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Nonlinear Modeling in Mathematical Physics: Complex Systems and Boundary Value Problems

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Introduction

A surge of advances in both experimental and theoretical techniques, has allowed in recent years to develop useful mathematical tools for the modeling of interesting systems in applied sciences.
The validation of models is generally based on their ability to predict realistic phenomena at a qualitative level. An appropriate quantitative analysis is of course required as well, through a comparison with reliable empirical data, whenever such data are available. To this end the equations describing the system have to be inclusive of suitable parameters whose values have to be fixed according to the experimental evidence.
The models discussed in this thesis are related to two important aspects of life-and-material science which require different mathematical techniques. Namely, in the following we discuss some mathematical models related to biological and medical applications.
A common aspect in the description of real-life phenomena is the emergence of an intrinsic nonlinearity which from a technical point of view cannot be studied through perturbation expansions about small amplitude linear approximation to the true solutions. Indeed, since the mid-1970s it has become increasingly evident that the assumption of quasi-linearity leads the theorist to miss qualitatively significant aspects.
The present thesis is divided in two parts. We first consider the description of complex living systems. Such description relays on a kinetic theory formalism, called kinetic theory of active particle (KTAP theory) which, as we explain later was developed to describe systems characterized by a large number of interacting "individuals" whose state is described not only by mathematical variables, but also by a new scalar variable called "activity". This new variable indicates the ability of each individual (active particle) to express a specific strategy. The macroscopic behavior of the whole system is a non-deterministic result of the nonlinear interactions among the active particles.
In the second chapter of the thesis the KTAP theory is described and two applications of the theory to "population dynamics" problems are presented. Namely, after general considerations related to the fundamental aspects of the mathemati-

cal framework, we discuss the case of a discrete vehicular traffic model and of an epidemics-spread model. The results presented are original contributions obtained in [20, 21, 32].
The third chapter of the thesis is instead devoted to the application of boundary value problems techniques to the modeling of a nonlinear diffusion phenomenon in medicine. More precisely, we first introduce a well known nonlinear diffusion-convection equation (Rosen - Fokas - Yorstos model) of great applicative relevance, and discuss the construction of the Dirichlet-to-Neumann map obtained in [17]. Next, we present recent results obtained in [19] where the phenomenon of drug diffusion in arterial tissues, after the drug is released by an arterial stent, is modeled through a moving boundary problem on a finite domain.
Finally, in Appendix A and Appendix B, we show some technical details of rigorous proofs related to theorems reported in the thesis.

Chapter 2

Complex systems

Complex living systems are systems constituted by a large number of individual components characterized at microscopic level by nonlinear interactions. The outcome of such interactions is described by stochastic games. The behavior of the system can thus be seen as the collective action of a large number of components that through their interactions give rise to a global outcome for the complex system. All of this happens without a central control or a leader. Moreover, all the components change their behavior through evolutionary processes in order to improve their chances of success or survival. Thus, the modeling of complex living systems requires to take into account all the interactions among the elements that compose the system under study, in order to determine the macroscopic evolution. This is achieved by the use of various models that adopt different methods corresponding to different scales. These models can be classified into:

Microscopic models: used to study, through ordinary differential equations, the dynamics of each individual particle.

Macroscopic models: used to study, through partial differential equations, the averages of the state of a large number of elements, to develop some locally averaged quantities suitable to describe the system.

Kinetic models: used to study, through integral differential equations, the behavior of groups of interacting particles through suitable probability distributions over the microscopic state. Macroscopic quantities in such models can be obtained by computing averages over the microscopic state space.

In this work we concentrate our attention on a mathematical framework adapt to describe kinetic models.

2.1 Kinetic theory

The statistical mechanics framework was first introduced by Ludwig Boltzmann in order to overcome the continuum approach in the study of fluid-dynamics.

2.1.1 The Boltzmann equation

Following the idea of Boltzmann we introduce the one-particle distribution function:

$$f = f(t, \mathbf{x}, \mathbf{v}) \;:\; \mathbb{R}_+ \times \Omega \times \mathbb{R}^3 \;\rightarrow\; \mathbb{R}_+$$

under the hypothesis that f is locally integrable. $\Omega \subset \mathbb{R}^3$ is the domain where the particles are free to move in all directions. Then, the number of particles in the volume $[\mathbf{x}, \mathbf{x} + d\mathbf{x}] \times [\mathbf{v}, \mathbf{v} + d\mathbf{v}]$ at the time t is defined with $f(t, \mathbf{x}, \mathbf{v})\, dvdx$. Moreover, for a system of only one kind of particle, integrating over the velocity, we define the number density:

$$n(t, \mathbf{x}) = \int_{\mathbb{R}^3} f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v};$$

on the other hand, integrating over the space and over the velocity, we obtain the total number of the particles:

$$N = \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, \mathbf{x}, \mathbf{v})\, d\mathbf{x}\; d\mathbf{v}.$$

Under the additional hypothesis that vf and $v^2 f$ are integrable we can define:

the mass density

$$\rho(t, \mathbf{x}) = mn(t, \mathbf{x})$$

where m is the mass of the particle, and

the mass velocity

$$\mathbf{U}(t, \mathbf{x}) = \frac{1}{n(t, \mathbf{x})} \int_{\mathbb{R}^3} vf(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v}.$$

In order to derive the evolution equation for the distribution function in the case of Boltzmann equation, we assume to be significant only the interactions between pairs of particles. This collisions are elastic and preserve mass, momentum and energy. Then the evolution equation is obtained trough the mass conservation equation. Along this way the **Boltzmann equation** in the case of absence of an external force is:

$$\frac{df}{dt}(t, \mathbf{x}, \mathbf{v}) = \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}}\right) f = J[f, f] = G[f, f] - L[f, f],$$

where $G[f,f]$ and $L[f,f]$ are respectively the gain and loss term that emerge due to the collision between a couple of particles:

$$G[f,f](t,\mathbf{x},\mathbf{v}) = \int_{\mathbb{R}^3\times\mathbb{S}^2_+} B(\mathbf{n},\mathbf{q})\, f(t,\mathbf{x},\mathbf{v}')\, f(t,\mathbf{x},\mathbf{w}')\, d\mathbf{n}\; d\mathbf{w}$$

and

$$L[f,f](t,\mathbf{x},\mathbf{v}) = f(t,\mathbf{x},\mathbf{v}) \int_{\mathbb{R}^3\times\mathbb{S}^2_+} B(\mathbf{n},\mathbf{q})\, f(t,\mathbf{x},\mathbf{w})\, d\mathbf{n}\; d\mathbf{w}.$$

In these equations:

$\mathbf{v},\mathbf{w}$ are the pre-collision velocities of the two interacting particles with $\mathbf{q} = \mathbf{w} - \mathbf{v}$,

$\mathbf{v}',\mathbf{w}'$ are the post-collision velocities of the two interacting particles with $\mathbf{q}' = \mathbf{w}' - \mathbf{v}'$, $\mathbf{v}' = \mathbf{v} + \mathbf{n}(\mathbf{n}\cdot\mathbf{q})$ and $\mathbf{w}' = \mathbf{w} - \mathbf{n}(\mathbf{n}\cdot\mathbf{q})$.

$\mathbf{n}$ is the versor along the bisector of the angle between q and q',

$\mathbb{S}^{\mathbf{2}}_+ = \{\mathbf{n} \in \mathbb{R}^3 : |\mathbf{n}| = 1,\ \mathbf{n}\cdot\mathbf{q} \le 0\}$,

$\mathbf{B}(\mathbf{n},\mathbf{q})$ is the collision kernel, see [25].

In this Subsection we have described a system of particles that interact in absence of external force fields. Boltzmann equation, indeed, is able to characterize also the case where external actions occur. Moreover, the mathematical framework provided takes into account only short range interactions. On the other hand, various physical systems involve long range interactions. In this case the appropriate model is given by **Vlasov equation** [70].

2.1.2 Kinetic theory of active particle

In the kinetic theory the particles taken into account are indistinguishable from each other. To overcome this problem, in recent years a mathematical approach has been developed to describe complex systems belonging to the domain of life sciences. A description of such systems requires the use of appropriate techniques and mathematical methods that differ substantially from those used for the description of the inert matter. The mathematical formalism is called Kinetic Theory of Active Particles (KTAP Theory); indeed in such formalism the complex system is characterized by a large number of interacting entities named "active particles". This means that the physical state of the particles belonging to the complex system is characterized not only by geometric and mechanics variables but also by a new variable named "activity". This variable characterizes the type of strategy

and the type of interactions that the particles of the complex system are able to develop. Indeed the "activity" has the role to differentiate the behavior of each particle; it takes a different meaning depending on the model.
The KTAP theory, reviewed in [10, 28], allows the derivation of evolution equations suitable to describe the time and space dynamics of appropriate probability distributions over the micro-scale state of a large system of interacting entities. The derivation of the said equations is based on suitable developments of the methods of the mathematical kinetic theory, while interactions are modeled by theoretical tools of the evolutionary game theory [62, 63]. The KTAP theory allowed the derivation of various models of practical interest in life science such as the description of crowds [69], the formulation of models of social and immune competition [12, 14, 39], the modeling of vehicular traffic flow [13] and of the spread of epidemics contrasted by immune defense [31].
Following [10] we now derive the mathematical framework for this theory.

Mathematical frameworks for continuous systems

Let us consider a system constituted by n subsystems labeled with the index $i = 1, \dots, n$ where the activity variable describe, for each subsystem, the main properties of its respective particles. Then the one-particle distribution function of the i-th subsystem is defined by

$$f_i = f_i\,(t, \mathbf{x}, \mathbf{v}, \mathbf{u}), \qquad i = 1, \dots, n,$$

where $\mathbf{x}$, $\mathbf{v}$ and $\mathbf{u}$ indicate respectively the position, the velocity and the activity of the particle and $f_i\,(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{x} d\mathbf{v} d\mathbf{u}$ denotes the number of active particles belonging to the i-th subsystem that at time t are in the elementary volume $[\mathbf{x}, \mathbf{x} + d\mathbf{x}] \times [\mathbf{v}, \mathbf{v} + d\mathbf{v}] \times [\mathbf{u}, \mathbf{u} + d\mathbf{u}] = D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_{\mathbf{u}}$. We point out that the distribution function for all subsystems is denoted by $\mathbf{f} = \{f_1, \dots, f_n\}$.
In this way, under suitable integrability hypothesis we can define some important quantities like:

the local size of the i-th subsystem

$$n_i\,[f_i]\,(t, \mathbf{x}) = \int_{D_{\mathbf{x}} \times D_{\mathbf{v}}} f_i\,(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{v}\; d\mathbf{u}, \tag{2.1}$$

the total density

$$n\,[\mathbf{f}]\,(t, \mathbf{x}) = \sum_{i=1}^{n} n_i\,[f_i]\,(t, \mathbf{x}), \tag{2.2}$$

the total size of the subsystem at $t = 0$

$$n_0 \left[\mathbf{f_0}\right](\mathbf{x}) = \sum_{i=1}^{n} n_{i0}(\mathbf{x}), \tag{2.3}$$

where n_{i0} is the local initial size of the i-th subsystem and $\mathbf{f_0} = \mathbf{f}(t=0)$,

the total size of the i-th subsystem

$$N_i(t) = \int_{D_{\mathbf{x}}} n_i(t, \mathbf{x})\, d\mathbf{x} \tag{2.4}$$

and

the total size of all subsystems

$$N(t) = \sum_{i=1}^{n} N_i(t). \tag{2.5}$$

Moreover, under suitable integrability properties, we can also calculate some macroscopic quantities like:

marginal densities of the distribution over the mechanical state

$$f_i^m(t, \mathbf{x}, \mathbf{v}) = \int_{D_{\mathbf{u}}} f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{u},$$

marginal densities of the distribution over the activity

$$f_i^a(t, \mathbf{u}) = \int_{D_{\mathbf{x}} \times D_{\mathbf{v}}} f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{x}\ d\mathbf{v},$$

mass velocity of particles

$$\mathbf{U}\left[f_i\right](t, \mathbf{x}) = \frac{1}{n_i\left[f_i\right](t, \mathbf{x})} \int_{D_{\mathbf{v}} \times D_{\mathbf{u}}} \mathbf{v} f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{v}\ d\mathbf{u}, \tag{2.6}$$

local activation

$$a_{ij} = a_j\left[f_i\right](t, \mathbf{x}) = \int_{D_{\mathbf{v}} \times D_{\mathbf{u}}} u_j f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{v}\ d\mathbf{u}, \tag{2.7}$$

local activation density

$$a_{ij}^d = \frac{a_j\left[f_i\right](t, \mathbf{x})}{n_i\left[f_i\right](t, \mathbf{x})} = \frac{1}{n_i\left[f_i\right](t, \mathbf{x})} \int_{D_{\mathbf{v}} \times D_{\mathbf{u}}} u_j f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u})\, d\mathbf{v}\ d\mathbf{u}, \tag{2.8}$$

global activation

$$\mathbf{A}_{ij} = \mathbf{A}_{ij} [f_i] (t) = \int_{D_\mathbf{x}} a_{ij} (t, \mathbf{x}) \, d\mathbf{x} \tag{2.9}$$

and

global activation density

$$\mathbf{A}^d_{ij} = \mathbf{A}^d_{ij} [f_i] (t) = \int_{D_\mathbf{x}} a^d_{ij} (t, \mathbf{x}) \, d\mathbf{x}. \tag{2.10}$$

Now we are ready to characterize the microscopic interactions between the particles. In this treatment we describe only the case of **conservative interactions**, namely interactions that don't modify the size of the subsystem but only the state of the particles. Moreover, we take into account only the case of **short range binary interactions**. In the interest of providing fuller information we should remark that this theory can be extended also to the case of **proliferative** or **destructive interactions** which generate the birth or the death of active particles. Furthermore, like in the continuous case, a mathematical framework appropriate to describe **long range mean field interactions** exists in the literature (see [10]).

In order to provide the dynamics of the interactions we consider the **microscopic state** of active particles $\mathbf{w} = \{\mathbf{x}, \mathbf{v}, \mathbf{u}\} \in D_\mathbf{w} = D_\mathbf{x} \times D_\mathbf{v} \times D_\mathbf{u}$ and we define three kind of particles: the **candidate** active particle with state $\mathbf{w}_*$, the **test** active particle with state $\mathbf{w}$ and the **field** active particle with state $\mathbf{w}^*$.
Moreover we consider the **encounter rate** between a particle belonging to the i-th subsystem with state $\mathbf{w}_*$ and a particle belonging to the j-th subsystem with state $\mathbf{w}^*$

$$\eta_{ij} = c_{ij} \delta (\mathbf{x}_* - \mathbf{x}^*) \, |\mathbf{v}_* - \mathbf{v}^*|$$

where c_{ij} is a constant and δ is the Dirac's function.
Finally we define the **transition probability density**

$$\varphi_{ij} (\mathbf{w}_*, \mathbf{w}^*; \mathbf{w}) : D_\mathbf{w} \times D_\mathbf{w} \times D_\mathbf{w} \;\to\; \mathbb{R}_+,$$

namely the probability that a candidate active particle belonging to the i-th subsystem with state $\mathbf{w}_*$, interacting with the field particle belonging to the j-th subsystem with state $\mathbf{w}^*$ falls into the state $\mathbf{w}$ of the test particle (remaining in the same subsystem). The latter definition requires an additional hypothesis:

$$\int_{D_\mathbf{w}} \varphi_{ij} (\mathbf{w}_*, \mathbf{w}^*; \mathbf{w}) \, d\mathbf{w} = 1, \quad \forall \mathbf{w}_*, \mathbf{w}^*, \quad \forall i, j. \tag{2.11}$$

The evolution equations of the system are the following:

$$\frac{df_i}{dt} = \frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = G_i\left[\mathbf{f}\right] - L_i\left[\mathbf{f}\right]$$

where

$$G_i\left[\mathbf{f}\right](t, \mathbf{x}, \mathbf{v}, \mathbf{u}) = \sum_{j=1}^{n} \int_{(D_{\mathbf{v}} \times D_{\mathbf{u}})^2} c_{ij} \left|\mathbf{v}_* - \mathbf{v}^*\right| \varphi_{ij}\left(\mathbf{w}_*, \mathbf{w}^*; \mathbf{w}\right)$$
$$\times f_i\left(t, \mathbf{x}, \mathbf{v}_*, \mathbf{u}_*\right) f_j\left(t, \mathbf{x}, \mathbf{v}^*, \mathbf{u}^*\right) d\mathbf{v}_*\, d\mathbf{v}^*\, d\mathbf{u}_*\, d\mathbf{u}^*$$

and

$$L_i\left[\mathbf{f}\right](t, \mathbf{x}, \mathbf{v}, \mathbf{u}) = f_i\left(t, \mathbf{x}, \mathbf{v}, \mathbf{u}\right) \sum_{j=1}^{n} \int_{D_{\mathbf{v}} \times D_{\mathbf{u}}} c_{ij} \left|\mathbf{v} - \mathbf{v}^*\right|$$
$$\times f_j\left(t, \mathbf{x}, \mathbf{v}^*, \mathbf{u}^*\right) d\mathbf{v}^*\, d\mathbf{u}^*$$

are the **gain** and the **loss** terms respectively.

Remark 2.1.1. *There is a particular case when the candidate particle belonging to the h-th subsystem with state $\mathbf{u}_*$ interacting with a particle belonging to the k-th subsystem with state $\mathbf{u}^*$ falls in i-th subsystem with state $\mathbf{u}$. In this case the* ***encounter rate*** *is defined by:*

$$\eta_{ij}^0 = \int_{D_{\mathbf{v}} \times D_{\mathbf{v}}} c_{ij} \left|\mathbf{v} - \mathbf{v}^*\right| P_j\left(\mathbf{v}^*\right) P_i\left(\mathbf{v}\right) d\mathbf{v}^* d\mathbf{v}$$

where $P(\mathbf{v})$ is the distribution function over the velocity variable, satisfying the normalization condition

$$\int_{D_{\mathbf{v}}} P_i\left(\mathbf{v}\right) d\mathbf{v} = 1.$$

Moreover we indicate by $\mathscr{B}_{hk}^i\left(\mathbf{u}_*, \mathbf{u}^*; \mathbf{u}\right)$ the ***transition probability density*** *and the additional hypothesis (2.11) becomes:*

$$\sum_{i=1}^{n} \int_{D_{\mathbf{u}}} \mathscr{B}_{hk}^i\left(\mathbf{u}_*, \mathbf{u}^*; \mathbf{u}\right) d\mathbf{u} = 1, \quad \forall \mathbf{u}_*, \mathbf{u}^*, \quad \forall h, k.$$

Assuming that:

$$f_i\left(t, \mathbf{v}, \mathbf{u}\right) = f_i^a\left(t, \mathbf{u}\right) P_i\left(\mathbf{v}\right),$$

the ***gain*** *term takes the form:*

$$G_i\left[\mathbf{f}\right](t, \mathbf{x}, \mathbf{v}, \mathbf{u}) = \sum_{h=1}^{n} \sum_{k=1}^{n} \eta_{hk}^0 \int_{D_{\mathbf{u}} \times D_{\mathbf{u}}} \mathscr{B}_{hk}^i\left(\mathbf{u}_*, \mathbf{u}^*; \mathbf{u}\right)$$
$$\times f_h^a\left(t, \mathbf{u}_*\right) f_k^a\left(t, \mathbf{u}^*\right) d\mathbf{u}_*\, d\mathbf{u}^*$$

*and the **loss** term takes the form:*

$$L_i\,[\mathbf{f}]\,(t,\mathbf{x},\mathbf{v},\mathbf{u}) = f_i^a\,(t,\mathbf{u}) \sum_{k=1}^{n} \eta_{ik}^0 \int_{D_\mathbf{u}} f_k^a\,(t,\mathbf{u}^*)\,d\mathbf{u}^*.$$

Mathematical frameworks for discrete systems

Let us now consider the mathematical framework for discrete systems suitable to describe some particular models that require a specific discretization of the variables.
We take into account a system constituted by n subsystems labeled with the index $i = 1, \ldots, n$ where the activity variable describes, for each subsystem, the main properties of its respective particles. In this case, the activity of the particles is expressed by a discrete grid:

$$I_\mathbf{u} = \{u_1, \ldots, u_r, \ldots, u_R\}.$$

Then the distribution function of the particles belonging to the i-th subsystem with state u_r is defined by

$$f_{ir} = f_{ir}\,(t,\mathbf{x},\mathbf{v}) = f_i\,(t,\mathbf{x},\mathbf{v};u_r) : [0,T] \times D_\mathbf{x} \times D_\mathbf{v} \;\rightarrow\; \mathbb{R}_+, \qquad i = 1, \ldots, n,$$

In this way we can obtain a mathematical framework for a discrete activity system and in (2.1)-(2.5), by replacing integrals with sums, we recover the quantities previously defined:

the local size of the i-th subsystem

$$n_i\,[f_i]\,(t,\mathbf{x}) = \sum_{r=1}^{R} \int_{D_\mathbf{v}} f_{ir}\,(t,\mathbf{x},\mathbf{v})\,d\mathbf{v},$$

the total density

$$n\,[\mathbf{f}]\,(t,\mathbf{x}) = \sum_{i=1}^{n} n_i\,[f_i]\,(t,\mathbf{x}),$$

the total size of the subsystem at $t = 0$

$$n_0\,(\mathbf{x}) = n\,(t = 0,\mathbf{x}),$$

where $n_{i0}\,(\mathbf{x}) = n_i\,(t = 0,\mathbf{x})$,

the total size of the i-th subsystem

$$N_i(t) = \int_{D_{\mathbf{x}}} n_i(t, \mathbf{x})\, d\mathbf{x}$$

and

the total size of all subsystems

$$N(t) = \sum_{i=1}^{n} N_i(t).$$

Moreover, along the same lines, from (2.6)-(2.10) we can calculate also some macroscopic quantities:

mass velocity of particles

$$\mathbf{U}[f_i](t, \mathbf{x}) = \frac{1}{n_i(t, \mathbf{x})} \sum_{r=1}^{R} \int_{D_{\mathbf{v}}} \mathbf{v} f_i^r(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v},$$

activation at time t in position x

$$a_{ir} = a_{ir}[f_{ir}](t, \mathbf{x}) = u_r \int_{D_{\mathbf{v}}} f_{ir}(t, \mathbf{x}, \mathbf{v})\, d\mathbf{v},$$

activation density

$$d_{ir} = d_{ir}[f_i](t, \mathbf{x}) = \frac{a_{ir}[f_{ir}](t, \mathbf{x})}{n_i[f_i](t, \mathbf{x})},$$

global activation

$$\mathbf{A}_{ir} = \mathbf{A}_{ir}[f_{ir}](t) = \int_{D_{\mathbf{x}}} a_{ir}(t, \mathbf{x})\, d\mathbf{x}$$

and

global activation density

$$\mathbf{D}_{ir} = \mathbf{D}_{ir}[f_i](t) = \int_{D_{\mathbf{x}}} d_{ir}(t, \mathbf{x})\, d\mathbf{x}.$$

If motivated by a specific application, we can discretize also the velocity variable:

$$I_{\mathbf{v}} = \{v_1, \ldots, v_s, \ldots, v_S\}$$

or the space variable:

$$I_{\mathbf{x}} = \{x_1, \ldots, x_l, \ldots, x_L\}.$$

The respectively distribution functions are:

$$f_{ikr}(t, \mathbf{x}) = f_i(t, \mathbf{x}, v_k, u_r)$$

and

$$f_{ilkr}(t) = f_i(t, x_l, v_k, u_r).$$

Like in the case of a discrete activity system, if we replace integrals with the sums in (2.1)-(2.5) and (2.6)-(2.10) we recover the quantities previously defined.
Now we are ready to characterize the microscopic interactions between the particles. Also in this treatment we describe only the case of conservative interactions. In particular, we take into account a mathematical framework for models where the microscopic state is identified by activity only. However, we underline that the other frameworks can be obtained following the same lines.

In order to provide the dynamics of the interactions we define three kind of particles: the **candidate** active particle with state u_p the **test** active particle with state u_r and the **field** active particle with state u_q.
Moreover, we consider the **encounter rate** η_{ij}^{pq} between a particle belonging to the i-th subsystem with state u_p and a particle belonging to the j-th subsystem with state u_q:

$$\eta_{ij}^{pq} = \eta_{ij}[\mathbf{f}](u_p, u_q)$$

We then define the **transition probability density**:

$$\mathscr{B}_{ij}^{pq}(r) = \mathscr{B}_{ij}(u_p, u_q; u_r)$$

namely the probability that a candidate active particle belonging to the i-th subsystem with state u_p, interacting with the field particle belonging to the j-th subsystem with state u_q falls into the state u_r of the test particle (remaining in the same subsystem). The latter definition requires an additional hypothesis:

$$\sum_{r=1}^{R} \mathscr{B}_{ij}^{pq}(r) = 1, \quad \forall i, j, \quad \forall p, q.$$

The evolution equations of the system have the form:

$$\frac{df_i^h}{dt} = G_{ih} - L_{ih}.$$

where

$$G_{ih} = \sum_{j=1}^{n} \sum_{p,q=1}^{R} \eta_{ij}^{pq} \mathscr{B}_{ij}^{pq}(r) f_{ip} f_{jq}$$

and

$$L_{ih} = f_{ih} \sum_{j=1}^{n} \sum_{q=1}^{R} \eta_{ij}^{hq} f_{jq}$$

are the **gain** and the **loss** terms respectively.

Remark 2.1.2. *Like in the continuous systems there is a particular case where the candidate particle belonging to the h-th subsystem with state u_p interacting with a particle belonging to the k-th subsystem with state u_q, falls in the i-th subsystem with state u_r. In this case we indicate by $\mathscr{B}_{hk}^{pq}(r,i)$ the* ***transition probability density*** *under the hypothesis*

$$\sum_{r=1}^{R} \sum_{i=1}^{n} \mathscr{B}_{hk}^{pq}(r,i) = 1, \quad \forall h,k, \quad \forall p,q.$$

The ***gain*** *term takes the form:*

$$G_{ir} = \sum_{h,k=1}^{n} \sum_{p,q=1}^{R} \eta_{hk}^{pq} \mathscr{B}_{hk}^{pq}(r,i) f_{hp} f_{kq}$$

and the ***loss*** *term takes the form:*

$$L_{ir} = f_{ir} \sum_{k=1}^{n} \sum_{q=1}^{R} \eta_{ik}^{rq} f_{kq}.$$

In the next two Sections we present two models described through the KTAP theory approach. More precisely in Section 2.2 an epidemic model adapt to study the spread of epidemics under the influence of risk perception obtained by De Lillo, Prioriello and myself is presented [32]. Section 2.3 is instead dedicated to a discrete vehicular traffic model influenced by the ability of the drivers, obtained by Burini, De Lillo and myself [20, 21].

2.2 Modeling of epidemics under the influence of risk perception

Modeling the epidemics of infectious diseases, motivated in the past a very extended literature, starting from the early studies of Kermack and McKendrick [53]. In [58] the authors present an interesting survey of mathematical models and analytical results, to be compared with laboratory data in order to understand epidemiological trends and to control the spread of infection and disease within human communities. On the other hand, in [24] the author analyzes and classifies epidemic models according to their mathematical structure. Two main classes are identified: one of them related to order preserving dynamical systems, the other one related to Lyapunov methods. The mathematical models discussed in [24, 58] are deterministic; however as pointed out also in [24], spontaneous stochastic fluctuations have to be taken into account in order to get a more realistic model, able to fit experimental data. Indeed, more recently several studies were devoted to the development of stochastic epidemic models, mainly in the framework of random networks [4, 7, 8, 16, 40, 48, 57, 71]. The present model proposes some new ideas developed in the context of the model discussed in [31]. In particular we focalize our attention on two fundamental issues:

- **Nonlinear interactions:** recent studies [28, 33] have introduced new concepts concerning nonlinear additivity of interactions. In our model the evolution of the system is ruled by nonlinear interactions between the active particles. The outcome of such interactions is described by stochastic games.

- **Risk perception:** it is assumed in this model that susceptible individuals may be aware of the risk to contract the infection [6]. According to the level of awareness they can take the necessary precautions.

In Subsection 2.2.1 is presented the mathematical structure able to describe the spread of epidemics. Subsection 2.2.2 describes the transitions probability densities with particular attention to the role of the risk perception awareness among healthy individuals. Subsection 2.2.3 is dedicated to the qualitative analysis of the model. Finally, Subsection 2.2.4 develops some simulations in order to show the evolution of the epidemics, starting from an initial situation.

2.2.1 Mathematical structure

Let us consider a large system of many interacting entities, called *active particles*, grouped into several different *functional subsystems*. Within the same subsystem,

each individual is characterized by a microscopic state called *activity*, with a different meaning in each functional subsystem.
The number of particles in the whole system is assumed to be constant.
The evolution of the system is determined by interactions between pairs belonging to the same subsystem or to different ones.
The system consists of four subsystems, also called populations, labelled by the index $i \in \{1, \ldots, 4\}$:

- i=1: doctors;
- i=2: susceptible individuals;
- i=3: individuals affected by the disease;
- i=4: healed individuals (these individuals cannot be infected again).

The activity is a discrete scalar variable $u \in [0, 1]$ describing, for each i-th population, the main properties of its respective individuals. In particular, it represents in the four distinct subsystems:

- i=1: the ability and the experience of doctors to treat the disease;
- i=2: the susceptibility (to contract the infection);
- i=3: the progression of the pathological state;
- i=4: getting back in shape.

Remark 2.2.1. *We assume that in the disease under consideration the severity of the pathological state is highest in the first stage of the disease. Specifically, for the third subsystem $u = 0$ and $u = 1$ correspond, respectively, to the highest and to the lowest levels of severity of the pathological state.*
We assume that the infectivity is constant, i.e. it is the same for all individuals of the third population.

In the following we assume that the activity of individuals is heterogeneously distributed in each functional subsystem and we introduce the set:

$$I_{\mathbf{u}} = \{u_1 = 0, ..., u_r, ..., u_m = 1\} .$$

The overall state is described by the probability distributions:

$$f_{ir} = f_i(t, u = u_r) : [0, T] \ \rightarrow \ \mathbb{R}^+ \qquad i \in \{1, ..., 4\} , \quad r = 1, \ldots, m.$$

The interaction terms are defined as follows:

- $\eta_{hk}^{pq} = \eta_{hk}\left[\mathbf{f}\right](u_p, u_q)$ is the encounter rate between the active particle of the h-th functional subsystem with state u_p and the active particle of the k-th functional subsystem with state u_q, where $h, k \in [1, \ldots, 4]$ and $p, q \in [1, \ldots, m]$.
- $\mathscr{B}_{hk}^{i}(r) = \mathscr{B}_{hk}^{i}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)$ is the probability that an active particle of the h-th subsystem, with state u_p ends up into the i-th subsystem with state u_r, after interacting with the active particle of the k-th subsystem, with state u_q.

Then, for $i = 1, \ldots, 4$ and for $r = 1, \ldots, m$, the evolution equations are given by:

$$\begin{aligned}\frac{d}{dt} f_{ir}(t) = Q_{ir}\left[\mathbf{f}\right](t) &= \sum_{h,k=1}^{4} \sum_{p,q=1}^{m} \eta_{hk}\left[\mathbf{f}\right](u_p, u_q) \mathscr{B}_{hk}^{i}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q) \\ &\times f_{hp}(t) f_{kq}(t) - f_{ir}(t) \sum_{k=1}^{4} \sum_{q=1}^{m} \eta_{ik}\left[\mathbf{f}\right](u_r, u_q) f_{kq}(t) \end{aligned} \tag{2.12}$$

where $\mathbf{f}$ denotes the set of all f_{ir} components of the probability density. In order to model the encounter rates we introduce a distance between the probability densities:

$$d\left(f_h, f_k\right)\left[\mathbf{f}\right](t) = \sum_{r=1}^{m} \sum_{r^*=1}^{m} \left| f_{hr}(t) - f_{kr^*}(t) \right|, \qquad h,\, k \in \{1, ..., 4\}.$$

The encounter rates are modeled according to:

$$\eta_{22}^{pq} = \eta_{14}^{pq} = \eta_{41}^{pq} = \eta_{24}^{pq} = \eta_{42}^{pq} = \eta_{44}^{pq} = \alpha_1, \tag{2.13}$$

$$\eta_{11}^{pq} = \alpha_2, \tag{2.14}$$

$$\eta_{12}^{pq} = e^{\frac{1}{1+(\alpha_3 u_q)}}, \tag{2.15}$$

$$\eta_{21}^{pq} = e^{\frac{1}{1+(\alpha_3 u_p)}}, \tag{2.16}$$

$$\eta_{13}^{pq} = e^{\frac{1}{\frac{1}{2}+(\alpha_3 u_q)}}, \tag{2.17}$$

$$\eta_{31}^{pq} = e^{\frac{1}{\frac{1}{2}+(\alpha_3 u_p)}}, \tag{2.18}$$

$$\eta_{23}^{pq} = e^{-\beta(1+u_p)(1+d(f_2,f_3))}, \tag{2.19}$$

$$\eta_{32}^{pq} = e^{-\beta(1+u_q)(1+d(f_2,f_3))}, \tag{2.20}$$

$$\eta_{33}^{pq} = \eta_{34}^{pq} = \eta_{43}^{pq} = \alpha_4, \tag{2.21}$$

where α_1,α_2,α_3,α_4 are positive constants and $0 < \beta < 1$ denotes the risk perception.

The above choice for the encounter rates, indicates that the encounter rate η_{12}^{pq} doctor/susceptible, increases when the value of the activity u_q decreases: indeed people at a low level of susceptivity are more induced to get immunized. On the other hand, the risk perception induces susceptible individuals to stay away from infected ones, which explains the encounter rates in (2.19) and (2.20) that are exponentially decreasing as the distance between the distribution is increasing. Finally the encounter rates in (2.17) and (2.18), corresponding to the interactions doctor/infected, tend to increase in the first stage of the illness, when the doctors are more invoked to prescribe the cure. In all other cases the encounter rates are assumed to be constant.

2.2.2 Transition probability density

Interactions modeled by the terms $\mathscr{B}_{hk}^{i}(r)$, are called stochastic games since the microscopic state of the active particles is known in probability and the output is identified by a transition probability density. The set of the transition probability densities is called table of games.
In order to describe the tables of games we need to introduce the following parameters:

doctors ability: $0 \leq \delta \leq 1$

intensity of the vaccine reaction: $0 \leq \gamma \leq 1$

infectivity: $0 \leq \chi \leq 1$.

Moreover, we consider the first order moment for $i = 1, ..., 4$ which we identify with the mean value:

$$\mathbb{E}_i^1[f_i](t) = \sum_{r=1}^{m} u_r f_{ir}(t),$$

and

$$B_i^p\left(\mathbb{E}_i^1[f_i]\right) = \varepsilon_i \left|\mathbb{E}_i^1[f_i] - u_p\right|,$$

which is proportional to the distance between the activity of the interacting particle p and the mean value $\mathbb{E}_i^1[f_i]$, with $p = 1, ..., m$ and $0 < \varepsilon_i \leq 1$.

Tables of games for $\mathscr{B}^i_{1k}(r)$, for $k = 1, ..., 4$. (doctors)

$$\underline{\mathbf{\mathscr{B}^i_{11}(r) = \mathscr{B}^i_{11}\,[f]\,(u_p \to u_r \mid u_p, u_q)}}$$

When a doctor with state u_p interacts with another doctor with state u_q, he can change his state, according to the following rules:

$$u_p < u_q \begin{cases} u_p \geq \mathbb{E}^1_1[f_1] \begin{cases} \mathscr{B}^1_{11}(r = p-1) & = 0 \\ \mathscr{B}^1_{11}(r = p) & = B^p_1 \\ \mathscr{B}^1_{11}(r = p+1) & = 1 - B^p_1 \\ \mathscr{B}^1_{11}(r \neq p-1, p, p+1) & = 0 \end{cases} \\ u_p < \mathbb{E}^1_1[f_1] \begin{cases} \mathscr{B}^1_{11}(r = p-1) & = 0 \\ \mathscr{B}^1_{11}(r = p) & = 1 - \dfrac{(\delta_1\,|u_q - u_p| + B^p_1)}{2} \\ \mathscr{B}^1_{11}(r = p+1) & = \dfrac{\delta_1\,|u_q - u_p| + B^p_1}{2} \\ \mathscr{B}^1_{11}(r \neq p-1, p, p+1) & = 0 \end{cases} \end{cases}$$

The above rules imply that when the ability of the doctor u_p is less then the ability of the doctor u_q, then if u_p is above the mean value, the transition $u_p \to u_{p+1}$ will be ruled by the comparison between the two terms $(1 - B^p_1)$ and B^p_1. When instead u_p is below the mean value, the transition $u_p \to u_{p+1}$ will be ruled by a comparison of terms involving a linear combination of B^p_1 and the activity distance.

$$u_p \geq u_q \begin{cases} \mathscr{B}^1_{11}(r = p-1) & = 0 \\ \mathscr{B}^1_{11}(r = p) & = 1 \\ \mathscr{B}^1_{11}(r = p+1) & = 0 \\ \mathscr{B}^1_{11}(r \neq p-1, p, p+1) & = 0 \end{cases}$$

When the ability u_p is greater or equal to the ability u_q the only possibility is that the value u_p does not change.

$$\underline{\mathbf{\mathscr{B}^{i}_{13}(r) = \mathscr{B}^{i}_{13}\,[f]\,(u_p \to u_r \mid u_p, u_q)}}$$

When a doctor with state u_p interacts with an individual with state u_q of the third subsystem, he can change his state, according with the following rules:

$$u_q < \mathbb{E}^1_3[f_3] \begin{cases} p < m \begin{cases} \mathscr{B}^1_{13}(r = p-1) & = 0 \\ \mathscr{B}^1_{13}(r = p) & = 1 - (\delta_1 B^q_3) \\ \mathscr{B}^1_{13}(r = p+1) & = \delta_1 B^q_3 \\ \mathscr{B}^1_{13}(r \neq p-1, p, p+1) & = 0 \end{cases} \\ p = m \begin{cases} \mathscr{B}^1_{13}(r = m) & = 1 \\ \mathscr{B}^1_{13}(r \neq m) & = 0 \end{cases} \end{cases}$$

$$u_q \geq \mathbb{E}^1_3[f_3] \begin{cases} \mathscr{B}^1_{13}(r = p-1) & = 0 \\ \mathscr{B}^1_{13}(r = p) & = 1 \\ \mathscr{B}^1_{13}(r = p+1) & = 0 \\ \mathscr{B}^1_{13}(r \neq p-1, p, p+1) & = 0 \end{cases}$$

The above table corresponds to the realistic assumption that doctors learn by taking care of their patients, indeed the ability of a doctor u_p, when the level of illness u_q is below the average, can only increase or remain the same according to the distance of u_q from the mean value.
For the case when the level of illness is above he mean value, the doctor ability u_p does not change anymore (because the doctor already knows which therapy is appropriate).

$$\underline{\mathbf{\mathscr{B}^{i}_{1k}(r) = \mathscr{B}^{i}_{1k}\,[f]\,(u_p \to u_r \mid u_p, u_q),\ \text{for } k = 2, 4}}$$

The interaction between an individual of the first subsystem with state u_p and an individual with state u_q of the second or fourth subsystems brings no change:

$$\begin{cases} \mathscr{B}^1_{1k}(r = p-1) & = 0 \\ \mathscr{B}^1_{1k}(r = p) & = 1 \\ \mathscr{B}^1_{1k}(r = p+1) & = 0 \\ \mathscr{B}^1_{1k}(r \neq p-1, p, p+1) & = 0 \end{cases}$$

The above table refers to interactions doctors/susceptile and doctors/healed, this kind of interactions do not imply any change of the activity u_p for the doctors.

Tables of games for $\mathscr{B}^i_{2k}(r)$, for $k = 1, ..., 4$. (susceptible individuals)

$$\underline{\mathscr{B}^{\mathbf{i}}_{\mathbf{2k}}(\mathbf{r}) = \mathscr{B}^{\mathbf{i}}_{\mathbf{2k}}\,[\mathbf{f}]\,(\mathbf{u_p} \to \mathbf{u_r} \mid \mathbf{u_p}, \mathbf{u_q}),\ \textbf{for } \mathbf{k = 2, 4}}$$

The interaction between an individual of the second subsystem with state u_p and an individual with state u_q of the second or fourth subsystem (susceptible/susceptible, or susceptible/hill) brings no change:

$$\begin{cases} \mathscr{B}^2_{2k}(r = p - 1) & = 0 \\ \mathscr{B}^2_{2k}(r = p) & = 1 \\ \mathscr{B}^2_{2k}(r = p + 1) & = 0 \\ \mathscr{B}^2_{2k}(r \neq p - 1, p, p + 1) & = 0 \end{cases}$$

$$\underline{\mathscr{B}^{\mathbf{i}}_{\mathbf{21}}(\mathbf{r}) = \mathscr{B}^{\mathbf{i}}_{\mathbf{21}}\,[\mathbf{f}]\,(\mathbf{u_p} \to \mathbf{u_r} \mid \mathbf{u_p}, \mathbf{u_q})}$$

We now consider the table referring to interactions between a susceptible and a doctor: we describe separately the case when a susceptible first encounters a doctor and takes the vaccine. We then have the following cases:

$$u_p < \mathbb{E}^1_2[f_2] \begin{cases} \mathscr{B}^4_{21}(r = m) & = 1 \\ \mathscr{B}^2_{21}(r = p) & = 0 \\ \mathscr{B}^4_{21}(r \neq m) & = 0 \\ \mathscr{B}^2_{21}(r \neq p) & = 0 \end{cases}$$

When the activity u_p (susceptivity) is below the average then the susceptible individual becomes immunized and he makes a transition to the state m of the last class.

Let us now consider the case when the susceptivity is above the mean value. We have the following table:

$$u_p \geq \mathbb{E}_2^1[f_2] \begin{cases} p < m \begin{cases} \mathscr{B}_{21}^4(r=m) & = 1 - \left(\left(1 - \tanh\left(\dfrac{1}{(1-\gamma)}\right)\right) B_2^p\right) \\ \mathscr{B}_{21}^2(r=p+1) & = \left(1 - \tanh\left(\dfrac{1}{(1-\gamma)}\right)\right) B_2^p \\ \mathscr{B}_{21}^2(r \neq p+1) & = 0 \\ \mathscr{B}_{21}^4(r \neq m) & = 0 \end{cases} \\ p = m \begin{cases} \mathscr{B}_{21}^4(r=m) & = 1 - \left(\left(1 - \tanh\left(\dfrac{1}{(1-\gamma)}\right)\right) B_2^p\right) \\ \mathscr{B}_{21}^3(r=1) & = \left(1 - \tanh\left(\dfrac{1}{(1-\gamma)}\right)\right) B_2^p \\ \mathscr{B}_{21}^4(r \neq m) & = 0 \\ \mathscr{B}_{21}^3(r \neq 1) & = 0 \end{cases} \end{cases}$$

From the above table we see that if the susceptivity is greater than the mean value, then $u_p \to u_{p+1}$ in the case of a small γ; when γ increases instead, the susceptible individual will be driven toward the healed class.
In the special case $p = m$ for small γ, the individuals will be driven to the first stadium of the third class (illness).

$$\underline{\mathscr{B}_{\mathbf{23}}^{\mathbf{i}}(\mathbf{r}) = \mathscr{B}_{\mathbf{23}}^{\mathbf{i}}\left[\mathbf{f}\right](\mathbf{u_p} \to \mathbf{u_r} \mid \mathbf{u_p}, \mathbf{u_q})}$$

$$u_p \geq \mathbb{E}_2^1[f_2] \begin{cases} p < m \begin{cases} \mathscr{B}_{23}^2(r=p-1) & = 0 \\ \mathscr{B}_{23}^2(r=p) & = 1 - e^{\chi-1} \\ \mathscr{B}_{23}^2(r=p+1) & = e^{\chi-1} \\ \mathscr{B}_{23}^2(r \neq p-1, p, p+1) & = 0 \end{cases} \\ p = m \begin{cases} \mathscr{B}_{23}^2(r=m) & = 1 - e^{\chi-1} \\ \mathscr{B}_{23}^3(r=1) & = e^{\chi-1} \\ \mathscr{B}_{23}^2(r \neq m) & = 0 \\ \mathscr{B}_{23}^3(r \neq 1) & = 0 \end{cases} \end{cases}$$

$$u_p < \mathbb{E}_2^1[f_2] \begin{cases} \mathscr{B}_{23}^2(r=p-1) & = 0 \\ \mathscr{B}_{23}^2(r=p) & = 1 - e^{((1-B_2^p)\chi)-1} \\ \mathscr{B}_{23}^2(r=p+1) & = e^{((1-B_2^p)\chi)-1} \\ \mathscr{B}_{23}^2(r \neq p-1, p, p+1) & = 0 \end{cases}$$

The above table refers to the interactions susceptible/ infected. When the susceptivity is above the mean value, the probability transition $u_p \to u_{p+1}$ increases as χ increases. For $p = m$ the transition refers to the first stadium of the third class. When u_p is below the mean value, the transition $u_p \to u_{p+1}$ is again driven by infectivity χ but now there is a dumping effect due to the distance from the mean value.

Tables of games for $\mathscr{B}^i_{3k}(r)$, for $k = 1, ..., 4$. (individuals affected by the disease)

$$\underline{\mathscr{B}^{\mathbf{i}}_{\mathbf{3k}}(\mathbf{r}) = \mathscr{B}^{\mathbf{i}}_{\mathbf{3k}}\,[\mathbf{f}]\,(\mathbf{u_p} \to \mathbf{u_r} \mid \mathbf{u_p}, \mathbf{u_q}),\ \textbf{for } \mathbf{k = 2, 3, 4}}$$

$$u_p \geq \mathbb{E}^1_3[f_3] \begin{cases} p < m \begin{cases} \mathscr{B}^3_{3k}(r = p-1) & = 0 \\ \mathscr{B}^3_{3k}(r = p) & = 1 - B^p_3 \\ \mathscr{B}^3_{3k}(r = p+1) & = B^p_3 \\ \mathscr{B}^3_{3k}(r \neq p-1, p, p+1) & = 0 \end{cases} \\ p = m \begin{cases} \mathscr{B}^3_{3k}(r = m) & = 0 \\ \mathscr{B}^4_{3k}(r = 1) & = 1 \\ \mathscr{B}^3_{3k}(r \neq m) & = 0 \\ \mathscr{B}^4_{3k}(r \neq 1) & = 0 \end{cases} \end{cases}$$

$$u_p < \mathbb{E}^1_3[f_3] \begin{cases} \mathscr{B}^3_{3k}(r = p-1) & = 0 \\ \mathscr{B}^3_{3k}(r = p) & = 1 \\ \mathscr{B}^3_{3k}(r = p+1) & = 0 \\ \mathscr{B}^3_{3k}(r \neq p-1, p, p+1) & = 0 \end{cases}$$

When we consider individuals affected by the disease (above table) we observe that when the level of illness is below the mean value, the activity u_p does not change. In all other cases the probability transition $u_p \to u_{p+1}$ increases as the distance B^p_3 from the mean value increases. We point out that in the special case $p = m$, the individuals end up in the healed individuals population.

$$\underline{\mathscr{B}^{\mathbf{i}}_{\mathbf{31}}(\mathbf{r}) = \mathscr{B}^{\mathbf{i}}_{\mathbf{31}}\left[\mathbf{f}\right]\left(\mathbf{u_p} \to \mathbf{u_r} \mid \mathbf{u_p}, \mathbf{u_q}\right)}$$

$$
\begin{cases}
u_p \geq \mathbb{E}^1_3[f_3] &
\begin{cases}
p < m &
\begin{cases}
u_q \geq \mathbb{E}^1_1[f_1] &
\begin{cases}
\mathscr{B}^3_{31}(r = p-1) & = 0 \\
\mathscr{B}^3_{31}(r = p) & = 0 \\
\mathscr{B}^3_{31}(r = p+1) & = 1 \\
\mathscr{B}^3_{31}(r \neq p-1, p, p+1) & = 0
\end{cases} \\
u_q < \mathbb{E}^1_1[f_1] &
\begin{cases}
\mathscr{B}^3_{31}(r = p-1) & = 0 \\
\mathscr{B}^3_{31}(r = p) & = B^q_1(1 - B^p_3) \\
\mathscr{B}^3_{31}(r = p+1) & = 1 - B^q_1(1 - B^p_3) \\
\mathscr{B}^3_{31}(r \neq p-1, p, p+1) & = 0
\end{cases}
\end{cases} \\
p = m &
\begin{cases}
\mathscr{B}^3_{31}(r = m) & = 0 \\
\mathscr{B}^4_{31}(r = 1) & = 1 \\
\mathscr{B}^3_{31}(r \neq m) & = 0 \\
\mathscr{B}^4_{31}(r \neq 1) & = 0
\end{cases}
\end{cases} \\
u_p < \mathbb{E}^1_3[f_3] &
\begin{cases}
u_q \geq \mathbb{E}^1_1[f_1] &
\begin{cases}
\mathscr{B}^3_{31}(r = p-1) & = 0 \\
\mathscr{B}^3_{31}(r = p) & = 0 \\
\mathscr{B}^3_{31}(r = p+1) & = 1 \\
\mathscr{B}^3_{31}(r \neq p-1, p, p+1) & = 0
\end{cases} \\
u_q < \mathbb{E}^1_1[f_1] &
\begin{cases}
\mathscr{B}^3_{31}(r = p-1) & = 0 \\
\mathscr{B}^3_{31}(r = p) & = 1 - (1 - B^q_1)(1 - B^p_3) \\
\mathscr{B}^3_{31}(r = p+1) & = (1 - B^q_1)(1 - B^p_3) \\
\mathscr{B}^3_{31}(r \neq p-1, p, p+1) & = 0
\end{cases}
\end{cases}
\end{cases}
$$

The above table describes the interactions between the individuals affected by the disease and the doctors. In the first case the degree of illness is above the mean value. Then the output of interaction depends both on the doctors ability and on the distance B^p_3 of the activity u_p from the mean value. The illness will tend to evolve toward the healed state as rapidly as B^p_3 increases and the distance B^q_1 decreases. In the second case, when u_p is below the mean value, we have the opposite behavior.

Tables of games for $\mathscr{B}^i_{4k}(r)$, for $k = 1, ..., 4$. (healed individuals)

$$\underline{\mathscr{B}^{\mathbf{i}}_{\mathbf{4k}}(\mathbf{r}) = \mathscr{B}^{\mathbf{i}}_{\mathbf{4k}}\left[\mathbf{f}\right](\mathbf{u_p} \to \mathbf{u_r} \mid \mathbf{u_p}, \mathbf{u_q}),\ \textbf{for } \mathbf{k = 1, 2, 3, 4}}$$

$$p \neq m \begin{cases} \mathscr{B}^4_{4k}(r = p-1) & = 0 \\ \mathscr{B}^4_{4k}(r = p) & = 0 \\ \mathscr{B}^4_{4k}(r = p+1) & = 1 \\ \mathscr{B}^4_{4k}(r \neq p-1, p, p+1) & = 0 \end{cases}$$

$$p = m \begin{cases} \mathscr{B}^4_{4k}(r = m-1) & = 0 \\ \mathscr{B}^4_{4k}(r = m) & = 1 \\ \mathscr{B}^4_{4k}(r = m+1) & = 0 \\ \mathscr{B}^4_{4k}(r \neq m-1, m, m+1) & = 0 \end{cases}$$

The last above table describes the interactions between healed individuals and individuals belonging to the other populations. As expected, the healed individuals proceed in their complete recovery and this is independent by the index i.

2.2.3 Qualitative analysis

In this Subsection the initial value (I.V.) problem for equation (2.12) is formulated. It is shown that the solution of such I.V. problem exists, it is unique and is a positive, regular function of time, of class $C^1([0, T])$.
We point out that the proof carried out in the following is different from the one reported in [28] which refers to a (I.V.) problem for a system where there are no migration phenomena between different classes.
In order to obtain the time evolution of the distribution functions $f_{ir}(t)$, $i \in \{1, \ldots, n\}$, we consider the I.V. problem:

$$\begin{cases} \dfrac{d}{dt} f_{ir}(t) = Q_{ir}\left[f\right](t), \qquad i = 1, \ldots, n, \quad r = 1, \ldots, m, \\ f_{ir}(0) = f_i(0, u_r), \end{cases} \tag{2.22}$$

where, due (2.12) we write:

$$\frac{d}{dt} f_{ir}(t) = Q_{ir}\left[\mathbf{f}\right](t) = \sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \eta_{hk}\left[\mathbf{f}\right](u_p, u_q) \mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)$$
$$\times f_{hp}(t) f_{kq}(t) - f_{ir}(t) \sum_{k=1}^{n} \sum_{q=1}^{m} \eta_{ik}\left[\mathbf{f}\right](u_r, u_q) f_{kq}(t).$$

We introduce the space:

$$X = \{f_i : [0,T] \to \mathbb{R},\ f_i \in C^1([0,T]), i = 1, \dots, n,\ T > 0\}$$

characterized with the norm:

$$\| f_i\,(t) \|_X = \sum_{r=1}^{m} |f_{ir}(t)|. \tag{2.23}$$

Moreover, we define the space $\mathbf{X} = X^n$ with the corresponding norm:

$$\|\mathbf{f}\,(t) \|_{\mathbf{X}} = \sum_{i=1}^{n} \|f_i(t)\|_X, \tag{2.24}$$

and introduce:

$$\mathbf{X}_+ = \{\mathbf{f} \in \mathbf{X} \mid f_i \geq 0,\ i = 1, \dots, n\}$$

The following theorem states a result of local existence and uniqueness for the solution of the I.V. problem (2.22).

Theorem 2.2.2. *Consider the I.V. problem (2.22) with* $\mathbf{f}_0 = \{f_1(0,u), \dots, f_n(0,u)\} \in \mathbf{X}_+$. *Assume that*

$$\eta_{h,k}^{p,q} \geq 0, \quad \mathscr{B}_{hk}^i(r) \geq 0, \quad \sum_{i=1}^{n}\sum_{r=1}^{m} \mathscr{B}_{hk}^i\,[\mathbf{f}]\,(u_p \to u_r \mid u_p, u_q) = 1 \quad \forall \mathbf{f}. \tag{2.25}$$

holds, together with the following hypotheses:

- *The encounter rate* η_{hk}^{pq} *satisfies the following condition:*

  $$\sum_{r=1}^{m} \eta_{hk}\,[\mathbf{f}]\,(u_p, u_q) \leq C,\ \forall\ h,k = 1 \dots, n\ \forall\ p,q \in \{1, \dots, m\}\ \textit{ and } \forall \mathbf{f} \in \mathbf{X}$$

  with C *a positive constant;*

- $\forall \mathbf{f}, \boldsymbol{g} \in \mathbf{X}$ *the probability* $\mathscr{B}_{hk}^i(r)$ *and the encounter rate* η_{hk}^{pq} *are Lipschitz continuous in* X, *that is,* $\forall\ p,q \in \{1, \dots, m\}$ *it results*
  $$\sum_{h,k,i=1}^{n}\sum_{r=1}^{m} \mid \mathscr{B}_{hk}^i\,[\mathbf{f}]\,(u_p \to u_r | u_p, u_q) - \mathscr{B}_{hk}^i\,[\mathbf{g}]\,(u_p \to u_r | u_p, u_q) \mid$$
  $$\leq L_1 \|\mathbf{f} - \mathbf{g}\|_{\mathbf{X}},$$
  $$\sum_{h,k=1}^{n}\sum_{r=1}^{m} \mid \eta_{hk}\,[\mathbf{f}]\,(u_p, u_q) - \eta_{hk}\,[\mathbf{g}]\,(u_p, u_q)| \leq L_2 \|\mathbf{f} - \mathbf{g}\|_{\mathbf{X}},$$
  with L_1, L_2 *positive constants.*

Then, there exist $T > 0$ and a unique solution $\mathbf{f}(t)$ in $\mathbf{X}$ for the I.V. problem (2.22) on the time interval $[0, T]$. Moreover $\mathbf{f}(t) \in \mathbf{X}_+$, $t \in [0, T]$.

Proof. We start observing that, since the interactions are assumed number conservative, see (2.25), it results that:

$$\frac{d}{dt} \sum_{i=1}^{n} \sum_{r=1}^{m} f_{ir}(t) = 0,$$

which implies:

$$\|\mathbf{f}(t)\|_{\mathbf{X}} = \|\mathbf{f}(0)\|_{\mathbf{X}}, \quad \text{for any } t \geq 0. \tag{2.26}$$

Therefore the solution of (2.22), if it exists, remains bounded in $\mathbf{X}$ for any time $t \geq 0$. The latter observation assures that the operator $Q_i[\mathbf{f}](t)$ in the right hand side of (2.22) is a closed map in $\mathbf{X}$.
Let us now prove that $Q_i[\mathbf{f}](t)$ is Lipschitz continuous in $\mathbf{X}$, i.e. given $\|\mathbf{f}\|_{\mathbf{X}}$ and $\|\mathbf{g}\|_{\mathbf{X}} \leq M$ it follows that:

$$\|Q_i[\mathbf{f}](t) - Q_i[\mathbf{g}](t)\|_{\mathbf{X}} \leq L\|\mathbf{f} - \mathbf{g}\|_{\mathbf{X}}, \tag{2.27}$$

with L a positive constant depending on M. Indeed, when (2.12) is used together with (2.23) and (2.24), for the right hand side of (2.27) we can write:

$$\sum_{i=1}^{n} \sum_{r=1}^{m} \Bigg| \Bigg[\sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \eta_{hk}[\mathbf{f}](u_p, u_q) \mathscr{B}^i_{hk}[\mathbf{f}](u_p \to u_r \mid u_p, u_q) f_{hp}(t) f_{kq}(t)$$

$$- f_{ir} \sum_{k=1}^{n} \sum_{q=1}^{m} \eta_{ik}[\mathbf{f}](u_r u_q) f_{kq}(t) \Bigg]$$

$$- \Bigg[\sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \eta_{hk}[\mathbf{g}](u_p, u_q) \mathscr{B}^i_{hk}[\mathbf{g}](u_p \to u_r \mid u_p, u_q) g_{hp}(t) g_{kq}(t)$$

$$- g_{ir} \sum_{k=1}^{n} \sum_{q=1}^{m} {}_ik[\mathbf{g}](u_r u_q) g_{kq}(t) \Bigg] \Bigg|$$

$$\leq \sum_{i=1}^{n} \sum_{r=1}^{m} \Bigg\{ \sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \big| {}_hk[\mathbf{f}](u_p, u_q) \mathscr{B}^i_{hk}[\mathbf{f}](u_p \to u_r \mid u_p, u_q) \, [f_{hp}(t) f_{kq}(t)$$

$$- g_{hp}(t) g_{kq}(t)] + g_{hp}(t) g_{kq}(t) \left[\eta_{hp}[\mathbf{f}](u_p, u_q) \mathscr{B}^i_{hk}[\mathbf{f}](u_p \to u_r \mid u_p, u_q) \right.$$

$$\left. - \eta_{hp}[\mathbf{g}](u_p, u_q) \mathscr{B}^i_{hk}[\mathbf{g}](u_p \to u_r \mid u_p, u_q) \right] \big|$$

$$\sum_{k=1}^{n}\sum_{q=1}^{m}|\eta_{ik}[\mathbf{f}](u_r,u_q)[f_{ir}(t)f_{kq}(t)-g_{ir}(t)g_{kq}(t)]$$

$$\left.+g_{ir}(t)g_{kq}(t)[\eta_{ik}[\mathbf{f}](u_r,u_q)-\eta_{ik}[\mathbf{g}](u_r,u_q)]|\right\}$$

$$\leq\sum_{i=1}^{n}\sum_{r=1}^{m}\left\{\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|\eta_{hk}[\mathbf{f}](u_p,u_q)\mathscr{B}_{hk}^{i}[\mathbf{f}](u_p\to u_r\mid u_p,u_q)f_{hp}(t)[f_{kq}(t)\right.\right.$$

$$-g_{kq}(t)]|+\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|\eta_{hk}[\mathbf{f}](u_p,u_q)\mathscr{B}_{hk}^{i}[\mathbf{f}](u_p\to u_r\mid u_p,u_q)g_{kq}(t)[f_{hp}(t)\right.$$

$$-g_{hp}(t)]|\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|g_{hp}(t)g_{kq}(t)\eta_{hp}[\mathbf{f}](u_p,u_q)\left[\mathscr{B}_{hk}^{i}[\mathbf{f}](u_p\to u_r\mid u_p,u_q)\right.\right.$$

$$\left.\left.-\mathscr{B}_{hk}^{i}[\mathbf{g}](u_p\to u_r\mid u_p,u_q)\right]\right|$$

$$\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|g_{hp}(t)g_{kq}(t)\mathscr{B}_{hk}^{i}[\mathbf{g}](u_p\to u_r\mid u_p,u_q)[\eta_{hk}[\mathbf{f}](u_p,u_q)\right.$$

$$-\eta_{hk}[\mathbf{g}](u_p,u_q)]|$$

$$+\sum_{k=1}^{n}\sum_{q=1}^{m}|\eta_{ik}[\mathbf{f}](u_r,u_q)f_{ir}(t)[f_{kq}-g_{kq}]|$$

$$+\sum_{k=1}^{n}\sum_{q=1}^{m}|\eta_{ik}[\mathbf{f}](u_r,u_q)g_{kq}(t)[f_{ir}-g_{ir}]|$$

$$\left.+\sum_{k=1}^{n}\sum_{q=1}^{m}|g_{ir}(t)g_{kq}(t)[eta_{ik}[\mathbf{f}](u_r,u_q)-\eta_{ik}[\mathbf{g}](u_r,u_q)]|\right\}$$

$$\leq 2m^2n^3CM\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}}+m^2n^3M^2CL_1\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}}+n^2m^2M^2L_2\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}}$$

$$+2n^2mCM\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}}+nmM^2L_2\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}}\leq L\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}},$$

that proves (2.27). Then, there follows the existence of a unique solution $\mathbf{f}(t)$ in $\mathbf{X}$ of (2.22) local in time. Next, the non negativity of the solution, in its domain of existence, is easily obtained along the same lines of the proof reported in [28]. Observing that the components $f_{ir}(t)$ of the solution satisfy the condition:

$$f_{ir}(t) \geq 0 \quad \forall i = 1, \ldots, n \quad \text{and} \quad \forall j = 1, \ldots, m \tag{2.28}$$

when $\mathbf{f}(0) \in \mathbf{X}_+$. We set:

$$R^i(f,f)(t) = \sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \eta_{hk} \left[\mathbf{f}\right] (u_p, u_q) \mathscr{B}^i_{hk} \left[\mathbf{f}\right] (u_p \to u_r \mid u_p, u_q) f_{hp}(t) f_{kq}(t),$$

$$S^i(f)(t) = \sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \eta_{ik} \left[\mathbf{f}\right] (u_r, u_q) f_{kq}(t).$$

Equation (2.12) can be rewritten as

$$\frac{d}{dt} f_{ir}(t) + f_{ir}(t) S^i(f)(t) = R^i(f,f)(t). \tag{2.29}$$

Now we call

$$\lambda_i(t) = \int_0^t S^i(f)(t^{'}) dt^i.$$

If f_{ir} is solution of (2.29), it then follows

$$\frac{d}{dt}(\exp(\lambda_i(t)) f_{ir}(t)) = \exp(\lambda_i(t)) R^i(f,f)(t)$$

which implies

$$f_{ir}(t) = \exp(-\lambda_i(t)) f_{ir}(0) + \int_0^t \left[\exp(\lambda_i(t^{'})) R^i(f,f)(t^{'})\right] dt^{'}. \tag{2.30}$$

The relation (2.30) allows us to conclude that, given $\mathbf{f}(0) \in \mathbf{X}_+$ and the positivity of the integral function, the function $f_{ir}(t)$ satisfies the condition of non-negativity (2.28) in its domain of existence. Moreover, when (2.28) is used together with (2.26), we obtain that the solution of (2.22) is uniformly bounded on any compact time interval $[0, T]$, $T > 0$. This latter observation leads immediately to the following result of global existence and uniqueness of the solution in $\mathbf{X}_+$ $\square$

Theorem 2.2.3. *Consider the I.V. problem (2.22) under the assumptions of the theorem 2.2.2. Then the solution* $\mathbf{f}(t)$ *exists and is unique for any finite time* $t \geq 0$.

2.2.4 Numerical simulations

The results of numerical simulations are shown in Figs.2.1, 2.2, 2.3, 2.4, where initial configurations for the populations distribution among the different activity classes ($m = 6$) are shown versus final and also intermediate Fig.2.1 configurations. In our simulations we used realistic initial values of the parameters, coming from the CIRI database [72] (Interuniversity Center Flu Research).
In Figures 2.1 - 2.4 we represent the different populations from top to bottom, re-

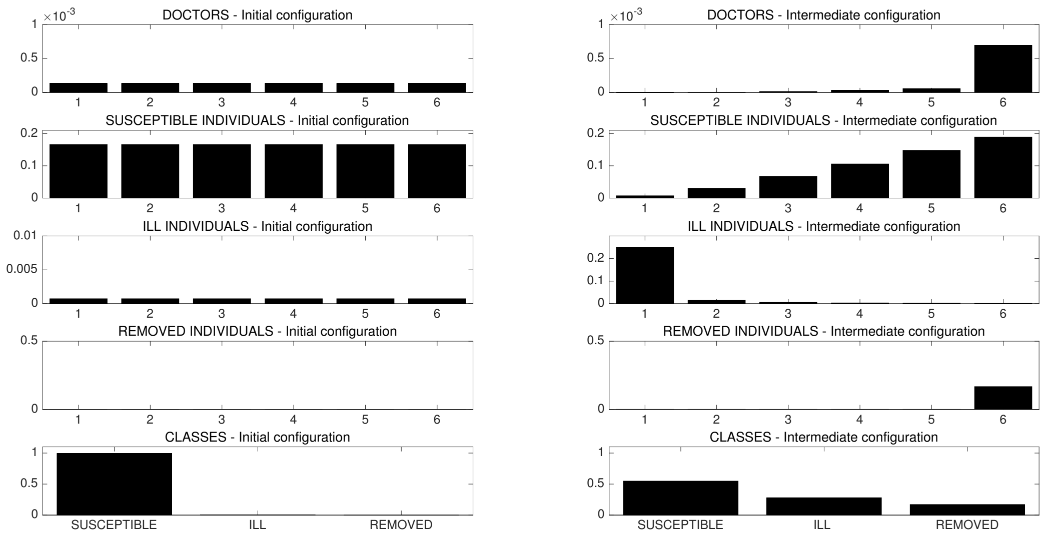

Figure 2.1: Initial (left) and intermediate (right) configurations for the populations distribution among the different activity classes. Here the parameters are fixed as $\alpha_1 = 0.9$, $\alpha_2 = 2.5$, $\alpha_3 = 0.5$, $\alpha_4 = 0.7$, $\gamma = 0.94$, $\delta = 0.9$, $\chi = 0.9$, $\beta = 0.23$.

porting on the left the initial values and on the right the final (asymptotic) values or intermediate values. The α_j parameters concerning the encounter rates (2.13) - (2.21) are fixed as $\alpha_1 = 0.9$, $\alpha_2 = 2.5$, $\alpha_3 = 0.5$, $\alpha_4 = 0.7$. Moreover, in Figures 2.1, 2.2, 2.3, we keep fixed the intensity of vaccine reaction $\gamma = 0.94$, the infectivity $\chi = 0.9$ and the doctors ability $\delta = 0.9$; we wish to observe how the evolution of the system changes by changing the risk perception parameter β.
In Fig.2.1,2.2 we put $\beta = 0.23$. The initial distribution for doctors, susceptible individuals and infective individuals are chosen to be uniform. In Fig.2.1 we look at the configuration taken at an intermediate time, while in Fig.2.2 we look at the configuration taken at the final (asymptotic) time. In Fig.2.1 we can follow the evolution of the epidemics, and see how the doctors progressively migrate to the

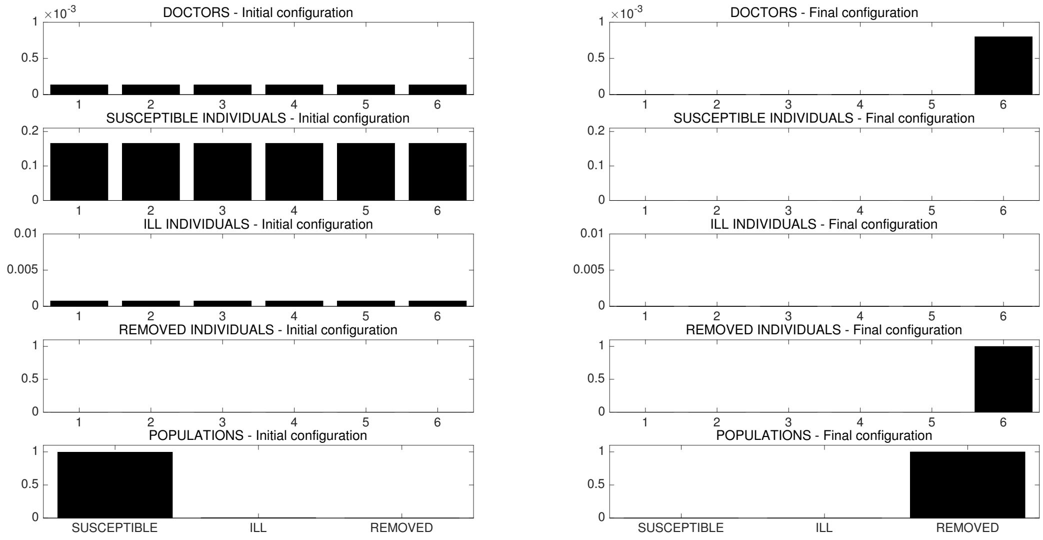

Figure 2.2: Initial (left) and asymptotic (right) configurations for the populations distribution among the different activity classes. Here the parameters are fixed as $\alpha_1 = 0.9$, $\alpha_2 = 2.5$, $\alpha_3 = 0.5$, $\alpha_4 = 0.7$, $\gamma = 0.94$, $\delta = 0.9$, $\chi = 0.9$, $\beta = 0.23$.

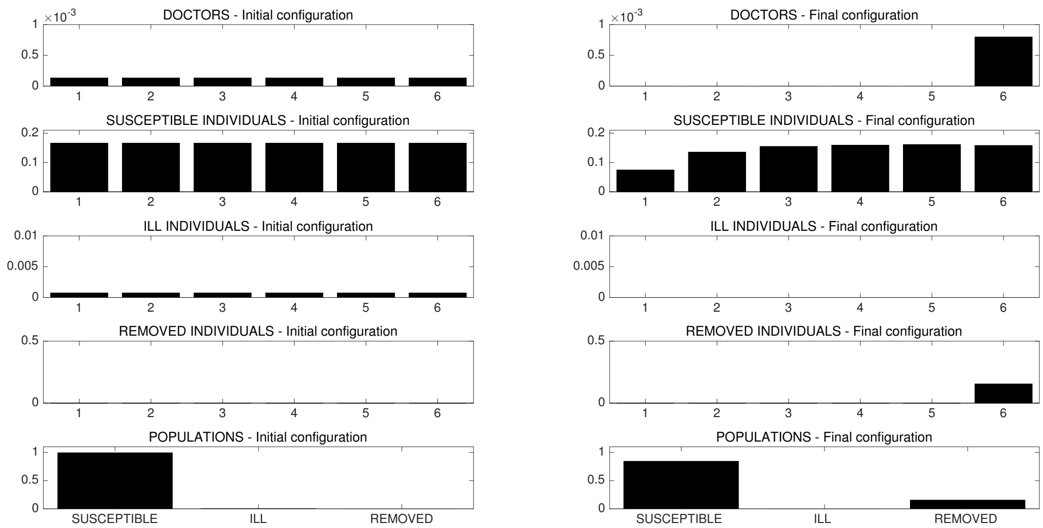

Figure 2.3: Initial (left) and asymptotic (right) configurations for the populations distribution among the different activity classes. Here the parameters are fixed as $\alpha_1 = 0.9$, $\alpha_2 = 2.5$, $\alpha_3 = 0.5$, $\alpha_4 = 0.7$, $\gamma = 0.94$, $\delta = 0.9$, $\chi = 0.9$, $\beta = 0.34$.

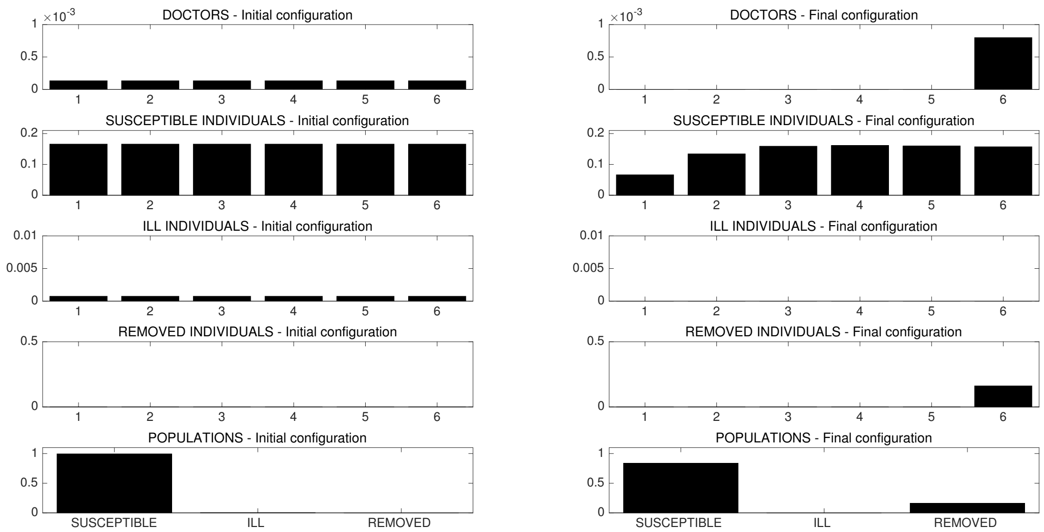

Figure 2.4: Initial (left) and asymptotic (right) configurations for the populations distribution among the different activity classes. Here the parameters are fixed as $\alpha_1 = 0.9$, $\alpha_2 = 2.5$, $\alpha_3 = 0.5$, $\alpha_4 = 0.7$, $\gamma = 0.94$, $\delta = 0.9$, $\chi = 0.1$, $\beta = 0.25$.

last class, while the susceptible individuals became part infected and part susceptible to the last stage. Also, the infected people start to migrate toward the removed population. In Fig.2.2 as expected, all the doctors migrate eventually in the last class. They learn from experience by treating many different cases and become expert both in prevention and in the handling of the epidemics. When we look at the second population, we see that there are no susceptible individuals in the corresponding final states. The same happens with the individuals affected by the disease. On the other hand, all the individuals of the two populations, susceptible + infective, make a migration in the last class of the removed population, which constitutes their final (asymptotic) state. In other words, the risk perception in this case is not big enough to prevent susceptible individuals from exposing themselves to the infection. It appears that all of them contract the disease, and then, as time goes on they end up in the removed population.
The situation is instead different in Fig.2.3 where the risk perception parameter β is higher ($\beta = 0.34$). The first population (doctors) has the same behavior as in Fig.2.2. Also the third population (infected individuals) has the same behavior as in Fig.2.2: all the individuals eventually end up in the last class of the removed population. More interesting is the evolution of the second population: looking carefully at the final values for the different classes of the susceptible population,

it appears that there are two migration phenomena. First of all, there are individuals with a low level of susceptibility which get immunized (vaccinated) and migrate into the removed population; then there are those who migrate to a different class (higher level of susceptibility) and either stay there or contract the disease and then, as time goes on, end up in the removed population. In our last figure we take now the risk perception at a lower level, $\beta = 0.25$, with a low level of infectivity $\chi = 0.1$ and a high reaction to the vaccine $\gamma = 0.94$. We start with uniform initial distribution for the different populations. When we look at the final (asymptotic) configuration we find a situation which is almost identical to the one corresponding to high risk perception $\beta = 0.34$, with high infectivity $\chi = 0.9$ and the same reaction to the vaccine $\gamma = 0.94$, shown in Fig.2.3. In other words, from the comparison of Fig.2.3 and Fig.2.4, it appears that a variation in χ (infectivity) of order $8 \cdot 10^{-1}$ has the same effect as a variation in β (risk perception) of order $9 \cdot 10^{-2}$. This implies that the evolution of the system toward the asymptotic configuration is much more influenced by the risk perception than by the infectivity of the disease.

2.3 Influence of drivers ability in a discrete vehicular traffic model

Traffic flow problems have been the subject of several investigations in the past due to their relevance in everyday-life applications [11, 50, 54]. From the mathematical point of view, traffic flow phenomena can be modeled at three different scales: microscopic [49], macroscopic [5, 26] and kinetic [11, 27, 42]. The microscopic description refers to vehicles individually identified and leads to system of ODEs, while continuum mechanics assumptions lead to macroscopic models stated in terms of PDEs corresponding to fluid dynamic equations [59, 68]. The approach offered by the kinetic theory, developed after the pioneer contribution by Prigogine and Herman [65], uses Boltzmann and/or Vlasov-type equations to model the complex system under consideration. The kinetic approach is indeed suitable for an aggregate representation of the distribution of vehicles, not necessarily focused on single car, while still allowing for a detailed characterization of the microscopic vehicle-to-vehicle dynamics.

Classically, in the kinetic representation of vehicular traffic along one-way road, the spatial position and speed of vehicles are assumed to be continuously distributed over the spatial and speed domains. However, this does not reflect correctly the physical reality of vehicular flow. Indeed, the number of vehicles along a road is normally not large enough for the continuity of the distribution function over the microscopic states to be an acceptable approximation (like in the classical kinetic theory of gases). Vehicles do not span continuously the whole set of admissible speeds and the actual distribution of vehicles in space, as well as that of their speeds, is strongly granular. Recently, discrete velocity models have been introduced [13, 27, 42], relaxing the hypothesis that the speed distribution is continuous, by introducing a lattice of discrete speeds.

In the present paper we make a step further, taking into account the activity variable u. This new variable is a measure of the driver ability to adapt to the traffic conditions and to elaborate his own strategy (in order to avoid collisions with other vehicles). Following the ideas of Daganzo [30] we define a discrete set of activity classes to differentiate the behavior of each driver.

In the next Subsection the mathematical framework of the KTAP theory suitable to describe a traffic model is introduced; the nonlinear interactions characterizing the system are discussed in Subsection 2.3.2, where the transition probability densities is also derived. Subsection 2.3.3 is dedicated to the qualitative analysis of the model; finally some numerical examples illustrating the behavior of our model are presented in Subsection 2.3.4. Our results show that the ability of the drivers influences the behavior both of the average velocity and of the flux as functions of the density of the vehicles. Moreover, it influences also the asymptotic configuration of the velocity distribution obtained for different values of the density. Finally, we underline that our model not only reproduces qualitatively the traffic phases already observed in previous studies, but also allows to get quantitative agreement with experimental evidence. Indeed, in the case of intermediate road conditions, we obtain an estimate of the critical density ρ_c corresponding to the transition from free to congested traffic flow, coincident with the one measured on the Venezia-Mestre highway [15].

2.3.1 Mathematical representation and structures

Let us consider a large system of interacting entities, called *active particles*, each active particle is the pair vehicle-driver which has its own driving ability, called *activity*.
Starting from the discrete kinetic model introduced by Delitala -Tosin [38], the hypothesis of granular traffic allow us to discretize the velocity variable v introducing in $D_{\mathbf{v}} = [0, 1]$ a grid $I_{\mathbf{v}} = \{v_i\}_{i=1}^n$ of the form

$$0 = v_1 < v_2 < \cdots < v_{n-1} < v_n = v_{max} ,$$

where v_{max} is the maximum speed allowed along the road.
The activity is represented by the discrete variable $u \in D_{\mathbf{u}} = [0, 1]$ and it is heterogeneously distributed over each *velocity class* v_i. Let us define in D_u a grid of activities $I_{\mathbf{u}} = \{u_r\}_{r=1}^m$ of the form

$$u_1 < u_2 < \cdots < u_{m-1} < u_m ,$$

where u_1 and u_m represent respectively the class of *incapable* and *experienced* drivers. The physical system is then described by the *distribution functions*

$$f_{ir} = f_i(t, u_r) : \mathbb{R}^+ \rightarrow \mathbb{R}^+,$$

$$\forall i = 1, \ldots, n; \; r = 1, \ldots, m$$

that, at time t, denote the number of vehicles which travel with velocity v_i and possess activity u_r. Moreover, we denote by N_{ir} the total number of vehicles with speed v_i and activity u_r, while the total number N_i of vehicles in the velocity class v_i is

$$N_i = \sum_{r=1}^{m} N_{ir}.$$

Similarly, the total number N_r of cars in the activity class u_r is

$$N_r = \sum_{i=1}^{n} N_{ir}.$$

According to this mathematical structure we can define the following macroscopic quantities:

- the *vehicles density*
$$\rho(t) = \sum_{i=1}^{n}\sum_{r=1}^{m} f_{ir}(t),$$
- the *vehicles flux*
$$q(t) = \sum_{i=1}^{n}\sum_{r=1}^{m} v_i f_{ir}(t),$$
- the *average velocity*
$$\overline{v}(t) = \frac{q(t)}{\rho(t)} = \frac{\sum_{i=1}^{n}\sum_{r=1}^{m} v_i f_{ir}(t)}{\sum_{i=1}^{n}\sum_{r=1}^{m} f_{ir}(t)},$$
- the *velocity variance*
$$\Delta(t) = \frac{1}{\rho(t)}\sum_{i=1}^{n}\sum_{r=1}^{m}(v_i - \overline{v}(t))^2 f_{ir}(t).$$

2.3.2 Modeling interactions

The relevant interactions are now considered at microscopic level: they involve three types of particles.

- *Test particle* whose state is ideally targeted by a hypothetical observer;
- *Candidate particle*, with velocity v_h and activity u_p. It is likely to change its current state to that of the test particle as a consequence of an interaction;
- *Field particle*, with velocity v_k and activity u_q. It is a generic particle of the system interacting with the candidate particle.

The test particle loses its state after the interaction.
The encounters among the vehicles are described in an essentially stochastic way, introducing the probability that a velocity transition occurs after an interaction between the candidate vehicle and the field vehicle located in front of it. We point out that such interactions are nonlinearly additive. Indeed, the outcome depends not only on the state of the two interacting vehicles, but also, as we will see in the following, on the state of all the other vehicles in the surrounding domain. Vehicles do not interact mechanically, they simply *see* each other and adjust their velocity

according to the behavioral rules coded in the transition probability density. The following *evolution equation* yield the overall description of the dynamics

$$\begin{aligned}\frac{d}{dt} f_{ir}(t) &= Q_{ir}\left[\mathbf{f}\right](t) \\ &= \sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \left[\eta_{hk}\left[\mathbf{f}\right](u_p, u_q) \mathscr{B}_{hk}^{i}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q) f_{hp}(t) f_{kq}(t)\right] \\ &\quad - f_{ir}(t) \sum_{k=1}^{n} \sum_{q=1}^{m} \eta_{ik}\left[\mathbf{f}\right](u_r, u_q) f_{kq}(t)\,, \end{aligned} \tag{2.31}$$

$$\forall i = 1, \ldots, n; \quad r = 1, \ldots, m\,,$$

where $\mathbf{f}$ is the set of all the probability distributions and

- $\eta_{hk}\left[\mathbf{f}\right](u_p, u_q)$ is the *encounter rate*, which gives the number of interactions between a candidate vehicle with velocity v_h and activity u_p and a field one with velocity v_k and activity u_q;
- $\mathscr{B}_{hk}^{i}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q) = \mathscr{B}_{hk}^{i}(r)$ is the *transition probability density* that a candidate vehicle adjusts its velocity to v_i after an interaction with a field vehicle.
  Accordingly, it must fulfill the following requirements:

$$\mathscr{B}_{hk}^{i}[\mathbf{f}] \geq 0, \qquad \sum_{i=1}^{n} \sum_{r=1}^{m} \mathscr{B}_{hk}^{i}[\mathbf{f}] = 1,$$
$$\forall h, k = 1, \ldots, n\,; \quad \forall p, q = 1, \ldots, m\,, \quad \text{for all } \mathbf{f}.$$

The transition probability density

The transition probability density $\mathscr{B}_{hk}^{i}(r)$ models the microscopic interactions among the vehicles. Here we not only consider the probability that a candidate particle changes its velocity after an interaction [38], but also that it changes its driving ability (activity). In the modeling of microscopic interactions important roles are played by the density ρ, intended as an indicator of the macroscopic local conditions of the traffic, and by the road conditions. This latter aspect is incorporated in the transition probability density via the parameter $\alpha \in [0, 1]$, whose lowest and highest values are related to bad and good road conditions respectively. Technically, the functional dependence of η_{hk} on $\mathbf{f}$ is achieved via $\rho = \sum_{i=1}^{n} \sum_{r=1}^{m} f_{ir}$; therefore, in the following we explicitly write $\eta[\rho]$ instead of $\eta_{hk}[\mathbf{f}]$. In particular, we consider an encounter rate inversely proportional to the mean free space locally found along the road. Observing that $\rho = 1$ represents the road capacity, we write

$$\eta\,[\rho] = \frac{1}{1-\rho}, \quad \text{with } \rho \in [0,1)\ ;$$

which implies that the local encounter rate increases as the density increases toward its limit threshold fixed by the road capacity.
In our model, let us consider:

- equally spaced velocity grid $I_{\mathbf{v}}$ of the form
$$v_i = \frac{i-1}{n-1}, \quad i = 1, \dots, n;$$
- equally spaced activity grid $I_{\mathbf{u}}$ of the form
$$u_r = \frac{r}{m}, \quad r = 1, \dots, m.$$

Three cases need to be dealt with, corresponding to candidate vehicles h traveling more slowly, or at the same speed, or faster than fields vehicles k.
In all three cases the variation of velocity depends both on the quality of the road α and on the density ρ. The relevant transition probability densities are shown below:

<u>Case I</u>: $\boldsymbol{v_h < v_k}$

If $u_p < u_q$:

$$p \neq m \begin{cases} \mathscr{B}_{hk}^{h}(r=p) & = [1-\alpha(1-\rho)]\,(1-|u_p-u_q|) \\ \mathscr{B}_{hk}^{h}(r=p+1) & = [1-\alpha(1-\rho)]\,|u_p-u_q| \\ \mathscr{B}_{hk}^{h+1}(r=p) & = \alpha(1-\rho)(1-|u_p-u_q|) \\ \mathscr{B}_{hk}^{h+1}(r=p+1) & = \alpha(1-\rho)|u_p-u_q| \\ 0, & otherwise \end{cases}$$

$$p = m \begin{cases} \mathscr{B}_{hk}^{h}(r=m) & = 1-[\alpha(1-\rho)] \\ \mathscr{B}_{hk}^{h+1}(r=m) & = \alpha(1-\rho) \\ 0, & otherwise. \end{cases}$$

In the above case we see that when the distance between the activities $|u_p - u_q|$ increases, then the candidate vehicle tends to increase its activity $u_p \to u_{p+1}$. At

the same time its velocity tends to increase $v_h \to v_{h+1}$ as the road conditions improve and as the density decreases.
In all other cases, the candidate vehicle tends to preserve its own velocity v_h and activity u_p.
If $u_p \geq u_q$:

$$p \neq 1 \begin{cases} \mathscr{B}_{hk}^{h}(r = p-1) & = [1-\alpha(1-\rho)]\,|u_p - u_q| \\ \mathscr{B}_{hk}^{h}(r = p) & = [1-\alpha(1-\rho)]\,(1-|u_p - u_q|) \\ \mathscr{B}_{hk}^{h+1}(r = p-1) & = \alpha(1-\rho)|u_p - u_q| \\ \mathscr{B}_{hk}^{h+1}(r = p) & = \alpha(1-\rho)(1-|u_p - u_q|) \\ 0, & otherwise \end{cases}$$

$$p = 1 \begin{cases} \mathscr{B}_{hk}^{h}(r = m) & = 1-[\alpha(1-\rho)] \\ \mathscr{B}_{hk}^{h+1}(r = m) & = \alpha(1-\rho) \\ 0, & otherwise. \end{cases}$$

In this case we observe the opposite behavior for what concerns the activity variable: as the distance $|u_p - u_q|$ increases the activity of the candidate vehicle tends to decrease $u_p \to u_{p-1}$. We observe instead the same behavior as before for what concerns the velocity: $v_h \to v_{h+1}$ as α increases and ρ decreases. In the limiting cases $p = 1$ and $p = m$ the probability densities only depend on α and ρ.

<u>Case II</u>: $v_h = v_k$

If $u_p < u_q, \quad h \neq 1,\, h \neq n$:

$$p \neq m \begin{cases} \mathscr{B}_{hk}^{h-1}(r = p) & = \alpha\rho(1-|u_p - u_q|) \\ \mathscr{B}_{hk}^{h-1}(r = p+1) & = \alpha\rho|u_p - u_q| \\ \mathscr{B}_{hk}^{h}(r = p) & = (1-\alpha)(1-|u_p - u_q|) \\ \mathscr{B}_{hk}^{h}(r = p+1) & = (1-\alpha)|u_p - u_q| \\ \mathscr{B}_{hk}^{h+1}(r = p) & = \alpha(1-\rho)(1-|u_p - u_q|) \\ \mathscr{B}_{hk}^{h+1}(r = p+1) & = \alpha(1-\rho)|u_p - u_q| \\ 0, & otherwise \end{cases}$$

$$p = m \begin{cases} \mathscr{B}_{hk}^{h-1}(r = m) & = \alpha\rho \\ \mathscr{B}_{hk}^{h}(r = m) & = (1-\alpha) \\ \mathscr{B}_{hk}^{h+1}(r = m) & = \alpha(1-\rho) \\ 0, & otherwise. \end{cases}$$

From the above table we can deduce that as the road conditions improve (α increases) and the density decreases, the velocity of the candidate vehicle tends to increase $v_h \to v_{h+1}$. As for the activity change as before, when the distance $|u_p - u_q|$ increases, the candidate vehicle tends to increase its activity $u_p \to u_{p+1}$, and viceversa.
Along the same lines is possible to discuss the tables corresponding to the limiting cases $h = 1$ and $h = n$ which are shown below.

$h = 1$:

$$p \neq m \begin{cases} \mathscr{B}_{11}^1(r = p) & = [1 - \alpha(1-\rho)]\,(1 - |u_p - u_q|) \\ \mathscr{B}_{11}^1(r = p+1) & = [1 - \alpha(1-\rho)]\,|u_p - u_q| \\ \mathscr{B}_{11}^2(r = p) & = \alpha(1-\rho)(1 - |u_p - u_q|) \\ \mathscr{B}_{11}^2(r = p+1) & = \alpha(1-\rho)|u_p - u_q| \\ 0, & otherwise \end{cases}$$

$$p = m \begin{cases} \mathscr{B}_{11}^1(r = m) & = 1 - [\alpha(1-\rho)] \\ \mathscr{B}_{11}^2(r = m) & = \alpha(1-\rho) \\ 0, & otherwise, \end{cases}$$

$h = n$:

$$p \neq m \begin{cases} \mathscr{B}_{nn}^{n-1}(r = p) & = \alpha\rho(1 - |u_p - u_q|) \\ \mathscr{B}_{nn}^{n-1}(r = p+1) & = \alpha\rho|u_p - u_q| \\ \mathscr{B}_{nn}^{n}(r = p) & = (1 - \alpha\rho)(1 - |u_p - u_q|) \\ \mathscr{B}_{nn}^{n}(r = p+1) & = (1 - \alpha\rho)|u_p - u_q| \\ 0, & otherwise \end{cases}$$

$$p = m \begin{cases} \mathscr{B}_{11}^1(r = m) & = \alpha\rho \\ \mathscr{B}_{11}^2(r = m) & = 1 - \alpha\rho \\ 0, & otherwise. \end{cases}$$

In the limiting case $p = m$ the probability densities only depend on α and ρ.
If $u_p \geq u_q$ the probability densities $\mathscr{B}_{hk}^i(r)$ depend also on the activity of the field vehicle:

$h \neq 1$, $h \neq n$:

$$p \neq 1 \begin{cases} \mathscr{B}_{hk}^{h-1}(r = p-1) & = \alpha\rho u_q |u_p - u_q| \\ \mathscr{B}_{hk}^{h-1}(r = p) & = \alpha\rho u_q (1 - |u_p - u_q|) \\ \mathscr{B}_{hk}^{h}(r = p-1) & = (1-\alpha) u_q |u_p - u_q| \\ \mathscr{B}_{hk}^{h}(r = p) & = (1-\alpha) u_q (1 - |u_p - u_q|) \\ \mathscr{B}_{hk}^{h+1}(r = p-1) & = \alpha(1-\rho) u_q |u_p - u_q| \\ \mathscr{B}_{hk}^{h+1}(r = p) & = \alpha(1-\rho) u_q (1 - |u_p - u_q|) \\ 0, & otherwise \end{cases}$$

$$p = 1 \begin{cases} \mathscr{B}_{hk}^{h-1}(r = 1) & = \alpha\rho u_q \\ \mathscr{B}_{hk}^{h}(r = 1) & = 1 - \alpha u_q \\ \mathscr{B}_{hk}^{h+1}(r = 1) & = \alpha(1-\rho) u_q \\ 0, & otherwise. \end{cases}$$

$h = 1:$

$$p \neq 1 \begin{cases} \mathscr{B}_{11}^{1}(r = p-1) & = [1 - \alpha(1-\rho)]\, u_q |u_p - u_q| \\ \mathscr{B}_{11}^{1}(r = p) & = [1 - \alpha(1-\rho)]\, u_q (1 - |u_p - u_q|) \\ \mathscr{B}_{11}^{2}(r = p-1) & = \alpha(1-\rho) u_q |u_p - u_q| \\ \mathscr{B}_{11}^{2}(r = p) & = \alpha(1-\rho) u_q (1 - |u_p - u_q|) \\ 0, & otherwise \end{cases}$$

$$p = 1 \begin{cases} \mathscr{B}_{11}^{1}(r = 1) & = 1 - [\alpha(1-\rho) u_q] \\ \mathscr{B}_{11}^{2}(r = 1) & = \alpha(1-\rho) u_q \\ 0, & otherwise, \end{cases}$$

$h = n:$

$$p \neq 1 \begin{cases} \mathscr{B}_{nn}^{n-1}(r = p-1) & = \alpha\rho u_q |u_p - u_q| \\ \mathscr{B}_{nn}^{n-1}(r = p) & = \alpha\rho u_q (1 - |u_p - u_q|) \\ \mathscr{B}_{nn}^{n}(r = p-1) & = (1-\alpha\rho) u_q |u_p - u_q| \\ \mathscr{B}_{nn}^{n}(r = p) & = (1-\alpha\rho) u_q (1 - |u_p - u_q|) \\ 0, & otherwise \end{cases}$$

$$p = 1 \begin{cases} \mathscr{B}_{11}^{1}(r = 1) & = \alpha\rho u_q \\ \mathscr{B}_{11}^{2}(r = 1) & = 1 - \alpha\rho u_q \\ 0, & otherwise. \end{cases}$$

The above table shows that as the distance $|u_p - u_q|$ increases, the activity of the candidate vehicle tends to decrease $u_p \to u_{p-1}$. For what concerns the velocity, instead, as α increases and ρ decreases, $v_h \to v_{h+1}$. In the limiting case $p = 1$ the probability densities not only depend on α and ρ, but also on the activity of the field vehicle u_q.

<u>Case III</u>: $v_h > v_k$

If $u_p < u_q$:

$$p \neq m \begin{cases} \mathscr{B}^h_{hk}(r = p) & = \alpha(1-\rho)(1 - |u_p - u_q|) \\ \mathscr{B}^h_{hk}(r = p+1) & = \alpha(1-\rho)|u_p - u_q| \\ \mathscr{B}^k_{hk}(r = p) & = [1 - \alpha(1-\rho)]\,(1 - |u_p - u_q|) \\ \mathscr{B}^k_{hk}(r = p+1) & = [1 - \alpha(1-\rho)]\,|u_p - u_q| \\ 0, & otherwise \end{cases}$$

$$p = m \begin{cases} \mathscr{B}^h_{hk}(r = m) & = \alpha(1-\rho) \\ \mathscr{B}^k_{hk}(r = m) & = 1 - [\alpha(1-\rho)] \\ 0, & otherwise. \end{cases}$$

If $u_p \geq u_q$ the variation of velocity depends also on the activity of the field vehicle:

$$p \neq 1 \begin{cases} \mathscr{B}^h_{hk}(r = p-1) & = \alpha(1-\rho)u_q|u_p - u_q| \\ \mathscr{B}^h_{hk}(r = p) & = \alpha(1-\rho)u_q(1 - |u_p - u_q|) \\ \mathscr{B}^k_{hk}(r = p-1) & = [1 - \alpha(1-\rho)u_q]\,|u_p - u_q| \\ \mathscr{B}^k_{hk}(r = p) & = [1 - \alpha(1-\rho)u_q]\,(1 - |u_p - u_q|) \\ 0, & otherwise \end{cases}$$

$$p = 1 \begin{cases} \mathscr{B}^h_{hk}(r = 1) & = \alpha(1-\rho)u_q \\ \mathscr{B}^k_{hk}(r = 1) & = 1 - [\alpha(1-\rho)u_q] \\ 0, & otherwise. \end{cases}$$

The above transition probability densities show the same behavior as in Case I for what concerns the activity change. Indeed when the distance between the activities $|u_p - u_q|$ increases, then the candidate vehicle tends to increase its activity $u_p \to u_{p+1}$, and viceversa. As for the velocity change instead, the candidate vehicle tends to uniform its velocity to v_k as the road conditions get worse (α decreases) and the density ρ increases. In the limiting cases $p = 1$ and $p = m$ we refer to Case II.

2.3.3 Qualitative analysis

In this Subsection the initial value (I.V.) problem for Eq.(2.31) is considered. It is shown that the solution of such I.V. problem exists is unique and is a positive, regular function of time, of class $C^1([0,T])$.
We start with

$$\begin{cases} \dfrac{d}{dt} f_{ir}(t) = Q_{ir}\left[\mathbf{f}\right](t), \qquad i = 1, \ldots, n; \quad r = 1, \ldots, m, \\ f_{ir}(0) = f_i(0, u_r), \end{cases} \tag{2.32}$$

where

$$\frac{d}{dt} f_{ir}(t) = Q_{ir}\left[\mathbf{f}\right](t) = \eta(\rho) \left[\sum_{h,k=1}^{n} \sum_{p,q=1}^{m} (\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q) \right.$$
$$\left. \times f_{hp}(t) f_{kq}(t) - f_{ir}(t) \sum_{k=1}^{4} \sum_{q=1}^{m} f_{kq}(t) \right]. \tag{2.33}$$

We introduce the space:

$$X = \left\{ f_i : [0,T] \to \mathbb{R},\ f_i \in C^1([0,T]), i = 1, \ldots, n,\ T > 0 \right\}$$

equipped with the norm:

$$\|f_i\|_X = \sum_{r=1}^{m} |f_{ir}(t)|. \tag{2.34}$$

Moreover, we introduce the space $\mathbf{X} = X^n$ equipped with the norm:

$$\|\mathbf{f}\|_{\mathbf{X}} = \sum_{i=1}^{n} \|f_i(t)\|_X, \tag{2.35}$$

and set:

$$\mathbf{X}_+ = \left\{ \mathbf{f} \in \mathbf{X} \mid f_i \geq 0, i = 1, \ldots, n \right\} .$$

The following theorem states a result of local existence and uniqueness for the solution of the I.V. problem (2.32).

Theorem 2.3.1. *Consider the I.V. problem (2.32) with* $\mathbf{f}_0 = \{f_1(0,u), \ldots, f_n(0,u)\} \in \mathbf{X}_+$. *Assume that*

$$\eta(\rho) \geq 0, \quad \mathscr{B}^i_{hk}(r) \geq 0, \quad \sum_{i=1}^{n} \sum_{r=1}^{m} \mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q) = 1 \quad \forall \mathbf{f}. \tag{2.36}$$

holds, together with the following hypotheses:

- *The encounter rate $\eta(\rho)$ satisfies the following condition:*

$$\eta(\rho) \leq C,$$

$\forall \mathbf{f}, \boldsymbol{g} \in \mathbf{X}$ the probability $\mathscr{B}^i_{hk}(r)$ and the encounter rate η^{pq}_{hk} are Lipschitz continuous in X, that is, $\forall\ p, q \in \{1, \ldots, m\}$ it results
$$\sum_{h,k,i=1}^{n} \sum_{r=1}^{m} \mid \mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r | u_p, u_q) - \mathscr{B}^i_{hk}\left[\mathbf{g}\right](u_p \to u_r | u_p, u_q) \mid$$
$$\leq L_1 \|\mathbf{f} - \mathbf{g}\|_{\mathbf{X}},$$
with L_1 a positive constant.

Then, there exist $T > 0$ and a unique solution $\mathbf{f}(t)$ in $\mathbf{X}$ for the I.V. problem (2.32) on the time interval $[0, T]$. Moreover $\mathbf{f}(t) \in \mathbf{X}_+$, $t \in [0, T]$.

Proof. We start observing that, since the interactions are assumed number conservative, see (2.36), it results that:

$$\frac{d}{dt} \sum_{i=1}^{n} \sum_{r=1}^{m} f_{ir}(t) = 0\,,$$

which implies:

$$\|\mathbf{f}(t)\|_{\mathbf{X}} = \|\mathbf{f}(0)\|_{\mathbf{X}}, \text{ for any } t \geq 0. \tag{2.37}$$

Therefore the solution of (2.32), if it exists, remains bounded in $\mathbf{X}$ for any time $t \geq 0$. The latter observation assures that the operator $Q_i\left[\mathbf{f}\right](t)$ in the right hand side of (2.32) is a closed map in $\mathbf{X}$.
Let us now prove that $Q_i\left[\mathbf{f}\right](t)$ is Lipschitz continuous in $\mathbf{X}$, i.e. given $\|\mathbf{f}\|_{\mathbf{X}}$ and $\|\mathbf{g}\|_{\mathbf{X}} \leq M$ it follows that:

$$\|Q_i\left[\mathbf{f}\right](t) - Q_i\left[\mathbf{g}\right](t)\|_{\mathbf{X}} \leq L \|\mathbf{f} - \mathbf{g}\|_{\mathbf{X}} \tag{2.38}$$

with L a positive constant depending on M. Indeed, when (2.33) is used together with (2.34) and (2.35), for the right hand side of (2.38) we can write:

$$\eta(\rho) \left\{ \sum_{i=1}^{n} \sum_{r=1}^{m} \left| \left[\sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q) f_{hp}(t) f_{kq}(t) \right.\right.\right.$$
$$\left. - f_{ir} \sum_{k=1}^{n} \sum_{q=1}^{m} f_{kq}(t) \right]$$
$$\left.\left. - \left[\sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \mathscr{B}^i_{hk}\left[\mathbf{g}\right](u_p \to u_r \mid u_p, u_q) g_{hp}(t) g_{kq}(t) - g_{ir} \sum_{k=1}^{n} \sum_{q=1}^{m} g_{kq}(t) \right] \right| \right\}$$

$$\leq \eta(\rho)\left\{\sum_{i=1}^{n}\sum_{r=1}^{m}\left\{\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)\left[f_{hp}(t)f_{kq}(t)\right.\right.\right.\right.$$

$$\left. -g_{hp}(t)g_{kq}(t)\right] + g_{hp}(t)g_{kq}(t)\left[\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)\right.$$

$$\left.\left.\left.\left. -\mathscr{B}^i_{hk}\left[\mathbf{g}\right](u_p \to u_r \mid u_p, u_q)\right]\right| + \sum_{k=1}^{n}\sum_{q=1}^{m}\left|\left[f_{ir}(t)f_{kq}(t) - g_{ir}(t)g_{kq}(t)\right]\right|\right\}\right\}$$

$$\leq \eta(\rho)\left\{\sum_{i=1}^{n}\sum_{r=1}^{m}\left\{\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)f_{hp}(t)\left[f_{kq}(t) - g_{kq}(t)\right]\right|\right.\right.$$

$$+ \sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)g_{kq}(t)\left[f_{hp}(t) - g_{hp}(t)\right]\right|$$

$$+ \sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\left|g_{hp}(t)g_{kq}(t)\left[\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)\right.\right.$$

$$\left.\left. -\mathscr{B}^i_{hk}\left[\mathbf{g}\right](u_p \to u_r \mid u_p, u_q)\right]\right|$$

$$\left.\left. + \sum_{k=1}^{n}\sum_{q=1}^{m}\left|f_{ir}(t)\left[f_{kq} - g_{kq}\right]\right| + \sum_{k=1}^{n}\sum_{q=1}^{m}\left|g_{kq}(t)\left[f_{ir} - g_{ir}\right]\right|\right\}\right\}$$

$$\leq 2m^3n^3CM\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}} + m^2M^2CL_1\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}} + 2n^2m^2CM\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}},$$

$$\leq L\|\mathbf{f}-\mathbf{g}\|_{\mathbf{X}}$$

that proves (2.38). Then, the existence of a unique solution $\mathbf{f}(t)$ in $\mathbf{X}$, local in time, to (2.32) follows. Non negativity of such a solution is easily obtained observing that the components $f_{ir}(t)$ of the solution satisfy the condition:

$$f_{ir} \geq 0 \quad \forall i = 1, \ldots, n \quad \text{and} \quad \forall r = 1, \ldots, m \tag{2.39}$$

when $\mathbf{f}(0) \in \mathbf{X}_+$. We set:

$$R^i(f,f)(t) = \eta(\rho)\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}\mathscr{B}^i_{hk}\left[\mathbf{f}\right](u_p \to u_r \mid u_p, u_q)f_{hp}(t)f_{kq}(t),$$

$$S(f)(t) = \eta(\rho)\sum_{h,k=1}^{n}\sum_{p,q=1}^{m}f_{kq}(t).$$

Equation (2.33) can be rewritten as

$$\frac{d}{dt}f_{ir}(t) + f_{ir}(t)S(f)(t) = R^i(f,f)(t). \tag{2.40}$$

Now we call

$$\lambda(t) = \int_0^t S(f)(t^{'})dt^{'}.$$

If f_{ir} is solution of (2.40), it then follows

$$\frac{d}{dt}(\exp(\lambda(t))f_{ir}(t)) = \exp(\lambda(t))R^i(f,f)(t)$$

which implies

$$f_{ir}(t) = \exp(-\lambda(t))f_{ir}(0) + \int_0^t \left[\exp(\lambda(t^{'}))R^i(f,f)(t^{'})\right] dt^{'}. \tag{2.41}$$

The relation (2.41) allows us to conclude that, given $\mathbf{f}(0) \in \mathbf{X}_+$ and the positivity of the integral function, the function $f_{ir}(t)$ satisfies the condition of non-negativity (2.39) in its domain of existence. Moreover, when (2.39) is used together with (2.37), we obtain that the solution to (2.32) is uniformly bounded on any compact time interval $[0,T]$, $T > 0$. This latter observation leads immediately to the following result of global existence and uniqueness of the solution in $\mathbf{X}_+$

Theorem 2.3.2. *Consider the I.V. problem (2.32) under the assumptions of the theorem 2.3.1. Then the solution $\mathbf{f}(t)$ exists and is unique for any finite time $t \geq 0$.*

2.3.4 Simulations

Numerical simulations of Eq.(2.31) have been carried out in order to analyze the behavior of the average velocity $\overline{v}$, the flux q and the velocity variance Δ as functions of the density ρ. Time integration has been performed via a standard fourth-order Runge-Kutta scheme, using a uniform velocity grid $I_v = \{v_i\}_{i=1}^5$ where $v_1 = 0, \ldots, v_5 = 1$ and a uniform activity grid $I_u = \{u_r\}_{r=1}^5$ where $u_1 = 1/5, \ldots, u_5 = 1$.
Figs.2.5, 2.6 show the diagrams of the average velocity, of the flux and the velocity variance as functions of the density, for three different values of the road conditions. In particular Fig.2.5 shows the behavior of driver-vehicle pairs with average driving ability, Fig.2.6 shows instead the behavior of pairs with maximum driving ability. Considering in particular the cases of intermediate and good road conditions ($\alpha = 0.7$ and $\alpha = 1$, respectively) Fig.2.5 and Fig.2.6 indicate that for low density the flux q is almost linearly increasing, in agreement with

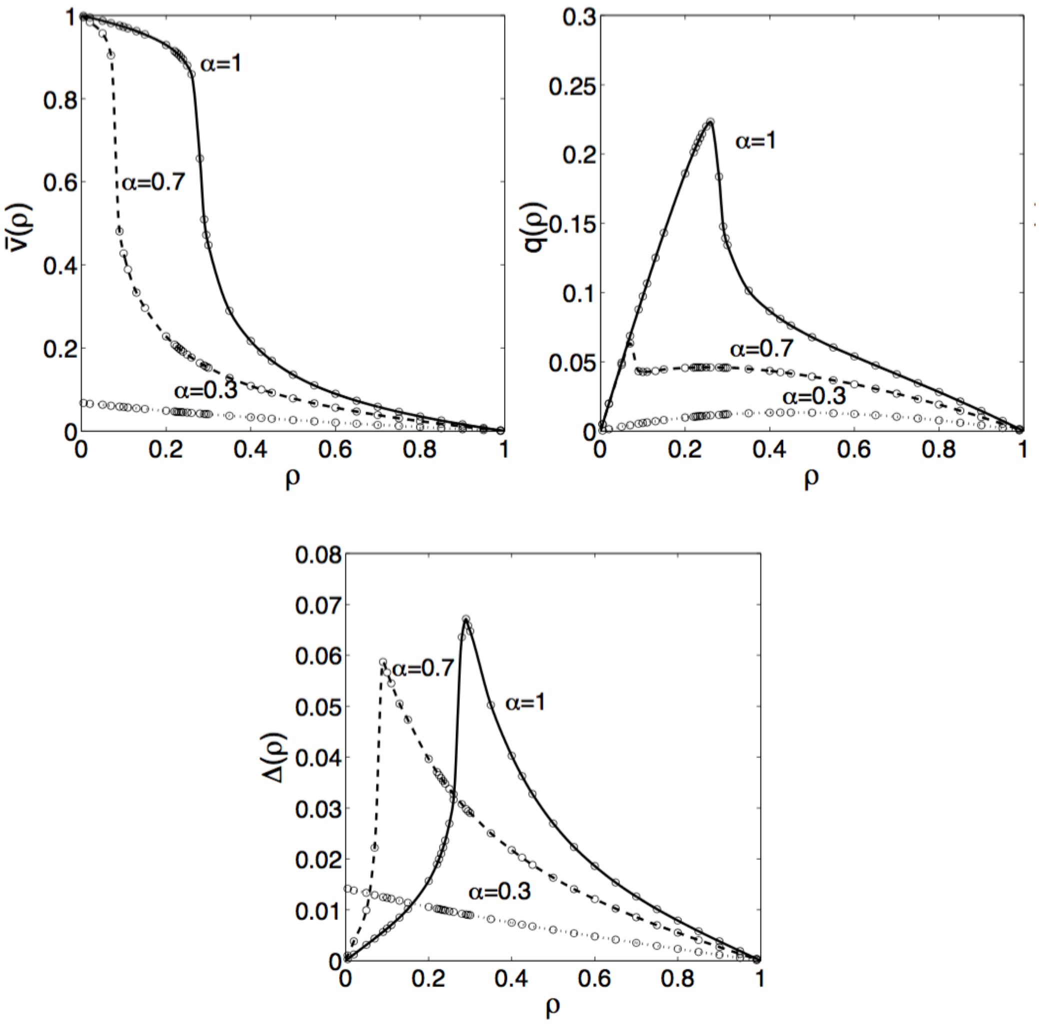

Figure 2.5: Diagrams for the average velocity (left), the macroscopic flux (right) and the velocity variance (bottom) as functions of the macroscopic density, obtained under various road conditions $\alpha = 0.3$, $\alpha = 0.7$, $\alpha = 1$ respectively. In this case the activity of the particles is uniformly distributed over each class.

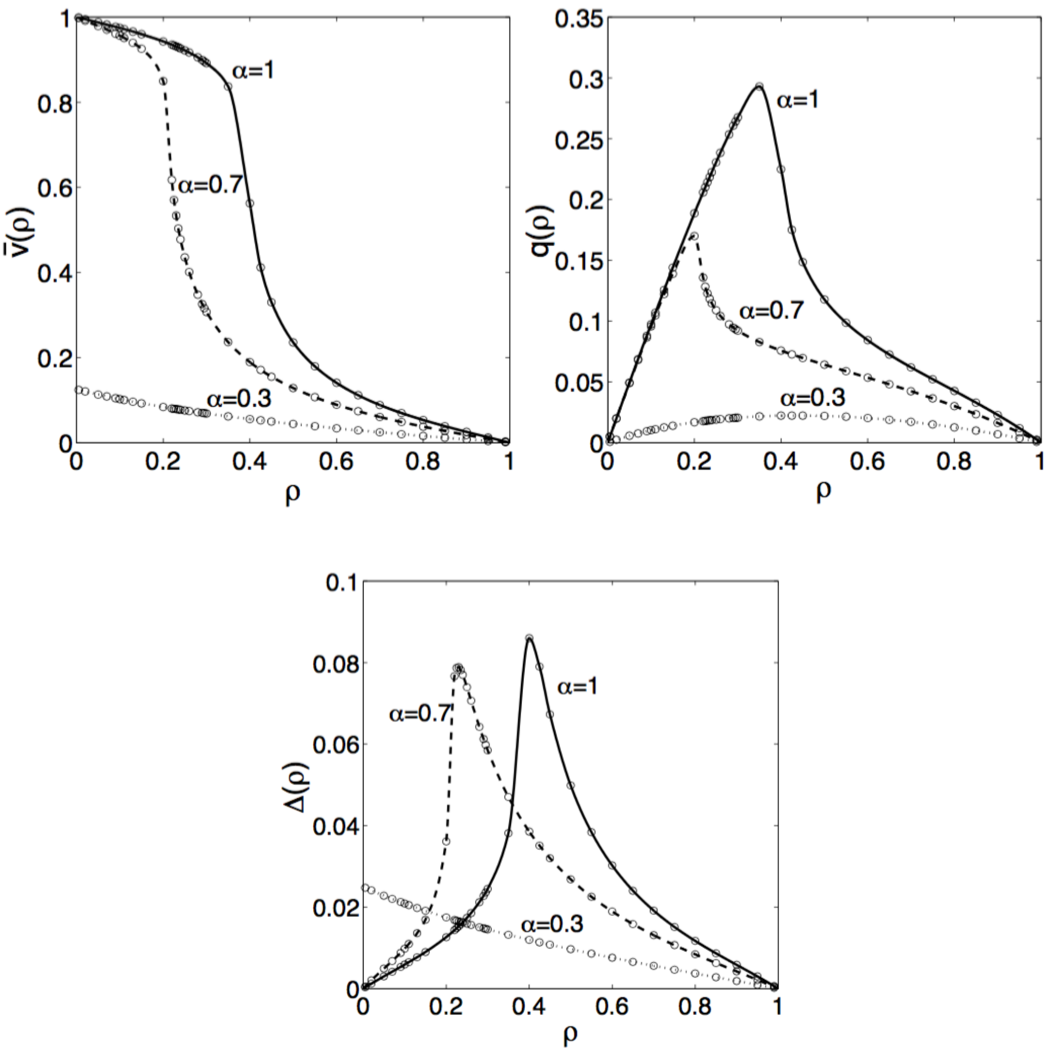

Figure 2.6: Diagrams for the average velocity (left), the macroscopic flux (right) and the velocity variance (bottom) as functions of the macroscopic density, obtained under various road conditions $\alpha = 0.3$, $\alpha = 0.7$, $\alpha = 1$ respectively. In this case the activity of the all particles is $u_5 = 1$.

experimental observations reported by Kerner [54] under free flow conditions. The subsequent flux behavior is then nonlinearly decreasing to zero, which suggests a critical change in the traffic regime for high density. Following [55], we define the congested traffic regime as the one characterized by average vehicle velocity lower then the minimum possible average velocity corresponding to free flow. In this respect the behaviors shown in Fig.2.5 and Fig.2.6 describe the well known phase transition from free to congested traffic flow, taking place once the vehicle density increases exceeding a critical value.

Such transition was mathematically studied in [26]. The ability of the model to reproduce qualitatively the observed traffic phases, is confirmed when we note that the maximum of the velocity variance Δ is located in correspondence of a density value very close to the critical one for which the change in the flux behavior is observed. The average velocity $\overline{v}$ in turn, for low densities takes values very close to the maximum allowed one, then drastically decreases approaching zero once the density exceeds the critical threshold value.

A comparison between Fig.2.5 and Fig.2.6 indicates that the decrease of the average velocity as the density increases is much faster for average driving ability (Fig.2.5) than for maximum ability (Fig.2.6). Similar considerations of course, apply to the comparison between the corresponding two diagrams of the flux as function of the density. Moreover, looking at the data reported in Fig.2.6 we can obtain an estimate of the critical density in the range $\rho_c \in [0.15, 0.2]$ for the case of intermediate road conditions ($\alpha = 0.7$) and maximum class of activity ($u_5 = 1$). This estimate is in agreement with experimental measurements of traffic flow made on the Venezia-Mestre highway [15].

In Fig.2.7 we report the initial and asymptotic configurations of the vehicle distribution in the velocity classes for three different values of the density. We observe that in the three cases taken into account, the initial distribution of the vehicles over the classes of velocity is uniform, but asymptotically the concentration of the vehicles N_i is different for low, intermediate and hight density. In particular, if $\rho = 0.6$ (the density is higher than the critical value $\rho_c = 0.28$) the highest concentration of the vehicles is in the lowest velocity classes ($N_1 > N_2 > N_3$). If the density is close to the critical value ($\rho = 0.29$) the concentration of the vehicles is in the central class (normal distribution type); if $\rho = 0.2$ the vehicles end up in the highest velocity classes ($N_5 > N_4 > N_3$).

To explain the role of the activity, Fig.2.8 shows the initial and asymptotic configurations of the distribution of the vehicles in the velocity/activity classes for $\rho = 0.6$ in the case of a uniform initial distribution. In the asymptotic configurations the vehicles are all in the intermediate activity class and this means that the drivers have the ability to adapt to the congested traffic conditions.

Fig.2.9 shows initial and asymptotic configurations of the vehicle activity, respec-

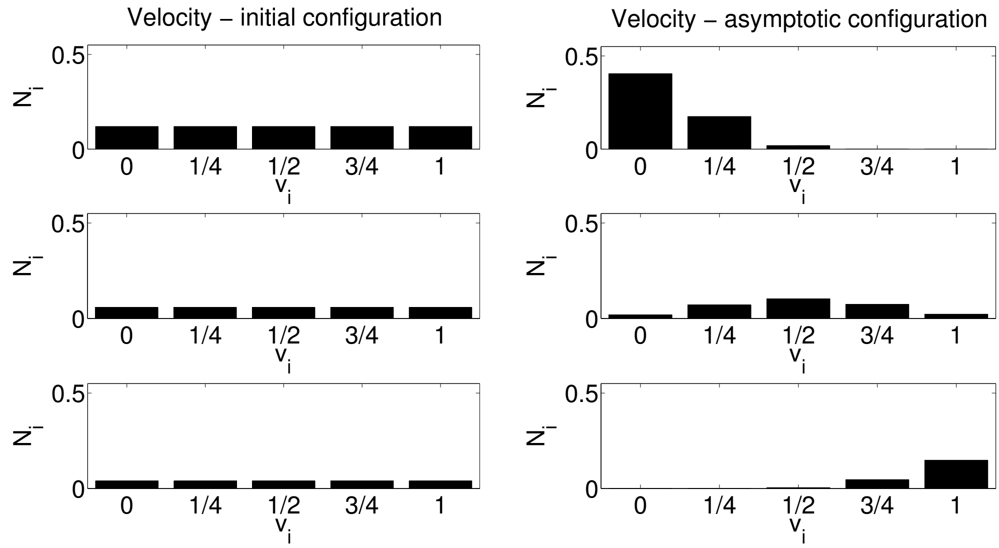

Figure 2.7: The asymptotic configuration of the velocity is shown for three possible values of the density (from bottom to top: $\rho = 0.2$, $\rho = 0.29$, $\rho = 0.6$) and $\alpha = 1$.

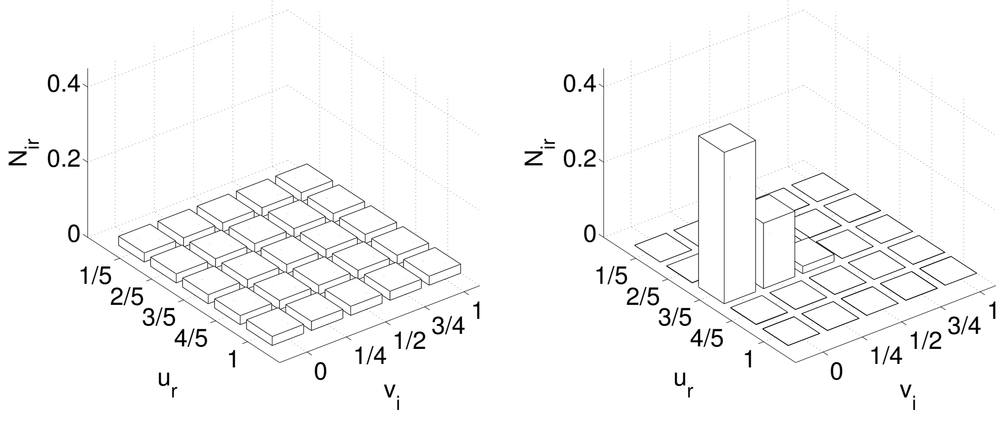

Figure 2.8: On the left the initial configuration and on the right the asymptotic configuration of the vehicles in the velocity/activity class, is shown for density $\rho = 0.6$ and good road conditions $\alpha = 1$.

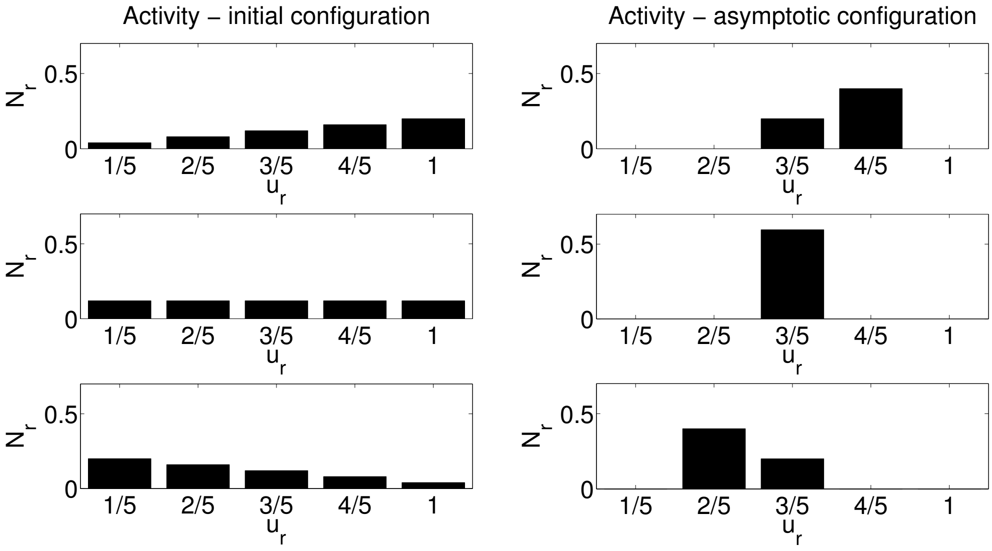

Figure 2.9: The asymptotic configuration of the activity is shown for the value of the density $\rho = 0.6$ and $\alpha = 1$.

tively. In this case we consider only one value of the density ($\rho = 0.6$) because the activity doesn't depend on ρ. The results show that asymptotically, the driving abilities tend to uniform to each other, converging in a single intermediate final class, in the case of a uniform initial distribution.

Chapter 3

Free boundary value problems

Initial Boundary Value Problems (IBV) for nonlinear partial differential equations (PDEs) have been the object of several studies in the past. Indeed such problems have great relevance both from a mathematical point of view and from the point of view of applications.
In the following, two main classes of nonlinear PDEs are identified, according to their integrability properties.
The first class is the class of S-integrable equations. Such equations are integrable via the spectral method also called inverse scattering method [3]. Important nonlinear models belonging to this class are:

- **the nonlinear Schrödinger equation**

$$i\psi_t + \psi_{xx} \left|\psi\right|^2 \psi = 0, \qquad \psi \equiv \psi\left(x, t\right),$$

whose principal application is the propagation of light in nonlinear optical fibers;

- **the Korteweg-de Vries equation**

$$\psi_t + 6\psi\psi_x + \psi_{xxx} = 0, \qquad \psi \equiv \psi\left(x, t\right),$$

originally used to describe the propagation of shallow water waves and

- **the Sine-Gordon equation**

$$\psi_{tt} - \psi_{xx} + \sin\psi = 0, \qquad \psi \equiv \psi\left(x, t\right),$$

which has several applications in solid state physics.
The second class is the class of C-integrable equations. Such equations are linearizable through an appropriate change of variables. Important examples in this class are:

- **the Burgers equation**

$$\psi_t + \psi\psi_x = \nu\psi_{xx} \qquad \psi \equiv \psi(x,t),$$

which is a fundamental model for turbulence phenomena and nonlinear dissipative phenomena;

- **the nonlinear diffusion-convection equation**

$$\psi_t = \psi^2 (\psi_{xx} - \psi_x) \qquad \psi \equiv \psi(x,t), \tag{3.1}$$

suitable to investigate the flow of two immiscible fluids through porous media. It is worth noticing that, according to [22], S-integrability is a weaker requirement than C-integrability i.e. C-integrable equations can be considered to be S-integrable equation but not viceversa. For example, the Nonlinear Schrödinger equation in $1 + 1$ dimensions is S-integrable but not C-integrable.
It is the object of this chapter to discuss Free Boundary Problems (FBP) for the nonlinear diffusion convection equation (3.1).
FBPs arise in several physical and biological applications. Indeed they occur in different contexts, e.g. surface dynamics in water waves, the internal evolution of the boundary between immiscible liquids, the motion of the boundary between two phases (Stefan problems) [41, 47]. In general, flow through porous media is an important source of FBP, frequently in connection with the filtration phenomena that occur in nature [29].
From the mathematical point of view, FBP are boundary value problems defined over a domain with a moving boundary [34, 35, 43]. The motion of such a boundary is unknown and has to be determined as part of the solution [45, 66].
The underlying difficulty in most of the mentioned FBP is that they require one to solve a nonlinear system. In some cases, for nonlinear evolution equations of diffusive type, it was possible to prove existence and uniqueness of solutions (at least for short time) and also to obtain some special explicit solutions such as an exact travelling wave in the case of the Burgers equation [1].
In the following Section we review the result obtained by Burini and De Lillo in [17] where an inverse IBV problem on a moving boundary for (3.1) is studied. Section 3.2 is instead devoted to the presentation of new results [19] (obtained by Burini, De Lillo and myself). We consider a model of drug propagation in the arterial tissues after the drug has been released by a stent expansion. Such model is described through a FBP on a finite interval for equation (3.1).

3.1 An inverse problem

Let us consider an IBV problem associated with the nonlinear diffusion-convection equation (3.1), over the domain $-\infty < x < s(t)$, $t > 0$, where $s(t)$ is known

$(s(0) = b > 0)$, with the initial datum

$$\vartheta(x, 0) = \vartheta_0(x) > 0, \qquad -\infty < x < b$$

$$\vartheta_0(b) = \beta_2 > 0$$

and boundary conditions:

$$\vartheta(s(t), t) = f(t),\ t > 0, \qquad f(0) = \beta_2 \tag{3.2a}$$

$$\vartheta(-\infty, t) = \beta_1, \qquad \vartheta_x(-\infty, t) = 0, \qquad t \geq 0. \tag{3.2b}$$

In the present case we assume β_1 and β_2 to be positive constants with $\beta_1 > \beta_2$ and the initial datum $\vartheta_0(x)$ to be a regular, bounded function of its argument $(\beta_2 \leq |\vartheta_0(x)| \leq \beta_1)$. The moving boundary $s(t)$ is assumed to be a continuously differentiable function of time, with $\dot{s}(t)$ bounded $(|\dot{s}(t)| \leq \alpha\,,\ \alpha$ a positive constant). In (3.2a), $f(t)$ is the Dirichlet datum defined as a given, integrable function of time.

The aim is to determine the unknown Neumann datum at the boundary, $g\,(t)$:

$$\vartheta_x(s(t), t) = g(t),\ t \geq 0. \tag{3.2c}$$

The Neumann datum has to be reconstructed from the knowledge of the Dirichlet datum $f\,(t)$ (Dirichlet-to-Neumann map).

This problem is a typical inverse moving boundary problem where the unknown boundary datum $g(t)$ has to be determined in order to be suitable with the motion of the boundary $s(t)$.

We start our analysis by introducing a change of the independent variable called hodograph transform

$$\vartheta(x, t) = \psi(z, t), \quad z \equiv z(x, t) \tag{3.3a}$$

and

$$z_x = \frac{1}{\vartheta}, \qquad z_t = \vartheta - \vartheta_x. \tag{3.3b}$$

Under this change of variables, the equation (3.1) becomes:

$$\psi_t = \psi_{zz} - 2\psi_z\psi \quad -\infty < z < \overline{z}(t), \tag{3.4}$$

which is the Burgers equation for the dependent variable $\psi\,(z, t)$ characterized by the initial datum

$$\psi(z, 0) = \psi(z_0) = \vartheta_0(x) \tag{3.5a}$$

where

$$z_0 \equiv z_0(x) = \int_0^x \frac{1}{\vartheta_0(x')}\, dx'. \tag{3.5b}$$

In the virtue of (3.3b) the moving boundary $\overline{z}(t)$, a-priori unknown, takes the form

$$\overline{z}(t) \equiv z(s(t),t) = \int_0^t [\vartheta(s(\tau),\tau) - \vartheta_x(s(\tau),\tau) + \frac{\dot{s}(\tau)}{\vartheta(s(\tau),\tau)}]d\tau$$

which, when (3.2a) and (3.2c) are used, becomes:

$$\overline{z}(t) = \int_0^t [f(\tau) - g(\tau) + \frac{\dot{s}(\tau)}{\vartheta(s(\tau),\tau)}]d\tau. \tag{3.6}$$

Moreover the boundary conditions (3.2a) and (3.2b) take the form:

$$\psi(\overline{z}(t),t) = \vartheta(s(t),t) = f(t), \tag{3.7a}$$

$$\psi_z(\overline{z}(t),t) = f(t)g(t), \tag{3.7b}$$

$$\psi(-\infty,t) = \beta_1, \qquad \psi_z(-\infty,t) = 0. \tag{3.7c}$$

The above relations (3.5a),(3.5b) and (3.7a)-(3.7c) imply that the the problem of constructing the Dirichlet-to-Neumann map for the nonlinear diffusion-convection equation (3.1) has now been mapped into a Neumann problem for the Burgers equation (3.4) on a moving boundary $\overline{z}(t)$. The motion of the boundary $\overline{z}(t)$ is unknown and has to be determined as part of the solution.
The approach to solve this problem is the same used in [1] to determine the solution of a Burgers-Stefan problem.
The first step is to introduce the generalized Hopf-Cole transformation

$$\psi(z,t) = \frac{\varphi(z,t)}{\left(C(t) - \int_{\overline{z}(t)}^{z} \varphi(z',t)\, dz'\right)}, \tag{3.8a}$$

$$\varphi(z,t) = C(t)\psi(z,t)exp\left[-\int_{\overline{z}(t)}^{z} \psi(z',t)\, dz'\right] \tag{3.8b}$$

with

$$C(0) = 1. \tag{3.8c}$$

Under the above transformation the Burgers equation (3.4) is mapped into the linear heat equation

$$\varphi_t = \varphi_{zz}, \tag{3.9}$$

with the compatibility condition

$$\dot{C}(t) = -\varphi_z(\overline{z}(t),t). \tag{3.10}$$

Moreover, from (3.5a) and (3.7a),(3.7b) equation (3.9) is characterized by the initial datum

$$\varphi(z,0) = \psi(z_0)exp\left[-\int_0^z \psi(z',0)\,dz'\right] \equiv \varphi_0(z), \tag{3.11}$$

and by the boundary data

$$\varphi_z(\overline{z}(t),t) = C(t)\left[f(t)g(t) - f^2(t)\right] \equiv h(t), \tag{3.12a}$$

$$\varphi(\overline{z}(t),t) = C(t)f(t). \tag{3.12b}$$

The second step is to solve the Neumann problem for equation (3.9) on the domain $-\infty < z < \overline{z}(t)$, with initial datum (3.11) and Neumann boundary datum (3.12a). Through the Laplace Transform

$$\mathcal{L}(\varphi(z,t)) \equiv \widehat{\varphi}(z,s) = \int_0^\infty e^{-st}\varphi(z,t)\,dt,$$

we obtain from (3.9) and (3.11) the equation

$$\hat{\varphi}_{zz} - s\widehat{\varphi} = -\varphi_0(z). \tag{3.13}$$

The boundary condition (3.12a) then becomes

$$\mathcal{L}(\varphi_z(\overline{z}(t),t)) = \int_0^\infty e^{-st}h(t)\,dt = \widehat{\varphi}_z(\overline{z}(t),s) \equiv H(s). \tag{3.14}$$

If (3.13) is solved with the boundary condition (3.14) one has

$$\begin{aligned}\hat{\varphi}(z,s) = {} & \frac{H(s)}{\sqrt{s}}\,e^{-\sqrt{s}(\overline{z}-z)} + \frac{1}{2\sqrt{s}}\,e^{-\sqrt{s}(\overline{z}-z)}\int_{-\infty}^{\overline{z}(0)} e^{-\sqrt{s}(\overline{z}-z')}\varphi_0(z'\,dz' \\ & - \frac{1}{2\sqrt{s}}\left[\int_{-\infty}^{z} e^{-\sqrt{s}(z-z')}\varphi_0(z')\,dz' + \int_z^{\overline{z}(0)} e^{-\sqrt{s}(z'-z)}\varphi_0(z')\,dz'\right]\end{aligned}$$

which, through the inverse Laplace transform, gives the solution of the linear equation (3.9) as

$$\begin{aligned}\varphi(z,t) = {} & \frac{1}{2\sqrt{\pi t}}\int_{-\infty}^{0} e^{-\frac{(z-z')^2}{4t}}\varphi_0(z')\,dz' \\ & - \frac{1}{2\sqrt{\pi t}}\int_{-\infty}^{0} e^{-\frac{(2\overline{z}-(z+z'))^2}{4t}}\varphi_0(z')\,dz' + \frac{1}{\sqrt{\pi}}\int_0^t \frac{e^{-\frac{(\overline{z}-z)^2}{4(t-t')}}}{\sqrt{t-t'}}\,h(t')\,dt'.\end{aligned} \tag{3.15}$$

From Eq.(3.15) we can note that $\varphi(z,t)$ is known once the Neumann datum $h(t)$ of the Burgers equation, is known.
We then introduce the fundamental Kernel of the heat equation

$$K(z-z',t-t') = \frac{1}{2\sqrt{\pi}}\,\frac{1}{\sqrt{t-t'}}\,e^{-\frac{(z-z')^2}{4(t-t')}}. \tag{3.16}$$

By taking the z-derivative of both sides in (3.15) and evaluating it as $z \to \overline{z}(t)$, the result is

$$\begin{aligned} h(t) = -\frac{2\varphi_0(0)\,e^{-\frac{\overline{z}^2}{4t}}}{\sqrt{\pi t}} &+ 4\int_{-\infty}^{0} K(\overline{z}(t)-z',t)\,\varphi_0'(z')\,dz' \\ &+ 4\int_0^t K_z(\overline{z}(t)-\overline{z}(t'),t-t')\,h(t')\,dt'. \end{aligned} \tag{3.17a}$$

where, due to (3.6), (3.7a), (3.10) and (3.12a), we can write

$$\overline{z}(t) = \int_0^t \frac{\dot{s}(t')}{f(t')}\,dt' - \int_0^t \frac{h(t')}{C(t')f(t')}\,dt'. \tag{3.17b}$$

The solution of the Neumann problem for the linear heat equation (3.9) has then been reduced to the solution of the nonlinear integral equation (3.17a), (3.17b). Once existence and uniqueness of the functions $h(t)$ is established for small time, $0 \le t < \sigma$, existence and uniqueness of $\varphi(z,t)$ for $0 \le t < \sigma$ then follows via (3.15). As a consequence, $\psi(z,t)$ via (3.8a), exists and is unique for $0 \le t < \sigma$, together with the solution of the original FBP for the nonlinear diffusion-convection equation (3.1).
Existence and uniqueness of $h(t)$ $(0 \le t < \sigma)$ are established through the following

Theorem 3.1.1. *We denote by S_M the closed sphere $||g_1|| \le M$ $(M > 0)$ in the Banach space of functions $h(t)$ continuous for $0 \le t < \sigma$ with the uniform norm $||h|| = l.u.b.|h(t)|$. On the sphere S_M we define the transformation*

$$w(t) = Th(t),$$

where $Th(t)$ coincides with the right hand side of (3.17a).
Then $h(t) = Th(t)$ exists and is the unique fixed point of T in S_M for $0 \le t < \sigma$.

The detailed proof of the above Theorem is reported in Appendix A.

3.2 A Free Boundary Problem on a Finite Domain in Nonlinear Diffusion

In this Section we formulate and solve a free boundary problem for a nonlinear diffusion convection equation (Rosen - Fokas - Yorstos equation) [44, 67], defined on a finite interval. Such equation describes fluid diffusion with convective effects in porous media and is suitable for the modeling of drug propagation in the arterial tissues, after the drug has been released by a stent expansion. Experimental and numerical studies on the modeling of drug release from arterial stents [60, 61], indeed indicate that the drug filtration process in the arterial wall takes place under the effect of convective and diffusive forces, and is influenced by the porosity of the medium [52, 64]. Moreover, sharp variations of the drug concentration, indicate the presence of nonlinear effects [51].
Such observation motivates the present study, which is based on a nonlinear evolution equation of diffusive type. This aspect constitutes a novelty with respect to previous analysis carried out in the framework of linear diffusive equations.
In the next Subsection we introduce the model and through a hodograph transform we map the FBP for the nonlinear diffusion-convection equation into a FBP for the Burgers equation. In Subsection 3.2.2 we reduce the FBP for the Burgers equation to a system of coupled nonlinear integral equations; existence and uniqueness of the solution for a small interval of time $0 \leq t < \sigma$, are proven in Subsection 3.2.3. Finally, in the last Subsection we show that the problem admits an exact solution corresponding to a travelling wave of the Burgers equation, moving at the same velocity as the two free boundaries of the interval.

3.2.1 The problem

We consider the nonlinear diffusion-convection equation

$$\theta_t = \theta^2 \left(D\theta_{xx} - \theta_x \right), \quad \theta = \theta(x,t), \quad t > 0 \tag{3.18}$$

over the finite interval $x \in [s_0(t), s_1(t)]$, $s_0(0) = 0$, $s_1(0) = L$ with initial datum

$$\theta(x,0) = \theta_0 > 0 \tag{3.19}$$

and boundary conditions

$$\theta(s_0(t), t) = \alpha, \tag{3.20a}$$

$$D\theta_x(s_0(t), t) - \theta(s_0(t), t) = -\dot{s}_0(t), \tag{3.20b}$$

$$\theta(s_1(t), t) = \beta, \tag{3.20c}$$

$$D\theta_x\left(s_1\left(t\right),t\right)-\theta\left(s_1\left(t\right),t\right)=-\dot{s}_1\left(t\right). \tag{3.20d}$$

Equation (3.18) is a well known model for fluid diffusion with convective effects in porous media [44, 67]; one and two-phase free boundary problems were solved for (3.18) and the Dirichlet-to-Neumann map on a moving boundary was recently obtained [17, 36, 37].
In the present case, using dimensionless variables, $\theta\left(x,t\right)$ denotes the concentration of the drug, which is assumed to be in a percolated phase, that propagates in the arterial wall after it has been released by a drug eluting stent; D is the coefficient of diffusivity of the drug in the medium.
Following the literature [52, 60, 61, 64] the initial concentration is assumed to be constant; we also assume the concentration to be constant at the two ends of the interval, with $\alpha>\beta>0$. The constant β could be very small or even zero due to the flux loss during the propagation. On the other hand, the boundary data (3.20b) and (3.20d) are the ones usually associated with free-boundary problems. Indeed, they are flux boundary conditions streaming from energy balance considerations[1, 37]. The functions $s_0\left(t\right)$ and $s_1\left(t\right)$ describe the motion of the free boundaries due to the profile of the fluid drug concentration moving in the arterial tissue. Such functions are unknown and have to be determined together with the solution $\theta\left(x,t\right)$.
In order to solve the Initial/Boundary Value (IBV) problem given by (3.18) with (3.19) and (3.20a)-(3.20d), we start our analysis by introducing the change of independent variables

$$\theta\left(x,t\right)=\psi\left(z,t\right),\quad z=z\left(x,t\right) \tag{3.21a}$$

with

$$\frac{\partial z}{\partial x}=\frac{1}{\theta\left(x,t\right)},\quad \frac{\partial z}{\partial t}=\theta(x,t)-D\theta_x(x,t), \tag{3.21b}$$

whose compatibility $\dfrac{\partial^2 z}{\partial x\partial t}=\dfrac{\partial^2 z}{\partial t\partial x}$ is guaranteed by (3.18).
Under the above tranformation, the IBV problem for Eq.(3.18), specified by condition (3.19) and (3.20a),(3.20b), takes the form:

$$\psi_t=D\psi_{zz}-2\psi\psi_z,\quad z_0\left(t\right)\le z\le z_1\left(t\right), \tag{3.22}$$

which is the Burgers equation for the dependent variable $\psi(z,t)$, with the initial datum

$$\psi\left(z,0\right)\equiv\psi_0\equiv\theta_0 \tag{3.23a}$$

and in the virtue of (3.21b),

$$z_0\left(t\right) = b_0 + \int_0^{s_0(t)} \frac{dx'}{\theta(x',t)}, \quad z_1\left(t\right) = b_1 + \int_0^{s_1(t)} \frac{dx'}{\theta(x',t)}. \tag{3.23b}$$

where b_0 and b_1 are arbitrary positive constants.
Moreover, under the change of variable (3.21a) and (3.21b), the boundary conditions (3.20a) and (3.20b) take the form:

$$\psi\left(z_0\left(t\right), t\right) = \alpha, \tag{3.24a}$$

$$D\psi_z\left(z_0\left(t\right), t\right) = -\alpha\dot{s}_0\left(t\right) + \alpha^2, \tag{3.24b}$$

$$\psi\left(z_1\left(t\right), t\right) = \beta, \tag{3.24c}$$

$$D\psi_z\left(z_1\left(t\right), t\right) = -\beta\dot{s}_1\left(t\right) + \beta^2. \tag{3.24d}$$

The above relations (3.23a),(3.23b) and (3.24a)-(3.24d) imply that the IBV problem for the nonlinear diffusion-convection equation (3.18) has now been mapped into a one-phase FBP for the Burgers equation (3.22) on the finite interval $z \in \left[z_0\left(t\right), z_1\left(t\right)\right]$; the motion of the boundaries $z_0\left(t\right)$ and $z_1\left(t\right)$ is unknown and has to be determined as part of the solution.
It is now expedient to use the Galilean Transformation

$$\begin{cases} z \to z - 2\beta t \\ \psi \to \psi - \beta \end{cases}$$

which leaves (3.22) invariant while changing (3.24a)-(3.24d) into

$$\psi\left(F_0\left(t\right), t\right) = \alpha - \beta, \tag{3.25a}$$

$$D\psi_z\left(F_0\left(t\right), t\right) = -\alpha\dot{s}_0\left(t\right) + \alpha^2, \tag{3.25b}$$

$$\psi\left(F_1\left(t\right), t\right) = 0, \tag{3.25c}$$

$$D\psi_z\left(F_1\left(t\right), t\right) = -\beta\dot{s}_1\left(t\right) + \beta^2, \tag{3.25d}$$

where

$$F_0\left(t\right) = z_0\left(t\right) - 2\beta t, \quad F_1\left(t\right) = z_1\left(t\right) - 2\beta t. \tag{3.25e}$$

In the next Subsection we will reduce the FBP for the Burgers equation (3.22) with boundary conditions (3.25a)-(3.25e) to a system of coupled nonlinear integral equation in one variable (time), which admit a unique solution for small time.

3.2.2 The Linear Heat Equation

Let us now introduce the generalized Hopf-Cole transformation [1, 23]

$$\psi(z,t) = \frac{\varphi(z,t)}{\left(C(t) - \frac{1}{D}\int_{F_1(t)}^{z}\varphi(z',t)\,dz'\right)}, \tag{3.26a}$$

$$\varphi(z,t) = C(t)\,\psi(z,t)\exp\left[-\frac{1}{D}\int_{F_1(t)}^{z}\psi(z',t)\,dz'\right], \tag{3.26b}$$

with the initial condition

$$C(0) = 1. \tag{3.26c}$$

Under the above transformation the Burgers equation (3.22) is mapped into the linear heat equation

$$\varphi_t = D\varphi_{zz} \tag{3.27}$$

with the compatibility condition [18]

$$\dot{C}(t) = -\varphi_z(F_1(t),t). \tag{3.28}$$

Moreover, from (3.23a) and (3.25a)-(3.25d), we obtain the following set of initial and boundary data for eq. (3.27)

$$\varphi_0(z) = \psi_0\exp\left[-\frac{\psi_0}{D}(z - F_1(0))\right], \tag{3.29a}$$

$$\varphi(F_0(t),t) = C(t)(\alpha-\beta)\exp\left[-\frac{1}{D}\int_{F_1(t)}^{F_0(t)}\psi(z'(t))\,dz'\right], \tag{3.29b}$$

$$\varphi(F_1(t),t) = 0, \tag{3.29c}$$

$$D\varphi_z(F_0(t),t) = C(t)\left(2\alpha\beta - \beta^2 - \alpha\dot{s}_0(t)\right)\times\exp\left[-\frac{1}{D}\int_{F_1(t)}^{F_0(t)}\psi(z',t)\,dz'\right], \tag{3.29d}$$

$$D\varphi_z(F_1(t),t) = C(t)\left(-\beta\dot{s}_1(t) + \beta^2\right). \tag{3.29e}$$

We now use (3.28) together with (3.29e) and the initial conditions $s_1(0) = L$, $C_1(0) = 1$; we get

$$C(t) = \exp\frac{\beta}{D}(s_1(t) - \beta t - L), \tag{3.30a}$$

which can be readily inverted as

$$s_1(t) = L + \beta t + \frac{D}{\beta}\ln\left[1 - \int_0^t \varphi_z(F_1(t'),t')\,dt'\right]. \tag{3.30b}$$

Let us now introduce the auxiliary function

$$B(t) = \frac{\varphi(F_0(t), t)}{\psi(F_0(t), t)}, \tag{3.31a}$$

which, due to (3.29b) and (3.26a) satisfies

$$B(t) = C(t) \exp\left[-\frac{1}{D}\int_{F_1(t)}^{F_0(t)} \psi(z', t)\, dz'\right], \tag{3.31b}$$

$$B(t) = C(t) - \frac{1}{D}\int_{F_1(t)}^{F_0(t)} \varphi(z', t)\, dz'. \tag{3.31c}$$

From (3.31b) we get the initial condition

$$B(0) = \exp\left[-\frac{1}{D}\int_{F_1(0)}^{F_0(0)} \psi_0(z', t)\, dz'\right] = \exp\left(\psi_0 \frac{L}{D}\right), \tag{3.32a}$$

where (3.25e) has been also used; from (3.31c) we obtain the time evolution

$$\dot{B}(t) = -\varphi_z(F_0(t'), t'). \tag{3.32b}$$

From (3.32b), when we use (3.31b) and (3.29d), we finally obtain

$$s_0(t) = 2\beta t + \frac{1}{\alpha}\left[-\beta^2 t - \psi_0 L + D \ln\left(\exp\left(\frac{\psi_0 L}{D}\right) - \int_0^t \varphi_z(F_0(t'), t')\, dt'\right)\right]. \tag{3.32c}$$

We are now ready to solve the FBP for the linear heat equation (3.27), with initial datum (3.29a) and boundary conditions (3.29b)-(3.29e).
In the following we put

$$\varphi_z(F_0(t), t) \equiv G_0(t)$$

$$\varphi_z(F_1(t), t) \equiv G_1(t).$$

We now introduce the fundamental kernel of the heat equation (3.27)

$$K(z, t) = \frac{1}{2\sqrt{\pi}} \frac{1}{\sqrt{Dt}} \exp\left(-\frac{z^2}{4Dt}\right),$$

and consider the Green's function on the half-plane $z > 0$:

$$H(z, t; \xi, \tau) = K(z, t; \xi, \tau) - K(-z, t; \xi, \tau).$$

Integrating the Green's identity

$$\frac{\partial}{\partial \xi}\left(H\frac{\partial \varphi}{\partial \xi}-\varphi\frac{\partial H}{\partial \xi}\right)-\frac{\partial}{\partial \tau}\left(H\varphi\right)=0$$

over the domain $F_0(\tau) \leq \xi \leq F_1(\tau)$, $0 < \varepsilon < \tau < t-\varepsilon$ and letting $\varepsilon \to 0$, after using $K(z-\xi,0)=\delta(z-\xi)$ and $\varphi(F_1(t),t)=0$ we get the solution of the heat equation as:

$$\begin{aligned}\varphi(z,t) &= \int_0^L H(z-\xi,t)\,\varphi_0(\xi)\,d\xi + (\alpha-\beta)\int_0^t H_\xi(z-F_0(\tau),t-\tau)\,B(\tau)\,d\tau \\ &- \int_0^t H(z-F_0(\tau),t-\tau)\,G_0(\tau)\,d\tau + \int_0^t H(z-F_1(\tau),t-\tau)\,G_1(\tau)\,d\tau; \qquad (3.33)\end{aligned}$$

where (3.31a) and (3.25a) have also been used.
Eq.(3.33) is telling us that $\varphi(z,t)$ is known once the boundary data $G_0(t)$ and $G_1(t)$ are known; indeed the function $B(t)$ in the second integral in the r.h.s. of (3.33) is related to $G_0(t)$ via (3.32b). We then take the z-derivative of both sides in (3.33) and evaluate it once as $z \searrow F_0(t)$ and a second time as $z \nearrow F_1(t)$.
By using the following results [46]

$$\begin{aligned}&\lim_{z\to F_i(t)}\frac{\partial}{\partial z}\int_0^t K(z-F_j(\tau),t-\tau)\,G_j(\tau)\,d\tau \\ &= \frac{1}{2}G_j(t) + \int_0^t K_z(F_i(t)-F_j(\tau),t-\tau)\,G_j(\tau)\,d\tau, \qquad i=0,1,\ j=0,1\end{aligned}$$

after introducing the Neumann function for the half plane $z>0$,

$$N(z,t,\xi,\tau) = K(z,t,\xi,\tau) + K(-z,t,\xi,\tau), \qquad (3.34)$$

we finally obtain the integral equation:

$$\begin{aligned}G_0(t) =& \frac{2}{3}\left[\varphi_0(0)-(\alpha-\beta)\,B(0)\right]N(F_0(t),t) + \frac{2}{3}\left[\int_0^L \varphi_0'(\xi)\,N(F_0(t)-\xi,t)\,d\xi\right. \\ &+ (\alpha-\beta)\int_0^t G_0(\tau)\,N(F_0(t)-F_0(\tau),t-\tau)\,d\tau \\ &- \int_0^t G_0(\tau)\,H_z(F_0(t)-F_0(\tau),t-\tau)\,d\tau \\ &\left.+ \int_0^t G_1(\tau)\,H_z(F_0(t)-F_1(\tau),t-\tau)\,d\tau + \frac{1}{2}G_1(t)\right], \qquad (3.35a)\end{aligned}$$

where

$$F_0(t) = z_0(t) - 2\beta t, \tag{3.35b}$$

and $z_0(t)$ is given by (3.23b) and (3.32c). Similarly, we obtain for $G_1(t)$ the nonlinear integral equation:

$$\begin{aligned} G_1(t) = 2\Big[\varphi_0(0) - (\alpha-\beta)B(0)\Big] N(F_1(t), t) + 2\Big[\int_0^L \varphi_0'(\xi) N(F_1(t)-\xi, t)\, d\xi \\ + (\alpha-\beta)\int_0^t G_0(\tau) N(F_1(t) - F_0(\tau), t-\tau)\, d\tau \\ - \int_0^t G_0(\tau) H_z(F_1(t) - F_0(\tau), t-\tau)\, d\tau \\ + \int_0^t G_1(\tau) H_z(F_1(t) - F_1(\tau), t-\tau)\, d\tau - \frac{1}{2}G_0(t)\Big], \end{aligned} \tag{3.36a}$$

with

$$F_1(t) = z_1(t) - 2\beta t, \tag{3.36b}$$

where $z_1(t)$ is given by (3.23b) and (3.30b).
The above equations (3.35a),(3.35b) and (3.36a),(3.36b) form a system of coupled nonlinear integral equations. The solution of the FBP for the linear heat equation (3.27) on the finite interval $F_0(t) \le z \le F_1(t)$, has been reduced to the solution of the system (3.35a),(3.35b) and (3.36a),(3.36b). We point out that (3.35b) and (3.36b) imply, via (3.32c) and (3.30b) respectively, that in the present case the relation between the motion of the boundaries $F_i(t)$ $(i = 0, 1)$ and the functions $G_i(t)$ $(i = 0, 1)$ is nonlinear. This is different from what usually happens in classical Stefan problems for the linear heat equation [46] where the corresponding relation is linear. The difference is of course due to the fact that the starting point of our analysis is a FBP for a nonlinear evolution equation.
Once existence and uniqueness of the functions $G_0(t)$ and $G_1(t)$ is established for small time, $0 \le t < \sigma$, existence and uniqueness of $\varphi(z,t)$ for $0 \le t < \sigma$ then there follows via (3.33). As a consequence, $\psi(z,t)$ via (3.26a), exists and is unique for $0 \le t < \sigma$, together with the solution of the original FBP for the nonlinear diffusion-convection equation (3.18).

3.2.3 Contraction mapping

Next we outline a method to prove the existence and uniqueness for $G_0(t)$ and $G_1(t)$, for $0 \le t < \sigma$. We denote by S_M the closed sphere $\|G_i\| \le M$ in the Banach

space of functions $G_i(t)$ $(i=0,1)$ continuous for $0 \le t < \sigma$, with the uniform norm $\|G_i\| = l.u.b. |G_i(t)|$ $(i=0,1)$.
The proof is obtained in two steps:
Step 1
On the sphere S_M define the transformation

$$w_i(t) = T_i G_i(t) \qquad i=0,1 \tag{3.37}$$

where $T_i G_i$, $i=0,1$, coincides with the right-hand side of (3.35a) and (3.36a) respectively.
Then, the first step is to prove that T is a closed mapping:

$$\|G_i\| \le M_i \Longrightarrow \|w_i\| \le M_i \qquad\qquad i=0,1.$$

In order to prove that T_i $(i=0,1)$ is a mapping of S_M into itself, we consider the case $i=0$ and first we evaluate some relevant bounds in the right hand side of (3.35a).
By using (3.29a), (3.32a), (3.25e), (3.23a) and (3.23b), we get

$$|\varphi_0(0)| < \|\psi_0\| e^{\left(\frac{|\psi_0|L}{D}\right)} \quad \text{and} \quad |B_0(0)| \le e^{\left(\frac{|\psi_0|L}{D}\right)}.$$

Moreover, from (3.32c) we obtain

$$\begin{aligned} |s_0(t)-s_0(\tau)| \le{} & \frac{(2\alpha\beta-\beta^2)}{\alpha}|t-\tau| \\ & + \left|\frac{D}{\alpha}\ln\left(1-e^{-\frac{\alpha s_0(t)+\psi_0 L+\beta^2\alpha t}{D}+\frac{2\alpha\beta t}{D}}\int_\tau^t G_0(t')\,dt'\right)\right| \\ \le{} & \frac{(2\alpha\beta-\beta^2)}{\alpha}|t-\tau| + 2\frac{D}{\alpha}\left|\int_\tau^t G_0(t')\,dt'\right| \le A_1|t-\tau|, \end{aligned} \tag{3.38}$$

$$A_1 \equiv \frac{(2\alpha\beta-\beta^2)}{\alpha} + 2\frac{M_0 D}{\alpha} \tag{3.39}$$

where we take $0 < t < \sigma_1$, with $\sigma_1 : e^{\frac{2\alpha\beta}{D}\sigma_1} \le 1$.

When (3.38) is used together with (3.35b) and (3.21b), we can also write

$$|F_0(t)-F_0(\tau)| \le \frac{A_1}{\beta}|t-\tau| + 2\beta|t-\tau| \equiv A_2|t-\tau| \tag{3.40}$$

where $A_2 \equiv \dfrac{A_1}{\beta} + 2\beta$.

Next, we estimate the bounds on the terms in the right hand side of (3.35a). First, we consider

$$\left|\frac{2}{3}\int_0^L \varphi_0'(\xi)\,N(F_0(t)-\xi,t)\,d\xi\right| \le \frac{2}{3}\|\varphi_0'\|\,|Erf(F_0(t))-Erf(F_0(t)-L)|$$

where $Erf(z)$ denotes the Error function

$$Erf(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-y^2}dy.$$

For the above term we then get

$$\left|\frac{2}{3}\int_0^L \varphi_0'(\xi)\,N(F_0(t)-\xi,t)\,d\xi\right| \le \frac{4}{3}\|\varphi_0'\| \equiv A_0. \tag{3.41}$$

For the estimate of the first term in (3.35a), we can write

$$\begin{aligned}
&\left|\frac{2}{3}(\varphi_0(0))-(\alpha-\beta)B(0)\right|\left|N(F_0(t),t)\right| \\
&< \frac{2}{3}\left(\|\psi_0\|e^{\left(\frac{\|\psi_0\|L}{D}\right)}+(\alpha-\beta)\,e^{\frac{\|\psi_0\|L}{D}}\right)\frac{1}{\sqrt{\pi Dt}}e^{-\frac{F_0^2(t)}{4Dt}} \\
&\le \frac{4}{3}e^{\left(\frac{\|\psi_0\|L}{D}\right)}(\|\psi_0\|+(\alpha-\beta))\frac{e^{-\frac{F_0^2(t)}{4Dt}}}{\sqrt{\pi Dt}} \le A_3\sqrt{\sigma_2},
\end{aligned} \tag{3.42}$$

with $\sigma_2 : A_3\sqrt{\sigma_2}\le 1, \quad 0<t<\sigma_2,$
where $A_3 \equiv \dfrac{16}{3}e^{\left(\frac{\|\psi_0\|L}{D}\right)}(\|\psi_0\|+\alpha-\beta)\sqrt{\dfrac{D}{\pi}\dfrac{1}{b_0^2}}$
The third term in the right hand side of (3.35a) can be estimated as

$$\begin{aligned}
&\left|\frac{2}{3}(\alpha-\beta)\int_0^t G_0(\tau)\,N((F_0(t)-F_0(\tau)),t-\tau)\,d\tau\right| \\
&\le \frac{4}{3}(\alpha-\beta)\frac{M_0}{\sqrt{\pi D}}\left|\int_0^t \frac{e^{-\frac{(F_0(t)-F_0(\tau))^2}{4(t-\tau)D}}}{2\sqrt{t-\tau}}d\tau\right| \le A_4\sqrt{\sigma_3},
\end{aligned} \tag{3.43}$$

with $\sigma_3 : A_4\sqrt{\sigma_3}\le 1,$
where $A_4 \equiv \dfrac{4}{3}\dfrac{(\alpha-\beta)}{\sqrt{D}}M_0.$
Next, we evaluate

$$\left|\frac{2}{3}\int_0^t G_0(\tau) H_z(F_0(t) - F_0(\tau), t-\tau)\, d\tau\right|$$
$$\leq \frac{1}{6}M_0\frac{1}{\sqrt{\pi}}\frac{1}{D^{3/2}}\left[A_2\left|\int_0^t \frac{exp\left(-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}\right)}{\sqrt{t-\tau}}\right|\right.$$
$$\left.+4D\left|\int_0^t \frac{1}{\sqrt{t-\tau}}\frac{d\tau}{(F_0(t)+F_0(\tau))}\right|\right] \leq A_5\sqrt{\sigma_4}, \tag{3.44}$$
$$A_5 \equiv \frac{M_0}{3\sqrt{\pi D}}\left(\frac{A_2}{D}+\frac{2}{b_0}\right)$$

where (3.40) has been used and we take $0 < t < \sigma_4$, with $\sigma_4 : A_5\sqrt{\sigma_4} < 1$. We finally evaluate

$$\left|\int_0^t G_1(\tau) H_z(F_0(t) - F_0(\tau), t-\tau)\, d\tau\right|$$
$$\leq \frac{M_1}{6}\frac{1}{\sqrt{\pi}}\frac{1}{D^{3/2}}\left[A_2\left|\int_0^t \frac{exp\left(-\frac{(F_0(t)-F_1(\tau))^2}{4D(t-\tau)}\right)}{\sqrt{t-\tau}}d\tau\right|\right.$$
$$\left.+4D\left|\int_0^t \frac{1}{\sqrt{t-\tau}}\frac{d\tau}{(F_0(t)+F_1(\tau))^2}\right|\right] \leq A_6\sqrt{\sigma_5}, \tag{3.45}$$
$$A_6 \equiv \frac{M_1}{3\sqrt{\pi D}}\left(\frac{A_2}{D}+\frac{4}{b_0+b_1}\right)$$

where the bound $|F_0(t) - F_1(\tau)| \leq A_2|t-\tau|$ has been used, with A_2 given by (3.40). Moreover in (3.45) we take $0 < t < \sigma_5$, with $\sigma_5 : A_6\sqrt{\sigma_5} \leq 1$. When the above estimates (3.41), (3.42), (3.43), (3.44) and (3.45) are taken into account, we finally obtain from (3.37) the following estimate

$$\|w_0\| < A_0 + \frac{1}{3}M_1 + A_3\sqrt{\sigma_2} + A_4\sqrt{\sigma_3} + A_5\sqrt{\sigma_4} + A_6\sqrt{\sigma_5}. \tag{3.46a}$$

We now define M_0 as $M_0 = A_0 + \frac{1}{3}M_1 + 1$ and get from (3.46a)

$$\|w_0\| < A_0 + \frac{1}{3}M_1 + A\sqrt{\sigma} \tag{3.46b}$$

with $A = \sum_{i=3}^{6} A_i$ and $\sigma \leq min(\sigma_2, \sigma_3, \sigma_4, \sigma_5) : A\sqrt{\sigma} < 1$. We can therefore conclude

$$\|w_0\| < M_0.$$

Thus the map is closed. The proof that is $\|w_1\| \leq M_1$, is of course analogous.
Step 2
We now prove that T_i, defined by (3.37), is a contraction mapping: i.e. given two solutions of (3.37) with $\|G_i - \overline{G}_i\| = \delta$, $\delta < 2M$, it follows that $\|T_i\left(G_i - \overline{G}_i\right)\| = \theta\delta$ with $0 \leq \delta < 1$.
We consider (3.32c) and evaluate the following estimate

$$\begin{aligned} |s_0(t) - \overline{s}_0(t)| &\leq \frac{D}{\alpha}\left|ln\left(1 - e^{-\frac{\overline{s}_0(t)\alpha + \psi_0 L + \beta^2 t}{D} + \frac{2\alpha\beta t}{D}}\int_0^t G_0(t') - \overline{G}_0(t')\,dt'\right)\right| \\ &\leq \frac{D}{\alpha}2e^{\frac{2\alpha\beta}{D}\sigma_1}\delta t \leq B_1\delta t, \qquad B_1 \equiv \frac{2D}{\alpha} \end{aligned} \tag{3.47}$$

where we take $0 < t < \sigma_1$, with $\sigma_1 : e^{\frac{2\alpha\beta}{D}\sigma_1} \leq 1$.
Also, when (3.47) is used, we can evaluate via (3.25e) the estimate

$$|F_0(t) - \overline{F}_0(t)| = |z_0(t) - \overline{z}_0(t)| \leq \lambda B_1 \delta t, \tag{3.48}$$

with $\lambda = \left\|\frac{1}{\theta}\right\|$.
Next, we evaluate the following bounds:

$$\begin{aligned} &\frac{2}{3}\left|\varphi_0(0) - (\alpha - \beta)B(0)\right|\frac{1}{\sqrt{\pi t D}}\left|e^{-\frac{F_0^2(t)}{4Dt}} - e^{\frac{\overline{F}_0^2(t)}{4Dt}}\right| \\ &< \frac{4}{3}e^{\left(\frac{\|\psi_0\|L}{D}\right)}\frac{|\|\psi_0\| + \alpha - \beta|}{\sqrt{\pi D t}}\frac{|F_0(t) - \overline{F}_0(t)||F_0(t) + \overline{F}_0(t)|}{|F_0(t)|^2} \\ &\leq \frac{8}{3}e^{\left(\frac{\|\psi_0\|L}{D}\right)}\frac{|\|\psi_0\| + \alpha - \beta|}{\sqrt{\pi D}}\frac{2R}{b^2}\lambda B_1\delta\sqrt{t} \leq B_2\delta\sqrt{\sigma_6}, \\ &\qquad\qquad B_2 \equiv \frac{8}{3}e^{\left(\frac{\|\psi_0\|L}{D}\right)}\frac{(\|\psi_0\| + \alpha - \beta)}{\sqrt{\pi D}}\frac{2R\lambda}{b^2}B_1 \end{aligned} \tag{3.49}$$

where we made use of (3.42) and (3.47); moreover the mean value theorem has also been applied and in (3.49) $R \equiv max\left\{|F_0(t)|, |\overline{F}_0(t)|\right\}$.
Next, we put

$$H_1 = \frac{2}{3}\int_0^L \varphi_0'(\xi)\left(N(F_0(t) - \xi, t) - N\left(\overline{F}_0(t) - \xi, t\right)\right) \tag{3.50}$$

where N denotes the Neumann function (3.34).
For the estimate of H_1 we put $\xi_0 = F_0(t) - 2t\|\psi_0\|$ and $\overline{\xi}_0 = \overline{F}_0(t) - 2t\|\psi_0\|$ in the integral in the right hand side of (3.50) getting

$$\begin{aligned} |H_1| &\leq \frac{4}{3}\frac{\|\varphi_0'\|}{\sqrt{\pi D t}}\left|\int_{-\xi_0}^{L-\xi_0} e^{-\frac{\varphi^2}{4Dt}}d\varphi - \int_{-\overline{\xi}_0}^{L-\overline{\xi}_0} e^{-\frac{\varphi^2}{4Dt}}d\varphi\right| \leq A_0\frac{2}{\sqrt{\pi t D}}\left|\xi_0 - \overline{\xi}_0\right| \\ &= \frac{2A_0}{\sqrt{\pi D t}}|F_0(t) - \overline{F}_0(t)| \leq B_3\delta\sqrt{\sigma_7}, \qquad B_3 \equiv \frac{2A_0}{\sqrt{\pi D}}\lambda B_1 \end{aligned} \tag{3.51}$$

where A_0 is given by (3.41) and (3.48) has also been used. Moreover, in (3.51) we choose $\sigma_7 : B_3\sqrt{\sigma_7} < 1$.
We now put

$$\begin{aligned} H_2 =& \frac{2}{3}(\alpha - \beta)\int_0^t \Big[G_0(\tau)\, N(F_0(t) - F_0(\tau), t-\tau) \\ &- \overline{G}_0(\tau)\, N\left(\overline{F}_0(t) - \overline{F}_0(\tau)\right), t-\tau\Big]d\tau \end{aligned}$$

and write

$$\begin{aligned} H_2 =& \frac{2}{3}(\alpha - \beta)\Bigg[\int_0^t \Big[\left(G_0(\tau) - \overline{G}_0(\tau)\right) N(F_0(t) - F_0(\tau), t-\tau)\Big]d\tau \\ &+ \int_0^t \Big[G_0(\tau)\big(N(F_0(t) - F_0(\tau), t-\tau) - N\left(\overline{F}_0(t) - \overline{F}_0(\tau), t-\tau\right)\big)\Big]d\tau\Bigg]. \end{aligned} \tag{3.52}$$

For the first integral in the right hand side of (3.52), we obtain the estimate

$$\begin{aligned} &\left|\int_0^t \left(G_0(\tau) - \overline{G}_0(\tau)\right) N(F_0(t) - F_0(\tau), t-\tau)\, d\tau\right| \\ &\leq \frac{4\delta}{\sqrt{\pi D}}\left|\int_0^t \frac{d\tau}{2\sqrt{t-\tau}}\right| \leq \frac{4\delta}{\sqrt{\pi D}}\sqrt{\sigma}. \end{aligned} \tag{3.53}$$

For the second integral in the right hand side of (3.52), we write

$$\begin{aligned} &\left|\int_0^t G_0(\tau)\left(N(F_0(t) - F_0(\tau), t-\tau) - N\left(\overline{F}_0(t) - \overline{F}_0(\tau), t-\tau\right)\right) d\tau\right| \\ &\leq \frac{2M}{\sqrt{\pi D}}\int_0^t \frac{1}{\sqrt{t-\tau}} e^{-\frac{(\overline{F}_0(t) - F_0(\tau))^2}{4D(t-\tau)}}\left|1 - e^{\frac{(F_0(t) - F_0(\tau))^2}{4D(t-\tau)} - \frac{(\overline{F}_0(t) - \overline{F}_0(\tau))^2}{4D(t-\tau)}}\right| d\tau. \end{aligned} \tag{3.54a}$$

We now define

$$\overline{Q} = -\frac{\left[\left(F_0(t) - F_0(\tau)\right)^2 - \left(\overline{F}_0(t) - \overline{F}_0(\tau)\right)^2\right]}{4D(t-\tau)} \tag{3.54b}$$

and obtain the estimate

$$\begin{aligned} |\overline{Q}| \leq & \frac{1}{4D|t-\tau|}\left|\left(\overline{F}_0(t) - F_0(t)\right) - \left(\overline{F}_0(\tau) - F_0(\tau)\right)\right| \\ & \times \left|\left(F_0(t) - F_0(\tau)\right) + \left(\overline{F}_0(t) - \overline{F}_0(\tau)\right)\right| \leq \frac{\lambda B_1}{2D|t-\tau|} A_2 \delta\sigma |t-\tau| \\ & \leq B_4 \delta\sigma, \qquad\qquad B_4 \equiv \frac{\lambda B_1 A_2}{2D} \end{aligned} \tag{3.54c}$$

where (3.40) and (3.48) have been used.
From (3.54a) we now have

$$\begin{aligned} & \left|\int_0^t G_0(\tau)\left(N\left(F_0(t) - F_0(\tau), t-\tau\right) - N\left(\overline{F}_0(t) - \overline{F}_0(\tau), t-\tau\right)\right) d\tau\right| \\ & \leq \frac{2M}{\sqrt{\pi D}} \int_0^t \frac{d\tau}{\sqrt{t-\tau}} |\overline{Q}| e^{|\overline{Q}|} \leq \frac{2M}{\sqrt{\pi D}} B_4 \delta \sigma^{3/2}. \end{aligned} \tag{3.54d}$$

we finally obtain from (3.52), (3.53) and (3.54d) the following estimate

$$\begin{aligned} |H_2| \leq \frac{2}{3}(\alpha - \beta)\left[\frac{4}{\sqrt{\pi D}}\delta\sqrt{\sigma} + \frac{2M}{\sqrt{\pi D}} B_4 \delta \sigma^{3/2}\right] & \leq B_5 \delta \sqrt{\sigma_8} \quad (\sigma_8 \leq 1) \\ B_5 \equiv \frac{2}{3}(\alpha - \beta)\left[\frac{4 + 2MB_4}{\sqrt{\pi D}}\right] & \end{aligned} \tag{3.55}$$

In order to evaluate the next estimate, we put

$$
\begin{aligned}
H_3 =& \frac{2}{3}\int_0^t \left[G_0(\tau) H_z\left(F_0(t)-F_0(\tau), t-\tau\right)\right. \\
&\left.-\overline{G}_0(\tau) H_z\left(\overline{F}_0(t)-\overline{F}_0(\tau), t-\tau\right)\right] d\tau \\
&= V_1 + V_2, \qquad (3.56a) \\
V_1 =& \frac{1}{6}\frac{1}{\sqrt{\pi}D^{3/2}}\int_0^t \left(G_0(\tau)-\overline{G}_0(\tau)\right)\frac{\left(F_0(\tau)-F_0(t)\right)}{(t-\tau)^{3/2}} e^{-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}} d\tau \\
&+\frac{1}{6}\frac{1}{\sqrt{\pi}D^{3/2}}\int_0^t \overline{G}_0(\tau)\left[\frac{\left(F_0(\tau)-F_0(t)\right)}{(t-\tau)^{3/2}} e^{-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}}\right. \\
&\left.-\frac{\left(\overline{F}_0(\tau)-\overline{F}_0(t)\right)}{(t-\tau)^{3/2}} e^{-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}}\right] d\tau, \qquad (3.56b) \\
V_2 =& -\frac{1}{6}\frac{1}{\sqrt{\pi}}\frac{1}{D^{3/2}}\int_0^t \left(\overline{G}_0(\tau)-G_0(\tau)\right)\frac{\left(\overline{F}_0(t)-\overline{F}_0(\tau)\right)}{(t-\tau)^{3/2}} e^{-\frac{(\overline{F}_0(t)+\overline{F}_0(\tau))^2}{4D(t-\tau)}} d\tau \\
&-\frac{1}{6}\frac{1}{\sqrt{\pi}}\frac{1}{D^{3/2}}\int_0^t G_0(\tau)\left[\frac{\left(\overline{F}_0(t)-\overline{F}_0(\tau)\right)}{(t-\tau)^{3/2}} e^{-\frac{(\overline{F}_0(t)+\overline{F}_0(\tau))^2}{4D(t-\tau)}}\right. \\
&\left.-\frac{\left(F_0(t)+F_0(\tau)\right)}{(t-\tau)^{2}} e^{-\frac{(F_0(t)+F_0(\tau))^2}{4D(t-\tau)}}\right] d\tau. \qquad (3.56c)
\end{aligned}
$$

In order to get an estimate for $|V_1|$, we use (3.40) in the right hand side of (3.56b) and write

$$
\begin{aligned}
|V_1| \leq& \frac{1}{6}\frac{A_2}{\sqrt{\pi}D^{3/2}}\delta\int_0^t \left|\frac{e^{-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}}}{\sqrt{t-\tau}}\right| d\tau \\
&+\frac{1}{6}\frac{A_2}{\sqrt{\pi}}\frac{M_0}{D^{3/2}}\int_0^t \left|\frac{e^{-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}}}{\sqrt{t-\tau}} - \frac{e^{-\frac{\left(\overline{F}_0(t)-\overline{F}_0(\tau)\right)^2}{4D(t-\tau)}}}{\sqrt{t-\tau}}\right| d\tau
\end{aligned}
$$

which in turn implies

$$
|V_1| \leq \frac{1}{3}\frac{A_2}{\sqrt{\pi}D^{3/2}}\delta\sqrt{t} + \frac{1}{6}\frac{A_2 M_0}{\sqrt{\pi}D^{3/2}}\int_0^t \left|\frac{e^{-\frac{(F_0(t)-F_0(\tau))^2}{4D(t-\tau)}}}{\sqrt{t-\tau}}\right| \left|1-e^{-|\overline{Q}|}\right| d\tau, \qquad (3.57)
$$

where $\overline{Q}$ is given by (3.54b).
Using $|1-e^{-\overline{Q}}| \leq \overline{Q}e^{|\overline{Q}|}$, together with (3.54c), from (3.57) we get

$$|V_1| \leq \frac{1}{3}\frac{A_2}{\sqrt{\pi}D^{3/2}}\left(\delta\sqrt{\sigma} + M_0 B_4 \delta \sigma^{3/2}\right), \qquad 0 < t < \sigma.$$

From the above relation we can write

$$|V_1| \leq B_6 \delta \sqrt{\sigma_9}, \qquad B_6 \equiv \frac{1}{3}\frac{A_2}{\sqrt{\pi}D^{3/2}}\left(1 + M_0 B_4\right) \tag{3.58}$$

with $\sigma_9 : B_6\sqrt{\sigma_9} \leq 1$.

The estimate of V_2 is somewhat more cumbersome; a detailed analysis is given in the Appendix B (see (B.1)-(B.4)). There obtains

$$|V_2| \leq B_7 \delta \sqrt{\sigma_{10}}, \qquad B_7\sqrt{\sigma_{10}} \leq 1. \tag{3.59}$$

When we go back to (3.56a), from (3.58) and (3.59) we finally obtain

$$|H_3| \leq B_8 \delta \sqrt{\sigma^*} \qquad B_8 = B_6 + B_7 \tag{3.60}$$

with $\sigma^* = min\{\sigma_9, \sigma_{10}\} : B_0\sqrt{\sigma^*} < 1$.
Our last task is to evaluate an upper bound for:

$$|H_4| = \frac{2}{3}\left|\int_0^t \left[G_1(\tau)\, H_z\left(F_1(t) - F_1(\tau), t-\tau\right) - \overline{G}_1(\tau)\, H_z\left(\overline{F}_1(t) - \overline{F}_1(\tau), t-\tau\right)\right] d\tau\right|.$$

Such bound can be obtained along the same lines followed to get the estimate on $|H_3|$. The only difference being that $G_0(t)\left(\overline{G}_0(t)\right)$ in (3.56a) is replaced by $G_1(t)\left(\overline{G}_1(t)\right)$ and $F_0(t)\left(\overline{F}_0(t)\right)$ is replaced by $F_1(t)\left(\overline{F}_1(t)\right)$. We can therefore write:

$$|H_4| \leq B_9 \delta \sqrt{\sigma^*}, \tag{3.61}$$

where B_9 is an appropriate constant.
We now go back to (3.37) and consider

$$|w_0 - \overline{w}_0| = |T_0\left(G_0 - \overline{G}_0\right)|,$$

with $T_0 G_0$ given by the right-hand side of (3.35a).
We put together the esimates given by (3.49), (3.51), (3.55), (3.60) and (3.61), obtaining

$$\frac{|w_0 - \overline{w}_0|}{\delta} < \overline{B}\sqrt{\sigma} + \frac{1}{3}; \qquad \overline{B} = B_2 + B_3 + B_5 + B_8 + B_9$$

where σ satisfies $\sigma < min\,(\sigma_6, \sigma_7, \sigma_8, \sigma^*)$ with $\overline{B}\sqrt{\sigma} \leq \frac{2}{3}$.
We can therefore conclude that

$$|w_0 - \overline{w}_0| \leq \delta\theta, \qquad \theta < 1, \qquad \theta = \overline{B}\sqrt{\sigma}$$

which in turn implies that T_0 is a contraction operator in δ_M. Thus, there exists a unique fixed point $G_0\,(t) = T_0 G_0\,(t)$ in δ_M for $0 \leq t < \sigma$. The proof for the case $i = 1$ of course follows along the same lines.
We have then proven existence and uniqueness of the solutions $G_0\,(t)$ and $G_1\,(t)$ (see (3.35a) and (3.36a)) for a small interval of time $0 \leq t < \sigma$.
In the next Subsection we concentrate our attention on a particular solution $\theta\,(x, t)$ of our original problem. Namely, we show that there exists a solution $\theta\,(x, t)$ corresponding to a travelling wave solution of the FBP for the Burgers equation (3.22).

3.2.4 A particular solution

We now turn our attention to a particular solution $\theta\,(x, t)$ of our problem. Namely, we show that there exists a solution $\theta\,(x, t)$ of the FBP for equation (3.18) corresponding to a travelling wave solution of the Burgers equation (3.22) specified by the boundary conditions (3.24a)-(3.24d).
The usual travelling wave solution of equation (3.22) reads

$$\psi\,(z, t) = u_1 + \frac{(u_2 - u_1)}{\left[1 + \exp \frac{1}{D}\Big((u_2 - u_1)\,(z - Vt - z_0)\Big)\right]} \tag{3.62a}$$

with

$$V = u_1 + u_2, \qquad u_2 > u_1. \tag{3.62b}$$

In the following we use the above solution on the interval $z_0\,(t) \leq z \leq z_1\,(t)$, determining the two constants u_1 and u_2; we assume both of them to be positive $(u_2 > u_1 > 0)$.
When we require the solution (3.62a) to satisfy the boundary condition (3.24a), we get

$$z_0\,(t) - Vt - z_0 = k_1, \tag{3.63}$$

k_1 arbitrary constant. Without loss of generality we put $k_1 = 0$ and then get from (3.24a)

$$2\alpha = u_1 + u_2; \tag{3.64}$$

which is the first constraint on u_1 and u_2. The boundary condition (3.24c) in turn gives

$$z_1(t) - Vt - z_0 = k_2, \tag{3.65}$$

k_2 arbitrary constant. Once we fix the value of k_2, we get from (3.24c) the second constraint to determine the constants u_1 and u_2:

$$\beta - u_1 = \frac{(u_2 - u_1)}{\left[1 + \exp\left(\frac{k_2}{D}(u_2 - u_1)\right)\right]}. \tag{3.66}$$

Moreover, we observe that (3.63) and (3.65) imply

$$\dot{z}_0(t) = \dot{z}_1(t) = V.$$

The above relation is telling us that the travelling wave and the two free boundaries are all moving to the right with the same constant velocity.
Let us now consider the two flux boundary conditions (3.24b) and (3.24d). For simplicity we put in the following $k_2 = 1$.
When the solution (3.62a) is used, together with (3.64), in (3.24b), there obtains

$$\dot{s}_0(t) = 2\alpha - \frac{u_1 u_2}{\alpha}, \tag{3.67a}$$

which is the constant velocity corresponding to the motion of the free boundary $s_0(t)$.
The boundary condition (3.24d), when (3.66) is also used, in turn gives

$$\dot{s}_1(t) = 2\alpha - \frac{u_1 u_2}{\beta}, \tag{3.67b}$$

which is the constant velocity of the free boundary $s_1(t)$. Due to the condition $\alpha > \beta$, (3.67a) and (3.67b) imply

$$\dot{s}_0 > \dot{s}_1.$$

Then, in the physical space $s_0(t) \leq x \leq s_1(t)$, the moving front solution is compatible with a constant velocity motion of the two boundaries, but $s_0(t)$ is moving faster then $s_1(t)$. This is not surprising, since in the modeling of drug propagation in the arterial tissues, one expects the diluted drug concentration to move faster close to the point where the drug has been released.
After a finite time the position of $s_0(t)$ coincides with $s_1(t)$, indicating that the moving front has spanned the whole interval of existence of the solution.

Finally, the solution of the FBP for the nonlinear diffusion-convection equation (3.18) is given in parametric form by

$$\theta\left(x,t\right)=\left(\frac{\partial z}{\partial x}\right)^{-1},$$

where, in virtue of (3.21b), z solves

$$x=\int_{z_0}^{z}\psi\left(z',t\right)dz',$$

with $\psi\left(z,t\right)$ given by (3.62a) together with (3.64) and (3.66).
In Fig.3.1 the moving front profile (3.62a) is shown at different times (dimen-

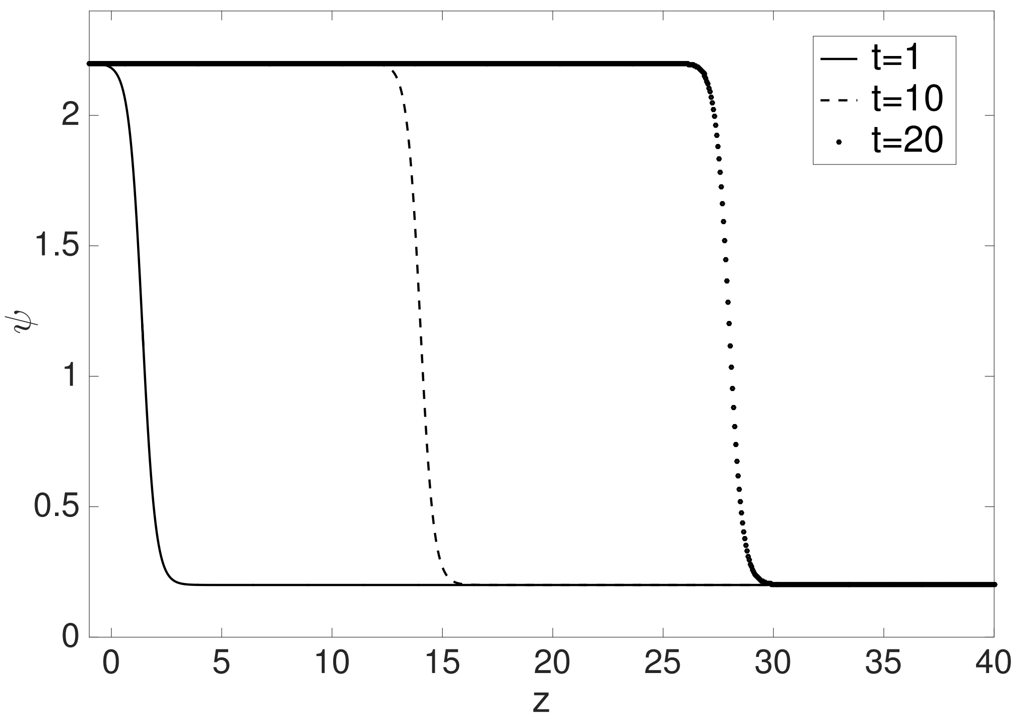

Figure 3.1: Nondimensional concentration profiles at three times: $t = 1$, $t = 10$, $t = 20$ (from the left to the right).

sionless units). Its behavior is in qualitative agreement with the corresponding concentration profiles reported in Fig.5 of [61].

Chapter 4

Conclusions

As pointed out in the Introduction, the aim of the present thesis is to discuss the applications of some useful mathematical techniques to problems which are relevant in life-and-material science. The models considered here all share the common feature of nonlinearity, which indeed characterizes the behavior and the time evolution of several real-life phenomena.
We first considered two applications related to population dynamics in the framework of the Kinetic Theory of Active Particles.
We started our analysis with a mathematical model suitable to describe the onset and the evolution of epidemics. The model is characterized by three fundamental parameters: the risk perception, the infectivity and the vaccine reaction. Our results show how such parameters influence both the onset and the evolution of the infective disease. In particular, as expected, the epidemic spread can be controlled by increasing the risk perception. At the same time we observe that an increase of the infectivity induces and promotes the diffusion of the infection.
The approach presented here can be further developed in order to include some important aspects. In particular:

- we believe that the mathematical structure should be generalized to open systems, incorporating birth and death processes;
- a space dependance of the model could be possibly derived through an asymptotic analysis of the microscopic model described by the kinetic theory approach. This would open the way to the description of propagation phenomena with finite velocity and also to relate the spread of epidemics to space dynamics of individuals affected by the pathology.

Next, we considered a traffic flow model based on microscopic interactions between active particles composed by a vehicle-driver pair. The outcome of such

interactions is stochastic and is called "Table of games". At the macroscopic scale we obtained physical quantities such as the average velocity and the flux, whose behavior is consistent with experimental evidence.
A further development of the ideas presented here includes of course the analysis of a traffic flow model on a network of interconnected roads, in order to obtain a more realistic mathematical description. Work along this lines is in progress.
Finally in the last model we studied a free boundary value problem for a nonlinear diffusion/convection model. From the mathematical point of view we proved existence and uniqueness of the solution for nonlinear evolution equation on a finite domain characterized by free boundaries. From the applicative point of view we developed a model suitable to describe drug diffusion in arterial tissues after the drug is released by an arterial stent.
Our proposal is to extend the diffusion/convection model developed in 2016. The previous analysis will be in the next future extended to the modeling of two layers system, with the first layer describing the drug dissolution-diffusion process which takes place in the coating of polymeric drug delivery devices.

Appendix A

In the following we report the proof of the of existence and uniqueness for the IBV problem associated with the nonlinear diffusion-convection equation (3.1), obtained in [17]. To analyze the existence properties of $h(t)$ for $0 \leq t < \sigma$ we first denote by S_M the closed sphere $||g_1|| \leq M \;\; (M > 0)$ in the Banach space of functions $h(t)$ continuous for $0 \leq t < \sigma$ with the uniform norm $||h|| = l.u.b.|h(t)|$. On the sphere S_M define the transformation

$$w(t) = Th(t), \tag{A.1}$$

where $Th(t)$ coincides with the right hand side of (3.17a).
The proof is obtained in two steps, the first step is to prove that T is a mapping of S_M into itself. By using (3.17b) we obtain

$$|\overline{z}(t)| \leq \frac{\alpha\sigma}{\beta_2}+\frac{1}{\beta_2}+\frac{M\sigma}{\beta_2} = \sigma\,\frac{\alpha+M}{\beta_2}+\frac{1}{\beta_2} \equiv \sigma\,B_1+\frac{1}{\beta_2}, \qquad \left(B_1 = \frac{\alpha+M}{\beta_2}\right); \tag{A.2}$$

moreover from (3.17b) we also obtain

$$\begin{aligned} |\overline{z}(t)-\overline{z}(t')| &\leq \frac{\alpha}{\beta_2}|t-t'| + \frac{2}{\beta_2}(1+M\sigma)\,\gamma\,|t-t'| = \frac{|t-t'|}{\beta_2}\left[\alpha+2\,(1+M\sigma)\,\gamma\right] \\ &\leq \frac{|t-t'|}{\beta_2}\left[\alpha+2\,(1+M)\,\gamma\right] \equiv B_2|t-t'|, \qquad \left(B_2 = \frac{\alpha+2\,(1+M)\,\gamma}{\beta_2}\right), \end{aligned} \tag{A.3}$$

with $\gamma \; : \; \gamma|t-t'| > 1$.
Now we evaluate some relevant bounds in the right hand side of (A.1). We first consider

$$\left|\frac{2\varphi_0(0)\,e^{-\frac{\overline{z}^2(t)}{4t}}}{\sqrt{\pi t}}\right| \leq 2\,||\varphi_0||\,\left|\frac{A_1\,\overline{z}^2(t)}{4t\sqrt{\pi t}}\right| < ||\varphi_0||\frac{A_1}{2\sqrt{\pi}}\left(B_1\,\sigma+\frac{1}{\beta_2}\right)^2\sqrt{\sigma}, \tag{A.4}$$

with $A_1 > 0 \; : \; A_1\dfrac{\overline{z}^2(t)}{4t} > 1$.
In the following we denote by A_i and by B_i, $i > 1$, appropriate positive constants

which do not depend on σ. For the estimate of the integral terms in the right hand side of (A.1), using (3.16), we can write

$$4\left|\int_{-\infty}^{0} K(\overline{z}(t)-z',t)\,\varphi_0'(z')\,dz'\right| \leq 2||\varphi_0'||\left|\int_{-\infty}^{0} \frac{1}{\sqrt{\pi t}}\,e^{-\frac{(\overline{z}(t)-z')^2}{4t}}\,dz'\right|$$
$$\leq 4\,||\varphi_0'|| \equiv A_2, \tag{A.5a}$$

and

$$4\left|\int_{0}^{t} K_z(\overline{z}(t)-\overline{z}(t'),t-t')\,h(t')\,dt'\right| \leq \frac{2M}{\sqrt{\pi t}}\left(\frac{\alpha+2\,(1+M\sigma)\,\gamma}{\beta_2}\right)\sigma \tag{A.5b}$$

where (A.3) has been used.

Using the inequalities (A.4), (A.5a) and (A.5b) in the right hand side of (A.1) we have the following bound

$$|w(t)| \leq A_2 + \frac{A_1}{2\sqrt{\pi}}\left(B_1\sigma+\frac{1}{\beta_2}\right)^2 ||\varphi_0||\sqrt{\sigma} + \frac{2M}{\sqrt{\pi}}\left(\frac{\alpha+2\,(1+M\sigma)\gamma}{\beta_2}\right)\sqrt{\sigma}, \tag{A.6}$$

with $M = A_2 + 1$.

Finally if we choose $\sigma = \ min(\sigma_1,\sigma_2)$ with $\sigma_1 : A_1\left(B_1\sigma_1+\frac{1}{\beta_2}\right)^2 ||\varphi_0||\sqrt{\sigma_1} < 2\sqrt{\pi}$ and $\sigma_2 : 2M\left(\frac{\alpha+2\,(1+M\sigma)\gamma}{\beta_2}\right)\sqrt{\sigma_2} < \sqrt{\pi}$, from (A.6) we can therefore conclude

$$|w(t)| < M.$$

Thus the mapping is closed.

The second step is to prove that T is a contraction mapping; i.e. given two solutions of (A.1) with $||h-\widehat{h}|| = \delta$ it follows that $||Th - T\widehat{h}|| \leq \vartheta\delta$ with $0 < \vartheta < 1$. For this purpose we take into account the function $P(t)$ defined as

$$P(t) = \frac{1}{C(t)}.$$

Using the properties of $C(t)$ we find

$$||P||_\infty = \sup_{t>0}|P(t)|.$$

From (3.17b), the following relevant bound is obtained:

$$|\overline{z}(t)-\widehat{\overline{z}}(t)| \leq \left|\int_0^t \frac{\dot{s}(t')}{f(t')}+\frac{\dot{\widehat{s}}(t')}{f(t')}\,dt'\right| + \left|\int_0^t \frac{\dot{C}(t')}{C(t')f(t')}+\frac{\dot{\widehat{C}}(t')}{\widehat{C}(t')f(t')}\,dt'\right|$$
$$\leq 2\,\frac{\alpha}{\beta_2}N_1\delta t + \frac{2M}{\beta_2}||P||_\infty N_1\delta t \equiv (A_3+A_4)\delta t \tag{A.7}$$

with $N_1 : N_1\delta > 1,\ A_3 = \dfrac{2\,\alpha\,N_1}{\beta_2},\ A_4 = \dfrac{2M||P||_\infty N_1}{\beta_2}$.
Moreover we obtain

$$\left|\dot{\overline{z}}(t) - \dot{\widehat{\overline{z}}}(t)\right| \leq (A_3 + A_4)\delta. \tag{A.8}$$

From (A.1) and (3.17a) we can write

$$w - \hat{w} = H_1 + H_2 + H_3, \tag{A.9a}$$

where,

$$H_1 = -\,2\varphi_0(0)\,\frac{\left(e^{-\frac{\overline{z}^2(t)}{4t}} - e^{-\frac{\widehat{\overline{z}}^2(t)}{4t}}\right)}{\sqrt{\pi t}}, \tag{A.9b}$$

$$H_2 = \frac{2}{\sqrt{\pi t}}\int_{-\infty}^{0} \varphi_0'(z')\left[e^{-\frac{(\overline{z}(t)-z')^2}{4t}} - e^{-\frac{(\widehat{\overline{z}}(t)-z')^2}{4t}}\right] dz', \tag{A.9c}$$

$$\begin{aligned} H_3 = &-2\int_0^t h(t')\,\frac{(\overline{z}(t) - \overline{z}(t'))}{(t-t')}\,K(\overline{z}(t) - \overline{z}(t'), t - t')\,dt' \\ &+2\int_0^t \widehat{h}(t')\,\frac{(\widehat{\overline{z}}(t) - \widehat{\overline{z}}(t'))}{(t-t')}\,K(\widehat{\overline{z}}(t) - \widehat{\overline{z}}(t'), t - t')\,dt', \end{aligned} \tag{A.9d}$$

with $K(z - z', t - t')$ given by (3.16).
From (A.9b) we obtain the estimate

$$|H_1| \leq 2||\varphi_0||\frac{1}{\sqrt{\pi t}}\left|e^{-\frac{\overline{z}^2(t)}{4t}} - e^{-\frac{\widehat{\overline{z}}^2(t)}{4t}}\right|. \tag{A.10}$$

Now the exponentials in the right hand side of (A.10), can be expanded in Taylor series:

$$\begin{aligned} \left|e^{-\frac{\overline{z}^2(t)}{4t}} - e^{-\frac{\widehat{\overline{z}}^2(t)}{4t}}\right| &\leq \sum_{n=1}^{+\infty}\left|\frac{\left(\frac{\overline{z}^2(t)}{4t}\right)^n - \left(\frac{\widehat{\overline{z}}^2(t)}{4t}\right)^n}{n!}\right| \\ &\leq \left|\frac{\overline{z}^2(t)}{4t} - \frac{\widehat{\overline{z}}^2(t)}{4t}\right|\sum_{n=1}^{+\infty}\left(\frac{1}{2}\right)^n < 2\left|\frac{\overline{z}^2(t)}{4t} - \frac{\widehat{\overline{z}}^2(t)}{4t}\right|. \end{aligned} \tag{A.11}$$

To get an estimate for $|H_1|$ we use (A.11) in the right hand side of (A.10), together with (A.7), and write

$$|H_1| \leq \frac{2||\varphi_0||\,(A_3 + A_4)}{\sqrt{\pi}}\,\delta\sqrt{\sigma} \equiv B_3\,\delta\sqrt{\sigma}. \tag{A.12}$$

From (A.9c) we can write

$$
\begin{aligned}
|H_2| \leq & 2\,\frac{||\varphi_0'||}{\sqrt{\pi t}}\left|\int_{-\infty}^{0}\left[e^{-\frac{(\overline{z}(t)-z')^2}{4t}} - e^{-\frac{(\widehat{\overline{z}}(t)-z')^2}{4t}}\right]dz'\right| \\
\leq & 2\,\frac{||\varphi_0'||}{\sqrt{\pi t}}\left|\int_{-\widehat{\overline{z}}(t)}^{-\overline{z}(t)} e^{-\frac{y^2}{4t}}\,dy\right| \leq 2\,\frac{||\varphi_0'||}{\sqrt{\pi t}}\,|\overline{z}(t)-\widehat{\overline{z}}(t)|.
\end{aligned} \tag{A.13}
$$

In order to evaluate the estimate of H_2 we use (A.7) in the right hand side of (A.13) and immediately recover

$$
|H_2| < 2\frac{||\varphi_0'||}{\sqrt{\pi}}\,(A_3+A_4)\,\delta\sqrt{\sigma} \equiv B_4\,\delta\sqrt{\sigma}. \tag{A.14}
$$

Our last task is to evaluate an upper bound for H_3:

$$
|H_3| \leq 2(|V_1|+|V_2|+|V_3|), \tag{A.15a}
$$

where,

$$
V_1 = -\int_0^t (h(t)-\widehat{h}(t'))\frac{(\overline{z}(t)-\overline{z}(t'))}{(t-t')}\,K(\overline{z}(t)-\overline{z}(t'),t-t')\,dt', \tag{A.15b}
$$

$$
V_2 = -\int_0^t \widehat{h}(t')\left[\frac{(\overline{z}(t)-\overline{z}(t'))}{(t-t')} - \frac{(\widehat{\overline{z}}(t)-\widehat{\overline{z}}(t'))}{(t-t')}\right]K(\overline{z}(t)-\overline{z}(t'),t-t')\,dt', \tag{A.15c}
$$

$$
\begin{aligned}
V_3 = & -\int_0^t \widehat{h}(t')\left[\frac{\widehat{\overline{z}}(t)-\widehat{\overline{z}}(t')}{(t-t')}\right]K(\overline{z}(t)-\overline{z}(t'),t-t') \\
& \times\left[1-e^{-\frac{(\widehat{\overline{z}}(t)-\widehat{\overline{z}}(t'))^2-(\overline{z}(t)-\overline{z}(t'))^2}{4(t-t')}}\right]dt's\,.
\end{aligned} \tag{A.15d}
$$

From (A.15b) and (A.3) we obtain

$$
\begin{aligned}
|V_1| \leq & \frac{\delta}{2\sqrt{\pi}\,\beta_2}\,[\alpha+2(1+M\sigma)\gamma]\left|\int_0^t \frac{1}{\sqrt{t-t'}}\,e^{-\frac{(\overline{z}(t)-\overline{z}(t'))^2}{4(t-t')}}\,dt'\right| \\
\leq & \frac{\delta\sqrt{\sigma}}{\sqrt{\pi}\beta_2}\,[\alpha+2(1+M\sigma)\gamma] < \frac{\delta\sqrt{\sigma}}{\sqrt{\pi}\beta_2}\,[\alpha+2(1+M)\gamma] \equiv B_4\,\delta\sqrt{\sigma}.
\end{aligned} \tag{A.16a}
$$

In order to evaluate the estimate of $|V_2|$ we take into account (A.15c), together with (A.2) and (A.8)

$$
|V_2| \leq \frac{M}{2\sqrt{\pi}}\int_0^t \left|\frac{(\overline{z}(t)-\widehat{\overline{z}}(t))-(\overline{z}(t')-\widehat{\overline{z}}(t'))}{(t-t')}\right|\,\frac{dt'}{\sqrt{t-t'}}.
$$

Now, using the mean value theorem, we obtain

$$|V_2| \leq \frac{M}{2\sqrt{\pi}} \int_0^\sigma |\dot{\overline{z}}(\theta) - \dot{\widehat{\overline{z}}}(\theta)| \, \frac{dt'}{\sqrt{t-t'}} < \frac{M}{\sqrt{\pi}} \, (A_3 + A_4) \, \delta \, \sqrt{\sigma} \equiv B_5 \, \delta \, \sqrt{\sigma}. \quad \text{(A.16b)}$$

For the estimate of V_3, we put in (A.15d)

$$\begin{aligned} Q &= - \, \frac{[(\widehat{\overline{z}}(t) - \widehat{\overline{z}}(t'))^2 - (\overline{z}(t) - \overline{z}(t'))^2]}{4(t-t')} \\ &= - \, \frac{1}{4(t-t')} [(\widehat{\overline{z}}(t) - \overline{z}(t)) - (\widehat{\overline{z}}(t') - \overline{z}(t'))][(\widehat{\overline{z}}(t) - \widehat{\overline{z}}(t')) - (\overline{z}(t) - \overline{z}(t'))] \end{aligned}$$

and using (A.3) and (A.7) we get

$$\begin{aligned} |Q| \leq & \frac{1}{4|t-t'|} \; [2(A_3 + A_4) \, \delta t] \left[2 \frac{|t-t'|}{\beta_2} (\alpha + 2(1 + M\,\sigma)\,\gamma) \right] \\ < & \frac{(A_3 + A_4)[\alpha + 2(1+M)\,\gamma]}{\beta_2} \, \delta \, \sigma = (A_3 + A_4) \, B_2 \, \delta \, \sigma. \end{aligned}$$

On the other hand, from (A.3) it also follows that

$$|Q| \leq \frac{4B_2^2 |t-t'|^2}{4|t-t'|} < B_2^2 \, \sigma < B_2, \qquad (B_2 \, \sigma < 1)\,.$$

From (A.15d), using the inequality $|1 - e^{-Q}| \leq |Q| e^{|Q|}$ [2] together with (A.3), we then obtain

$$\begin{aligned} |V_3| \leq & \frac{1}{2\sqrt{\pi}} \, M \int_0^t \left| \frac{\widehat{\overline{z}}(t) - \widehat{\overline{z}}(t')}{t - t'} \right| \, \frac{|1 - e^{-Q}|}{\sqrt{t-t'}} \, dt' \\ < & \frac{MB_2}{\sqrt{\pi}} \, |Q| e^{|Q|} \, \sigma < \frac{MB_2^2}{\sqrt{\pi}} \, (A_3 + A_4) \, e^{B_2} \, \delta \, \sigma \sqrt{\sigma}, \end{aligned}$$

which gives :

$$|V_3| < B_6 \, \delta \, \sqrt{\sigma}, \quad \text{(A.16c)}$$

where

$$B_6 = B_2^2 \, (A_3 + A_4) \quad \text{and} \quad \frac{M}{\sqrt{\pi}} \, e^{B_2} \, \sigma < 1.$$

From (A.15a) and (A.16a)-(A.16c) we then get:

$$|H_3| < 2(B_4 + B_5 + B_6) \, \delta \sqrt{\sigma} \equiv B_7 \, \delta \sqrt{\sigma}. \quad \text{(A.17)}$$

Finally, we go back to (A.9a) and put together the estimates given by (A.13), (A.14) and (A.17) obtaining

$$\frac{||w - \widehat{w}||}{\delta} < (B_3 + B_4 + B_7)\sqrt{\sigma} \equiv B_8\sqrt{\sigma}.$$

We can therefore conclude that T is a contraction operator in S_M. By the fixed point theorem in a Banach space [9, 56], there exists a unique fixed point
$h(t) = Th(t)$ in S_M for $0 \leq\ t <\ \sigma$.
We now observe that existence of the Neumann datum $h(t)$ of the linear heat equation for small times, imply existence and uniqueness of both the solution of the linear problem $\varphi(z,t)$ and of the function $C(t)$ (see (3.10)). From (3.12a), the Neumann datum $g(t)$ of the nonlinear diffusion-convection equation is therefore determined in terms of the Dirichlet datum $f(t)$ as

$$g(t) = \frac{h(t)}{C(t)f(t)} + f(t),$$

which is the explicit form of the Dirichlet-to-Neumann map for (3.1).

Appendix B

From (3.56c) we easily get

$$\begin{aligned}|V_2|\leq & \frac{2}{3}\frac{\delta}{\sqrt{\pi D}}\left|\int_0^t \frac{1}{\sqrt{t-\tau}}\frac{d\tau}{\left(\overline{F}_0\left(t\right)+\overline{F}_0\left(\tau\right)\right)}\right| \\ & +\frac{2}{3}\frac{M_0}{\sqrt{\pi D}}\left|\int_0^t \frac{1}{\sqrt{t-\tau}}\left[\frac{1}{\left(\overline{F}_0\left(t\right)+\overline{F}_0\left(\tau\right)\right)}-\frac{1}{\left(F_0\left(t\right)+F_0\left(\tau\right)\right)}\right]d\tau\right|.\end{aligned} \tag{B.1}$$

The above relation implies

$$\begin{aligned}|V_2|\leq & \frac{2}{3}\frac{\delta}{\sqrt{\pi D}}\frac{1}{b}\sqrt{t} \\ & +\frac{2}{3}\frac{M_0}{\sqrt{\pi D}}\int_0^t \frac{1}{\sqrt{t-\tau}}\frac{\left(|F_0\left(t\right)-\overline{F}_0\left(t\right)|+|F_0\left(\tau\right)-\overline{F}_0\left(\tau\right)|\right)}{|\overline{F}_0\left(t\right)+\overline{F}_0\left(\tau\right)||F_0\left(t\right)+F_0\left(\tau\right)|}d\tau.\end{aligned} \tag{B.2}$$

By using (3.48) in the second term of (B.2), we get

$$|V_2| \leq \frac{2}{3}\frac{1}{\sqrt{\pi D}}\frac{1}{b}\left(\delta\sqrt{\sigma}+\frac{M_0\lambda}{b}B_1\delta\sigma^{3/2}\right), \tag{B.3}$$

where is $0 \leq \tau < t < \sigma$.
From (B.3) we can therefore conclude

$$|V_2| \leq B_7\delta\sqrt{\sigma_{10}}, \qquad B_7 = \frac{2}{3}\frac{1}{\sqrt{\pi D}}\frac{1}{b}\left(1+\frac{M_0\lambda B_1}{b}\right) \tag{B.4}$$

with $\sigma_{10} : B_7\sqrt{\sigma_{10}} \leq 1$, which coincides with (3.59).

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