The joy and pain of skew symmetry

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Skew symmetry is good for you! More specifically, once a derivative is discretised with a skew-symmetric matrix, a numerical PDE scheme displays a range of favourable features: it is stable and various structural features of the original equation are preserved.

It is easy to design skew-symmetric differentiation matrices in tandem with periodic boundary conditions, e.g. using spectral collocation, and the first part of the talk will be devoted to a detailed study of the discretisation of the semiclassical Schrödinger equation using asymptotic splittings. Our main tools are a free Lie algebra of operators, palindromic Zassenhaus splitting and the symmetric BCH formula.

In the second part of the talk we consider Dirichlet boundary conditions, and this is the instant the pain kicks in. Using finite differences on a uniform grid, the highest order of a skew-symmetric differentiation matrix is just two! We will derive detailed necessary conditions for a non-uniform grid so that a skew-symmetric differentiation matrix of given order exists and prove that they can be always realised by a banded matrix. We will also discuss the state of the art in the construction and properties of such matrices.