REGULARIZATION OF SINGULAR SOURCES FOR PSIC COMPUTATIONS OF PARTICLE-LADEN FLOWS WITH SHOCKS

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Approval of the Review Committee

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Abstract

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by

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In this dissertation we develop a high-order regularization technique with optimal scaling to approximate singular sources expressed as one single Dirac-delta or weighted summation of Dirac-deltas. We consider the numerical solution of hyperbolic conservation laws arising in the simulation of shocked particle-laden flows with the particle-source-in-cell (PSIC) method. In one dimension, the regularization technique is based on a class of compactly-supported piecewise polynomials plus an optimal scaling of the width of the support. We show that the regularization approximates the singular source with the desired order of accuracy and smoothness (number of continuous derivatives). We establish a theoretical criterion to choose an optimal scaling in the regularization that leads to formal order of convergence of the numerical scheme, away from the singularities, in the solution of the hyperbolic conservation laws. We validate our criterion by solving a linear and a nonlinear (Burgers) scalar hyperbolic conservation law with a singular source, as well as the nonlinear Euler equations with singular sources, a system of hyperbolic conservation laws governing compressible fluid dynamics with shocks and particles. A Chebyshev collocation method (spectral) discretizes the spatial derivatives in the scalar equation tests. A multidomain high-order resolution hybrid spectral-WENO method discretizes the Euler equations. In the future, we aim to enhance the accuracy of the PSIC method by using the proposed regularization technique with optimal scaling.
Dedication

I dedicate this dissertation to my parents, Alix Solano and Henry Suarez, and wife, Lorenna Perez.
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List of Acronyms

CFL Courant–Friedrich–Lewy
ENO Essentially Non-Oscillatory
MR Multiresolution
ODE(s) Ordinary Differential Equation(s)
PDE(s) Partial Differential Equation(s)
PSIC Particle-Source-In-Cell
SIAC Smoothness-Increasing Accuracy-Conserving
TVD Total Variation Diminishing
WENO Weighted Essentially Non-Oscillatory
Chapter 1

Introduction

This dissertation focuses on the high-order approximation of solutions of hyperbolic conservation laws with singular sources, arising in the simulation of shocked particle-laden flows with the particle-source-in-cell (PSIC) method [29].

The full analysis of fluid particle interaction at high speeds involve the computation of the complete flow over each particle, the tracking of individual solid or liquid complex particle boundaries along their paths, and the tracking of shock waves in the moving frame. These individual computational components are difficult to resolve and are currently barely within reach, even with the latest advances of computational technologies. The combined interaction between flows with shocks and particles has an immense complexity, scale range and size, that can currently potentially be analyzed only in highly idealized situations with a few particles. Therefore, simplified models for the particle and the particle interactions with the shock containing carrier flow are required to handle more realistic applications of shocked particle-laden flows.

The PSIC method facilitates affordable computations of real geometries, while accurately representing individual particle dynamics. It is a particle-mesh type algorithm where the continuum model is approximated on a static mesh, while the particle dynamics are traced along their path in a Lagrangian frame. The static mesh solution and the dynamic particle-mesh solution are subsequently coupled through interpolation.

In the PSIC model for simulation of particle-laden flows with shocks, the carrier flow is governed by a system of hyperbolic conservation laws with singular sources,
whereas kinematic equations govern the particle motion. The singular source, expressed as weighted summation of Dirac-deltas, represents the effect of the particles on the carrier flow.

One of the difficulties to achieve high-order of accuracy in the PSIC simulation is the singularity of the source term. The presence of the Dirac-delta can disrupt the convergence rate of the numerical schemes. Indeed, recent work has shown that a nonstationary singular source term can induce nonphysical oscillations in the numerical solution of a one-dimensional linear advection equation with high-order methods [31, 32]. For a nonstationary singular source that is moving in time, one has to consider the effect of the movement of the singular source between discrete grid points on the solution. As the singular source moves from one grid point toward the other at certain velocity, the location of the singularity is mostly between two discrete grid points at a given time. Under this situation, the singular source function cannot be represented accurately, resulting in numerical oscillations.

In numerical implementations, singular sources are approximated most commonly by low-order interpolants, i.e., top-hat or piecewise linear functions. Their lack of smoothness results in instability and Gibbs type phenomena that affect accuracy and introduce noise in the source term. Many of these undesirable effects can be reduced by using high-order interpolants.

A promising candidate for the higher-order approximation of singular source term is proposed by Tornberg [55]. She suggest a regularization technique based on a class of high-order, compactly-supported piecewise polynomials. The regularization technique provides a high-order approximation to the Dirac-delta whose overall accuracy is controlled by the number of vanishing moments and continuous derivatives (smoothness).

Typically, regularization techniques are based on the replacement of the Dirac-delta with a smooth function in a small regularization zone around the singularities. While this strategy introduces errors in the regularization zone, outside the regularization zone it can be expected that the accuracy of the numerical scheme, the smoothness of
the regularization, and the size of the regularization zone, determine the accuracy of
the solution.

An outstanding issue in the high-order regularization of the Dirac-delta is the size
of the regularization zone. Ideally, it should be:

- Wide enough to ensure that the respective approximation is sufficiently cap-
tured by the spatial grid.

- As narrow as possible to correctly approximate the singular nature of the source.

On uniform grids, it has been shown that the optimal scaling (size of the regulariza-
tion zone) should be proportional to the grid spacing $15$. However, on non-uniform
unstructured grids this has not been fully established.

The PSIC method, in addition to the source singularity, needs to capture the fine
scale and delicate structures of the physical phenomena such as shock interaction
with vortices or acoustic waves. If both complicated smooth structure and shocks are
present in the carrier flow, then there are good arguments to support the development
of high-order resolution schemes over lower order methods, which are usually sta-
ble, but contain large numerical diffusion which smears out the shock profile. Such
high-order accurate methods include spectral methods $34$ and the weighted essen-
tially non-oscillatory (WENO) scheme $49$. Spectral methods are non-dispersive,
non-dissipative and therefore, well fitted to resolve the flow in non-shocked regions.
The WENO scheme is a successful high-order resolution method used to capture
large gradients and shocks. Not only they are better at propagating waves over long
distance and time, but they do so with dramatically reduced resources, for exam-
ple, a coarser grid and increased efficiency. For a given accuracy, high-order methods
thus allow for faster prototyping of an engineering design of a shocked particle-laden
system.

This chapter presents the general and specific objectives, the contributions and
organization of the dissertation.
The chapter is divided in three sections. In Section 1.1, we formulate the objectives of the dissertation. In Section 1.2, we state the research contributions. In Section 1.3, the structure and content of the manuscript is presented.

1.1 Objectives

We seek to improve the accuracy of the PSIC method based on a high-order resolution multidomain hybrid spectral-WENO scheme, by introducing a high-order regularization technique with optimal scaling to approximate the singular Dirac-delta in source term on general grids. We will focus in the following tasks:

1. Numerical solution of one-dimensional linear and nonlinear hyperbolic conservation laws.
   a) Single particle case (one Dirac-delta in the source term).
      • Development of a theoretical background for regularization techniques in the approximation of the Dirac-delta.
         – Establishment of theoretical criteria to construct high-order accurate approximations with optimal scaling.
         – Assessment of high-order regularization techniques in the numerical solution for scalar problems and system of equations.
   b) Multiple particles case (weighted summation of Dirac-deltas).
      • Assessment of high-order regularization techniques in capturing particle interfaces and particle clustering.
         – Testing and validation of the high-order regularization techniques in the numerical solution of scalar problems.

2. Verification of accuracy of the spectral method for the scalar problems, and the high-order resolution PSIC algorithm for nonlinear systems.
1.2 Contributions

The main contribution of this dissertation is the development of a theoretical criterion to estimate the optimal scaling parameter for a high-order regularization technique based on a class of compactly supported polynomials in the approximation of the singular Dirac-delta. Specifically, the high-order regularization with optimal scaling

- leads to high-order of accuracy away from the singularity in the numerical solution of hyperbolic conservation laws with the singular Dirac-delta and the weighted summation of Dirac-deltas in the source term;
- provides a consistent and accurate representation of the Dirac-delta on general grids;
- provides a high-order of accurate representation of Lebesgue integrable functions (at smooth parts) through the operation of convolution;
- allows the use of the high-order, non-dispersive and non-dissipative spectral method to compute smooth solutions; and
- makes feasible the development of the PSIC multidomain high-order resolution hybrid spectral-WENO scheme for particle-laden flow with shocks, ensuring a consistent and stable coupling between the Eulerian and Lagragian frame in the PSIC model.

1.3 Outline

The dissertation is organized into five chapters. Chapters 1 to 4 start with an introduction to the topic in question, detailing the respective content and structure in the last two paragraphs.
Chapter 1 presents the motivation, objectives and contributions of the dissertation in the context of simulation of particle-laden flows with shocks with the PSIC method; concretely, in the numerical solution of hyperbolic conservation laws with the Dirac-delta in the source term.

Chapter 2 highlights some of the major developments in shock-capturing schemes for hyperbolic conservation laws, with special emphasis on a high-order multidomain resolution hybrid spectral-WENO scheme.

Chapter 3 contains the main contribution of the dissertation, i.e., a high-order regularization technique with optimal scaling to approximate the Dirac-delta on general grids. It provides the mathematical framework necessary to define the Dirac-delta and its basic properties, and to develop high-order accurate and consistent approximations. Specifically, the high-order regularization and optimal scaling to approximate the Dirac-delta (weighted summation of Dirac-deltas) are presented in Theorem 8 and Proposition 1 (Theorem 11 and Proposition 3), respectively.

Chapter 4 presents a numerical evaluation of the high-order regularization technique with optimal scaling, in the solution of hyperbolic conservation laws with Dirac-delta sources.

Chapter 5 summarizes the results and conclusions of the numerical experiments, and provides the scope for future work.
Chapter 2

Numerical Methods for Hyperbolic Conservation Laws

The general form of a $d$-dimensional system of hyperbolic conservation laws is

$$\frac{\partial}{\partial t} Q(x, t) + \sum_{i=1}^{d} \frac{\partial}{\partial x_i} F_i(Q) = S(Q, x, t), \quad (2.1)$$

where $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$, $Q : \mathbb{R}^d \times (0, \infty) \rightarrow \mathbb{R}^q$ represents the $q \in \mathbb{N}$ conserved quantities, $F_i : \mathbb{R}^q \rightarrow \mathbb{R}^q$ is the flux function and the respective Jacobian matrix has $q$ real and distinct eigenvalues (hyperbolicity condition), and $S : \mathbb{R}^{q+d} \times [0, \infty) \rightarrow \mathbb{R}^q$ is the source term.

In many physical systems, the system of partial differential equations (PDEs) in (2.1) describes some of the fundamental conservation laws of certain basic quantities such as mass, momentum, and energy \[2, 14, 29, 36\].

A classical solution of (2.1) is a $C^1 (\mathbb{R}^d \times (0, \infty))$ function $Q$ that satisfies the respective PDE. The main difficulty in solving this problem is the development of discontinuities (shocks) in $Q$ beyond some finite time interval, even when the initial condition, the fluxes, and the source term, are very smooth functions. The shock formation is due to the nonlinearity in the flux function and the absence of dissipation terms with regularizing effect \[4\]. In order to illustrate this fact, consider the following one-dimensional and scalar Cauchy problem:
\begin{equation}
\begin{cases}
\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{Q^2}{2} \right) = 0, \\
Q(x,0) = \arctan(x),
\end{cases}
\tag{2.2}
\end{equation}

for \((x,t) \in \mathbb{R} \times [0, \infty)\). By using the method of characteristics [38], it can be shown that the classical solution of (2.2) for \(t < 1\) is given implicitly by

\begin{equation}
\begin{cases}
x = x_0 + \arctan(x_0)t, \\
Q(x,t) = \arctan(x_0),
\end{cases}
\end{equation}

and the discontinuity in \(Q\) emerges beyond \(t = 1\) at \(x = 0\). The solution of (2.2) at \(t = 0, 0.25, 0.5, 0.75, 1\), is shown in Figure 1.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{solution_plots.png}
\caption{Plots of the solution to (2.2) at \(t = 0, 0.25, 0.5, 0.75, 1\).}
\end{figure}

In the presence of shock discontinuities, the tools of differential calculus must be amended, and the solution has to be considered in a generalized sense (distribution) [4]. For an extensive discussion of capturing of shocks, we refer to [4, 18, 36, 49].

Traditional low order numerical methods include the first order Godunov and Roe schemes [19, 44]. They can resolve the discontinuities monotonically without spurious numerical oscillations; however, they often smear some of these discontinuities and contain relatively large numerical dissipation in the smooth part of the solution.

High-resolution approaches represented by the monotone upwind scheme for conservation laws, the total variation diminishing (TVD) schemes and the piecewise parabolic method [7, 22, 57], are usually second order accurate in smooth regions and can resolve discontinuities monotonically with a sharper transition than first or-
der schemes. They are often the best choice in terms of a balance between computational cost and desired resolution, especially for problems with solutions dominated by shocks or other discontinuities with relatively simple structures between these discontinuities.

A successful class of high-order high-resolution methods is given by the essentially non-oscillatory (ENO) and WENO schemes [49]. ENO uses adaptative stencils to obtain information from smooth regions when discontinuities are present, allowing the achievement of high-order accuracy right up to discontinuities. One problem with the ENO scheme is the freely adaptive stencil, which could change even by a round-off the type perturbation near zeroes of the solution and its derivatives, leading to a loss of accuracy for certain functions [51]. To overcome this difficulty, WENO schemes were designed to get optimal accuracy through the use of a dynamic set of stencils, where a nonlinear convex combination of lower-order polynomials adapts either to a higher-order approximation at smooth parts of the solution, or to an upwind spatial discretization that avoids interpolation across discontinuities and provides the necessary dissipation for shock capturing. The numerical dissipation can be reduced by increasing the number of points, as well as the order of the WENO scheme which, however, it makes the scheme computationally expensive. This also means waste of computational effort since it would not change the situation of well resolved structures in the smooth regions of the solution.

In order to increase computational efficiency, efforts have been made in the literature to develop high-order resolution hybrid schemes to approximate the solution of hyperbolic conservation laws using high- and low-order methods in smooth regions and near shocks, respectively. For example, Costa and Don [9] present a hybrid central-WENO finite difference scheme to solve one-dimensional shock-turbulence interaction problems, that switches between a sixth order central finite difference scheme and a fifth order WENO scheme through a high-order multiresolution (MR) analysis, [23]. The MR analysis detects the large gradient regions of the numerical solution and captures shocks with the WENO scheme, while in smooth regions, the
solution is computed with the more efficient and accurate central finite difference scheme.

We have assessed the performance of a three-dimensional version of the hybrid central-WENO-Z finite difference scheme in parallel computations of circular sonic jet injection in a Mach 2.1 supersonic cross flow with air [14]. Figure 2 (right) shows the iso-surface of the Mach number at time \( t = 3 \) computed by the hybrid scheme. The hybrid scheme captures the long time evolution of large scale structures (bow shock, barrel shock, reflected shock and expansion plume) as well as small scale eddy structures (vortical rollups along the slip line), illustrated in Figure 2 (left), in an accurate and efficient manner. The hybrid central-WENO finite difference scheme showed to be more computationally efficient, reducing the CPU time needed to perform large scale numerical experiments and giving improvement in the overall accuracy over the WENO scheme.

![Figure 2](image)

**Figure 2:** Schematic of flow features in a sonic injection in a supersonic cross stream flow (left) and iso-surface of the Mach number at time \( t = 3 \) computed by the hybrid scheme (right).

The non-dissipative nature of central difference schemes makes them good candidates to resolve smooth solutions. However, the finite difference scheme is known to be dispersive, meaning that the phase velocity in the finite difference grid is not the same as the phase velocity in the continuous physical domain.

Costa, Don, Gottlieb and Sendersky [10, 11] have addressed the issue described in the paragraph above, by conjugating the non-dispersive spectral method with the high-order WENO scheme. The main idea of the multidomain hybrid spectral-WENO
scheme is to partition the physical domain into equal sized sub-domains. Sub-domains containing discontinuities are treated with the high-order WENO scheme on an equidistant grid avoiding Gibbs phenomena. Sub-domains containing smooth parts of the solution are treated with Chebyshev spectral methods increasing numerical efficiency and ensuring a small dispersion error. Each sub-domain is switched to the other discretization based on the high-order MR analysis \([23]\) on the temporal evolution of the solution. This hybrid scheme was tested in one- and two-dimensional problems in the numerical solution of nonlinear hyperbolic conservation laws arising in simulation of compressible flow, shock-vortex interaction and the Richtmyer-Meshkov instabilities, showing its computational efficiency and accuracy compared with the WENO scheme.

We seek to improve the accuracy of a high-order resolution PSIC method in the simulation of particle-laden flows with shocks \([29]\), based on the effective and computational efficient multidomain hybrid spectral-WENO scheme \([10, 11]\) for the solution of nonlinear systems of hyperbolic conservation laws with nonstationary Dirac-delta sources. Specifically, we are interested in obtaining spectral accuracy in smooth parts of the solution as well as a high-order (resolution) essentially nonoscillatory representation of the shock discontinuities using the WENO scheme.

This chapter presents the main three individual high-order components of the multidomain hybrid spectral-WENO scheme, including the spectral Chebyshev collocation method, WENO-Z and MR schemes. Without loss of generality, we shall concentrate on the discussion of the semi-discrete (discrete in space, continuous in time) representation of the one-dimensional and scalar hyperbolic conservation law

\[
\frac{\partial}{\partial t} Q(x, t) + \frac{\partial}{\partial x} F(Q) = 0,
\]

on a bounded spatial domain, in absence of boundary conditions. The resulting system of ordinary differential equations (ODE(s)) after the spatial discretization can be advanced in time via the third order TVD Runge–Kutta scheme \([21]\). The extension of the spatial discretization to systems with higher dimensions and nonzero source
terms is straightforward by using tensor product of functions and the method of lines to solve the respective semi-discretized form of (2.3) [5, 49]. A detailed explanation about the computational implementation of the multidomain hybrid scheme can be found in [10, 11].

The chapter is divided in three sections. In Section 2.1, we present the spectral Chebyshev collocation method with Gauss–Lobatto points, the respective error estimates, and the exponential filtering for enhancing the accuracy. In Section 2.2, we introduce the improved fifth order finite difference based WENO-Z scheme. In Section 2.3, we review the MR analysis, which is used to determine the smoothness of the solution in the computational domain, and to maintain the high-order nature of the multidomain hybrid scheme, by switching between the spectral Chebyshev collocation and WENO-Z schemes.

2.1 Chebyshev Collocation Method

Let \( w : [a, b] \rightarrow \mathbb{R} \) be a nonnegative integrable function which vanishes at most finitely many times in the interval. Consider the Hilbert space

\[
L^2_w[a, b] \overset{\text{def}}{=} \left\{ u : \int_a^b u^2(x) w(x) \, dx < \infty \right\},
\]

with the usual inner product

\[
\langle u_1, u_2 \rangle_w \overset{\text{def}}{=} \int_a^b u_1(x) u_2(x) w(x) \, dx,
\]

and the respective norm

\[
\| u_1 \|_w \overset{\text{def}}{=} \langle u_1, u_1 \rangle_w^{1/2},
\]

for all \( u_1, u_2 \in L^2_w[a, b] \).
The spectral approximation of a function \( Q(\cdot, t) \in L^2_w([a, b]) \), for each \( t > 0 \), is based on the series expansion

\[
Q(x, t) = \sum_{k=0}^{\infty} \hat{Q}_k(t) \phi_k(x), \quad x \in [a, b],
\]

(2.5)

where \( \{\phi_k\}_{k \geq 0} \) represents an orthogonal basis of \( L^2_w([a, b]) \) with respect to the inner product defined in (2.4), and the expansion coefficients are given by

\[
\hat{Q}_k(t) \equiv \frac{1}{\tilde{\gamma}_k} \int_a^b Q(x, t) \phi_k(x) w(x) \, dx, \quad \tilde{\gamma}_k \equiv \frac{1}{\langle \phi_k, \phi_k \rangle_w} \int_a^b \phi_k^2(x) w(x) \, dx.
\]

In the context of spectral theory of operators, the series expansion (2.5) is known as a generalized Fourier series, and the orthogonal basis is obtained by solving Sturm–Liouville problems with suitable separated or periodic boundary conditions [5, 42].

The spectral approximation is obtained by truncation of (2.5) and the use of quadrature rules to approximate the expansion coefficients \( \hat{Q}_k(t) \). Concretely, if \( \tilde{Q}_k(t) \) and \( \tilde{\gamma}_k \) are the respective approximations to \( \hat{Q}_k(t) \) and \( \tilde{\gamma}_k \) through a quadrature rule with nodes \( \{x_j\}_{j=0}^N \) and discrete weights \( \{w_j\}_{j=0}^N \), then

\[
\tilde{Q}_k(t) = \frac{1}{\tilde{\gamma}_k} \sum_{j=0}^{N} Q(x_j, t) \phi_k(x_j) w_j, \quad \tilde{\gamma}_k = \sum_{j=0}^{N} \phi_k^2(x_j) w_j,
\]

and the spectral approximation, denoted by \( Q^N(x, t) \), is defined as

\[
Q^N(x, t) \equiv \sum_{k=0}^{N} \tilde{Q}_k(t) \phi_k(x), \quad = \sum_{k=0}^{N} \left( \frac{1}{\tilde{\gamma}_k} \sum_{j=0}^{N} Q(x_j, t) \phi_k(x_j) w_j \right) \phi_k(x),
\]

\[
= \sum_{j=0}^{N} Q(x_j, t) \left( w_j \sum_{k=0}^{N} \frac{1}{\tilde{\gamma}_k} \phi_k(x_j) \phi_k(x) \right).
\]
The spectral Chebyshev–Gauss–Lobatto method corresponds to the particular choice of the Chebyshev polynomials $T_k(x) = \cos(k \arccos(x))$ as an orthogonal basis for $L^2_{\text{w}}([-1, 1])$ with the weight function $w(x) = (1 - x^2)^{-\frac{1}{2}}$, and the quadrature rule with Gauss–Lobatto nodes and discrete weights

$$x_j = -\cos\left(\frac{\pi j}{N}\right), \quad w_j = \frac{\pi}{c_j N},$$

where $c_0 = c_N = 2$, and $c_j = 1$ for $j = 1, \ldots, N - 1$.

The Chebyshev–Gauss–Lobatto approximation can be expressed as a global interpolation polynomial

$$Q^N(x, t) = \sum_{j=0}^{N} Q(x_j, t) l_j(x), \quad (2.6)$$

where $l_j(x) = \frac{(-1)^{N+j+1}(1 - x^2) dT_N}{c_j N^2(x - x_j)}$ is the $j$th Lagrange polynomial satisfying

$$l_j(x_i) = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

The derivative $\frac{\partial Q}{\partial x}$ at each Gauss–Lobatto node is approximated by differentiating (2.6), i.e.,

$$\left.\frac{\partial Q^N}{\partial x}\right|_{x=x_i} = \sum_{j=0}^{N} D_{ij} Q(x_j, t), \quad i = 0, 1, \ldots, N,$$

where $D_{ij} \overset{\text{def}}{=} \left.\frac{d}{dx} l_j\right|_{x=x_i}$ is the $(N + 1) \times (N + 1)$ matrix representing the discrete spectral derivative operator, and whose entries are

$$D_{ij} = \begin{cases} \frac{-2N^2 + 1}{6}, & i = j = 0, \\ \frac{1}{2 c_i} \sin\left(\frac{(i+j)\pi}{2N}\right) \sin\left(\frac{(i-j)\pi}{2N}\right), & i \neq j, \\ \frac{x_i}{2 \sin^2\left(\frac{\pi}{N}\right)}, & i = j \text{ and } 1 \leq i, j \leq N - 1, \\ \frac{2N^2 + 1}{6}, & i = j = N. \end{cases}$$
In the numerical solution of the one-dimensional and scalar hyperbolic conservation law (2.3), the collocation approach in the Chebyshev spectral method, leads to the respective PDE to be satisfied exactly by (2.6), at the Gauss–Lobatto nodes. Thus, we obtain the following semi-discrete representation of (2.3):

$$\frac{d}{dt} Q^N(x_i, t) + \sum_{i=0}^{N} D_{ij} F(Q^N(x_i, t)) = 0.$$ 

Interpolation error estimates in the $L^2_w([-1, 1])$ norm for the spectral approximation (2.6) can be established, provided that the existence of $p \in \mathbb{N}$ such that $\frac{\partial^i Q(\cdot, t)}{\partial x^i} \in L^2_w([-1, 1])$ for $i = 0, \ldots, p$ and each $t > 0$. Indeed,

$$\|Q - Q^N\|_{w} \leq \kappa N^{-p}\|Q\|_{w,p},$$

$$\left\| \frac{\partial Q}{\partial x} - \frac{\partial Q^N}{\partial x} \right\|_{w} \leq \kappa N^{1-p}\|Q\|_{w,p},$$

where $\kappa$ denotes a constant independent of $N$ and $\|Q\|_{w,p} \overset{\text{def}}{=} \left( \sum_{i=0}^{p} \left\| \frac{\partial^i Q}{\partial x^i} \right\|_{w}^2 \right)^{\frac{1}{2}}$. In addition, if $Q(x, t) \in C^0([-1, 1] \times (0, \infty))$, then

$$\max_{x \in [-1, 1]} |Q(x, t) - Q^N(x, t)| \leq \kappa N^{\frac{1}{2}-p}\|Q\|_{w,p}.$$ 

Exponential decay of the interpolation error, i.e., faster decay than any negative power of $N$, can be achieved when $Q \in C^\infty([-1, 1] \times (0, \infty))$. This property, known as spectral convergence, ensures that

$$\|Q - Q^N\|_{w} \leq \kappa \exp(-\eta N),$$

for some $\eta > 0$. Proof of these error estimates can be found in [5, 54].

The interpolation error estimates rely on the smoothness of the function to be approximated. If the function has a discontinuity, even at one point, the spectral approximation will be affected by the Gibbs phenomenon [27]. Consequently, the polynomial interpolant (2.6) will exhibit an oscillatory behavior near the discontinuity,
reducing the global order of convergence to first order. However, convergence of the spectral method in approximating discontinuous functions can be enhanced by using a filter function [27].

The convergence of the infinite series (2.5) depends on the rate of decay of the expansion coefficients [5]. In the spectral interpolation of functions with discontinuities, a slow decay of the respective coefficients is possible [34]. A filter function modifies the expansion coefficients to speed up the rate of decay, and thus to improve the accuracy of the spectral approximation.

A filter of order q is a real and even function \( \sigma : \mathbb{R} \rightarrow \mathbb{R} \) in \( C^q(\mathbb{R}) \) with the following properties:

\[
\begin{align*}
\sigma(\eta) &= 0, & |\eta| > 1, \\
\sigma(0) &= 1 \quad \text{and} \quad \sigma(\pm 1) = 0, \\
\sigma^{(i)}(0) &= \sigma^{(i)}(\pm 1) = 0, & i = 1, \ldots, q - 1.
\end{align*}
\]

The respective filtered polynomial interpolant is

\[
Q^N_{\sigma}(x, t) = \sum_{j=0}^{N} Q(x_j, t) l^\sigma_j(x),
\]

where

\[
l^\sigma_j(x) \overset{\text{def}}{=} w_j \sum_{k=0}^{N} \sigma \left( \frac{k}{N} \right) \frac{1}{\tilde{\gamma}_k} T_k(x_j) T_k(x), \quad \tilde{\gamma}_k = \sum_{j=0}^{N} T^2_k(x_j) w_j.
\]

A more convenient way to express the action of the filter at each grid point is through the filter matrix \( M_{ij} \overset{\text{def}}{=} I^\sigma_j(x_i) \), i.e., by taking the filtered expansion as

\[
Q^N_{\sigma}(x_i, t) = \sum_{j=0}^{N} M_{ij} Q(x_j, t).
\]

In the context of hyperbolic conservation laws, a very common choice is the exponential filter

\[
\sigma(\eta) = \exp(-\alpha \eta^q),
\]
where \( a \overset{\text{def}}{=} -\log(\epsilon) \), with \( \epsilon \) denoting the machine zero. The use of this filter helps both to mitigate the Gibbs phenomenon and to introduce the necessary artificial dissipation for hyperbolic problems \([20]\). Additionally, different alternatives to filter spectral approximations are discussed in \([27]\).

### 2.2 Weighted Essentially Non-Oscillatory Scheme

We consider the characteristics based WENO-Z scheme of order \( 2r - 1 \), in the semi-discretization of (2.3). We present the explicit formula for a fifth order scheme, i.e., \( r = 3 \). Extension to a higher order WENO-Z scheme is straightforward as explained in \([6]\).

Consider a uniform grid defined by the cell centers \( x_i = i \Delta x \) and the cell boundaries \( x_{i \pm \frac{1}{2}} = x_i \pm \Delta x/2 \) for \( i = 0, \ldots, N \), where \( \Delta x \) represents the uniform grid spacing. The semi-discretized form of (2.3) is

\[
\frac{dQ_i(t)}{dt} = -\frac{\partial F(Q)}{\partial x} \bigg|_{x=x_i}, i = 0, \ldots, N, \tag{2.7}
\]

where \( Q_i(t) \) denotes a numerical approximation to the point value \( Q(x_i, t) \).

To form the flux differences across the uniformly spaced cells and to obtain high-order numerical fluxes consistent with the hyperbolic conservation law, a conservative finite difference formulation is required at the cell boundaries. We implicitly define the numerical flux function \( h(x, t) \) as

\[
F(Q(x, t)) = \frac{1}{\Delta x} \int_{x - \frac{\Delta x}{2}}^{x + \frac{\Delta x}{2}} h(\xi, t) \, d\xi,
\]
such that the spatial derivative in (2.7) is approximated by a conservative finite difference formula at the cell boundaries $x_{i \pm \frac{1}{2}}$, i.e.,

$$\frac{dQ_i(t)}{dt} = -\frac{1}{\Delta x} \left(h_{i+\frac{1}{2}} - h_{i-\frac{1}{2}}\right),$$

where $h_{i \pm \frac{1}{2}} \overset{\text{def}}{=} h(x_{i \pm \frac{1}{2}}, t)$. High-order polynomial interpolations to $h_{i \pm \frac{1}{2}}$ are computed using the known cell-averaged values $F_j \overset{\text{def}}{=} F(Q_j(t))$ for $j = i - r + 1, \ldots, i + r - 1$.

The $2r - 1$ order WENO scheme uses a $(2r - 1)$-points global stencil, which is subdivided into $r$ substencils $\{S_0, S_1, \ldots, S_{r-1}\}$ with each substencil containing $r$ grid points and a global stencil $S^{2r-1} = \bigcup_{i=0}^{r-1} S_i$. For $r = 3$, the 5-points global stencil, hereafter named $S^5$, is subdivided into three 3-points substencils $\{S_0, S_1, S_2\}$ (see Figure 3).

![Figure 3: The computational uniformly spaced grid $x_i$ and the 5-points stencil $S^5$, composed of three 3-points substencils $S_0, S_1, S_2$, used for the fifth-order WENO reconstruction step.](image)

The $2r - 1$ degree polynomial approximation

$$\tilde{F}_{i \pm \frac{1}{2}} = h_{i \pm \frac{1}{2}} + O(\Delta x^{2r-1})$$

is built through the convex combination of the lower $r$ degree polynomial $\tilde{F}^k(Q(x,t))$ in substencils $S_k$ at the cell boundaries $x_{i \pm \frac{1}{2}}$, i.e.,

$$\tilde{F}_{i \pm \frac{1}{2}} = \sum_{k=0}^{r-1} \omega_k \tilde{F}^k \left(Q_{i \pm \frac{1}{2}}(t)\right),$$
where
\[
\hat{F}_k \left( Q_{i+\frac{1}{2}}(t) \right) = \sum_{j=0}^{r-1} c_{kj} F_{i-k+j}, \quad i = 0, \ldots, N.
\]

The \( c_{kj} \) are Lagrangian interpolation coefficients \cite{50} and \( \omega_k \) are normalized nonlinear weights, which will be described below.

The regularity of the \( r - 1 \) degree interpolation polynomial approximation \( \hat{F}_k (Q(x,t)) \) at the substencil \( S_k \) is measured by the lower order local smoothness indicators \( \beta_k \), which are given by
\[
\beta_k = \sum_{i=1}^{r-1} \Delta x^{2l-1} \int_{x_i-\frac{1}{2}}^{x_{i+\frac{1}{2}}} \left( \frac{\partial^l}{\partial x^l} \hat{F}_k (Q(x,t)) \right)^2 \, dx, \quad k = 0, \ldots, r - 1.
\]

For \( r = 3 \), the \( \beta_k \) in terms of the cell averaged values \( F_i \) are given explicitly by
\[
\begin{align*}
\beta_0 &= \frac{13}{12} (F_{i-2} - 2F_{i-1} + F_i)^2 + \frac{1}{4} (F_{i-2} - 4F_{i-1} + 3F_i)^2, \\
\beta_1 &= \frac{13}{12} (F_{i-1} - 2F_i + F_{i+1})^2 + \frac{1}{4} (F_{i-1} - F_{i+1})^2, \\
\beta_2 &= \frac{13}{12} (F_i - 2F_{i+1} + F_{i+2})^2 + \frac{1}{4} (3F_i - 4F_{i+1} + F_{i+2})^2.
\end{align*}
\]

The WENO-Z scheme makes use of the higher order information obtained from a global optimal order smoothness indicator \( \tau_{2r-1} \) which is built as a linear combination of \( \beta_k \), i.e.,
\[
\tau_{2r-1} = \left| \sum_{k=0}^{r-1} c_k \beta_k \right|,
\]
where \( c_k \) are given constants \cite{3, 6}. For \( r = 3 \), one has \( \tau_5 = |\beta_0 - \beta_2| \), which is of order \( O(\Delta x^5) \).

Systems of hyperbolic conservation laws admit a complete set of right and left eigenvectors for the Jacobian matrix associated to the fluxes \cite{4}. Following \cite{3, 6}, the approximated eigenvalues and eigenvectors can be obtained via the Roe averaged Jacobian. The first order global Lax-Friedrichs flux can be used as the low order building block for the high-order reconstruction step of the WENO scheme.
After projecting the positive and negative fluxes on the characteristic fields via the left eigenvectors, the high-order WENO reconstruction step is applied to obtain the high-order approximation at the cell boundaries using the surrounding cell-centered values, which are then projected back into the physical space via the right eigenvectors and added together to form a high-order numerical flux at the cell-interfaces. The conservative difference of the reconstructed high-order fluxes can then be computed for the inviscid flux.

### 2.3 Multiresolution Analysis

The MR analysis measures the smoothness of the solution at each grid point at a given time and quantifies smoothness through an MR coefficient. Since the spectral Chebyshev–Gauss–Lobatto and WENO-Z schemes are both high-order schemes, the measure of smoothness of the solution must also be of high-order in order to differentiate a high-frequency wave from a large gradient or shock so that the appropriate numerical spatial scheme (spectral for high-frequency wave or WENO-Z for shocks) can be applied at a given spatial location and at a given time. To do so, the high-order multilevel MR algorithm by Harten [22] is employed to detect the smooth and rough parts of the solution.

Given an initial number of grid points $N_0$ and grid spacing $\Delta x_0$, we shall consider a set of nested dyadic grids up to level $L < \log_2(N_0)$,

$$G^k = \left\{ x_j^k : j = 0, \ldots, N_k \right\}, \quad 0 \leq k \leq L,$$

where $x_j^k = j\Delta x_k$ with $\Delta x_k = 2^k\Delta x_0$, $N_k = 2^{-k}N_0$ and the cell averages of the function $Q(x,t)$ at $x_j^k$

$$\bar{Q}_j^k(t) = \frac{1}{\Delta x_k} \int_{x_{j-1}^k}^{x_j^k} Q(x,t) \, dx.$$
Let $\tilde{Q}_{2j-1}^k(t)$ be the approximation to $\bar{Q}_{2j-1}^k(t)$ by a unique polynomial of degree $2s$ that interpolates $\bar{u}_{j+l}^k(t)$ for $|l| \leq s$ at $x_{j+l}^k$, where $r = 2s + 1$ is the order of approximation.

The approximation error (or MR coefficients) $d_j^k = \bar{Q}_{2j-1}^k - \tilde{Q}_{2j-1}^k$, at the $k$ level and the grid point $x_j$, has the property that if $Q(x,t)$ has $p - 1$ continuous spatial derivatives and a jump discontinuity at its $p$ derivative, then

$$d_j^k \approx \begin{cases} \left[ \frac{\partial^p Q}{\partial x^p} \right] \Delta x_k^p, & p \leq r, \\ \frac{\partial^r Q}{\partial x^r} \Delta x_k^r, & p > r, \end{cases}$$

where $[\cdot]$ denotes the jump in the discontinuity of the function.

The MR coefficient $d_j^k$ measures how close the data at the finer grid $\{x_k^{k-1}\}$ can be interpolated by the data at the coarser grid $\{x_j^k\}$. From (2.8) it follows that

$$\left|d_{2j}^{k-1}\right| \approx 2^{\bar{p}} \left|d_j^k\right|, \quad \bar{p} = \min\{p, r\},$$

which implies that away from discontinuities, the MR coefficients $\{d_j^k\}$ diminish in magnitude with the refinement of the grid at smooth parts of the solution; close to discontinuities, they remain the same size, independent of the order $r = 2s + 1$ and level $k$ of MR analysis. Examples of the performance of the high-order multilevel MR analysis in detecting discontinuities in the solution of systems of hyperbolic conservation laws, can be found in [9].
Chapter 3

Singular sources

In the context of nonlinear hyperbolic conservation laws, the presence of shocks in the solution, no matter how smooth the initial condition is, makes it impossible to define classical solutions for all time, i.e., a smooth function that satisfies the respective differential equation. The standard way of extending the admissible set of solutions (allowing discontinuities) is through the theory of distributions [4, 18].

The theory of distributions, introduced by Laurent Schwartz in [47], is fundamental in the study of generalized solutions to hyperbolic conservation laws. It extends the function concept and the differentiation operation by introducing a class of objects, called distributions, which are infinitely differentiable and satisfy the usual formal rules of calculus under a generalized differentiation.

One of the most important examples of distributions is the Dirac-delta. It was introduced by Paul Dirac as a generalized function, in an effort to create the mathematical tools for the development of quantum field theory [13]. Its introduction was preceded by the practical use of another standard discontinuous function, the Heaviside function, introduced by Oliver Heaviside for operational calculus in electromagnetic theory [24, 25, 26]. The Dirac-delta represents an essential tool in the study of many areas of applied mathematics and theoretical physics, including operational calculus for electromagnetic problems, the development of generalized derivatives and generalized solutions to hyperbolic differential equations, and generalized Fourier transforms [17, 35].

In one dimension, the Dirac-delta is often defined as a generalized singular function $\delta$, satisfying the following properties:
(i) \[ \delta(x) = \begin{cases} 0, & x \neq 0, \\ \infty, & x = 0. \end{cases} \]

(ii) If \( \phi : \mathbb{R} \to \mathbb{R} \) is any function which is continuous in a neighborhood of the point \( x = 0 \), then
\[
\int_{\mathbb{R}} \delta(x)\phi(x) \, dx = \phi(0).
\]

This definition is generalized in the sense that properties (i) and (ii) are inconsistent with the classical definition of a function and an integral. The property \( \delta(0) = \infty \) represents the singularity of the Dirac-delta.

From the point of view of the theory of distributions, \( \delta \) can be represented by a parametric family of smooth functions \( \{ f_\varepsilon(x) : \varepsilon > 0 \} \) on \( \mathbb{R} \) with compact support \( [-\varepsilon, \varepsilon] \), satisfying properties (i) and (ii) as long as \( \varepsilon \to 0^+ \). Thus, given \( \varepsilon > 0 \), the singularity at \( x = 0 \) is removed by approximating \( \delta \) with a smooth function on the support. This technique is known as regularization, \( \varepsilon \) is the scaling parameter, and \( [-\varepsilon, \varepsilon] \) is the regularization zone.

The regularization techniques are very useful in the discretization of the Dirac-delta. However, the choice of scaling parameter constitutes an issue for the representation of \( \delta \) on general grids. Specifically, the high-order smoothing of singularities requires a wide regularization zone, whereas a narrow area is desirable to accurately mimic the properties of the singular source. A scaling parameter \( \varepsilon > 0 \), that satisfies both requirements, we will call optimal.

The development of regularization techniques with optimal scaling has been restricted to uniform grids, by taking the width of the regularization zone proportional to the grid spacing [15]. On nonuniform unstructured grids, the optimal scaling is not trivially defined. Typically, some form of projection or mapping on a uniform grid is used [28, 30].

A number of approaches based on the theory of distributions can be formulated to regularize the Dirac-delta in the numerical solution of hyperbolic conservation laws with high-order methods. Top-hat and piecewise linear functions are widely used;
however, their lack of smoothness produces Gibbs oscillations in spectral solutions [53].

Jung and Don [31, 32] proposed a direct discretization, where the Dirac-delta is expressed as the derivative of the Heaviside function and the discrete derivative is determined based on a spectral differentiation operator. In unsteady test problems with nonstationary source terms, Jung and Don show an inherent oscillatory behavior due to the discrete nature of the approximation of the singular source on the collocation grid.

Abe, Natsuhiko and Itatani [1] present a high-order spline interpolation on uniform grids where the $k$th order spline is a $C^{k-1}(\mathbb{R})$ piecewise compactly supported polynomial, constructed by convolution of the zero order spline. The spline’s approximation order is limited to second order of accuracy for all $k \geq 1$. Ryan and Shu [46] consider the smoothness-increasing accuracy-conserving (SIAC) filter to enhance the accuracy of the discontinuous Galerkin methods in the numerical solution of scalar hyperbolic equations. The SIAC filter is constructed from a linear combination of splines of order $k + 1$ and reach a $(2k + 1)$th order of accuracy. Monaghan uses in [40] a limit form of Richardson extrapolation to obtain a higher-order accurate approximation than the splines, which are commonly used in particle methods for hydrodynamics [39]. These regularization techniques disrupt the convergence rate of spectral methods in the solution of hyperbolic conservation laws with singular sources [53].

A promising candidate for the approximation of Dirac-delta is proposed by Tornberg [55]. She suggests the use of compactly supported piecewise mixed polynomials. The mixed polynomial has a desired order of accuracy and a specified number of zero moments, smoothness, and it integrates to unity. The polynomials are mixed in the sense that they are expressed as the product of two polynomials controlling independently the moment and smoothness conditions.

This chapter contains the main contribution of the doctoral dissertation. It presents a high-order accurate regularization technique, with the proper scaling on general grids, in the discretization of time-dependent singular Dirac-delta sources for the
numerical solution of hyperbolic conservation laws with high-order methods. Concretely, the regularization is based on the mixed polynomial approximation [55] and for the scaling parameter, we introduce a theoretical criterion that establishes a lower bound on the size of the regularization zone (optimal scaling) that has to be satisfied to achieve optimal order of convergence. The proposed regularization technique has been assessed in the numerical solution of scalar and systems of hyperbolic equations with Dirac-delta sources, leading to high-order accurate representations of the source at smooth parts and full convergence order away from the singularities in the discrete solution of hyperbolic conservation laws [52, 53].

The chapter is divided into four sections. In Section 3.1 we introduce the basic fundamentals of the theory of distributions, including the definition of the space of distributions and the respective algebraic operations, differentiation and convolution of distributions, and convergence of sequences of distributions, that are necessary to define and formally establish the mathematical properties of the one-dimensional Dirac-delta distribution, and that provide the theoretical support in the developing of approximations to this particular distribution. In Section 3.2, we present the theoretical approach—Theorem 8 (Mixed polynomials) and Proposition 1 (Optimal scaling for delta-sequences)—that has been used in the development of a high-order accurate regularization technique. Section 3.3 is devoted to the smoothing of piecewise functions using the mixed polynomial, with an optimal scaling parameter—Theorem 11 (Smoothing), and Proposition 3 (Optimal scaling for smoothing). In Section 3.4, we present the definition of the Dirac-delta distribution in higher dimensions, and a theoretical result—Theorem 12 (Tensor product of distributions)—that supports the extension of the proposed regularization to higher dimensions.
3.1 Distributions in one dimension

The definition of distribution requires the introduction of two concepts: the space of test functions and linear functionals on it, which are presented in Definition 1 and Definition 2, respectively. We then define distribution in Definition 3.

**Definition 1** (Space of test functions). The space of test functions, denoted by $\mathcal{D}(\mathbb{R})$, is the set of all $C^\infty(\mathbb{R})$ functions whose support is a compact subset of $\mathbb{R}$.

**Definition 2** (Linear functionals). A linear functional on $\mathcal{D}(\mathbb{R})$ is a linear map from $\mathcal{D}(\mathbb{R})$ to $\mathbb{R}$, i.e., a map $T : \mathcal{D}(\mathbb{R}) \to \mathbb{R}$ such that

$$T[\phi + \alpha \psi] = T[\phi] + \alpha T[\psi],$$

for all $\phi, \psi \in \mathcal{D}(\mathbb{R})$ and $\alpha \in \mathbb{R}$.

**Definition 3** (Distribution). A linear functional $T$ on $\mathcal{D}(\mathbb{R})$ is said to be a distribution if $T$ is continuous with the usual topology of $\mathcal{D}(\mathbb{R})$. The space of all distributions in $\mathbb{R}$ is denoted by $\mathcal{D}^\ast(\mathbb{R})$.

On finite-dimensional vector spaces, every linear functional is continuous. In infinite dimensions, the characterization of continuity is not trivial and theoretical criteria are necessary.

The space of test functions is an infinite-dimensional vector space with respect to the usual definitions of addition and scalar multiplication of real functions. A useful criterion to establish the continuity of a linear functional on $\mathcal{D}(\mathbb{R})$, in terms of the norm

$$\|\phi\|_N \overset{\text{def}}{=} \max \left\{ |\phi^{(i)}(x)| : x \in \mathbb{R}, 0 \leq i \leq N \right\},$$

where $N$ denotes a nonnegative integer and $\phi^{(i)}$ is the $i$th derivative of $\phi \in \mathcal{D}(\mathbb{R})$, is given in Theorem 1.

**Theorem 1** (Characterization of distributions). Let $T$ be a linear functional on $\mathcal{D}(\mathbb{R})$. Then, the following conditions are equivalent:

1 The topology is fully described in [45].
(i) \( T \in \mathcal{D}^*(\mathbb{R}) \).

(ii) To every compact set \( \Omega \subset \mathbb{R} \) corresponds a constant \( \kappa < \infty \) and a nonnegative integer \( N \) such that the inequality

\[
|T[\phi]| \leq \kappa \|\phi\|_N
\]

holds for every \( \phi \in C^\infty(\mathbb{R}) \) with support contained in \( \Omega \).

Proof. See [45].

An important example of a distribution is the Dirac-delta. It is the most fundamental distribution in many mathematical areas with physical applications [37]. Its formal definition is given in Definition 4.

Definition 4 (Dirac-delta distribution). The Dirac-delta is the distribution defined by

\[
\delta : \mathcal{D}(\mathbb{R}) \rightarrow \mathbb{R} \\
\phi \mapsto \delta[\phi] \overset{\text{def}}{=} \phi(0).
\]

The Dirac-delta is clearly a linear map on \( \mathcal{D}(\mathbb{R}) \), and the continuity can be easily proved using Theorem 1. Indeed, let \( \phi \) be as in condition (ii) of the respective theorem, then

\[
|\delta[\phi]| = |\phi(0)| \leq \|\phi\|_0.
\]

The basic operations on distributions are vector addition and scalar multiplication defined on \( \mathcal{D}^*(\mathbb{R}) \). Given \( T, W \in \mathcal{D}^*(\mathbb{R}) \) and \( \alpha \in \mathbb{R} \), the distributions

\[
T + W : \mathcal{D}(\mathbb{R}) \rightarrow \mathbb{R} \\
\phi \mapsto (T + W)[\phi] \overset{\text{def}}{=} T[\phi] + W[\phi]
\]

and

\[
\alpha T : \mathcal{D}(\mathbb{R}) \rightarrow \mathbb{R} \\
\phi \mapsto \alpha T[\phi] \overset{\text{def}}{=} T[\alpha \phi],
\]
represent the addition and scalar multiplication, respectively. In addition, the multiplication of distributions by smooth functions can be defined according to Definition 5.

**Definition 5 (Multiplication by smooth functions).** Given \( f \in C^\infty(\mathbb{R}) \) and \( T \in D^*(\mathbb{R}) \), the product of \( f \) by \( T \) is defined as the distribution

\[
f \cdot T : D(\mathbb{R}) \rightarrow \mathbb{R} \\
\phi \mapsto f \cdot T[\phi] \overset{\text{def}}{=} T[f \phi].
\]

A straightforward extension of the definition of product of continuous functions to multiplication of two distributions is impossible \([48]\). Moreover, there are a large variety of other possible definitions with no natural or canonical candidate \([8]\).

In the classical sense, the solution of partial differential equations is treated within the framework of the \( C^i(\mathbb{R}) \) functions, for \( i \in \mathbb{Z}_{\geq 0} \). These spaces possess a canonical structure given by the chain of inclusions

\[ C^\infty(\mathbb{R}) \subset \cdots \subset C^i(\mathbb{R}) \subset \cdots \subset C^0(\mathbb{R}) \subset L^1_{\text{loc}}(\mathbb{R}), \quad i \in \mathbb{N}, \]

where only the elements of \( C^\infty(\mathbb{R}) \) are indefinitely differentiable in the classical sense. However, every \( f \in L^1_{\text{loc}}(\mathbb{R}) \) can be represented in \( D^*(\mathbb{R}) \) through a regular distribution, as presented in Definition 6.

**Definition 6 (Regular distributions).** Given a locally integrable function \( f : \mathbb{R} \rightarrow \mathbb{R} \), the regular distribution generated by \( f \) is

\[
T_f : D(\mathbb{R}) \rightarrow \mathbb{R} \\
\phi \mapsto T_f[\phi] \overset{\text{def}}{=} \int_{\mathbb{R}} f(x)\phi(x) \, dx.
\]

In Definition 6, the linearity of \( T_f \) is evident and the continuity follows from the fact that

\[
|T_f[\phi]| = \left| \int_{\Omega} f(x)\phi(x) \, dx \right| \leq \left( \int_{\Omega} |f(x)| \, dx \right) \|\phi\|_0,
\]
with $\phi$ and $\Omega$ as in condition (ii) of Theorem 1.

The theory of distributions aims at eliminating the limitations of the classical notion of differentiability for a function, by introducing the distributions and a generalized differentiation.

The differentiation of distributions is presented in Definition 7. With this generalized operation, every distribution is infinitely differentiable, although no longer in the classical sense.

**Definition 7 (Differentiation).** Given $T \in \mathcal{D}^\ast(\mathbb{R})$ and $i \in \mathbb{Z}_{\geq 0}$, the $i$th derivative of $T$ is defined as the distribution

$$D^i : \mathcal{D}(\mathbb{R}) \rightarrow \mathbb{R}$$

$$\phi \mapsto D^i T[\phi] \overset{\text{def}}{=} (-1)^i T[\phi^{(i)}],$$

where $\phi^{(i)}$ denotes the $i$th derivative of $\phi$ in the classical sense.

Using Definition 7, it can be shown that the generalized first order derivative of the Heaviside function

$$H(x) = \begin{cases} 0, & x < 0, \\ \frac{1}{2}, & x = 0, \\ 1, & x > 0, \end{cases}$$

is the Dirac-delta distribution. Indeed, let $T_H$ be the regular distribution generated by (3.1), then

$$D^1 T_H[\phi] \overset{\text{def}}{=} -\int_0^\infty \phi^{(1)}(x) \, dx = \phi(0) = \delta[\phi],$$

for all $\phi \in \mathcal{D}(\mathbb{R})$.

The basic rules of differentiation of distributions are presented in Theorem 2. Specifically, the theorem establishes the following: (i) commutativity of the differential operator, (ii) linearity of the differential operator, (iii) a generalized Leibniz’s product rule and (iv) a formula for the derivative of regular distributions, showing that the generalized and classical derivative coincide for sufficiently smooth functions.
Theorem 2 (Differentiation rules). Suppose $T, W \in D^*(\mathbb{R})$, $f \in C^\infty(\mathbb{R})$ and $g \in C^M(\mathbb{R})$ for some $M \in \mathbb{Z}_{\geq 0}$. Then, for all $i, j \in \mathbb{Z}_{\geq 0}$ and $\alpha \in \mathbb{R}$

(i) $D^i D^j T = D^{i+j} T = D^j D^i T$.

(ii) $D^i (T + \alpha W) = D^i T + \alpha D^i W$.

(iii) $D^i (f \cdot T) = \sum_{l \leq i} \binom{i}{l} f^{(i-l)} \cdot D^l T$.

(iv) $D^l T_g = T_{g(l)}$ for $l = 0, \ldots, M$.

Proof. See [45].

The convergence of sequences in $D^*(\mathbb{R})$ is characterized by the weak topology induced by $D(\mathbb{R})$, which is introduced in Definition 8.

**Definition 8 (Weak convergence).** A sequence $\{T_n\}_{n \in \mathbb{N}} \subset D^*(\mathbb{R})$ converges to $T \in D^*(\mathbb{R})$ in the weak topology of $D^*(\mathbb{R})$ if

$$\lim_{n \to \infty} T_n[\phi] = T[\phi],$$

for all $\phi \in D(\mathbb{R})$. In other words, the weak topology of $D^*(\mathbb{R})$ is the topology of the pointwise convergence.

For instance, the Dirac-delta can be represented as the limit of regular distributions $T_{f_n}$, by taking the sequence of real functions

$$f_n(x) \overset{\text{def}}{=} nf(nx), \quad (3.2)$$

where $f \in D(\mathbb{R})$, $f \geq 0$ and $\int_\mathbb{R} f(x) \, dx = 1$ [45]. An example of such a function $f$ is

$$f(x) = \begin{cases} 
  x \exp \left( - \left( 1 - x^2 \right)^{-1} \right), & |x| < 1, \\
  0, & |x| \geq 1,
\end{cases}$$
with $\kappa$ a constant such that $\int_{-1}^{1} f(x) \, dx = 1$. Moreover, the distributional derivatives of the Dirac-delta can be represented through this limit process, based on Theorem 3.

**Theorem 3** (Limit of distributional derivatives). Suppose $\{T_n\}_{n \in \mathbb{N}} \subset \mathcal{D}^*(\mathbb{R})$ and

$$T[\phi] = \lim_{n \to \infty} T_n[\phi]$$

exist for every $\phi \in \mathcal{D}(\mathbb{R})$. Then $T \in \mathcal{D}^*(\mathbb{R})$, and

$$\lim_{n \to \infty} D^i T_n[\phi] = D^i T[\phi],$$

for every $i \in \mathbb{Z}_{\geq 0}$.

**Proof.** See [45]. \hfill \Box

The operation of convolution with distributions is very useful in the development of regularization techniques, and fundamental solutions for differential equations using Fourier transforms [17, 35].

Starting from convolutions of two functions, the convolution of a distribution and a $\mathcal{D}(\mathbb{R})$ function, and the convolution of two distributions, will be defined.

If $h : \mathbb{R} \to \mathbb{R}$ is a function and $x \in \mathbb{R}$, the translation $\tau_x h$ and the reflection $\hat{h}$ are the functions defined by

$$(\tau_x h)(y) \overset{\text{def}}{=} h(y - x),$$

$$\hat{h}(y) \overset{\text{def}}{=} h(-y),$$

for $y \in \mathbb{R}$. Now, let $f$ and $g$ be integrable functions on $\mathbb{R}$, then the convolution of $f$ and $g$, denoted by $f * g$, is the function defined by

$$(f * g)(x) \overset{\text{def}}{=} \int_{\mathbb{R}} f(y)g(x - y) \, dy = \int_{\mathbb{R}} f(y)((\tau_x \hat{g})(y)) \, dy.$$
The translation of a distribution, and the convolution of distributions with $\mathcal{D}(\mathbb{R})$ functions, are presented in Definition 9 and Definition 10, respectively.

**Definition 9 (Translation).** The translation of $T \in \mathcal{D}^*(\mathbb{R})$ is the distribution

$$\tau_x T : \mathcal{D}(\mathbb{R}) \longrightarrow \mathbb{R}$$

$$\phi \longmapsto \tau_x T[\phi] \overset{\text{def}}{=} T[\tau_x \phi].$$

**Definition 10 (Convolution between distributions and test functions).** Let $T \in \mathcal{D}^*(\mathbb{R})$ and $\phi \in \mathcal{D}(\mathbb{R})$. The convolution of $T$ and $\phi$ is defined as the function

$$(T \ast \phi)(x) \overset{\text{def}}{=} T[\tau_x \hat{\phi}] \text{ for } x \in \mathbb{R}.$$

Theorem 4 states the following properties of the convolution between distributions and $\mathcal{D}(\mathbb{R})$ functions: (i) Commutativity of the convolution with translations, (ii) associativity of the convolution and (iii) regularization of distributions by convolution.

**Theorem 4 (Properties of convolution between distributions and test functions).** Suppose $T \in \mathcal{D}^*(\mathbb{R})$ and $\phi, \psi \in \mathcal{D}(\mathbb{R})$. Then

(i) $\tau_x (T \ast \phi) = (\tau_x T) \ast \phi = T \ast (\tau_x \phi)$ for all $x \in \mathbb{R}$.

(ii) $T \ast (\phi \ast \psi) = (T \ast \phi) \ast \psi$.

(iii) $T \ast \phi \in C^\infty(\mathbb{R})$ and

$$(T \ast \phi)^{(i)} = (\mathcal{D}^iT) \ast \phi = T \ast \phi^{(i)}$$

for every $i \in \mathbb{N}$.

**Proof.** See [45].

One of the notable properties of the Dirac-delta distribution is that it behaves as a unit element for the convolution, i.e.,

$$\delta \ast \phi = \phi,$$
for all $\phi \in D(\mathbb{R})$. Moreover, if $\{f_n(x)\}_{n \in \mathbb{N}} \subset D(\mathbb{R})$ is the sequence of real functions in (3.2) that generates a sequence of regular distributions converging to $\delta$, then

$$\lim_{n \to \infty} T * f_n = T \text{ in } D^*(\mathbb{R}),$$

(3.3)

for all $T \in D^*(\mathbb{R})$ [45]. Therefore, property (iii) in Theorem 4 and (3.3) imply that every distribution is a uniform limit of a sequence of infinitely differentiable functions (regularization).

The convolution of two distributions can be defined, assuming that at least one of the distributions has compact support. Under that additional assumption

$$T \in D^*(\mathbb{R}) \text{ and } \phi \in D(\mathbb{R}) \implies T * \phi \in D(\mathbb{R}).$$

The support of a distribution, and the convolution of two distributions, are presented in Definition 11 and Definition 12, respectively.

**Definition 11** (Support of a distribution). The support of $T \in D^*(\mathbb{R})$ is the smallest closed set $\Omega \subset \mathbb{R}$ which satisfies the condition

$$\phi \in D(\mathbb{R}) \text{ and support of } \phi \text{ contained in } \mathbb{R} - \Omega \implies T[\phi] = 0.$$

**Definition 12** (Convolution of two distributions). Suppose $T, V \in D^*(\mathbb{R})$, and at least one of these two distributions has compact support. Then, the convolution of $T$ and $W$ is the distribution defined by

$$T * V : D(\mathbb{R}) \longrightarrow \mathbb{R} \quad \phi \longmapsto (T * V)[\phi] \stackrel{\text{def}}{=} (T * (V * \hat{\phi}))(0).$$

In Theorem 5, the following properties of the convolution between distributions are enunciated: (i) commutativity of the convolution, (ii) associativity of the convolution, (iii) the distributional derivative can be regarded as convolutions with derivatives of
the Dirac-delta distribution and (iv) commutativity of the convolution with differentiation.

**Theorem 5** (Properties of convolution between distributions). Suppose $T, V, W \in \mathcal{D}^*(\mathbb{R})$. Then

(i) If at least one of the distributions $T, V$ has compact support, then

$$T * V = V * T.$$  

(ii) If at least two of the distributions $T, V, W$ have compact support, then

$$(T * V) * W = T * (V * W).$$  

(iii) If $\delta$ is the Dirac-delta distribution and $i \in \mathbb{Z}_{\geq 0}$, then

$$\mathcal{D}^i T = (\mathcal{D}^i \delta) * T.$$  

In particular, $T = \delta * T$.

(iv) If at least one of the distributions $T, V$ has compact support, then

$$\mathcal{D}^i (T * V) = (\mathcal{D}^i T) * V = T * \mathcal{D}^i V,$$

for every $i \in \mathbb{Z}_{\geq 0}$.

**Proof.** See [45].
3.2 Regularization of the Dirac-delta

In Section 3.1 it was shown that the Dirac-delta is the distribution defined by

\[ \delta : \mathcal{D}(\mathbb{R}) \rightarrow \mathbb{R} \]
\[ \phi \mapsto \delta[\phi] \overset{\text{def}}{=} \phi(0). \]

and its distributional derivative is the regular distribution \( T_H \), generated by the Heaviside function in (3.1).

The Dirac-delta can be represented as the limit of an infinite converging sequence of regular distributions. Such sequences are called delta-sequences and to generate them, we build on Theorem 6.

**Theorem 6 (Delta-sequences).** Let \( f \) be a nonnegative locally integrable function in \( \mathbb{R} \) such that \( \int_{\mathbb{R}} f(x) \, dx = 1 \) and let \( \{T^f_n\}_{n \in \mathbb{N}} \) be the sequence of regular distributions defined by

\[ T^f_n[\phi] \overset{\text{def}}{=} \int_{\mathbb{R}} \delta^f_n(x) \phi(x) \, dx \text{ for } \phi \in \mathcal{D}(\mathbb{R}), \]

where \( \delta^f_n(x) \overset{\text{def}}{=} nf(nx) \). Then \( \{\delta^f_n\}_{n \in \mathbb{N}} \) is a delta-sequence, i.e.,

\[ \lim_{n \to \infty} T^f_n[\phi] = \delta[\phi], \]

for all \( \phi \in \mathcal{D}(\mathbb{R}). \)

**Proof.** See [33].

In Theorem 6, \( f \) is known as the generating function of the delta-sequence. Sometimes, instead of \( \delta^f_n(x) \), \( T^f_n[\phi] \) and \( n \to \infty \), it is convenient to use the parametric family of functions.
\begin{align*}
\delta^f_\varepsilon(x) & \overset{\text{def}}{=} \frac{1}{\varepsilon} f \left( \frac{x}{\varepsilon} \right), \\
T^f_\varepsilon[\phi] & \overset{\text{def}}{=} \int_{\mathbb{R}} \delta^f_\varepsilon(x) \phi(x) \, dx,
\end{align*}

for the scaling parameter \( \varepsilon \to 0^+ \).

In practical applications, \( f \) is commonly selected as an even function with a maximum value at \( x = 0 \), which concentrates nonzero values in the neighborhood of the origin. The compactness of the support is a desired property because in practical approximations of \( \delta \) functions on grids it reduces the number of numerical evaluations on \( f \). However, these properties and the positiveness of \( f \) (according to Theorem 6) are not necessary conditions to generate delta-sequences. Counterexamples of functions that do not satisfy those properties but generate delta-sequences are given and plotted in Figure 4.

![Figure 4: Delta-sequences generated by the function \( f \) with scaling parameter \( \varepsilon = 0.1 \).](image)

In Theorem 7, we present an improved version of Theorem 6, eliminating the restriction of positiveness on \( f \) and establishing a necessary condition (vanishing moments) to obtain any desired order of accuracy in the approximation to the Dirac-delta distribution.

**Theorem 7** (Moment conditions on delta-sequences). Let \( f \) be a locally integrable function satisfying the condition \( \int_{\mathbb{R}} f(x) \, dx = 1 \) with \( m \in \mathbb{N} \) vanishing moments, i.e.,

\[
(i) \quad \int_{\mathbb{R}} x^i f(x) \, dx = 0 \quad \text{for} \quad i = 1, \ldots, m.
\]
(ii) \( 0 < \left| \int_{\mathbb{R}} x^{m+1} f(x) \, dx \right| < \infty. \)

Then, \( \delta^f_\epsilon(x) \) is \((m + 1)\)th order accurate delta-sequence.

Proof. The Taylor’s theorem on \( \phi \in \mathcal{D}(\mathbb{R}) \) leads to
\[
\phi(x) = \phi(0) + \sum_{i=1}^{m} \frac{\phi^{(i)}(0)}{i!} x^i + \frac{\phi^{(m+1)}(\xi)}{(m + 1)!} x^{m+1},
\]
for some \( \xi \) between 0 and \( x \). Thus,
\[
\lim_{\epsilon \to 0^+} T^f_\epsilon[\phi] = \phi(0) + \left( \frac{\phi^{(m+1)}(\xi)}{(m + 1)!} \int_{\mathbb{R}} x^{m+1} f(x) \, dx \right) \lim_{\epsilon \to 0^+} \epsilon^{m+1} = \phi(0).
\]

Under the assumptions of Theorem 7, the delta-sequence reaches a certain order of accuracy if the integral \( T^f_\epsilon[\phi] \) is computed exactly. However, the quadrature rules typically used in numerical approximations introduce errors. More precisely, if \( Q \left( \delta^f_\epsilon \phi \right) \) denotes the numerical approximation of \( T^f_\epsilon[\phi] \), through a quadrature rule, the quadrature error in the approximation of \( \delta[\phi] \) by \( Q \left( \delta^f_\epsilon \phi \right) \) can be expressed as
\[
\delta[\phi] - Q \left( \delta^f_\epsilon \phi \right) = \left( \delta[\phi] - T^f_\epsilon[\phi] \right) + \left( T^f_\epsilon[\phi] - Q \left( \delta^f_\epsilon \phi \right) \right). \tag{3.4}
\]
The accuracy of the first term in (3.4) is \( \mathcal{O}(\epsilon^{m+1}) \) whereas the second term depends on the quadrature rule. Ideally, the accuracy of the second term is \( \mathcal{O}(\epsilon^{m+1}) \), so that it is accurate with order comparable to the first term. Using this as a criteria, we restrict the second term to estimate the scaling parameter \( \epsilon \) and preserve the accuracy established in Theorem 7.

Based on a specific family of quadrature rules, in Proposition 1, we propose the following theoretical result in choosing the optimal scaling parameter \( \epsilon \), keeping the accuracy of the delta-sequence in Theorem 7.
Proposition 1 (Optimal scaling for delta-sequences). Let \( f \in C^k([a,b]) \) be a function satisfying the hypothesis in Theorem 7, \( \phi \in D(\mathbb{R}) \) with compact support \([a,b] \subset \mathbb{R}\), and \( Q \) a quadrature rule on \([a,b]\) with \( N+1 \) nodes such that the quadrature error satisfies one of the following conditions:

\[
|T_\varepsilon^f [\phi] - Q(\delta_\varepsilon^f \phi)| \leq \kappa N^{-k} \left| (\delta_\varepsilon^f \phi)^{(k)}(\xi) \right| \text{ for } \xi \in (a,b), \quad (3.5)
\]

or

\[
|T_\varepsilon^f [\phi] - Q(\delta_\varepsilon^f \phi)| \leq \kappa N^{-k} \left\| (\delta_\varepsilon^f \phi)^{(k)} \right\|_{L^1_w(a,b)}, \quad (3.6)
\]

where \( \kappa \in \mathbb{R}_{>0} \) and \( w(x) \) denote a constant and a nonnegative weight function, respectively. Then, by taking the optimal scaling parameter \( \varepsilon = O\left(N^{-k/(m+k+2)}\right) \), the quadrature error (3.4) will be \( O(e^{m+1}) \).

Proof. By the Leibnitz rule, it follows that the \( k \)th derivative of \( \delta_\varepsilon^f \phi \) with \( x \in (a,b) \) is

\[
(\delta_\varepsilon^f \phi)^{(k)}(x) = \sum_{i=0}^{k} \binom{k}{i} (\delta_\varepsilon^f)^{(i)}(x) \phi^{(k-i)}(x)
= \sum_{i=0}^{k} \binom{k}{i} \frac{1}{\varepsilon^{i+1}} f^{(i)}(\frac{x}{\varepsilon}) \phi^{(k-i)}(x),
\]

and the continuity of the derivatives leads to

\[
\left| (\delta_\varepsilon^f \phi)^{(k)}(x) \right| \leq \frac{\tilde{C}}{\varepsilon^{k+1}}, \quad \varepsilon \in \mathbb{R}_{>0}, \quad \varepsilon \in (0,1).
\]

Thus, for \( \varepsilon = O\left(N^{-k/(m+k+2)}\right) \) we have

\[
|T_\varepsilon^f [\phi] - Q(\delta_\varepsilon^f \phi)| \leq \tilde{C} \frac{N^{-k}}{\varepsilon^{k+1}} = \tilde{C} \varepsilon^{m+1}, \quad \tilde{C} \in \mathbb{R}_{>0}.
\]

\( \square \)

According to Proposition 1, the smoothness on \( f \) is required in the convergence of the numerical integration. Some examples of quadrature rules that satisfy the condition (3.5) in Proposition 1 are the composite version of trapezoidal, midpoint, and
Simpson and Newton–Cotes rules \[43\]. Condition (3.6) is satisfied by the Clenshaw–Curtis quadrature \[56\].

In Table 1 we present some of the most common delta-sequences $\delta^f_\epsilon$ in the literature \[1, 33, 39, 46\], specifying the generating function ($f$), number of vanishing moments ($m$), smoothness ($C^k(\mathbb{R})$), and compact support ([a, b]). $W_n$ denotes the $n$th degree piecewise polynomial in $C^{n-1}(\mathbb{R})$ known as cardinal B-spline, defined as

$$W_n(x) \overset{\text{def}}{=} (W_0 \ast W_{n-1})(x) = \int_\mathbb{R} W_0(x - y)W_{n-1}(y) \, dy \text{ for } n \in \mathbb{N},$$

where

$$W_0(x) \overset{\text{def}}{=} \begin{cases} 1, & |x| \leq \frac{1}{2}, \\ 0, & |x| > \frac{1}{2}, \end{cases}$$

and the coefficients $c_i$ in the expression for $K_n$ are chosen such that

$$\sum_{i=-n}^{n} c_i \int_\mathbb{R} W_n(x)(x+i)^q \, dx = \begin{cases} 1, & q = 0, \\ 0, & q = 1, \ldots, 2n. \end{cases}$$

<table>
<thead>
<tr>
<th>$f$</th>
<th>$m$</th>
<th>$k$</th>
<th>[a, b]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$</td>
<td>1</td>
<td>$\infty$</td>
<td>$\times$</td>
</tr>
<tr>
<td>$\frac{1}{2} \exp(-</td>
<td>x</td>
<td>)$</td>
<td>1</td>
</tr>
<tr>
<td>$\frac{1}{\sqrt{\pi}} (\frac{3}{2} - x^2) \exp(-x^2)$</td>
<td>3</td>
<td>$\infty$</td>
<td>$\times$</td>
</tr>
<tr>
<td>$(\pi(x^2 + 1))^{-1}$</td>
<td>1</td>
<td>$\infty$</td>
<td>$\times$</td>
</tr>
<tr>
<td>$\frac{1}{2} \text{sech}^2(x)$</td>
<td>1</td>
<td>$\infty$</td>
<td>$\times$</td>
</tr>
<tr>
<td>$W_n(x) \overset{\text{def}}{=} W_{n-1} \ast W_0$</td>
<td>1</td>
<td>$n - 1$</td>
<td>$\left[\frac{-n+1}{2}, \frac{n+1}{2}\right]$</td>
</tr>
<tr>
<td>$K_n(x) \overset{\text{def}}{=} \sum_{i=-n}^{n} c_i W_n(x-i)$</td>
<td>2$n$</td>
<td>$n - 1$</td>
<td>$\left[\frac{-3n+1}{2}, \frac{3n+1}{2}\right]$</td>
</tr>
</tbody>
</table>

Table 1: Generating function ($f$), number of vanishing moments ($m$), smoothness ($C^k(\mathbb{R})$), and compact support ([a, b]) for the delta-sequence $\delta^f_\epsilon(x) \overset{\text{def}}{=} \frac{1}{\epsilon} f\left(\frac{x}{\epsilon}\right)$.

In order to control the overall accuracy in the approximation, we propose the use of the optimal scaling given in Proposition 1 with a compactly supported delta-sequence that has any variable number of vanishing moments and smoothness. Specifically, we
consider the piecewise mixed polynomials presented in [55], which are characterized by Theorem 8.

**Theorem 8** (Mixed polynomials). Given integers \(m \geq 0\) and \(k \geq -1\), there exists a polynomial \(P_{m}^{k} : [-1, 1] \rightarrow \mathbb{R}\) which is uniquely determined by the following conditions:

(i) \(\int_{-1}^{1} P_{m}^{k}(\xi) \, d\xi = 1\).

(ii) \((P_{m}^{k})^{(i)}(\pm 1) = 0\) for \(i = 0, \ldots, k\).

(iii) \(\int_{-1}^{1} \xi^{i} P_{m}^{k}(\xi) \, d\xi = 0\) for \(i = 1, \ldots, m\).

It is a polynomial of degree \(2(\lfloor \frac{m}{2} \rfloor + k + 1)\), containing only even powers of \(\xi\). Moreover,

\[
\delta_{\varepsilon}^{m, k}(x) \equiv \begin{cases} \frac{1}{\varepsilon} P_{m}^{k}(\frac{x}{\varepsilon}), & |x| \leq \varepsilon, \\ 0, & |x| > \varepsilon \end{cases}
\]

is a \((m + 1)\)th order accurate delta-sequence in \(C^{k}(\mathbb{R})\) with compact support \([-\varepsilon, \varepsilon]\).

**Proof.** See [55]. \(\square\)

The polynomials \(P_{m}^{k}\) in Theorem 8 are mixed in the sense that they are expressed as the product of two polynomials controlling independently the moment and smoothness conditions [55]. Indeed, they have the general form

\[
P_{m}^{k}(\xi) = c w_{k}(\xi) Q(\xi), \quad Q(\xi) = 1 - \sum_{j=1}^{\lfloor \frac{m}{2} \rfloor} \langle 1, r_{2j} \rangle_{w_{k}} r_{2j}(\xi),
\]

where \(\langle \cdot, \cdot \rangle_{w_{k}}\) denotes the usual weighted inner product on \(C^{0}([-1, 1])\) with positive weight function \(w_{k}(\xi) = (1 - \xi^{2})^{k+1}\), \(\{r_{j}\}_{j=1}^{m}\) is an orthonormal basis for span \(\{\xi^{j}\}_{j=1}^{m}\) associated to \(\langle \cdot, \cdot \rangle_{w_{k}}\), and \(c = 1/\langle Q, 1 \rangle_{w_{k}}\). In addition, the delta-sequence induces the following \(C^{k+1}(\mathbb{R})\) approximation to the Heaviside function:

\[
H_{\varepsilon}^{m, k}(x) \equiv \int_{-\infty}^{x} \delta_{\varepsilon}^{m, k}(\xi) \, d\xi = \int_{-\varepsilon}^{x} \delta_{\varepsilon}^{m, k}(\xi) \, d\xi.
\]
An equivalent and more practical representation of $H_{\epsilon}^{m,k}$ is presented in Theorem 9.

**Theorem 9 (Regularized Heaviside function).** Given integers $m \geq 0$ and $k \geq 0$, there exists a polynomial $R_{m,k} : [-1, 1] \rightarrow \mathbb{R}$ which is uniquely determined by the following conditions:

(i) $R_{m,k}(-1) = 0$ and $R_{m,k}(1) = 1$.

(ii) $(R_{m,k})^{(i)}(\pm 1) = 0$ for $i = 1, \ldots, k + 1$.

(iii) $\int_{-1}^{1} \xi^i R_{m,k}(\xi) \, d\xi = \frac{1}{i+1}$ for $i = 0, \ldots, m - 1$.

Moreover, $R_{m,k}$ can be expressed as

$$R_{m,k}(\xi) = \frac{1}{2} + r_{m,k}(\xi),$$

where $r_{m,k}$ is a polynomial of degree $2 \left\lfloor \frac{m+1}{2} \right\rfloor + 2k + 1$ containing only odd powers of $\xi$ and

$$H_{\epsilon}^{m,k}(x) = \begin{cases} 
1, & x > \epsilon, \\
R_{m,k} \left( \frac{x}{\epsilon} \right), & |x| \leq \epsilon, \\
0, & x < -\epsilon.
\end{cases} \quad (3.9)$$

**Proof.** See [55]. \qed

In Table 2 and Figures 5 and 6, we present the essential coefficients and factors of the generating polynomials with $\delta_{\epsilon}^{m,k}$ and $H_{\epsilon}^{m,k}$ for $m = 1, 3, 5$ and $k = 0, 1, 2$. 

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Table 2: Constant $c$, polynomials $Q$ and $r_{m,k}$ to generate $P_{m,k}$, $R_{m,k}$ in (3.8), (3.9), respectively.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$k$</th>
<th>$c$</th>
<th>$Q(\xi)$</th>
<th>$r_{m,k}(\xi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>$\frac{3}{4}$</td>
<td>1</td>
<td>$\frac{3\xi - \xi^3}{4}$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$\frac{15}{16}$</td>
<td>1</td>
<td>$\frac{15\xi - 10\xi^3 + 3\xi^5}{16}$</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$\frac{35}{32}$</td>
<td>1</td>
<td>$\frac{35\xi^3 - 35\xi + 21\xi^2 - 9\xi^7}{32}$</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>$\frac{45}{32}$</td>
<td>$1 - \frac{7}{5}\xi^2$</td>
<td>$\frac{45\xi - 50\xi^3 + 21\xi^5}{32}$</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>$\frac{105}{64}$</td>
<td>$1 - 3\xi^2$</td>
<td>$\frac{105\xi - 175\xi^3 + 147\xi^5 - 45\xi^7}{64}$</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>$\frac{945}{512}$</td>
<td>$1 - \frac{11}{30}\xi^2$</td>
<td>$\frac{945\xi - 2100\xi^3 + 2646\xi^5 - 1620\xi^7 + 385\xi^9}{512}$</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>$\frac{525}{256}$</td>
<td>$1 - 6\xi^2 + \frac{33}{5}\xi^4$</td>
<td>$\frac{525\xi - 1225\xi^3 + 1323\xi^5 - 495\xi^7}{256}$</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>$\frac{4725}{2048}$</td>
<td>$1 - \frac{22}{15}\xi^2 + \frac{143}{15}\xi^4$</td>
<td>$\frac{4725\xi - 14700\xi^3 + 23814\xi^5 - 17820\xi^7 + 5005\xi^9}{2048}$</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>$\frac{10395}{4096}$</td>
<td>$1 - \frac{26}{95}\xi^2 + \frac{13}{95}\xi^4$</td>
<td>$\frac{10395\xi - 40425\xi^3 + 87318\xi^5 - 98010\xi^7 + 55059\xi^9 - 122885\xi^{11}}{4096}$</td>
</tr>
</tbody>
</table>

Figure 5: Polynomial $P_{m,k}$ for $m = 1, 3, 5$, $k = 2$ (left) and $k = 0, 1, 2$, $m = 3$ (right).
3.3 Smoothing of piecewise functions

The mixed polynomial presented in Theorem 8 can be used to regularized discontinuities of Lebesgue integrable functions that are smooth on compact subsets of $\mathbb{R}$, with arbitrary accuracy and smoothness, through the operation of convolution. This approach is particularly relevant in the representation of singular sources arising in the numerical simulation of particle-laden flows with shocks [29].

Concretely, given $S \in L^1(\mathbb{R})$, let $S^{m,k}_\epsilon$ be the function defined by the convolution

$$S^{m,k}_\epsilon(x) \overset{\text{def}}{=} (S * \delta^{m,k}_\epsilon)(x) = \int_{\mathbb{R}} S(\xi) \delta^{m,k}_\epsilon(x - \xi) \, d\xi = \int_{x-\epsilon}^{x+\epsilon} S(\xi) \delta^{m,k}_\epsilon(x - \xi) \, d\xi. \quad (3.10)$$

Then, $S^{m,k}_\epsilon(x)$ is a $C^k(\mathbb{R})$ class function that converges to $S$ in the $L^1(\mathbb{R})$ sense. This follows from Proposition 2 and Theorem 10, a classical result of real analysis.

**Proposition 2.** Suppose that $f \in L^1(\mathbb{R})$, $g \in C^k(\mathbb{R})$ and the derivatives $g^{(i)}$ are bounded for $i = 0, \ldots, k$. Then $f * g \in C^k(\mathbb{R})$ and $(f * g)^{(i)} = f * g^{(i)}$.

**Proof.** See [16].

**Theorem 10.** Let $\varphi \in L^1(\mathbb{R})$ such that $\int_{\mathbb{R}} \varphi(\xi) \, d\xi = 1$ and let $\varphi_\epsilon(x) \overset{\text{def}}{=} \frac{1}{\epsilon} \varphi\left(\frac{x}{\epsilon}\right)$. If $f \in L^1(\mathbb{R})$, then $f * \varphi_\epsilon$ converge to $f$ in the $L^1(\mathbb{R})$ norm as $\epsilon \to 0^+$.  

Figure 6: Polynomial $R^{m,k}$ for $m = 1, 3, 5, k = 2$ (left) and $k = 0, 1, 2, m = 3$ (right).
Proof. See [16].

An arbitrary order of accuracy in the approximation of $S$ by (3.10) can be achieved locally, according to the number of vanishing moments $m$. We establish this result in Theorem 11.

**Theorem 11 (Smoothing).** Let $S \in L^1(\mathbb{R})$ and let $[a,b] \subset \mathbb{R}$ be a compact set. If $S \in C^m([a,b])$ and $S^{(m+1)}$ exists and is bounded on $(a,b)$, then $S^{m,k}_\epsilon$ converges pointwise to $S$ on $(a,b)$ as $\epsilon \to 0^+$. Moreover,

$$S^{m,k}_\epsilon(x) - S(x) = O(\epsilon^{m+1}) \text{ for } x \in (a + \epsilon, b - \epsilon). \quad (3.11)$$

**Proof.** Let $\epsilon > 0$ be sufficiently small such that $\epsilon < \frac{b-a}{2}$. Expanding $S$ in a Taylor series on $\zeta \in [a,b]$, around $x \in (a + \epsilon, b - \epsilon)$, we obtain

$$S^{m,k}_\epsilon(x) = \sum_{j=0}^{m} \frac{S^{(j)}(x)}{j!} \int_{a}^{b} (\zeta - x)^j \delta^{m,k}_\epsilon(\zeta - x) \, d\zeta \quad + \quad \frac{1}{(m+1)!} \int_{a}^{b} (\zeta - x)^{m+1} \delta^{m,k}_\epsilon(\zeta - x) S^{(m+1)}(\zeta) \, d\zeta,$$

for some $\zeta$ between $\zeta$ and $x$. Note that since $[-\epsilon,\epsilon] \subset (a - x, b - x)$,

$$\int_{a}^{b} (\zeta - x)^i \delta^{m,k}_\epsilon(\zeta - x) \, d\zeta = \epsilon^i \int_{-1}^{1} |\xi|^i P^{m,k}(\xi) \, d\xi = \begin{cases} 1, & i = 0, \\ 0, & i = 1, \ldots, m, \end{cases}$$

and therefore

$$|S(x) - S^{m,k}_\epsilon(x)| \leq \frac{\kappa \epsilon^{m+1}}{(m+1)!} \int_{-1}^{1} |\xi|^m |P^{m,k}(\xi)| \, d\xi,$$

for some constant $\kappa \in \mathbb{R}_+$. \hfill \square

In computational implementations, the use of numerical integration to evaluate (3.10) is required. The main challenge is to preserve the $(m+1)$th order of accuracy.
established in (3.11), when \( S^m_k \) is replaced by an approximation \( \tilde{S}^m_k \) computed with a quadrature formula. According to Theorem 11, the error estimation

\[
\left| S(x) - \tilde{S}^m_k(x) \right| \leq \underbrace{\left| S(x) - S^m_k(x) \right|}_{\mathcal{O}(\varepsilon^{m+1}) \text{ by (3.11)}} + \left| S^m_k(x) - \tilde{S}^m_k(x) \right|,
\]

shows that the desired order of accuracy can be reached by imposing the following condition on the quadrature error:

\[
S^m_k(x) - \tilde{S}^m_k(x) = \mathcal{O}(\varepsilon^{m+1}) \text{ for } x \in (a + \varepsilon, b - \varepsilon). \tag{3.12}
\]

Generally, the quality of the approximation resulting from quadrature rules depends on continuity, the number of continuous derivatives and the magnitude of the integrand. Observe that

\[
\frac{\partial^i \left( S(\xi) \delta^m_k(x - \xi) \right)}{\partial \xi^i} = \frac{1}{\varepsilon^{l+1}} \frac{\partial^i \left( S(\xi) P^m_k \left( \frac{x - \xi}{\varepsilon} \right) \right)}{\partial \xi^i},
\]

for any integer \( i \geq 0 \) and \( \xi \in (x - \varepsilon, x + \varepsilon) \). Thus, an arbitrarily small choice of the scaling parameter \( \varepsilon \) might affect the validity of (3.12).

In Proposition 3, we shall introduce an optimal scaling parameter that preserves the \((m + 1)\)th order of accuracy in (3.12). Without loss of generality, suppose that \( \tilde{S}^m_k \) is computed using the composite Newton–Cotes formulas (closed) [12] on \( N_p \) subintervals \( \left\{ [\xi_i, \xi_{i+1}] \right\}_{i=0}^{N_p-1} \) given by the points

\[
\xi_0 = a < \xi_1 < \cdots < \xi_{N_p} = b,
\]
where $q$ is a nonnegative integer denoting the degree of exactness of the quadrature rule, $\alpha_{ij}$ are the quadrature weights, $h_i = (\xi_{i+1} - \xi_i) / q$, $\kappa$ is a constant independent of the integrand and $h_i$, and $\zeta_i \in (\xi_i, \xi_{i+1})$.

**Proposition 3** (Optimal scaling for smoothing). Under the hypotheses in Theorem 11, suppose that $m, k \geq 2$ and let $q \leq \min\{m, k\} - 1$ be the degree of exactness in the Newton–Cotes quadrature rule. Then

$$S(x) - S^{m,k}_\varepsilon(x) = O(\varepsilon^{m+1}) \text{ for } x \in (a + \varepsilon, b - \varepsilon),$$

provided that the optimal scaling parameter $\varepsilon = O \left( \left( \sum_{i=0}^{N_p-1} h_i^{q+2} \right)^{1/(m+q+3)} \right)$.

**Proof.** From (3.13), it follows that

$$S^{m,k}_\varepsilon(x) - S^{m,k}_\varepsilon(x) = \kappa \sum_{i=0}^{N_p-1} h_i^{q+2} \frac{\partial^{q+1} \left( S(\xi) \delta^{m,k}_\varepsilon(x - \zeta) \right)}{\partial \xi^{q+1}} \bigg|_{\xi = \xi_i}.$$ 

In [53], it has been proven that

$$\frac{\partial^{q+1} \left( S(\xi) \delta^{m,k}_\varepsilon(x - \zeta) \right)}{\partial \xi^{q+1}} \bigg|_{\zeta = \xi_i} = O \left( \frac{1}{\varepsilon^{q+2}} \right) \text{ for } i = 0, \ldots, N_p - 1;$$

and hence, (3.12) leads to the proposed optimal scaling parameter. \qed
3.4 Extension to higher dimensions

Let $\mathcal{D}(\mathbb{R}^d)$ be the set of $C^\infty(\mathbb{R}^d)$ functions $\varphi: \mathbb{R}^d \to \mathbb{R}$ whose support is compact and contained in $\mathbb{R}^d$. The space of distributions in $\mathbb{R}^d$, denoted by $\mathcal{D}^*(\mathbb{R}^d)$, is defined as the set of all continuous linear functionals $T: \mathcal{D}(\mathbb{R}^d) \to \mathbb{R}$.

The generalized differentiation for distributions is presented in Definition 13. Under this operation, every distribution has derivatives of all orders.

**Definition 13 (Differentiation in several variables).** Given $T \in \mathcal{D}^*(\mathbb{R}^d)$ and $i = (i_1, \ldots, i_d) \in \mathbb{Z}^d$ a $d$-tuple of nonnegative integers, the $i$th partial derivative of $T$ is defined as the distribution

$$\partial^i T : \mathcal{D}(\mathbb{R}^d) \longrightarrow \mathbb{R}$$

$$\varphi \longmapsto \partial^i T[\varphi] \overset{\text{def}}{=} (-1)^{|i|} T[\partial_1^{i_1} \cdots \partial_d^{i_d} \varphi],$$

where $|i| \overset{\text{def}}{=} i_1 + \cdots + i_d$, and $\partial_j^{i_j}$ is the usual partial differential operator, i.e.,

$$\partial_j^{i_j} \varphi(x) \overset{\text{def}}{=} \frac{\partial^{i_j} \varphi}{\partial x_j^{i_j}},$$

$$\partial_1^{i_1} \cdots \partial_d^{i_d} \varphi(x) \overset{\text{def}}{=} \frac{\partial^{|i|} \varphi}{\partial x_1^{i_1} \cdots \partial x_d^{i_d}},$$

for $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$.

Based on Theorem 12, the high-order regularization technique with optimal scaling to approximate the one-dimensional Dirac-delta distribution, presented in Section 3.2, can be extended to higher dimensions by tensor product.

**Theorem 12 (Tensor product of distributions).** Let $T_x \in \mathcal{D}^*(\mathbb{R}^d)$ and $V_y \in \mathcal{D}^*(\mathbb{R}^q)$. Then, there exist a unique distribution $W_{x,y} \in \mathcal{D}^*(\mathbb{R}^{d+q})$ satisfying

$$W_{x,y}[\varphi(x) \psi(y)] = T_x[\varphi(x)] V_y[\psi(y)],$$

for $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$ and $y = (y_1, \ldots, y_q) \in \mathbb{R}^q$. 

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for all $\phi \in D(\mathbb{R}^d)$ and $\psi \in D(\mathbb{R}^q)$. Moreover, this unique distribution, known as tensor product of $T_x$ and $V_y$, is defined by

$$(T_x \otimes V_y)[\phi(x,y)] \overset{\text{def}}{=} T_x[V_y[\phi(x,y)]] = V_y[T_x[\phi(x,y)]] ,$$

for every $\phi \in D(\mathbb{R}^{p+q})$.

**Proof.** See [17].

The Dirac-delta in $D^*(\mathbb{R}^d)$ is the distribution defined by

$$\delta_{x_1,\ldots,x_d} : D(\mathbb{R}^d) \longrightarrow \mathbb{R}$$

$$\phi \longmapsto \delta_{x_1,\ldots,x_d}[\phi(x_1,\ldots,x_d)] \overset{\text{def}}{=} \phi(0,\ldots,0) .$$

(3.14)

Now, Theorem 12 allows us to represent $\delta_{x_1,\ldots,x_d}$ as the tensor product of one-dimensional Dirac-delta distributions, i.e.,

$$\delta_{x_1,\ldots,x_d} = \bigotimes_{i=1}^{d} \delta_{x_i} ,$$

where

$$\delta_{x_i}[\phi(x_1,\ldots,x_{i-1},x_i,x_{i+1},\ldots,x_d)] = \phi(x_1,\ldots,x_{i-1},0,x_{i+1},\ldots,x_d) .$$

Moreover, if $\{f_n(\xi)\}_{n \in \mathbb{N}}$ is a sequence of real functions such that the regular distribution

$$T_{f_n}[\phi] \overset{\text{def}}{=} \int_{\mathbb{R}} f_n(\xi)\phi(\xi) \, d\xi \text{ for } \phi \in D(\mathbb{R}) ,$$

converges pointwise to the one-dimensional Dirac-delta distribution, then

$$T_{f_n(x_1),\ldots,f_n(x_d)}[\phi] \overset{\text{def}}{=} \int_{\mathbb{R}^d} \left(\prod_{i=1}^{d} f_n(x_i)\right) \phi(x_1,\ldots,x_d) \, dx_1 \cdots dx_d \text{ for } \phi \in D(\mathbb{R}^d) ,$$

defines a distribution in $D^*(\mathbb{R}^d)$ that converges pointwise to $\delta_{x_1,\ldots,x_d}$.
We propose to approximate the Dirac-delta in (3.14) by using the tensor product of the one-dimensional regularization $\delta^{m,k}_\varepsilon$ in Theorem 8 and the respective cartesian product of the regularization zone $[-\varepsilon, \varepsilon]$, where $\varepsilon$ is the optimal scaling in Proposition 1. However, an error analysis of this approach has not been fully established.
Chapter 4

Numerical Experiments

Computations of shocked particle-laden flows in a PSIC framework (described in Chapter 1) are typically restricted to second order accuracy at best. The main components of the PSIC method are the following:

(i) Solution of hyperbolic conservation laws governing the carrier flow (Eulerian frame).

(ii) Integration of ODEs for particle’s position and velocity (Lagrangian frame).

(iii) Interpolation of the flow properties at the particle’s position.

(iv) Evaluation of weighted summation of Dirac-delta sources to account particle’s effect on the carrier flow.

High-order schemes for computations of (i), (ii), and (iii), are available in the literature (see Chapter 2). However, the high-order accurate representation of (iv) (i.e., the singular source term) on nonuniform grids has not been fully accomplished (see Chapter 3), causing difficulties to develop high-order PSIC methods.

In the PSIC framework, the singular source term is expressed as

\[ S(x,t) \overset{def}{=} \sum_{i=0}^{N_p} \frac{W(x,\xi_i(t))}{n(\xi_i(t))} \delta(x - \xi_i(t)) \]  \hspace{1cm} (4.1)

for \((x,t) \in \mathbb{R}^d \times [0,\infty)\); where \(\xi_i : [0,\infty) \rightarrow \mathbb{R}^d\) denotes the position of the \(i\)th particle at time \(t\), \(n(\xi_i(t))\) is the number density of the \(i\)th particle, \(W\) is a weight function describing the influence of each particle onto the carrier flow, and \(\delta\) is the Dirac-delta distribution.
The presence of the Dirac-delta in (4.1) leads to sharp particle interface discontinuities in the source term. This is illustrated in Figure 7, for a distribution of isolated particles (single particle case) and clustered particles (multiple particles case). The discontinuous interfaces may yield to nonphysical oscillations in the solution or low order of accuracy away of the singularities, even considering only one particle (see Chapter 3).

\[ S(x, t) \]

Clustered particle

Single particle

\( x \)

Figure 7: One-dimensional representation of particle interface discontinuities in the singular source term (4.1).

We propose to use the high-order regularization technique in Theorem 8 (Theorem 11) with the optimal scaling parameter in Proposition 1 (Proposition 3) to regularize the Dirac-delta in (4.1) with high-order of accuracy away from the singularities in the numerical solution of hyperbolic conservation laws.

This chapter shows numerical results in the solutions of a linear and a nonlinear scalar hyperbolic conservation law with a singular source, as well as the nonlinear Euler equations with singular sources, a system of hyperbolic conservation laws governing compressible fluid dynamics with shocks and particles. The Chebyshev collocation method (spectral) discretizes the spatial derivatives in the scalar equation tests. A multi-domain hybrid spectral-WENO method discretizes the Euler equations.
The chapter is divided into two sections. In Section 4.1, we present numerical results for both, scalar and systems of hyperbolic conservation laws with a single and nonstationary singular source term. In Section 4.2, we assess the accuracy of the Chebyshev collocation method and the high-order regularization technique in the solution of an advection and inviscid Burgers equation with a weighted summation of Dirac-delta sources with stationary singularities.

4.1 Single Particle

Singular Advection Equation

Consider the first order advection PDE:

\[
\begin{aligned}
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= \delta \left( x + \frac{t}{4} \right), \\
u(x, 0) &= \sin(\pi x) , \\
u(-1, t) &= \sin(\pi (-1 - t))
\end{aligned}
\]

with \((x, t) \in [-1, 1] \times [0, 2]\) and a nonstationary singular source term given by the Dirac-delta distribution, whose analytical solution in the distributional sense (it satisfies the PDE when the respective distributional derivatives are taken) is

\[
u(x, t) = \sin(\pi (x - t)) + \frac{4}{5} \left( H \left( x + \frac{t}{4} \right) - H(x - t) \right),
\]

where \(H\) denotes the Heaviside function in (3.1).

The respective regularized problem is obtained by substituting \(\delta\) with an approximation based on a regularization technique. The respective analytical solution of the regularized PDE becomes

\[
u_\epsilon(x, t) = \sin(\pi (x - t)) + \frac{4}{5} \left( H_\epsilon \left( x + \frac{t}{4} \right) - H_\epsilon(x - t) \right),
\]
where \( H_\epsilon \) denotes the regularized Heaviside function induced by the approximate Dirac-delta. We will study the accuracy of the Chebyshev collocation method in the solution of the regularized problem, compared with the analytical solution of (4.2). For time integration up to \( t = 2 \), we will use the third order TVD Runge–Kutta scheme with a time step \( \Delta t = \frac{\lambda}{N^2} \) and \( \lambda = 0.5 \) representing the Courant–Friedrich–Lewy (CFL) number. The inflow boundary flux at \( x = -1 \) is implemented at each Runge–Kutta stage.

The pointwise error in the numerical solution of (4.2) is separated into two parts: a regularization error and a spectral interpolation error, i.e.,

\[
u(x,t) - u_\epsilon^N(x,t) = (u(x,t) - u_\epsilon(x,t)) + (u_\epsilon(x,t) - u_\epsilon^N(x,t)),
\]

where the first term in the right hand side is the regularization error and the second term is the spectral interpolation error. The pointwise error is dominated by the first term inside the regularization zone and the spectral interpolation error outside of that zone.

In problem (4.2), the classical convergence results for spectral methods do not apply, as these rely on the regularity of the source term. Lack of smoothness in the regularization of \( \delta \) can lead to instabilities and Gibbs type phenomena that affect the accuracy of the numerical scheme. Therefore, with the regularization techniques, it can be expected that the global accuracy of the numerical scheme outside the regularization zone depends solely on the accuracy in smooth parts of the solution. A regularization with \( k \) continuous derivatives leads to a regularized Heaviside function in \( C^{k+1}(\mathbb{R}) \), and thus, the expected order of convergence in the spectral interpolation of (4.4) is \((k+1)\)th order [5].

First, we consider some of the approximations presented in Table 1: the top-hat function \( W_0(x) \), the high-order accurate SIAC filter \( K_3(x) \) and the Gaussian function \( f(x) \overset{\text{def}}{=} \frac{1}{\sqrt{\pi}} \left( \frac{3}{2} - x^2 \right) \exp(-x^2) \). The top-hat function and the SIAC filter have to be defined on a uniform grid; therefore, following the procedure in [28], they are numerically evaluated on \( N + 1 \) equidistant points and subsequently projected onto
the spectral grid through first and third order central Lagrange interpolation, respectively. The Gaussian function is directly evaluated on the spectral grid. Theoretically, the scaling parameter $\varepsilon$ of the regularization of the delta-sequence should be chosen sufficiently small in order to obtain an accurate representation of the Dirac-delta. Based on $[15, 31, 32, 46]$, we take the optimal scaling $\varepsilon = \frac{4}{N}$ for all these regularization techniques.

Figure 8 shows the spectral solution when $\delta$ is regularized with the top-hat function. The lack of smoothness in the source term yields a solution with Gibbs oscillations.

![Figure 8: Analytical and spectral solution to (4.2) at $t = 2$ for $N = 30, 60, 120, 240, 480$, when $\delta$ is regularized with the top-hat function and the optimal scaling $\varepsilon = \frac{4}{N}$.](image)

Figures 9 and 10 show the spectral solution (left) and the pointwise error (right) when $\delta$ is regularized with the high-order accurate SIAC filter $K_3(x)$ and the Gaussian function, respectively. In both cases, the spectral approximation converges to the analytical solution, performing a sharp capture of the jump discontinuity with an increasing $N$. However, the spectral solution does not reach the expected formal order of convergence under grid refinement. These results show that the smoothness in the regularized source term is not a necessary condition in obtaining high-order accurate spectral solutions.
Using the same scaling $\varepsilon = \frac{4}{N}$, let us consider our proposed high-order regularization $\delta_m^k$ presented in Theorem 8, choosing particularly $m = 3$ vanishing moments and $k = 2$ continuous derivatives. The moment condition ensures a high-order accurate representation of the Dirac-delta, whereas the smoothness determines high-order convergence ($(k+1)$th order) of the spectral solution to the analytical one in (4.3), outside of the regularization zone. However, as shown in Figure 11, the spectral solution exhibits an oscillatory behavior.
Figure 11: Analytical and spectral solution to (4.2) at $t = 2$ for $N = 30$, when $\delta$ is regularized with $\delta^{m,k}_\epsilon$ and scaling parameter $\epsilon = \frac{4}{N}$.

Instead of using $\epsilon = \frac{4}{N}$, we use the optimal scaling as proposed in Proposition 1. Figure 12 shows a comparison between the analytical and spectral solutions at $t = 2$ for $N = 30, 60, 120, 240, 480$. In contrast to the high-order accurate SIAC filter and Gaussian function, the spectral solution performs an excessive smoothing of the jump discontinuity contained within the regularization zone $\mathcal{R}_\epsilon \equiv \left[ -\frac{1}{2} - \epsilon, -\frac{1}{2} + \epsilon \right]$ for large $N$. However, as illustrated in Figure 13 and Table 3, on $Q_\epsilon \equiv [-1, 1] - \mathcal{R}_\epsilon$ (outside of the regularization zone), the regularization with the optimal scaling leads to a high-order accurate spectral solution according to the asymptotic behavior of the interpolation error, i.e., $O(N^{-2.92})$.

Figure 12: Analytical and spectral solution (left), and pointwise error (right) to (4.2) at $t = 2$ for $N = 30, 60, 120, 240, 480$, when $\delta$ is regularized with $\delta^{3,2}_\epsilon$ and the optimal scaling $\epsilon = N^{-2/7}$. 
Figure 13: Error in $\| \cdot \|_{L^2_w}$ norm and linear regression to estimate convergence order on $Q_\epsilon$ to (4.2) at $t = 2$, when $\delta$ is regularized with $\delta^3_\epsilon$ and the optimal scaling $\epsilon = N^{-2/7}$.

<table>
<thead>
<tr>
<th>N</th>
<th>$\epsilon$</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.37</td>
<td>×</td>
</tr>
<tr>
<td>60</td>
<td>0.31</td>
<td>2.67</td>
</tr>
<tr>
<td>120</td>
<td>0.25</td>
<td>3.01</td>
</tr>
<tr>
<td>240</td>
<td>0.20</td>
<td>3.08</td>
</tr>
<tr>
<td>480</td>
<td>0.17</td>
<td>2.73</td>
</tr>
</tbody>
</table>

Table 3: Optimal scaling $\epsilon$ and convergence order $p$ in $\| \cdot \|_{L^2_w}$ norm of the spectral solution on $Q_\epsilon$ to (4.2) at $t = 2$, when $\delta$ is regularized with $\delta^3_\epsilon$.

Singular Inviscid Burgers Equation

Let us consider the following Riemann problem for the inviscid Burgers equation with a nonstationary singular source term:

\[
\begin{cases}
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( \frac{u^2}{2} \right) = \delta \left( x + \frac{t}{4} \right), \\
u(x,0) = \frac{1}{4} + H(x), \\
u(-1,t) = \frac{1}{4},
\end{cases}
\]  

(4.5)
and \((x,t) \in [-1,1] \times [0,2]\). This problem admits a solution in the distributional sense given by

\[
u(x,t) = \frac{1}{4} + H \left( x + \frac{t}{4} \right).
\]

It consists of a discontinuity traveling to the left with speed \(\frac{1}{4}\), according to the generalized Rankine–Hugoniot condition for hyperbolic conservation laws with singular source terms [41].

For this problem, we compute the spectral solution of the respective regularized problem with the same setup as given for the problem in Section 4.2. Figure 14 shows the analytical solution, the spectral solution, and the pointwise error for the Burgers equation. Similarly to Section 4.2, choosing the optimal scaling parameter \(\varepsilon = N^{-2/7}\), we compute a numerical solution which regularizes the jump discontinuity at \(x = \frac{1}{2}\) on the regularization zone \(R_{\varepsilon}\) and is approximately \(O(N^{-3.2})\) convergent on \(Q_{\varepsilon}\), as illustrated in Figure 15 and Table 4.

![Figure 14: Analytical and spectral solution (left), and pointwise error (right) to (4.5) at \(t = 2\) for \(N = 30, 60, 120, 240, 480\), when \(\delta\) is regularized with \(\delta_{\varepsilon}^{3,2}\) and the optimal scaling \(\varepsilon = N^{-2/7}\).](image)

\[\begin{array}{cccccc}
N & 30 & 60 & 120 & 240 & 480 \\
\varepsilon & 0.37 & 0.31 & 0.25 & 0.20 & 0.17 \\
p & \times & 2.90 & 3.74 & 2.81 & 3.01 \\
\end{array}\]

Table 4: Optimal scaling \(\varepsilon\) and convergence order \(p\) in \(\|\cdot\|_{L^2}^{3,2}\) norm of the spectral solution on \(Q_{\varepsilon}\) to (4.5) at \(t = 2\), when \(\delta\) is regularized with \(\delta_{\varepsilon}^{3,2}\).
Figure 15: Error in $\| \cdot \|_{L_2}$ norm and linear regression to estimate convergence order on $Q_\varepsilon$ to (4.5) at $t = 2$, when $\delta$ is regularized with $\delta_\varepsilon^{3,2}$ and the optimal scaling $\varepsilon = N^{-2/7}$.

Singular System of Euler Equations

For a more rigorous and realistic example, we consider the numerical solution of a one-dimensional coupled system of conservation laws arising in the simulation of particle dispersion in a shocked flow [29], where the carrier flow is governed by the Euler equations for gas dynamics with a singular source term, and the particle motion is modeled through kinematic equations.

The governing equations for the carrier flow are

$$\frac{\partial}{\partial t} Q(x,t) + \frac{\partial}{\partial x} F(Q) = S(x,t),$$

(4.6)

where:

$$Q \overset{\text{def}}{=} \begin{bmatrix} \rho, \rho u, E \end{bmatrix},$$

$$F(Q) \overset{\text{def}}{=} \begin{bmatrix} \rho u, \rho u^2 + P, (E + P)u \end{bmatrix},$$

$$S(x,t) \overset{\text{def}}{=} \begin{bmatrix} 0, \frac{m_p}{\tau_p} (u(x_p,t) - v_p) \delta(x - x_p), 0 \end{bmatrix}$$

with the equation of state for ideal gas:

$$P = (\gamma - 1) \left( E - \frac{1}{2} \rho u^2 \right), \quad \gamma = 1.4.$$
In these equations, \((4.6)\) represents the conservation of mass, momentum, and total energy for the fluid. The source term \(S\) accounts for the effect of momentum and energy generated by an individual particle of mass \(m_p\), whose position \(x_p(t)\) and velocity \(v_p(t)\) are governed by the following equations:

\[
\begin{align*}
\frac{dx_p}{dt} &= v_p, \\
\frac{dv_p}{dt} &= \frac{u(x_p, t) - v_p}{\tau_p},
\end{align*}
\]

where \(\tau_p\) is the particle response time. In particular, we take \(m_p = 1\) and \(\tau_p = 1\).

The initial Riemann data of a Mach 3 shock flow for \((4.6)\) is given by

\[
\begin{bmatrix}
\rho, \ u, \ P
\end{bmatrix} = \begin{cases}
\begin{bmatrix}
3.857143, \ 2.629369, \ 10.333333
\end{bmatrix}, & -5 \leq x < 0, \\
\begin{bmatrix}
1, \ 0, \ 1
\end{bmatrix}, & 0 \leq x \leq 15,
\end{cases}
\]

and the initial conditions for \((4.7)\) are \(\begin{bmatrix} x_p(0), \ v_p(0) \end{bmatrix} = \begin{bmatrix} -3, \ 0 \end{bmatrix}\).

In contrast to Sections 4.2 and 4.1, the numerical solution of the Euler equations requires the use of nonlinear shock capturing schemes to avoid Gibbs oscillations produced by the spectral solution around the shocks. We developed a high-order multidomain scheme which approximates the nonlinear system of hyperbolic conservation laws \((4.6)\) with the multidomain hybrid spectral-WENO method as described in \([10, 11]\), combined with a hybrid spectral-ENO interpolation to compute the velocity of the fluid at the particle position \(x_p\) in \((4.7)\). The high-order MR analysis \([23]\) is used to switch between the spectral and ENO/WENO schemes \([49]\) when a certain level of tolerance is reached. The overall goal of the hybridization is to reduce the computational cost required by the ENO/WENO schemes, approximating the solution with the spectral method in regions where it is sufficiently smooth.

In the numerical experiments, the physical domain is divided into twenty subdomains as follows:

\([-5, 15] = \bigcup_{i=1}^{20} [i-6, i-5] , \]
where initially, the subdomains $[-1, 0]$ and $[0, 1]$ will be using the fifth order ENO/WENO schemes and spectral scheme in the remainder. The number of grid points on each spectral and WENO subdomain is denoted by $N_S$ and $N_W$, respectively. A sixth order MR analysis with tolerance level for the multiresolution coefficient equal to $5 \times 10^{-3}$ for switching is used. Time integration up to $t = 3.5$ is performed with the third order TVD Runge–Kutta scheme and a CFL number equal to 0.5. The approximation of the singular source is carried out by $\delta_3^2$, taking the optimal scaling $\epsilon = (N_S - 1)^{-2/7}$ and $\epsilon = (N_W - 1)^{-2/7}$ for the hybrid and WENO schemes, respectively. Due to the absence of an analytical solution, we compare the numerical approximations computed with the hybrid and WENO schemes.

The solution for the fluid variables are expected to be a right-moving shock with large gradients generated by the singular source along the locus $x = x_p(t)$. Figure 16 shows the numerical solution for the density computed with the hybrid at $t = 0.5$ and $t = 1$, indicating the respective numerical scheme (spectral or WENO). Figure 17 shows the numerical solution for the density computed with the hybrid ($N_S = 15, 31, 61$ and $N_W = 31, 61, 121$) and WENO ($N_W = 121$) schemes at $t = 3.5$. As time evolves, the singular source generates a large gradient at $x = x_p(0)$ which moves to the right (slower than the particle) and is located approximately at $x = -2.32$. In addition, for $t \in (0, 1.4]$, a large gradient at the particle position is observed. The hybrid scheme uses the WENO method for computation around these singularities, as well as for the tracking of the initial shock at $x = 0$. The approximations obtained with the hybrid and WENO schemes for the density and particle position are in very close agreement.
In the numerical simulation of particle-laden flow with shocks, the WENO scheme is ideally suited for computations of a shock wave interacting with a cloud of particles due to the complicated shock structure of the problem, and the importance of preserving high orders of accuracy to resolve the small scale interactions [29]. On subdomains with single particles away from the cloud and shocks we would like to perform computations with the more efficient spectral method and avoid the computationally expensive MR analysis for switching. However, the hybrid scheme might switch to WENO near these single particles.

In order to explore the viability of this modification on the hybrid scheme and improve its computational efficiency, we modify the hybrid scheme such that it does not switch to WENO on subdomains with single particles where there is no shock.
The numerical solution for the density computed with the modified hybrid scheme is shown in Figure 18. In contrast to the solution computed with the hybrid scheme at $t = 3.5$ (left in Figure 17), it can be observed that a different location of the jump discontinuity is created by the singular source at $x = -2.32$, with respect to the solution computed by the WENO scheme. However, the computations for the particle position (right in Figure 18) with these modified-hybrid and WENO schemes are very similar.

![Figure 18: Numerical solution for the density at $t = 3.5$ (left) and particle position, computed with the modified-hybrid and WENO schemes for $N_S = 15, 31, 61$, $N_W = 31, 61, 121$.](image)

### 4.2 Multiple Particles

**Singular Advection Equation**

Consider the following first order advection PDE on the domain $(x, t) \in [-1, 1] \times [0, 2]$:

$$
\begin{align*}
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= \frac{3 \cos(5\pi x)}{s(x)} \left( H \left( x + \frac{3}{10} \right) - H \left( x - \frac{3}{10} \right) \right), \\
\quad s(x) &= \begin{cases} 
N_S = 15, N_W = 31 \\
N_S = 31, N_W = 61 \\
N_S = 61, N_W = 121 
\end{cases} \\
\quad u(x, 0) &= \sin(\pi x), \\
\quad u(-1, t) &= \sin(\pi(-1 - t)),
\end{align*}
$$

(4.8)
where $H$ denotes the Heaviside function in (3.1) and $S \in C^0([-1,1])$ denotes the singular source term, whose first order derivative is discontinuous at $x = \pm \frac{3}{10}$. The analytical solution to (4.8) is the $C^0([-1,1])$ function

$$u(x,t) = \sin(\pi(x - t)) + \int_{x-t}^{x} S(\xi) \, d\xi, \quad (4.9)$$

which has discontinuous first order derivatives at $x = \pm \frac{3}{10} + t$.

In (4.8), the source term leads to first order singularities in the analytical solution (4.9). When approximating (4.8) with a Chebyshev collocation method combined with a third order TVD Runge–Kutta scheme, spectral accuracy is prevented by Gibbs oscillations, as illustrated in Figure 19, where $u^N(x,2)$ denotes the spectral solution at $t = 2$ using $N + 1$ Gauss–Lobatto nodes with the CFL condition $\Delta t = 0.5/N^2$.

![Figure 19: Analytical and spectral solution (left), and pointwise error (right) to (4.8) at $t = 2$ for $N = 60, 120, 240, 480$, without regularization of $S$.](image)

To suppress the Gibbs phenomenon, we shall henceforth approximate the singular source term $S$ by the smooth function $S_{\varepsilon}^{m,k} \in C^k([-1,1])$ in (3.13), using the composite Simpson quadrature rule on $N_p + 1$ nonuniform points given by

$$\xi_i = \frac{3}{10} \sin \left( \pi \left( -\frac{1}{2} + \frac{i}{N_p} \right) \right) \text{ for } i = 0, \ldots, N_p,$$

and the optimal scaling parameter $\varepsilon$ in Proposition 3. Without loss of generality, we consider $N_p + 1 = 2000$ (see Figure 20). The same accuracy can be obtained by
using a more accurate quadrature rule with fewer points, for instance, a five points
Newton–Cotes quadrature rule with $N_P + 1 = 300$.

We assess accuracy within three separate zones of the spatial domain $\Omega \overset{\text{def}}{=} [-1, 1]$, i.e.,

$$\mathcal{P}_\varepsilon \overset{\text{def}}{=} \left( \xi_0 + \varepsilon, \xi_{N_P} - \varepsilon \right),$$

$$\mathcal{R}_\varepsilon \overset{\text{def}}{=} \left[ \xi_0 - \varepsilon, \xi_0 + \varepsilon \right] \cup \left[ \xi_{N_P} - \varepsilon, \xi_{N_P} + \varepsilon \right],$$

$$\mathcal{Q}_\varepsilon \overset{\text{def}}{=} \Omega - (\mathcal{P}_\varepsilon \cup \mathcal{R}_\varepsilon).$$ (4.10) (4.11)

Specifically, $\mathcal{P}_\varepsilon$ contains the particles $\{\xi_i\}_{i=0}^{N_P}$. On $\mathcal{R}_\varepsilon$, the singularities in $S$ are re-
moved by using a smooth function (polynomial). Within $\mathcal{Q}_\varepsilon$, the compactness of the
support in $\delta_{\varepsilon}^{m,k}$ (see Theorem 8) implies that $S$ and $\tilde{S}_{\varepsilon}^{m,k}$ are equal.

Let us now study the accuracy of the spectral method applied to (4.8) when $S$ is replaced by the regularization $\tilde{S}_{\varepsilon}^{k,A}$ shown in Figure 20 (left), compared with the analytical solution (4.9). The spectral solution computed with $N + 1$ Gauss–Lobatto
nodes using the regularized source term will be denoted by $u_N^{\varepsilon}(x,t)$. Since $\tilde{S}_{\varepsilon}^{m,k} \in C^k([-1, 1])$, we expect to have a convergence of $O \left( N^{-(k+1)} \right)$ on $\mathcal{P}_\varepsilon \cup \mathcal{Q}_\varepsilon$ with the
regularization of the singular source term. On $\mathcal{R}_\varepsilon$, the regularization error clearly
will cause a loss of accuracy.

![Figure 20: Singular source, regularized source for $m = 7$, $k = 4$ and optimal scaling $\varepsilon = 6.6 \times 10^{-2}$ (left), and pointwise error (right) on $N + 1$ spectral points.](image)
In Figure 21, the analytical and spectral solution (left) and the respective pointwise error (right) at \( t = 2 \) are shown. The regularization improves the accuracy of the spectral solution on \( P_\varepsilon \cup Q_\varepsilon \) with grid refinement, as opposed to Figure 19, where the spectral solution was computed without regularization of \( S \). Figure 22 shows the convergence order on \( P_\varepsilon \) (left) and \( Q_\varepsilon \) (right), which has been estimated using linear regression to fit the respective \( L^2 \) error. The convergence is faster than \( O \left( N^{-(k+1)} \right) \) (superconvergence), i.e., \( O \left( N^{-6.45} \right) \) and \( O \left( N^{-7.71} \right) \) on \( P_\varepsilon \) and \( Q_\varepsilon \), respectively.

![Figure 21: Analytical and spectral solution (left), and pointwise error (right) to (4.8) at \( t = 2 \) for \( N = 60, 120, 240, 480 \), when \( S \) is regularized with \( S^7_\varepsilon \) and the optimal scaling \( \varepsilon = 6.6 \times 10^{-2} \).](image)

![Figure 22: Error in \( \| \cdot \|_{L^2} \) norm and linear regression to estimate convergence order on \( P_\varepsilon \) (left) and \( Q_\varepsilon \) (right) to (4.8) at \( t = 2 \), when \( S \) is regularized with \( S^7_\varepsilon \) and the optimal scaling \( \varepsilon = 6.6 \times 10^{-2} \).](image)

Fixing \( k \), the accuracy of the spectral solution is controlled by \( m \) and the optimal scaling \( \varepsilon \). For \( k = 4 \), the expected \( O \left( N^{-(k+1)} \right) \) convergence on \( P_\varepsilon \cup Q_\varepsilon \) requires at least \( m = 7 \) vanishing moments. By increasing \( m \), a more accurate representation
of the singular source on $P_\epsilon$, through the regularization, is obtained. However, the optimal scaling $\epsilon$ increases as long as $m$ does it, so that an arbitrary large choice of $m$ can lead to a violation of the condition $\epsilon < \frac{3}{10}$ (see proof in Theorem 11), i.e., an increase in the size of the regularization zone $R_\epsilon$ where high-order of accuracy will not be reached. In terms of accuracy of the spectral solution, superconvergence is observed for $m \geq 7$. Results for $m = 1, 5, 9, 13, 17$ and $k = 4$ are summarized in Table 5.

| $m$ | $\epsilon$ | $\log_{10}|S(x) - S^{m,k}(x)|$ on $P_\epsilon$ | Conv. order on $P_\epsilon$ | Conv. order on $Q_\epsilon$ |
|-----|-------------|-----------------------------------------------|-----------------------------|-----------------------------|
| 1   | $6.5 \times 10^{-3}$ | $O \left(10^{-4}\right)$ | 1.56 | 2.36 |
| 5   | $4.0 \times 10^{-2}$ | $O \left(10^{-7}\right)$ | 5.42 | 6.66 |
| 9   | $9.5 \times 10^{-2}$ | $O \left(10^{-9}\right)$ | 7.48 | 8.00 |
| 13  | $1.5 \times 10^{-1}$ | $O \left(10^{-11}\right)$ | 7.32 | 8.21 |
| 17  | $2.1 \times 10^{-1}$ | $O \left(10^{-14}\right)$ | 8.15 | 8.60 |

Table 5: Number of vanishing moments $m$, optimal scaling $\epsilon$, pointwise error in the regularization of the source term on $P_\epsilon$, and convergence order of the spectral solution on $P_\epsilon$ and $Q_\epsilon$ to (4.8) at $t = 2$, when $S$ is regularized with $S^{m,4}$.

**Singular Inviscid Burgers Equation**

We now consider the inviscid Burgers equation on the domain $(x,t) \in [0,2] \times [0,2]$

\[
\begin{aligned}
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( \frac{u^2}{2} \right) &= S(x - 1), \\
\quad u(x,0) &= x, \\
\quad u(0,t) &= 0.
\end{aligned}
\]  

(4.12)

where $S$ is the singular source term in (4.8). The smooth initial data was chosen such that the corresponding homogeneous problem does not develop shock discontinuities caused by the nonlinearity of the flux function.
In analogy with what was done in Section 4.2, we shall evaluate the accuracy of the Chebyshev collocation method with \( N+1 \) Gauss–Lobatto nodes in the solution of (4.12) on the zones of the spatial domain \( \Omega \overset{\text{def}}{=} [0, 2] \) defined in (4.10) and (4.11), when \( S \) is regularized by \( S^\mu_{\varepsilon,k} \), using the composite Simpson quadrature rule and \( N_p + 1 = 2000 \) nonuniform points \( \xi_i = 1 + \frac{3}{10} \sin \left( \pi \left( -\frac{1}{2} + \frac{i}{N_p} \right) \right) \) for \( i = 0, \ldots, N_p \).

We compute the spectral solution at \( t = 2 \) with a 12th order exponential filter for stabilization, taking \( N = 100, 200, 300, 400 \). Due to the absence of analytical solution, the respective error is estimated by comparison with a spectral solution \( \tilde{u}_\varepsilon(x, 2) \) on a finer grid (\( N = 500 \)).

The spectral solution (left) and pointwise error (right) for \( m = 13, k = 4 \) and optimal scaling \( \varepsilon = 1.5 \times 10^{-1} \), are shown in Figure 23. The spectral solution exhibits an oscillatory behavior around \( x = \frac{7}{10} \) (where the first derivative of \( S \) is discontinuous), which decays as \( N \) increases. The convergence on \( P_\varepsilon \) and \( Q_\varepsilon \) is approximately \( O\left( N^{-5.34} \right) \) and \( O\left( N^{-5.61} \right) \), respectively (see Figure 24). The expected \( O\left( N^{-(k+1)} \right) \) requires at least \( m = 13 \) vanishing moments. Table 6 summarizes results for \( m = 5, 9, 13, 17 \) and \( k = 4 \). In contrast to the results in Section 4.2, superconvergence as \( m \) increases is not observed.

![Figure 23](image-url)  
**Figure 23:** Spectral solution (left), and pointwise error (right) to (4.12) at \( t = 2 \) for \( N = 100, 200, 300, 400 \), when \( S \) is regularized with \( S^\mu_{13,4} \) and the optimal scaling \( \varepsilon = 1.5 \times 10^{-1} \).
Figure 24: Error in $\| \cdot \|_{L^2}$ norm and linear regression to estimate convergence order on $P_\varepsilon$ (left) and $Q_\varepsilon$ (right) to (4.12) at $t = 2$, when $S$ is regularized with $S^{13,4}_\varepsilon$ and the optimal scaling $\varepsilon = 1.5 \times 10^{-1}$.

<table>
<thead>
<tr>
<th>$k$ = 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$</td>
</tr>
<tr>
<td>---</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>9</td>
</tr>
<tr>
<td>13</td>
</tr>
<tr>
<td>17</td>
</tr>
</tbody>
</table>

Table 6: Number of vanishing moments $m$, optimal scaling $\varepsilon$, pointwise error in the regularization of the source term on $P_\varepsilon$, and convergence order of the spectral solution on $P_\varepsilon$ and $Q_\varepsilon$ to (4.12) at $t = 2$, when $S$ is regularized with $S^{m,A}_\varepsilon$. 

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Chapter 5

Conclusions and Future Work

A regularization technique with optimal scaling based on piecewise polynomials with compact support, has been proposed to approximate Dirac-delta sources on general grids, in the numerical solution of hyperbolic conservation laws arising in the simulation of particle-laden flows with shocks with the PSIC method.

Specifically, we consider two cases. First, a single nonstationary Dirac-delta source (single particle case) in the numerical solution of a linear advection equation with smooth initial data, a Riemann problem for the inviscid Burgers equation, and the Euler equations in gas dynamics for simulation of shocked particle-laden flows. Second, the weighted summation of stationary Dirac-delta sources (multiple particles case) in the numerical solution of a linear advection and inviscid Burgers equations with smooth initial data.

In the single particle case, the numerical experiments were focused in the study of the accuracy of Chebyshev collocation method in the solution of the advection and Burgers problems, and a comparison between the multi-domain hybrid spectral-WENO and WENO schemes in the solution of the Euler equations.

For the advection and Burgers problems, we have shown that regardless of the smoothness on the approximation to the singular source, an arbitrary choice for the scaling parameter of the regularized delta-sequence can produce numerical oscillations in the spectral solution. However, our criterion to select the optimal scaling leads to high-order accurate spectral solutions outside of the regularization zone, according to the asymptotic behavior of the spectral interpolation error. The accuracy of the spectral method is controlled by the smoothness of the regularization whereas
the number of vanishing moments determine the accuracy in the representation of
the Dirac-delta distribution.

In the numerical solution of the Euler equations, the hybrid scheme is in good
agreement with the WENO method under grid refinement. The modified-hybrid
scheme, which uses only the spectral method to compute the solution at the particle
position, produces a numerical solution with a small deviation from the WENO in
capturing the location of a large gradient generated by the singular source at the
initial position of the particle.

In the multiple particles case, we assess the accuracy of the regularization and
the Chebyshev collocation method under the assumption of a clustered distribution
of Dirac-delta singularities. The regularization approximates the source term with
high-order of accuracy away from the singularities, according to the number of van-
ishing moments, smoothness and the optimal scaling parameter. The regularization
leads to the expected order of accuracy in the spectral solution of both problems away
from the singularities, at a certain number of vanishing moments. In particular, su-
perconvergence was observed in the linear advection problem as long as the number
of vanishing moments increases.

The results corresponding to the single particle and multiple particles case illus-
trate the viability of the regularization technique with optimal scaling to respectively
represent the contribution of isolated and clustered particles, in the particle-laden
flow simulation with the PSIC method. However, this ideal particle distribution can
be altered by the influence of the carrier flow, scattering the particles and creating a
sparse distribution.

Future work aims to represent the singular source term with a sparse distribution
of particles by modifying the weights in the multiple particles cases, while preserving
the accuracy in the studied cases in this dissertation.
Bibliography


