informatics mathematics

Erwan Faou
Directeur de recherche
INRIA
Ecole Normale Supérieure de Rennes
Campus de Ker Lann
35170 Bruz
France

Rennes, December 18, 2018

Subject: Report on the Habilitation thesis *Advanced computational methodologies for evolutionary differential equations*, presented by Karolina Kropielnicka.

The manuscript presented by K. Kropielnicka summarizes and describes some of her works done since her PhD in view of obtaining the Habilitation degree. Six main results are presented in details, referring to six publications in some of the best journals in numerical analysis.

This resumé is very well written, lively and nice to read. The results presented can be divided into four main parts: Works on finite difference methods (which is one of the activities of K. Kropielnicka following her PhD thesis), results on highly oscillatory delay systems, a work on population dynamics (involving the discretization of nonlocal operators) and several works on numerical methods for quantum dynamics (in semi-classical context and/or with time dependent potentials).

The first work entitled *Implicit difference methods for parabolic FDE on cylindrical domains* deals with linear parabolic partial differential equations (PDEs) with non constant coefficients (both in time and space) and evolving on an arbitrary bounded domain. In this study, K. Kropielnicka proposes a discretization by finite differences which - to my opinion - is a field that still deserves a lot of attention as it is probably the most flexible techniques for discretizing PDEs *in general.* She proposes to use a linearly implicit scheme. In this paper, a non trivial treatment of the approximation of derivatives near the boundary is given and convergence results are given.

The second work *Efficient computation of delay differential equations with highly oscillatory terms* deals with modulated Fourier expansions of solutions to highly oscillatory delay equations. These systems are linear delay systems (*i.e.* the differential system of equation depends in a non local way on the time) forced by highly oscillatory terms depending on a single high frequency ω. For such systems, it is natural to search for an expansion of the solution as an asymptotic superposition of slowly varying profiles depending periodically of the high frequency. Such expansion is classical for systems of ordinary differential equations, but much less studied for delay equations, in particular in the context of numerical analysis.

Postponing the analysis of the third paper that I prefer to group with the fith and sixth papers, the fourth paper, *The escalator boxcar train method for a system of age-structured equations*, deals with non local differential systems typically arising in mathematical biology. The model can be seen as an infinite dimensional Lotka-Volterra system and the goal of the work is to extend a numerical method derived by biologists. The method is in essence a particle methods extended to a case where two species are nonlinearly interacting and the difficulty is thus here to approximate this nonlinear interaction in a consistent way.

E.F.

Finally, K. Kropielnicka presents three works devoted to the numerical analysis of time-dependent Schrödinger equations in different settings (semi-classical, time dependent). The first paper entitled *Effective approximation for the semiclassical Schrödinger equation* proposes a completely new type of numerical approximation. It is based on a algorithm inspired by the Zassenhaus splitting which is a representation of the exact solution (at least formally) in terms of product of exponentials, as in the famous Baker-Campbell-Hausdorff formula. However, taking into account the semi-classical structure of the problem, it turns out that this Zassenhaus splitting behaves extremely well with respect to the small semi-classical parameter (in some sense it is an asymptotic splitting). This work is extremely interesting and original. Let me mention that the problem of computing the solution of the time-dependent Schrödinger equation in the semi-classical regime is known to be very difficult and very competitive.

In the work *Magnus-Lanczos methods with simplified commutators for the Schrödinger equation with a time-dependent potential*, the case of a linear time-dependent Schrödinger equation with a time dependent potential is considered, and a method based on Magnus expansion is proposed. However, the main point is here to reduce the number of commutators in the expansion by introducing anti-commutators terms simplifying a lot the implementation from the algebraic point of view. Eventually, the same problem but in the semi-classical regime is studied in the last paper *Efficient methods for linear Schrödinger equation in the semiclassical regime with time-dependent potential*, where the combination of the previous method and the Zassenhaus splitting is studied, yielding to new efficient integrators.

The collection of works presented by K. Kropielnicka constitutes an original and high level collection of achievements in the research fields of applied mathematics and numerical analysis. Some of these realizations are published in the highest level journals in numerical analysis, and constitute major developments in highly competitive domains. Moreover, these results are sources of many projects presented by K. Kropielnicka in the last part of her manuscript, evidencing the scientific interests of her work and the high potential of her mathematical activity. For these reasons, there is no doubt that K. Kropielnicka possesses the capacity of conducting research at a high international level, and I recommend her without hesitation for the Habilitation degree.

(E. Faou)