Chapter 1

Introduction

This thesis contains most — though not all — scientific findings during my doctoral position at the institute of *Computational Mathematics* at the *Technische Universität Braunschweig* starting in April 2016. Its focus lies on the numerical treatment of hyperbolic conservation laws (CLs). Among all partial differential equations (PDEs), CLs are a particularly important, yet challenging subclass. Their importance results from the fact that they can be used to model many phenomena in the natural and engineering sciences. In fact, CLs in the form of the Euler equations were among the first PDEs to be written down [Eul57]. Since then, they have had broad application in physics as well as in other fields, such as chemistry, biology, geology, and engineering. Their challenging nature, on the other hand, stems from the well-known observation that solutions of CLs can develop spontaneous shock discontinuities, even in finite time and for smooth initial states. This observation was first made by Riemann in his ground breaking work on the propagation of waves of finite amplitude in air [Rie60]. As a consequence, the numerical treatment of CLs involves many different fields from mathematics as well as physics, which can all be quite challenging themselves. At the same time, the study of CLs has therefore always yielded new and fruitful connections between originally separated scientific fields. Most notable for this thesis are the many synergies between the numerical treatment of CLs and the field of image processing, where the treatment of image edges closely resembles (shock) discontinuities in the context of CLs. Here, we ourselves, will adapt certain objects from image processing (so-called edge sensors) to develop novel shock capturing procedures for the numerical treatment of CLs. Including these novel procedures, the contributions of this thesis can be roughly divided up into three parts:

1. Construction and investigation of stable high order quadrature rules (QRs) for the numerical integration of experimental data.
2. Development of conservative and (energy/entropy) stable high order methods for CLs.
3. Design and analysis of shock capturing procedures to stabilize high order methods for CLs in the presence of shock discontinuities.

A complete list of all publications related to this thesis can be found at the end of this chapter. In what follows, we shortly outline these contributions and their role in the current state of science, while providing an overview for the subsequent material of this thesis.

Fundamentals

The fundamentals regarding CLs as well as numerical preliminaries needed for their numerical treatment can be found in chapters 2 and 3. Readers which are already familiar with numerical methods for hyperbolic CLs and the related fields of numerical analysis, e. g., orthogonal polynomials and numerical integration, should be able to skip these two chapters.

Numerical integration of experimental data

The first novel contribution of this thesis can be found in chapters 4 and 5. In these chapters, we investigate and develop new stable high order QRs for the numerical integration of experimental data. The problem of measuring areas and volumes has always been present in everyday life. Thus, one can argue that numerical integration is as old as mathematics itself and dates back at least to the ancient Babylonians and Egyptians [BM11, Son16]. Since then, the mathematical field of numerical integration has matured considerably. Today, numerical integration describes the problem of recovering a continuous integral over a function f by using only a finite number of function evaluations $f(x_n)$, $n = 1, \dots, N$. At least in one dimension — as considered here — there exist many excellent QRs by now, e. g., Gaussian QRs. So one might ask, what there is left for us to do in this thesis. However, it should be stressed that most of these QRs, especially the highly efficient ones, assume very specific distributions for the quadrature points x_n. Yet, experimental measurements are often performed at equidistant or even scattered points. In many applications, it is therefore impractical — if not even impossible — to obtain data to fit known QRs. In this thesis, we tackle this problem by investigating and further developing a class of QRs first proposed by Wilson [Wil70b, Wil70a] in 1970. The idea behind this approach is to formulate the well-known exactness conditions as an underdetermined least squares (LS) problem. Then, the remaining degrees of freedom can be used to also ensure stability of the QR. In principle, this approach is independent of the distribution of the quadrature points x_n and can therefore be used to construct stable high order QRs for experimental data. So far, stability of the resulting QRs has been proven by Wilson for the simple case of an unweighted integral $\int f(x) \, \mathrm{d}x$. In Chapter 4, we extend this result to weighted integrals $\int f(x)\omega(x) \, \mathrm{d}x$ including a positive weight function ω. This result can also be found in the publication [Gla19a] which resulted from this thesis. An extension to general weight functions is provided in Chapter 5. In the process of developing stable high order QRs for this case, we also discuss different stability concepts which arise when considering general weight functions. To the best of our knowledge, some of these concepts (e. g. sign-consistency) have not been considered before. Hence, the findings of Chapter 5 resulted in the publication [Gla19d]. Besides yielding to new insight regarding the stability of QRs (possibly including nonpositive weight functions), the resulting stable high order QRs are used in the subsequent chapters (and [GÖ20]) to construct stable high order methods for numerically solving CLs.

Stable high order methods for hyperbolic conservation laws

Actual numerical methods for hyperbolic CLs $\partial_t u + \partial_x f(u) = 0$ are first addressed Chapter 6. There, we present two state-of-the-art high order methods, namely the discontinuous Galerkin (DG) and the flux reconstruction (FR) method. While the DG method is derived from a weak (integral) form of the underlying CL, the FR method directly emerges from the differential form of the CL. Yet, both schemes essentially build up on a piecewise polynomial approximation of the solution u in space and can be classified as discontinuous spectral element (SE) methods. It should be stressed that in both schemes, the piecewise polynomial approximations are usually obtained by polynomial interpolation on Gauss–Legendre (GLe) or Gauss-Lobatto (GLo) points. In Chapter 7, we discuss two high order methods which, to the best of our knowledge, have not been proposed before.

The first method, presented in Chapter 7.1, builds up on the usual DG method but extends its stable discretization from GLe and GLo points to equidistant and even scattered points. The basic idea in our construction of this method is to replace usual interpolation polynomials by more general discrete least squares (DLS) approximations (resulting from orthogonal projections with respect to a discrete inner product). Moreover, the corresponding discrete inner product as well as the QR used to replace exact integrals occurring in the weak form of the CL are derived from the LS-QRs developed in the previous Chapter 4. The material presented in Chapter 7.1 resulted in the publication [GÖ20].

In Chapter 7.2, we start by investigating so-called radial basis function (RBF) methods. These methods use a global approximation of the solution u by RBFs and can therefore be classified as spectral methods. RBFs have become a powerful tool in multivariate interpolation and approximation theory since they are easy to implement, allow arbitrary scattered data, and can be spectrally accurate. As a consequence they are also often used to numerically solve PDEs. Unfortunately, Platte and Driscoll [PD06] have demonstrated that their application to CLs can yield unstable schemes in the presence of boundary conditions (BCs). Here, we show that this only holds true if RBFs are applied too naively to CLs. By carefully investigating their stability properties, we are able to develop new conservative and stable RBF methods for CLs by constructing them from a weak integral form of the CL and incorporating BCs via numerical fluxes. The material presented in this chapter resulted the publication [GG19b].

Shock capturing procedures

Probably the most outstanding challenge for numerically solving CLs lies in the famous Gibbs–Wilbraham phenomenon [HH79, Ric91, GS97]. This phenomenon was first discovered by Wilbraham [Wil48] in 1848 and rediscovered by Gibbs [Gib98, Gib99] in 1899 and essentially describes the inability of high order (polynomial) approximations to represent discontinuous functions, due to spurious oscillations around the discontinuities. In the context of high order methods for CLs, these spurious oscillations arise in the presence of shock discontinuities and often yield the numerical method to break down. As a consequence, many researchers have proposed different techniques to 'smooth out' these oscillations and to stabilize high oder numerical methods in the presence of shock discontinuities. In chapters 8, 9, and 10 we investigate and propose three different shock capturing procedures to do so for (discontinuous) SE methods. Furthermore, in Chapter 11 we build up on some of our findings and develop new promising artificial viscosity (AV) operators to stabilize (modern) finite difference (FD) methods.

We start our investigation of shock capturing methods for SE methods in Chapter 8 by revisiting the well-known AV method. This method has first been proposed in the context of classical FD schemes by von Neumann and Richtmyer [vNR50] during the *Manhattan project* at *Los Alamos National Laboratory* during the 1940's. It utilizes the well-known effect of dissipative mechanisms on (shock) discontinuities; when viscosity is incorporated, discontinuities in the solution are smeared out, yielding surfaces of discontinuities to be replaced by thin layers in which the solution varies (possibly rapidly but) continuously. Since then, AV methods have been adapted and refined by many researchers, especially in the context of discontinuous Galerkin spectral element methods (DGSEMs). In Chapter 8, we revisit the most commonly used variants of the AV method in DG methods [PP06, KWH11]. We also provide an investigation with respect to conservation and entropy stability which allows us to formulate clear criteria for the AV method which have to be satisfied in order for the AV method to preserve certain physical properties of the underlying CL. This material, presented in Chapter 8.3, resulted in the publication [GNJA$^+$19]. Moreover, we address a strong connection to the technique of modal filtering as well as the discretization of AV methods by so-called summation by parts (SBP) operators. SBP operators allow to mimic integration by parts on a discrete level and can therefore be used to preserve many properties of the exact solution also for the (discrete) numerical solution. Even though they are an active field of research in the FD community since the work [KS77] of Kreiss and Scherer in 1977, their application to SE methods has only been initiated in 2013 by Gassner [Gas13]. In Chapter 8.6, we show how these can be utilized to construct conservative and stable discretizations of the AV method for SE methods. This analysis resulted in the publication [RGÖS18]. Additional publication which are connected to the material presented in Chapter 8 are [GÖRS16, GÖS18, ÖGR18, ÖGR19].

In Chapter 9, we then propose a new type of shock capturing in SE methods by ℓ^1 regularization. In many application, the solutions u of CLs might be discontinuous, but still piecewise smooth. In one dimension, this means that the exact solution only contains a finite number of jump discontinuities which are connected by smooth profiles. Thus, considering the jump function $[u]$ of the solution, $[u](x) \neq 0$ only holds for this finite set of jump discontinuities and $[u]$ is said to be sparse. Our idea in this chapter is to mimic this behavior of the exact solution also for the numerical solution. This is achieved by first approximating $[u]$ by certain high order edge sensors (HOES), originally proposed in the field of image processing [AGY05], and to enhance sparsity in this approximation by applying ℓ^1 regularization. It is shown in Chapter 9 that this technique, in fact, can enhance usual DG methods. It should be noted that similar investigations have been performed in [SGP17b] and [GHL19]. Yet, this thesis and the related publication [GG19a] are the first works to develop this idea in the context of SE methods. Here, we demonstrate that these methods allow some distinct advantages, such as element-to-element variations in the corresponding ℓ^1 optimization problem, yielding increased efficiency and accuracy of the method.

Another new type of shock capturing in SE methods is proposed and carefully investigated in Chapter 10. This time, the procedure is derived from some classical results in approximation theory and consists of going over from the original (polluted) approximation of u to a convex combination of the original approximation and its so-called Bernstein reconstruction. Our idea builds up on classical Bernstein operators — first introduced by Bernstein [Ber12a] in 1912 to provide a constructive proof of the famous Weierstrass approximation theorem [Wei85] — and we are able to prove that the resulting procedure is total variation diminishing (TVD) and preserves monotone (shock) profiles. Furthermore, the procedure can be modified to not just preserve but also to enforce certain bounds for the solution, such as positivity. Numerical tests demonstrate that the proposed shock capturing procedure is able to stabilize and enhance SE approximations in the presence of shocks. To the best of our knowledge, a similar approach has not been proposed before and the material presented in Chapter 10 resulted in the publication [Gla19c].

Finally, in Chapter 11, we come back to AV methods, this time in the context of modern high order FD methods though. Usual AV methods for FD methods essentially distribute viscosity equally over the whole computational domain [MSN04] or element — if a multi element/block structure is used. Here, we adapt the HOES introduced in Chapter 9 for ℓ^1 regularization and use them to construct novel AV operators which adapt themselves to the smoothness of the numerical solution. In particular, the resulting AV operators are able to calibrate the amount of viscosity and its distribution to the location of possible (shock) discontinuities. Moreover, we discuss their discretization by SBP operators. As a result, these operators are shown to preserve conservation, stability, and accuracy (in smooth regions) of the underlying method. The material presented in this final chapter resulted in the publication [Gla19b].

List of related publications

1. J. Glaubitz:
   High order edge sensor steered artificial viscosity operators.
   Submitted, 2019.