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Dissertation Thesis Abstract

Effective Methods of Numerical Solution for Some Problems with an Implicitly Given Interface

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ABSTRACT

Dynamic interfaces arise in a wide range of modern applications and require careful numerical treatment. A robust approach to modeling their evolution are the level set methods, where the interface is implicitly represented as the zero level set of a function. While these methods naturally handle topological changes and can operate on structured grids, they introduce significant computational challenges when combined with the unconditionally stable implicit time discretizations. In particular, the governing Hamilton-Jacobi and Hamilton-Jacobi-Bellman-type equations are nonlinear, often curvature dependent, and difficult to solve efficiently, especially in higher dimensions.

This thesis develops numerical methods aimed at increasing the effectiveness of level-set-based simulations by improving the trade-off between accuracy, stability, and computational cost. First, we introduce an efficient upwind-based scheme for curvature-driven motion, compatible with fast sweeping solvers, and supported by a detailed stability analysis. Second, we propose a compact high-order scheme that leverages a partial inverse Lax-Wendroff procedure to achieve high-resolution and reduced oscillations with minimal computational overhead. Finally, we present a novel predictor-corrector method achieving third-order accuracy in both space and time, which remains stable and non-oscillatory for arbitrary Courant numbers and extends naturally to higher dimensions.

All proposed methods use implicit time discretization to ensure unconditional stability, with spatial discretizations carefully constructed to retain computational efficiency by minimizing or avoiding the need for costly implicit solvers.

ABSTRAKT

Dynamické rozhrania sa vyskytujú v mnohých moderných aplikáciách a vyžadujú si dôkladné numerické spracovanie. Robustným prístupom k modelovaniu ich vývoja sú metódy úrovňových množín (level set metódy), kde je rozhranie implicitne reprezentované ako množina nultej úrovne funkcie. Hoci táto metóda prirodzene zvláda topologické zmeny a funguje na štruktúrovaných mriežkach, prináša značné výpočtové problémy, špeciálne pri použití bezpodmienečne stabilných implicitných časových diskretizácií. Napríklad, riadiace rovnice Hamiltonovho-Jacobiho a Hamiltonovho-Jacobiho-Bellmanovho typu sú nelineárne, často závislé od zakrivenia rozhrania a je náročné ich efektívne riešiť, najmä vo vyšších dimenziách.

Táto práca sa zaoberá vývojom numerických metód zameraných na zvýšenie efektívnosti riešenia pomocou metód úrovňových množín zlepšením kombinácie presnosti, stability a výpočtovej náročnosti. Najprv predstavíme novú efektívnu schému založenú na takzvanej upwind aproximácií pre pohyb riadený krivosťou, kompatibilnú s rýchlymi metódami pre riešenie systémov rovníc, ako napríklad takzvaná fast sweeping metóda, a podrobne popíšeme analýzu stability tejto metódy. Po druhé, navrhneme kompaktnú schému vyššieho rádu presnosti, ktorá využíva čiastočnú inverznú Lax-Wendroffovu procedúru na dosiahnutie vyššej presnosti a zníženie oscilácií s minimálnymi výpočtovými nákladmi. Nakoniec predstavíme novú metódu prediktora a korektora, ktorá dosahuje presnosť tretieho rádu v priestore aj čase, zostáva stabilná, zabraňuje osciláciam v gradiente riešenia, a to pre ľubovoľné Courantovo číslo. Navzše je prirodzene rozšíriteľná na viacdimenzionálne modely.

Všetky navrhnuté metódy používajú implicitnú časovú diskretizáciu kvôli zabezpečeniu bezpodmienečnej stability, pričom priestorová diskretizácia je starostlivo zostavená tak, aby sa zachovala výpočtová efektívnosť minimalizovaním potreby nákladných implicitných riešiteľov.

Contents

1

Introduction

Dynamic interfaces play a crucial role in the world of modern mathematical applications across all spatial dimensions. A robust approach to modeling their evolution is the level set methods [14, 16], where the interface is implicitly represented as the zero level set of a function. Although these methods naturally handle topological changes and can operate on structured grids, they introduce significant computational challenges when combined with the unconditionally stable implicit time discretizations. In particular, the governing Hamilton-Jacobi [15, 18] and Hamilton-Jacobi-Bellman-type equations [4, 9] are nonlinear, often curvature dependent, and difficult to solve efficiently, especially in higher dimensions.

Throughout this thesis, we present various methods, all of which are based on implicit time discretization, motivated by its unconditional stability. To counterbalance the associated computational cost, we design efficient spatial discretizations that, in most cases for linear problems, allow the numerical solution to be expressed explicitly using precomputed values or values from the previous time step.

First, we propose an Eulerian numerical scheme in structured grids to solve the advection-dominated evolution of implicit interfaces, as introduced in [11]. This scheme addresses models in which the interface velocity partially depends on the curvature. It combines standard upwind finite differences for advection with non-traditional upwind differences for the curvature term, enhancing efficiency in upwind-based solvers like the fast sweeping method. A key component is the detailed stability analysis presented in [10].

The second part focuses on higher-order approximations of some representative models in the class of the Hamilton-Jacobi equation. We introduce a new compact, high-resolution finite difference scheme based on [7] and extended in [12] through a non-traditional partial inverse Lax-Wendroff procedure. The scheme achieves higher-order accuracy and unconditional stability, effectively eliminating non-physical oscillations in the solution gradient for any Courant number. Its approximation stencil includes a compact, purely upwind implicit part, enabling efficiency comparable to first-order schemes and compatibility with fast upwind-based solvers such as the fast sweeping method. However, the scheme's ability to reduce oscillations remains somewhat Courant number dependent, and its extension to higher dimensions proves cumbersome.

Lastly, inspired by [6, 13] and motivated by certain drawbacks of our compact scheme, we propose a new predictor-corrector-based finite difference method. It achieves up to third-order accuracy in both space and time for smooth solutions and, when combined with appropriate limiters, effectively suppresses non-physical oscillations regardless of the Courant number. Despite its high-order accuracy, the implicit part of the stencil remains equivalent to that of a first-order scheme, similarly to our compact scheme, and the approach extends naturally to higher dimensions.

2

Upwind Schemes for Forced Mean Curvature Flow

We are interested in solving two dimensional forced mean curvature flow in the form:

$$\partial_t \phi + a(1 - \epsilon(\kappa)\kappa)|\nabla \phi| = 1, \qquad (2.1)$$

with the initial condition $\phi(\boldsymbol{x}, t) = \phi^0(\boldsymbol{x})$, $\boldsymbol{x} \in \mathbb{R}^2$, $t \in [0, T]$ and we suppose the initial position of the interface is given by a closed curve $\partial\Omega^-$. The boundary conditions are given as:

$$\phi(\boldsymbol{\gamma}, t) = 0\,,\ \boldsymbol{\gamma} \in \partial\Omega^-\,,\ t > 0\,. \qquad (2.2)$$

In our study, the time variable can be viewed as an (artificial) relaxation time for the purpose of obtaining (or estimating) a stationary solution to the modified eikonal equation:

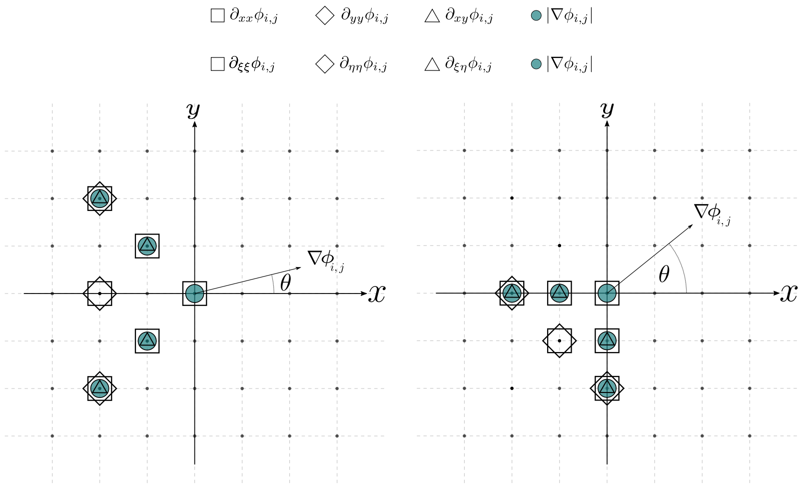
$$a(1 - \epsilon(\kappa)\kappa)|\nabla T| = 1, \quad T(\gamma) = 0, \quad \gamma \in \Gamma_0. \qquad (2.3)$$

Our aim is to propose an Eulerian type of numerical finite difference approximation on structured grids for the above-mentioned advection-dominated level set equations [11] that is upwind in both the advective and the diffusive term. Moreover, we use fast sweeping method to solve the resulting system of equations.

In order to follow the upwind principle in the discretization and the subsequent use of the fast sweeping method, to efficiently solve equation (2.1), we need to know the direction of the characteristics determined by the advection, which in the case of equation (2.1) is equivalent to the gradient direction.

Therefore, we introduce a deciding parameter θ defined as the angle between the iteratively estimated numerical gradient computed using the standard Rouy-Tourin scheme.

The partial derivatives in the resulting scheme are approximated using standard and newly developed finite differences, designed to complement each other and resulting into a fully upwind stencil, visualized in Figure 2.1.



(a) Stencil for $-22.5° < \theta < 22.5°$ (b) Stencil for $22.5° < \theta < 67.5°$

Figure 2.1: Local stencils for the approximation of the advective term and the second-order derivatives for different values θ.

We performed multiple experiments aiming to test the method's accuracy and efficiency.

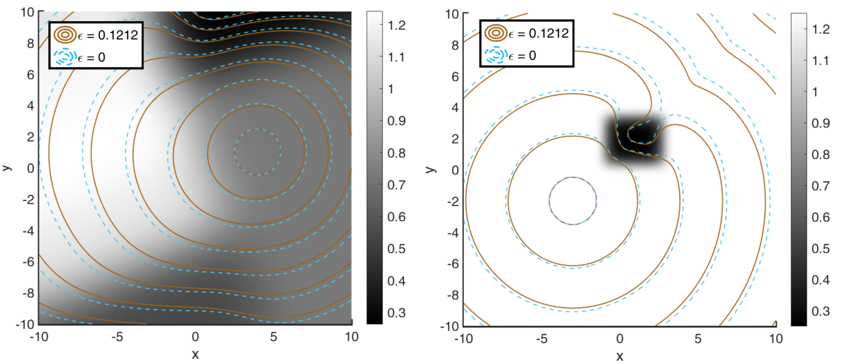
We can see in Table 2.1 that the number of fast sweeping iterations does not increase significantly with mesh refinement. This is an expected property of upwind schemes.

Furthermore we present results of an experiment inspired

N	L_2 norm	EOC_{L_2}	L_∞ norm	EOC_{L_∞}	$k\#$
21	0.107520		0.005115		3
41	0.032069	1.745	0.00174	1.556	3
81	0.010229	1.649	0.000612	1.507	4

Table 2.1: The results (L_2 norm, L_∞ norm , EOC (experimental order of convergence), total number of fast sweeping iterations ($k\#$)), of experiment involving nonuniform curvature, solved as stationary solution.

by a real-life application [1, 2], which models the spread of a forest fire.



(a) Combustibility map 1

(b) Combustibility map 2

Figure 2.2: Comparison of isocontour shapes for solution with $\epsilon = 0$ and $\epsilon = 0.1212$. There are isocontours of the first arrival time $t \in \{0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20\}$ in the figure (a) and $t \in \{0, 2, 4, 6, 8, 10, 12\}$ in the figure (b). The smallest circle in both figures is the zero isocontour.

3

Compact High-Resolution Schemes

We present a novel compact high-resolution scheme for some representative equation of the family of Hamilton-Jacobi equations designed to efficiently produce stable, non-oscillatory solutions. The method relies on a compact stencil that is upwind in its implicit part, allowing for high accuracy and robustness while preserving computational efficiency. The development and analysis of this scheme have been published in [12].

Consider the following advection equation in one-dimensional space:

$$\partial_t \phi(x_i, t^n) + u(x_i)\, \partial_x \phi(x_i, t^n) = 0, \quad \phi(x_i, 0) = \phi^0(x_i), \quad (3.1)$$

with given boundary conditions $\phi(x_0, t^n) = \phi_0(t^n)$ if $u_0 > 0$ and $\phi(x_{N-1}, t^n) = \phi_{N-1}(t^n)$ if $u_{N-1} < 0$.

To derive a compact high-resolution finite difference scheme for equation (3.1), we employ the Lax-Wendroff procedure [5, 8, 19], which systematically incorporates higher-order terms to improve accuracy and stability. This approach is also used when developing an unconditionally stable implicit scheme [3, 8].

We obtain a compact implicit numerical scheme of second-order accuracy which for the linear advection equation can be written as follows:

$$\phi_i^n + |c_i|\Bigg(\phi_i^n - \phi_{i\mp1}^n + \frac{1-\omega_i^n}{2}\left(\phi_{i\pm1}^{n-1} - \phi_i^{n-1} - \phi_i^n + \phi_{i\mp1}^n\right) \qquad (3.2)$$

$$+ \frac{\omega_i^n}{2}\left(\phi_i^{n-1} - \phi_{i\mp1}^{n-1} - \phi_{i\mp1}^n + \phi_{i\mp2}^n\right)\Bigg) = \phi_i^{n-1},$$

where $\pm = \operatorname{sign}(c_i)$ and $\mp = -\operatorname{sign}(c_i)$. This scheme is oscillation-free for Courant numbers smaller than 1. To avoid issues and ensure non-oscillatory behavior for larger Courant numbers, we propose a new method derived via a non-standard formulation, the partial inverse Lax-Wendroff procedure. The general form of the final scheme can be written as follows:

$$\phi_i^n + |c_i|\left(\phi_i^n - \phi_{i\mp1}^n\right) + \frac{1}{2c_i}(c_i - c_{i\mp1})(\phi_i^n - \phi_i^{n-1}) \qquad (3.3)$$

$$+\frac{1-\alpha_i^n}{2}\left(\phi_{i\mp1}^{n+1} - \phi_{i\mp1}^n - \phi_i^n + \phi_i^{n-1}\right).$$

$$+\frac{\alpha_i^n}{2}\left(\phi_{i\mp1}^n - \phi_{i\mp1}^{n-1} - \phi_i^{n-1} + \phi_i^{n-2}\right) = \phi_i^{n-1},$$

where $\pm = \operatorname{sign}(c_i)$ and $\mp = -\operatorname{sign}(c_i)$.

We can combine both schemes into one non-oscillatory framework:

$$\phi_i^n + |c_i|\big(\phi_i^n - \phi_{i\mp1}^n\big) + \frac{|c_i^{super}|}{2c_i^2}|c_i - c_{i\mp1}|(\phi_i^n - \phi_i^{n-1})$$

$$+ \frac{|c_i^{sub}|}{2}\left[\omega_i^n\Big(\cdots\Big) + (1-\omega_i^n)\Big(\cdots\Big)\right] \qquad (3.4)$$

$$+ \frac{|c_i^{super}|}{2|c_i|}\left[\alpha_i^n\Big(\cdots\Big) + (1-\alpha_i^n)\Big(\cdots\Big)\right] = \phi_i^{n-1},$$

where α_i^n and ω_i^n are chosen using WENO (Weighted Essentially Non-Oscillatory) approach, $c_i^{sub} = \operatorname{sign}(c_i)\min\{|c_i|, 1\}$ and $c_i^{super} = c_i - c_i^{sub}$.

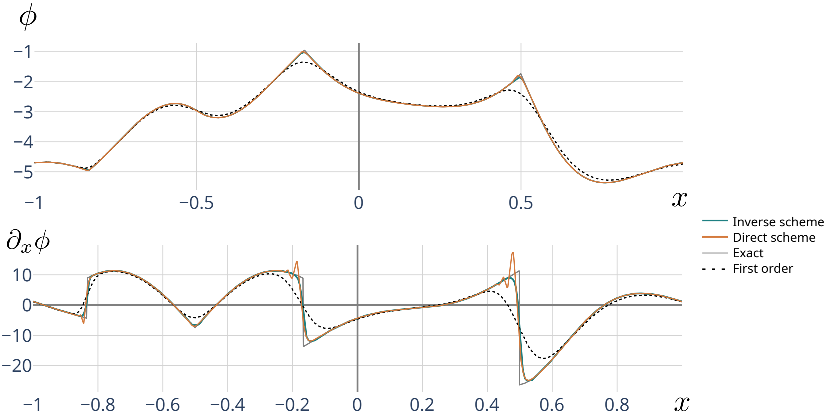


Figure 3.1: Solutions of the linear advection equation with constant velocity and non-smooth initial condition.

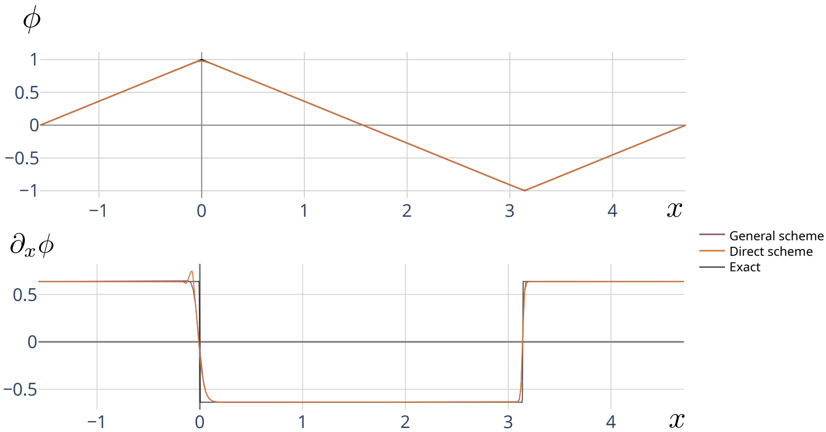


Figure 3.2: Solutions of the advection equation with variable velocity and the non-smooth initial condition.

We test the proposed schemes on a series of examples. We solve a one-dimensional linear advection equation with a given constant velocity. We test the behavior of numerical schemes in the presence of discontinuities in its gradient. The results can be seen in Figure 3.1. Although the direct scheme gives slightly more accurate numerical solutions, it clearly has an oscillatory approximation of its space derivative.

Furthermore, we performed a test of the general non-oscillatory framework on an example with variable velocity $u(x) = \cos(x)$ and non-smooth initial condition; see Figure 3.2. Clearly, the novel compact WENO method produced better results with respect to oscillatory behavior in both the low- and high-velocity regions.

4

Local implicit predictor-corrector method

Efficiency should not be understood narrowly as a low computational cost alone. It must be evaluated in the broader context of the method's overall behavior. The core of this chapter focuses on the development of a novel predictor-corrector scheme that was designed to be locally implicit, higher-order accurate in both space and time, and easily extendable into higher dimensions. In addition, when combined with ENO or WENO, the scheme reduces non-physical oscillations regardless of the Courant number.

To illustrate the key ideas and practical implementation of the proposed method, we begin with a simple representative model problem: one-dimensional linear advection. We propose a novel method designed to efficiently solve the following problem:

$$\tilde{\boldsymbol{u}} \cdot \tilde{\nabla}\phi = 0, \quad \tilde{\nabla} = (\partial_t, \partial_x), \quad \tilde{\boldsymbol{u}} = (1, u) \tag{4.1}$$

with given inflow boundary conditions $\phi(x, 0) = \phi^0(x)$ and $\phi(x_{in}, t) = g(t)$.

The novel method that can be summarized in the following set of steps.

1. We begin by predicting values $\phi_i^{n-1,(1)}, \phi_{i-1}^{n,(1)}, \phi_i^{n,(1)}, \phi_{i+1}^{n-1,(1)}$ using a first-order accurate finite difference scheme. We adopt the convention that a superscript (p) denotes a predictor of order p, where $p = 1, 2$.

2. Next, we compute the predictor $\phi_i^{n,(2)}$ using the second-order accurate upwind finite difference scheme employing the previously computed predictors.

$$\phi_i^{n,(2)} = \frac{1}{1+c_i}\left(\phi_i^{n-1} - \frac{1}{2}\left(\phi_i^{n,(1)} - \phi_i^{n-1,(1)} + \phi_i^{n-1} + \phi_i^{n-2}\right)\right.$$
$$\left. + c_i\left(\phi_{i-1}^{n} - \frac{1}{2}\left(\phi_i^{n,(1)} - \phi_{i-1}^{n,(1)} - \phi_{i-1}^{n} + \phi_{i-2}^{n}\right)\right)\right) \tag{4.2}$$

3. In addition, we compute the "future" predicted values $\phi_{i+1}^{n,(2)}, \phi_i^{n+1,(2)}$ in both space and time following a similar strategy.

   During the space–time marching process, the values $\phi_{i+1}^{n,(2)}$ and $\phi_i^{n+1,(2)}$ will be overwritten in subsequent iterations. To maintain third-order accuracy of the final scheme, these values must be temporarily stored and, in the next iteration, reused as previously computed approximations, that is to say, as the value $\phi_i^{n,(2)}$ assessed in the previous step. We will denote the stored values as $\varphi_{i+1}^{n,(2)}$ and $\psi_i^{n+1,(2)}$.

4. Finally, we compute the corrector using the scheme

$$\phi_i^{n,(3)} = \frac{1}{1+c_i}\left(\phi_i^{n-1} - \frac{1-\alpha_i^n}{2}\left(\phi_i^{n+1,(2)} - \phi_i^{n,(2)}\right.\right.$$
$$\left. -\psi_i^{n,(2)} + \phi_i^{n-1}\right) - \frac{\alpha_i^n}{2}\left(\phi_i^{n,(2)} - \phi_i^{n-1,(2)} - \phi_i^{n-1} + \phi_i^{n-2}\right)$$
$$+ c_i\left(\phi_{i-1}^{n} - \frac{1-\omega_i^n}{2}\left(\phi_{i+1}^{n,(2)} - \phi_i^{n,(2)} - \varphi_i^{n,(2)} + \phi_{i-2}^{n}\right)\right.$$
$$\left.\left. - \frac{\omega_i^n}{2}\left(\phi_i^{n,(2)} - \phi_{i-1}^{n,(2)} - \phi_{i-1}^{n} + \phi_{i-2}^{n}\right)\right)\right) \tag{4.3}$$

which is generally second-order accurate and appears to achieve third-order accuracy when $\alpha_i^n = \omega_i^n = 0$, although this has so far only been observed experimentally.

Furthermore, the parameters α_i^n and ω_i^n can be selected based on smoothness indicators, for example, using an ENO-type scheme [17].

We perform a test on an example with a non-smooth initial condition

$$\phi^0(x) = \begin{cases} 4(x-0.25), & \text{if } 0.25 \le x \le 0.5, \\ -4(x-0.75), & \text{if } 0.5 < x \le 0.75, \\ 0, & \text{otherwise.} \end{cases} \tag{4.4}$$

and a constant velocity $u(x) = 1$, with the Courant number $c_i = 5$.

We compare the results of the proposed third-order accurate method (lPC) and a complementing ENO lPC variant; see Figure 4.1. We observe that the ENO lPC method successfully eliminates non-physical oscillations in the gradient of the solution.

We also present solutions to one-dimensional linear advection with variable velocity $u(x) = 1 + 3/4\cos(x)$. The numerical solutions at the final time $T = 8\pi/\sqrt{7}$ are shown in Figure 4.2. The ENO lPC method effectively reduces non-physical oscillations in the gradient, both in regions of low velocity $u(x)$ (near $x = \pi$) and high velocity (around $x = 0$), without requiring additional limiting.

We performed a similar test on a two-dimensional advection equation with constant velocity $\boldsymbol{v}(x,y) = (-1.5, 1.5)$ with equivalent non-smooth initial condition in the shape of a pyramid

$$\phi^0(x,y) = \max(-\max(|x-1.5|, |y+1.5|) + 2, 0.0). \tag{4.5}$$

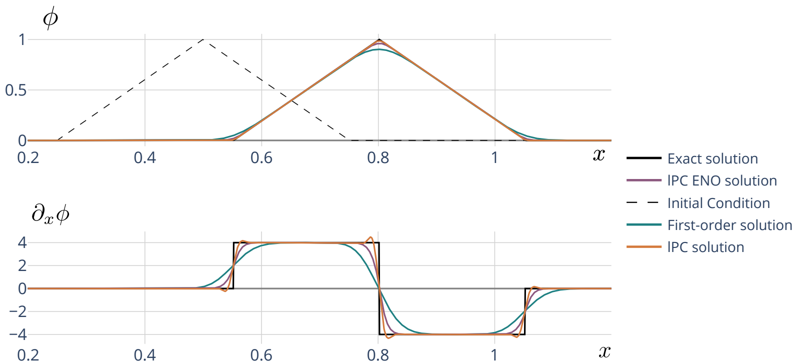


Figure 4.1: Comparison of solution ϕ (up) and $\partial_x \phi$ (down) obtained by the first-order accurate method, lPC end ENO lPC methods on a non-smooth example (4.4).

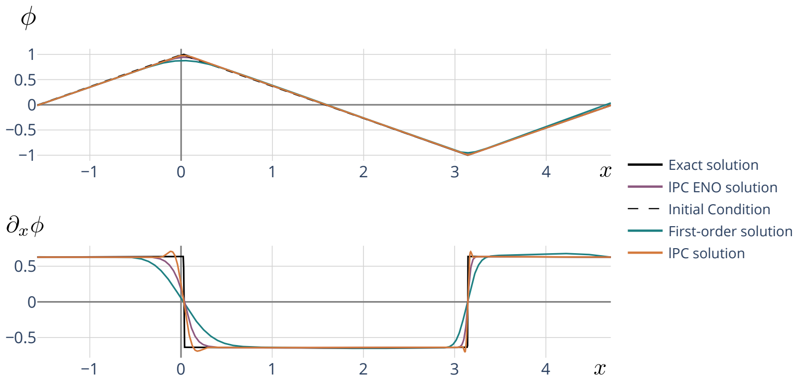


Figure 4.2: Numerical solutions of the advection equation with variable velocity and the initial condition (**??**) computed with the lPC and ENO lPC methos.

Again, ENO lPC was able to recover the solution with no significant non-physical oscillations in the gradient of the solution; see Figure 4.3.

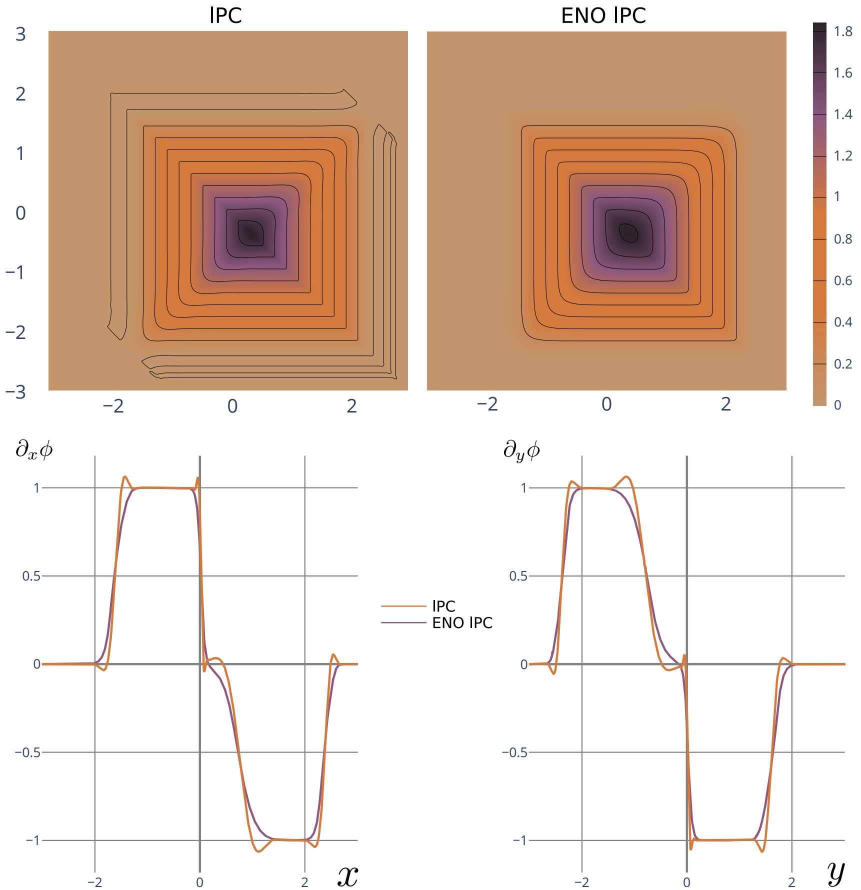


Figure 4.3: Visual comparison of lPC and ENO lPC method results for the two-dimensional example with non-smooth initial condition (4.5). The top row shows contour plots of the solutions, while the bottom row displays their respective gradient profiles along a selected slice.

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