A Symposium on Splitting Methods for Differential Equations

Institut de Matemàtiques i Aplicacions de Castelló

Universitat Jaume I, Castelló (Spain)

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Abstracts

Fourier-Hermite methods for perturbed harmonic oscillator problems

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We consider the numerical integration of the Gross–Pitaevskii and Schrödinger equation with a potential trap given by a harmonic potential or a small perturbation to it. Splitting methods are frequently used with Fourier techniques since the system can be split into the kinetic and remaining part, and each part can be solved efficiently using Fast Fourier Transforms. To split the system into the quantum harmonic oscillator problem and the remaining part allows to get higher accuracies in many cases, but it requires to change between Hermite basis functions and the coordinate space. We show how to build new methods which combine the advantages of using Fourier methods while solving the harmonic oscillator exactly.

Splitting methods for the Schrödinger equation

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The time-dependent Schrödinger equation plays an essential role to understand non-relativistic atomic and molecular processes. This is a linear partial differential equation with a very particular structure with many preserved quantities. Geometric numerical integration has been developed during the last years leading to new numerical methods which preserve most qualitative properties of the exact solution. Some of these methods can also be applied to the Schrödinger equation. The analysis of this particular equation allows, in many cases, to build new methods tailored for different problems (depending on the dimension, the potential, the regularity, etc.), leading in many cases to improved qualitative and quantitative results. In this talk we review different families of splitting methods and present new methods which can be considered as polynomial approximations to compute the action of the exponential on a vector. We show the relation of the new splitting methods with Taylor and Chebyshev approximations. We compare their performance on some numerical examples.

This is joint work with Fernando Casas and Ander Murua.

Splitting methods with processing in path integral Monte Carlo simulations

Fernando Casas

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Processed splitting methods are particularly well adapted to carry out path integral Monte Carlo (PIMC) simulations: since one is mainly interested in estimating traces of operators, only the kernel of the method is necessary to approximate the thermal density matrix. Unfortunately, they suffer the same drawback as standard, non-processed integrators: kernels of effective order greater than two necessarily involve some negative coefficients. This problem can be circumvented, however, by incorporating modified potentials into the composition, thus rendering schemes of higher effective order. Here we analyze a family of fourth-order schemes recently proposed in the PIMC setting, paying special attention to their linear stability properties, and justify their observed behavior in practice.

Composition and splitting methods with complex times for (complex) parabolic equations

Philippe Chartier

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This is a joint work with Sergio Blanes, Fernando Casas and Ander Murua.

The instability of splitting algorithms in solving complex and non-linear equations

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Splitting algorithms, when applied to simple and linear systems, enjoyed great success in being structure preserving and stable. This is not the case when there are multiple time scales and nonlinarities. This talk will show that instabilities will arise and persist if the underlying spectrum of the system in non-analytic in the splitting component of the algorithm. Thus despite symplecticity or unitarity, the resulting algorithms may not be stable no matter how small the time step. Thus the application of splitting algorithms in these cases requires further improvements. These points will be illustrated in the use of multiple time step algorithms and in solving the nonlinear Schrödinger equation.

New strategies for multi-scale reaction wave : splitting methods coupled with space adaptative multiresolution and parareal algorithm.

Stéphane Descombes

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In this talk I will described a new strategy to solve very big systems of ODE coming from the discretization of PDE with multiple scales. We will see that it is possible to couple optimized methods and save up a lot of computations.

Splitting and composition schemes and energy preservation for separable Hamiltonians

Fasma Diele and Brigida Pace

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We consider a new class of splitting and composition schemes for the numerical integration of separable Hamiltonians. We compose, at each step, symplectic maps of a given order which depend on a parameter. The parameter is chosen in order to minimize the error in the preservation of the energy. In correspondence of parameters which nullify the error we have methods which exactly preserve the energy of the system. The proposed symmetric methods applied on several examples of non linear oscillators reveal their superiority in the preservation of the energy when compared with the optimal methods given in literature.

Backward error analysis for splitting methods applied to Hamiltonian PDEs

Erwan Faou

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Multi-product operator splitting as a general method of solving differential equations: Theory and Application

Juergen Geiser

Department of Mathematics
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This is a joint work with Siu A. Chin.

Adapting splitting methods to stellar dynamics: a wishlist

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Energy-preserving numerical integration methods

Reinout Quispel

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An exploration of exponentially transformed splitting methods for highly oscillatory wave equations

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Highly oscillatory wave equations, such as the paraxial Helmholtz equation, have been used frequently in modelling propagation of the light from the lens to the focal region. It is evident that numerical approximations of solutions of such equations contain crucial light information in focal regions even when the f-number is small. In this talk, we will present two correlated splitting schemes for fast and effective computations of highly oscillatory wave solutions. The exponentially transformation based difference schemes offer oscillation-free ways for solving oscillatory equations and are asymptotically stable.

Are exponential operator splitting methods favourable for the time integration of evolutionary problems involving critical parameters?

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In this talk, the error behaviour of exponential operator splitting methods for evolutionary problems is investigated. In particular, an exact local error representation that is suitable in the presence of critical parameters is deduced. Essential tools in the theoretical analysis including time-dependent Schrödinger equations in the semi-classical regime as well as parabolic initial-boundary value problems with high spatial gradients are an abstract formulation of differential equations on function spaces and the formal calculus of Lie-derivatives. The general mechanism is exposed for linear problems on the basis of the least technical example method, the first-order Lie–Trotter splitting. The conclusion that exponential operator splitting methods are favourable for the time-integration of linear Schrödinger equations in the semi-classical regime with Wentzel–Kramers–Brillouin initial condition under the time stepsize restriction $h = \mathcal{O}(\sqrt[p]{\varepsilon})$, where $0 < \varepsilon \ll 1$ denotes the critical parameter and p the order of the splitting method, is confirmed by a numerical example.

This is a joint work with Stéphane Descombes.

Splitting methods with complex coefficients

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We explain how the use of complex coefficients with positive real parts (instead of real coefficients) permits to derive high-order splitting methods and composition methods that overcome the classical order barrier 2 for non-reversible problems (e.g. reaction-diffusion equations). We give details on the construction of such high-order methods. In particular, using the idea of symmetry, we show how one can achieve order 6 with only $s = 6$ compositions per time step, although the minimal number of compositions for solving the order conditions up to order 6 is in fact $s = 7$. This is a joint work with François Castella, Philippe Chartier and Stéphane Descombes.