

Splitting methods and some of its applications: from Celestial Mechanics to Quantum Optimal Control

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An important number of differential equations are originated from as diverse research areas as celestial mechanics, quantum mechanics, Hybrid Monte Carlo, control, etc., and Geometric Numerical Integrators (GNIs) [6, 8] have shown to be very useful to solve them. In particular, splitting methods are frequently used as GNIs since they are easy to use and show good performance [3, 7].

To build efficient methods it is important to analyse the algebraic structure of the problem to be solved as well as the relevant contributions to the error and computational cost: the accuracy desired (in energy or in positions), the stability, the computational cost, to consider long or short time integrations, etc. We review splitting methods through applications on a set of different problems:

- Numerical integration of the Solar System backward in time: for some studies it is desired to get very high accuracy in positions over long time integrations. This is a near integrable system and a number of different classes of methods are developed for perturbed oscillating problems like symplectic exponentially fitting methods or explicit symplectic extended RKN methods. However, it is easy to show that these methods are equivalent to splitting methods [1]. The Lie algebra associated to splitting methods allow a relatively simple way to obtain the order conditions as well as to analyse which are the relevant ones that contribute to the error in positions over long time integrations, etc. [2].

- Hybrid Monte Carlo methods: it requires the numerical integration of separable classical Hamiltonian systems where relatively low accuracy suffices (but good stability is desired to allow for large time steps) being the error in energy the most relevant aspect [5].

- Quantum Mechanics: it requires in some cases the integration of PDEs from medium to high accuracy and the symplectic methods used for classical Hamiltonian systems can also be used (see [3] and references therein). Different splitting methods that preserve either unitarity or symplecticity [4] have shown to be useful.

- Quantum Optimal Control: it requires, in some cases, the numerical integration of coupled non-linear Schrödinger equations with boundary conditions. Second order splitting methods have shown to be highly efficient methods used as the basic methods at each forward and backward iteration in the solution of the boundary value problem [9]. Can we obtain more efficient splitting methods to solve these problems with respect to the convergence of the iterations, computational cost, accuracy, storage requirements, etc.?

In this talk we present a review on splitting methods mainly focusing in our recent works on splitting methods for the previous problems and we present, for the brainstorming discussion, the open problem on how to look for more efficient splitting methods in quantum optimal control.

References

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