Computing the Schrödinger equation with no fear of commutators

Arieh Iserles a.iserles@damtp.cam.ac.uk
University of Cambridge, UK
Coauthors: Philipp Bader (Valencia) and Karolina Kropielnicka (Cambridge & Gdańsk)

Abstract

The discretization of a linear Schrödinger equation is difficult due to the presence of a small parameter which induces high oscillations. A standard approach consists of a spectral semidiscretization, followed by an exponential splitting. This, however, is sub-optimal, because the exceedingly high precision in space discretization is marred by low order of the time solver. It turns out, however, that once we employ spectral collocation in place of a conventional spectral method, the size of nested commutators becomes small, and this allows to boost significantly the order of space discretization.

In this talk we consider formally objects in the free Lie algebra spanned by the Laplacian and by a multiplication by the potential. We demonstrate that only a very small proportion of commutators survives once the exponential is split by using a symmetric version of the Zassenhaus splitting. Since the size of these commutators remains small once derivatives are appropriately replaced with spectral collocation derivative matrices, this approach, in tandem with Krylov subspace techniques for rapid computation of a matrix exponential, results in an affordable and precise discretization of the linear Schrödinger equation.

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