Introduction

Many physical problems can be formulated in terms of linear or nonlinear partial differential equations. As the analytical solution is usually unknown in the case of a realistic modelling of complex engineering applications, numerical methods are indispensable.

There exist various approaches to solve partial differential equations numerically. Depending on the type of the equation, the dimension of the problem, the complexity of its boundary conditions, and the smoothness of its solution, it may be advantageous to use either finite differences or weighted residual methods (e.g., spectral and pseudospectral methods, wavelets, discontinuous Galerkin methods, finite elements, finite volumes). Finite volume schemes are well suited to discretize conservation laws, e.g., in aerodynamics, because they inherently provide flux conservation even on arbitrary meshes. Finite elements are widely employed in mechanical engineering because of their ability to resolve complex-shaped structures with a relatively high accuracy. The more general discontinuous Galerkin method allows for discontinuities between the discretization elements. The adaptive multiresolution potential of wavelet schemes is particularly advantageous if the qualitative structure of the solution varies strongly in the considered domain, e.g., if it has one or a few isolated sharp spikes or shock waves and a relatively smooth shape elsewhere.

For problems with simple geometries and globally smooth solutions, (pseudo-)spectral and finite difference methods are very efficient. Spectral and pseudospectral methods offer an excellent convergence, but are computationally not very fast due to their global stencil. In contrast, finite difference methods have a fixed stencil width that makes them computationally fast, but also limits their order of convergence with respect to the grid spacing τ.

In this work, it is shown that the computational speed of finite differences can be combined with the excellent accuracy of spectral methods, resulting in *quasi-spectral finite differences*. The corresponding finite difference weights are derived either by spectral interpolation or weighted least-squares optimization, with the *relative frequency window width* $\vartheta \in (0,1)$. In the case of spectral interpolation, it is required that for certain a-priori chosen discrete frequencies $\phi_l \in [-\vartheta\pi, \vartheta\pi]$, the finite differentiation of harmonic functions $e^{i\phi_l t/\tau}$ is exact. In the case of weighted least-squares optimization, the finite differentiation error for harmonic functions $e^{i\varphi t/\tau}$ is minimized with respect to some scalar-product induced norm representing an integral or a discrete sum over frequencies $\varphi \in [-\vartheta\pi, \vartheta\pi]$. One of the theoretical results of this work states that for each weighted least-squares problem there exists a *unique* equivalent spectral interpolation problem with interpolation frequencies $\phi_l \in [-\vartheta\pi, \vartheta\pi]$. Important tools for this proof are newly discovered Haar systems from combinations of algebraic and trigonometric monomials.

As expected from their construction, these quasi-spectral finite difference formulae possess a relatively uniform accuracy when applied to harmonic functions $e^{i\varphi t/\tau}$ with normalized angular frequencies $\varphi \in [-\vartheta\pi, \vartheta\pi]$. In contrast, standard Taylor-optimized finite differences, based on exactness for algebraic monomials up to the highest possible degree, have the maximal possible order of consistency in the low-frequency limit $\varphi \to 0$, but a strongly increasing error for higher frequencies. Thus, for solutions having a wide rectangular-shaped spectrum of relevant frequencies, the quasi-spectral finite differences can be substantially more accurate. For the first time, it is proven that the optimal order of consistency of the Taylor approach can also be achieved by such quasi-spectral finite differences if the relative frequency window width ϑ is chosen sufficiently small in comparison to the grid spacing τ.

Important technical examples for functions with rectangular-shaped frequency spectra are *wavelength division multiplexing* (WDM) signals. These are superpositions of a number of different carrier frequencies (wavelength channels), each modulated by an envelope carrying information to be transmitted to the receiver. As this modulation technique is predestinated for a very efficient utilization of the huge bandwidth of optical fibers, it is the preferred format for metropolitan, long-haul and intercontinental optical fiber networks, which are indispensable to cover the rapid growth of the internet data traffic. For the optimization of the network parameters, extensive numerical simulations are required.

The propagation of the signals in optical fibers can be modeled by the one-dimensional *nonlinear Schrödinger equation* (NLSE). Compared to most other applications for this equation, e.g., quantum mechanics and plasma physics, the time and space variables are interchanged. Hence, the corresponding initial value problem has boundary conditions at time points (in a retarded Galilei-transformed time frame moving with group velocity) and is integrated in space along the fiber. Important analytical solutions are the so-called *solitons*. They have a spatially periodic shape and are often used to compare the accuracy of different numerical solvers for the NLSE.

For the propagation of WDM signals over long-haul distances of hundreds to thousands of kilometers, the computation times are tremendous and therefore critical. Thus, the improved efficiency from the proposed quasi-spectral finite difference methods is not only convenient but also necessary to allow for a more economic optimization of fiber-optic system parameters.

This work is organized as follows: Chap. 1 gives an overview of previously published work on quasi-spectral finite differences and solvers for the nonlinear Schrödinger equation and highlights the main achievements of the present work. A detailed derivation of the nonlinear Schrödinger equation from Maxwell's equations is presented in Chap. 2, including a short presentation of low-order soliton solutions. In Chap. 3, the consistency of quasi-spectral finite difference formulae is proven and compared to the standard Taylor approach. Furthermore, it is shown that, for each weighted least-squares problem, there exists a *unique* equivalent spectral interpolation problem. This is proven employing Haar systems from combinations of algebraic and trigonometric monomials, which cannot be found yet in the literature to the best of the author's knowledge. A key tool is a certain lemma on the arccos function. After applying the finite differences for the temporal differentiation, numerical methods for the spatial integration of the resulting semidiscrete nonlinear system are presented and analyzed in Chap. 4. The efficiency of the new methods for the propagation of solitons and practically relevant WDM signals is demonstrated in Chap. 5. A brief summary and outlook conclude the main part of the work. Appendix A gives a short introduction to (weighted) least-squares approximations and Haar systems. Appendix B summarizes the frequently employed Fourier transform equivalences. Alternative semidiscretization techniques are presented in Appendix C. Appendix D states some well-known and repeatedly applied theorems.