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Adjoint computational methods for 2D inverse design of linear transport equations on unstructured grids

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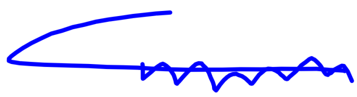
Abstract

In this work, we look at the inverse design issue of the linear transport equation in 2D heterogeneous media with a source term and an unbounded time and space dependant coefficient. Using a regularization methodology and the method of characteristics, we verify the existence and uniqueness of the solution of the linear transport problem as well as the adjoint problem which allowed us to define the inverse design problem. On unstructured grids, we create numerical techniques based on gradient-adjoint methodologies, with the flow equation solved using the Lax-Friedrich scheme for the first order and Muscl for the second order to ensure sufficient accuracy when solving the sensitivity or adjoint equation. Here, the case of Doswell frontogenesis will be examined.

Keywords: Linear transport; Inverse design; Lax-Friedrich and MUSCL schemes; Gradient descent method.

Declaration

I, the undersigned, hereby declare that the work contained in this essay is my original work, and that any work done by others or by myself previously has been acknowledged and referenced accordingly.



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Contents

Abstract **i**

1 Introduction **1**

2 Preliminaries **4**

2.1 Notations 4

2.2 Bochner spaces 4

2.3 Weak topology and weak convergence 6

2.4 Weak* topology and Banach-Alaoglu theorem 7

3 Time-dependent linear transport equation **8**

3.1 Existence and uniqueness of solution for linear transport with bounded coefficients . . . 8

3.2 Existence and uniqueness of linear transport with unbounded coefficients 10

3.3 Inverse problem design and the Adjoint problem of the transport equation 13

4 Numerical approach to the continuous 2D inverse design problem **16**

4.1 Preliminaries and second order MUSCL method 16

4.2 Numerical scheme of time-dependent linear transport equation 17

4.3 Adjoint numerical scheme 19

5 Simulations and Interpretation **21**

6 Conclusions and Perspectives **23**

Acknowledgements **24**

References **26**

1. Introduction

The subject matter of Partial Differential Equations (PDEs) is of fundamental importance in the study and understanding of natural phenomena in the mathematical and numerical view points. Historically, the first equations studied were those that arose from problems of mathematical physics, build dynamics, phase transition, and geometry. Today, those problems are still important, but more areas of science and technology require advanced study of PDEs, its controllability, associated inverse problem design, and numerical analysis.

The advent of modern numerical analysis has contributed a great deal to the development of the subject. Nowadays, numerical schemes are used to compute approximate solutions, because in general the equations of interest do not have solutions that can be obtained in close form. However, the numerical computations have to be supported by theoretical studies, going from the abstract existence theorems, regularity, and sharp error estimates. This interplay between theory and applications is one of the most attractive features and the most challenging of the subject.

More recently, one observes an extensive literature on the control and inverse design of partial differential equations. When dealing with some models, most often, the analysis requires careful mathematical and numerical analysis. This Master thesis is devoted to analyze the problem of inverse design of linear hyperbolic time-dependent transport equations in 2D heterogeneous media. We are interested in developing numerical algorithms based on gradient-adjoint methodologies on unstructured grids. Adjoint methods have been successfully

Implemented and associated with the optimal control design in [14]. As an application of this method to the time-independent linear transport equation one can point out the most recent work of Morales and Enrique Zuazua [22] , which is the main motivation of our current work. As further applications, we also mention [6, 7, 26, 30] and references therein.

To fix ideas, we consider the problem of inverse design aiming to identify the initial datum so that the solution, at the final time, is close to a given final target. To be more precise, given a finite time $T > 0$, $\Omega \subset \mathbb{R}^2$ and a target function $u^* = u^*(x, y)$ at $t = T$, we consider the functional J to be minimized over a suitable class of initial data $\mathcal{U}_{ad}$, defined by

$$J(u_0) = \frac{1}{2}\int_\Omega |u(T) - u^*(s)|^2 \, \mathrm{d}s. \tag{1.0.1}$$

Here, the function u solves the time-dependent linear transport equation

$$\frac{\partial u(x,y,t)}{\partial t} + \nabla \cdot (vu) = g, \quad u(x,y,0) = u_0, \tag{1.0.2}$$

where $v = v(x, y, t)$ is a time-dependent velocity field of propagation.

Motivated by the study of our optimal control and design problem, we are rather interested in the case when v may be unbounded, with at most a linear growth at infinity. More precisely, we assume

$$\begin{cases} g \in L^1\left([0,T]; L^2(\Omega)\right) & \text{and} \quad u_0 \in L^2(\Omega) \\ v \in L^1\left([0,T]; C^1(\Omega)\right), & \text{with} \quad \nabla v \in L^1\left([0,T]; C_b^0(\Omega)\right). \end{cases} \tag{1.0.3}$$

Thus, the problem under consideration reads: To find $u_{0,\min} \in \mathcal{U}_{ad}$ such that

$$J\left(u_{0,\min}\right)=\min_{u_0\in\mathcal{U}_{ad}} J\left(u_0\right).$$

The initial datum u_0 will be assumed to belong to a suitable class called class admissible and denoted by $\mathcal{U}_{ad}$. As observed in [22] , this problem can be easily addressed by simply solving the transport equation backwards in time because of the time reversibility of the model. But such a simple approach fails as soon as the model involves nonlinearities (leading to shock discontinuities) or diffusive terms, making the system time-irreversible.

The inverse design problem under consideration is one of the classical optimization problems which is often addressed in the context of optimal control theory, aerodynamic design, robust control theory based on the concepts of observability, optimality and controllability for linear and non-linear equations and systems of equations (see, for example [8, 13, 31, 32, 33]). Indeed, as stated in [22] , the use of adjoint equations and gradient methods for this purposes is widely justified via the minimization of a functional or cost function [15, 29], resulting a suitable way of analysing the sensitivity of a complex dynamical system [19] . As we will see, the existence of minimizers can be established under some natural assumptions on the class of admissible data, using the well-posedness and compactness properties of solutions of the time-dependent linear transport equation (1.0.2). The uniqueness of the minimizers is true here, in general, due, in particular, to the possible strong assumption on the vector field v in the solutions of (1.0.2).

Although this work is devoted to this particular choice of the J, that can also be handled by other methods, as, for instance, by backward resolution of the equation out of the final target, most of our analysis and numerical algorithms can be adapted to many other functionals and control problems, that would require to implement descent algorithms, which is one of the main content of the present work. Note that, when minimizing the functional (1.0.1), we are looking for an initial datum u_0 so that the solution of the conservation law reaches, or gets as close as possible to, the final target u^*. Thus, the problem can be viewed as a controllability one, the control being the initial datum. The problem can be recast in terms of identifying the set of reachable states at the final time $t = T$ for the semigroup generated by the conservation law.

It is worthwhile emphasising that optimization methods in particular, the best representative gradient descent method, need some information about the gradient of the function to be minimized, which will be closest related to the resolution of the adjoint variables. As pointed in [22], two approaches have divided the research community when trying to solve backwards in time the adjoint equation or system of equations: the continuous and the discrete version. While in the continuous approach the set of adjoint equations is derived analytically and then discretized and solved by means of a certain numerical method, the discrete approach consist of a straightforward algebraic manipulation to achieve the discretized version of the adjoint equation from the original numerical methods used for the primitive flow equations. Since the discrete approach forces the use of the discrete adjoint problem of the flow solver to numerically solve the adjoint equation, the continuous approach is adopted due to its valuable flexibility of using different solvers for the flow and adjoint equations.

In this thesis, we are thus interested in the development of gradient descent methods with the aid of the adjoint equation that can be easily deduced

$$\begin{cases} -\partial_t p - v\nabla p = f, & \text{in} \quad \mathbb{R}^2\times(0,T),\\ p(x,y,T)=p^T(x,y), & \text{on} \quad \mathbb{R}^2, \quad P^T(x,y)=u(x,y,T)-u^*(x,y). \end{cases} \tag{1.0.4}$$

Here, $p = p(x, y, t)$ is the adjoint variable. We assume that the data p_0, v, and f verifies the assumptions in (1.0.3), where u_0 is replaced by p_0. Here, $u(x, y, T) := u^*(x, y)$ for all $x,\ y \in \mathbb{R}^2$.

As noted in [22], we shall see that to achieve a good match with the continuous solutions, high order numerical schemes need to be used for the forward state (1.0.2). Here, we shall use a second order scheme. Our main objective is to test the convenience of using the same order of accuracy when solving the adjoint equation or, by contrast, to employ a low order one. When implementing the gradient descent iterations, the numerical scheme employed for solving the adjoint equation determines the direction of descent. Hence, different solvers for the adjoint system provide different results that can be compared in terms of accuracy and efficiency.

A gradient-adjoint iterative method is based on iterating a loop where the equation of state (1.0.2) is solved in a forward sense while the adjoint equation, which is of hyperbolic nature as well, is solved backwards in time. The adequate resolution of this loop is the main question addressed in this work, paying attention not only to accuracy but also to reducing its computational complexity.

It is worth noticing that several cases of transport equations have already been treated. In particular, in [22], the authors study adjoint computational methods for $2D$ inverse design linear transport equations on unstructured grids but do not take into account the source term, and also provide numerical methods for unstructured grids using gradient-adjoint approaches. The particularity of our work lies in the fact that we are interested in the inverse question of the transport equation with an unbounded velocity vector depending on time and space. We also involve a source term. To address the problem, our work is articulated as follows:

In Chapter 2, we recall the basic notions of functional analysis such as weak and weak-$*$ topology, weak time derivative, and the Banach-Alaoglu theorem.

Chapter 3 is devoted to proving the existence and uniqueness of the transport problem, using the regularization technique and the method of characteristics.Then, we define the inverse and adjoint problems.

We close with Chapter 4 and Chapter 5, which deal with the numerical scheme. Indeed, we use here the first-order Lax-Friedrich scheme combined with the second-order Muscl (Van-Leer) scheme to build a numerical scheme for the approximation of the solution to our problem. The implementation is done using Matlab software in the chapter which is crucial for the discretization of the domain using the Delaunay mesh and the calculation of the solution in each mesh.

2. Preliminaries

In this chapter, we recall some basic notions, definitions, and concepts in Functional Analysis such as Lebesgue and Banach spaces, weak and weak$-*$topology and convergence, weak time derivative and Banach-Alaoglu theorem.

2.1 Notations

The notation used throughout this thesis is given below.

Given $k \in \mathbb{N}$, we denote by $C^k(X)$ the space of all k-times continuously differentiable functions defined on X and by $C_b^k(X)$ the subspace of $C^k(X)$ formed by functions which are uniformly bounded together with all their derivatives up to the order k. We endow $C_b^k(X)$ with the $W^{k,\infty}-$norm as follows

$$\| v \|_{C_b^k(X)} := \sum_{|\alpha| \leq k} \| D^\alpha v \|_{L^\infty},$$

where $\alpha \in \mathbb{N}^d$ is a multi-index, with $|\alpha| := \sum_{i=1}^d \alpha_i$ and

$$D^\alpha f := \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}},$$

denoting the weak α-th derivative.

Next, we consider the $(u_n)_{n\geq 1}$ sequence of X; this sequence is uniformly bounded in X if there exists some constant k such that

$$\| u_n \|_X \leq k, \qquad \forall n \in \mathbb{N}.$$

Here, for X a Banach space and X^* its predual, we denote by $C_*\big([0,T];X\big)$ the set of measurable functions $f : [0,T] \longrightarrow X$ which are continuous with respect to the weak topology. Namely, for any $u \in X^*$, the function $x \longmapsto \langle u, f(x)\rangle_{X^* \times X}$ is continuous over $[0,T]$.

2.1.1 Definition (Family of mollifiers)**.** Let a function $L \in C_c^\infty(\mathbb{R}^d)$ with $L = 1$ for $|x| \leq 1$ and $L = 0$ for $|x| \geq 2$, L radially decreasing and such that $\displaystyle\int_{\mathbb{R}^d} L = 1$. For all $n \in \mathbb{N}$, the family $(L_n)_n$ define by

$$L_n := n^d L(nx)$$

is called family of standard mollifiers.

2.2 Bochner spaces

In this section, we recall the essentials of the integration theory of Banach space-valued functions.These spaces will appear very often in this project. For more details about Bochner spaces see for example [12]. In particular, we refer the interested reader to the book Analysis in Banach Spaces [18].

2.2.1 Definition. Let X be a measurable space and X, Y Banach spaces. A function $f : S \longrightarrow \mathcal{L}(X,Y)$ is called strongly measurable (respectively, strongly μ-measurable) if for all $x \in X$ the Y-valued function $f_x : s \mapsto f(s)x$ is strongly measurable (respectively strongly μ-measurable).

Let X be separable Banach space. We consider mapping

$$t \in [0,T] \mapsto y(t) \in X.$$

We extend the concept of measurability, integrability, and weak differentiability.

2.2.2 Definition (Bochner integral)**.** We have

1. For a simple function $s(t) = \sum_{i=1}^{m} 1_{E_i}(t) y_i$, we define the integral

$$\int_0^T s(t)dt = \sum_{i=1}^{m} y_i \mu\left(E_i\right),$$

where $\mu\left(E_i\right)$ is the Lebesgue measure of E_i.

2. We say that $f : [0,T] \longrightarrow X$ is Bochner-integrable if there exists a subsequence (s_k) of simple functions such that $s_k(t) \to f(t)$ a.e. and

$$\int_0^T \|f\|_X \mathrm{d}t \to 0 \text{ as } k \to +\infty.$$

3. If f is Bochner integrable we define

$$\int_0^T f(t)\mathrm{d}t := \lim_{k\to 0} \int_0^T s_k(t)\mathrm{d}t.$$

For $m \in \mathbb{N}$ and $1 \le p \le +\infty$, we denote with $W^{m,p}(\Omega)$ the usual Sobolev space of L^{p-}functions with all the derivatives up to the order m in L^p; we also set $H^m(\Omega) := W^{m,2}(\Omega)$. For $1 \le p < +\infty$, let $W^{-m,p}(\Omega)$ denote the dual space of $W^{m,p}(\Omega)$. For any $p \in [1,+\infty]$, the space $L^p_{\mathrm{loc}}(\Omega)$ is the set formed by all functions which belong to $L^p\left(K\right)$, for any compact subset K of Ω.

Furthermore, we make use of the so-called Bochner spaces. Given a Banach space $(X, \|\cdot\|_X)$ and a fixed time $T > 0$, we define for $1 \le p < \infty$, and a generic representative function $u = u(x,t)$, the spaces

$$L^p([0,T];X) \quad \text{with norm} \quad \|u\|_{L^p_T(X)} := \left(\int_0^T \|u(\cdot,t)\|_X^p dt\right)^{\frac{1}{p}},$$

and

$$L^\infty([0,T];X) \quad \text{with norm} \quad \|u\|_{L^\infty([0,T];X)} := \operatorname{ess}\sup_{t\in[0,T]} \|u(\cdot,t)\|_X.$$

Further, for $m \in \mathbb{N}$ and a function $u = u(t)$, we define $C^m([0,T];X)$ with the norm

$$\|u\|_{C^m([0,T];X)} := \sum_{k=0}^{m} \max_{t\in[0,T]} \left\| \frac{\mathrm{d}^k}{\mathrm{d}t^k} u(t) \right\|_X.$$

2.2.3 Definition ([20])**.** Let $y \in L^1(0,T;X)$. We say that $v \in L^1(0,T;X)$ is the weak derivative of y, written $\dot{y} := v$ if

$$\int_0^T \dot{\varphi}(t) y(t)\mathrm{d}t = \int_0^T \varphi(t) v(t)\mathrm{d}t, \quad \forall \varphi \in \mathcal{C}_c^\infty(0,T).$$

Moreover, one can define the Bochner dual space analogy as for L^p spaces.

2.2.4 Theorem ([20]). *For $1 \leq p < +\infty$ the dual space of $L^p(0,T;X)$ can isometrically be identified with $L^q\left(0,T;X^*\right), \frac{1}{p}+\frac{1}{q}=1$, by means of the pairing*

$$\langle v, y\rangle_{L^q(0,T;X^*),L^p(0,T;X)} = \int_0^T \langle v(t), y(t)\rangle_{X^*,X} \mathrm{d}t.$$

If H is a Hilbert space then $L^2(0,T;H)$ is a Hilbert space with inner product

$$(y, v) := \int_0^T (v(t), y(t))_H \mathrm{d}t$$

.

Given two operators u and v, we use the standard symbol $[u,v]$ to denote their commutator:

$[u,v] := uv - vu.$

2.3 Weak topology and weak convergence

Let us recall the concept of the weak topology, since we will use it several times through this project. Let V a Banach Space and f a linear functional of V^*. We define the functional

$$\begin{aligned} F_f : V &\to \mathbb{R} \\ v &\mapsto \langle f, v\rangle. \end{aligned}$$

2.3.1 Definition ([20]). The weak topology on V is the coarsest topology associated to the family $(F_v)_{v\in V^*}$.

The sequences in V which converge to an element in V in the weakly topology are called weakly convergent sequences. We will write

$$v_n \rightharpoonup v,$$

for indicating that the sequence $v_n \in V$ weakly converges to $v \in V$.

2.3.2 Proposition ([4]). Let v_n be a sequence in V whose limit is v also in V. Then,

(a) $v_n \to v$ weakly in $\sigma(V,V^*)$ if and only if $\langle f, v_n\rangle \to \langle f, v\rangle$ for all $f \in V^*$.

(b) If $v_n \to v$ strongly, then $v_n \to v$ weakly in $\sigma(V,V^*)$.

(c) If $v_n \to v$ weakly in $\sigma(V,V^*)$, then $\|v_n\|_V$ is bounded and $\|v\|_V \leq \liminf \|v_n\|_V$.

(d) If $v_n \to v$ weakly in $\sigma(V,V^*)$ and if $f_n \to f$ strongly in V^*, then $\langle f_n, v_n\rangle \to \langle f, v\rangle$.

2.3.3 Remark. Every weakly open (resp. closed) set is strongly open (resp. closed) and the converse is false in infinite dimension. However, if the set is convex, then the equivalence holds.

We shall call a weakly sequentially compact set if such set is compact with respect to the weak topology.

2.4 Weak* topology and Banach-Alaoglu theorem

So far we have introduced two topologies for a the dual space V^* of a Banach space V. These topologies are: the strong topology associated to the norm on V and the weak topology on V^* obtained by performing on V^* the construction of the previous section.

In this section we are going to define and present some important results on the weak* topology.

2.4.1 Definition ([20]). Let V be a Banach space, then the weak* topology on its dual, V^*, is the weakest (coarsest) topology on V^* that makes continuous all functionals of the form

$$\varphi_x : V^* \to \mathbb{R}$$
$$f \mapsto \varphi_x(f) := \langle f, v \rangle.$$

to the scalars.

2.4.2 Definition ([20]). Suppose that the normed space where we want to work, V, itself is the dual of some Banach space, i.e., $V = X^*$. A sequence $(f_n) \subset V$ converges in weak*-sense or in the weak topology to $f \in V$, if

$$\langle f_n, x \rangle \to \langle f, x \rangle$$

for any $x \in X$ and we will denote it by $f_n \overset{*}{\to} f$.

As in the weak topology, we have the following result.

2.4.3 Proposition. Let f_n be a sequence in V whose limit is f also in V. Then,

(a) $f_n \overset{*}{\to} f$ if and only if $\langle f_n, v \rangle \to \langle f, v \rangle$ for all $v \in V$.

(b) If $f_n \to f$, then $f_n \to f$. If $f_n \to f$, then $f_n \overset{*}{\to} f$.

(c) If $f_n \overset{*}{\to} f$, then $\|f_n\|_{V^*}$ is bounded and $\|f\|_{V^*} \leq \liminf \|f_n\|_{V^*}$.

(d) If $f_n \overset{*}{\to} f$ and if $v_n \to v$ strongly in V, then $\langle f_n, v_n \rangle \to \langle f, v \rangle$.

Proof. Similar to the proof Proposition [4]. □

This concept allow us to introduce the following theorem

2.4.4 Theorem (Banach-Alaoglu theorem). *Let V be a normed space and V^* its dual. Then, the closed unit ball of V^* is weakly* compact, i.e., it is compact on the weak* topology.*

Proof. One can find the proof in [4]. □

2.4.5 Corollary. As a consequence we have that, if $\|f_n\|_{L^1(0,T;V)} \leq C$ uniformly where C is a constant and V is a Banach space, then there exists a subsequence f_{n_k} such that

$$f_{n_k} \overset{*}{\to} f \text{ in } L^\infty(0, T; V).$$

3. Time-dependent linear transport equation

In this chapter, our objective is to establish the proof of existence and uniqueness of the linear time-dependent transport with unbounded coefficients and for that we will first do it in the framework where the drift function v is bounded and then use the regularization techniques for the general case [2, 3]. The idea of the result here follows from [2].

We consider the following time-dependent linear transport problem in $\mathbb{R}^d$

$$\begin{cases} \partial_t u + \operatorname{div}\big(v(x,t)u(x,t)\big) = g(x,t) & \text{in} \quad \mathbb{R}^d \times [0,T], \\ u(x,0) = u_0(x) \quad \text{on} \quad \mathbb{R}^d. \end{cases} \tag{3.0.1}$$

Whenever attempting to solve (3.0.1), we need to have in mind its weak formulation. Namely, for all $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times [0,T[)$, by multiplying the first equation in (3.0.1) by the test function ϕ, we obtain by integrating successively on $\mathbb{R}^d$ and over $[0,T]$, the following weak formulation

$$\int_0^T \int_{\mathbb{R}^d} \phi \, \partial_t u \, \mathrm{dx} \, \mathrm{dt} + \int_0^T \int_{\mathbb{R}^d} \phi \, \operatorname{div}\left(v(x,t)u(x,t)\right) \, \mathrm{d}x \, \mathrm{dt} = \int_0^T \int_{\mathbb{R}^d} \phi \, g(x,t) \, \mathrm{d}x \, \mathrm{dt},$$

therefore, using Green's formula we have

$$-\int_0^T \int_{\mathbb{R}^d} u \, \partial_t \phi \, \mathrm{d}x \, \mathrm{dt} - \int_0^T \int_{\mathbb{R}^d} u \, v.\nabla\phi \, \mathrm{d}x \, \mathrm{dt} = \int_0^T \int_{\mathbb{R}^d} g \, \phi \, \mathrm{d}x \, \mathrm{dt} + \int_{\mathbb{R}^d} u_0 \, \phi(0) \mathrm{d}x. \tag{3.0.2}$$

The solution of this equation is classical, at least in the case of the bounded drift function v.

Motivated by the study of our optimal control and design problem, we are rather interested in the case when v may be unbounded, with at most a linear growth at infinity. More precisely, we assume

$$\begin{cases} g \in L^1\left([0,T]; L^2\left(\mathbb{R}^d\right)\right) \quad \text{and} \quad u_0 \in L^2\left(\mathbb{R}^d\right), \\ \\ v \in L^1\left([0,T]; C^1\left(\mathbb{R}^d\right)\right), \quad \text{with} \quad \nabla v \in L^1\left([0,T]; C_b^0\left(\mathbb{R}^d\right)\right). \end{cases} \tag{3.0.3}$$

3.0.6 Remark. Notice that hypotheses in (3.0.3) imply, in particular, that $v(\cdot,t)$ has at most linear growth in space at infinity. Indeed, there exists a positive constant C, such that for every $(x,t) \in \mathbb{R}^d \times [0,T]$, one has

$$|v(x,t)| < Ck(t)(1+|x|), \quad \text{for} \quad k(t) = \|\nabla v\|_{L^\infty(\mathbb{R}^d)} \in L^1\left([0,T]\right). \tag{3.0.4}$$

The condition of at most linear growth at infinity can be proved to be somehow sharp for well-posedness. We use an important statement proved by DiPerna and Lions in [10].

3.1 Existence and uniqueness of solution for linear transport with bounded coefficients

In this section, the aim is to prove the existence and uniqueness of (3.0.1) assuming that, v is a bounded drift.

In the context with bounded coefficients, the solution is given by the characteristic method

$$u\left(X(\xi,t),t\right)=\left[u_0(\xi)+\int_0^t g(s)\exp\left(\int_0^s \nabla v\left(X(\xi,l),l\right)\mathrm{d}l\right)\mathrm{d}s\right]\exp\left(-\int_0^t \nabla v\left(X(\xi,s),s\right)\mathrm{d}s\right) \tag{3.1.1}$$

where the characteristic curves are defined by $X:\mathbb{R}^d\times[0,T]\longrightarrow\mathbb{R}^d$.

Here, we will show that (3.1.1) is a unique weak solution of

$$-\int_0^T\int_{\mathbb{R}^d} u\,\partial_t\phi\,\mathrm{d}x\,\mathrm{d}t-\int_0^T\int_{\mathbb{R}^d} u\,v.\nabla\phi\,\mathrm{d}x\,\mathrm{d}t=\int_0^T\int_{\mathbb{R}^d} g\,\phi\,\mathrm{d}x\,\mathrm{d}t+\int_{\mathbb{R}^d} u_0\,\phi(0)\,\mathrm{d}x, \tag{3.1.2}$$

for any $\phi\in\mathcal{C}_c^\infty(\mathbb{R}^d\times[0,T[)$. This will allow us to conclude directly on the existence and uniqueness of the problem (3.0.1) using the fact that there is equivalence between the solution of the variational problem and the one of the initial problem under the hypothesis that the solution is regular.

Concerning the existence of the solution, by replacing (3.1.1) in the variational problem (3.1.2), and using the Green's formula, we have

$$-\int_0^T\int_{\mathbb{R}^d} u\,\partial_t\phi\,\mathrm{d}x\,\mathrm{d}t=\int_{\mathbb{R}^d} u_0(\xi)\,\phi(0)+\int_0^T\int_{\mathbb{R}^d} g(x,t)\mathrm{d}x\,\mathrm{d}t+\int_0^T\int_{\mathbb{R}^d} -\nabla v\,u\,\phi\,\mathrm{d}x\,\mathrm{d}t, \tag{3.1.3}$$

and

$$-\int_0^T\int_{\mathbb{R}^d} u\,v.\nabla\phi\,\mathrm{d}x\,\mathrm{d}t=\int_0^T\int_{\mathbb{R}^d}\nabla(uv)\,\phi\,\mathrm{d}x\,\mathrm{d}t. \tag{3.1.4}$$

So by combining (3.1.3) and (3.1.4), we have the desired equality.

The result about uniqueness is given by the following proposition.

3.1.1 Proposition. For every function $f\in\mathcal{D}([0,T[\times\mathbb{R}^d)$, there exists $\phi\in\mathcal{C}_c^1([0,T]\times\mathbb{R}^d)$ such that $\frac{\partial\varphi}{\partial t}+v.\nabla\varphi=f$ with $v\in\mathcal{C}^1([0,T]\times\mathbb{R}^d)$, a vector field.

Let u_1 and u_2 be two weak solutions of (3.1.2), our objective is to show that $u_1=u_2$. We proceed as follows. Setting $w=u_1-u_2$, we have from (3.1.2):

$$-\int_0^T\int_{\mathbb{R}^d} w\,\partial_t\phi\,\mathrm{d}x\,\mathrm{d}t-\int_0^T\int_{\mathbb{R}^d} w\,v.\nabla\phi\,\mathrm{d}x\,\mathrm{d}t=0 \tag{3.1.5}$$

is zero almost everywhere.

From (3.1.5), we have

$$\int_0^T\int_{\mathbb{R}^d} w\left(\frac{\partial\phi}{\partial t}+v.\nabla\phi\right)\mathrm{d}x\,\mathrm{d}t=0.$$

Therefore, $w=0$ almost everywhere.

In addition, u satisfies the energy estimate,

$$\|u\|_{L^2(\mathbb{R}^d)}\le C\left(\|u_0\|_{L^2(\mathbb{R}^d)}+\int_0^t\|g(\tau)\|_{L^2(\mathbb{R}^d)}\,\mathrm{d}\tau\right)\exp\left(C\int_0^t\|\nabla v(\tau)\|_{C_b^0(\mathbb{R}^d)}\,\mathrm{d}\tau\right).$$

3.2 Existence and uniqueness of linear transport with unbounded coefficients

In this section, we give a self-contained presentation of it proof.Indeed, the idea of the proof is as follows: We simplify our problem by truncating it to a family of linear transport equations with constrained coefficients, to which the classical theory applies. Then we reach the approximation parameter's limit, demonstrating convergence to a solution of the original equation. Finally, we explore questions of time regularity and uniqueness.The idea follows from [2, 3].

3.2.1 Existence. The first step is to construct a suitable truncation of the drift function. For this purpose, let us introduce a smooth cut-off function $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ such that χ is radially decreasing, $\chi(x) = 1$ for $|x| \leq 1$ and $\chi(x) = 0$ for $|x| \geq 2$. For all real $\Lambda > 0$, we define

$$v_\Lambda(x,t) := \chi\left(\frac{x}{\Lambda}\right) v(x,t). \tag{3.2.1}$$

Notice that, by (3.0.3), we can check that $v_\Lambda \in L^1\left([0,T]; C_b^1\left(\mathbb{R}^d\right)\right)$ for all $\Lambda > 0$. Moreover, in view of Remark 3.0.6, it holds that

$$(\nabla v_\Lambda)_\Lambda \in L^1\left([0,T]; C_b^0\left(\mathbb{R}^d\right)\right), \quad \text{with} \quad \|\nabla v_\Lambda\|_{L^1([0,T];L^\infty(\mathbb{R}^d))} \leq C, \tag{3.2.2}$$

for a suitable constant $C > 0$ independent of Λ. Indeed, let $A \subset \mathbb{R}^d$ and denote by $\mathbf{1}_A$ the characteristic function of A and by $B(x,r)$ the ball in $\mathbb{R}^d$ centered at x with radius $r > 0$, we compute

$$\begin{aligned}
\|\nabla v_\Lambda\|_{L^\infty(\mathbb{R}^d)} &= \left\| \frac{1}{\Lambda}\nabla\chi\left(\frac{x}{\Lambda}\right) v + \chi\left(\frac{x}{\Lambda}\right)\nabla v \right\|_{L^\infty(\mathbb{R}^d)}, \\
&\leq \|\nabla v\|_{L^\infty(\mathbb{R}^d)} + \frac{C}{\Lambda}\left\|v\mathbf{1}_{B(0,2\Lambda)}\right\|_{L^\infty(\mathbb{R}^d)} \\
&\leq C.
\end{aligned}$$

At this point, for each fixed $\Lambda > 0$, we consider the truncated problem

$$\begin{cases} \partial_t u + \operatorname{div}(v_\Lambda u) = g, & \text{in} \quad \mathbb{R}^d \times [0,T], \\ u(x,0) = u_0, & \text{on} \quad \mathbb{R}^d, \end{cases} \tag{3.2.3}$$

which possesses a unique weak solution $u_\Lambda \in C\left([0,T]; L^2(\mathbb{R}^d)\right)$ according to previous section.

Moreover, each u_Λ satisfies the energy estimate

$$\|u_\Lambda\|_{L^2(\mathbb{R}^d)} \leq C\left(\|u_0\|_{L^2(\mathbb{R}^d)} + \int_0^t \|g(\tau)\|_{L^2(\mathbb{R}^d)}\,\mathrm{d}\tau\right)\exp\left(C\int_0^t \|\nabla v_\Lambda(\tau)\|_{C_b^0(\mathbb{R}^d)}\,\mathrm{d}\tau\right). \tag{3.2.4}$$

Thanks to (3.2.2), we deduce the uniform bounds

$$(u_\Lambda)_\Lambda \subset L^\infty\left([0,T]; L^2\left(\mathbb{R}^d\right)\right) \tag{3.2.5}$$

As a result of (3.2.5), we learn about the existence of a $u \in L^\infty\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$ such that, up to the extraction of a subsequence, one has

$$u_\Lambda \overset{*}{\rightharpoonup} u \quad \text{in} \quad L^\infty\left([0,T]; L^2\left(\mathbb{R}^d\right)\right).$$

Our next aim is to show that u actually solves problem (3.0.1) in the weak form, (3.0.3). For this reason, we need pass to the limits as $\Lambda \longrightarrow +\infty$, into the weak formulation of problem (3.2.3).

Indeed, we start by recalling that u_Λ is a weak solution to (3.2.3) for any $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times [0,T[)$, we have

$$-\int_0^T \int_{\mathbb{R}^d} u_\Lambda\, \partial_t\phi \,\mathrm{d}x\,\mathrm{d}t - \int_0^T \int_{\mathbb{R}^d} u_\Lambda v_\Lambda.\nabla\phi \,\mathrm{d}x\,\mathrm{d}t = \int_0^T \int_{\mathbb{R}^d} g\,\phi\,\mathrm{d}x\,\mathrm{d}t + \int_{\mathbb{R}^d} u_0\,\phi(0)\mathrm{d}x. \quad (3.2.6)$$

The only term which presents some difficulties is the term $u_\Lambda v_\Lambda$, and thus we focus on it. We start by proving the following lemma

3.2.2 Lemma. For all compact set $K \subset \mathbb{R}^d$, it holds that

$$\|v_\Lambda - v\|_{L^1([0,T];L^\infty(K))} \longrightarrow 0 \quad as \quad \Lambda \longrightarrow +\infty.$$

Proof. Let $K \subset \mathbb{R}^d$ be a compact set; and let $R > 0$ such that $K \subset B(0,R)$. The claim of the lemma follows then by observing that, by definition, for all $\Lambda \geq R+1$, one has $v_\Lambda(t) \equiv v(t)$ over K, for almost every $t \in [0,T]$. □

3.2.3 Theorem. *Let $T > 0$ and let v, u_0, g satisfy hypothesis (3.0.3). Then, there exists a unique solution $u \in C\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$ to problem (3.0.1). Moreover, there exists a constant $C > 0$, independent of v, u_0, g and T, such that the following estimate holds true for any $t \in [0,T]$:*

$$\|u(t)\|_{L^2(\mathbb{R}^d)} \leq C\left(\|u_0\|_{L^2(\mathbb{R}^d)} + \int_0^t \|g(\tau)\|_{L^2(\mathbb{R}^d)}\,\mathrm{d}\tau\right)\exp\left(C\int_0^t \|\nabla v(\tau)\|_{C_b^0(\mathbb{R}^d)}\,\mathrm{d}\tau\right). \quad (3.2.7)$$

Let K be the support in x of ϕ, where ϕ is the test function appearing in (3.2.6).

Thanks to uniform bound, to the strong convergence of v_Λ to v in $L^1\left([0,T];L^\infty\left(K\right)\right)$ and the weak -* convergence of u_Λ to u in $L^\infty\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$, we finally deduce that $(u_\Lambda v_\Lambda)_\Lambda$ is uniformly bounded in $L^1\left([0,T];L^\infty\left(K\right)\right)$, (given by Lemma 3.2.2) and $u_\Lambda v_\Lambda \overset{*}{\rightharpoonup} uv$ in that space in the limit when $\Lambda \longrightarrow +\infty$.

Thus, we have proven that the limit function u is a weak solution to (3.0.1). It is worth noticing that thanks to (3.2.4), the uniform bounds (3.2.6) and lower semicontinuity of the norm, we also deduce that u verifies the energy estimate (3.2.4).

It remains to prove uniqueness of solutions and their time regularity.

3.2.4 Time regularity and uniqueness. Before doing so, we recall the following lemma.

3.2.5 Lemma ([10])**.** Let $(\rho_n)_n$ be a family of mollifiers defined above 2.1.1. For all $n \in \mathbb{N}$, define the operator L_n, acting on tempered distributions over $[0,T] \times \mathbb{R}^d$, by the formula

$$L_n u := \rho_n *_x u,$$

where the symbol $*_x$ means that the convolution is taken only with respect to space variable. For given $u \in L^\infty\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$ and $v \in L^1\left([0,T];C^1\left(\mathbb{R}^d\right)\right)$ such that $\nabla v \in L^1\left([0,T];C_b\left(\mathbb{R}^d\right)\right)$, we set for all $n \in \mathbb{N}$ and $1 \leq j \leq d$,

$$\begin{aligned} S_n^j(u) &:= \partial_j\left([v, L_n]u\right), \\ &:= \partial_j\left(\left(vL_n - L_n v\right)u\right). \end{aligned}$$

Then, for all j fixed, we have $(S_n^j)_n \subset L^1\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$. Moreover, for $n \longrightarrow +\infty$, we have the strong convergence $S_n^j \longrightarrow 0$ in $L^1\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$.

3.2.6 Proposition. Let $T > 0$ and take $n \in \mathbb{N}$. Let $u \in L^\infty\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$ be a weak solution to (3.0.1) under hypotheses (3.0.3). Then, $u \in C\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$ and it verifies the energy estimate (3.2.4).

Proof. With the same notations as in Lemma 3.2.5, let us define $u_n := L_n u$.

Notice that $(u_n)_n \subset L^\infty\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$. Furthermore, u_n satisfies the equation

$$\partial_t u_n + \operatorname{div}(v u_n) = g_n + \rho_n \quad \text{with} \quad (u_n)\big|_{t=0} = L_n(u_0) \tag{3.2.8}$$

where we have set $S_n := \operatorname{div}\left([v, L_n]u\right)$. Notice that one has $\|L_n u_0\|_{L^2(\mathbb{R}^d)} \le C\|u_0\|_{L^2(\mathbb{R}^d)}$ and $\|g_n\|_{L^1([0,T];L^2(\mathbb{R}^d))} \le \|g\|_{L^1([0,T];L^2(\mathbb{R}^d))}$. Furthermore, when $n \longrightarrow +\infty$, we have the strong convergence properties $g_n \longrightarrow g$ in $L^1\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$ and $L_n u_0 \longrightarrow u_0$ in $L^2\left(\mathbb{R}^d\right)$. In addition, by Lemma 3.2.5, we see that $\|S_n\|_{L^1([0,T];L^2(\mathbb{R}^d))} \le C$ and $S_n \longrightarrow 0$ in $L^1\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$.

Next, it is worth noticing that (3.2.8) implies the property $(\partial_t u_n)_n \subset L^1\left([0,T]; H^{-1}_{\text{loc}}\right)$ which in turn gives us the uniform embedding $(u_n)_n$ in $C\left([0,T]; H^{-1}_{\text{loc}}\right)$. From this latter property, combined with density argument and the uniform boundedness of $(u_n)_n$ in $L^\infty\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$, we deduce that $(u_n)_n$ is uniformly bounded in $C_*\left([0,T]; X\right)$, Which is the set of measurable function u: $[0,T] \to X$ which are continuous with respect to the weak topology.

Next, let us take the L^2- scalar product of (3.2.8) by u_n. We have

$$\langle \partial_t u_n + \operatorname{div}(a u_n), u_n \rangle = \langle g_n + S_n, u_n \rangle,$$

that is,

$$\langle \partial_t u_n, u_n \rangle + \langle \operatorname{div}(a u_n), u_n \rangle - \langle S_n, u_n \rangle = \langle g_n, u_n \rangle.$$

Therefore,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_n\|^2_{L^2(\mathbb{R}^d)} + \frac{1}{2}\int_{\mathbb{R}^d} \operatorname{div}(a)|u_n|^2 \mathrm{d}x = \int_{\mathbb{R}^d} g_n u_n \mathrm{d}x, \tag{3.2.9}$$

which implies that, for all $n \in \mathbb{N}$, one has $\|u_n(t)\|_{L^2(\mathbb{R}^d)} \in C\left([0,T]\right)$, thanks to this property, together with the fact that $u_n \in C_*\left([0,T], L^2\left(\mathbb{R}^d\right)\right)$, after writing

$$\|u_n(t+h) - u_n(t)\|^2_{L^2(\mathbb{R}^d)} = \|u_n(t+h)\|^2_{L^2(\mathbb{R}^d)} + \|u_n(t)\|^2_{L^2(\mathbb{R}^d)} - 2\langle u_n(t+h), u_n(t)\rangle_{L^2(\mathbb{R}^d)\times L^2(\mathbb{R}^d)},$$

one immediately deduces that for all $n \in \mathbb{N}$, u_n belongs to $C\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$. Since the right hand side goes to zeros as h goes to zero.

Moreover, by straightforward computations from (3.2.9), we also infer the following inequality:

$$\begin{aligned}
\|u_n(t)\|_{L^2(\mathbb{R}^d)} \le C \exp\left(C\int_0^t \|\operatorname{div} v(\tau)\|_{L^\infty(\mathbb{R}^d)} \mathrm{d}\tau\right) \times \\
\left(\|L_n u_0\|_{L^2(\mathbb{R}^d)} + \int_0^t \left(\|g_n(\tau)\|_{L^2(\mathbb{R}^d)} + \|S_n(\tau)\|_{L^2(\mathbb{R}^d)}\right)\mathrm{d}\tau\right), \\
\le C \exp\left(C\int_0^t \|\operatorname{div} v(\tau)\|_{L^\infty(\mathbb{R}^d)} \mathrm{d}\tau\right)\left(\|u_0\|_{L^2(\mathbb{R}^d)} + \int_0^t \|g_n(\tau)\|_{L^2(\mathbb{R}^d)} \mathrm{d}\tau\right),
\end{aligned}$$

for all $t \in [0,T]$, thanks to the Gronwall's lemma also to the previous properties on $(L_n u_0)_n$, $(g_n)_n$, and $(S_n)_n$. In view of this energy estimate, we deduce that $(u_n)_n$ is uniformly bounded in $C\left([0,T]; L^2\left(\mathbb{R}^d\right)\right)$.

Next, by similar argument, using the fact that $(L_n u_0)_n$, $(g_n)_n$, and $(S_n)_n$ are strongly convergent in the respective functional spaces, we can deduce that $(u_n)_n$ is a Cauchy sequence in $C\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$. To prove this, we take $m<n$ and consider the difference $\delta_m^n u := u_n - u_m$. Then, $\delta_m^n u$ fulfils

$$\partial_t \delta_m^n u + \operatorname{div}(v\delta_m^n u) = \delta_m^n g + \delta_m^n S, \quad \text{with} \quad (\delta_m^n u)\big|_{t=0} = u_0^n - u_0^m, \tag{3.2.10}$$

where we defined $\delta_m^n g = g^n - g^m$ and $\delta_m^n S = S^n - S^m$.

Foremost, we proceed by applying the energy estimates to (3.2.10) and obtain

$$\begin{aligned} \|\delta_m^n u\|_{L^\infty([0,T];L^2(\mathbb{R}^d))} \leq C\exp\left(C\|\operatorname{div}(v)\|_{L^1([0,T];L^\infty(\mathbb{R}^d))}\right)\times \\ \left(\|\delta_m^n u_0\|_{L^2(\mathbb{R}^d)} + \|\delta_m^n g\|_{L^1([0,T];L^2(\mathbb{R}^d))} + \|\delta_m^n S\|_{L^1([0,T];L^2(\mathbb{R}^d))}\right). \end{aligned} \tag{3.2.11}$$

Hence, we can conclude thanks to the fact that $(L_n u_0)_n$, $(g_n)_n$, $(S_n)_n$ are strongly convergent in the respective functional spaces and thus they are in particular, Cauchy sequences. Proving our claim. To finish with the proof, we deduce that the limit u of the sequence $(u_n)_n$ belongs to $C\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$, and the convergence $u_n \longrightarrow u$ is strong in this space.

Finally, passing the limit in the left-hand side of (3.2.11) we see that u verifies the energy estimate (3.2.7).

We conclude this part by noticing that the stability and uniqueness are direct consequences of Corollary 3.2.7. □

3.2.7 Corollary. Let v as in (3.0.1) and fix $T>0$, for $i=1,2$ take an initial datum $u_0^i \in L^2\left(\mathbb{R}^d\right)$ and an external force $g^i \in L^1\left([0,T],L^2\left(\mathbb{R}^d\right)\right)$ and let $u^i \in L^\infty\left([0,T];L^2\left(\mathbb{R}^d\right)\right)$ be a corresponding solution to (3.0.1). Then, define $\delta u_0 = u_0^1 - u_0^2$, $\delta g = g^1 - g^2$ and $\delta u = u^1 - u^2$, the following estimate holds true for all $t\in[0,T]$, for some constant C independent of the data and the respective solutions:

$$\|\delta u(t)\|_{L^2(\mathbb{R}^d)} \leq C\exp\left(C\int_0^t \|\nabla v(\tau)\|_{C_b^0(\mathbb{R}^d)}\,\mathrm{d}\tau\right)\left(\|\delta u_0\|_{L^2(\mathbb{R}^d)} + \int_0^t \|\delta g(\tau)\|_{L^2(\mathbb{R}^d)}\,\mathrm{d}\tau\right). \tag{3.2.12}$$

Proof. It is worth noticing that, by taking the difference of the equations satisfied by u^1 and u^2, one deduces that $\delta u \in L^\infty\left([0,T],L^2(\mathbb{R}^d)\right)$ is a weak solution to the following

$$\begin{cases} \partial_t(\delta u) + \operatorname{div}(v\delta u) = \delta g & \text{in } \mathbb{R}^d\times(0,T], \\ \delta u_{|t=0} = \delta u_0 & \text{on } \mathbb{R}^d. \end{cases}$$

Then, Proposition 3.2.6 applies and, gives us the claimed estimates (3.2.12) □

3.3 Inverse problem design and the Adjoint problem of the transport equation

In this part we will give a brief description of the inverse problem [17] with some illustrative examples and we will establish the adjoint equation of the transport problem.

3.3.1 Inverse problem and examples. As pointed out in [1], two problems are inverses of each other if the formulation of one of them implies the other. In a simpler way, an inverse problem consists in determining the causes by knowing the effects. Thus, this problem is the inverse of the so-called direct problem which consists in deducing the effects knowing the causes. The prediction of the future state of a physical system knowing its present state is a reasonable example of a direct problem; thus among the inverse problems we can have the determination of the parameters of the system knowing a part of its evolution, commonly called identification of the parameters is the main concern in the continuation of our work.

In the context where we focus on the conservative linear transport scalar equation (3.0.1), with a time and space dependent heterogeneous vector field $v = v(x, y, t)$, and a source term $g = g(x, y, t)$; the inverse design problem is defined as follows:

Given $\Omega \subseteq \mathbb{R}^2$ and a target function $u^* = u^*(x, y)$ at $t = T$, to determine the initial condition u_0 such that $u(x, y, T) \equiv u^*(x, y)$ for all $x,\ y \in \Omega$.

But we can rewrite the inverse design problem as optimal control problem, consisting on the minimization of the cost function

$$J(u_0) = \frac{1}{2}\int_{\Omega} |u(x, y, T) - u^*(x, y)|^2 \mathrm{d}s. \tag{3.3.1}$$

.

3.3.2 The Adjoint problem of the transport equation. The characterization of set controls with optimality conditions requires the solution of an adjoint linear transport problem. In preparation for that discussion, and to complete the analysis of this present part, we consider the following problem

$$\begin{cases} \partial_t p + v.\nabla p = g \ \text{ in } \ \Omega \times [0, T], \\ u(T) - u^* \equiv u(x, y, T), \ \text{ on } \ \Omega. \end{cases} \tag{3.3.2}$$

We assume that the data p_0, v, and g verifies the assumptions in (3.0.3) , where u_0 is replaced by p_0.

We point out that the weak formulation of (3.3.2) now reads as follows : for all $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^d \times [0, T[)$

$$-\int_0^T\int_{\mathbb{R}^d} p\ \partial_t\phi - \int_0^T\int_{\mathbb{R}^d} p\ v.\nabla\phi - \int_0^T\int_{\mathbb{R}^d} p\ \mathrm{div}(v)\ \phi = \int_0^T\int_{\mathbb{R}^d} g\ \phi + \int_{\mathbb{R}^d} p_0\ \phi(0). \tag{3.3.3}$$

From (3.3.2), we have the following well-posedness, analogous to Theorem 3.2.3.

3.3.3 Theorem. *Fix $T > 0$, and let the data v, p_0, and g satisfy the assumptions stated above. Then, there exists a unique solution $p \in C\left([0, T]; L^2\left(\mathbb{R}^d\right)\right)$ to (3.3.2). Moreover, there exists a constant $C > 0$, independent of p_0, v, g, p, and T, such that the following estimate holds for any $t \in [0, T]$:*

$$\|p(t)\|_{L^2(\Omega)} \leq C\left(\|p_0\|_{L^2(\Omega)} + \int_0^t \|g(\tau)\|_{L^2(\Omega)}\, d\tau\right) \exp\left(C\int_0^t \left(\|\nabla v(\tau)\|_{C_b^0}\right) d\tau\right). \tag{3.3.4}$$

The proof is analogous to the one given for Theorem 3.2.3, so it is omitted here. In particular, the regularization procedure and the energy estimate work the same way. We only point out the fact that passing the limit in the weak formulation (3.3.4) at step n of the regularization procedure requires some attention in the terms

$$-\int_0^T\int_{\Omega} p^n \mathrm{div}(v^n)\ \phi.$$

Notice that the integral is in fact performed on the compact set $K := \mathrm{supp}\ \phi$ where supp refers to support of the function ϕ. On the other hand, thanks to uniform bounds, $p^n \overset{*}{\rightharpoonup} p$ in $L^\infty\left([0, T]; L^\infty\left(K\right)\right)$, for some p belonging to the space; so in particular the weak$-^*$ convergence holds true in $L^\infty\left([0,T];L^\infty(K)\right)$. This previous argument shows that we can pass to the limit in the weak formulation of the approximated problems and gather that the limit point p of the sequence $(p^n)_n$ solves (3.3.3).

3.3.4 Optimisation methods and classical result of convergence(Gradient descent method). In practical applications, and in order to perform numerical computations and simulations, one has to replace the above continuous optimization problem and methods by discrete approximations. Then, it is natural to consider a discretization of (1.0.2) and the functional J. If this is done in an appropriate way, the discrete optimization problem has minimizers that are often taken, for small enough mesh-sizes, as approximations of the continuous minimizers. This is the so-called discrete or direct approach: **Discretize first and then optimize** . There are however few results in the context of hyperbolic conservation laws proving rigorously the convergence of the discrete optimal controls towards the continuous ones, as the mesh-size goes to zero. In this part, our aim is to minimize the cost function defined by (3.3.1). We chose the gradient descent method whose iterative algorithm is given by minimizing the cost function define by (3.3.1), the optimisation method chosen is the gradient descent method whose the iterative algorithm is given by

$$\begin{cases} u_0^{k+1} = u_0^k - \varepsilon \nabla J^k, \\ u_0^0 = 0, \end{cases} \tag{3.3.5}$$

for $k \geq 0$, where $\nabla J^k(u_0) = p^k(0)$ denotes the descent direction, p is the solution of the backround in time problem, and $\varepsilon > 0$ the step.

The following theorem guarantee us a result of convergence of the method.

3.3.5 Theorem ([11])**.** *Let $J \in C^1$ from $\mathbb{R}^n$ to $\mathbb{R}$, x^* a minimum of J. If*

1. *J is α-elliptique, that means there exists $\alpha > 0$,such that for all $x, y \in \mathbb{R}^n$*

$$\langle \nabla J(x) - \nabla J(y), (x-y) \rangle \geq \alpha \left\| x - y \right\|^2;$$

2. *∇J is Lipschitz, that means there exists $M > 0$, such that for all $x, y \in \mathbb{R}^n$*

$$\left\| \nabla J(x) - \nabla J(y) \right\| \leq M \left\| x - y \right\|.$$

Furthermore, if there is $a, b \in \mathbb{R}$ such that $0 < a < \varepsilon^{(k)} < b < \frac{2b}{M^2}$, for all $k \geq 0$ then the gradient method define by

$$x^{(k+1)} = x^{(k)} - \varepsilon^{(k)} \nabla J^{(k)},$$

converge for all choice of $x^{(0)}$ of geometric ways there exist β in $]0,1[$

$$\left\| x^{(k+1)} - x^* \right\| \leq \beta^k \left\| x^{(k)} - x^* \right\|.$$

If $\varepsilon^{(k)} = \varepsilon$ fixed, then, we talk about gradient descent method.

Proof. One can find the proof in [9]. □

4. Numerical approach to the continuous 2D inverse design problem

This chapter is devoted to the numerical schemes to the continuous 2D inverse design problem which will be used in the next chapter of this thesis, and in particular for the simulation of the so called Doswell frontogenesis problem. The Doswell frontogenesis problem symbolizes the presence of horizontal temperature gradients and fronts in the context of meteorological dynamics.

A stable scheme need to be derived for this convected dominated flow, with the ability of vortex-type profile capturing. Beside this, the convection part needs in most cases to involve a numerical dissipation which is as small as possible. Two type of numerical schemes are considered. The Lax-Friedrich and the Monotone Upstream Scheme for Conservation Laws (MUSCL) in order to have a good accuracy in space and time for the flow equation and its associated adjoint problem. While the flow equation is solved by means of a second order upwind scheme so to guarantee sufficient accuracy, the necessity of using the same order of approximation when solving the sensitivity or adjoint equation is examined.

This chapter is organized in three sections. We start with Section 4.1 where we focus on the description of main numerical aspects for spatial resolution of a simpler model, the Finite volume Euler model. In this section one will be guided through the presentation of the Finite volume space-time mesh and the second order MUSCL method. Next, in Section 4.2, we shall focus on numerical schemes for the time dependent flow equation. Here, the discrete version of the problem is then analysed. In particular, two schemes are presented, which will be the basis of the numerical experiments: a First and Second Order scheme, both implemented on unstructured grids.

The last part of this chapter, that is Section 4.3, is dedicated to the implementation of these upper mentioned schemes to adjoint equation. Here, we care about the signs in the upwind discretization in view of the fact that the sense of time is to be reversed.

4.1 Preliminaries and second order MUSCL method

The celebrated Godunov method builds fluxes between cells in which all unknown variables are considered as constant. This results in a first-order accurate scheme, is known to be not enough accurate for most applications in fluid dynamic. Due to the rather poor approximation of the true solution within a cell, higher order versions of Godunov's method have been developed that yield more accurate approximations. In this regards,

in order to improve the method, Van Leer has proposed ([27, 28]) to reconstruct a linear interpolation of the variables inside each cell and to introduce in the Riemann solver the boundary values of these interpolations. This approach has the advantage that, the slopes used for linear reconstruction can be limited in order to represent the variable without introducing new extrema. The resulting Monotone Upstream Scheme for Conservation Laws (MUSCL) method produces positive second-order schemes and was modified by S. Hancock, hence generally referred to as MUSCL-Hancock method [16, 28]. The MUSCL-Hancock method is a predictor-corrector- type scheme, meaning that at first a less accurate approximation to the numerical solution is computed, which is then corrected by a different numerical method. We describe now an extension of MUSCL to unstructured triangulations with dual cells. The MUSCL ideas also applies to reconstructions which are different on each interface between cells, or equivalently on each edge.

4.1.1 Definition (Finite volume space-time mesh)**.** The finite volume space-time mesh is defined by the couple $(\mathcal{T}, \{t_i\}_{1\leq i\leq N})$,where the family $\{t_i\}_{1\leq i\leq N}$ is a subdivision of the interval $[0, T]$ such that

$$0 = t_0 < t_1 < t_2 < \cdots < t_N < t_{N+1} = T,$$

and we denote $t_{i+1} - t_i = \Delta t$, for all $i \in \{0, 1, 2, \cdots, N\}$ representing the time step following [22] for the purpose of stability.

In addition, the mesh $\mathcal{T}$ "Finite volume" is made of control or cell volume K which are polygons (in our context, we restrict ourselves to the case of triangles) forming a partition of the domain such that $\overline{\Omega} = \bigcup_{K\in\mathcal{T}} \overline{K}$ with $\mathring{K} \cap \mathring{L} = \emptyset$ with $K \neq L$ for all $K, L \in \mathcal{T}$.

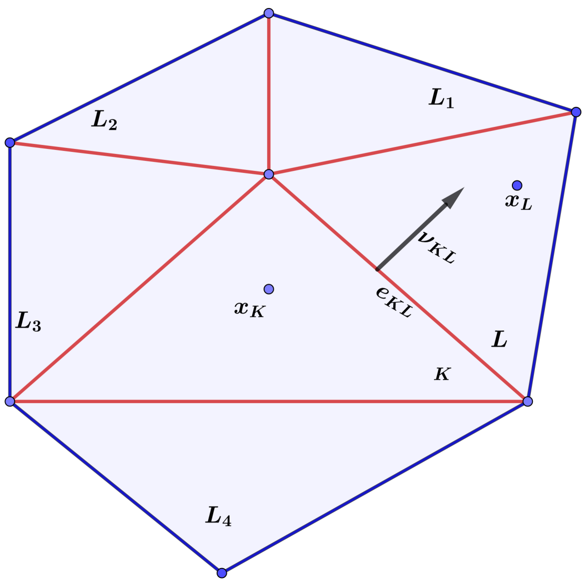

Figure 4.1: Triangular Mesh

Developing stable high-order methods in a time-dependent linear transport equation will be the topic of the remaining chapter. In doing so, the basic principles of the numerical methods will be shown for two dimensional spatial dimension. We follow the idea developed in [21, 22].

4.2 Numerical scheme of time-dependent linear transport equation

The purpose of this section is to explicitly define the two numerical schemes that will be applied throughout this thesis.

In order to obtain the numerical solution based on the finite volume approach, we integrate this (3.0.1) on the space-time mesh $K \times [t_n, t_{n+1}]$. We have

$$\int_{t_n}^{t_{n+1}} \int_K \partial_t u \,\mathrm{d}t\,\mathrm{d}s + \int_{t_n}^{t_{n+1}} \int_K \mathrm{div}[v(x, y, t)u(x, y, t)]\mathrm{d}t\,\mathrm{d}s = \int_{t_n}^{t_{n+1}} \int_K g(x, y, t)\,\mathrm{d}t\,\mathrm{d}s, \quad (4.2.1)$$

and using Green's theorem, (4.2.1) becomes

$$\int_K u(x,y,t_{n+1})\mathrm{d}s - \int_K u(x,y,t_n)\mathrm{d}s + \int_{t_n}^{t_{n+1}}\int_{\partial K} f.\nu \ \mathrm{d}S \ \mathrm{d}t = \int_{t_n}^{t_{n+1}}\int_K g(x,y,t)\mathrm{d}t \ \mathrm{d}s, \quad (4.2.2)$$

where $f = vu$ is the flux, $\partial K = \bigcup_{\sigma\in\varepsilon_K}\sigma$ denotes the boundary of K, ν its unit normal vector and ε_K the set of edges of K.

Thus, (4.2.2) becomes

$$\int_K u(x,y,t_{n+1})\mathrm{d}s - \int_K u(x,y,t_n)\mathrm{d}s + \int_{t_n}^{t_{n+1}}\sum_{\sigma\in\varepsilon_K}\int_\sigma f.\nu_\sigma \ \mathrm{d}S \ \mathrm{d}t = \int_{t_n}^{t_{n+1}}\int_K g(x,y,t) \ \mathrm{d}t \ \mathrm{d}s, \quad (4.2.3)$$

that means,

$$\int_K u(x,y,t_{n+1})\mathrm{d}s - \int_K u(x,y,t_n)\mathrm{d}s + \int_{t_n}^{t_{n+1}}\left(\sum_{L\in\mathcal{V}(K)}\int_{e_{KL}} f.\nu_{KL}\mathrm{d}S\right)\mathrm{d}t = \int_{t_n}^{t_{n+1}}\int_K g(x,y,t) \ \mathrm{d}t \ \mathrm{d}s, \quad (4.2.4)$$

where $\mathcal{V}(K)$ denotes the set of neighbouring cells of K: That means, L is in $\mathcal{V}(K)$ if $L\in\mathcal{T}$ and $K\cap L = e_{KL}$. The meaning of each variable is clarifies by the figure (4.1).

Afterwards, two numerical schemes are proposed: the Lax-Friedrich for the first order and the second order based on MUSCL scheme with limiter flux the one Van-Leer.

4.2.1 First Order Scheme(Lax-Friedrich Scheme). The First Order scheme can be formulated by considering the spatially-averaged value of the variable $u(x,y,t_n)$ at each cell K with $|K|=$ area of the cell K. That is

$$u_K^n = \frac{1}{|K|}\int_K u(x,y,t_n)\mathrm{d}s, \quad (4.2.5)$$

and the flux through an edge e_{KL}

$$\int_{e_{KL}} f.\nu_{KL}\mathrm{d}S = |e_{KL}|\phi(u_K,u_L,\nu_{KL}), \quad (4.2.6)$$

where $\phi(u_K,u_L,\nu_{KL})$ is the numerical flux through the edge e_{KL} associated to the cell K, and it is an approximation of $f.\nu_{KL}$ on the edge e_{KL}. By replacing in (4.2.4) u_K^n and e_{KL} by their approximate values given in (4.2.5) and (4.2.6), we have

$$|K|\left[u_K^{n+1} - u_K^n\right] + \int_{t_n}^{t_{n+1}}\sum_{L\in\mathcal{V}(K)}|e_{KL}|\phi(u_K,u_L,\nu_{KL}) = \int_{t_n}^{t_{n+1}}\int_K g(x,y,t) \ \mathrm{d}t \ \mathrm{d}s, \quad (4.2.7)$$

that means,

$$|K|\left[u_K^{n+1} - u_K^n\right] + \Delta t\sum_{L\in\mathcal{V}(K)}|e_{KL}|\phi(u_K^n,u_L^n,\nu_{KL}) = \Delta t|K|g_K^n, \quad (4.2.8)$$

where

$$g_K^n = \frac{1}{\Delta t|K|}\int_{t_n}^{t_{n+1}}\int_K g(x,y,t) \ \mathrm{d}t \ \mathrm{d}s.$$

Therefore, we have

$$u_K^{n+1} = u_K^n - \frac{\Delta t}{|K|}\sum_{L\in\mathcal{V}(K)}|e_{KL}|\phi(u_K^n,u_L^n,\nu_{KL}) + \Delta t g_K^n, \quad (4.2.9)$$

where $\phi(u_K^n, u_L^n, \nu_{KL})$ is the numerical flux whose expression is given according Lax-Friedrich [5] by

$$\phi(u_K^n, u_L^n, \nu_{KL}) = \frac{1}{2}\left[(v_K^n.\nu_{KL})\, u_K^n + (v_L^n.\nu_{KL})\, u_L^n\right] - \lambda(u_K^n - u_L^n), \tag{4.2.10}$$

with $v_K^n = v(x_k, t_n)$ and λ a positive constant to ensure the stability of the system.

4.2.2 Remark. From [5], we deduce that the first order schemes give a poor approximation and induce high viscosity effect and the second order scheme provides a better approximation and manages to reduce the viscous smoothing effect in the vicinity of the shocks.

4.2.3 Second Order Scheme(MUSCL Van-Leer). The second order scheme is based on the MUSCL approach [27]. According to [25] this approach is routinely used in practice today. Indeed, it allows the construction of very high order methods, fully discrete, semi-discrete and also implicit methods.

Starting from the Lax-Friedrich scheme, the MUSCL method consists to reconstruct the solution u_K^n at each cell K in the following way

$$\tilde{u}_K^n = u_K^n + \sigma_K^n x_K.\left(\frac{x_K + x_L}{2}\right). \tag{4.2.11}$$

In this work, the limiter proposed by Van Leer [24] is define by

$$\sigma_K^n = \begin{cases} 0, & \text{if } r \leq 0, \\ \frac{2r}{1+r}, & \text{if } r \geq 0, \end{cases} \tag{4.2.12}$$

where r represents the ratio of successive gradients on the solution mesh.

Therefore, to obtain a second order approach using the MUSCL method (Van Leer's), we start by substitute the numerical flux $\phi(u_K^n, u_L^n, \nu_{KL})$ by $\phi(\tilde{u}_K^n, \tilde{u}_L^n, \nu_{KL})$. Thus, (4.2.10) becomes

$$\begin{aligned}\phi(\tilde{u}_K^n, \tilde{u}_L^n, \nu_{KL}) = \frac{1}{2}\Bigg[(v_K^n.\nu_{KL})\left[u_K^n + \sigma_K^n x_K.\left(\frac{x_K + x_L}{2}\right)\right] + (v_L^n.\nu_{KL})\left[u_L^n + \sigma_L^n x_L.\left(\frac{x_K + x_L}{2}\right)\right]\Bigg] \\ + \lambda\left[(u_K^n - u_L^n) - \left(\frac{x_K + x_L}{2}\right)(u_K^n\sigma_K^n - u_L^n\sigma_L^n)\right].\end{aligned} \tag{4.2.13}$$

Then, our numerical scheme is given by

$$u_K^{n+1} = u_K^n - \frac{\Delta t}{|K|}\sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(\tilde{u}_K^n, \tilde{u}_L^n, \nu_{KL}) + \Delta t g_K^n, \tag{4.2.14}$$

with $u_K^0 = \frac{1}{|K|}\int_K u(x, t_0)\mathrm{d}x.$

4.3 Adjoint numerical scheme

The main objective of this Section is to apply the same numerical scheme techniques described in Section 4.2 for the flow equation. It is worth noticing that $\mathrm{div}(vp) = v\nabla p + p\nabla v$, and it follows that (3.3.2) can be expressed in a conservative divergence as

$$\begin{cases} \partial_t p + \mathrm{div}(vp) - p\nabla v = g & \text{in } \Omega \times [0, T], \\ p(x, T) = u(x, T) - u^*(x), & \text{on } \quad \Omega, \end{cases} \tag{4.3.1}$$

where we observe an extra of two terms related to the divergence of the velocity field appears. By integrating (4.3.1) on $K \times [t_n, t_{n+1}]$, we have

$$\int_{t_n}^{t_{n+1}} \int_K (\partial_t p + \mathrm{div}(vp))\,\mathrm{d}t\,\mathrm{d}s - \int_{t_n}^{t_{n+1}} \int_K p\,\nabla v\,\mathrm{d}s\,\mathrm{d}t = \int_K \int_{t_n}^{t_{n+1}} g(x,y,t)\mathrm{d}s\,\mathrm{d}t. \tag{4.3.2}$$

Assuming backward resolution of this adjoint equation, we consider the following time linearization

$$\int_{t_n}^{t_{n+1}} \int_K p\,\nabla v\,\mathrm{d}s\,\mathrm{d}t \simeq \Delta t \int_K (p.\nabla v)^{n+1}\mathrm{d}s. \tag{4.3.3}$$

This assumption allows us to formulate the numerical scheme for the adjoint equation in a similar way to that proposed for the flow equation. Thus, applying the Lax-Friedrich scheme on (4.3.3), the adjoint equation is given by

$$|K|\left[p_K^{n+1} - p_K^n\right] + \Delta t \sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(p_K^n, p_L^n, \nu_{KL}) - \Delta t\, p_K^{n+1} \sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(v_K^n, v_L^n, \nu_{KL}) = \Delta t|K|\left[g_K^n\right],$$

that means,

$$p_K^{n+1}\left[1 - \underbrace{\frac{\Delta t}{|K|}\sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(v_K^n, v_L^n, \nu_{KL})}_{DV}\right] = p_K^n - \frac{\Delta t}{|K|}\sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(p_K^n, p_L^n, \nu_{KL}) + \Delta t\, g_K^n. \tag{4.3.4}$$

Applying the MUSCL (Van-Leer) scheme for the flow equation given in (4.3.4), we obtain

$$p_K^{n+1}\left[1 - \underbrace{\frac{\Delta t}{|K|}\sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(\tilde{v}_K^n, \tilde{v}_L^n, \nu_{KL})}_{DV}\right] = -\frac{\Delta t}{|K|}\sum_{L\in\mathcal{V}(K)} |e_{KL}|\phi(\tilde{p}_K^n, \tilde{p}_L^n, \nu_{KL}) + \Delta t\, g_K^n, \tag{4.3.5}$$

where $\phi(\tilde{p}_K^n, \tilde{p}_L^n, \nu_{KL})$ is defined as in (4.2.13). The underlined term named DV are related to the divergence of the velocity field and we will take this null term in the simulations as in [22].

5. Simulations and Interpretation

In this chapter, we will done some numerical simulation on the Matlab software. Moreover, We will start doing some easy example especially in the case of the Doswell frontogenesis test which was first introduced (in a direct sense) in Doswell [11, 22].

For the numerical experiments and most clarity, we have consider the domain $\Omega = [-5, 5]^2 \subseteq \mathbb{R}^2$ for the space that we discretized into 200 uniform triangles (following the Delaunay uniform mesh in [23]) which can be seen in the Figure 5.1 (for 32 triangles by example) and $[0, 4]$ for the time. .

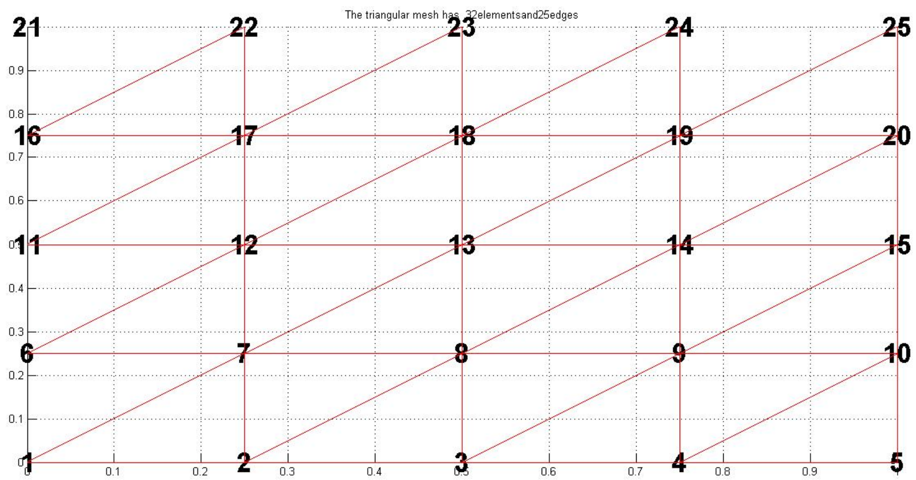

Figure 5.1: Triangular mesh with 32 triangles and 25 edges

Afterwards, we will need to know an exact solution of the problem

$$\begin{cases} \partial_t u + \operatorname{div}\big(v(x, y, t)u(x, y, t)\big) = g(x, y, t) \quad \text{in} \quad \Omega \times [0, 4], \\ u(x, y, 0) = u_0(x, y) \quad \text{on} \quad \Omega. \end{cases} \tag{5.0.1}$$

For simplicity, we are interested in the case where v depends on space. Through the initial condition given in [22] by

$$u(x, y, 0) = \tanh(y); \tag{5.0.2}$$

which is advected under the velocity field

$$v(x, y, t) = (-yf(r), xf(r)) \quad f(r) = \frac{1}{r} v_0 \left(\frac{1}{\cosh}\right)^2 (r) \tanh(r) \; ; v_0 = 2.59807, \tag{5.0.3}$$

where $r = \sqrt{x^2 + y^2}$.

An exact solution of (5.0.1) can be given by

$$u(x, y, t) = \tanh\left(y \cos(f(r)t) - x \sin(f(r)t)\right) + \sin(f(r)t), \tag{5.0.4}$$

with the source term

$$g(x, y, t) = f(r) \cos(f(r)t) + \operatorname{div}\left(v \sin(f(r)t)\right). \tag{5.0.5}$$

and

$$u(x, y, t) = \tanh\left(y \cos(f(r)t) - x \sin(f(r)t)\right), \tag{5.0.6}$$

without the source term.

This allow us to formulate the inverse design problem. Given the exact value of the solution at time $t = 4$, that means, given (5.0.4) or (5.0.6) as the target function at $t = T = 4$, we seek to recover by a computer version of the gradient-adjoint methodology described above, an accurate and efficient approximation of the initial data (5.0.2).

The exact initial and target conditions are shown in Figure 5.2 and Figure 5.3 in the case of the presence of a source term or not (respectively)for the value of $T = 4\ s$

Figure 5.2: Doswell frontogenesis with source term: initial condition u_0 (left) and target function u_T (right),

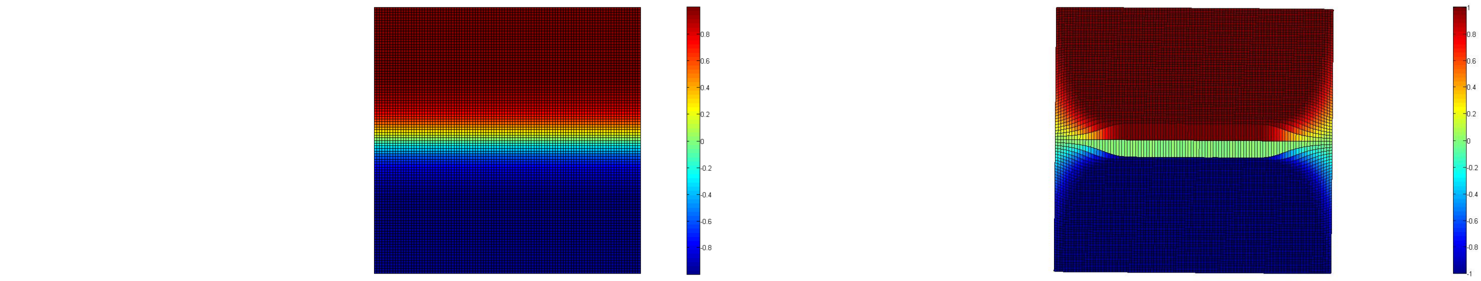

Figure 5.3: Doswell frontogenesis without source term: initial condition u_0 (left) and target function u_T (right).

We can see in both cases that the target solution has a vortex-like profile as in [22].

6. Conclusions and Perspectives

In this thesis, we studied the inverse design 2D of linear transport equation with unbounded coefficient on unstructured grids and we developed some numerical experiment by comparing two Finite volume method numerical schemes (Lax-Friedrich and MUSCL Van-Leer).

For the theoretical study, before to establish the inverse design of transport equation, we showed the existence and uniqueness of the problem in the general case (with unbounded coefficient). For establish that, we used the regularisation technique knowing that the case where we have bounded coefficient is easy to prove thank, to the characteristic method; once this has been done, we have defined the adjoint problem which also has a unique solution. The second part of this thesis was related with the numerical treatment of the inverse problem of the linear transport equation . First, we discretized the direct problem and adjoint problem by using two numerical scheme, Lax-Friedrich for the first order and MUSCL Van-Leer for the second order on a space time mesh finite volume where the polygons are uniform triangles follows Delaunay mesh, secondly used the numerical scheme defined above on the gradient descent method for obtain the wished numerical results for the initial condition, target solution of direct problem. With this thesis , we opened two ways for the future work, the simulation by taking into account that the coefficient is bounded on uniform and non-uniform delaunay mesh.

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