michael Hintermüller, Peter A. Markowich, Christof Sparber

We present a mathematical framework for optimal bilinear control of nonlinear Schrödinger equations of Gross-Pitaevskii type. We prove existence of an optimal control and derive the first-order optimality system. Finally we propose a numerical solution method based on a Newton type iteration and present numerical simulations of several coherent quantum control problems.

$\longrightarrow \infty \diamond \infty \longleftarrow$

Favourable space and time discretisations for low-dimensional nonlinear Schrödinger equations

Mechthild Thalhammer
University of Innsbruck, Austria
mechthild.thalhammer@uibk.ac.at

In this talk, I shall address the issue of efficient numerical methods for the space and time discretisation of low-dimensional nonlinear Schrödinger equations such as systems of coupled time-dependent Gross-Pitaevskii equations arising in quantum physics for the description of multi-component Bose-Einstein condensates. For the considered class of problems, a variety of contributions confirms the favourable behaviour of pseudo-spectral and higher-order exponential operator splitting methods regarding efficiency and accuracy. However, in the absence of an adaptive local error control in space and time, the reliability of the numerical solution and the performance of the space and time discretisation strongly depends on the experienced scientist selecting the space and time grid in advance, I will exemplify different approaches for the reliable time integration of Gross-Pitaevskii systems on the basis of a local error control for splitting methods. A convergence result for full discretisations by higher-order time-splitting and different pseudo-spectral methods (Fourier, Hermite, Sine) provides the theoretical basis.

$\longrightarrow \infty \diamond \infty \longleftarrow$