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Dissertation Thesis Abstract

Implicit numerical methods for some scalar hyperbolic equations

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ABSTRACT

This thesis presents a novel approach to solving hyperbolic partial differential equations by developing a higher order compact implicit numerical schemes based on the finite volume method. Unlike traditional explicit schemes, which are often limited by stringent stability requirements, the proposed implicit method allows for larger time steps without sacrificing stability.

To ensure high resolution results and prevent nonphysical oscillations, the scheme integrates Essentially Non-Oscillatory (ENO) and Weighted Essentially Non-Oscillatory (WENO) spatial reconstructions along with nonlinear flux limiting in time. The method is further enhanced to accommodate space-dependent velocities, and to be used to solve nonlinear transport problems characterized by various sorption isotherms with a focus on the Freundlich type of isotherm, which are important in modeling contaminant migration in porous media and in applications such as liquid chromatography. Computational efficiency is achieved through the implementation of a fast sweeping method, significantly reducing the computational effort typically associated with implicit solvers.

The effectiveness of the developed schemes is demonstrated on representative linear and nonlinear problems in one and two dimensions; and also on transport equations with nonlinear sorption isotherms. We demonstrate the effectiveness of high resolution methods in minimizing oscillations near discontinuities, thereby increasing the accuracy of the solution.

Keywords: hyperbolic problems; conservation law; higher order accuracy; compact implicit scheme; advection equation; Burgers equation; transport problem; sorption isotherm; Freundlich isotherm.

ABSTRACT

Táto dizertačná práca prezentuje nový prístup k riešeniu hyperbolických parciálnych diferenciálnych rovníc prostredníctvom vývoja kompaktných implicitných numerických schém vyššieho rádu presnosti založených na metóde konečných objemov. Na rozdiel od tradičných explicitných schém, ktoré sú často obmedzené prísnymi požiadavkami na stabilitu, navrhovaná implicitná metóda umožňuje používať väčšie časové kroky bez straty stability.

Na zabezpečenie vysokého rozlíšenia výsledkov a prevenciu nefyzikálnych oscilácií, schéma integruje priestorové rekonštrukcie typu ENO (Essentially Non-Oscillatory) a WENO (Weighted Essentially
Non-Oscillatory), spolu s nelineárnym limiterom toku v čase. Metóda je ďalej rozšírená tak, aby zohľadňovala rýchlosti závislé od priestorovej veličiny a aby mohla byť použitá na riešenie nelineárnych transportných problémov charakterizovaných rôznymi sorpčnými izotermami, so zameraním na Freundlichovu izotermu. Tá je dôležitá pri modelovaní migrácie kontaminantov v pórovitých médiách a v aplikáciách, ako je kvapalinová chromatografia. Výpočtová efektivita je dosiahnutá pomocou implementácie *fast sweeping* metódy, čím sa výrazne znižuje výpočtová náročnosť typická pre riešenie implicitných schém.

Účinnosť vyvinutých schém je demonštrovaná na reprezentatívnych lineárnych a nelineárnych problémoch v jednej a dvoch dimenziách, ako aj na rovniciach reprezentujúcich transport s nelineárnymi sorpčnými izotermami. Taktiež práca prezentuje, že metódy s vysokým rozlíšením efektívne minimalizujú oscilácie v blízkosti nespojitostí, čím zvyšujú presnosť riešenia.

Kľúčové slová: hyperbolické rovnice; zákon zachovania; schémy vyššieho rádu presnosti; kompaktná implicitná schéma; rovnica advekcie; Burgersova rovnica; sorpčná izoterma; Freundlichova izoterma.

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1

Introduction

When numerically solving time-dependent partial differential equations (PDEs), a key decision is the choice of time discretization—explicit or implicit. Explicit methods, are simple and computationally cheap but require stability-based restrictions on time steps. Implicit methods, while unconditionally stable, involve solving algebraic systems, which can be costly.

The main difference between explicit and implicit time discretization methods is significantly relaxed in the case when the term with the time derivative in the PDE is nonlinear. In such cases, even explicit time discretization methods can lead to algebraic equations for the values of the numerical solution.

Many numerical methods apply time and space discretizations separately, often using spatial semi-discretization to reduce PDEs to systems of ODEs. However, preserving structural properties of hyperbolic PDEs often necessitates a more integrated approach.

Concerning implicit methods (or their combinations with explicit methods), we can mention the class of Runge-Kutta (RK) methods used for hyperbolic problems in [1, 3, 4, 6, 14, 21–24]. Furthermore, it is recognized that further improvements can be achieved if, contrary to standard RK methods, not only the values of the right-hand side function are used, but also its derivatives. This approach is realized in the development of two- or multi-derivative RK methods [26, 28], available also in the form of implicit methods [15, 33]. Although all these methods are very well developed, their application is not straightforward

if certain structural properties of the solution for hyperbolic equations are to be preserved not only by space discretization but also by the time discretization.

The idea of implicit time discretization using the LW procedure involving the mixed spatial-temporal derivatives [10, 12, 13] can be used not only to enhance the stability of the method but also to improve the solvability of the resulting algebraic systems.

In this thesis, we extend the approach of solving hyperbolic problems by extending the compact implicit numerical scheme in several important directions, building upon a previous work such as [13]. The presented schemes are based on the finite volume method, which provides enhanced flexibility, particularly for problems involving nonuniform grids [27], in contrast to the finite difference method that is generally restricted to uniform grids. A significant methodological improvement over earlier studies [13, 19] is the avoidance of the fractional time step method. By eliminating this approach, we remove time splitting errors that can undermine accuracy [18] and instead introduce a more universal scheme with a newly developed solution procedure.

To avoid unphysical oscillations, this thesis proposes a high resolution form of the compact implicit scheme using an Essentially Non-Oscillatory (ENO) and a Weighted Essentially Non-Oscillatory (WENO) reconstruction in space [27], and a nonlinear limiting in time using a flux limiter. We treat here a space dependent velocity situations and relate the computations of parameters in the numerical scheme with theoretical results on a preservation of non-negative coefficients in the final numerical scheme. To further increase the efficiency of the method, we apply the procedures with the approach to compute the parameters in the ENO and WENO approximations. We implement the fast sweeping method with proper orderings of unknowns in each Gauss-Seidel iteration to avoid a large

number of iterations being used.

In this work, we also apply such a numerical schemes to the transport equation with nonlinear sorption isotherms. Such models are used to describe the transport of contaminants in porous media when contaminant adsorption on pore skeletons must be taken into account [11]. Other interesting applications of such models are in liquid chromatography technology [16]. We show that to solve related representative mathematical models, the computational cost of the compact implicit scheme is comparable to explicit schemes, but with the clear advantage of no stability requirement for the implicit scheme.

The main purpose of this study, is to show that, following these guidelines, the resulting compact implicit scheme can deliver accurate numerical solutions for representative scalar hyperbolic equations. The main motivation is to show that if the method is used as an implicit, a good accuracy can be obtained in standard numerical experiments that is significantly improved with respect to the implicit first order accurate scheme. Consequently, the dominant criterion for the choice of time steps is the accuracy of numerical resolution for the solution phenomena that are of interest, and no restriction on the time step is required due to the stability requirement that might be related to some uninteresting phenomena. In this initial study, we do not compute numerical examples in which such stability requirements are presented, which we plan to do in our subsequent research.

2

Scalar conservation law in one-dimensional space

This chapter presents the development and analysis of compact implicit finite volume schemes for one-dimensional scalar conservation laws. These equations, fundamental in modeling transport and wave phenomena, often require robust numerical methods due to the presence of discontinuities and nonlinearities.

2.1 Mathematical model and finite volume method

We consider two representative choices of scalar hyperbolic equations [18], one in a form of a linear advection equation with a space dependent velocity

$$\partial_t u + \partial_x (v(x)u) = 0\,,$$

and the second one being the nonlinear autonomous hyperbolic equation

$$\partial_t u + \partial_x f(u) = 0\,,$$

with $u = u(x,t)$ being the unknown function for $x \in (x_L, x_R) \subset R$ and $t \in (0,T)$. The initial conditions are prescribed by $u(x,0) = u^0(x)$ and we use the Dirichlet boundary conditions which will be described later together with a physical interpretation.

Firstly, we will focus on the advection equation (2.1) with a given velocity. We can identify the unknown function u with a concentration of a tracer that is dissolved in a fluid flowing with the given velocity.

The numerical discretization to solve the equation (2.1) is done in space and time using the notation $t^n = n\tau$, $n = 0, 1, ...N$ for a chosen number of time steps N and $\tau > 0$, and the spatial discretization is based on the finite volume method [18]. The computational domain is divided into finite volumes with a regular grid in the form $I_i = (x_{i-1/2}, x_{i+1/2})$, where $x_{i-1/2} = x_L + (i-1)h$ with $i = 1, 2, ..., M$ for the chosen M and $h = (x_R - x_L)/M$.

To obtain the numerical scheme, we use the finite volume method [18] obtaining the scheme

$$h\bar{u}_i^{n+1} - h\bar{u}_i^n + \tau v_{i+1/2}\bar{u}_{i+1/2}^{n+1/2} - \tau v_{i-1/2}\bar{u}_{i-1/2}^{n+1/2} = 0. \tag{2.1}$$

The scheme (2.1) is exact and it emphasizes the conservation law behind the equation. It states that the difference of the mass of the tracer in the volume I_i at two different times is only due the mass entering and/or leaving the volume through its boundary points.

The numerical solution is obtained from (2.1) by approximating the values $\bar{u}_{i+1/2}^{n+1/2}$ using $U_{i+1/2}^{n+1/2} \approx \bar{u}_{i+1/2}^{n+1/2}$ [18, 27] and $U_i^n \approx \bar{u}_i^n$. Consequently, the numerical scheme takes the form

$$U_i^{n+1} - U_i^n + \frac{\tau}{h}(v_{i+1/2}U_{i+1/2}^{n+1/2} - v_{i-1/2}U_{i-1/2}^{n+1/2}) = 0\,. \tag{2.2}$$

To complete the description of the numerical scheme, we have to define the values $U_{i+1/2}^{n+1/2}$ using the numerical values U_i^n and U_i^{n+1}.

In case of considering the nonlinear hyperbolic equation (2.1), the numerical scheme takes the form

$$U_i^{n+1} - U_i^n + \frac{\tau}{h}(F_{i+1/2} - F_{i-1/2}) = 0, \tag{2.3}$$

where, again, $U_i^n \approx \bar{u}_i^n$.

2.2 First order accurate implicit numerical scheme

The advection equation (2.1) includes explicitly defined velocity, for which we can easily treat separately positive and negative values. In particular, we apply the splitting of the velocity, which is performed as

$$v = v^+ + v^-, \qquad \text{with } v^+ := \max(0, v),\ v^- := \min(0, v)\,. \tag{2.4}$$

Similarly, for the nonlinear equation (2.1), it is beneficial if one can split the flux into positive and negative values, with the definition

$$f = f^+ + f^-, \qquad \text{with } \frac{df^+(u)}{du} \geq 0,\ \frac{df^-(u)}{du} \leq 0\,. \tag{2.5}$$

2.3 Fast sweeping method

The different approach to the fractional step method is to use the full numerical scheme (2.2) and (2.3) and to implement the iterative fast sweeping method to obtain a numerical solution of a better accuracy. To obtain the implicit numerical scheme, we follow the standard approaches [7, 18, 27] and we use the upwind approach proposing approximations $U_{i+1/2}^{n+1/2,\pm} \approx u(x_{i+1/2}, t^{n+1/2})$, which correspond to numerical values obtained by linear reconstructions in related finite volumes, namely $U_{i+1/2}^{n+1/2,-}$ in I_i and $U_{i+1/2}^{n+1/2,+}$ in I_{i+1}, as we explain later. Together with the splitting (2.4), the scheme will become

$$\begin{aligned} U_i^{n+1} - U_i^n + \frac{\tau}{h}\Big[& v_{i+1/2}^+ U_{i+1/2}^{n+1,-} - v_{i-1/2}^+ U_{i-1/2}^{n+1,-} \\ & + v_{i+1/2}^- U_{i+1/2}^{n+1,+} - v_{i-1/2}^- U_{i-1/2}^{n+1,+} \Big] = 0\,. \end{aligned} \tag{2.6}$$

In the case of the first order scheme, we obtain

$$U_i^{n+1} - U_i^n + \frac{\tau}{h}\Big[v^+_{i+1/2}U_i^{n+1} - v^+_{i-1/2}U_{i-1}^{n+1} + v^-_{i+1/2}U_{i+1}^{n+1} - v^-_{i-1/2}U_i^{n+1}\Big] = 0\,. \tag{2.7}$$

The approach of the fast sweeping method indicates that the scheme is solved iteratively, with each fast sweeping iteration corresponding to a single Gauss-Seidel iteration applied sequentially in alternating index directions across the computational domain. Specifically, we "*sweep*" from each end of the domain as follows:

$$\text{First sweep:} \quad i = 1, \ldots, M-1, \tag{2.8}$$

$$\text{Second sweep:} \quad i = M-1, \ldots, 1. \tag{2.9}$$

At each of these "*sweeps*", we solve (2.7) using the Gauss-Seidel method. Namely, let $U_i^{n+1,0} = U_i^n$ and to obtain $U_i^{n+1,k} \approx U_i^{n+1}$ for $k > 0$ we express this value from

$$\Big(1 + \frac{\tau}{h}\Big[v^+_{i+1/2} - v^-_{i-1/2}\Big]\Big)\, U_i^{n+1,k} = U_i^n + \frac{\tau}{h}\Big[v^+_{i-1/2}U_{i-1}^{n+1,*} - v^-_{i+1/2}U_{i+1}^{n+1,*}\Big]\,, \tag{2.10}$$

where $* = k$ if the value $U_{i\pm1}^{n+1,k+1}$ is available, otherwise $* = k-1$.

Generally, to reduce the absolute error of the solution, more than two fast sweeping iterations (positive and negative) may be required for each computational time step. Note that in the case of $v(x) > 0$, only the first sweep is necessary (2.8) (*positive sweep*). Conversely, when $v(x) < 0$, the second sweep alone is sufficient (2.9) (*negative sweep*). The number of required iterations depends on the problem's complexity. For higher order accuracy or nonlinear problems involving challenging features such as shocks, the iteration count increases, especially for problems in several dimensions.

In case of solving the nonlinear problem (2.3), to construct the numerical fluxes, we follow the same proposition [7, 18, 27] of the approximations $U_{i+1/2}^{n+1/2,\pm} \approx u(x_{i+1/2}, t^{n+1/2})$.

Having such values, one has to choose a proper numerical flux function $H = H(u^-, u^+)$ of two arguments [18, 27], and one defines

$$F_{i+1/2} = H(U_{i+1/2}^{n+1/2,-}, U_{i+1/2}^{n+1/2,+})\,. \tag{2.11}$$

For our purposes, we choose the Godunov flux H defined by

$$H(u^-, u^+) = \begin{cases} \min\limits_{u^- \le u \le u^+} f(u) & \text{if } u^- \le u^+ \\ \max\limits_{u^+ \le u \le u^-} f(u) & \text{if } u^- > u^+ \end{cases}, \tag{2.12}$$

with the simplest first order accurate numerical scheme using the approximations

$$U_{i+1/2}^{n+1/2,-} = U_i^{n+1}\,, \qquad U_{i+1/2}^{n+1/2,+} = U_{i+1}^{n+1}\,, \tag{2.13}$$

which creates the full scheme without fractional time splitting and can be solved using the fast sweeping method described in this chapter. Note that it is necessary to deal with the nonlinearity in the flux term. To solve this, at each of the *"sweeps"*, we solve the scalar nonlinear algebraic equation (2.3) for each index i using Newton's method.

2.4 Second order accurate compact implicit numerical scheme

One of the approaches to approximate the values $U_{i+1/2}^{n+1/2}$ up to the second order of accuracy [7], is using the parameter $\omega \in [0, 1]$, getting the compact implicit numerical approximation

$$U_{i+1/2}^{n+1/2} = U_i^{n+1} - \frac{1}{2}\big(\omega(U_{i-1}^{n+1} - U_i^n) + (1-\omega)(U_i^{n+1} - U_{i+1}^n)\big)\,. \tag{2.14}$$

Notice that we have managed to obtain a compact stencil as the value U_{i+1}^{n+1} in (2.14) is canceled. This is also a substantial

difference from the approach given in [7]. Two particular choices of the parameter $\omega \in [0,1]$ do not use the full stencil in (2.14) which we later conveniently use for the ENO approximation [27].

The compact implicit numerical scheme for solving linear advection equation for cases with positive velocity ($v > 0$) eventually looks like

$$\begin{aligned} U_i^{n+1} - U_i^n + \frac{\tau}{h}\Big[v_{i+1/2}\Big(U_i^{n+1} - \frac{1}{2}\big(\omega(U_{i-1}^{n+1} - U_i^n) + (1-\omega)(U_i^{n+1} - U_{i+1}^n)\big)\Big) \\ -v_{i-1/2}\Big(U_{i-1}^{n+1} - \frac{1}{2}\big(\omega(U_{i-2}^{n+1} - U_{i-1}^n) + (1-\omega)(U_{i-1}^{n+1} - U_i^n)\big)\Big)\Big] = 0\,. \end{aligned} \tag{2.15}$$

The scheme is unconditionally stable in the case of constant speed for any $\omega \geq 0$ as proved in [13] using von Neumann stability analysis.

Observe that the term u_{i+1}^{n+1} from (2.35) and (2.36) is canceled in (2.15). This indicates that for such cases, the solution can be obtained directly using only one fast sweeping iteration for $i = 2, 3, \ldots, M-1$. This necessitates, as visible in (2.15), some extension of the boundary conditions.

In case of solving the equation (2.1) with the velocity that changes the sign, very similarly, we obtain the numerical approximation of $u(x_{i+1/2}, t^{n+1/2})$ as

$$U_{i+1/2}^{n+1/2,+} = U_{i+1}^{n+1} - \frac{1}{2}\big(\omega(U_{i+2}^{n+1} - U_{i+1}^n) + (1-\omega)(U_{i+1}^{n+1} - U_i^n)\big)\,. \tag{2.16}$$

As the scheme expands to include both positive and negative velocity values using two different schemes with distinct upwind approaches, we also need to extend the parameter ω as $\boldsymbol{\omega} = (\omega^+, \omega^-)$ and the scheme becomes

$$\begin{aligned} U_i^{n+1} - U_i^n + \frac{\tau}{h}\Big[v_{i+1/2}^+\big(U_i^{n+1} - \frac{1}{2}\big(\omega^+(U_{i-1}^{n+1} - U_i^n) + (1-\omega^+)(U_i^{n+1} - U_{i+1}^n)\big)\big) \\ -v_{i-1/2}^+\big(U_{i-1}^{n+1} - \frac{1}{2}\big(\omega^+(U_{i-2}^{n+1} - U_{i-1}^n) + (1-\omega^+)(U_{i-1}^{n+1} - U_i^n)\big)\big) \\ +v_{i+1/2}^-\big(U_{i+1}^{n+1} - \frac{1}{2}\big(\omega^-(U_{i+2}^{n+1} - U_{i+1}^n) + (1-\omega^-)(U_{i+1}^{n+1} - U_i^n)\big)\big) \\ -v_{i-1/2}^-\big(U_i^{n+1} - \frac{1}{2}\big(\omega^-(U_{i+1}^{n+1} - U_i^n) + (1-\omega^-)(U_i^{n+1} - U_{i-1}^n)\big)\big)\Big] = 0\,, \end{aligned} \tag{2.17}$$

which, again, may be solved using the fast sweeping method described in Section 2.3 which consists of two *sweeps*

$$\text{First sweep:} \quad i = 2, 3, \ldots, M-2\,, \tag{2.18}$$

$$\text{Second sweep:} \quad i = M-2, M-3, \ldots, 2\,. \tag{2.19}$$

When solving the nonlinear equation, to finalize the second order accurate compact implicit scheme, we express the numerical fluxes in (2.3) using (2.11) with the numerical approximations $U_{i+1/2}^{n+1/2,\pm}$ from (2.14), and (2.16); and we solve it using the fast sweeping method using two sweeps (2.18), (2.19).

2.5 High resolution schemes

For discontinuous initial conditions or when shocks are present in the solution, unphysical oscillations may occur in numerical solutions if the numerical methods from the previous section with a fixed parameter are used.

To avoid such oscillations, we choose the values of the parameters $\boldsymbol{\omega}$ in each numerical flux differently, i.e., depending on the numerical solution [13, 27].

Let $\boldsymbol{\omega}^{\pm} = \boldsymbol{\omega}_i^{\pm} \in [0,1]$ for each I_i be the free parameter that we want to determine. Notice that the values $\boldsymbol{\omega} = (\omega_i^+, \omega_i^-)$ may change for each time step, which we do not focus on in the notation.

As it is known from the literature [1, 7, 13, 23, 24], unphysical oscillations can occur not only due to an inappropriately fixed choice of space reconstruction, but also due to the fixed time reconstruction. Therefore, similarly to [13], we add another numerical parameter $\boldsymbol{l} = (\boldsymbol{l}^{\pm}) = (l^+, l^-)$, which, if necessary, can limit the second order space reconstruction to the first order form of the scheme that produces numerical solutions free of unphysical oscillations. Again, the parameter $\boldsymbol{l}$ is defined in each I_i in the form $l_i^+, l_i^- \in [0,1]$. Notice again that the values

$\boldsymbol{l}$ also change at each time step, which we do not emphasize in the notation.

In summary, the approximation of $U_{i+1/2}^{n+1/2,\pm}$ will transform into the form

$$U_{i+1/2}^{n+1/2,-} = U_i^{n+1} - \frac{l_i^-}{2}\left(\omega_i^-(U_{i-1}^{n+1} - U_i^n) + (1-\omega_i^-)(U_i^{n+1} - U_{i+1}^n)\right),$$
$$U_{i+1/2}^{n+1/2,+} = U_{i+1}^{n+1} - \frac{l_{i+1}^+}{2}\left(\omega_{i+1}^+(U_{i+2}^{n+1} - U_{i+1}^n) + (1-\omega_{i+1}^+)(U_{i+1}^{n+1} - U_i^n)\right). \quad (2.20)$$

The high resolution scheme is then defined by (2.2), and (2.3) with (2.11), with the face values given in (2.20).

Concerning the space reconstruction, we present in the next sections two standard choices - the simplest Essentially Non-Oscillatory (ENO) method and a variant of the Weighted ENO (WENO) method. The value of $\boldsymbol{\omega}$ for the ENO approximation will depend on the following ratios $\boldsymbol{r} = (r_i^+, r_i^-)$ which will be defined for each finite volume I_i as

$$r_i^- = \frac{U_{i-1}^{n+1} - U_i^n}{U_i^{n+1} - U_{i+1}^n}, \qquad r_i^+ = \frac{U_{i+1}^{n+1} - U_i^n}{U_i^{n+1} - U_{i-1}^n}, \quad (2.21)$$

while the WENO approximation will depend on the nominators and denominators in the definitions of $\boldsymbol{r}$. Clearly, due to the dependence of $\boldsymbol{r}$ on unknown values of the numerical solution, an iterative procedure shall be proposed [13, 23] to compute the parameters $\boldsymbol{\omega}$.

Once the solution dependent values of $\boldsymbol{\omega}$ are computed, they are used for the definition of the parameters l_i^-

$$l_i^- = \min\left\{1, \max\left\{0, \left(\omega_i^- + \frac{1-\omega_i^-}{r_i^-}\right)^{-1}\left(\frac{2}{C} + l_{i-1}^-(\omega_{i-1}^- r_{i-1}^- + 1 - \omega_{i-1}^-)\right)\right\}\right\}, \quad (2.22)$$

with C being the local Courant like number. The l_{i+1}^+ in (2.20) is defined analogously.

Additionally to (2.22), we also require $\boldsymbol{l}_i^\pm = 0$ if $\boldsymbol{r}_i^\pm < 0$. Note that the ratios in $\boldsymbol{r}$ (2.21) take negative values only near the extrema of numerical solutions.

2.6 Third order accurate compact implicit numerical scheme

In this section, we focus on deriving a compact implicit numerical scheme of third order accuracy for cases involving smooth solutions [29, 30]. The derivation is mainly concerned with formulating the term $U^{\cdot,\pm}_{i+1/2}$ in different time steps with a third order accuracy. Specifically, it is necessary to use two Gauss points, $t^n + s_1\tau$ and $t^n + s_2\tau$, with the parameters s_1 and s_2 defined later in the text, and to approximate the values $u(x_{i+1/2}, t)$ in $t = t^{n+s_1} = t^n + s_1\tau$ and $t = t^{n+s_2} = t^n + s_2\tau$.

The derivation differs, but remains straightforward for the positive and negative cases (denoted by the index $\pm$). For simplicity, we will detail only the derivation for the values $U^{\cdot,-}_{i+1/2}$. Similarly, we can address the values $U^{\cdot,+}_{i+1/2}$, for which we will provide only the final definitions.

Firstly, we will focus on giving detailed derivation of the scheme to solve the nonlinear equation and later we will give details to the linear advection equation (2.1).

For the numerical approximation, we use the Gaussian quadrature [20] to obtain the third order accuracy. Namely, we take

$$F_{i+1/2} \approx \bar{f}_{i+1/2} \approx \frac{1}{2}\left(f(u(x_{i+1/2}, t^n + s_1\tau)) + f(u(x_{i+1/2}, t^n + s_2\tau))\right), \tag{2.23}$$

with parameters s_1 and s_2 being

$$s_1 = \frac{1}{2}(1 - \frac{1}{\sqrt{3}}) \quad \text{and} \quad s_2 = \frac{1}{2}(1 + \frac{1}{\sqrt{3}}). \tag{2.24}$$

To approximate $u(x_{i+1/2}, t^n + s\tau)$, we truncate the Taylor series

$$u(x, t^n + s\tau) = u(x, t^{n+1}) - s\tau\partial_t u(x, t^{n+1}) + \frac{s^2\tau^2}{2}\partial_{tt} u(, t^{n+1}) + \mathcal{O}(\tau^3). \tag{2.25}$$

Denoting $\bar{s} = \frac{1}{2\sqrt{3}}$ then the time approximations using Taylor

series can be written in the form

$$U_{i+1/2}^{n+s_1} = U_{i+1/2}^{n+1/2-\bar{s}} = U_{i+1/2}^{n+1} - \left(\frac{1}{2}+\bar{s}\right)\tau\partial_t U_{i+1/2}^{n+1} + \left(\frac{1}{2}+\bar{s}\right)^2\frac{\tau^2}{2}\partial_{tt}U_{i+1/2}^{n+1},$$
$$U_{i+1/2}^{n+s_2} = U_{i+1/2}^{n+1/2+\bar{s}} = U_{i+1/2}^{n+1} - \left(\frac{1}{2}-\bar{s}\right)\tau\partial_t U_{i+1/2}^{n+1} + \left(\frac{1}{2}-\bar{s}\right)^2\frac{\tau^2}{2}\partial_{tt}U_{i+1/2}^{n+1}. \quad (2.26)$$

Now, the first, second, and third terms in (2.26) will be approximated in space using the reconstruction polynomial p_k^{n+1} with $k = 3, 2, 1$, respectively. Before doing so, we have to replace the time derivatives with space (or mixed) derivatives. First, we use the Taylor series to approximate the first time derivative

$$\tau\partial_t U_{i+1/2}^{n+1} = (U_{i+1/2}^{n+1} - U_{i+1/2}^{n}) + \frac{\tau^2}{2}\partial_{tt}U_{i+1/2}^{n+1}, \quad (2.27)$$

and express $\partial_{tt}U_{i+1/2}^{n+1}$ using the Lax-Wendroff procedure

$$\partial_{tt}u(x_{i+1/2}, t^{n+1}) = -\partial_{tx}f(u(x_{i+1/2}, t^{n+1})), \quad (2.28)$$

with the mixed derivative approximated by a standard finite difference scheme

$$\tau h\partial_{tx}f(u(x_{i+1/2}, t^{n+1})) \approx f(U_i^{n+1}) - f(U_{i-1}^{n+1}) - f(U_i^n) + f(U_{i-1}^n). \quad (2.29)$$

Putting together (2.26) - (2.29), we get the approximation

$$U_{i+1/2}^{n+1/2\pm\bar{s}} = U_{i+1/2}^{n+1} \quad (2.30)$$
$$- (\tfrac{1}{2}\mp\bar{s})(U_{i+1/2}^{n+1} - U_{i+1/2}^{n}) \quad (2.31)$$
$$+ ((\tfrac{1}{2}\mp\bar{s}) - (\tfrac{1}{2}\mp\bar{s})^2)\frac{\tau}{2h}(f(U_i^{n+1}) - f(U_{i-1}^{n+1}) - f(U_i^n) + f(U_{i-1}^n)). \quad (2.32)$$

Using the quadratic and linear polynomial in (2.30) and (2.31), respectively, we obtain

$$U_{i+1/2}^{n+1/2\pm\bar{s}} = p_3^{n+1}(x_{i+1/2}) - (\tfrac{1}{2}\mp\bar{s})(p_2^{n+1}(x_{i+1/2}) - p_2^n(x_{i+1/2}))$$
$$+ ((\tfrac{1}{2}\mp\bar{s})\mp(\tfrac{1}{2}-\bar{s})^2)(f(U_i^{n+1}) - f(U_{i-1}^{n+1}) - f(U_i^n) + f(U_{i-1}^n)). \quad (2.33)$$

For the polynomial $p_3^{n+1}(x_{i+1/2})$ we obtain [27]

$$p_3^{n+1}(x_{i+1/2}) = \frac{1}{3}U_{i+1}^{n+1} + \frac{5}{6}U_i^{n+1} - \frac{1}{6}U_{i-1}^{n+1}\,. \tag{2.34}$$

Furthermore, we use p_2^{n+1}

$$p_1^{n+1}(x_{i+1/2}) = (1-\omega)U_{i+1}^{n+1} + \omega U_i^{n+1}\,, \tag{2.35}$$

$$p_2^{n+1}(x_{i+1/2}) = \frac{\omega}{2}(3U_i^{n+1} - U_{i-1}^{n+1}) + \frac{1-\omega}{2}(U_i^{n+1} + U_{i+1}^{n+1})\,. \tag{2.36}$$

with different values $\boldsymbol{\omega}_\pm$ to cancel the term U_{i+1}^{n+1} in (2.34) when used in (2.33). To do so, we must solve two simple equations

$$\frac{1}{3} - \Big(\frac{1-\omega_+}{2}\Big)\Big(\frac{1}{2} - \bar{s}\Big) = 0\,, \quad \frac{1}{3} - \Big(\frac{1-\omega_-}{2}\Big)\Big(\frac{1}{2} + \bar{s}\Big) = 0\,, \tag{2.37}$$

where we obtain the values $\omega_+ = \frac{1+\sqrt{3}}{-3+\sqrt{3}}$ and $\omega_- = \frac{-1+\sqrt{3}}{3+\sqrt{3}}$.

The numerical scheme with the third order accuracy, can then be expressed in the form of (2.3) with

$$F_{i+1/2} = \frac{1}{2}\big[H(U_{i+1/2}^{n+1/2-\bar{s},-}, U_{i+1/2}^{n+1/2-\bar{s},+}) + H(U_{i+1/2}^{n+1/2+\bar{s},-}, U_{i+1/2}^{n+1/2+\bar{s},+})\big]\,, \tag{2.38}$$

with function H in (2.12), where

$$\begin{aligned} U_{i+1/2}^{n+1/2\mp\bar{s},-} = {} & U_i^{n+1} + \frac{1}{12}\big[(-3 \pm 3\sqrt{3})U_i^{n+1} + (-3 \mp \sqrt{3})U_{i-1}^{n+1} \\ & + (1 \pm \sqrt{3})U_{i-1}^{n} + (1 \mp 3\sqrt{3})U_i^n + 4U_{i+1}^n\big] \\ & + \big((\tfrac{1}{2} \mp \bar{s}) - (\tfrac{1}{2} \mp \bar{s})^2\big)\frac{\tau}{2h}\big[f(U_i^{n+1}) - f(U_{i-1}^{n+1}) - f(U_i^n) + f(U_{i-1}^n)\big]\,. \end{aligned} \tag{2.39}$$

Using analogously the upwind approach, one can straightforwardly determine the values $U_{i+1/2}^{n+1/2,+}$. The problem is solved using the fast sweeping method described in Section 2.3.

3

Scalar conservation law in two-dimensional space

This chapter introduces a novel approach for the numerical solution of two-dimensional conservation laws, focusing on a compact implicit discretization scheme that enables the use of fast algebraic solvers, such as the fast sweeping method also mentioned in Chapter 2.

We consider two representative scalar hyperbolic partial differential equations in two-dimensional case. First, we consider the nonlinear hyperbolic equation in the form

$$\partial_t u + \nabla \cdot \boldsymbol{f}(u) = 0, \tag{3.1}$$

with $\boldsymbol{f}(u) = (f(u), g(u))$ being the vector flux function, so (3.1) can be written in the form

$$\partial_t u + \partial_x f(u) + \partial_y g(u) = 0 \tag{3.2}$$

with $u = u(x, y, t)$ being the unknown function for $t \in (0, T)$ and $x \in (x_L, x_R) \subset R$, $y \in (y_L, y_R) \subset R$. The initial condition is defined by $u(x, y, 0) = u^0(x, y)$ and the Dirichlet boundary conditions, if prescribed, are denoted by

$$\begin{aligned} u(x_L, y, t) &= u_{x_L}(y, t), \quad u(x, y_L, t) = u_{y_L}(x, t) \\ u(x_R, y, t) &= u_{x_R}(y, t), \quad u(x, y_R, t) = u_{y_R}(x, t)\,. \end{aligned} \tag{3.3}$$

In case of dealing with the linear advection equation in two dimensions, the $\boldsymbol{f}$ in (3.1) is present in the form $\boldsymbol{f} = \vec{v}u$ and the equation becomes

$$\partial_t u + \partial_x(vu) + \partial_y(wu) = 0\,, \tag{3.4}$$

where $\vec{v}$ represents the velocity field $\vec{v} = \vec{v}(x, y) = (v(x, y), w(x, y))$ which is a known function.

3.1 Numerical scheme and finite volume method

Firstly, we will describe the derivation for the (3.2).

The discretization is done in space and time using the following notation. We denote $t^n = n\tau$, $n = 0, 1, ...N$ for a chosen N and $\tau > 0$ with $t^{n+1/2} = t^n + \tau/2$. The spatial discretization is based on the finite volume method [2, 8, 18]. For simplicity of the notation, we assume a squared computational domain $(x, y \in (x_L, x_R))$ that is divided into finite volumes of the form $I_{i,j} = (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2})$ with the regular square grid, where $x_{i-1/2} = x_L + (i-1)h$ and $y_{j-1/2} = x_L + (j-1)h$ with $i, j = 1, 2, ..., M$ for the chosen M and $h = (x_R - x_L)/M$.

The main idea behind the finite volume method is to integrate the differential equation (3.2) over $I_{i,j} \times (t^n, t^{n+1})$, obtaining the exact form

$$\bar{u}_{i,j}^{n+1} - \bar{u}_{i,j}^{n} + \frac{\tau}{h}(\bar{f}_{i+1/2,j} - \bar{f}_{i-1/2,j}) + \frac{\tau}{h}(g_{i,j+1/2} - g_{i,j-1/2}) = 0\,. \tag{3.5}$$

To obtain a numerical scheme, of the second order of accuracy, we consider midpoint quadrature rules. Using $U_{i,j}^{n+1} \approx \bar{u}_{i,j}^{n+1} \approx u(x_i, y_j, t^{n+1})$ and numerical fluxes

$$F_{i+1/2,j} \approx \bar{f}_{i+1/2,j} \approx f(u(x_{i+1/2}, y_j, t^{n+1/2}))\,,$$
$$G_{i,j+1/2} \approx \bar{g}_{i,j+1/2} \approx g(u(x_i, y_{j+1/2}, t^{n+1/2}))\,,$$

the numerical scheme takes then the form

$$U_{i,j}^{n+1} - U_{i,j}^{n} + \frac{\tau}{h}(F_{i+1/2,j} - F_{i-1/2,j}) + \frac{\tau}{h}(G_{i,j+1/2} - G_{i,j-1/2}) = 0\,. \tag{3.6}$$

To construct the numerical fluxes F, G in, we follow standard approaches [7, 18, 27], also mentioned in Chapter 2, and

the only need is to propose the approximations $U^{n+1/2,\pm}_{i+1/2,j} \approx u(x_{i+1/2}, y_j, t^{n+1/2})$ and $U^{n+1/2,\pm}_{i,j+1/2} \approx u(x_i, y_{j+1/2}, t^{n+1/2})$ that correspond to numerical values obtained by linear reconstructions in related finite volumes, namely $U^{n+1/2,-}_{i+1/2,j}$ in $I_{i,j}$ and $U^{n+1/2,+}_{i+1/2,j}$ in $I_{i+1,j}$, and analogously for $U^{n+1/2,\pm}_{i,j+1/2}$. Having such values and properly chosen numerical flux function $H = H(u^-, u^+)$ of two arguments [18, 27], one defines

$$F_{i+1/2,j} = H(U^{n+1/2,-}_{i+1/2,j}, U^{n+1/2,+}_{i+1/2,j}), \tag{3.7}$$

and similarly for the flux $G_{i,j+1/2}$,

$$G_{i,j+1/2} = H(U^{n+1/2,-}_{i,j+1/2}, U^{n+1/2,+}_{i,j+1/2}). \tag{3.8}$$

For our purposes, we choose the Godunov flux H defined by

$$H(u^-, u^+) = \begin{cases} \min\limits_{u^- \le u \le u^+} h(u) & \text{if } u^- \le u^+ \\ \max\limits_{u^+ \le u \le u^-} h(u) & \text{if } u^- > u^+ \end{cases}, \tag{3.9}$$

where $h = f$ for (3.7) and $h = g$ for (3.8).

Note that the simplest first order accurate numerical scheme uses the approximations

$$\begin{aligned} U^{n+1/2,-}_{i+1/2,j} &= U^{n+1}_{i,j}, & U^{n+1/2,+}_{i+1/2,j} &= U^{n+1}_{i+1,j}, \\ U^{n+1/2,-}_{i,j+1/2} &= U^{n+1}_{i,j}, & U^{n+1/2,+}_{i,j+1/2} &= U^{n+1}_{i,j+1}. \end{aligned} \tag{3.10}$$

3.2 Second order accurate compact implicit numerical scheme

In this section, we present the parametric form of the second order accurate scheme in time and space that is later used also in the framework of high resolution schemes. As discussed above, one has to define the approximations $U^{n+1/2,\pm}_{i+1/2,j}$ and $U^{n+1/2,\pm}_{i,j+1/2}$

based on the upwind approach. The approximations then look like

$$U^{n+1/2,-}_{i+1/2,j} = U^{n+1}_{i,j} - \frac{1}{2}\left(\omega^{x,-}(U^{n+1}_{i-1,j} - U^{n}_{i,j}) + (1-\omega^{x,-})(U^{n+1}_{i,j} - U^{n}_{i+1,j})\right), \quad (3.11)$$

$$U^{n+1/2,-}_{i,j+1/2} = U^{n+1}_{i,j} - \frac{1}{2}\left(\omega^{y,-}(U^{n+1}_{i,j-1} - U^{n}_{i,j}) + (1-\omega^{y,-})(U^{n+1}_{i,j} - U^{n}_{i,j+1})\right). \quad (3.12)$$

Notice that we have managed to obtain a compact stencil as the values $U^{n+1}_{i+1,j}$ and $U^{n+1}_{i,j+1}$ in (3.11) and (3.12) are canceled. This is also the substantial difference to the approach given in [7]. Two particular choices of parameters $\omega^{x,-} \in [0,1]$ and $\omega^{y,-} \in [0,1]$ do not use the full stencil in (3.11) and (3.12) that we use later conveniently for ENO approximation [27]. In particular, with the value $\omega^{x,-} = 0$ and $\omega^{y,-} = 0$ we create in (3.11) and (3.12) a *"central"* kind of discretization and for $\omega^{x,-} = 1$ (and $\omega^{y,-} = 1$) the *"upwind"* one.

Very similarly, one obtains the numerical approximations of $U^{n+1/2,+}_{i+1/2,j}$ and $U^{n+1/2,+}_{i,j+1/2}$ as

$$\begin{aligned} U^{n+1/2,+}_{i+1/2,j} &= U^{n+1}_{i+1,j} - \frac{1}{2}\left(\omega^{x,+}(U^{n+1}_{i+2,j} - U^{n}_{i+1,j}) + (1-\omega^{x,+})(U^{n+1}_{i+1,j} - U^{n}_{i,j})\right), \\ U^{n+1/2,+}_{i,j+1/2} &= U^{n+1}_{i,j+1} - \frac{1}{2}\left(\omega^{y,+}(U^{n+1}_{i,j+2} - U^{n}_{i,j+1}) + (1-\omega^{y,+})(U^{n+1}_{i,j+1} - U^{n}_{i,j})\right). \end{aligned} \quad (3.13)$$

To finalize the second order accurate compact implicit scheme for the nonlinear problem (3.2), we express the numerical fluxes in (3.6) using (3.7) and (3.8) with the numerical approximations $U^{n+1/2,\pm}_{i+1/2,j}, U^{n+1/2,\pm}_{i,j+1/2}$ from (3.11), (3.12), and (3.13).

The discretization schemes create a system of algebraic equations that can be solved, again, iteratively, using the fast sweeping method mentioned in Chapter 2.

3.3 Fast sweeping method in 2D

The approach of the fast sweeping method indicates that the scheme is solved iteratively, with alternating index directions

across the computational domain [19, 34]. In particular, for two-dimensional case, we use four different "*sweeps*" from each corner of a rectangular domain:

$$\begin{aligned}
&\text{First sweep:} && i = 2, ..., M-2\,, \quad j = 2, ..., M-2 \\
&\text{Second sweep:} && i = M-2, ..., 2\,, \quad j = 2, ..., M-2 \\
&\text{Third sweep:} && i = M-2, ..., 2\,, \quad j = M-2, ..., 2 \\
&\text{Fourth sweep:} && i = 2, ..., M-2\,, \quad j = M-2, ..., 2
\end{aligned} \tag{3.14}$$

or, alternatively, when applying the first order accurate scheme, the sweeps are performed from $i/j = 1$ to $i/j = M - 1$ (or opposite direction) because of the smaller stencil used in scheme.

4

Transport problem with sorption isotherm

In this Chapter, we are interested in numerical solution of nonlinear transport equations in a conservative form [31] where the time derivative in the model is applied to a nonlinear function of the solution.

Such models are used to describe the transport of contaminants in porous media when contaminant adsorption on pore skeletons must be taken into account [11]. Other interesting applications of such models are in liquid chromatography technology [16]. We show that to solve related representative mathematical models, the computational cost of the compact implicit scheme is comparable to explicit schemes, but with the clear advantage of no stability requirement for the implicit scheme.

4.1 Mathematical model and numerical scheme

We consider the representative nonlinear transport problem in the form

$$\partial_t F(u) + \partial_x u = 0, \tag{4.1}$$

with $u = u(x,t) \geq 0$ being the unknown function for $t \in (0,T)$ and $x \in (x_L, x_R) \subset R$. The initial condition is defined by

$$u(x,0) = u^0(x)\,. \tag{4.2}$$

As $F'(u) > 0$ for $u \in R$, the Dirichlet boundary condition is defined only at the left boundary,

$$u(x_L, t) = u_{x_L}(t)\,, \tag{4.3}$$

and no boundary condition is required at the right boundary.

The mathematical model can represent the transportation of contaminant [5, 9, 11, 17] or liquids in chromatography [16, 25] with the sorption isotherm

$$\Psi(u) = F(u) - u\,. \tag{4.4}$$

One of the most frequently encountered type of (nonlinear) sorption isotherms is the Freundlich type,

$$\Psi(u) = au^p\,, \quad a, p > 0\,. \tag{4.5}$$

In this paper, we will focus on a single choice $a = 1$.

The solution to (4.1) discussed in this paper is based on the theoretical results [18], which ensure the existence and uniqueness of so-called entropy solutions for hyperbolic problems. Such theoretical framework has been established for hyperbolic equations in the form

$$\partial_t q + \partial_x f(q) = 0\,, \tag{4.6}$$

that can be obtained with the transformation

$$q = F(u)\,,\ u = f(q)\,, \tag{4.7}$$

where $f = F^{-1}$ is the inverse function of F.

In general, the function f may not be available analytically. In the case where f is known, the problem can be readily addressed using established methods for hyperbolic problems [18].

The equation (4.1) may be extended using the velocity $v(x)$, known for each value of x, into the form

$$\partial_t F(u) + \partial_x(v(x)u) = 0\,, \tag{4.8}$$

where the velocity may take on both positive and negative values and the Dirichlet boundary condition will be extended also to the right boundary

$$u(x_R, t) = u_{x_R}(t)\,. \tag{4.9}$$

The numerical discretization to solve the equation (4.8) is done in space and time using the notation $t^n = n\tau$, $n = 0, 1, ...N$ for a chosen N and $\tau > 0$, and the spatial discretization is based on the finite volume method [18]. The computational domain is divided into finite volumes with a regular grid in the form $I_i = (x_{i-1/2}, x_{i+1/2})$, where $x_{i-1/2} = x_L + (i-1)h$ with $i = 1, 2, ..., M$ for the chosen M and $h = (x_R - x_L)/M$.

To obtain the numerical scheme, we use the finite volume method, [18]. To solve (4.8), we need to treat the positive and negative velocities separately as in 2.4

After integrating the differential equation (4.8) over $I_i \times (t^n, t^{n+1})$, we obtain the scheme

$$\bar{q}_i^{n+1} - \bar{q}_i^n + \frac{\tau}{h}(v_{i+1/2}\bar{u}_{i+1/2}^{n+1/2} - v_{i-1/2}\bar{u}_{i-1/2}^{n+1/2}) = 0\,. \tag{4.10}$$

The numerical solution of (4.10) is obtained by approximating the values $\bar{u}_{i+1/2}^{n+1/2}$ using $U_{i+1/2}^{n+1/2} \approx \bar{u}_{i+1/2}^{n+1/2}$ [18, 27] and $Q_i^n \approx \bar{q}_i^n$. The numerical scheme takes the form

$$Q_i^{n+1} - Q_i^n + \frac{\tau}{h}(v_{i+1/2}U_{i+1/2}^{n+1/2} - v_{i-1/2}U_{i-1/2}^{n+1/2}) = 0\,. \tag{4.11}$$

To complete the description of the numerical scheme, we have to define the values $U_{i+1/2}^{n+1/2}$ using the numerical values U_i^n and $Q_i^{n+1} = F(U_i^{n+1})$.

4.2 First order accurate numerical scheme

For convenience and a comparison, we give notation for the first order accurate explicit and implicit numerical schemes. To obtain the first order accurate explicit numerical scheme, we use the upwind approach together with the velocity splitting, and the scheme [18] will become

$$Q_i^{n+1} = Q_i^n - \frac{\tau}{h}\Big[v_{i+1/2}^+ U_i^n - v_{i-1/2}^+ U_{i-1}^n + v_{i+1/2}^- U_{i+1}^n - v_{i-1/2}^- U_i^n\Big], \tag{4.12}$$

where the explicit structure of the scheme is clearly evident.

It is important to note that when employing an explicit numerical scheme (4.12), the challenge of solving the nonlinear problem does not vanish and is still present in terms $Q_i^{n+1} = F(U_i^{n+1})$. The nonlinearity $F(u) = u + u^p$ still requires resolution, which necessitates the use of an iterative method to obtain the solution, such as Newthon's method, together with the necessity to adhere to the stability restrictions imposed by explicit numerical schemes.

In case of using the implicit numerical scheme, one gets

$$Q_i^{n+1} - Q_i^n + \frac{\tau}{h}\Big[v_{i+1/2}^+ U_i^{n+1} - v_{i-1/2}^+ U_{i-1}^{n+1} + v_{i+1/2}^- U_{i+1}^{n+1} - v_{i-1/2}^- U_i^{n+1}\Big] = 0\,, \tag{4.13}$$

where the nonlinearity is readily apparent in the previously mentioned relation $Q_i^{n+1} = F(U_i^{n+1})$.

The discretization scheme creates a system of algebraic equations (4.13) that can be solved iteratively, using the fast sweeping method [34].

4.3 Second order accurate compact implicit numerical scheme

In this section, we will focus on the derivation of the second order accurate compact implicit numerical scheme and its high resolution formulation. We will start with assuming only $v > 0$.

To obtain the second order of accuracy [7] of (4.11), the derivation is very similar to the one described in Section 2.4 obtaining the approximation for $U_{i+1/2}^{n+1/2}$ (2.14)

$$U_{i+1/2}^{n+1/2} = U_i^{n+1} - \frac{1}{2}\big(\omega_i(U_{i-1}^{n+1} - U_i^n) + (1-\omega_i)(U_i^{n+1} - U_{i+1}^n)\big)\,. \tag{4.14}$$

To deal with the oscillations that may arise due to discontinuities in the solution, again, we propose a high resolution form of the scheme. Such scheme incorporates a variable parameter ω and a limiter l to control numerical oscillations and to ensure stability [13, 32]. By adapting ω and employing the limiter l, the scheme effectively balances accuracy and non-oscillatory behavior near discontinuities. Consequently, the proposed method (for cases with $v > 0$) is transformed into the following form,

$$\begin{aligned} Q_i^{n+1} - Q_i^n + \frac{\tau}{h}\Big[v_{i+1/2}\Big(U_i^{n+1} - \frac{l_i}{2}\big(\omega_i(U_{i-1}^{n+1} - U_i^n) + (1-\omega_i)(U_i^{n+1} - U_{i+1}^n)\big)\Big) \\ - v_{i-1/2}\Big(U_{i-1}^{n+1} - \frac{l_{i-1}}{2}\big(\omega_{i-1}(U_{i-2}^{n+1} - U_{i-1}^n) + (1-\omega_{i-1})(U_{i-1}^{n+1} - U_i^n)\big)\Big)\Big] = 0\,. \end{aligned} \tag{4.15}$$

Again, it is necessary to handle the nonlinearity present in Q, since $Q = F(U)$, and to determine the values of ω and l. To do that, we use the ENO or WENO approximations, together with the iterative procedure.

In case of solving the equation (4.8) with the velocity that changes the sign, we need to extend the values $\boldsymbol{\omega} = (\omega^+, \omega^-)$

and $\boldsymbol{l} = (l^+, l^-)$ and the scheme becomes

$$\begin{aligned} Q_i^{n+1} - Q_i^n + \frac{\tau}{h}\Big[& v^+_{i+1/2}(U_i^{n+1} - \frac{l_i^+}{2}(\omega_i^+(U_{i-1}^{n+1} - U_i^n) + (1-\omega_i^+)(U_i^{n+1} - U_{i+1}^n))) \\ & -v^+_{i-1/2}(U_{i-1}^{n+1} - \frac{l_{i-1}^+}{2}(\omega_{i-1}^+(U_{i-2}^{n+1} - U_{i-1}^n) + (1-\omega_{i-1}^+)(U_{i-1}^{n+1} - U_i^n))) \\ & +v^-_{i+1/2}(U_{i+1}^{n+1} - \frac{l_{i+1}^-}{2}(\omega_{i+1}^-(U_{i+2}^{n+1} - U_{i+1}^n) + (1-\omega_{i+1}^-)(U_{i+1}^{n+1} - U_i^n))) \\ & -v^-_{i-1/2}(U_i^{n+1} - \frac{l_i^-}{2}(\omega_i^-(U_{i+1}^{n+1} - U_i^n) + (1-\omega_x^-)(U_i^{n+1} - U_{i-1}^n)))\Big] = 0\,, \end{aligned} \tag{4.16}$$

which, again, may be solved using the fast sweeping method.

5

Conclusion

The thesis presents a development of implicit numerical schemes for hyperbolic problems which are of a high order of accuracy, unifying methodologies across linear and nonlinear scalar conservation laws in one and two dimensions.

Central to this research is the derivation of the compact implicit schemes that are based on the finite volume method combined with Taylor series expansions. These schemes are distinguished by their use of compact stencils, which reduce the number of grid points required for spatial discretization while maintaining high order accuracy.

The schemes show flexibility, adapting both smooth and discontinuous solutions for linear and nonlinear problems. High resolution techniques with limiters ensure physically plausible solutions together with Essentially Non-Oscillatory (ENO) and Weighted ENO (WENO) methods, effectively reducing oscillations near discontinuities through the careful optimization of parameters. This is further examined in nonlinear transport problems, such as those involving Freundlich sorption isotherms, where implicit methods outperform explicit counterparts in stability and efficiency, particularly at high Courant numbers.

In one-dimensional problems, the integration of the Lax-Wendroff procedure enables a single time-step approach by resolving mixed space-time derivatives, enhancing computational efficiency to create the third order accurate scheme. For two-dimensional cases, the compact stencil design simplifies algebraic systems, allowing iterative solutions via the fast sweeping

method and nonlinear Gauss-Seidel techniques without compromising stability.

Validation through extensive numerical experiments underline the accuracy and convergence of the proposed schemes. The second order methods exhibit the expected rate of convergence for smooth cases and perform well in scenarios involving discontinuities, yielding the desired increase in precision. The third order extension of the scheme achieves the anticipated convergence rates for smooth solutions.

The implicit framework eliminates the restrictive time-step constraints characteristic of explicit methods. Computational efficiency is further enhanced by the fast sweeping method, which reduces the algebraic complexity of multi-dimensional systems.

The practical implications of this work include environmental hydrology, materials science, and contaminant transport modeling, where accurate and stable simulations are critical. Future research directions include extending these schemes to systems of coupled equations. Furthermore, validation using experimental data from real-world applications will improve the selection of parameters and the predictive accuracy, thereby strengthening the connection between theoretical models and industrial practice.

By combining innovative techniques with computational efficiency, this thesis establishes a framework for compact implicit methods that offers a balanced approach to accuracy, stability, and performance in solving a broad class of hyperbolic problems.

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