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Kurzfassung

In dieser Arbeit behandeln wir Netzwerkstrukturen in biologischen Systemen. Wir untersuchen, wie sich eine Flüssigkeit in einem porösen Medium verhält, welches die Intensität und Fließrichtung beeinflusst. Das Verhalten der Flüssigkeit wird durch den sogenannten Permeabilitätstensor bestimmt, dessen Wirkung auf den Gradienten des Druckes die Richtung des Flusses bestimmt. Der Permeabilitätstensor hängt normalerweise von der Konduktivität des Mediums ab, welche beschreibt, wie einfach es für die Flüssigkeit ist, in einem Punkt zu fließen und was die beste Richtung dafür ist.

Zuerst demonstrieren wir Murray's Gesetz für ein diskretes Modell mit einem allgemeinen metabolischen Koeffizienten und verallgemeinern es dann für ein kontinuierliches System durch Grenzwertbildung des diskreten Modells auf einem rechteckigen Gitter. Danach reinterpretieren wir Murray's Gesetz für die stationären Zustände eines kontinuierlichen Systems, das durch phänomenologische Überlegungen motiviert wird.

In der Arbeit untersuchen wir außerdem ein kontinuierliches Modell, das auch die Evolution des Permeabilitätstensors als einen formalen L^2 -Gradientenflusses eines Energiefunktional, das aus einem Diffusionsterm, einem metabolischen sowie einem kinetischen Term besteht, berücksichtigt. Wir werden auch hier die stationären Zustände und die Konvexität diskutieren. Weiters präsentieren wir eine formale Herleitung dieses Systems in zwei Dimensionen als Limes des diskreten Netzwerkmodells, das auf einer unstrukturierten Triangulation definiert ist, indem die Länge der Kanten gegen Null geht.

Als letztes präsentieren wir die ersten Resultate einer noch nicht finalisierten Arbeit, in der wir eine Energie für die skalare Konduktivität betrachten, die eine diffusen, einen kinetischen und einen metabolischen Term aufweist. Insbesondere hoffen wir, die Existenz einer Γ -Konvergenz in diesem Fall zeigen zu können.

Abstract

In this thesis we study the formation of network structures in biological systems. To be more precise, we consider a fluid moving through a porous medium, which influences the movement of the fluid both in direction and intensity. The flux of the fluid is governed by the so-called permeability tensor, whose action on the gradient of the pressure gives the direction of the flux. The permeability tensor usually depends on the conductivity of the medium, which describes how easy it is for the fluid to move in a point and what is the best direction to do so.

We first demonstrate Murray's law for a discrete model with general metabolic coefficient and then generalise the law for a continuous system, which was obtained from the continuous limit of the discrete model on a rectangular mesh. We proceed by reinterpreting Murray's law for the steady states of a vector model, derived from phenomenological considerations.

As a next step, we study a continuous model which takes into consideration the evolution of the permeability tensor as a formal L^2 -gradient flow of an energy functional, consisting of a diffusion term, a metabolic and a kinetic term. We investigate its convexity and the properties of the steady states. Moreover, we present a formal derivation of this system in two dimensions as a limit of the discrete network model defined on an unstructured triangulation as the maximal length of the edges goes to zero.

Lastly, we present the first results of a work in progress, which considers an energy for a scalar conductivity that contains a diffusive term, a kinetic part and a metabolic one. In particular, we aim to prove the existence of a Γ -limit for this energy, as the diffusion coefficient goes to zero.

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1 Introduction

Planar reticular networks are ubiquitous in nature and engineering; few examples include for instance the arterial vasculature in the mammalian neocortex, urban street grids, or the vascular network of plant leaves [58]. Robust networks are built on a complex trade-off between cost, transport efficiency, and fault tolerance. They are constantly adapting to the environment and they are the result of successive rounds of evolutionary selection. Thus, they have reached a point at which cost, efficiency, and resilience are balanced. Moreover, they often develop without centralized control [70].

An interesting example is given by the vascular system. It constitutes a complex organised structure that conducts oxygen and nutrition to almost all the tissues in the body, efficiently removes waste products, and it is used by cells of the immune system to quickly transport leukocytes to an inflammation site [21]. Despite the fact that certain features of the vascular system vary with different functional requirements at different locations (for example a difference in the blood pressure), the overall general architecture and cellular composition of blood vessels is the same throughout all the cardiovascular system [50]. Moreover, it has been observed that a common mechanism guides the development of blood vessels and nerves and therefore the two systems share a similar branched structure [22].

A second important example is represented by the design and function of leaf venation, central to the well functioning of the plant. The vein xylem transports water from the roots to the leaves, while the phloem transports sugars from the leaves to the rest of the plant. Leaf venation systems vary strongly across different plant lineages, but many species show an articulated reticulation. Despite the diversities, the vein structures share key architectural elements, e.g. a hierarchy of vein orders based on vein diameter and branching, which forms a reticulate mesh. This structure evolves early in angiosperms and confers a high transport capacity relative to construction cost [60,61]. Together with the transport of nutrients and water for photosynthesis and transpiration, leaf veins provide mechanical support to orient the leaf towards light [53]. The influence of the external environment could bring one of the branches to break, causing the death of a whole part of the system. In order to protect themselves from such damages, these structures often develop loops in the networks [60]. Moreover, it has been suggested that loops may also arise as an adaptation to the varying water demands in different areas of the leaf [59].

The diversity and complexity of the processes that lead to the formation of similar structures in diverse biological systems exerts a broad interest in recent research, due to their numerous and useful applications in medicine or engineering. Because of this, many models have been developed in the last years in various mathematical fields.

Traditionally, many studies of transportation networks are set in a discrete framework. In [9], the authors analyse optimal shapes of steady states in a discrete setting, in dependence of the cost function adopted to describe the process of transporting material. They prove that the shape (convexity or concavity) of the cost function for local transportation of material impacts directly on the topology (the presence or absence of loops) of the emergent networks that minimise the total cost of transportation. In [30] a discrete model for auxin transportation in leaves venation is introduced; it is numerically shown that in this framework are generated structures that connect a source and sink for the auxin with a mid-vein, producing branching in the patterns. Discrete mathematical models support also important biological observations, such as that fluctuations in the flux can give rise to a

different class of optimal structures, which contain loops while retaining the hierarchical organization of trees [18, 57]. Moreover, in [41] the authors mathematically prove that loops can arise also as a result of resilience to damage .

Continuous models are often easier to analyse and simulate than discrete ones and are often obtained as a mean-field approximation of a two-dimensional lattice-based discrete model [54]. For a comparison of non-linear mean-field models derived from discrete-to-continuum approaches see for example [47]. Alternatively, to describe the angiogenesis, the cellular mechanism that remodels the primitive embryonic vasculature into a mature vascular structure, various chemotaxis models have been suggested ([28, 71]). For example, in [65] the authors (supported by experimental observations) proposed a model based on the assumption that cells communicate via a chemoattraction factor. An interesting model for angiogenesis has been suggested in [1]. Here the authors focus the attention on the blood flow, instead of the cells forming the vessels, and assimilate the tissue to a porous medium in which blood moves under the influence of a pressure gradient. The blood velocity is assumed to follow Darcy's law. A review of different models for angiogenesis can be found in [63].

Recently, hybrid models have been developed, using a continuous approach to represent certain quantities of interest (e.g., the concentration of a drug), and discrete or stochastic methods to describe the behaviour of other quantities, for example cells ([7, 8, 49, 68, 72]). This approach allows to better analyse the interplay between the micro and macro-scale behaviours.

In this thesis we analyse various models of biological transportation network in porous media. The fluid movement is influenced by the presence of the medium, both in its direction and intensity. In this setting, the hydraulic conductivity represents an important physical variable. It models the ability of vascular plants, soil, or rock to let the fluid pass through the pores and fractures of the medium at a particular time scale. It is related to physical properties such as particle size distribution, shapes of the particles, effective porosity, and it changes depend on the properties of the porous medium, as well as density and viscosity of the liquid [64].

The hydraulic conductivity over a control volume can be either isotropic or anisotropic. In the first case, the values of the hydraulic conductivity are independent of the direction; therefore, this quantity is mathematically represented as scalar. However, this quantity may be not homogeneous in space, since the medium may consist of different materials. Conversely, if the conductivity over a volume differs for different directions, the hydraulic conductivity is said to be anisotropic. In general, a porous medium may be homogeneous and nevertheless anisotropic, or it may be heterogeneous and yet isotropic at each location. In most cases, mediums exhibit both heterogeneity and anisotropy [81]. For example, different orientation of non-symmetric particles produces flow channels parallel to their main plane, which allows the fluid to flow with little resistance. However, in the direction perpendicular to the flat surface of particles the flux must detour and take more tortuous and longer paths [10, Chapter 5] . In the case of soil, a stratified medium might consist of layers of clay, silt, and sand. In each layer an homogeneous and isotropic conductivity could be defined at a local-scale, but at a macroscopic scale the hydraulic conductivity becomes anisotropic. In order for a stratified formation of this kind to be qualified as an anisotropic homogeneous medium, the thickness of the individual layers should be much smaller than the length of interest [81]. In many aquifers fractures produce very high flux in the direction along them, while the permeability of the rock in the direction normal to the fractures is much smaller. In some rocks the flow of water through them dissolves the rock, creating channels that develop mainly in the direction of the flow, giving an anisotropic medium with a very high permeability in the general direction of these channels [10, Chapter 5].

How the flow direction is influenced by the conductivity of the system is mathematically described by Darcy's law, a fundamental principle in the studying of fluid flow in porous medium. It assumes that

the conductivity influences the flux q by acting on the gradient of the pressure ∇p through a matrix called *permeability tensor* $\mathbb{P}$, via the formula

$$q = -\mathbb{P}\nabla p.$$

If the medium is isotropic, the permeability tensor assumes the form $r(x)\mathbb{I}$, where $\mathbb{I}$ is the identity matrix and $r(x) \geq 0$ is a scalar quantity. If the conductivity is anisotropic, the permeability tensor is represented by a symmetric, positive semi-definite matrix. For a more detailed description of this phenomenon, we refer to [10].

In the following section, we will introduce three mathematical models that have been developed in the last years to describe this phenomenon. The first one is a discrete model introduced by Hu and Cai [39]. The same authors proposed also a continuous model, which has lately been analysed in the series of papers [2, 3, 33, 34]. The third one is a continuous tensor model, in which the conductivity is represented by a diagonal matrix. The model has been introduced in [31, 32] and was obtained as the Γ -limit of the discrete model as the length of the edges of the graph goes to zero, in the particular case in which the graph is a rectangular equidistant grid.

In Section 1.2 we give an overview of what will be in more detailed presented in Chapter 2. This consists of a work carried out with Professor Peter Markowich and Jan Haskovec, published in [35], in which we generalise the so called Murray's law for the three models mentioned above.

Section 1.3 introduces what will be presented in details in Chapter 3. This collects the results of the work published with Professor Peter Markowich and Jan Haskovec in [36], where we introduce a new model in which the conductivity assumes the more general shape of a symmetric positive semi-definite matrix.

Lastly, Section 1.4 summarises the results obtained until this moment in collaboration with Professor Christian Schmeiser and Professor Benedikt Wirth. The goal of this work is to prove Γ -convergence of the energy corresponding to a scalar model to a suitable one in which the minimisers recover the tree-shaped support we would expect in the studied biological phenomena.

1.1 Introduction of the three models

In the discrete setting, the edges of a graph represent the pipes of the system in which the fluid moves. Since the direction is dictated by the pipes, the conductivity is represented by a scalar function defined on the edges. In a continuous setting, in which the fluid can in principle move freely in any direction, the presence of the medium influence the flux both in intensity and in the direction. In this case the conductivity is assumed to be a vector-valued variable, pointing in the easiest direction in which the fluid can move. All the models share the same basic assumptions, focusing on the interplay between the conductivity and the flux of the fluid. Indeed, the conductivity is assumed to minimise in time the sum of a kinetic and a metabolic term, while the flux is at each time oriented following the Darcy's law.

In Section 1.1.1 we introduce the discrete model, proposed by Hu and Cai, describing the evolution of the conductivity along a fixed graph. Section 1.1.2 is dedicated to the presentation of the continuous model, first introduced in [38], in which the conductivity is represented by a vector-valued function. Finally, Section 1.1.3 of this introduction describes a continuous model constructed as the Γ -limit of the discrete model defined on a rectangular grid.

1.1.1 A discrete description

The microscopic model considered in this section was first introduced by Hu and Cai in [39], and reformulated in [3].

Let $G = (\mathbb{V}, \mathbb{E})$ be a connected undirected graph, where $\mathbb{E}$ denotes the finite set of the edges (which represent the branches of the network) and $\mathbb{V}$ the set of nodes of size $N = |\mathbb{V}|$. We assume that no vertex is connected to itself, and that for every couple of vertices $i, j \in \mathbb{V}$ there exists at most one edge connecting them. Such edge is denoted by $(i, j) \in \mathbb{E}$. Since the graph is assumed to be undirected, (i, j) and (j, i) refer to the same edge. In each vertex $i \in \mathbb{V}$ we define the unknown fluid pressure $P_i \in \mathbb{R}$, and we introduce the strength of the external flow source ($S_i > 0$) or sink ($S_i < 0$). This quantity is prescribed a priori and it is assumed to be constant in time.

On every edge we define the conductivity $C_{ij} = C_{ji} \geq 0$, and denote by $L_{ij} = L_{ji} > 0$ the edge length. This is a datum of the model and is constant in time. The drop of pressure between the vertex $i \in \mathbb{V}$ and $j \in \mathbb{V}$ is denoted by

$$(\Delta P)_{ij} := P_j - P_i.$$

Note that this quantity is antisymmetric, i.e. $(\Delta P)_{ij} = -(\Delta P)_{ji}$. The oriented flux (flow rate) from vertex $j \in \mathbb{V}$ to $i \in \mathbb{V}$ is denoted by Q_{ij} , and, as for the pressure, it satisfies $Q_{ij} = -Q_{ji}$.

We assume that the flux satisfies Darcy's law, linking on each edge its intensity to the pressure drop and the conductivity via the formula

$$Q_{ij} := C_{ij} \frac{P_j - P_i}{L_{ij}} \quad \text{for all } (i, j) \in \mathbb{E}. \quad (1.1)$$

Moreover, we assume that in each node $i \in \mathbb{V}$ the inflow and outflow flux balance the external source (or sink), i.e. the Kirchhoff law holds

$$- \sum_{j \in \mathcal{N}(i)} C_{ij} \frac{P_j - P_i}{L_{ij}} = S_i \quad \text{for all } i \in \mathbb{V}. \quad (1.2)$$

Here $\mathcal{N}(i) \subset \mathbb{V}$ denotes the set of vertices connected to $i \in \mathbb{V}$ through an edge, i.e.,

$$\mathcal{N}(i) := \{j \in \mathbb{V} : (i, j) \in \mathbb{E}\}.$$

For each fixed vector of conductivities $C = (C_{ij})_{(i,j) \in \mathbb{E}}$, the Kirchhoff law (1.2) can be rewritten as a linear system of equations for the vector of pressures $P = (P_i)_{i \in \mathbb{V}}$. A necessary condition for the solvability of the equation is the global mass conservation

$$\sum_{i \in \mathbb{V}} S_i = 0.$$

With this assumption, the system (1.2) has been proven to be solvable if and only if the graph with edge weights $C = (C_{ij})_{(i,j) \in \mathbb{E}}$ is connected [3]. In this context, only edges with positive conductivities $C_{ij} > 0$ are taken into account (i.e., edges with zero conductivities are discarded). The solution vector $P = (P_i)_{i \in \mathbb{V}}$ is unique up to an additive constant. Finally, we denote by $Q_{ij}[C]$ the corresponding fluxes, uniquely defined via (1.1).

The conductivities' evolution in time is assumed to follow an energy optimisation process, where the cost functional is defined as the sum of a kinetic term and a metabolic energy along all the edges. More precisely, the energy is defined as

$$\mathcal{E}[C] := \sum_{(i,j) \in \mathbb{E}} \left(\frac{Q_{ij}[C]^2}{C_{ij}} + \frac{\nu}{\gamma} C_{ij}^\gamma \right) L_{ij}, \quad (1.3)$$

where $\nu > 0$ is the so-called metabolic coefficient and the metabolic cost on each edge is assumed to be proportional to the $\gamma > 0$ power of the conductivity. Indeed, it has been observed that the metabolic cost to maintain the system is proportional to a power of the conductivity. In particular, the assumption $\gamma = 1/2$ well approximates the case of blood vessel systems (we recall that in a three-dimensional tube the conductivity is proportional to fourth power of the tube radius, while the metabolic cost scales quadratically with the radius, see [51]). For models of plant leaf venation the effective value of γ lies typically between $1/2$ and 1 (see e.g. [38, 39]), since the metabolic cost is proportional to the number of small tubes, and hence proportional to C_{ij} , while the metabolic loss of the photosynthetic power is proportional to the area of the venation cells, which is linked to $C_{ij}^{1/2}$. The evolution in time of the conductivities is defined as the gradient flow of the energy (1.3) under the constraint of the Kirchhoff's law (1.2), leading to the ODE system

$$\frac{dC_{ij}}{dt} = \left(\frac{Q_{ij}^2}{C_{ij}^2} - \nu C_{ij}^{\gamma-1} \right) L_{ij} \quad \text{for } (i, j) \in \mathbb{E}. \quad (1.4)$$

The authors in [39] showed that the optimal networks generated by (1.4) have a loopless tree structure. Global existence of solutions of the ODE model first proposed in [39] was shown in [31].

1.1.2 A continuous vector-valued model

Inspired by the derivation of the discrete model, Hu and Cai proposed in [38] a continuous model, which has lately been analysed in the sequence of papers [2, 3, 33, 34]. A phenomenological derivation is given in [3], and we present here the main steps.

Let $\Omega \in \mathbb{R}^d$ be a bounded domain occupied by a porous medium in which a fluid is moving, and let

the function $S : \Omega \rightarrow \mathbb{R}$ represent the external sources and sinks. The fluid is assumed to satisfy a local mass conservation law, i.e.

$$\operatorname{div} q = S \quad \text{in } \Omega, \quad (1.5)$$

where $q : \Omega \rightarrow \mathbb{R}^d$ denotes the flux of the fluid.

Moreover, we denote by $m : \Omega \rightarrow \mathbb{R}^d$ the vector conductivity of the medium. Indeed, the presence of a, anisotropic medium influences the orientation and the intensity on the flux, aligning it in a direction that is a priori different from the one of the pressure gradient. This is mathematically modelled via the continuous Darcy's law for slow flow in porous media [73], i.e.

$$q = -\mathbb{P}[m]\nabla p,$$

where $p : \Omega \rightarrow \mathbb{R}$ denotes the fluid pressure, and $\mathbb{P}[m] : \Omega \rightarrow \mathbb{R}^{d \times d}$ is the *permeability tensor*. This tensor specifies the way the medium influences the flux, and it is assumed to be dependent on the conductivity. Loosely speaking, this quantity represents at each point the "easiest" direction in which the fluid could move. The permeability tensor is defined as a symmetric, positive semi-definite matrix and its eigenvectors yield the principal directions of flow, while the eigenvalues represent the principal permeabilities. The authors [38] suggested the following structure for the permeability tensor

$$\mathbb{P}[m] := m \otimes m.$$

Note that $\mathbb{P}[m]$ admits the eigenvalue $|m|^2$ with corresponding eigenvector m , and 0 with eigenvectors orthogonal to m . Thus, it represents conduction along the direction m with conductivity $|m|^2$, while there is no conduction in directions perpendicular to m . Consequentially, we locally identify the network conductivity with the principal eigenvalue of $\mathbb{P}$, i.e., $C_i \simeq |m|^2$ in the neighbourhood of a node $i \in \mathbb{V}$. Equation (1.5) becomes

$$-\nabla \cdot ((m \otimes m)\nabla p) = S. \quad (1.6)$$

A necessary assumption for the existence of solutions is the assumption that $\int_{\Omega} S \, dx = 0$. Note that the strong degeneracy of (1.6) leads to a solvability issue. For this reason, in [2, 33, 34] the authors suggested the regularisation

$$-\operatorname{div} [(r\mathbb{I} + m \otimes m)\nabla p] = S, \quad (1.7)$$

where $\mathbb{I}$ is the identity matrix and $r : \Omega \rightarrow \mathbb{R}$, with $r(x) \geq r_0 > 0$ is a scalar function describing the isotropic background permeability of the medium. Equation (1.7) is uniformly elliptic. Equipped with homogeneous Neumann boundary condition, i.e.,

$$n \cdot \mathbb{P}[m]\nabla p = 0 \quad \text{on } \partial\Omega,$$

where $n = n(x)$ denotes the outer unit normal vector to $\partial\Omega$, equation (1.7) admits a solution which is unique up to an additive constant. The flux is instead uniquely defined by the relation $q = -\mathbb{P}[m]\nabla p$. Since, as we mentioned, the local anisotropic conductivity of the network is identified with $|m|^2$, the continuous analogue of the discrete energy functional (1.3) reads

$$\mathcal{E}[m] = \int_{\Omega} \nabla p[m] \cdot \mathbb{P}[m]\nabla p[m] + \frac{\nu}{\gamma} |m|^{2\gamma} \, dx,$$

where $p[m]$ denotes a solution to the Poisson equation (1.7) and $\mathbb{P}[m] := rI + m \otimes m$.

Note that the new permeability tensor admits m and $m^\perp$ as eigenvectors, as does the previous one. However, the corresponding eigenvalues now are $r(x) + |m|^2$ and $r(x)$ respectively. This suggests that in the direction orthogonal to m the flow "feels" the background permeability $r(x)$, allowing flux in that direction, while the principal permeability is increased by $|m|^2$ in the direction of the conductivity vector m .

The final energy considered in this model is given by

$$\mathcal{E}[m] = \int_{\Omega} D^2 |\nabla m|^2 + c^2 (\nabla p[m] \mathbb{P}[m] \nabla p) + \frac{|m|^{2\gamma}}{\gamma} dx, \quad (1.8)$$

where the diffusion term has been added to model the propagation of the network, the middle term represent the kinetic energy and the last one corresponds to the metabolic cost of the system. The evolution of the conductivity is defined as the L^2 -gradient flow of this energy, leading the function m to satisfy

$$\partial_t m = D^2 \Delta m + c^2 (m \cdot \nabla p) \nabla p - |m|^{2\gamma-2} m.$$

The first term on the right-hand side represents the random effect (Brownian process) in the network structure. The term $(m \cdot \nabla p) \nabla p$ is called *activation term* and models the driving force in the direction of the pressure gradient, while the last term is an algebraic relaxation term, corresponding to the functional derivative of the metabolic cost.

The model was first analysed in [2], and a proof of the existence of global weak solutions in the case $\gamma \geq 1$ was given in [33]. An extension of this result to the case $\gamma \geq \frac{1}{2}$, together with numerical results, was given in [34].

1.1.3 A diagonal model

First suggested in [31], the authors in [32] proved the rigorous continuous limit of the constrained discrete energy (1.3) functional defined on rectangular equidistant grid, as the edge lengths go uniformly to zero, in the case $\gamma > 1$. The discrete energy was rewritten as a sequence of integral functions which Γ -converges to the continuous energy functional

$$\mathcal{E}[c] := \int_{\Omega} \nabla p \cdot c \nabla p + \frac{\nu}{\gamma} |c|^\gamma dx,$$

where $\nu > 0$ represents again the metabolic coefficient.

The energy functional $\mathcal{E}[c]$ is defined on the set of non-negative diagonal tensor fields $c : \Omega \rightarrow \mathbb{R}^{d \times d}$

$$c = \begin{pmatrix} c^1 & & \\ & \ddots & \\ & & c^d \end{pmatrix}, \quad (1.9)$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain and $|c|^\gamma$ is defined as $\sum_{k=1}^d |c^k|^\gamma$. The scalar pressure $p : \Omega \rightarrow \mathbb{R}$ of the fluid occupying the domain Ω is defined as the solution to the Poisson equation

$$-\nabla \cdot (c \nabla p) = S. \quad (1.10)$$

As for the vector-valued model, the function $S = S(x)$ represents the external sources and sinks in the domain and it is assumed to satisfy $\int_{\Omega} S dx = 0$. Let us observe that in this case the permeability tensor can be identified with $\mathbb{P}[c] = c$, which is a symmetric, positive semi-definite matrix. The diagonal structure of the tensor was inherited from the squared structure of the grid on which the

discrete model was defined. The Poisson equation (1.10) is possibly strongly degenerate since the eigenvalues of the permeability tensor (1.9) may vanish. As done for equation (1.7), the authors introduced a regularisation

$$\mathbb{P}[c] := r\mathbb{I} + c, \quad (1.11)$$

where now the permeability tensor assumes the form

$$-\nabla \cdot (\mathbb{P}[c] \nabla p) = S. \quad (1.12)$$

The scalar function $r = r(x) \geq r_0 > 0$ is a prescribed positive function that models the isotropic background permeability of the medium, and $\mathbb{I} \in \mathbb{R}^{d \times d}$ denotes the unit matrix. The equation (1.12) is equipped with no-flux boundary condition

$$n \cdot \mathbb{P}[c] \nabla p = 0 \quad \text{on } \partial\Omega,$$

where $n = n(x)$ denotes the outer unit normal vector to $\partial\Omega$. Since only nonnegative diagonal tensor fields $c = c(x)$ are admitted, equation (1.11) is uniformly elliptic and coercive, thus, it admits solutions which are unique up to an additive constant.

In order to describe the network propagation, in [31] the authors added a diffusion term which represents the random effects in the network structure, giving the updated energy

$$\mathcal{E}[c] := \int_{\Omega} D^2 |\nabla c|^2 + \nabla p \cdot c \nabla p + \frac{\nu}{\gamma} |c|^\gamma \, dx. \quad (1.13)$$

The evolution of the conductivity has been defined as the L^2 - gradient flow of the energy (1.13), under the constraint (1.12), i.e. for every component of the diagonal matrix c ,

$$\partial_t c_i = D^2 \Delta c_i + (\partial_{x_i} p)^2 - \nu |c_i|^{\gamma-2} c_i.$$

A proof of global existence of weak solutions for such a problem has been given in [31], while in [43] the regularity properties of solutions to the corresponding Dirichlet-Neumann initial-boundary value problem in dimension $d \leq 3$ was investigated.

1.2 Murray's law

In 1926 Murray proposed a law that predicts the thickness of branches in a biological network, based on the assumption that the cost for transport and maintenance of the medium is minimised. The law has been observed in vascular and respiratory system [75], xylem in plants, and the respiratory system of insects [48, 55, 66]. In [48] the authors showed that measurements of plant xylem satisfy Murray's optimum, assuming that the structure does not have an additional support function for the plant.

In such systems, large vessels are more suitable to minimise the cost of the transport of a bulk flux across relatively large distances, while the smaller ones minimise the metabolic cost the system has to pay to maintain the structure. Murray's law is based on the idea that, although the biological world presents many diversities in the anatomical structures and physiological functions, in the "ideal" tissue large and small vessels should be connected in a way that optimises simultaneously the transport and the maintenance cost [66].

Let us consider a single tube in which a fluid with laminar flow is moving. We assume that the pumping power E_p satisfies Joule's law, i.e.

$$E_p = Q\Delta P,$$

where Q is the volumetric flux and ΔP is the pressure difference between the entry and exit point of the tube. According to the Hagen-Poiseuille law for laminar flow in a three-dimensional tube, the flux can be expressed as follows

$$Q = \frac{\pi R^4}{8\mu L} \Delta P,$$

where $R > 0$ denotes the radius of the tube, $L > 0$ its length, and $\mu > 0$ the dynamic viscosity of the fluid. Therefore, the pumping term can be written in terms of the flux as

$$E_p = \frac{8\mu L}{\pi R^4} Q^2,$$

suggesting that a bigger radius would reduce the cost of transportation.

Furthermore, the metabolic cost E_m is assumed to be proportional to the number of cells in the tube [51], which is assumed to be proportional to the tube volume, giving

$$E_m = \nu\pi LR^2,$$

where the proportionality constant $\nu > 0$ is called *metabolic coefficient*. Notice that in this case, a smaller radius would decrease the volume and therefore the metabolic cost. The total energy is defined as the sum of these two terms, reading

$$E := E_p + E_m = \frac{8\mu L}{\pi R^4} Q^2 + \nu\pi LR^2.$$

As mentioned before, the system is assumed to minimise this energy, leading to the relation between the flow rate and the tube radius

$$Q = \sqrt{\frac{\pi^2 \nu}{16\mu}} R^3. \tag{1.14}$$

Thus, in an optimal situation the flux is proportional to the third power of the radius ([51]).

We now focus our attention on a bifurcation point of the network, where we assume that a parenting

branch split into n children branches. Let us denote by $Q_0 > 0$ the flow rate of the parent branch, with $Q_1, Q_2, \dots, Q_n > 0$ the flow rate of the children branches, and by $R_0 > 0$ and $R_1, R_2, \dots, R_n > 0$ the respective radii. We assume total mass conservation in the node, i.e.

$$Q_0 = \sum_{i=1}^n Q_i.$$

The relation between radii and fluxes (1.14) allows us to rewrite the flux balance in terms of the radii, obtaining the relation

$$R_0^3 = \sum_{i=1}^n R_i^3,$$

which is known as the classical Murray's law for laminar blood flow [51, 52].

The law can also be interpreted in terms of the conductivity. Indeed, it has been observed that for a three-dimensional laminar flow the edge conductivities $C_i > 0$ are proportional to R_i^4 (see [56]). Therefore, the law can be rewritten as

$$C_0^{3/4} = \sum_{i=1}^n C_i^{3/4}. \quad (1.15)$$

The above formula represents the classical 3/4-law for optimal ratio of conductivities in three-dimensional branching edges with laminar flow [51, 52].

Chapter 2 contains the work done in collaboration with Professor Peter Markowich and Jan Haskovec, in [35], where we present a generalisation of this law for the discrete model introduced in Section 1.1.1, as well as for both the continuous vector model presented in Section 1.1.2 and the diagonal tensor model described in Section 1.1.3. We give in the following subsections an overview of these results.

Murray's law for the discrete model

In [35] we first present a reinterpretation of Murray's law for the discrete model (1.4), considering the more general case of sources or sinks situated in correspondence of the nodes of the graph. Following the strategy adopted by Murray, we first consider in each node $i \in \mathbb{V}$ Kirchhoff's law

$$-\sum_{j \in \mathcal{N}(i)} Q_{ij} = S_i,$$

which in this case models flux balance in presence of an external source (or sink). We recall that by $\mathcal{N}(i)$ we denote the collection of nodes connected via an edge to i .

By optimising the energy (1.3), we observe that on each edge the flux and the conductivity satisfy

$$|Q_{ij}| = \nu C_{ij}^{\frac{\gamma+1}{2}}.$$

The flux balance assumption in the node $i \in \mathbb{V}$ can then be written as

$$\sqrt{\nu} \sum_{j \in \mathcal{N}^+(i)} C_{ij}^{\frac{\gamma+1}{2}} + S_i = \sqrt{\nu} \sum_{j \in \mathcal{N}^-(i)} C_{ij}^{\frac{\gamma+1}{2}} \quad \text{for all } i \in \mathbb{V}.$$

This formulation generalises Murray's law to the case in which external sources and sinks are present, and to the more general setting in which the metabolic cost is proportional to a general power of the conductivity. The case $\gamma = 1/2$ recovers the well-known 3/4 law mentioned in equation (1.15).

Murray's law for the vector model

We proceed to analyse the continuous model introduced in Section 1.1.2 in the case zero diffusion coefficient. The energy then reads

$$\mathcal{E}[m] = \int_{\Omega} c^2 (\nabla p[m] \mathbb{P}[m] \nabla p) + \frac{|m|^{2\gamma}}{\gamma} dx,$$

where we recall that the pressure satisfies the constraint

$$-\operatorname{div} [(r\mathbb{I} + m \otimes m) \nabla p] = S. \quad (1.16)$$

The corresponding Euler-Lagrange equation of the energy is then

$$(\nabla p \otimes \nabla p)m = \nu |m|^{2\gamma-2} m.$$

This suggests that there exists a measurable set $\mathcal{A} \subset \Omega$, on which the conductivity m is non-zero, and on which the vector m and ∇p are aligned. In particular it holds

$$\nu |m|^{2(\gamma-1)} = |\nabla p|^2 \quad \text{on } \mathcal{A}.$$

The gradient of the pressure can then be rewritten as follow

$$\nabla p = (\chi_{\mathcal{A}^+} - \chi_{\mathcal{A}^-}) \sqrt{\nu} |m|^{\gamma-2} m \quad \text{on } \mathcal{A}, \quad (1.17)$$

where we define $\mathcal{A}^+ = \{x \mid \nabla p \cdot m > 0\}$ and $\mathcal{A}^- = \{x \mid \nabla p \cdot m < 0\}$.

In [33] it was shown that steady states for which m is null on a set of positive Lebesgue measure are linearly unstable. We then adopt in the following the assumption that $\operatorname{meas}\{x \in \Omega, |m| = 0\} = 0$.

Let us now consider an open subset $\Lambda \subset \Omega$ with boundary $\partial\Lambda \in C^{0,1}$. Following the strategy adopted for the discrete case, we consider the flux balance equation, that in the continuous setting is given by the Poisson equation (1.16). Integrating it on the set Λ and using the relation between ∇p and m described in (1.17), we obtain

$$\begin{aligned} & -\sqrt{\nu} \int_{\partial\Lambda^+} (r + |m|^2) |m|^{\gamma-2} |m \cdot n| ds \\ & + \sqrt{\nu} \int_{\partial\Lambda^-} (r + |m|^2) |m|^{\gamma-2} |m \cdot n| ds = \int_{\Lambda} S dx, \end{aligned}$$

where $\partial\Lambda^+ := \{x \in \partial\Lambda : n(x) \cdot \nabla p(x) > 0\}$ and $\partial\Lambda^- := \{x \in \partial\Lambda : n(x) \cdot \nabla p(x) < 0\}$. This is Murray's law for the linearly stable solutions of the phenomenological continuous model in the case where there is no diffusion coefficient.

In this thesis we present the result in more details, and also extend it to the case with positive diffusion coefficient, as well as to the case in which the vector conductivity assumes value zero on a set with positive measure.

Murray's law for the diagonal model

In [31] the authors derived the formal continuous limit of the discrete model (1.2), (1.3) on rectangular equidistant grids, and the rigorous limit passage was studied in the paper [32]. The resulting continuous energy functional reads

$$\mathcal{E}[c] := \int_{\Omega} \nabla p \cdot c \nabla p + \frac{\nu}{\gamma} |c|^\gamma dx,$$

where $\nu > 0$ is the metabolic coefficient $\nu > 0$ and we assume the exponent $\gamma > 1$. As mentioned, the energy functional $\mathcal{E}[c]$ is defined on the set of nonnegative diagonal tensor fields $c = c(x)$ on a bounded domain $\Omega \subset \mathbb{R}^d$, and the scalar pressure $p : \Omega \rightarrow \mathbb{R}$ of the fluid is subject to the Poisson equation

$$-\nabla \cdot (c \nabla p) = S, \quad (1.18)$$

equipped with no-flux boundary condition on $\partial\Omega$. The datum $S = S(x)$ represents the intensity of sources and sinks in Ω . Due to the possible degeneracy of equation (1.18), in [31] the authors introduced the following regularisation

$$-\operatorname{div} [(r\mathbb{I} + c)\nabla p] = S. \quad (1.19)$$

It can be shown that the Euler-Lagrange equations for each component c^k of the diagonal tensor are

$$(\partial_{x_k} p)^2 - \nu |c^k|^{\gamma-1} = 0, \quad \text{for } k = 1, \dots, d.$$

The partial derivatives of the pressure can then be written in dependence of the conductivity diagonal tensor as

$$\partial_{x_k} p = (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) \sqrt{\nu} |c^k|^{\frac{\gamma-1}{2}}, \quad \text{for } k = 1, \dots, d,$$

where for each component $k = 1, \dots, d$ the disjoint Lebesgue-measurable set $\mathcal{A}_k^+$ (resp. $\mathcal{A}_k^-$) is defined as $\mathcal{A}_k^+ = \{x \mid \partial_{x_k} p(x) c^k(x) \geq 0\}$ (resp. $\mathcal{A}_k^- = \{x \mid \partial_{x_k} p(x) c^k(x) \leq 0\}$).

Let $\Lambda \subset \Omega$ be an open subset with boundary $\partial\Lambda \in C^{0,1}$. By plugging this new formulation of the pressure into the Poisson equation (1.19), we can rewrite it in terms of the conductivity, and by integrating it on the set Λ we obtain

$$-\sqrt{\nu} \int_{\partial\Lambda} \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) |c^k|^{\frac{\gamma-1}{2}} (r + c^k) n_k \, ds = \int_{\Lambda} S \, dx. \quad (1.20)$$

We recall that the flux is defined as the vector $q = -(rI + c)\nabla p$, and we define the inflow and outflow segments of $\partial\Lambda$ as

$$\partial\Lambda^+ := \{x \in \partial\Lambda : n(x) \cdot q(x) < 0\}, \quad \partial\Lambda^- := \{x \in \partial\Lambda : n(x) \cdot q(x) > 0\}.$$

We can then write equation (1.20) as

$$\begin{aligned} & -\sqrt{\nu} \int_{\partial\Lambda^+} \left| \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) |c^k|^{\frac{\gamma-1}{2}} (r + c^k) n_k \right| \, ds \\ & + \sqrt{\nu} \int_{\partial\Lambda^-} \left| \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) |c^k|^{\frac{\gamma-1}{2}} (r + c^k) n_k \right| \, ds = \int_{\Lambda} S \, dx. \end{aligned}$$

This is Murray's law for the continuous model, in which the two terms on the left-hand side represent the difference of in- and outgoing fluxes through the boundary $\partial\Lambda$, which is balanced by the volume integral of the external in- and outflows $S = S(x)$.

As done for the vector model, a generalisation of this law for the model considering a diffusion term is presented in [35].

1.3 A Tensor Model

The second chapter of this thesis contains results archived with Professor Peter Markowich and Jan Haskovec, and published in [36]. We derive a PDE model describing the evolution in time of the permeability tensor. Its derivation is strongly inspired by the one presented in Section 1.1.2. Let $\Omega \subset \mathbb{R}^d$ be a bounded domain occupied by a porous medium, and a fluid moving through it. We denote by $q : \Omega \rightarrow \mathbb{R}^d$ the flux of the fluid, and by $S : \Omega \rightarrow \mathbb{R}$ the density of external sources and sinks. This function is assumed to be constant in time, and satisfying $\int_{\Omega} S \, dx = 0$. Moreover, we assume that the local mass conservation law holds, i.e.

$$\nabla \cdot q = S \quad \text{in } \Omega.$$

Because of the presence of the medium, the space in which the fluid moves is not isotropic, influencing the direction in which the fluid goes. We model this effect via the Darcy's law for slow flow in porous media (see [73]). The influence of the medium on the flux intensity and direction is modelled via the action of a matrix, called *permeability tensor*, on the gradient of the pressure. The permeability tensor is defined as a symmetric, positive semi-definite matrix, and its eigenvectors yield the principal directions of flow. We assume the tensor to be of the form

$$\mathbb{P}[\mathbb{C}] = r\mathbb{I} + \mathbb{C},$$

where $r\mathbb{I}$ describes the isotropic influence of the medium, while the matrix-valued variable $\mathbb{C} : \Omega \rightarrow \mathbb{R}^{d \times d}$ describes the anisotropic conductivity of the substrate and is assumed to be symmetric and positive semi-definite. This term can be interpreted as a generalisation of the matrix $m \otimes m$ introduced in the vector model studied in [3] and briefly introduced in Section 1.1.2. Darcy's law then reads

$$q = -\mathbb{P}[\mathbb{C}] \nabla p,$$

where $p : \Omega \rightarrow \mathbb{R}$ denotes the scalar pressure of the fluid.

The mass conservation law in terms of the pressure and the permeability tensor reads

$$-\nabla \cdot [(r\mathbb{I} + \mathbb{C}) \nabla p] = S,$$

equipped with homogeneous Neumann boundary conditions

$$n \cdot \mathbb{P}[\mathbb{C}] \nabla p = 0 \quad \text{on } \partial\Omega,$$

where n denote the outer unit normal vector to $\partial\Omega$. For each fixed symmetric positive semi-definite matrix $\mathbb{C}$, this equation admits a solution p , unique up to an additive constant, while the flux $q = -\mathbb{P}[\mathbb{C}] \nabla p$ is uniquely defined.

We recall that in the vector model presented in Section 1.1.2, the conductivity of the system was identified with the quantity $|m|^2 = |m \otimes m|$, where in the right-hand side $|\cdot|$ denotes the Frobenius norm. We mentioned that the matrix $r\mathbb{I} + \mathbb{C}$ can be read as a generalisation of the previous permeability tensor $r\mathbb{I} + m \otimes m$, thus it is natural to identify the local conductivity of the network with $|\mathbb{C}|$.

We introduce the energy

$$\mathcal{E}[\mathbb{C}] = \int_{\Omega} \frac{D^2}{2} |\nabla \mathbb{C}|^2 + \nabla p[\mathbb{C}] \cdot \mathbb{P}[\mathbb{C}] \nabla p[\mathbb{C}] + M(\mathbb{C}) \, dx.$$

The first term represents random effects in the network structure. The second one models the kinetic energy, while the last part generalises the metabolic cost the system has to pay to maintain the network structure. We assume $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ to be an increasing function satisfying $M(0) = 0$. Notice that the case $M(s) = s^\gamma$ corresponds to the assumptions made in the vector-valued model (1.8). The evolution in time of the matrix $\mathbb{C}$ is defined as the L^2 -gradient flow of such energy, leading to the equation

$$\partial_t \mathbb{C} = D^2 \Delta \mathbb{C} + \nabla p \otimes \nabla p - \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C}.$$

In [36] we present a formal derivation from the discrete model in a 2D setting. Moreover, we show that for convex metabolic cost functions M the energy functional is convex. For a strictly convex metabolic function M and $D > 0$, we prove the existence of unique steady states using standard arguments from calculus of variations. Indeed, contrarily to the vector-field model, a convex metabolic term leads to a convex energy, due to the linear dependence on the matrix $\mathbb{C}$ in Darcy's law, which was instead quadratic in the vector setting.

We also study the steady states of the system, both for $D > 0$ and $D = 0$.

1.4 A Γ -convergence

The last chapter of this thesis consists of a preliminary study of a PDE model describing the formation of network structures in which a diffusion coefficient is present. The aim of this work is to understand structural properties of the minimisers, by proving a Γ -convergence of the corresponding energies to a suitable limit as the diffusion coefficient D tends to zero.

We consider a fluid moving through a porous medium in the space $\Omega \subset \mathbb{R}^d$, which is assumed to be a bounded domain with regular boundary. We introduce the functions $u : \Omega \rightarrow \mathbb{R}$, that represents the scalar conductivity of the system, and $p : \Omega \rightarrow \mathbb{R}$ the pressure of the fluid. The evolution in time of the conductivity is described by the equation

$$\partial_t u = D^2 \Delta u + c^2 u |\nabla p|^2 - |u|^{2\gamma-2} u, \quad (1.21)$$

where the diffusion term represents random effects in the network structure, the second term models the influence of the fluid on the system, and the last term represents the functional derivative of the metabolic cost to maintain the network.

For any given u , the pressure function is defined as the solution to the equation

$$-\operatorname{div} [(r + u^2) \nabla p] = S, \quad (1.22)$$

equipped with homogeneous Neumann boundary conditions. The function $S : \Omega \rightarrow \mathbb{R}$ models the presence of external sources or sinks, and it is assumed to be constant in time with mean zero, i.e. $\int_{\Omega} S \, dx = 0$. Under these assumptions, equation (1.22) admits a solution, which is unique up to an additive constant.

Equation (1.21) can be interpreted as the L^2 -gradient flow of the energy

$$\tilde{\mathcal{E}}[u] = \int_{\Omega} \frac{D^2}{2} |\nabla u|^2 + c^2 \nabla p (r + u^2) \nabla p + \frac{|u|^{2\gamma}}{\gamma} \, dx.$$

1.4.1 Connection with the vector model

In the model introduced in Section 1.1.2, the vector variable m represents the conductivity of the system, and the pressure of the fluid satisfies

$$-\operatorname{div} [(r \mathbb{I} + m \otimes m) \nabla p] = S,$$

where S has been introduced above. The evolution in time of the vector-conductivity was defined as the L^2 -gradient of the energy

$$\tilde{\mathcal{E}}[m] = \frac{1}{2} \int_{\Omega} D^2 |\nabla m|^2 + c^2 \nabla p (r \mathbb{I} + m \otimes m) \nabla p + \frac{|m|^{2\gamma}}{\gamma} \, dx,$$

where the second term of the energy represents the kinetic energy and the last one the metabolic cost that has to be paid to maintain the system. The model was inspired by the discrete one presented in Section 1.1.1. However, in the discrete setting the diffusion term was not present and it was added in the continuous case to model the propagation of the network support in space. Indeed, in the discrete setting the network structure was fixed a priori and just the loss of the edges was possible. When the diffusion coefficient is neglected, the steady states satisfy

$$(m \cdot \nabla p) \nabla p = |m|^{2\gamma-2} m. \quad (1.23)$$

This suggests that, in absence of the diffusion term, the directions of the conductivity and the pressure gradient are aligned. Moreover, since for every given solution (m, p) of (1.23), the couple $(-m, p)$ is also a solution, we can assume that the conductivity and the pressure gradient point in the same direction, i.e. $m \cdot \nabla p \geq 0$.

Taking this into account, and denoting the absolute value of the conductivity by $u = |m|$, equation (1.4.1) can be rewritten in terms of the new variable as

$$-\operatorname{div}[(r + u^2)\nabla p] = S, \quad (1.24)$$

while the equation for the steady states reads

$$u|\nabla p|^2 = -|u|^{2\gamma-2}u. \quad (1.25)$$

Solutions of equation (1.25) can be interpreted as the steady states of the L^2 -gradient flow of the energy

$$\tilde{\mathcal{E}}[u] = \frac{1}{2} \int_{\Omega} c^2 \nabla p (r + u^2) \nabla p + \frac{|u|^{2\gamma}}{\gamma} \, dx,$$

where p is a solution to equation (1.24).

Inspired by what has been previously done for the vector model (see for example [3] and other works), we add again a diffusion term in the energy, which models randomness in the formation of the network structure.

The new energy is then

$$\tilde{\mathcal{E}}_D[u] = \frac{1}{2} \int_{\Omega} D^2 |\nabla u|^2 + c^2 \nabla p (r + u^2) \nabla p + \frac{|u|^{2\gamma}}{\gamma} \, dx,$$

where the pressure p satisfies (1.24). This leads to the diffusive equation

$$\partial_t u = D^2 \Delta u + u|\nabla p|^2 - |u|^{2\gamma-2}u.$$

Although solutions of this equation do not coincide with the time evolution of $|m|$, we expect that for small values of the diffusion coefficient D the steady states of this equation can represent a good approximation of the ones of the vector model. Under the assumption $\gamma > \frac{1}{2}$, the existence of global solutions can be proven following the strategy adopted for the vector model in [33].

In Chapter 4, we assume no regularisation of the Poisson equation, which hence reads

$$-\operatorname{div}[(u^2)\nabla p] = S.$$

Moreover, we introduce the new flux variable $q : \Omega \rightarrow \mathbb{R}^d$ defined as $q := -u^2 \nabla p$, which is assumed to satisfy

$$\operatorname{div} q = S. \quad (1.26)$$

In our work we aim to study the Γ -convergence, as the diffusion D coefficient goes to zero, of a rescaled version of the energy written in the new variable, which reads

$$\tilde{\mathcal{E}}_D[u] = D^{\frac{\gamma-1}{2}} \frac{1}{2} \int_{\Omega} D^2 |\nabla u|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \, dx,$$

under the constraint (1.26). The rescaling is performed to ensure that all the terms have the same magnitude.

In order to obtain the result, we put the problem in the more general setting of vector measures, which will be introduced in details in the chapter.

It has been shown that a vector measure q satisfying the constraint $\operatorname{div} q = S^+ - S^-$ can be decomposed as

$$q = \lambda_q \theta_q \mathcal{H}^1 \llcorner \Sigma_q + q^\perp,$$

where $\Sigma_q \subset \mathbb{R}^d$ is a 1-rectifiable set, and $q^\perp$ is a diffusive measure (see [67]). We aim to prove that the limit energy assumes the form

$$\mathcal{E}[q] = \begin{cases} \int_{\Sigma_q} \tau(\lambda_q(x)) \, d\mathcal{H}^1, & \text{if } q^\perp = 0, \\ +\infty & \text{otherwise.} \end{cases}$$

where τ is a positive, subadditive function. Minimisers of energies of this type are known to show interesting structures in their support. More details and a more precise definition of the mathematical setting will be given in Chapter 4. In this part of the thesis, we give a brief introduction to the concept of Γ -convergence and some basic results in the field of Optimal Network Transportation. We proceed identifying the suitable cost τ needed to define the limit energy, and we present a proof of the Γ -liminf inequality. The two more steps needed to prove convergence of the minimisers, i.e. equicoercivity and the Γ -limsup inequality, are still object of study and will be treated in future work.

The results contained in this chapter are part of a work in progress done in collaboration with Christian Schmeiser and Benedikt Wirth.

1.5 Declaration of Authorship

Chapter 2 is a joint work with Jan Haskovec (King Abdullah University of Science and Technology) and Professor Peter Markowich, published in Mathematical Models and Methods in Applied Sciences (2019) (see [35]).

Chapter 3 also consists also of a joint work with Jan Haskovec (King Abdullah University of Science and Technology) and Professor Peter Markowich and has been published in Communications in Mathematical Sciences (see [36]).

Chapter 4 contains results obtained so far in an ongoing collaboration with Professor Christian Schmeiser and Professor Benedikt Wirth (Department of Mathematics, University of Münster).

All of these works are based on discussions and exchange of ideas with my co-authors.

2 Murray's law

2.1 Introduction

Murray's law is a basic physical principle for transportation networks which predicts the thickness or conductivity of branches, such that the cost for transport and maintenance of the transport medium is minimized. This law is observed in the vascular and respiratory systems of animals, xylem in plants, and the respiratory system of insects [55, 66]. In [48] the authors showed that their measurements of plant xylem are conform with Murray's optimum as long as the structure does not have an additional support function for the plant. It is also a powerful biomimetics design tool in engineering and has been applied in the design of microfluidic devices, self-healing materials, batteries, photocatalysts, and gas sensors; see, e.g., Refs. [4], [23], [69], [82].

Murray's original analysis [51, 52] is based on the assumption that the radii inside a lumen-based system are such that the work for transport and upkeep is minimized. Larger vessels lower the expended energy for transport (pumping power), but increase the overall volume of blood in the system, which requires metabolic support. Murray's law reflects the optimum balancing of the pumping power versus metabolic expenditure. Assuming laminar flow in a single tube, the pumping power E_p is given by the Joule's law,

$$E_p = Q\Delta P,$$

where Q is the volumetric flux and ΔP is the pressure difference between the entry and exit of the tube. According to the Hagen-Poiseuille law for laminar flow in a three-dimensional tube,

$$Q = \frac{\pi R^4}{8\mu L} \Delta P, \quad (2.1)$$

where $R > 0$ is the radius of the tube, $L > 0$ its length, and $\mu > 0$ the dynamic viscosity of the fluid. Therefore, we have

$$E_p = \frac{8\mu L}{\pi R^4} Q^2.$$

Furthermore, we assume that the metabolic cost E_m is proportional to the number of blood cells in the tube [51], and that is proportional to the tube's volume,

$$E_m = \nu\pi LR^2,$$

where the proportionality constant $\nu > 0$ is called the metabolic coefficient. This gives for the total energy

$$E := E_p + E_m = \frac{8\mu L}{\pi R^4} Q^2 + \nu\pi LR^2. \quad (2.2)$$

The condition of maximum economy work, for a given flow Q and length L , translate in the condition

$$\frac{d}{dR} E = -\frac{16\mu L}{\pi R^5} Q^2 + 2\nu\pi LR.$$

The total energy is then minimized if the following relation between the flow rate and the tube radius is verified,

$$Q = \sqrt{\frac{\pi^2 \nu}{16\mu}} R^3. \quad (2.3)$$

In a branching node with a parent branch with flow rate $Q_0 > 0$ and children branches with flow rates $Q_1, Q_2, \dots, Q_n > 0$, we have the flux balance

$$Q_0 = \sum_{i=1}^n Q_i.$$

Using (2.3), we obtain for the respective radii $R_0 > 0$ and $R_1, R_2, \dots, R_n > 0$,

$$R_0^3 = \sum_{i=1}^n R_i^3, \quad (2.4)$$

which is the classical Murray's law for laminar blood flow [51, 52]. It can be also expressed in terms of the edge conductivities $C_i > 0$, which for three-dimensional laminar flow are proportional to R_i^4 , see Ref. [56], therefore

$$C_0^{3/4} = \sum_{i=1}^n C_i^{3/4}. \quad (2.5)$$

The above formula represents the classical 3/4-law for optimal ratio of conductivities in 3D branching edges with laminar flow [51, 52]. It clearly demonstrates the nonlinear nature of optimal network conductivity models, in particular, the nonlinear (and nonconvex) dependence of the total energy (2.2) on the edge conductivity.

In his derivation Murray assumed that the major metabolic cost was given by the blood, neglecting the thin walls of blood vessels. However, in the case of plants, the xylem water is cheap, while the cost of the conduit walls is higher. In [66] the author showed that the same law applies considering also the metabolic cost of the walls, assuming that their thickness is proportional to the internal radius of the vessel.

In [74] the authors analysed the optimal diameter of vessels in an engineering vascular network, giving particular attention at the point where the network bifurcates. Taking into consideration both the mass of the internal fluid and the walls of the vessels, and assuming as Sherman did that the thickness of the walls is proportional to the internal radius, the authors showed that the same relationship as (2.4) between the radii can be obtained as a result of a mass optimization process.

The first goal of this chapter is to show the validity of a generalization of the Murray's law (2.5) for general transportation networks with multiple branching nodes (Section 2.2). Then, in Section 2.3, we consider a continuum limit of the discrete model on a rectangular mesh, and derive an analogue of the discrete Murray's law for the continuum PDE system. Finally, in Section 2.4 we consider another continuum model for biological transportation networks, derived from phenomenological considerations, and show that a continuum version of Murray's law holds also for the linearly stable solutions of this model. The calculations made in Sections 2.3 and 2.4 are formal, however, they can be justified by assuming sufficient regularity of the steady state solutions of the respective continuum PDE systems. Details will be provided in the respective Sections.

2.2 Murray's law for the discrete network model

The microscopic model considered in this section was first introduced by Hu and Cai in [39], and reformulated in [3]. We consider a given undirected connected graph $G = (\mathbb{V}, \mathbb{E})$, consisting of a finite set of vertices (branching nodes) $\mathbb{V}$ of size $N = |\mathbb{V}|$ and a finite set of edges $\mathbb{E}$. Any pair of vertices is connected by at most one edge, which represents a tube (channel), and no vertex is connected to itself. We denote the edge between vertices $i \in \mathbb{V}$ and $j \in \mathbb{V}$ by $(i, j) \in \mathbb{E}$. Since the graph is undirected, (i, j) and (j, i) refer to the same edge. For each edge $(i, j) \in \mathbb{E}$ of the graph G we consider its length and its conductivity, denoted by $L_{ij} = L_{ji} > 0$ and $C_{ij} = C_{ji} \geq 0$, respectively. The edge lengths $L_{ij} > 0$ are given as a datum and fixed for all $(i, j) \in \mathbb{E}$. With each vertex $i \in \mathbb{V}$ there is associated the fluid pressure $P_i \in \mathbb{R}$. The pressure drop between vertices $i \in \mathbb{V}$ and $j \in \mathbb{V}$ connected by an edge $(i, j) \in \mathbb{E}$ is denoted by

$$(\Delta P)_{ij} := P_j - P_i.$$

Note that the pressure drop is antisymmetric, i.e., by definition, $(\Delta P)_{ij} = -(\Delta P)_{ji}$. The oriented flux (flow rate) from vertex $j \in \mathbb{V}$ to $i \in \mathbb{V}$ is denoted by Q_{ij} ; again, we have $Q_{ij} = -Q_{ji}$. For the three-dimensional laminar flow, conductance (transportation capacity) C_{ij} of an edge $(i, j) \in \mathbb{E}$ is proportional to the fourth power of its diameter [56]. Then, (2.1) is reformulated in terms of the conductivities as

$$Q_{ij} := C_{ij} \frac{P_j - P_i}{L_{ij}} \quad \text{for all } (i, j) \in \mathbb{E}. \quad (2.6)$$

The flux balance in each vertex is expressed in terms of the Kirchhoff law

$$- \sum_{j \in \mathcal{N}(i)} Q_{ij} = S_i \quad \text{for all } i \in \mathbb{V},$$

which can be rewritten in terms of pressure differences thanks to relation (2.6)

$$- \sum_{j \in \mathcal{N}(i)} C_{ij} \frac{P_j - P_i}{L_{ij}} = S_i \quad \text{for all } i \in \mathbb{V}. \quad (2.7)$$

Here $\mathcal{N}(i) \subset \mathbb{V}$ denotes the set of vertices connected to $i \in \mathbb{V}$ through an edge, i.e.,

$$\mathcal{N}(i) := \{j \in \mathbb{V} : (i, j) \in \mathbb{E}\},$$

and $S = (S_i)_{i \in \mathbb{V}}$ is the prescribed strength of the external flow source ($S_i > 0$) or sink ($S_i < 0$) in node $i \in \mathbb{V}$. Clearly, a necessary condition for the solvability of (2.7) is the global mass conservation

$$\sum_{i \in \mathbb{V}} S_i = 0, \quad (2.8)$$

which we shall assume in the sequel. Given the vector of conductivities $C = (C_{ij})_{(i,j) \in \mathbb{E}}$, the Kirchhoff law (2.7) is a linear system of equations for the vector of pressures $P = (P_i)_{i \in \mathbb{V}}$. With the global mass conservation (2.8), the linear system (2.7) is solvable if and only if the graph with edge weights $C = (C_{ij})_{(i,j) \in \mathbb{E}}$ is connected [3], where only edges with positive conductivities $C_{ij} > 0$ are taken into account (i.e., edges with zero conductivities are discarded). Note that the solution vector $P = (P_i)_{i \in \mathbb{V}}$ is unique up to an additive constant. The corresponding fluxes, which we denote by $Q_{ij}[C]$, are then calculated uniquely from (2.6).

The conductivities C_{ij} are subject to an energy optimization and adaptation process, where, in analogy to (2.2), the cost functional is a sum of pumping and metabolic energies over all edges of the graph,

$$\mathcal{E}[C] := \sum_{(i,j) \in \mathbb{E}} \left(\frac{Q_{ij}[C]^2}{C_{ij}} + \frac{\nu}{\gamma} C_{ij}^\gamma \right) L_{ij}. \quad (2.9)$$

Here we consider a generalization where the metabolic energy is proportional to a power $\gamma > 0$ of the respective edge conductivity. We have $\gamma = 1/2$ for blood vessel systems (recall that in a three-dimensional tube the conductivity is proportional to fourth power of the tube radius, while the metabolic cost scales quadratically with the radius, see Ref. [51]). For models of plant leaf venation the metabolic cost is proportional to the number of small tubes, which is proportional to C_{ij} , and the metabolic cost is due to the effective loss of the photosynthetic power at the area of the venation cells, which is proportional to $C_{ij}^{1/2}$. Consequently, the effective value of γ typically used in models of leaf venation in plants lies between 1/2 and 1, see, e.g., Refs. [38], [39]. Again, $\nu > 0$ is the so-called metabolic coefficient.

The derivation of the Murray's law for critical points of the energy functional (2.9), constrained by the Kirchhoff law (2.7), is based on the following explicit formula for the derivative of the pumping term in (2.9) with respect to the conductivities, derived in Ref. [31]. We restate its proof here for the sake of completeness.

Lemma 2.1. *Let $C = (C_{ij})_{(i,j) \in \mathbb{E}}$ be a vector of nonnegative conductivities such that the underlying graph is connected if only edges with strictly positive conductivities are taken into account. Let $Q_{ij}[C]$ be given by (2.6), where $P = (P_i)_{i \in \mathbb{V}}$ is a solution of the linear system (2.7) with the vector of conductivities C . Then, for any fixed $(k, l) \in E$ we have*

$$\frac{\partial}{\partial C_{kl}} \sum_{(i,j) \in E} \frac{Q_{ij}[C]^2}{C_{ij}} L_{ij} = -\frac{Q_{kl}[C]^2}{C_{kl}^2} L_{kl}. \quad (2.10)$$

Proof. Since

$$\frac{\partial}{\partial C_{kl}} \sum_{(i,j) \in E} \frac{Q_{ij}[C]^2}{C_{ij}} L_{ij} = -\frac{Q_{kl}[C]^2}{C_{kl}^2} L_{kl} + 2 \sum_{(i,j) \in E} \frac{Q_{ij}[C]}{C_{ij}} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} L_{ij},$$

it is sufficient to show that

$$\sum_{(i,j) \in E} \frac{Q_{ij}[C]}{C_{ij}} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} L_{ij} = 0.$$

Let $\mathbb{A} = (\mathbb{A}_{ij})$ denote the adjacency matrix of the graph $G = (\mathbb{V}, \mathbb{E})$, i.e. its coefficients are defined by

$$\mathbb{A}_{ij} = \begin{cases} 0 & \text{if } (i, j) \notin \mathbb{E}, \\ 1 & \text{if } (i, j) \in \mathbb{E}. \end{cases}$$

Note that G is an undirected graph, implying $\mathbb{A}_{ij} = \mathbb{A}_{ji}$. Due to the symmetry of C_{ij} and L_{ij} and

antisymmetry of Q_{ij} we have

$$\begin{aligned}
2 \sum_{(i,j) \in E} \frac{Q_{ij}[C]}{C_{ij}} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} L_{ij} &= \sum_{i=1}^n \sum_{j=1}^n \mathbb{A}_{ij} \left(\frac{P_j - P_i}{L_{ij}} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} \right) L_{ij} \\
&= \sum_{j=1}^n P_j \sum_{i=1}^n \mathbb{A}_{ij} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} - \sum_{i=1}^n P_i \sum_{j=1}^n \mathbb{A}_{ij} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} \\
&= -2 \sum_{i=1}^n P_i \sum_{j=1}^n \mathbb{A}_{ij} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} \\
&= -2 \sum_{i=1}^n P_i \frac{\partial}{\partial C_{kl}} \sum_{j \in N(i)} Q_{ij}.
\end{aligned}$$

By the definition of the flow rate Q_{ij} in (2.6) and Kirchhoff's law (2.7) we have

$$- \sum_{j \in N(i)} Q_{ij} = \sum_{j \in N(i)} C_{ij} \frac{P_j - P_i}{L_{ij}} = S_i,$$

and since the sources/sinks S_i are fixed, we conclude

$$\sum_{(i,j) \in E} \frac{Q_{ij}[C]}{C_{ij}} \frac{\partial Q_{ij}[C]}{\partial C_{kl}} L_{ij} = 0.$$

■

Using the identity (2.10), it is straightforward to calculate the derivative of the energy (2.9), constrained by the Kirchhoff law (2.7), with respect to the edge conductivities,

$$\frac{\partial}{\partial C_{ij}} \mathcal{E}[C] = - \left(\frac{Q_{ij}[C]^2}{C_{ij}^2} - \nu C_{ij}^{\gamma-1} \right) L_{ij}.$$

Since any critical point of $\mathcal{E}[C]$ satisfies

$$\frac{\partial}{\partial C_{ij}} \mathcal{E}[C] = 0 \quad \text{for all } (i, j) \in \mathbb{E},$$

we have

$$Q_{ij}[C]^2 = \nu C_{ij}^{\gamma+1} \quad \text{for all } (i, j) \in \mathbb{E}. \quad (2.11)$$

Now, the Kirchhoff law (2.7) written in terms of the fluxes $Q_{ij} := Q_{ij}[C]$ reads

$$\sum_{j \in \mathcal{N}(i)} Q_{ij} + S_i = 0 \quad \text{for all } i \in \mathbb{V}. \quad (2.12)$$

Let us write the set of neighbors $\mathcal{N}(i)$ of the node $i \in \mathbb{V}$ as the disjoint union $\mathcal{N}(i) = \mathcal{N}^+(i) \cup \mathcal{N}^-(i)$, based on the flow directions along the respective edges, i.e.,

$$\mathcal{N}^+(i) := \{j \in \mathcal{N}(i) : Q_{ij} \geq 0\}, \quad \mathcal{N}^-(i) := \{j \in \mathcal{N}(i) : Q_{ij} < 0\}.$$

Then, we can rewrite (2.12) as

$$\sum_{j \in \mathcal{N}^+(i)} Q_{ij} + S_i = \sum_{j \in \mathcal{N}^-(i)} (-Q_{ij}) \quad \text{for all } i \in \mathbb{V},$$

and, further,

$$\sum_{j \in \mathcal{N}^+(i)} |Q_{ij}| + S_i = \sum_{j \in \mathcal{N}^-(i)} |Q_{ij}| \quad \text{for all } i \in \mathbb{V}.$$

Using (2.11), we arrive at

$$\sqrt{\nu} \sum_{j \in \mathcal{N}^+(i)} C_{ij}^{\frac{\gamma+1}{2}} + S_i = \sqrt{\nu} \sum_{j \in \mathcal{N}^-(i)} C_{ij}^{\frac{\gamma+1}{2}} \quad \text{for all } i \in \mathbb{V}. \quad (2.13)$$

This is the (generalized) Murray's law for the discrete model (2.7), (2.9). Recall that for the case of three-dimensional blood vessel systems we have $\gamma = 1/2$, which leads to the power $\frac{\gamma+1}{2} = \frac{3}{4}$, so that (2.13) becomes a direct generalization of the classical Murray's law (2.5).

2.3 Murray's law for the continuum limit model on rectangular grids

In Ref. [31] the formal continuum limit of the discrete model (2.7), (2.9) for $\gamma > 1$ on rectangular equidistant grids was derived; the rigorous limit passage was studied in the consequent paper [32]. The resulting continuum energy functional is of the form

$$\mathcal{E}[c] := \int_{\Omega} \nabla p \cdot c \nabla p + \frac{\nu}{\gamma} |c|^\gamma dx, \quad (2.14)$$

with the metabolic coefficient $\nu > 0$ and the exponent $\gamma > 1$. The energy functional $\mathcal{E}[c]$ is defined on the set of nonnegative diagonal tensor fields $c = c(x)$ on a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$,

$$c = \begin{pmatrix} c^1 & & \\ & \ddots & \\ & & c^d \end{pmatrix}. \quad (2.15)$$

The symbol $|c|^\gamma$ is defined as $\sum_{k=1}^d |c^k|^\gamma$. The scalar pressure $p = p(x)$ of the fluid occupying the domain Ω is subject to the Poisson equation

$$-\nabla \cdot (c \nabla p) = S, \quad (2.16)$$

equipped with no-flux boundary condition on $\partial\Omega$, and the datum $S = S(x)$ represents the intensity of sources and sinks in Ω . Let us point out that the Poisson equation (2.16) is possibly strongly degenerate since the eigenvalues (i.e., diagonal elements) of the permeability tensor (2.15) may vanish. To overcome this problem, we follow Ref. [31] and introduce a regularization of (2.16) of the form

$$-\nabla \cdot (\mathbb{P}[c] \nabla p) = S, \quad (2.17)$$

with the permeability tensor

$$\mathbb{P}[c] := rI + c, \quad (2.18)$$

where $r = r(x) \geq r_0 > 0$ is a prescribed function that models the isotropic background permeability of the medium, and $I \in \mathbb{R}^{d \times d}$ is the unit matrix. Again, (2.17) is equipped with the no-flux boundary condition

$$n \cdot \mathbb{P}[c] \nabla p = 0 \quad \text{on } \partial\Omega, \quad (2.19)$$

where $n = n(x)$ denotes the outer unit normal vector to $\partial\Omega$. Then, the weak formulation of the boundary value problem (2.17)–(2.19) with a test function $\phi \in C^\infty(\Omega)$ reads

$$\int_{\Omega} \nabla \phi \cdot (rI + c) \nabla p \, dx = \int_{\Omega} S \phi \, dx. \quad (2.20)$$

Clearly, since we only admit nonnegative diagonal tensor fields $c = c(x)$, (2.20) is uniformly elliptic and it has solutions unique up to an additive constant. The energy functional (2.14) needs to be updated as

$$\mathcal{E}[c] := \int_{\Omega} \nabla p \cdot \mathbb{P}[c] \nabla p + \frac{\nu}{\gamma} |c|^\gamma \, dx. \quad (2.21)$$

We now calculate the Euler-Lagrange equations corresponding to critical points of the functional (2.21) constrained by (2.20).

Lemma 2.2. *The Euler-Lagrange equations for the constrained energy minimization problem (2.20), (2.21) read*

$$(\partial_{x_k} p)^2 - \nu |c^k|^{\gamma-1} = 0, \quad \text{for } k = 1, \dots, d. \quad (2.22)$$

Proof. We calculate the first variation of $\mathcal{E}$ in the direction ϕ , where ϕ denotes a diagonal matrix with entries $\phi^1, \dots, \phi^d$, such that $c + \varepsilon \phi$ is nonnegative. Using the expansion

$$p[c + \varepsilon \phi] = p_0 + \varepsilon p_1 + \mathcal{O}(\varepsilon^2),$$

we have

$$\begin{aligned} & \left. \frac{d}{d\varepsilon} \mathcal{E}[c + \varepsilon \phi] \right|_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon} \int_{\Omega} (\nabla p_0 + \varepsilon \nabla p_1) (rI + c + \varepsilon \phi) (\nabla p_0 + \varepsilon \nabla p_1) + \nu \frac{|c + \varepsilon \phi|^\gamma}{\gamma} \, dx \\ &= \frac{d}{d\varepsilon} \int_{\Omega} \nabla p_0 (rI + c) \nabla p_0 + \varepsilon [\nabla p_1 (rI + c) \nabla p_0 + \nabla p_0 (rI + c) \nabla p_1] + \mathcal{O}(\varepsilon^2) + \nu \frac{|c + \varepsilon \phi|^\gamma}{\gamma} \, dx \\ &= \sum_{k=1}^d \int_{\Omega} (\partial_{x_k} p_0)^2 \phi^k + 2(r + c^k) (\partial_{x_k} p_0) (\partial_{x_k} p_1) + \nu |c^k|^{\gamma-2} c^k \phi^k \, dx. \end{aligned} \quad (2.23)$$

Using p_0 as a test function in (2.20) with the permeability tensor $\mathbb{P}[c + \varepsilon \phi] = rI + c + \varepsilon \phi$ gives

$$\sum_{k=1}^d \int_{\Omega} (r + c^k + \varepsilon \phi^k) (\partial_{x_k} p_0)^2 + \varepsilon (r + c^k) (\partial_{x_k} p_0) (\partial_{x_k} p_1) \, dx = \int_{\Omega} S p_0 \, dx + \mathcal{O}(\varepsilon^2).$$

Subtracting the identity

$$\sum_{k=1}^d \int_{\Omega} (r + c^k) (\partial_{x_k} p_0)^2 \, dx = \int_{\Omega} S p_0 \, dx,$$

we obtain

$$\sum_{k=1}^d \int_{\Omega} (\partial_{x_k} p_0)^2 \phi^k + (r + c^k) (\partial_{x_k} p_0) (\partial_{x_k} p_1) \, dx = 0.$$

Plugging this into (2.23) gives

$$\frac{d}{d\varepsilon} \mathcal{E}[c + \varepsilon\phi] \Big|_{\varepsilon=0} = \sum_{k=1}^d \int_{\Omega} \left[-(\partial_{x_k} p_0)^2 + \nu |c^k|^{\gamma-1} \right] \phi^k dx,$$

and (2.22) follows. ■

From (2.22) it follows that for $k = 1, \dots, d$ there exist disjoint Lebesgue-measurable sets $\mathcal{A}_k^+, \mathcal{A}_k^-$ such that $\Omega = \mathcal{A}_k^+ \cup \mathcal{A}_k^-$ for all $k = 1, \dots, d$ and

$$\partial_{x_k} p = (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) \sqrt{\nu} |c^k|^{\frac{\gamma-1}{2}}, \quad \text{for } k = 1, \dots, d. \quad (2.24)$$

Note that by assumption $c_k \geq 0$. Let us now choose an open subset $\Lambda \subset \Omega$ with boundary $\partial\Lambda \in C^{0,1}$ and use the characteristic function of Λ as the test function ϕ in (2.20). This formal calculation can be justified by using a smoothened version of the characteristic function and passing to the limit, adopting the assumption that the flux $q := -(rI + c)\nabla p$ is locally Lipschitz continuous on Λ . Then the generalized Green's formula by De Giorgi-Federer [25] gives

$$- \int_{\partial\Lambda} n \cdot (rI + c) \nabla p ds = \int_{\Lambda} S dx, \quad (2.25)$$

where $n = n(x)$ denotes the outward unit normal vector to $\partial\Lambda$, and $s = s(x)$ is the $(d-1)$ -dimensional measure on $\partial\Lambda$. Using (2.24), we arrive at

$$-\sqrt{\nu} \int_{\partial\Lambda} \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) |c^k|^{\frac{\gamma-1}{2}} (r + c^k) n_k ds = \int_{\Lambda} S dx. \quad (2.26)$$

We define the inflow and outflow segments of $\partial\Lambda$ as

$$\partial\Lambda^+ := \{x \in \partial\Lambda : n(x) \cdot q(x) < 0\}, \quad \partial\Lambda^- := \{x \in \partial\Lambda : n(x) \cdot q(x) > 0\},$$

with the flux $q = -(rI + c)\nabla p$. Then, (2.26) can be written in the form

$$\begin{aligned} & -\sqrt{\nu} \int_{\partial\Lambda^+} \left| \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) |c^k|^{\frac{\gamma-1}{2}} (r + c^k) n_k \right| ds \\ & + \sqrt{\nu} \int_{\partial\Lambda^-} \left| \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) |c^k|^{\frac{\gamma-1}{2}} (r + c^k) n_k \right| ds = \int_{\Lambda} S dx. \end{aligned}$$

This is the Murray's law for the continuum model (2.17)–(2.21). The two terms on the left-hand side represent the difference of in- and outgoing fluxes through the boundary $\partial\Lambda$, which is balanced by the volume integral of the external in- and outflows $S = S(x)$. Note the analogy with the Murray's law for the discrete system (2.13).

Let us remark that the above formal calculation becomes rigorous if we assume sufficient regularity of the flux $q = -(rI + c)\nabla p$, in particular, we need q to be locally Lipschitz continuous on Λ . In the next Section we construct solutions in the energy space which are less regular; the proof of higher regularity is beyond the scope of this paper and we postpone it to a future work.

2.3.1 Construction of solutions

From (2.22) it follows that

$$c^k = \nu^{-\frac{1}{\gamma-1}} (\partial_{x_k} p)^{\frac{2}{\gamma-1}} \quad \text{for } k = 1, \dots, d.$$

Inserting this into (2.17), we obtain

$$-\sum_{k=1}^d \partial_{x_k} \left(\left(r + \nu^{-\frac{1}{\gamma-1}} (\partial_{x_k} p)^{\frac{2}{\gamma-1}} \right) \partial_{x_k} p \right) = S.$$

The weak formulation of this nonlinear elliptic equation, equipped with a no-flux boundary condition, reads

$$\int_{\Omega} \sum_{k=1}^d \left(r + \nu^{-\frac{1}{\gamma-1}} (\partial_{x_k} p)^{\frac{2}{\gamma-1}} \right) (\partial_{x_k} p) (\partial_{x_k} \phi) \, dx = \int_{\Omega} S \phi \, dx \quad (2.27)$$

for all test functions $\phi \in C^\infty(\Omega)$. For $\gamma > 1$ solutions can be constructed by the direct method of calculus of variations.

Lemma 2.3. *The relation (2.27) correspond to the Euler-Lagrange equation for the minimisers of the energy*

$$\mathcal{F}[p] := \int_{\Omega} \left(\sum_{k=1}^d \frac{r}{2} |\partial_{x_k} p|^2 + \nu^{-\frac{1}{\gamma-1}} \frac{\gamma-1}{2\gamma} |\partial_{x_k} p|^{\frac{2\gamma}{\gamma-1}} \right) \, dx - \int_{\Omega} p S \, dx. \quad (2.28)$$

Proof. We consider ϕ a smooth test function, and we evaluate

$$\begin{aligned} & \frac{d}{d\varepsilon} \mathcal{F}[p + \varepsilon \phi] = \\ &= \frac{d}{d\varepsilon} \int_{\Omega} \left(\sum_{k=1}^d \frac{r}{2} |\partial_{x_k} p + \varepsilon \partial_{x_k} \phi|^2 + \nu^{-\frac{1}{\gamma-1}} \frac{\gamma-1}{2\gamma} |\partial_{x_k} p + \varepsilon \partial_{x_k} \phi|^{\frac{2\gamma}{\gamma-1}} \right) \, dx - \int_{\Omega} S (p + \varepsilon \phi) \, dx \\ &= \int_{\Omega} \sum_{k=1}^d \left(r |\partial_{x_k} p + \varepsilon \partial_{x_k} \phi| \frac{\partial_{x_k} p + \varepsilon \partial_{x_k} \phi}{|\partial_{x_k} p + \varepsilon \partial_{x_k} \phi|} \partial_{x_k} \phi + \nu^{-\frac{1}{\gamma-1}} |\partial_{x_k} p + \varepsilon \partial_{x_k} \phi|^{\frac{\gamma+1}{\gamma-1}} \frac{\partial_{x_k} p + \varepsilon \partial_{x_k} \phi}{|\partial_{x_k} p + \varepsilon \partial_{x_k} \phi|} \partial_{x_k} \phi \right) \, dx \\ & \quad - \int_{\Omega} S \phi \, dx \\ &= \int_{\Omega} \sum_{k=1}^d \partial_{x_k} \phi \left(r \partial_{x_k} p + \nu^{-\frac{1}{\gamma-1}} |\partial_{x_k} p|^{\frac{1}{\gamma-1}} \partial_{x_k} p \right) \, dx - \int_{\Omega} S \phi \, dx, \end{aligned}$$

which is exactly the relation (2.27) ■

Lemma 2.4. *Let $\gamma > 1$. For every $S \in L^2(\Omega)$ there exists a unique solution $p \in H^1(\Omega)$ of (2.27) satisfying $\int_{\Omega} p(x) \, dx = 0$.*

Proof. We consider the functional $\mathcal{F} : H^1(\Omega) \rightarrow \mathbb{R}$ by

$$\mathcal{F}[p] := \int_{\Omega} \left(\sum_{k=1}^d \frac{r}{2} |\partial_{x_k} p|^2 + \nu^{-\frac{1}{\gamma-1}} \frac{\gamma-1}{2\gamma} |\partial_{x_k} p|^{\frac{2\gamma}{\gamma-1}} \right) \, dx - \int_{\Omega} p S \, dx.$$

Since $\frac{2\gamma}{\gamma-1} > 2$ for $\gamma > 1$, the functional $\mathcal{F}$ is uniformly convex on $H^1(\Omega)$. Moreover, a straightforward application of the Poincaré inequality provides coercivity on the set $H^{1,0}(\Omega) := \{p \in H^1(\Omega); \int_{\Omega} p(x) dx = 0\}$. The classical theory (see, e.g., Ref. [24]) provides the existence of a unique minimizer $p \in H^{1,0}(\Omega)$. Since, as proved in Lemma 2.3, (2.28) is the Euler-Lagrange equation for the minimizer of $\mathcal{F}$, p is the unique solution in $H^{1,0}(\Omega)$ of (2.27). ■

Let us note that (2.27) is independent of the choice of the sets $\mathcal{A}_k^+$, $\mathcal{A}_k^-$ in (2.24), and so is the solution p constructed in Lemma 2.4. We can therefore write, for $k = 1, \dots, d$,

$$\mathcal{A}_k^+ = \{x \in \Omega : \partial_{x_k} p(x) > 0\}, \quad \mathcal{A}_k^- = \{x \in \Omega : \partial_{x_k} p(x) < 0\}.$$

2.3.2 Murray law for the continuum model with diffusion

Following Ref. [31], we equip the model with a linear diffusive term that accounts for random fluctuations in the medium. In particular, we update the energy functional (2.21) to

$$\mathcal{E}[c] := \int_{\Omega} \frac{D^2}{2} |\nabla c|^2 + \nabla p \cdot \mathbb{P}[c] \nabla p + \frac{\nu}{\gamma} |c|^\gamma dx, \quad (2.29)$$

where $D^2 > 0$ is the diffusivity constant and the symbol $|\nabla c|^2$ is defined as $\sum_{k=1}^d |\nabla c^k|^2$. The permeability tensor is given by (2.18), i.e., $\mathbb{P}[c] = rI + c$. As can be easily checked following the steps of the proof of Lemma 2.2, the Euler-Lagrange equations corresponding to critical points of the functional (2.29) constrained by the Poisson equation (2.20) read

$$(\partial_{x_k} p)^2 + D^2 \Delta c^k - \nu |c^k|^{\gamma-1} = 0, \quad \text{for } k = 1, \dots, d.$$

Note that for sufficiently regular critical points of (2.29), (2.20) we have $\nu |c^k|^{\gamma-1} - D^2 \Delta c^k \geq 0$ almost everywhere on Ω . Then it follows that for $k = 1, \dots, d$ there exist disjoint Lebesgue-measurable sets $\mathcal{A}_k^+$, $\mathcal{A}_k^-$ such that $\Omega = \mathcal{A}_k^+ \cup \mathcal{A}_k^-$ for all $k = 1, \dots, d$ and

$$\partial_{x_k} p = (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) \left(\nu |c^k|^{\gamma-1} - D^2 \Delta c^k \right)^{1/2}, \quad \text{for } k = 1, \dots, d. \quad (2.30)$$

As before we choose an open subset $\Lambda \subset \Omega$ with boundary $\partial\Lambda \in C^{0,1}$, and using (2.30) in (2.25), we obtain

$$- \int_{\partial\Lambda} \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) (r + c^k) \left(\nu |c^k|^{\gamma-1} - D^2 \Delta c^k \right)^{1/2} n_k ds = \int_{\Lambda} S dx, \quad (2.31)$$

where $n = n(x)$ denotes the outward unit normal vector to $\partial\Lambda$, and $s = s(x)$ is the $(d-1)$ -dimensional measure on $\partial\Lambda$. We define the inflow and outflow segments of $\partial\Lambda$ as

$$\partial\Lambda^+ := \{x \in \partial\Lambda; n(x) \cdot q(x) < 0\}, \quad \partial\Lambda^- := \{x \in \partial\Lambda; n(x) \cdot q(x) > 0\},$$

where we denoted the flux $q := -(rI + c)\nabla p$. Then, (2.31) can be written in the form

$$\begin{aligned} & - \int_{\partial\Lambda^+} \left| \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) (r + c^k) \left(\nu |c^k|^{\gamma-1} - D^2 \Delta c^k \right)^{1/2} n_k \right| ds \\ & + \int_{\partial\Lambda^-} \left| \sum_{k=1}^d (\chi_{\mathcal{A}_k^+} - \chi_{\mathcal{A}_k^-}) (r + c^k) \left(\nu |c^k|^{\gamma-1} - D^2 \Delta c^k \right)^{1/2} n_k \right| ds \\ & = \int_{\Lambda} S dx. \end{aligned}$$

This is the Murray's law for the continuum model (2.29) constrained by the Poisson equation (2.20).

2.4 Murray's law for the phenomenological continuum model

In this Section we consider the continuum model briefly proposed in Ref. [38] and analyzed in Refs. [33], [34], [2]. Its phenomenological derivation, carried out in Ref. [3], assumes that the network domain $\Omega \subset \mathbb{R}^d$ is occupied by a porous medium with the permeability tensor

$$\mathbb{P}[m] := m \otimes m \quad (2.32)$$

with $m = m(x) \in \mathbb{R}^d$ a smooth vector field on $\mathbb{R}^d$. Note that $\mathbb{P}[m]$ has the eigenvalue $|m|^2$ with eigenvector m , and 0 with eigenvectors orthogonal to m . Thus, it represents conduction along the direction m with conductivity $|m|^2$, while there is no conduction in directions perpendicular to m . Consequently, we locally identify the network conductivity with the principal eigenvalue of $\mathbb{P}$, i.e., $C_i \simeq |m|^2$ in the neighborhood of a node $i \in \mathbb{V}$. Assuming quasi-incompressibility of the fluid, i.e., constant fluid density along particle trajectories, we have the local mass conservation law

$$\nabla \cdot q = S \quad \text{in } \Omega, \quad (2.33)$$

where $q = q(x) \in \mathbb{R}^d$ is the flux and $S = S(x)$ is the density of external sources and sinks; see Ref. [3] for details. Assuming the validity of Darcy's law for slow flow in porous media [73], we have

$$q = -\mathbb{P}[m] \nabla p,$$

where $p = p(x)$ is the fluid pressure. Combining with (2.33) and (2.32), we arrive at the Poisson equation

$$-\nabla \cdot ((m \otimes m) \nabla p) = S. \quad (2.34)$$

Let us point out the possible strong degeneracy of (2.34), leading to solvability issues. That is why in Refs. [33], [34], [2] the following regularization was considered,

$$-\nabla \cdot ((rI + m \otimes m) \nabla p) = S, \quad (2.35)$$

where I is the identity matrix and the scalar function $r = r(x) \geq r_0 > 0$ describes the isotropic background permeability of the medium. Then, (2.35) is uniformly elliptic and, equipped with suitable boundary conditions, solvable. We shall assume no flux through the boundary $\partial\Omega$, i.e., equip (2.35) with the homogeneous Neumann boundary condition

$$n \cdot \mathbb{P}[m] \nabla p = 0 \quad \text{on } \partial\Omega,$$

where $n = n(x)$ denotes the outer unit normal vector to $\partial\Omega$. Then the solution $p = p(x)$ is unique up to an additive constant and the flux $q = -\mathbb{P}[m] \nabla p$ is defined uniquely.

The local conductivity of the network being identified with $|m|^2$, the continuum analogue of the discrete energy functional (2.9) is

$$\mathcal{E}[m] = \int \nabla p[m] \cdot \mathbb{P}[m] \nabla p[m] + \frac{\nu}{\gamma} |m|^{2\gamma} dx, \quad (2.36)$$

where $p[m]$ denotes a solution of the Poisson equation (2.35) and $\mathbb{P}[m] := rI + m \otimes m$.

Lemma 2.5. *The Euler-Lagrange equations for the constrained energy minimization problem (2.35), (2.36) read*

$$(\nabla p \otimes \nabla p)m - \nu |m|^{2(\gamma-1)}m = 0. \quad (2.37)$$

Proof. We calculate the first variation of $\mathcal{E}$ given by (2.36) in the direction $\phi = \phi(x) \in \mathbb{R}^d$. Using the expansion

$$p[m + \varepsilon\phi] = p_0 + \varepsilon p_1 + \mathcal{O}(\varepsilon^2),$$

we have

$$\begin{aligned} & \left. \frac{d}{d\varepsilon} \mathcal{E}[m + \varepsilon\phi] \right|_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon} \int (\nabla p_0 + \varepsilon \nabla p_1) [rI + m \otimes m + \varepsilon (m \otimes \phi + \phi \otimes m)] (\nabla p_0 + \varepsilon \nabla p_1) + \frac{\nu}{\gamma} |m + \varepsilon\phi|^{2\gamma} dx \\ &= \frac{d}{d\varepsilon} \int \nabla p_0 (rI + m \otimes m) \nabla p_0 \\ &+ \varepsilon [\nabla p_0 (rI + m \otimes m) \nabla p_1 + \nabla p_0 (m \otimes \phi + \phi \otimes m) \nabla p_1 + \nabla p_1 (rI + m \otimes m) \nabla p_0] \\ &+ \frac{\nu}{\gamma} |m + \varepsilon\phi|^{2\gamma} + \mathcal{O}(\varepsilon^2) dx \\ &= \int_{\Omega} 2r \nabla p_0 \cdot \nabla p_1 + 2(\nabla p_0 \cdot m)(\nabla p_1 \cdot m) \\ &+ 2(\nabla p_0 \cdot m)(\nabla p_0 \cdot \phi) + 2\nu |m|^{2(\gamma-1)} m \cdot \phi dx. \end{aligned} \tag{2.38}$$

Multiplication of the Poisson equation (2.35) by p_0 and integration by parts, taking into account the no-flux boundary condition, gives

$$\begin{aligned} & \int_{\Omega} r |\nabla p_0|^2 + |m \cdot \nabla p_0|^2 + \varepsilon r \nabla p_0 \cdot \nabla p_1 + \varepsilon (\nabla p_0 \cdot m)(\nabla p_1 \cdot m) + 2\varepsilon (\nabla p_0 \cdot m)(\nabla p_0 \cdot \phi) dx \\ &= \int_{\Omega} S p_0 dx + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Subtracting the identity

$$\int_{\Omega} r |\nabla p_0|^2 + |m \cdot \nabla p_0|^2 dx = \int_{\Omega} S p_0 dx,$$

obtained by testing (2.35) with p_0 , we get

$$\int_{\Omega} r \nabla p_0 \cdot \nabla p_1 + (\nabla p_0 \cdot m)(\nabla p_1 \cdot m) dx = -2 \int_{\Omega} (\nabla p_0 \cdot m)(\nabla p_0 \cdot \phi) dx.$$

Plugging this into (2.38) gives

$$\left. \frac{d}{d\varepsilon} \mathcal{E}[m + \varepsilon\phi] \right|_{\varepsilon=0} = 2 \int_{\Omega} [-(\nabla p_0 \otimes \nabla p_0) m + \nu |m|^{2(\gamma-1)} m] \cdot \phi dx.$$

■

Interpreting (2.37) as an eigenvalue-eigenvector problem for the matrix $\nabla p \otimes \nabla p$, and noting that the matrix has the eigenvalues $|\nabla p|^2$ (with unit eigenvector $\frac{\nabla p}{|\nabla p|}$) and zero (with unit eigenvector $\frac{\nabla p^\perp}{|\nabla p^\perp|}$), there exists a measurable set $\mathcal{A} \subset \Omega$ such that m is a real multiple of ∇p on $\mathcal{A}$ and zero otherwise. Moreover, we have

$$\nu |m|^{2(\gamma-1)} = |\nabla p|^2 \quad \text{on } \mathcal{A}.$$

Therefore, there exist disjoint measurable sets $\mathcal{A}^+$, $\mathcal{A}^-$ such that $\mathcal{A}^+ \cup \mathcal{A}^- = \mathcal{A}$ and

$$\nabla p = (\chi_{\mathcal{A}^+} - \chi_{\mathcal{A}^-})\sqrt{\nu}|m|^{\gamma-2}m \quad \text{on } \mathcal{A}, \quad (2.39)$$

where $\chi_{\mathcal{A}^+}$, resp., $\chi_{\mathcal{A}^-}$ are the characteristic functions of the sets $\mathcal{A}^+$, resp., $\mathcal{A}^-$. For $\gamma = 1$ we define $\frac{m}{|m|} := 0$ for $m = 0$. Note that the measurable sets $\mathcal{A}^+$, $\mathcal{A}^-$ can be chosen arbitrarily and each choice gives a solution of the Euler-Lagrange equations (2.37).

In Ref. [33], Theorem 7 and Remark 6, it was shown that if $\text{meas}(\mathcal{A}) < \text{meas}(\Omega)$, i.e., if $m = 0$ on a set of positive Lebesgue measure, then the solution (m, p) is linearly unstable for the gradient flow system corresponding to (2.35)–(2.36). In other words, a necessary condition for asymptotic stability of the gradient flow system linearized at (m, p) is that $\text{meas}(\mathcal{A}) = \text{meas}(\Omega)$. We adopt this assumption for the sequel, since only the linearly stable steady states are likely to be observed in the nature or as results of numerical simulations.

Let us now choose an open subset $\Lambda \subset \Omega$ with boundary $\partial\Lambda \in C^{0,1}$ and integrate (2.35) over Λ , using the Green's theorem,

$$-\int_{\partial\Lambda} n \cdot (rI + m \otimes m) \nabla p \, ds = \int_{\Lambda} S \, dx, \quad (2.40)$$

where $n = n(x)$ denotes the outward unit normal vector to $\partial\Lambda$, and $s = s(x)$ is the $(d-1)$ -dimensional measure on $\partial\Lambda$. Here we assumed that the flux $q := -(rI + m \otimes m) \nabla p$ is locally Lipschitz continuous on Λ , so that the generalized Green's formula by De Giorgi-Federer [25] can be applied. We define the inflow and outflow segments of $\partial\Lambda$ as

$$\partial\Lambda^+ := \{x \in \partial\Lambda; n(x) \cdot q(x) < 0\}, \quad \partial\Lambda^- := \{x \in \partial\Lambda; n(x) \cdot q(x) > 0\},$$

with the flux $q := -(rI + m \otimes m) \nabla p$. Note that due to (2.39) we have

$$q = -(rI + m \otimes m) \nabla p = -(rI + |m|^2) \nabla p \quad \text{on } \mathcal{A},$$

so that $\text{sign}(n \cdot q) = -\text{sign}(n \cdot \nabla p)$ and we can equivalently (and slightly more elegantly) define the inflow and outflow segments in terms of ∇p only,

$$\partial\Lambda^+ := \{x \in \partial\Lambda; n(x) \cdot \nabla p(x) > 0\}, \quad \partial\Lambda^- := \{x \in \partial\Lambda; n(x) \cdot \nabla p(x) < 0\}.$$

Inserting then (2.39) into (2.40) we obtain

$$\begin{aligned} & -\sqrt{\nu} \int_{\partial\Lambda^+} (r + |m|^2) |m|^{\gamma-2} |m \cdot n| \, ds \\ & + \sqrt{\nu} \int_{\partial\Lambda^-} (r + |m|^2) |m|^{\gamma-2} |m \cdot n| \, ds = \int_{\Lambda} S \, dx. \end{aligned} \quad (2.41)$$

This is the Murray's law for the linearly stable solutions of the phenomenological continuum model (2.35)–(2.36). Clearly, the two terms on the left-hand side represent the difference of in- and outgoing fluxes through the boundary $\partial\Lambda$, which is balanced by the volume integral of the external in- and outflows $S = S(x)$ on the right-hand side. Note the analogy with the Murray's law for the discrete system (2.13).

Remark 2.6. *Should the restriction to only consider linearly stable states be relaxed, i.e., should it be admitted that $\text{meas}(\mathcal{A}) < \text{meas}(\Omega)$, then (2.41) must be modified. Namely, since we have no information about ∇p on the complement $\mathcal{A}^c$ of $\mathcal{A}$ in Ω , (2.41) needs to be rewritten as*

$$\begin{aligned} & -\sqrt{\nu} \int_{\mathcal{A} \cap \partial\Lambda^+} (r + |m|^2) |m|^{\gamma-2} |m \cdot n| \, ds - \int_{\mathcal{A}^c \cap \partial\Lambda^+} r |\nabla p \cdot n| \, ds \\ & + \sqrt{\nu} \int_{\mathcal{A} \cap \partial\Lambda^-} (r + |m|^2) |m|^{\gamma-2} |m \cdot n| \, ds + \int_{\mathcal{A}^c \cap \partial\Lambda^-} r |\nabla p \cdot n| \, ds = \int_{\Lambda} S \, dx, \end{aligned}$$

where we used the fact that $m \equiv 0$ on $\mathcal{A}^c$.

Let us again remark that the central assumption for the above calculations to be rigorously valid is that the flux $q = -(rI + m \otimes m)\nabla p$ is locally Lipschitz continuous on Λ .

2.4.1 Construction of solutions

We provide a short overview of rigorous existence results for the system (2.35), (2.37) that were obtained in Refs. [33] and [34]. Interpreting equation (2.37) as an eigenvalue problem for the matrix $\nabla p \otimes \nabla p$, we have the following expression for $m = m(x)$,

$$m(x) := (\chi_{\mathcal{A}_+}(x) - \chi_{\mathcal{A}_-}(x)) \nu^{\frac{1}{2(1-\gamma)}} |\nabla p(x)|^{\frac{2-\gamma}{\gamma-1}} \nabla p(x), \quad (2.42)$$

where $\mathcal{A}_+ \subseteq \Omega$ and $\mathcal{A}_- \subseteq \Omega$ are measurable disjoint sets. Inserting (2.42) into (2.35) gives

$$-\nabla \cdot \left[\left(rI + \nu^{\frac{1}{1-\gamma}} |\nabla p(x)|^{\frac{2}{\gamma-1}} \chi_{\mathcal{A}_+ \cup \mathcal{A}_-}(x) \right) \nabla p(x) \right] = S, \quad (2.43)$$

subject to the no-flux boundary condition. Solutions of (2.43) for $\gamma > 1$ are constructed by the direct method of calculus of variations.

Lemma 2.7. *Let $\gamma > 1$. Then for any $S \in L^2(\Omega)$ and for any pair of measurable disjoint sets $\mathcal{A}_+, \mathcal{A}_- \subseteq \Omega$ there exists a unique (up to an additive constant) weak solution $p \in H^1(\Omega) \cap W^{1,2\gamma/(\gamma-1)}(\mathcal{A}_+ \cup \mathcal{A}_-)$ of (2.43).*

Proof. The proof has been presented in Theorem 6 of Ref. [33], we present here the main steps. Let $\mathcal{A} = \mathcal{A}_+ \cup \mathcal{A}_-$, and we define the functional $\mathcal{F} : H_0^1 \rightarrow \mathbb{R} \cup \infty$,

$$\mathcal{F}[p] = \int_{\Omega} \frac{r}{2} |\nabla p|^2 dx + \int_{\mathcal{A}} \nu^{\frac{1}{1-\gamma}} \frac{\gamma-1}{2\gamma} |\nabla p|^{\frac{2\gamma}{\gamma-1}} dx - \int_{\Omega} S p dx.$$

The functional $\mathcal{F}$ is uniformly convex, and coercive with respect the weak-convergence of the space $H_0^1(\Omega)$. The classical theory (see for example Ref. [24]) provides the existence of a unique minimiser $p \in H_0^1(\Omega)$, which is also the unique solution of the equation (2.43). ■

In the case $\gamma = 1$, (2.37) reads

$$(\nabla p \otimes \nabla p)m = \nu m,$$

i.e., m is either the zero vector or an eigenvector of the matrix $\nabla p \otimes \nabla p$ with eigenvalue $\nu > 0$. The spectrum of $\nabla p \otimes \nabla p$ consists of zero and $|\nabla p|^2$, so that $m \neq 0$ is only possible if $|\nabla p|^2 = \nu$. Therefore, for every stationary solution there exists a measurable function $\lambda = \lambda(x)$ such that

$$m(x) = \lambda(x) \chi_{\{|\nabla p|^2 = \nu\}}(x) \nabla p(x)$$

and p solves the highly nonlinear Poisson equation

$$-\nabla \cdot \left[\left(1 + \lambda(x)^2 \chi_{\{c^2 |\nabla p|^2 = \nu\}}(x) \right) \nabla p \right] = S. \quad (2.44)$$

In Ref. [34], Section 4.2, it was shown that (2.44) is equivalent to the free boundary problem

$$-\nabla \cdot \left[(1 + a(x)^2) \nabla p \right] = S, \quad p \in H_0^1(\Omega), \quad (2.45)$$

$$|\nabla p(x)|^2 \leq \nu, \quad \text{a.e. on } \Omega, \quad (2.46)$$

$$a(x)^2 \left[|\nabla p(x)|^2 - \nu \right] = 0, \quad \text{a.e. on } \Omega, \quad (2.47)$$

for some measurable function $a^2 = a(x)^2$ on Ω which is the Lagrange multiplier for the condition (2.46). Solutions of (2.45)–(2.47) can be obtained as minimizers of the energy functional

$$\mathcal{F}[p] := \int_{\Omega} \left(\frac{|\nabla p|^2}{2} - Sp \right) dx$$

on the set $\{p \in H_0^1(\Omega), c^2|\nabla p|^2 \leq 1 \text{ a.e. on } \Omega\}$, or using the penalty method; see Section 4.2 of Ref. [34] for details.

Finally, for $1/2 \leq \gamma < 1$ the above approach fails due to the singularity of the term $|\nabla p(x)|^{\frac{2-\gamma}{\gamma-1}} \nabla p(x)$ at $|\nabla p| = 0$ and the resulting non-boundedness from below of the associated functional. However, stationary solutions can be constructed by “cutting off” small values of $|\nabla p|$, see Section 4.3 of Ref. [34] for details.

2.4.2 Murray’s law for the phenomenological continuum model with diffusion

Following Refs. [33] and [34], we equip the model with a linear diffusive term that accounts for random fluctuations in the medium. In particular, we update the energy functional (2.36) to

$$\mathcal{E}[m] = \int \frac{D^2}{2} |\nabla m|^2 + \nabla p[m] \cdot \mathbb{P}[m] \nabla p[m] + \frac{\nu}{\gamma} |m|^{2\gamma} dx, \quad (2.48)$$

where $D^2 > 0$ is the diffusivity constant, $p[m]$ denotes a solution of the Poisson equation (2.35) and $\mathbb{P}[m] = rI + m \otimes m$. With a similar proof to the one of Lemma 2.5, the Euler-Lagrange equations corresponding to critical points of the functional (2.48) constrained by the Poisson equation (2.35) read

$$(\nabla p \otimes \nabla p)m = -D^2 \Delta m + \nu |m|^{2(\gamma-1)} m.$$

Note that for sufficiently regular critical points of (2.48), (2.35) we have $(-D^2 \Delta m + \nu |m|^{2(\gamma-1)} m) \cdot m \geq 0$ almost everywhere in Ω . Let us denote

$$\mathcal{A} := \left\{ x \in \Omega; (-D^2 \Delta m(x) + \nu |m|^{2(\gamma-1)} m(x)) \cdot m(x) > 0 \right\}.$$

Then, there exist disjoint measurable sets $\mathcal{A}^+$, $\mathcal{A}^-$ such that $\mathcal{A}^+ \cup \mathcal{A}^- = \mathcal{A}$ and

$$\nabla p = (\chi_{\mathcal{A}^+} - \chi_{\mathcal{A}^-}) \left(\nu |m|^{2\gamma} - D^2 m \cdot \Delta m \right)^{-1/2} \left(\nu |m|^{2(\gamma-1)} m - D^2 \Delta m \right) \quad \text{on } \mathcal{A}, \quad (2.49)$$

where $\chi_{\mathcal{A}^+}$, resp., $\chi_{\mathcal{A}^-}$ are the characteristic functions of the sets $\mathcal{A}^+$, resp., $\mathcal{A}^-$. On the set $\mathcal{A}^c$ we have $(\nabla p \otimes \nabla p)m = 0$, which is equivalent to $m \cdot \nabla p = 0$.

Let us now choose an open subset $\Lambda \subset \Omega$ with boundary $\partial\Lambda \in C^{0,1}$ and define the inflow and outflow segments of $\partial\Lambda$ as

$$\partial\Lambda^+ := \{x \in \partial\Lambda; n(x) \cdot q(x) < 0\}, \quad \partial\Lambda^- := \{x \in \partial\Lambda; n(x) \cdot q(x) > 0\},$$

where we denoted the flux $q := -(rI + m \otimes m)\nabla p$. Using (2.49) in (2.40) leads to

$$\begin{aligned}
& - \int_{\mathcal{A} \cap \partial\Lambda^+} \left(\nu |m|^{2\gamma} - D^2 m \cdot \Delta m \right)^{-1/2} \left| n \cdot (rI + m \otimes m) \left(\nu |m|^{2(\gamma-1)} m - D^2 \Delta m \right) \right| \, ds \\
& - \int_{\mathcal{A}^c \cap \partial\Lambda^+} r |\nabla p \cdot n| \, ds \\
& + \int_{\mathcal{A} \cap \partial\Lambda^-} \left(\nu |m|^{2\gamma} - D^2 m \cdot \Delta m \right)^{-1/2} \left| n \cdot (rI + m \otimes m) \left(\nu |m|^{2(\gamma-1)} m - D^2 \Delta m \right) \right| \, ds \\
& + \int_{\mathcal{A}^c \cap \partial\Lambda^-} r |\nabla p \cdot n| \, ds \\
& = \int_{\Lambda} S \, dx.
\end{aligned}$$

This is the Murray's law for the phenomenological continuum model (2.36) constrained by the Poisson equation (2.35).

3 Tensor PDE model of biological network formation

3.1 Introduction

In this paper we study the tensor PDE system modeling formation of biological transportation networks,

$$-\operatorname{div} [(r\mathbb{I} + \mathbb{C})\nabla p] = S, \quad (3.1)$$

$$\frac{\partial \mathbb{C}}{\partial t} - D^2 \Delta \mathbb{C} - c^2 \nabla p \otimes \nabla p + \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C} = 0, \quad (3.2)$$

for the scalar pressure field $p = p(t, x) \in \mathbb{R}$ of the fluid transported within the network and the conductance (permeability) tensor $\mathbb{C} = \mathbb{C}(t, x) \in \mathbb{R}^{d \times d}$ with $d \leq 3$ the space dimension. We assume the validity of Darcy's law for slow flow in porous media, connecting the flux q of the fluid with the gradient of its pressure via the action of the permeability tensor $\mathbb{P}[\mathbb{C}]$,

$$q = -\mathbb{P}[\mathbb{C}]\nabla p.$$

The total permeability tensor is assumed to be of the form $\mathbb{P}[\mathbb{C}] := r\mathbb{I} + \mathbb{C}$, where the scalar function $r = r(x) \geq r_0 > 0$ describes the isotropic background permeability of the medium, while the conductance tensor $\mathbb{C}$ tends to align the flux along its eigenvectors. The source/sink distribution $S = S(x)$ in the mass conservation equation (3.1) is to be supplemented as an input datum and is assumed to be independent of time. The diffusivity parameter $D \geq 0$ in (3.2) measures the effect of random fluctuations in the network, and the activation parameter $c^2 > 0$ controls the strength of the network formation feedback loop. This corresponds to a kinetic term in the respective energy functional and represents the influence that the fluid movement has on the formation of the network structure. The last term in (3.2) is the functional derivative of the metabolic function $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$, which describes the dependence of the metabolic cost of maintaining the network on its transportation capacity. Here and in the sequel we shall denote

$$|\mathbb{C}| := \sqrt{\sum_{i=1}^d \sum_{j=1}^d \mathbb{C}_{ij}^2} = \sqrt{\mathbb{C} : \mathbb{C}}$$

the Frobenius norm of the matrix $\mathbb{C}$.

We pose (3.1), (3.2) on a bounded domain $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$, subject to homogeneous Dirichlet boundary conditions on $\partial\Omega$ for $\mathbb{C}$ and homogeneous Neumann boundary condition for p ,

$$\mathbb{C}(t, x) = 0, \quad \nu(x) \cdot \mathbb{P}[\mathbb{C}]\nabla p(t, x) = 0 \quad \text{for } x \in \partial\Omega, \ t \geq 0, \quad (3.3)$$

with $\nu = \nu(x)$ the outer normal vector to $\partial\Omega$, and subject to the initial condition for $\mathbb{C}$,

$$\mathbb{C}(t = 0, x) = \mathbb{C}^0(x) \quad \text{for } x \in \Omega, \quad (3.4)$$

with $\mathbb{C}^0 = \mathbb{C}^0(x)$ symmetric and positive semidefinite almost everywhere in Ω . In order for (3.1) to be solvable subject to (3.3) we assume $S = S(x)$ to have vanishing mean, i.e.,

$$\int_{\Omega} S(x) \, dx = 0. \quad (3.5)$$

The system (3.1)–(3.2) was introduced in [40]. Its fundamental structural property is that it represents the constrained L^2 -gradient flow associated with the energy functional

$$E_D[\mathbb{C}] := \int_{\Omega} \frac{D^2}{2} |\nabla \mathbb{C}|^2 + c^2 \nabla p[\mathbb{C}] \cdot \mathbb{P}[\mathbb{C}] \nabla p[\mathbb{C}] + M(|\mathbb{C}|) \, dx, \quad (3.6)$$

where $p[\mathbb{C}]$ is the unique solution (up to an additive constant) of the Poisson equation (3.1) subject to the homogeneous Neumann boundary condition (3.3). In Section 3.3 we show that for convex metabolic cost functions M the energy functional is convex. Based on this fact, we construct unique solutions of (3.1)–(3.2), both with $D > 0$ and $D = 0$, as the corresponding gradient flows. Finally, in Section 3.4 we study steady states of the system (3.1)–(3.2). For a strictly convex metabolic function M and $D > 0$, existence of unique steady states follows from standard arguments of the calculus of variations. For $D = 0$ and M being a power-law with exponent $\gamma > 1$, the steady state problem reduces to a p -Laplacian equation which, again by standard arguments, has unique solutions. The situation is significantly different for the borderline case $\gamma = 1$, i.e., for linear metabolic cost. Here one arrives at a highly nonlinear free-boundary problem separating the region where $\mathbb{C} = 0$ from the region with positive definite $\mathbb{C}$. Existence and uniqueness of solutions of this problem was shown in [34].

A variant of the system (3.1)–(3.2) was proposed in [39], where the local permeability (conductance) of the porous medium is described in terms of a vector field $m = m(t, x) \in \mathbb{R}^d$. The model is obtained by considering (3.6) with $D = 0$ and imposing $\mathbb{C}$ to be the rank-one tensor $\mathbb{C} := m \otimes m$. This leads to the energy functional

$$\tilde{E}_0[m] := \int_{\Omega} c^2 \nabla p[m] \cdot (r\mathbb{I} + m \otimes m) \nabla p[m] + M(|m|^2) \, dx, \quad (3.7)$$

where $p = p[m]$ is the unique solution of the Poisson equation

$$-\operatorname{div} [(r\mathbb{I} + m \otimes m) \nabla p] = S$$

subject to no-flux boundary condition on $\partial\Omega$. Note that the total permeability tensor $\tilde{\mathbb{P}}[m] := r\mathbb{I} + m \otimes m$ has the principal directions (eigenvectors) $m/|m|$ and, resp., $m^\perp$ with eigenvalues $r(x) + |m|^2$ and, resp., $r(x)$. This means that the flow "feels" only the background permeability $r(x) > 0$ in the directions orthogonal to m , while the principal permeability is increased by $|m|^2$ in the direction of the conductance vector m . Re-introducing the Dirichlet integral $\frac{D^2}{2} \int_{\Omega} |\nabla m|^2 \, dx$ into (3.7) and taking the formal gradient flow with respect to the L^2 -topology leads to the system

$$-\operatorname{div} [(r\mathbb{I} + m \otimes m) \nabla p] = S, \quad (3.8)$$

$$\frac{\partial m}{\partial t} - D^2 \Delta m - c^2 (m \cdot \nabla p) \nabla p + 2M'(|m|^2)m = 0. \quad (3.9)$$

Detailed mathematical analysis of the system (3.8)–(3.9) with $M(s) := s^\gamma$ was carried out in the series of papers [2, 3, 33, 34] and in [42, 79, 80], while its various other aspects were studied in [16, 31, 32, 35, 38].

The system (3.1)–(3.2) can be seen as a more general model than (3.8)–(3.9), not restricting the network permeability tensor to be a rank-one tensor product. Moreover, under appropriate assumptions on the parameters, (3.1)–(3.2) is obtained as the formal continuum limit of a sequence of discrete

graph problems, as we shall demonstrate in Section 3.2 below. On the other hand, the system (3.8)–(3.9) can be linked to the discrete problem by considering macroscopic physical laws of fluid flow in porous media, in particular, Darcy’s law and the Carmen-Kozeny equation; see [3, Section 2.3] for details.

The paper is structured as follows. In Section 3.2 we provide a formal derivation of the tensor PDE model (3.1)–(3.2) as a continuum limit of the discrete model on a sequence of unstructured regular graphs. In Section 3.3 we prove the convexity of the energy (3.6) for convex metabolic cost functions M , and construct solutions of the corresponding gradient flow, both with $D > 0$ and $D = 0$. In Section 3.4 we study steady states of the system (3.1)–(3.2), both with $D > 0$ and $D = 0$.

3.2 Formal derivation from the discrete model in 2D

A particular instance of the system (3.1)–(3.2) with diagonal permeability tensor $\mathbb{C}$ was derived formally in [31] from the discrete network formation model [38]. The system was derived as a formal L^2 -gradient flow of the continuum energy functional (3.6), obtained as a limit of a sequence of discrete problems under refinement of the network, with geometry restricted to rectangular networks in 2D. In [32] the process was carried out rigorously, in terms of the Γ -limit of a sequence of discrete energy functionals with respect to the strong L^2 -topology.

The goal of this Section is to provide a formal derivation of the continuum energy functional (3.6) as a limit of discrete energy functionals posed on a sequence of *unstructured* triangulations of a bounded domain $\Omega \subset \mathbb{R}^2$, i.e., without the restriction on rectangular geometries that was imposed in [31, 32]. The corresponding rigorous limit procedure will be studied in a future work.

The discrete model is posed on a sequence of undirected graphs $\mathbb{G}^h = (\mathbb{V}^h, \mathbb{E}^h)$, $h > 0$, consisting of finite sets of vertices $\mathbb{V}^h$ and edges $\mathbb{E}^h$. Each edge $(i, j) \in \mathbb{E}^h$, connecting the vertices i and $j \in \mathbb{V}^h$, has a fixed, prescribed length $L_{ij} = L_{ji} > 0$ with $L_{ij} = O(h)$, where the limit $h \rightarrow 0$ is under investigation. Its conductivity is denoted by $\mathcal{C}_{ij} = \mathcal{C}_{ji} \geq 0$. Each vertex $i \in \mathbb{V}^h$ has associated the pressure $P_i \in \mathbb{R}$ of the material flowing through it. The local mass conservation in each vertex is expressed in terms of the Kirchhoff law

$$-\sum_{j \in \mathcal{N}(i)} \mathcal{C}_{ij} \frac{P_j - P_i}{L_{ij}} = S_i \quad \text{for all } i \in \mathbb{V}^h, \quad (3.10)$$

where $\mathcal{N}(i)$ denotes the set of vertices connected to $i \in \mathbb{V}^h$ through an edge. Moreover, $S = (S_i)_{i \in \mathbb{V}^h}$ is the prescribed vector of strengths of flow sources ($S_i > 0$) or sinks ($S_i < 0$). Given the vector of conductivities $\mathcal{C} = (\mathcal{C}_{ij})_{(i,j) \in \mathbb{E}^h}$, the Kirchhoff law (3.10) is a linear system of equations for the vector of pressures $P = (P_i)_{i \in \mathbb{V}^h}$. A necessary condition for its solvability is the global mass balance

$$\sum_{i \in \mathbb{V}^h} S_i = 0,$$

whose validity we assume in the sequel. Then, the linear system (3.10) is solvable if and only if the graph with edge weights $\mathcal{C} = (\mathcal{C}_{ij})_{(i,j) \in \mathbb{E}^h}$ is connected [3], where only edges with positive conductivities $\mathcal{C}_{ij} > 0$ are taken into account (i.e., edges with zero conductivities are discarded). Note that the solution is unique up to an additive constant.

The conductivities $\mathcal{C}_{ij}$ are subject to a minimization process with the energy functional

$$E^h[\mathcal{C}] := \sum_{(i,j) \in \mathbb{E}^h} \left(\mathcal{C}_{ij} \frac{(P_j - P_i)^2}{L_{ij}^2} + M(\mathcal{C}_{ij}) \right) L_{ij}, \quad (3.11)$$

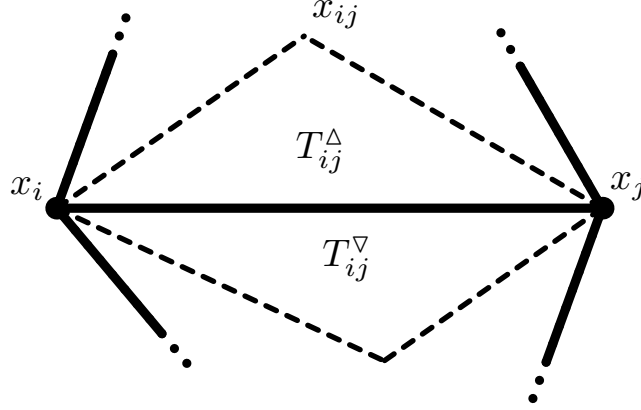


Figure 3.1: Edge $e_{ij} \in \mathbb{E}^h$ (horizontal solid line) and its adjacent diamond $\diamond_{ij}$ (quadrilateral delimited by dashed line). The diamond consists of the triangle T_{ij}^Δ , spanned by the vertices x_i , x_j and x_{ij} , and the triangle T_{ij}^∇ .

where $\mathcal{C} = (\mathcal{C}_{ij})_{(i,j) \in \mathbb{E}^h}$ denotes the vector of edge conductivities, and the sum is taken over unoriented edges, i.e., the edge (i, j) is considered identical with (j, i) and is counted only once. The first term in the summation describes the (physical) pumping power necessary for transporting the material through the network, while the second term describes the metabolic cost of maintaining the network structure, with the metabolic function $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$. It is remarkable that, despite the nonlocal character of the Kirchhoff law (3.10), the gradient flow of the energy (3.11) constrained by (3.10) can be written explicitly in terms of an ODE system for the conductivities $\mathcal{C}_{ij}$,

$$\frac{d\mathcal{C}_{ij}}{dt} = \left(\frac{(P_j - P_i)^2}{L_{ij}^2} - M'(\mathcal{C}_{ij}) \right) L_{ij} \quad \text{for } (i, j) \in \mathbb{E}^h. \quad (3.12)$$

This system, introduced in [39] and studied in more detail in [16], represents an adaptation model which dynamically responds to local information and can naturally incorporate fluctuations in the flow.

Let us assume that the graphs $\mathbb{G}^h = (\mathbb{V}^h, \mathbb{E}^h)$ represent a sequence of finite regular triangulations [20] of a bounded, polygonal domain Ω in 2D, and denote $x_i \in \mathbb{R}^2$ the location of the vertex $i \in \mathbb{V}^h$. For convenience, in the sequel we shall use both notations $(i, j) \in \mathbb{E}^h$ to address edges by the indices of their adjacent vertices, and $e_{ij} \in \mathbb{E}^h$ to address the linear segment in $\mathbb{R}^2$ connecting them (i.e., the set of all convex combinations of x_i and x_j). For each (unoriented) edge $e_{ij} \in \mathbb{E}^h$ we denote by $\diamond_{ij} \subset \mathbb{R}^2$ the adjacent closed diamond, i.e.,

$$\diamond_{ij} := \left\{ x \in \Omega; \text{dist}(x, e_{ij}) \leq \text{dist}(x, \tilde{e}) \text{ for all } \tilde{e} \in \mathbb{E}^h \right\}.$$

Since the graph $\mathbb{G}^h = (\mathbb{V}^h, \mathbb{E}^h)$ represents a triangulation of Ω , the diamonds are quadrilaterals; for edges e_{ij} belonging to the boundary $\partial\Omega$ the definition of $\diamond_{ij}$ has to be adjusted accordingly, such that the corresponding diamond is a quadrilateral too. For each $i \in \mathbb{V}^h$ we denote U_i the union of diamonds adjacent to the vertex x_i ,

$$U_i := \bigcup_{j \in \mathcal{N}(i)} \diamond_{ij}.$$

Each diamond $\diamond_{ij}$ consists of two triangles sharing the edge e_{ij} , which we denote T_{ij}^Δ and T_{ij}^∇ , see Fig. 3.1. Let us denote $\mathcal{T}^h$ the collection of all such triangles, i.e.,

$$\mathcal{T}^h := \{T_{ij}^\Delta; (i, j) \in \mathbb{E}^h\} \cup \{T_{ij}^\nabla; (i, j) \in \mathbb{E}^h\}. \quad (3.13)$$

Clearly, $\mathcal{T}^h$ represents a triangulation of the domain Ω .

The main idea of our construction is to map the vector of discrete edge conductivities $\mathcal{C} = (\mathcal{C}_{ij})_{(i,j) \in \mathbb{E}^h}$ onto the set of piecewise constant tensor fields on Ω through the mapping $\mathbb{Q}^h$ defined as

$$\mathbb{Q}^h[\mathcal{C}](x) := \mathcal{C}_{ij} \frac{(x_i - x_j) \otimes (x_i - x_j)}{|x_i - x_j|^2} \quad \text{for all } x \in \diamond_{ij}. \quad (3.14)$$

I.e., $\mathbb{Q}^h[\mathcal{C}]$ is a constant rank-one tensor on each diamond $\diamond_{ij}$, with principal direction (eigenvector) parallel to the edge e_{ij} and the corresponding eigenvalue equal to the conductivity $\mathcal{C}_{ij}$. Note that under the assumption $\mathcal{C}_{ij} > 0$ for all $(i, j) \in \mathbb{E}$, the tensor $\mathbb{Q}^h[\mathcal{C}]$ is uniformly positive definite on Ω .

Our strategy is, by means of the mapping $\mathbb{Q}^h$, to establish a connection between a properly rescaled version of the discrete energy functional (3.11) and its continuum counterpart (3.6). Since we only carry out formal arguments in this section, we set $D := 0$ for simplicity, and also remove the regularization in the permeability tensor $\mathbb{P}[\mathcal{C}]$, i.e., set $r := 0$ so that $\mathbb{P}[\mathcal{C}] = \mathcal{C}$. The continuum energy reads then

$$\mathcal{E}[\mathbb{C}] := \int_{\Omega} c^2 \nabla p[\mathbb{C}] \cdot \mathbb{C} \nabla p[\mathbb{C}] + M(|\mathbb{C}|) \, dx, \quad (3.15)$$

where $p[\mathbb{C}] \in H^1(\Omega)$ is the unique solution (up to an additive constant) of the Poisson equation (3.1) with the uniformly positive definite permeability tensor $\mathbb{C} \in L^\infty(\Omega)$, subject to the homogeneous Neumann boundary condition (3.3). Following the strategy of [32], the connection between the properly rescaled version of the discrete (3.11) and continuum (3.15) energy functionals will be established through an "intermediate" functional $\mathcal{E}^h$, where $p[\mathbb{C}]$ is replaced by a solution of a finite element discretization of the Poisson equation.

3.2.1 Finite element discretization of the Poisson equation and validity of the Kirchhoff law

We consider the first order H^1 -finite element approximation of the Poisson equation (3.1) with uniformly positive definite permeability tensor $\mathbb{Q}^h[\mathcal{C}]$,

$$-\nabla \cdot (\mathbb{Q}^h[\mathcal{C}] \nabla p) = S \quad (3.16)$$

subject to the no-flux boundary condition on $\partial\Omega$. We denote W^h the space of continuous, piecewise linear functions on the triangulation $\mathcal{T}^h$ introduced in (3.13), i.e.,

$$W^h := \left\{ \psi \in C(\Omega); \psi \text{ linear on each } T \in \mathcal{T}^h \right\}.$$

The finite element discretization of (3.16) reads then

$$\int_{\Omega} \nabla \psi^h \cdot \mathbb{Q}^h[\mathcal{C}] \nabla p^h \, dx = \int_{\Omega} S \psi^h \, dx \quad \text{for all } \psi^h \in W^h. \quad (3.17)$$

Using standard arguments (coercivity and continuity of the corresponding bilinear form) we construct a solution $p^h \in W^h$ of (3.17), unique up to an additive constant; without loss of generality we fix

$\int_{\Omega} p^h dx = 0$. The solution is represented by its vertex values $P_i^h := p^h(x_i)$, $i \in \mathbb{V}$ and the value of ∇p^h , which is constant on each triangle $T \in \mathcal{T}^h$.

Let us now fix $i \in \mathbb{V}$ and denote $\psi_i^h \in W^h$ a test function supported on the union U_i of diamonds adjacent to the vertex x_i . Since $\mathbb{Q}^h[\mathcal{C}]$ is constant on each diamond $\diamond_{ij}$, we have

$$\int_{\Omega} \nabla \psi_i^h \cdot \mathbb{Q}^h[\mathcal{C}] \nabla p^h dx = \sum_{j \in \mathcal{N}(i)} \mathcal{C}_{ij} \int_{\diamond_{ij}} \nabla \psi_i^h \cdot \frac{(x_i - x_j) \otimes (x_i - x_j)}{|x_i - x_j|^2} \nabla p^h dx.$$

Since ∇p^h is constant on each $T \in \mathcal{T}^h$, the Taylor expansion gives

$$p^h(x_i) - p^h(x_j) = \nabla p^h \cdot (x_i - x_j) \quad \text{for all } (i, j) \in \mathbb{E}^h, \quad (3.18)$$

and, consequently,

$$\begin{aligned} \int_{\diamond_{ij}} \nabla \psi_i^h \cdot \frac{(x_i - x_j) \otimes (x_i - x_j)}{|x_i - x_j|^2} \nabla p^h dx &= \int_{\diamond_{ij}} \nabla p^h \cdot \frac{x_i - x_j}{|x_i - x_j|} \nabla \psi_i^h \cdot \frac{x_i - x_j}{|x_i - x_j|} dx \\ &= \frac{p^h(x_i) - p^h(x_j)}{|x_i - x_j|} \int_{\diamond_{ij}} \nabla \psi_i^h \cdot \frac{x_i - x_j}{|x_i - x_j|} dx. \end{aligned}$$

Now, for each triangle $T \subset U_i$, we denote its spanning vertices x_i , x_j and x_{ij} , and define ψ_i^h by prescribing the vertex values

$$\psi_i^h(x_i) = 1, \quad \psi_i^h(x_j) = 0, \quad \psi_i^h(x_{ij}) = 0.$$

This leads to the explicit formula for ψ_i^h on each T ,

$$\psi_i^h(x) := n_{ij}^T \cdot (x - x_j) \quad \text{for } x \in T,$$

where the vector n_{ij}^T is such that

$$n_{ij}^T \cdot (x_{ij} - x_j) = 0, \quad n_{ij}^T \cdot (x_i - x_j) = 1.$$

Obviously, such vector exists (and is unique) for any non-collinear triplet (x_i, x_j, x_{ij}) . Since $\nabla \psi_i^h \equiv n_{ij}^T$ on each T , we have

$$\int_T \nabla \psi_i^h \cdot \frac{x_i - x_j}{|x_i - x_j|} dx = \frac{n_{ij}^T \cdot (x_i - x_j)}{|x_i - x_j|} \text{vol}(T) = \frac{\text{vol}(T)}{L_{ij}}.$$

Finally, recalling that each $\diamond_{ij}$ consists of two triangles (sharing the edge $e_{ij} \in \mathbb{E}^h$), we have

$$\int_{\Omega} \nabla \psi_i^h \cdot \mathbb{Q}^h[\mathcal{C}] \nabla p^h dx = \sum_{j \in \mathcal{N}(i)} \mathcal{C}_{ij} \frac{p^h(x_i) - p^h(x_j)}{L_{ij}} \frac{\text{vol}(\diamond_{ij})}{L_{ij}}.$$

Therefore, denoting

$$S_i^h := \int_{U_i} S \psi_i^h dx \quad \text{for all } i \in \mathbb{V}, \quad (3.19)$$

we have the following proposition.

Proposition 3.1. *Let $S \in L^2(\Omega)$ with $\int_{\Omega} S dx = 0$ and let S_i be given by (3.19). Let $\mathcal{C}_{ij} > 0$ for all $(i, j) \in \mathbb{E}^h$ and denote $P_i^h := p^h(x_i)$, with p^h being the solution of the discretized Poisson equation (3.17). Then we have, for all $i \in \mathbb{V}$,*

$$-\sum_{j \in \mathcal{N}(i)} \mathcal{C}_{ij} \frac{P_j^h - P_i^h}{L_{ij}} \frac{\text{vol}(\diamond_{ij})}{L_{ij}} = S_i. \quad (3.20)$$

Note that (3.20) is a rescaled version of the Kirchhoff law (3.10) by the factor $\frac{\text{vol}(\diamond_{ij})}{L_{ij}}$.

3.2.2 Semi-discrete energy functional

For uniformly positive definite permeability tensors $\mathbb{C} \in L^\infty(\Omega)$ we introduce the semi-discrete energy functional

$$\mathcal{E}^h[\mathbb{C}] = \int_{\Omega} \nabla p^h[\mathbb{C}] \cdot \mathbb{C} \nabla p^h[\mathbb{C}] + M(|\mathbb{C}|) \, dx, \quad (3.21)$$

where $p^h[\mathbb{C}] \in W^h$ the unique solution of the FEM-approximation of the Poisson equation (3.17) with the permeability tensor $\mathbb{C}$. We show that the value of $\mathcal{E}^h$ evaluated at the piecewise constant tensor $\mathbb{Q}^h[\mathbb{C}]$ can be identified with the value of the rescaled version of the discrete energy functional (3.11), given by

$$\bar{E}^h[\mathcal{C}] = \sum_{(i,j) \in \mathbb{E}^h} \frac{\text{vol}(\diamond_{ij})}{L_{ij}} \left(\mathcal{C}_{ij} \frac{(P_i^h - P_j^h)^2}{L_{ij}} + M(\mathcal{C}_{ij}) \right) L_{ij}. \quad (3.22)$$

Proposition 3.2. *For any vector of positive conductivities $\mathcal{C} = (\mathcal{C}_{ij})_{(i,j) \in \mathbb{E}^h}$ we have*

$$\bar{E}^h[\mathcal{C}] = \mathcal{E}^h[\mathbb{Q}^h[\mathcal{C}]], \quad (3.23)$$

with the rescaled discrete energy functional $\bar{E}^h$ defined in (3.22) and the semi-discrete energy $\mathcal{E}^h$ given by (3.21).

Proof. First, we note that, for $x \in \diamond_{ij}$,

$$|\mathbb{Q}^h[\mathcal{C}](x)| = \mathcal{C}_{ij} \left| \frac{(x_i - x_j) \otimes (x_i - x_j)}{|x_i - x_j|^2} \right| = \mathcal{C}_{ij}.$$

Consequently, for the metabolic term we have

$$\begin{aligned} \int_{\Omega} M(|\mathbb{Q}^h[\mathcal{C}]|) \, dx &= \sum_{(i,j) \in \mathbb{E}^h} \int_{\diamond_{ij}} M(|\mathbb{Q}^h[\mathcal{C}]|) \, dx \\ &= \sum_{(i,j) \in \mathbb{E}^h} \int_{\diamond_{ij}} M(\mathcal{C}_{ij}) \, dx = \sum_{(i,j) \in \mathbb{E}^h} \text{vol}(\diamond_{ij}) M(\mathcal{C}_{ij}), \end{aligned}$$

where, again, the sum is taken over unoriented edges so that each $(i, j) \equiv (j, i)$ is counted only once.

For the pumping term we have

$$\int_{\Omega} \nabla p^h \cdot \mathbb{Q}^h[\mathcal{C}] \nabla p^h \, dx = \sum_{(i,j) \in \mathbb{E}^h} \mathcal{C}_{ij} \int_{\diamond_{ij}} \nabla p^h \cdot \frac{(x_i - x_j) \otimes (x_i - x_j)}{|x_i - x_j|^2} \nabla p^h \, dx.$$

Using (3.18) again, we have

$$\int_{\diamond_{ij}} \nabla p^h \cdot \frac{(x_i - x_j) \otimes (x_i - x_j)}{|x_i - x_j|^2} \nabla p^h \, dx = \int_{\diamond_{ij}} \frac{|\nabla p^h \cdot (x_i - x_j)|^2}{|x_i - x_j|^2} \, dx = \text{vol}(\diamond_{ij}) \frac{(p^h(x_i) - p^h(x_j))^2}{|x_i - x_j|^2},$$

so that, denoting again $P_i := p^h(x_i)$,

$$\int_{\Omega} \nabla p^h \cdot \mathbb{Q}^h[\mathcal{C}] \nabla p^h \, dx = \sum_{(i,j) \in \mathbb{E}} \mathcal{C}_{ij} \frac{\text{vol}(\diamond_{ij})}{L_{ij}} \frac{(P_i^h - P_j^h)^2}{L_{ij}}.$$

■

Following the strategy of [32], we would proceed by proving the Γ -convergence of the sequence of functionals $\mathcal{E}^h$ towards $\mathcal{E}$ as $h \rightarrow 0$. In [32] this was carried out for the special case of $\mathbb{G}^h$ being a rectangular grid, and the mapping $\mathbb{Q}^h$ was constructed to generate piecewise constant diagonal permeability tensors $\mathbb{C}$ with diagonal elements corresponding to the conductivities of the horizontal and vertical edges. This peculiar construction facilitated the proof of Γ -convergence of the sequence $\mathcal{E}^h$ with respect to the norm topology of $L^2(\Omega)$. However, in our setting, the sequence $\mathbb{Q}^h[\mathcal{C}]$ given by (3.14) does not converge in the norm topology as $h \rightarrow 0$. Indeed, considering the special case of $\mathbb{G}^h$ being a regular triangulation of Ω , with, say, $\mathcal{C}_{ij} = 1$ for all $(i, j) \in \mathbb{E}^h$, the sequence $\mathbb{Q}^h[\mathcal{C}]$ is a sequence of periodic functions on Ω , which clearly does not converge in any norm topology. Instead, we only have weak convergence, which poses significant analytical challenges for proving the Γ -convergence. In particular, the so-called weak-strong lemma for the Poisson equation, see [32, Lemma 1], which is a fundamental ingredient of the proof, cannot be directly applied. Consequently, new approaches need to be developed to address this problem, which will be subject of future work. In this paper we only prove the following formal link between the (rescaled) discrete energy $\overline{\mathcal{E}}^h[\mathcal{C}]$ and its continuum counterpart $\mathcal{E}$.

Proposition 3.3. *Let $\mathcal{C} = (\mathcal{C}_{ij})_{(i,j) \in \mathbb{E}^h}$ be a vector of positive conductivities on $\mathbb{E}^h$. Then*

$$\overline{\mathcal{E}}^h[\mathcal{C}] = \mathcal{E}^h[\mathbb{Q}^h[\mathcal{C}]] = \mathcal{E}[\mathbb{Q}^h[\mathcal{C}]] + O(h^2), \quad (3.24)$$

with respect to the $H_0^1(\Omega)$ -topology, with the discrete energy functional $\overline{\mathcal{E}}^h$ defined in (3.22), the semi-discrete functional $\mathcal{E}^h$ defined in (3.21) and the continuum energy $\mathcal{E}$ defined in (3.15).

Proof. Since $\mathcal{C}$ has all positive entries, $\mathbb{C} := \mathbb{Q}^h[\mathcal{C}]$ is a symmetric, uniformly positive definite tensor field with $\mathbb{C} \in L^\infty(\Omega)$. Let us define the bilinear form $B : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}$,

$$B(u, v) = \int_{\Omega} \nabla u \cdot \mathbb{C} \nabla v \, dx.$$

Clearly, B induces a seminorm on $H^1(\Omega)$,

$$|u|_B := \sqrt{B(u, u)} \quad \text{for } u \in H^1(\Omega).$$

With this notation we have

$$\int_{\Omega} \nabla p \cdot \mathbb{C} \nabla p \, dx = |p|_B^2.$$

We now proceed along the lines of standard theory of the finite element method (proof of Céa's Lemma in the energy norm, see, e.g., [17]). Due to the Galerkin orthogonality

$$B(p - p^h, \psi) = 0 \quad \text{for all } \psi \in W^h, \quad (3.25)$$

we have, noting that $p^h \in W^h$,

$$|p|_B^2 - |p^h|_B^2 = |p - p^h|_B^2.$$

Then, again by (3.25) and by the Cauchy-Schwartz inequality, we have for all $\psi \in W^h$,

$$|p - p^h|_B^2 = B(p - p^h, p - \psi) \leq |p - p^h|_B |p - \psi|_B,$$

and, consequently,

$$\left| p - p^h \right|_B \leq \inf_{\psi \in W^h} |p - \psi|_B.$$

Then, by standard results of approximation theory, see, e.g., [17], we have $\inf_{\psi \in W^h} |p - \psi|_B = O(h)$ and, consequently,

$$\mathcal{E}[\mathbb{C}] - \mathcal{E}^h[\mathbb{C}] = |p|_B^2 - |p^h|_B^2 = \left| p - p^h \right|_B^2 = O(h^2).$$

An application of Proposition 3.2 gives the claim (3.24). ■

Finally, let us note that both the energy functional (3.22) and, resp., the Kirchhoff law (3.20) are rescaled by the same factor $\frac{\text{vol}(\diamond_{ij})}{L_{ij}^2}$ with respect to their original definitions (3.11) and, resp., (3.10). Consequently, the constrained gradient flow corresponding to the system (3.20), (3.22) still admits an explicit description in terms of the ODE

$$\frac{d\mathcal{C}_{ij}}{dt} = \left(\frac{(P_j - P_i)^2}{L_{ij}^2} - M'(\mathcal{C}_{ij}) \right) \text{vol}(\diamond_{ij}) \quad \text{for } (i, j) \in \mathbb{E}^h,$$

which is a rescaled version of (3.12).

3.3 Energy dissipation structure, convexity and gradient flow

A fundamental structural property of the system (3.1)–(3.2) is that it represents the constrained $L^2(\Omega)$ -gradient flow associated with the energy functional (3.6). The gradient flow structure implies the following energy relation, established in [40].

Proposition 3.4. *The energy (3.6) is nonincreasing along smooth solutions of (3.1)–(3.2) and satisfies*

$$\frac{d}{dt} E_D[\mathbb{C}(t)] = - \int_{\Omega} \left| \frac{\partial \mathbb{C}(t)}{\partial t}(t, x) \right|^2 dx.$$

Proof. The proof is obtained by an obvious modification of [33, Lemma 1]. We present here the main steps. Taking into consideration the relationship

$$\int_{\Omega} \nabla p(r\mathbb{I} + \mathbb{C}) \nabla p dx = \int_{\Omega} S p dx,$$

by adding a multiple of it, we can rewrite the energy as

$$E_D[\mathbb{C}(t)] = \int_{\Omega} \frac{D^2}{2} |\nabla \mathbb{C}|^2 + M(|\mathbb{C}|) - c^2 \nabla p(r\mathbb{I} + \mathbb{C}) \nabla p + 2c^2 S p dx.$$

We then evaluate

$$\begin{aligned} \frac{d}{dt} E_D[\mathbb{C}(t)] &= \int_{\Omega} D^2 \nabla \mathbb{C} : \nabla(\partial_t \mathbb{C}) + \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C} : \partial_t \mathbb{C} \\ &\quad - \nabla p \mathbb{C} \nabla p - 2 [\nabla \partial_t p (r\mathbb{I} + \mathbb{C}) \nabla p - S \partial_t p] dx, \end{aligned}$$

where we used the symmetry of the matrix $rI + \mathbb{C}$. Considering the equivalence $\int_{\Omega} \nabla \partial_t p (r\mathbb{I} + \mathbb{C}) \nabla p - S \partial_t p = 0$, and that $\mathbb{C}(t)$ is the solution of equation (3.2), we obtain the thesis. $\blacksquare$

A major observation is that if the metabolic cost function is convex and nondecreasing, then the energy functional E_D is convex. Let us denote $H_+^1(\Omega)$ the set of symmetric, positive semidefinite matrix-valued functions with entries in $H^1(\Omega)$. Obviously, $H_+^1(\Omega)$ is a closed, convex subset of $H^1(\Omega)$.

Proposition 3.5. *Let Ω be a bounded domain in $\mathbb{R}^d$ and denote C_{Ω} the corresponding Poincaré constant. Let $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ be such that*

$$\frac{M'(s)}{s} \geq -D^2 C_{\Omega} \quad \text{if } M''(s) \geq \frac{M'(s)}{s}, \quad (3.26)$$

$$M''(s) \geq -D^2 C_{\Omega} \quad \text{if } M''(s) < \frac{M'(s)}{s}. \quad (3.27)$$

Then the energy functional E_D given by (3.6) is convex on $H_+^1(\Omega)$. Moreover, if (3.26), (3.27) hold with sharp inequalities on the left-hand side, then E_D is strictly convex.

Proof. Using $p = p[\mathbb{C}]$ as a test function in the weak formulation of (3.1), one has

$$\int_{\Omega} \nabla p \cdot \mathbb{P}[\mathbb{C}] \nabla p \, dx = \int_{\Omega} S p \, dx,$$

so that the energy can be written as

$$E_D[\mathbb{C}] = \int_{\Omega} \frac{D^2}{2} |\nabla \mathbb{C}|^2 + M(|\mathbb{C}|) + c^2 S p[\mathbb{C}] \, dx.$$

By elementary calculation, the second-order variation of the first two terms above in direction $\Phi \in H_+^1(\Omega)$ reads

$$D^2 \int_{\Omega} |\nabla \Phi|^2 \, dx + \int_{\Omega} M''(|A|) \left| \frac{A}{|A|} : \Phi \right|^2 + \frac{M'(|A|)}{|A|} \left(|\Phi|^2 - \left| \frac{A}{|A|} : \Phi \right|^2 \right) \, dx.$$

Using $\frac{\delta p[\mathbb{C}, \Phi]}{\delta \mathbb{C}}$ as a test function in the weak formulation of (3.1) and calculating the first-order variation in direction $\Phi \in H_+^1(\Omega)$ gives

$$\begin{aligned} \frac{\delta^2}{\delta \mathbb{C}^2} \int S p[\mathbb{C}; \Phi] \, dx &= \int_{\Omega} \nabla \frac{\delta p}{\delta \mathbb{C}} \cdot (r\mathbb{I} + \mathbb{C}) \nabla \frac{\delta p}{\delta \mathbb{C}} \, dx \\ &+ \int_{\Omega} \nabla \frac{\delta^2 p}{\delta \mathbb{C}^2} \cdot (r\mathbb{I} + \mathbb{C}) \nabla p + \nabla \frac{\delta p}{\delta \mathbb{C}} \cdot \Phi \nabla p \, dx, \end{aligned}$$

where here and in the sequel we use the short-hand notation $\frac{\delta p}{\delta \mathbb{C}}$ for $\frac{\delta p[\mathbb{C}, \Phi]}{\delta \mathbb{C}}$. The first-order variation of the weak formulation of the Poisson equation (3.1) in direction $\Phi \in H_+^1(\Omega)$ with test function $\phi \in H^1(\Omega)$ reads

$$\int_{\Omega} \nabla \phi \cdot (r\mathbb{I} + \mathbb{C}) \nabla \frac{\delta p}{\delta \mathbb{C}} + \nabla \phi \cdot \Phi \nabla p \, dx = 0, \quad (3.28)$$

and using $\frac{\delta p}{\delta \mathbb{C}}$ as a test function we obtain the identity

$$\int_{\Omega} \nabla \frac{\delta p}{\delta \mathbb{C}} \cdot \Phi \nabla p \, dx = - \int_{\Omega} \nabla \frac{\delta p}{\delta \mathbb{C}} \cdot (r\mathbb{I} + \mathbb{C}) \nabla \frac{\delta p}{\delta \mathbb{C}} \, dx.$$

We now again take a variation of (3.28) in direction $\Phi \in H_+^1(\Omega)$ and use the pressure p as a test function, which leads to

$$\int_{\Omega} \nabla p \cdot (r\mathbb{I} + \mathbb{C}) \nabla \frac{\delta^2 p}{\delta \mathbb{C}^2} dx = -2 \int_{\Omega} \nabla p \cdot \Phi \nabla \frac{\delta p}{\delta \mathbb{C}} dx.$$

Consequently, we arrive at

$$\frac{\delta^2}{\delta \mathbb{C}^2} \int_{\Omega} Sp[\mathbb{C}; \Phi] dx = 2 \int_{\Omega} \nabla \frac{\delta p}{\delta \mathbb{C}} \cdot (r\mathbb{I} + \mathbb{C}) \nabla \frac{\delta p}{\delta \mathbb{C}} dx,$$

and, finally,

$$\begin{aligned} \frac{\delta^2 E_D[\mathbb{C}; \Phi]}{\delta \mathbb{C}^2} &= D^2 \int_{\Omega} |\nabla \Phi|^2 dx + \int_{\Omega} M''(|A|) \left| \frac{A}{|A|} : \Phi \right|^2 + \frac{M'(|A|)}{|A|} \left(|\Phi|^2 - \left| \frac{A}{|A|} : \Phi \right|^2 \right) dx \\ &+ 2c^2 \int_{\Omega} \nabla \frac{\delta p}{\delta \mathbb{C}} \cdot (r\mathbb{I} + \mathbb{C}) \nabla \frac{\delta p}{\delta \mathbb{C}} dx. \end{aligned}$$

Obviously, the last term is nonnegative. Using the Poincaré inequality for the first term of the right-hand side and denoting C_{Ω} the Poincaré constant for Ω , we have

$$\frac{\delta^2 E_D[\mathbb{C}; \Phi]}{\delta \mathbb{C}^2} \geq \int_{\Omega} \left(D^2 C_{\Omega} + \frac{M'(|A|)}{|A|} \right) |\Phi|^2 dx + \int_{\Omega} \left(M''(|A|) - \frac{M'(|A|)}{|A|} \right) \left| \frac{A}{|A|} : \Phi \right|^2 dx.$$

Denoting Ω^+ the set where $M''(|A|) - \frac{M'(|A|)}{|A|} \geq 0$, and Ω^- its complement in Ω , we have

$$\frac{\delta^2 E_D[\mathbb{C}; \Phi]}{\delta \mathbb{C}^2} \geq \int_{\Omega^+} \left(D^2 C_{\Omega} + \frac{M'(|A|)}{|A|} \right) |\Phi|^2 dx + \int_{\Omega^-} \left(D^2 C_{\Omega} + M''(|A|) \right) |\Phi|^2 dx,$$

where we used $\left| \frac{A}{|A|} : \Phi \right| \leq |\Phi|$. Clearly, conditions (3.26), (3.27) imply the convexity of E_D , which is strict if the inequalities on the left-hand side of (3.26), (3.27) are sharp. ■

Remark 3.6. *Let us consider the generic case of M being the power-law $M(s) = s^{\gamma}/\gamma$ with exponent $\gamma > 0$, as discussed in [39] and the subsequent works. Then $M'(s)/s = s^{\gamma-2}$, so that condition (3.26) is implicitly verified for all $s > 0$. Condition (3.27) is verified if and only if $\gamma \geq 1$. Consequently, E_D is strictly convex for every $\gamma \geq 1$ and $D > 0$. For $D = 0$ it is strictly convex for $\gamma > 1$ and convex for $\gamma = 1$.*

3.3.1 Existence and uniqueness of gradient flow

For a metabolic function M verifying the condition (3.26), (3.27), we prove the existence and uniqueness of weak solutions of the system (3.1)–(3.2) by an application of the standard theory of convex gradient flows on Hilbert spaces, see, e.g., [6, 62]. Before we proceed with the proof, we establish two auxiliary lemmas. In the sequel we shall denote by $\dot{H}^1(\Omega)$ the closed subspace of $H^1(\Omega)$ of functions with vanishing mean.

Lemma 3.7. *Let $\mathbb{C} \in L^2(\Omega)^{d \times d}$ be a matrix-valued function, positive semidefinite almost everywhere on Ω , and let $S \in L^2(\Omega)$ with $\int_{\Omega} S(x) dx = 0$. Then the Poisson equation (3.1) admits a unique weak solution $p \in \dot{H}^1(\Omega)$. Moreover, it holds*

$$\|\nabla p\|_{L^2(\Omega)} \leq C_{\Omega} \|S\|_{L^2(\Omega)}, \quad (3.29)$$

where C_{Ω} denotes the Poincaré constant on Ω .

Proof. In order to obtain L^∞ bound on the matrix $r\mathbb{I} + \mathbb{C}$, we consider the regularized problem

$$-\operatorname{div}[(r\mathbb{I} + \mathbb{C} * \eta_\varepsilon)\nabla p] = S, \quad (3.30)$$

where η is a radially symmetric function, with compact support and integral 1, and $\eta_\varepsilon := \frac{1}{\varepsilon^d} \eta(\frac{\cdot}{\varepsilon})$. For every fixed $\varepsilon > 0$, we define on the space $\dot{H}^1(\Omega)$ the bilinear form

$$B_\varepsilon(u, v) := \int_\Omega \nabla v (rI + \mathbb{C} * \eta_\varepsilon) \nabla u \, dx,$$

which is, thanks to the regularization, coercive and continuous. This imply the existence of a unique solution $p_\varepsilon \in \dot{H}^1(\Omega)$ for the equation (3.30). Moreover it holds, for every ε ,

$$\|\nabla p_\varepsilon\|_{L^2(\Omega)} \leq C \|S\|_{L^2(\Omega)}.$$

The sequence $\{p_\varepsilon\}$ is then uniformly bounded in $\dot{H}^1(\Omega)$. It exists then an element $p \in \dot{H}^1(\Omega)$ such that, up to a subsequence, p_ε converges weakly to such point p . We now prove that this element is a solution for the equation (3.1).

Let $\phi \in C^\infty(\Omega)$ be a test function, we want to pass the limit in the relation

$$\int_\Omega \nabla \phi (r\mathbb{I} + \mathbb{C} * \eta_\varepsilon) \nabla p_\varepsilon \, dx = \int_\Omega S \phi.$$

The first term converges because of the definition of weak convergence. Moreover, since the sequence $\{\mathbb{C} * \eta_\varepsilon\}$ converges strongly to $\mathbb{C}$ in the L^2 -norm, and $\{\nabla p_\varepsilon\}$ weakly converges to ∇p , the term $\int \nabla \phi \mathbb{C} * \eta_\varepsilon \nabla p_\varepsilon \, dx$ converges, for every ϕ , to $\int \nabla \phi \mathbb{C} \nabla p \, dx$. The equation (3.1) admits then a solution in the space $\dot{H}^1(\Omega)$.

Uniqueness follows from the uniform positive definiteness of the matrix $r\mathbb{I} + \mathbb{C}$. ■

Lemma 3.8. *Let $(\mathbb{C}_k)_{k \in \mathbb{N}}$ be a sequence of symmetric and positive semidefinite matrix-valued functions on a bounded domain $\Omega \subset \mathbb{R}^d$. Let the sequence $\mathbb{C}_k$ converge to $\mathbb{C}$ in the norm topology of the space $L^2(\Omega)^{d \times d}$ as $k \rightarrow \infty$. Then there exists a subsequence of $\sqrt{\mathbb{C}_k}$ converging to $\sqrt{\mathbb{C}}$ in the norm topology of $L^4(\Omega)^{d \times d}$.*

Proof. As the sequence $\mathbb{C}_k$ converges in the norm topology of $L^2(\Omega)$ to $\mathbb{C}$, there exists a subsequence converging almost everywhere on Ω to $\mathbb{C}$. As the operation of taking the principal square root is continuous on the set of positive semidefinite matrices, see p. 411 of [37], a subsequence of $\sqrt{\mathbb{C}_k}$ converges pointwise almost everywhere to $\sqrt{\mathbb{C}}$.

Symmetry of $\mathbb{C}_k$ implies symmetry of $\sqrt{\mathbb{C}_k}$, giving

$$|\sqrt{\mathbb{C}_k}|_2 = \varrho(\sqrt{\mathbb{C}_k}) = \sqrt{\varrho(\mathbb{C}_k)} = \sqrt{|\mathbb{C}_k|_2}, \quad (3.31)$$

where $|\cdot|_2$ denotes the spectral norm and $\varrho(\cdot)$ the spectral radius. Consequently, the boundedness of $\mathbb{C}_k$ in $L^2(\Omega)^{d \times d}$ implies boundedness of $\sqrt{\mathbb{C}_k}$ in $L^4(\Omega)^{d \times d}$ and there is a subsequence of $\sqrt{\mathbb{C}_k}$ converging weakly in $L^4(\Omega)^{d \times d}$ to $\sqrt{\mathbb{C}}$; identification of the limit is due to the almost everywhere convergence. Moreover, (3.31) implies that

$$\lim_{k \rightarrow \infty} \|\sqrt{\mathbb{C}_k}\|_{L^4(\Omega)} = \lim_{k \rightarrow \infty} \sqrt{\|\mathbb{C}_k\|_{L^2(\Omega)}} = \sqrt{\|\mathbb{C}\|_{L^2(\Omega)}} = \|\sqrt{\mathbb{C}}\|_{L^4(\Omega)}.$$

By uniform convexity of $L^4(\Omega)^{d \times d}$, Proposition 3.32 of [15] implies then the strong convergence of $\sqrt{\mathbb{C}_k}$ to $\sqrt{\mathbb{C}}$ in $L^4(\Omega)^{d \times d}$. ■

In the sequel, let us denote $H_{0,+}^1(\Omega)$ the space of symmetric, positive semidefinite tensor-valued functions with entries in $H^1(\Omega)$ and vanishing traces on $\partial\Omega$.

Proposition 3.9 (Existence and uniqueness of gradient flows). *Let $r > 0$, $D > 0$, $S \in L^2(\Omega)$ satisfying (3.5) and $\mathbb{C}^0 \in H_{0,+}^1(\Omega)$, symmetric and positive semidefinite almost everywhere in Ω , and such that $E_D[\mathbb{C}^0] < \infty$. Moreover, let the metabolic cost function $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ verify the conditions (3.26) and (3.27). Then, the problem (3.1)–(3.4) admits a unique global weak solution $\mathbb{C} \in H^1((0, \infty); L^2(\Omega)) \cap L^2((0, \infty); H_{0,+}^1(\Omega))$ with $E_D[\mathbb{C}] \in L^\infty(0, \infty)$. Moreover, $\mathbb{C} = \mathbb{C}(t, x)$ is symmetric positive semidefinite for almost all $x \in \Omega$ and $t \geq 0$, and satisfies the energy inequality*

$$E_D[\mathbb{C}(t)] + \int_0^t \int_\Omega \left| \frac{\partial \mathbb{C}}{\partial t}(s, x) \right|^2 dx ds \leq E_D[\mathbb{C}^0] \quad \text{for all } t \geq 0. \quad (3.32)$$

Proof. The energy functional (3.6) is proper and, according to Proposition 3.5, convex on $H_{0,+}^1(\Omega)$. Lower semicontinuity with respect to the $H^1(\Omega)$ -topology is obvious for the diffusive term $\int_\Omega \frac{D^2}{2} |\nabla \mathbb{C}|^2 dx$ and the metabolic term $\int_\Omega M(|\mathbb{C}|) dx$. To show lower semicontinuity of the activation term $\int_\Omega \nabla p[\mathbb{C}] \cdot \mathbb{P}[\mathbb{C}] \nabla p[\mathbb{C}] dx$, we choose a sequence $\mathbb{C}_k \in L^2(\Omega)$ converging to $\mathbb{C} \in L^2(\Omega)$. Denoting p_k the unique weak solution of the Poisson equation (3.1) with permeability tensor $\mathbb{C}_k$, constructed in Lemma 3.7, and using in as a test function, we have

$$\int_\Omega r |\nabla p_k|^2 + \nabla p_k \cdot \mathbb{C}_k \nabla p_k dx = \int_\Omega S p_k dx.$$

Then, we estimate, using the Cauchy-Schwartz and Poincaré inequalities,

$$\begin{aligned} \int_\Omega \left| \sqrt{\mathbb{C}_k} \nabla p_k \right|^2 dx &= \int_\Omega \nabla p_k \cdot \mathbb{C}_k \nabla p_k dx \leq \int_\Omega S p_k dx \\ &\leq \|S\|_{L^2(\Omega)} \|p_k\|_{L^2(\Omega)} \\ &\leq C_\Omega \|S\|_{L^2(\Omega)} \|\nabla p_k\|_{L^2(\Omega)}, \end{aligned}$$

where C_Ω is the Poincaré constant for Ω . Due to the bound (3.29), we obtain uniform boundedness of the sequence $\sqrt{\mathbb{C}_k} \nabla p_k$ in $L^2(\Omega)$. Consequently, up to a possible extraction of a subsequence, $\sqrt{\mathbb{C}_k} \nabla p_k$ converges weakly in $L^2(\Omega)$. The limit is identified due to the strong convergence of $\sqrt{\mathbb{C}_k}$ to $\sqrt{\mathbb{C}}$ provided by Lemma 3.8 and the weak convergence of ∇p_k to ∇p . Then, the lower-semicontinuity of the L^2 -norm gives

$$\int_\Omega \left| \sqrt{\mathbb{C}} * \eta \nabla p \right|^2 dx \leq \liminf_{k \rightarrow \infty} \int_\Omega \left| \sqrt{\mathbb{C}_k} * \eta \nabla p_k \right|^2 dx.$$

Consequently, we have the lower semicontinuity for the energy functional,

$$E[\mathbb{C}] \leq \liminf_{k \rightarrow \infty} E[\mathbb{C}_k].$$

Then, by the Rockafellar theorem, the subdifferential ∂E is a maximal monotone operator on $H_{0,+}^1(\Omega)$, which in turn implies the existence and uniqueness of solutions of the system (3.1)–(3.4), see, e.g., [15].

To check for preservation of positive definiteness, let us fix an arbitrary vector $\xi \in \mathbb{R}^d$ and define $u(t, x) := \xi \cdot \mathbb{C}(t, x) \xi$. From (3.2) we obtain

$$\frac{\partial u}{\partial t} - D^2 \Delta u + \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} u = |\xi \cdot \nabla p|^2 \geq 0,$$

and the maximum principle for linear parabolic problems (see, e.g., [24]) implies that $u \geq 0$ if $u(t = 0) \geq 0$. Consequently, the positive semidefiniteness of the initial datum $\mathbb{C}^0$ is preserved by (3.2). $\blacksquare$

Let us note that the proof of Proposition 3.9 can be easily adapted to the case $D = 0$, i.e., no diffusion, by changing the topology to $L^2(\Omega)$. Then, we obtain the following result.

Proposition 3.10. *Let $r > 0$, $S \in L^2(\Omega)$ satisfying (3.5) and $\mathbb{C}^0 \in L^2(\Omega)$, symmetric and positive semidefinite almost everywhere in Ω , and such that $E_0[\mathbb{C}^0] < \infty$. Let the metabolic cost function $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ verify the conditions (3.26) and (3.27).*

Then the problem (3.1)–(3.4) with $D = 0$ admits a unique global weak solution $\mathbb{C} \in H^1((0, \infty); L^2(\Omega))$, symmetric and positive semidefinite for almost all $x \in \Omega$ and $t \geq 0$, with $E_0[\mathbb{C}] \in L^\infty(0, \infty)$ and satisfying the energy inequality (3.32) with $D = 0$.

Proof. Convexity of E_0 follows from Proposition 3.5, with conditions (3.26), (3.27) verified due to the monotonicity and convexity of M . Lower semicontinuity of E_0 with respect to the norm L^2 -topology follows along the steps of the proof of Proposition 3.9. $\blacksquare$

Finally, let us observe that for suitable choices of the metabolic cost function M , uniform positive definiteness of the tensor $\mathbb{C}$ is preserved at least locally in time along the solutions of (3.2) with $D \geq 0$.

Proposition 3.11. *Let $M(s) = \frac{1}{\gamma}|s|^\gamma$ with $1 \leq \gamma < 2$, $D \geq 0$ and let ∇p be given with $\nabla p \in L^\infty((0, \infty); L^2(\Omega))$. Let $\mathbb{C}^0 \in L^2(\Omega)$, symmetric and uniformly positive definite in Ω . Then there exists $T > 0$ such that $\mathbb{C} = \mathbb{C}(t, x)$, the solution of (3.2)–(3.4), is uniformly positive definite in Ω for $t < T$.*

Proof. Let us fix an arbitrary unit vector $\xi \in \mathbb{R}^d$ and define $u(t, x) := \xi \cdot \mathbb{C}(t, x)\xi$. For the Frobenius norm we have $|\mathbb{C}| \leq \lambda_{\max}(\mathbb{C})$, where $\lambda_{\max}(\mathbb{C})$ denotes the principal eigenvalue of $\mathbb{C}$. Consequently, with $|\xi| = 1$ we have

$$|\mathbb{C}| \geq \lambda_{\max}(\mathbb{C}) \geq \xi \cdot \mathbb{C}\xi = u$$

and since $\gamma < 2$,

$$\frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} = |\mathbb{C}|^{\gamma-2} \leq u^{\gamma-2}.$$

From (3.2) we then obtain

$$\begin{aligned} \frac{\partial u}{\partial t} &= D^2 \Delta u + |\xi \cdot \nabla p|^2 - \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} u \\ &\geq D^2 \Delta u - u^{\gamma-1}. \end{aligned} \tag{3.33}$$

Clearly, the solution $v = v(t)$ of the initial value problem

$$\frac{dv}{dt} = -v^{\gamma-1}, \quad v(0) = \inf_{x \in \Omega} u(0, x)$$

is a subsolution for (3.33), as long as it exists. For $\gamma = 1$ we obviously have $\frac{dv}{dt} = -1$. A simple calculation reveals that

$$v(t) = (v(0) - (2 - \gamma)t)^{\frac{1}{2-\gamma}}$$

for $t \leq \frac{v(0)}{2-\gamma}$. Consequently, we have

$$u(t, x) \geq \left(\inf_{x \in \Omega} u(0, x) - (2 - \gamma)t \right)^{\frac{1}{2-\gamma}}$$

on this time interval. We conclude that if $\mathbb{C}^0$ is uniformly positive definite in Ω , then this property is preserved on sufficiently small time intervals. ■

Proposition 3.11 allows us to drop the regularization of the permeability tensor in (3.1) if $M(s) = \frac{1}{\gamma}|s|^\gamma$ with $1 \leq \gamma < 2$. In this case we may consider the system (3.1)–(3.4) with $r = 0$ and $D \geq 0$, and the uniform positive definiteness of $\mathbb{C} = \mathbb{C}(t, x)$ provided by Proposition 3.11 guarantees existence of solutions (at least) locally in time. Moreover, for $\gamma = 2$, a straightforward modification of the proof of Proposition 3.11 yields preservation of positive definiteness globally in time, and thus global solutions with $r = 0$.

3.4 Steady states

In this section we discuss existence and uniqueness of steady states of the system (3.1)–(3.2). We first provide a result for the case $D > 0$, and then carry out a more explicit construction for the case $D = 0$. Let us recall that we denoted $H_{0,+}^1(\Omega)$ the space of symmetric, positive semidefinite tensor-valued functions with entries in $H^1(\Omega)$ and vanishing traces on $\partial\Omega$.

Proposition 3.12. *Let $r > 0$, $D > 0$ and $S \in L^2(\Omega)$ satisfying (3.5). Moreover, let the metabolic cost function $M : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ be nonnegative and continuous. Then there exists a steady state of the system (3.1)–(3.2) in $H_{0,+}^1(\Omega)$.*

Moreover, if M satisfies conditions (3.26), (3.27), then the gradient flows constructed in Proposition 3.9 converge towards a steady state as $t \rightarrow \infty$.

The steady state is unique if M satisfies conditions (3.26), (3.27) with sharp inequalities on the left-hand side.

Proof. We apply the direct method of calculus of variations on the closed, convex set $H_{0,+}^1(\Omega)$. Since the energy E_D given by (3.6) is, by definition, nonnegative, we have an infimising sequence $(\mathbb{C}_n)_{n \in \mathbb{N}} \subset H_{0,+}^1(\Omega)$. With $D > 0$ and the Poincaré inequality, the energy E_D is coercive on $H_{0,+}^1(\Omega)$ due to the presence of the Dirichlet integral. Consequently, there exists a subsequence of $(\mathbb{C}_n)_{n \in \mathbb{N}}$ converging weakly to some $\mathbb{C} \in H_{0,+}^1(\Omega)$ and, due to compact embedding, strongly in $L^2(\Omega)$. Clearly, the Dirichlet integral $\frac{D^2}{2} \int_{\Omega} |\nabla \mathbb{C}_n|^2 dx$ in the definition of E_D is weakly lower semicontinuous. Due to the strong convergence of $\mathbb{C}_n$ in $L^2(\Omega)$ and the assumed continuity of M , we can pass to the limit in the metabolic term $\int_{\Omega} M(|\mathbb{C}_n|) dx$. Finally, we refer to the proof of Proposition 3.9 where lower semicontinuity of the activation term $\int_{\Omega} \nabla p[\mathbb{C}_n] \cdot \mathbb{P}[\mathbb{C}_n] \nabla p[\mathbb{C}_n] dx$ was shown with respect to the $L^2(\Omega)$ topology. Consequently, we have

$$E_D[\mathbb{C}] \leq \liminf_{n \rightarrow \infty} E_D[\mathbb{C}_n],$$

and $\mathbb{C} \in H_{0,+}^1(\Omega)$ is a global minimizer of E_D , i.e., a steady state of the system (3.1)–(3.2). The minimizer is unique if E_D is strictly convex, which, according to Proposition 3.5, is the case when conditions (3.26), (3.27) hold with sharp inequalities on the left-hand side.

Finally, the convergence of the gradient flow towards a steady state follows from the convexity and coercivity of E_D by standard theory, see, e.g., [6].

■

Next, let us study the case $D = 0$. Then, the stationary version of (3.2) reads

$$c^2 \nabla p \otimes \nabla p = m(|\mathbb{C}|) \mathbb{C}, \quad (3.34)$$

where we introduced the notation $m(s) := M'(s)/s$. Consequently, $\mathbb{C}$ is a multiple of $\nabla p \otimes \nabla p$,

$$\mathbb{C} = \lambda \nabla p \otimes \nabla p,$$

and inserting into (3.34), noting that $|\nabla p \otimes \nabla p| = |\nabla p|^2$, gives

$$m(|\lambda| |\nabla p|^2) = \frac{c^2}{\lambda}.$$

Assuming invertibility of m , we have

$$|\nabla p|^2 = \frac{1}{|\lambda|} m^{-1} \left(\frac{c^2}{\lambda} \right).$$

Consequently, denoting $g(\lambda) := \frac{1}{|\lambda|} m^{-1} \left(\frac{c^2}{\lambda} \right)$ and assuming its invertibility, we arrive at $\lambda = g^{-1}(|\nabla p|^2)$ and

$$\mathbb{C} = g^{-1}(|\nabla p|^2) \nabla p \otimes \nabla p,$$

where p solves the nonlinear Poisson equation

$$-\nabla \cdot \left(\left[r + g^{-1}(|\nabla p|^2) |\nabla p|^2 \right] \nabla p \right) = S.$$

Let us now consider the generic case of M being the power-law $M(s) = s^\gamma/\gamma$ with exponent $\gamma > 0$, as discussed in [39] and the subsequent works. Then, the functions $m = m(s)$ and $g = g(\lambda)$, introduced above, are both invertible if and only if $\gamma > 1$, and we easily calculate

$$g^{-1}(\lambda) = c^{\frac{2}{\gamma-1}} \lambda^{-\frac{\gamma-2}{\gamma-1}}.$$

Inserting this expression into the Poisson equation (3.1), we obtain the p -Laplacian equation

$$-\nabla \cdot \left(\left[r + c^{\frac{2}{\gamma-1}} |\nabla p|^{\frac{2\gamma}{\gamma-1}} \right] \nabla p \right) = S, \quad (3.35)$$

subject to the homogeneous Neumann boundary condition on $\partial\Omega$.

Proposition 3.13. *For any $S \in L^2(\Omega)$ and $\gamma > 1$ there exists a unique weak solution $p \in \overline{H}^1(\Omega) \cap W^{1, \frac{2\gamma}{\gamma-1}}(\Omega)$ of (3.35) subject to the homogeneous Neumann boundary condition on $\partial\Omega$.*

Proof. We define the functional $\mathcal{F} : \overline{H}^1(\Omega) \rightarrow \mathbb{R} \cup \{+\infty\}$,

$$\mathcal{F}[p] := \int_{\Omega} r |\nabla p|^2 + c^{\frac{2}{\gamma-1}} |\nabla p|^{\frac{2\gamma}{\gamma-1}} dx - \int_{\Omega} p S dx, \quad (3.36)$$

and $\mathcal{F}[p] := +\infty$ if $\nabla p \notin L^{\frac{2\gamma}{\gamma-1}}$. Then $\mathcal{F}$ is uniformly convex since $\frac{2\gamma}{\gamma-1} > 2$ for $\gamma > 1$. Coercivity follows from the Poincaré inequality on $\overline{H}^1(\Omega)$. Then the classical theory (see, e.g., [24]) provides the

existence of a unique minimizer for (3.36). We conclude by observing that (3.35) is the Euler-Lagrange equation corresponding to the minimization problem (3.36). ■

The situation is significantly different for the case $M(s) = s$, i.e., $\gamma = 1$. Then $m(s) = s^{-1}$ and $g(\lambda) \equiv c^{-2}$, thus not invertible. In fact, the stationary version of (3.2) reads

$$c^2 \nabla p \otimes \nabla p = \frac{\mathbb{C}}{|\mathbb{C}|},$$

which implies that for almost all $x \in \Omega$ either $\mathbb{C}(x) = 0$ or $c^2 |\nabla p(x)|^2 = 1$. In the latter case, $\mathbb{C} = \lambda \nabla p \otimes \nabla p$ with $\lambda > 0$. Consequently, similarly as in [33, Remark 7], there exists a positive, measurable function $\lambda = \lambda(x)$ such that

$$\mathbb{C}(x) = \lambda(x) \chi_{\{c|\nabla p|=1\}}(x) \nabla p(x) \otimes \nabla p(x),$$

where $\chi_{\{c|\nabla p|=1\}}$ denotes the characteristic function of the set $\{x \in \Omega; c|\nabla p(x)| = 1\}$, and $p = p(x)$ solves the highly nonlinear Poisson equation

$$-\nabla \cdot \left(\left[r + \frac{\lambda}{c^2} \chi_{\{c|\nabla p|=1\}} \right] \nabla p \right) = S.$$

subject to the homogeneous Neumann boundary condition on $\partial\Omega$. This problem was studied in [34, Section 4.2], where it was shown that its solutions can be constructed as the free-boundary problem

$$-\nabla \cdot \left[(1 + a(x)^2) \nabla p \right] = S, \quad p \in H_0^1(\Omega), \quad (3.37)$$

$$c^2 |\nabla p(x)|^2 \leq 1, \quad \text{a.e. on } \Omega, \quad (3.38)$$

$$a(x)^2 \left[c^2 |\nabla p(x)|^2 - 1 \right] = 0, \quad \text{a.e. on } \Omega, \quad (3.39)$$

for some measurable function $a^2 = a(x)^2$ on Ω which is the Lagrange multiplier for the condition (3.38). The function $\lambda = \lambda(x)$ can be chosen as $\lambda(x) := ca(x)$.

Moreover, in [34, Section 4.2.1], it was shown that solutions of (3.37)–(3.39) are minimizers of the energy functional

$$\mathcal{J}[p] := \int_{\Omega} \left(\frac{|\nabla p|^2}{2} - Sp \right) dx$$

on the set $\mathcal{M} := \{p \in H^1(\Omega), c^2 |\nabla p|^2 \leq 1 \text{ a.e. on } \Omega\}$. Existence and uniqueness of minimizers was established in [34, Lemma 5]. An alternative approach is to consider the penalized problem

$$-\nabla \cdot \left[\left(1 + \frac{(|\nabla p_{\varepsilon}|^2 - 1/c^2)_+}{\varepsilon} \right) \nabla p_{\varepsilon} \right] = S, \quad p_{\varepsilon} \in H^1(\Omega),$$

where $A_+ := \max(A, 0)$ denotes the positive part of A , and pass to the limit $\varepsilon \rightarrow 0$, see [34, Section 4.2.2]

3.5 Steady states in 1D with $D = 0$

The system (3.1)–(3.2) with $D = 0$ in the spatially one-dimensional setting, i.e., $\Omega := (0, 1)$, reads

$$-\partial_x((r + \mathbb{C})\partial_x p) = S, \quad (3.40)$$

$$\partial_t \mathbb{C} - c^2 (\partial_x p)^2 + \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C} = 0. \quad (3.41)$$

Let us recall that the weak solution, constructed as the gradient flow in Proposition (3.9), remains nonnegative for almost all $t > 0$ and $x \in (0, 1)$. Denoting $B(x) := -\int_0^x S(y) dy$ and integrating (3.40) on the interval $(0, x)$, taking into account the homogeneous Neumann boundary condition $\partial_x p(0) = 0$, we obtain

$$\partial_x p = \frac{B(x)}{r + \mathbb{C}}. \quad (3.42)$$

Note that due to the assumption (3.5), we have $B(1) = -\int_0^1 S(y) dy = 0$, and, consequently, $\partial_x p(1) = 0$, so that the homogeneous Neumann boundary condition for p is satisfied at $x = 1$ as well.

Inserting (3.42) into (3.41), we obtain

$$\partial_t \mathbb{C} = \frac{c^2 B(x)^2}{(r + \mathbb{C})^2} - \frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C}. \quad (3.43)$$

For further discussion, let us again adopt the generic choice $M(s) = s^\gamma/\gamma$ with the metabolic exponent $\gamma > 0$. We first study the case $\gamma \neq 1$. Then, $\frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C} = |\mathbb{C}|^{\gamma-2} \mathbb{C}$, and recalling that $\mathbb{C} \geq 0$, we have $\frac{M'(|\mathbb{C}|)}{|\mathbb{C}|} \mathbb{C} = \mathbb{C}^{\gamma-1}$. Therefore, steady states of (3.43) are characterized as solutions of the algebraic equation

$$(r + \mathbb{C})^2 \mathbb{C}^{\gamma-1} = c^2 B(x)^2. \quad (3.44)$$

A simple calculation reveals that if $\gamma > 1$ the left-hand side of (3.43) is a strictly increasing function of $\mathbb{C}$, vanishing at $\mathbb{C} = 0$. Therefore, for a given profile $B = B(x)$, there exists a unique steady state $\mathbb{C} = \mathbb{C}(x)$ of (3.43) on $\Omega = (0, 1)$, obtained as the unique solution of (3.44) for each $x \in (0, 1)$. Another simple calculation reveals that this solution is asymptotically stable. It is instructive to compare this result with [33, Section 6.1] for the one-dimensional version of the model (3.8)–(3.9), where for $\gamma > 1$ one has the unstable trivial steady state $m = 0$ and a pair of stable states $\pm m_s \neq 0$.

For $\gamma \in (0, 1)$ the left-hand side of (3.43) has the unique minimum $r_\gamma := \left(\frac{2}{1+\gamma}\right)^2 \left(\frac{1-\gamma}{1+\gamma}\right)^{\gamma-1} r^{\gamma+1}$ on $(0, \infty)$. Consequently:

- If $c^2 B(x)^2 > r_\gamma$, then (3.43) has two positive steady states $0 < \mathbb{C}_1 < \mathbb{C}_2$, where $\mathbb{C}_1$ is unstable and $\mathbb{C}_2$ is asymptotically stable.
- If $c^2 B(x)^2 = r_\gamma$, then (3.43) has one steady state, asymptotically stable from the right-hand side and unstable from the left.
- If $c^2 B(x)^2 < r_\gamma$, then (3.43) has no steady state and its solution, starting from a positive initial value, decays to zero in finite time.

Let us note that when $\gamma \in (0, 1)$ and $\mathbb{C}$ reaches zero, the right-hand side of (3.44) blows up and the equation loses validity. From the modeling point of view, it makes sense to extend the solution $\mathbb{C}$ by zero past this point; the transport of material in the (one-dimensional) structure is then due to the background permeability $r > 0$ only.

For $\gamma = 1$ equation (3.44) is to be interpreted as the inclusion

$$\frac{c^2 B(x)^2}{(r + \mathbb{C})^2} \in \text{sign}(\mathbb{C}),$$

where

$$\text{sign}(\mathbb{C}) = \begin{cases} \{1\} & \text{for } \mathbb{C} > 0, \\ [0, 1] & \text{for } \mathbb{C} = 0. \end{cases}$$

Obviously, $\mathbb{C}(x) > 0$ is only possible if $c|B(x)| > r$. Consequently, the steady state is of the form $\mathbb{C}(x) = (c|B(x)| - r)^+$, where $x^+ := \max\{0, x\}$. Note that the total permeability is then $\mathbb{C}(x) + r = \max\{c|B(x)|, r\}$ so that in the region where $c|B(x)| < r$ the transport of material is by the background permeability $r > 0$ of the medium. Again, this may be compared with [33, Section 6.1] for the model (3.8)–(3.9), where for $\gamma = 1$ there is a pair of nonzero stable steady states $\pm m_s \neq 0$ if and only if $c|B(x)|$ is large enough. On the other hand, for small $c|B(x)|$ one has only the trivial steady state $m = 0$, which is stable.

4 A Γ -convergence result

4.1 Introduction

This chapter consists of a preliminary stage of a study, dedicated to understand the behaviour of the steady states of a model describing the formation of biological network structures. In particular, we consider a scalar function u , denoting the scalar conductivity of a system in which a fluid is moving through a porous medium, and a function p denoting the pressure of the fluid. The pressure is supposed to satisfy Darcy's law, while the evolution of the conductivity is defined as the L^2 -gradient flow of an energy, in which both a kinetic and a metabolic term appear. To be more precise, we introduce the energy

$$\tilde{\mathcal{E}}_D[u] = \frac{1}{2} \int_{\Omega} D^2 |\nabla u|^2 + c^2 \nabla p (r + u^2) \nabla p + \frac{|u|^{2\gamma}}{\gamma} dx,$$

where the diffusivity represents randomness in the material, the second term is the kinetic part, and the last one is the metabolic cost. The pressure solves

$$-\operatorname{div} \left[(r + u^2) \nabla p \right] = S,$$

where S denotes the sources and sinks of the system, and it is assumed to satisfy $\int S dx = 0$. We equip the equation with homogeneous Neumann boundary conditions. Thus, the solution is unique (up to an additive constant). Such a model is strongly inspired by the vector one presented in [33], where the authors studied a similar model, in which the conductivity was represented by a vector function. The model has also quickly been described in the introduction to this thesis in Section 1.1.2.

The goal of this work is to prove a Γ -convergence result of the energy in a 2-dimensional setting, as the diffusion coefficient D goes to zero. If this result would be achieved, we may manage to recover the tree structure observed in numerous biological network systems.

In this chapter, we first present a quick idea of the connection between this model and the one studied in [3], and give a small overview on the basic results of Γ -convergence and the theory of Optimal Transportation Networks. We then formally introduce the model, the setting in which we will work, and finally we prove the Γ -liminf inequality. To prove the full result of Γ -convergence, we would need to show also the limsup inequality, as well as equicoercivity of the energies. However, as mentioned above, the content of this chapter is still a work in progress, and these two last steps are still object of study.

4.1.1 Connection with the vector model

The authors in [39] presented a discrete description of the formation of biological transportation networks. In this work the authors consider a fixed network, and describe the evolution of the conductance on the graph, under the assumption that the system minimises simultaneously the kinetic energy of the fluid moving through the system, and the metabolic cost that needs to be paid to maintain it. The same authors proposed a continuum version of this model, which was then analysed by other authors in a sequence of works (see for instance [2, 3, 33, 34]).

The continuous model describes the movement of a fluid through a porous medium in the space

$\Omega \subset \mathbb{R}^2$. The vector variable m represents the conductivity of the system, while the pressure of the fluid satisfies a Darcy type elliptic equation,

$$-\operatorname{div}[(r\mathbb{I} + m \otimes m)\nabla p] = S, \quad (4.1)$$

where S here represents the sources and sinks of the system, and is assumed to have mean zero. The evolution in time of the conductivity is defined as the L^2 -gradient flow of the energy

$$\tilde{\mathcal{E}}[m] = \frac{1}{2} \int_{\Omega} D^2 |\nabla m|^2 + c^2 \nabla p (r\mathbb{I} + m \otimes m) \nabla p + \frac{|m|^{2\gamma}}{\gamma} dx,$$

where the second term of the energy represents the kinetic energy, and the last one the metabolic cost that has to be paid to maintain the system. The diffusion term was not part of the discrete model and it has been added to model the propagation of the network support in space. Indeed, this property was not present in the discrete description, where no new edges could be formed from the initial state.

The evolution of the conductivity is described by the equation

$$\partial_t m = D^2 \Delta m + (m \cdot \nabla p) \nabla p - |m|^{2\gamma-2} m,$$

where p is a solution of the constraint (4.1).

If the diffusion term is removed, the steady states satisfy

$$(m \cdot \nabla p) \nabla p = |m|^{2\gamma-2} m. \quad (4.2)$$

This suggest that in absence of the diffusion term the directions of the conductivity and the pressure gradient are aligned. Moreover, since for every given (m, p) solution of (4.2), the couple $(-m, p)$ is also a solution, we can assume that the conductivity and the pressure gradient point in the same direction, i.e. $m \cdot \nabla p \geq 0$.

Taking this into consideration and denoting the absolute value of the conductivity by $u = |m|$, the Poisson equation can be rewritten in terms of the new variable as

$$-\operatorname{div}[(r + u^2)\nabla p] = S, \quad (4.3)$$

while the equation for the steady states reads

$$u|\nabla p|^2 = -|u|^{2\gamma-2} u. \quad (4.4)$$

Solutions of equation (4.4) can be interpreted as the steady states of the L^2 -gradient flow of the energy

$$\tilde{\mathcal{E}}[u] = \frac{1}{2} \int_{\Omega} c^2 \nabla p (r + u^2) \nabla p + \frac{|u|^{2\gamma}}{\gamma} dx,$$

where p is a solution of (4.3).

Inspired by what has been previously done for the vector model in [3] and other works, we add a diffusion term in the energy to this new model. As for the vector model, the absence of such a term would prevent the growth of the network, allowing just the loss of support.

The new energy reads

$$\tilde{\mathcal{E}}_D[u] = \frac{1}{2} \int_{\Omega} D^2 |\nabla u|^2 + c^2 \nabla p (r + u^2) \nabla p + \frac{|u|^{2\gamma}}{\gamma} dx,$$

where the pressure p now satisfies (4.3). This leads to the diffusive equation

$$\partial_t u = D^2 \Delta u + u |\nabla p|^2 - |u|^{2\gamma-2} u.$$

We remark that solutions of this equation do not coincide with the time evolution of $|m|$. However, we expect that for small values of the diffusion coefficient D , the steady states of this equation can represent a good approximation of the ones of the vector model. Under the assumption $\gamma > \frac{1}{2}$, the existence of global solutions can be proven following the strategy adopted for the vector model in [33].

In this work, and from this point on in all the chapter, the function r will be assumed to be zero.

4.1.2 Optimal Transportation Networks

A first model for transportation was given by the Monge-Kantorovich framework, with the goal of describing how to move a pile of sand from a place to another with the least work possible. However, this model only takes into consideration the starting and ending point of the transported mass, and not the path it may follow. In reality, natural structures and human constructions such as pipes systems or roads are built on the main assumption that transporting mass on a common street is often more convenient than moving them separately, giving birth to structures that resemble more a tree, rather than a set of strait lines.

The Gilbert-Steiner model

A first attempt to model this is represented by the so called Gilbert-Steiner model. Indeed, in his work [29], Gilbert proposed a model in which each edge of a graph is associated with a capacity, that morally represents "how much flux the edge can carry". He then introduces a function cost per unit length, here denoted by τ , that is assumed to be positive, increasing, and subadditive, i.e. satisfying $\tau(a) + \tau(b) \geq \tau(a+b) \geq \max\{\tau(a), \tau(b)\}$. In particular, the function τ is assumed to be $\tau(\lambda) = \lambda^\alpha$, for $\alpha \in (0, 1)$. In this way, transporting a bigger amount of mass on the same edge may result more efficient, even when moving along a longer route.

In [29] Gilbert considered atomic positive measures S^+ and S^- with same mass, and introduced the concept of *irrigated graphs*, i.e. a weighted oriented graph G with straight edges. The weight function $w : G \rightarrow (0, \infty)$ satisfies Kirchhoff's law and models the intensity of the flux on the edge per unit length. The graph is said to *irrigate* S^+ and S^- if it satisfies the constraint $\text{div } G = S^+ - S^-$ in the distributional sense. The Gilbert energy of the graph G is defined as

$$M^\alpha(G) = \sum_{e \in E(G)} w(e)^\alpha \text{length}(e).$$

The so called Gilbert-Steiner problem consists in minimising the energy $M^\alpha(G)$ among all the graphs irrigating the measures S^+ and S^- .

The Xia's model

A more general setting was proposed by Xia in [76], who extended the choice of the sources and sinks to general positive Radon measures (with same mass) with compact support in $\Omega \subset \mathbb{R}^d$. The main idea was to approximate the sources and sinks with a sequence of atomic measures, and define the transportation between S^+ and S^- loosely speaking as the limit of the graphs obtained in the previous setting. In particular, a *transport path* between two Radon measures S^+ and S^- is defined as a vector measure T , for which there exist two sequences of atomic measures S_n^+ and S_n^- , and a sequence of finite graphs G_n irrigating them, such that $S_n^+ \rightarrow S^+$, $S_n^- \rightarrow S^-$, and $G_n \rightarrow T$ as vector measures. The corresponding energy of the transport path T is then defined as

$$M^\alpha(T) = \inf \{ \liminf_{n \rightarrow \infty} M^\alpha(G_n) \},$$

where the infimum is taken over all the suitable sequences $\{S_n^+, S_n^-\}$ and G_n . The cost to transport the measure S^+ to S^- is then defined as the infimum over every transport path between the measures. For more details we refer to [76, 77, 78]. In these works the author showed many structural and regularity properties of the optimal transport paths. Note that a restriction on the exponent of the cost function τ is required, to ensure the existence of an optimal transport path, in particular $\alpha \in (1 - \frac{1}{d}, 1)$.

The Maddalena-Solimini model

The authors Maddalena, Morel and Solimini in [46] proposed a different approach, which seems at first unrelated to the others. In their work the source is assumed to be concentrated on a single point $S^+ = \delta_S$. The authors then consider particles moving from the source to the support of the sink measure S^- along trajectories called fibres. They introduce a general probability space Y which parametrises the particles. For the sake of simplicity Y is represented by $[0, 1]$. At time zero the particles are located in the initial point S , and $\chi(y, t)$ represents the location of the particle $y \in Y$ at time t . The fibre of a single particle $y \in Y$ is denoted by $\chi(y, \cdot)$. Two fibres are said to belong to the same branch at time t , if $\chi(y, s) = \chi(y', s)$ for all $s \leq t$. For each particle $y \in Y$ a stopping time function $T(y)$ is introduced, and the energy is defined as

$$\int_Y \int_0^{T(y)} |[y]_t|^{\alpha-1} dt dy,$$

where $[y]_t$ denotes the branch of the particle y , and $|[y]_t|$ its measure.

For completeness we mention that in [11] the authors extended the previous formalism to the case in which the source consists of any positive Radon measure, introducing the concept of *traffic plans*, i.e. probability measures on the set of Lipschitz paths.

A more general setting

These models, all developed in different settings, have been proven to be equivalent in case of finite atomic measures in [44], and later in a more general setting in [45]. In [12] the authors present a detailed overview of the cited models and their properties.

Our work is set in a more general framework proposed in [14]. The authors introduced a new formulation of the transport network problem, which extends the previous models. In this setting, a broader class of cost functions can be considered, which are now assumed to be positive, subadditive, and lower-semicontinuous. In particular, the strict concavity of the cost is no longer required.

It has been shown in [67] that a flux between two probability measures S^+ and S^- , i.e. a measure q satisfying the constraint $\operatorname{div} q = S^+ - S^-$, can be decomposed into $q = \lambda_q \theta_q \mathcal{H}^1 \llcorner \Sigma_q + q^\perp$, where $\Sigma_q \subset \mathbb{R}^d$ is a 1-rectifiable set, and $q^\perp$ is a diffusive measure. The authors then define the energy as

$$E[q] = \int_{\Sigma_q} \tau(\lambda_q(x)) d\mathcal{H}^1 + \tau'(0)|q^\perp|(\mathbb{R}^d).$$

Notice that in case $\tau'(0) = +\infty$ every minimiser admitting a finite cost is automatically supported on a 1-rectifiable set. More details about the contest will be given in the following sections.

Structure of the minimisers

Interesting properties on the structure of the optimal points of the minimisation problems have been proven. Indeed, it has been showed that, for $\alpha \in (1 - \frac{1}{d}, 1)$, outside the support of the source and sink measures, the minimisers' support assume the structure of a finite graph. Moreover, the number of branches at any point is bounded from above by a constant $\mathcal{N}(\alpha, d)$, depending only on the dimension of the space and the cost exponent α .

An example was studied by Xia in [76], analysing the behaviour of optimal minimisers in the case of two sources and a single sink. The shape obtained is the so called *Y shape*, proving that it is more convenient to first transport mass together and just in a second moment to split it. Moreover, the author proved that the branching point, as well as the angles between the branches, depend only on the exponent α and on the masses transported on the edges.

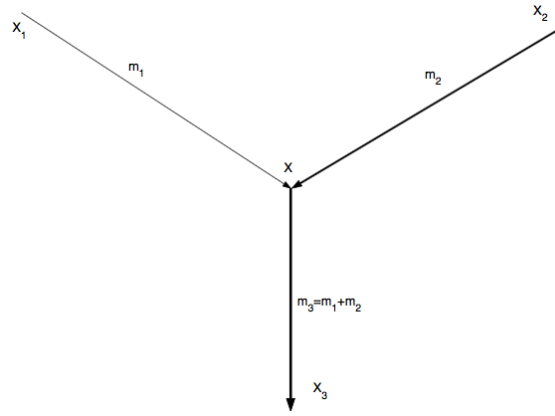


Figure 4.1: Two sources, one sink. Picture taken from [76]

Another interesting example consists of a single source point, and a sink that is represented by the Lebesgue measure on an interval. Numerical simulations made by Xia in the same article showed that also in this case the minimiser assume the tree structure, separating into smaller branches as the support approaches the sink. A detailed overview of these results, as well as other simulations and properties of minimisers, can be for example found in [12].

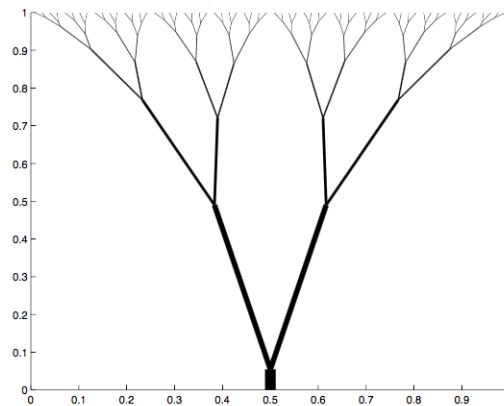


Figure 4.2: One source, sink on a segment. Picture taken from [76]

4.1.3 Γ -convergence

The concept of Γ -convergence has been introduced by De Giorgi at the beginning of the 1970s to describe a notion of convergence for variational problems. It studies the asymptotic behaviour of minimum problems depending on a parameter ε , denoted here by

$$\min\{F_\varepsilon(u) : u \in X_\varepsilon\}. \quad (4.5)$$

The idea is to focus the attention on an easier problem, defined on a new space X and independent from the parameter, denoted here by

$$\min\{F(u) : u \in X\}. \quad (4.6)$$

Important characteristics of the of the solutions of the Problem 4.5 could follow by studying the new functional. The Γ -convergence is a way to require convergence of minimisers and of the values of the minima minimum values of (4.5), and their continuous perturbation, to the ones of (4.6) (with the same continuous perturbation).

A priori, the space in which the problems are defined may differ in dependence of the parameter. A first essential step is to identify a suitable space X , large enough to contain all the domains X_ε , and to extend the functionals on this space. This can be done by identifying the functionals with their extension

$$\tilde{F}_\varepsilon(u) = \begin{cases} F_\varepsilon(u) & \text{if } u \in X_\varepsilon, \\ +\infty & \text{otherwise.} \end{cases}$$

In order to get convergence of the of the minimisers, it is useful to prove that they belong to a common compact set. This could be achieved by assuming compactness of the sublevels sets, leading to the following definition:

Definition 4.1. *The functionals $\{F_\varepsilon\}$ satisfy the equi-coercivity property if, for each $t \in \mathbb{R}$ there exists a compact set $K_t \subset X$ such that $\{u, F_\varepsilon(u) \leq t\} \subset K_t$.*

However, since the goal is to recover convergence just for the minimisers, the requirement can be relaxed to

Definition 4.2. *The sequence $\{F_\varepsilon\}$ is called equi-mildly coercive if there exists a non-empty, compact set $K \subset X$ such that $\inf_X F_\varepsilon = \inf_K F_\varepsilon$ for each ε .*

We now introduce the definition of Γ -convergence in a metric setting. However, the definition can be extended to general topological spaces (see [19]).

Definition 4.3. *Let (X, d) be a metric space. Let $\{F_\varepsilon\}$ be a sequence of functionals defined on X , such that $F_\varepsilon : X \rightarrow \bar{\mathbb{R}} := \mathbb{R} \cup +\infty$. We say that the sequence $\{F_\varepsilon\}$ Γ -converges to the functional $F : X \rightarrow \bar{\mathbb{R}}$ if the following two properties hold:*

- (Liminf inequality) *For every point $u \in X$ and every sequence $\{u_\varepsilon\}$ converging to u it holds*

$$F(u) \leq \liminf_{\varepsilon} F_\varepsilon(u_\varepsilon).$$

- (Limsup inequality) *For every element $u \in X$ there exists a sequence $\{\bar{u}_\varepsilon\}$ converging to u such that*

$$F(u) \geq \limsup_{\varepsilon} F_\varepsilon(\bar{u}_\varepsilon).$$

Such sequence is called recovery sequence.

The functional F is called Γ -limit of $\{F_\varepsilon\}$.

If the sequence $\{F_\varepsilon\}$ is equi-mildly coercive and Γ -converges to a functional F , the converges of the minima is recovered. Indeed, the following theorem holds:

Theorem 4.4. *Let (X, d) be a metric space, $\{F_\varepsilon\}$ be a sequence of equi-mildly coercive functions on X , and $F = \Gamma\text{-}\lim F_\varepsilon$. Then, the functional F admits at least a minimum, and it holds*

$$\min_X F = \lim_{\varepsilon} \inf_X F_\varepsilon.$$

Moreover, if u_ε is a precompact sequence such that $\lim_{\varepsilon} F_\varepsilon(u_\varepsilon) = \lim_{\varepsilon} \inf F_\varepsilon(u_\varepsilon)$, every limit of a subsequence of $\{u_\varepsilon\}$ is a minimum point for F .

A proof of this result can be found in [13].

Remark 4.5. *The choice of the space X and the topology defined on it play an important role. Indeed, a balance is needed between a stronger topology, which would make the $\liminf$ inequality easier to verify, and a weaker one, which would help in the proof of the equi-coerciveness, as well as to find the recovery sequence required for the $\limsup$ inequality.*

A detailed explanation of Γ -convergence, as well as many interesting examples of possible applications can be found in the books of Braides (see [13]) and Dal Maso (see [19]). We briefly introduce here a couple of examples that may be useful to better understand the strategy of our work.

Example 1: gradient theory of phase transitions. The first example aims to describe the behaviour of two immiscible fluids in a container. It has been observed that the fluids distribute themselves in a way that minimises the interface between them. For the sake of simplicity, we will illustrate it in a one dimensional setting.

Let $\Omega = (a, b)$ be an interval. The function $u : \Omega \rightarrow \{0, 1\}$ describes the presence of the fluids: it assumes the value 0 in the points where the first fluid is located, and 1 where the second fluid is. Also, we require that $\int_{\Omega} u \, dx = m$, which models the assumption that the masses of the fluids are fixed. We also introduce a so called *double-well potential*, a continuous function $W : \mathbb{R} \rightarrow \mathbb{R}$ with minima in 0 and 1 which grows at least linearly as $|x| \rightarrow \infty$.

The situation above can be described by the minimising problem

$$\min \left\{ \int_{\Omega} W(u) \, dx, \text{ s.t. } \int_{\Omega} u \, dx = m \right\}.$$

However, this formulation admits many different solutions, and does not take into consideration the minimisation of the interface. A way to solve this problem is to penalise high values of the integral of the derivative, forcing the function u to be "as constant as possible", since a point of discontinuity can be interpreted as a "steep" jump from the values 0 and 1. The adapted problem can be formulated as follows:

$$\min \left\{ \int_{\Omega} W(u) + \varepsilon^2 |u'|^2 \, dx, \int_{\Omega} u \, dx = m \right\}.$$

However, as the parameter ε gets smaller it gets harder to detect the behaviour of the minimisers. The energy is then rescaled by a factor $\frac{1}{\varepsilon}$,

$$\min \left\{ \int_{\Omega} \frac{1}{\varepsilon} W(u) + \varepsilon |u'|^2 \, dx, \int_{\Omega} u \, dx = m \right\}.$$

In this way the contribution of the two terms are of the same order along the minimising sequences. Indeed, the first term brings the function u to assume values in the set $\{0, 1\}$, while the second term minimises the number of interfaces. Indeed, it has been shown that, as ε tends to zero, this problem Γ -converges to the *minimal interface problem*

$$\min \left\{ \text{Per}(\{u = 0\}, \Omega), \quad u : \Omega \rightarrow \{0, 1\}, \quad \int_{\Omega} u \, dx = m \right\},$$

where $\text{Per}(A, \Omega)$ denotes the perimeter of A in Ω (see for example [13]).

The nature of the two problems changes deeply: the first one takes into consideration smooth functions, while the limit functional is defined on discontinuous functions. However, they are deeply connected.

Example 2: Approximation of free-discontinuity problems. Let us consider a class of problems in the world of Calculus of Variations in which the unknowns are a pair (u, K) , where K belongs to a class of closed hypersurfaces in an open set $\Omega \subset \mathbb{R}^d$, and $u : \Omega \rightarrow \mathbb{R}^m$. An important example coming from the theory of Image Reconstruction is given by the Mumford-Shah functional,

$$E(u, K) = \int_{\Omega \setminus K} |\nabla u|^2 \, dx + c_1 \text{length}(K) + c_2 \int_{\Omega \setminus K} |u - g|^2 \, dx,$$

Here $d = 2, m = 1$, the function g models an input picture, u is the unknown restored image, K represents the main contour of the subject in the picture, and c_1, c_2 are contrast parameters. The first term has the goal to smooth the image, while the last term, called *fidelity term*, forces the function to stay as close as possible to the input image. Solving numerically these kind of problems presents many difficulties due to the presence of an unknown surface of discontinuity K .

It has been proven that the Ambrosio-Tortorelli functional approximates this problem. They introduced an auxiliary variable v and defined the functional

$$G_{\varepsilon}(u, v) = \int_{\Omega} v^2 |\nabla u|^2 \, dx + \frac{1}{2} \int_{\Omega} \varepsilon |\nabla v|^2 + \frac{1}{\varepsilon} (1 - v)^2 \, dx + c_2 \int_{\Omega} |u - g|^2 \, dx,$$

where u and v are regular functions and $0 \leq v \leq 1$. The idea behind this approximation was inspired by the phase transition model. Indeed, the function v approaches $1 - \chi_K$, forcing the surface of K to be as small as possible, while the last term still forces the function u to be as close as possible to the input image g , and the first term tries to force u to be smooth outside the set K .

4.1.4 The model

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain. We look for a conductance $u : \Omega \rightarrow \mathbb{R}$ and a pressure function $p : \Omega \rightarrow \mathbb{R}$ minimising the energy

$$\int_{\Omega} \left(D^2 |\nabla u|^2 + c^2 u^2 |\nabla p|^2 + \frac{|u|^{2\gamma}}{\gamma} \right) \, dx,$$

under the constraint $-\text{div}(u^2 \nabla p) = S$. The function $S \in \mathcal{M}(\Omega)$ describes the distribution of sources and sinks and the exponent $\gamma \in \left(\frac{1}{2}, 1\right)$ is fixed.

We define the flux $q = -u^2 \nabla p$ and reformulate the energy in the equivalent form

$$\mathcal{E}_D[q, u] = \left\{ \int_{\Omega} \left(D^2 |\nabla u|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \right) \, dx \mid \text{div}(q) = S \right\}. \quad (4.7)$$

Indeed, the relation between flux and pressure is recovered in Section 4.2 by calculating the Euler-Lagrange equations. The goal of this chapter is to show Γ -convergence of a rescaled version of the energy (4.7) as the diffusion coefficient approaches zero, to a suitable energy (its precise structure is deduced in Section 4.2). As seen in Section 4.1.2, the minimisers of such energy consists of measures with support on a 1-rectifiable countable set. We saw in Section 4.1.3 that Γ -convergence of the energies and equicoercivity would imply convergences of the minimisers. For our problem this would mean that the steady states recover the tree-structure shape the model wants to describe, as the coefficient D approaches zero.

As mentioned before, every divergence-measure vector field can be decomposed as $q = \lambda_q \theta_q \mathcal{H}^1 \llcorner \Sigma_q + q^\perp$ (see [67]). In the rest of the chapter, we first identify the correct non-decreasing cost function $\tau : \mathbb{R} \rightarrow \mathbb{R}^+$, such that the rescaled energy $D^\alpha \mathcal{E}_D(q)$ Γ -converges to $\mathcal{E}(q) := \int_{\Sigma_q} \tau(\lambda_q) d\mathcal{H}^1$. In Section 4.3 we introduce the precise setting of the problem, and in Section 4.4 we prove the Γ -liminf result. The remaining steps are still objects of investigation.

4.2 Identification of the cost function τ

Loosely speaking, the cost function $\tau(\lambda)$ represents the price to pay to transport a fixed flux λ_q on a length unit, and mathematically can be read as the integral of the energy in the direction orthogonal to the pipe.

This section is dedicated to formally identify the candidate for the cost in the limit energy. In order to do so, we start assuming that the minimisers of such energy consist of measures supported on a countable 1-rectifiable support. We denote by $\hat{q}$ one of these minimisers. Moreover, we assume that the Γ -limit result holds, and that the minimisers of the problem (4.7) converges to $\hat{q}$.

In these formal computations, we focus our attention on a single brunch of the minimiser $\hat{q}$, away from the nodes of the edge; the idea is that such points contribute in minimal part to the integral value, and by "zooming" enough close, we can imagine the edge to be a line. Without loss of generality, we suppose that the flux points upwards and lies on the line $\Sigma = \{x_1 = 0\}$, i.e. that it assumes the form

$$\hat{q} = \hat{\lambda} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \mathcal{H}^1 \llcorner \Sigma,$$

where $\hat{\lambda}$ denotes the flux magnitude.

Besides, we suppose the minimiser (q, u) of the problem (4.7) to be both symmetric with respect to the origin, and monotonically decreasing on $\mathbb{R}^+$. Indeed, if this would not be the case, we could apply simultaneously to both variables a map that would make the variable u symmetric. This would decrease the term $\int_{\mathbb{R}} |\nabla u|^2 dx$ (thanks to the Pólya–Szegő inequality), and leave the other two terms unchanged. At this point, with this fix u , we observe that a symmetrical flux q carrying the same mass would also decrease the energy. The diffusive flux is described as

$$q(x) = \lambda(x_1) \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where λ is assumed symmetric with respect the origin, and monotonically decreasing on the positive half-line. Also, we assume that it transports the same quantity of mass of the limit flux $\hat{q}$, bringing

$$\int_{\mathbb{R}} \lambda(x_1) dx_1 = \hat{\lambda}.$$

The minimum energy that can be paid to transport the flux is given by

$$\tau(\hat{\lambda}) = \inf \left\{ D^{-\alpha} \int_{\mathbb{R}} \left(D^2 |u'|^2 + c^2 \frac{|\lambda|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \right) dx_1 \mid \int_{\mathbb{R}} \lambda(x_1) dx_1 = \hat{\lambda}, \quad u, \lambda \geq 0 \right\}.$$

We now rescale the energy and the variables, in a way that the terms of the energy have the same magnitude, and that keeps the intensity of the flux fixed. We define

$$\begin{aligned} y &= D^{-\beta} x_1 \\ \xi &= D^\beta \lambda \\ \zeta &= D^\delta u. \end{aligned}$$

The energy rewritten in the new variables reads

$$\tau(\hat{\lambda}) = D^{\beta-\alpha} \inf \left\{ \int_{\mathbb{R}} \left(D^{2-2\delta-2\beta} |\zeta'|^2 + D^{2\delta-2\beta} c^2 \frac{|\xi|^2}{\zeta^2} + D^{-2\delta\gamma} \frac{\zeta^{2\gamma}}{\gamma} \right) dy \mid \int \xi dy = \hat{\lambda}, \quad \xi, \zeta \geq 0 \right\}.$$

to archive our goal, we assume $\alpha = \frac{1-\gamma}{2}$, $\beta = \frac{\gamma+1}{2}$ and $\delta = \frac{1}{2}$. We point out that the new flux still satisfies $\int \xi dy = \hat{\lambda}$. With the new variables, the cost can then be calculated independently from the diffusion coefficient, meaning

$$\tau(\hat{\lambda}) = \inf \left\{ \int_{\mathbb{R}} \left(|\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{\zeta^{2\gamma}}{\gamma} \right) dy \mid \int_{\mathbb{R}} \xi dy = \hat{\lambda}, \quad \xi, \zeta \geq 0 \right\}. \quad (4.8)$$

The corresponding Lagrangian, taking into consideration the flux constraint $\int_{\mathbb{R}} \xi dy = \hat{\lambda}$, is

$$\mathcal{L} = \int_{\mathbb{R}} \left(|\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{\zeta^{2\gamma}}{\gamma} - \mu \xi \right) dy + \mu \hat{\lambda}, \quad (4.9)$$

where μ denotes the Lagrangian multiplier. The corresponding Euler-Lagrange equation, with respect to the variable ξ , reads

$$\xi = \frac{\mu}{2c^2} \zeta^2. \quad (4.10)$$

Plugging this relation into the Lagrangian, we obtain

$$\begin{aligned} \mathcal{L} &= \int_{\mathbb{R}} \left(|\zeta'|^2 + \frac{\mu^2 \zeta^2}{4c^2} + c^2 \frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2 \zeta^2}{2c^2} \right) dy + \mu \hat{\lambda} \\ &= \int_{\mathbb{R}} \left(|\zeta'|^2 + \frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2}{4c^2} \zeta^2 \right) dy + \mu \hat{\lambda}. \end{aligned}$$

The Euler-Lagrange equation with respect to the ζ variable reads

$$-2\zeta'' + 2\zeta^{2\gamma-1} - \frac{\mu^2}{2c^2} \zeta = 0.$$

Multiplying this relation by ζ' and integrating, we obtain that ζ' satisfies

$$(\zeta')^2 = \frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2 \zeta^2}{4c^2} + e_0.$$

Since we are considering minimisers that carry a finite flux $\hat{\lambda}$, we assume $e_0 = 0$, getting the equation

$$(\zeta')^2 = \frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2 \zeta^2}{4c^2}. \quad (4.11)$$

The values of ζ that annul its derivatives are $\zeta_0 = 0$ and $\zeta_{max} = \left(\frac{4c^2}{\gamma\mu^2}\right)^{\frac{1}{2(1-\gamma)}} = \left(\frac{4c^2}{\gamma}\right)^{\frac{1}{2(1-\gamma)}} \mu^{\frac{1}{\gamma-1}}$.

Using the flux constraint we can determine the Lagrange multiplier

$$\int_{\mathbb{R}} \frac{\mu}{2c^2} \zeta^2 dx = \hat{\lambda},$$

which has to be positive since we assumed $\hat{\lambda} > 0$. Let us observe that the function ζ depends on the Lagrange multiplier μ in a non-trivial way.

Since ζ^2 is also symmetric with respect to the origin, and decreasing on $[0, \infty)$, it holds

$$\begin{aligned} \int_{\mathbb{R}} \zeta^2 dx &= 2 \int_0^\infty \zeta^2 dx = 2 \int_0^{\zeta_{max}} \frac{\zeta^2}{\zeta'} d\zeta = \\ &= 2 \int_0^{\zeta_{max}} \frac{\zeta^2}{\sqrt{\frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2 \zeta^2}{4c^2}}} d\zeta. \end{aligned}$$

Changing variables $\zeta = \mu^{\frac{1}{\gamma-1}} v$, we get

$$2 \int_0^{\zeta_{max}} \frac{\zeta^2}{\sqrt{\frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2 \zeta^2}{4c^2}}} d\zeta = 2\mu^{\frac{3-\gamma}{\gamma-1}} \int_0^{v_{max}} \frac{v^2}{\sqrt{\frac{v^{2\gamma}}{\gamma} - \frac{v^2}{4c^2}}} dv = 2\mu^{\frac{3-\gamma}{\gamma-1}} C'(\gamma),$$

where $v_{max} = \left(\frac{4c^2}{\gamma}\right)^{\frac{1}{2(1-\gamma)}}$, and $C'(\gamma)$ is a constant independent from $\hat{\lambda}$ and μ , defined as

$$C'(\gamma) = \int_0^{v_{max}} \frac{v^2}{\sqrt{\frac{v^{2\gamma}}{\gamma} - \frac{v^2}{4c^2}}} dv.$$

The value of $C'(\gamma)$ is finite for every $\gamma \in \left(\frac{1}{2}, 1\right)$. We then rewrite the flux constraint as

$$2\mu^{\frac{2}{\gamma-1}} C'(\gamma) = 2c^2 \hat{\lambda},$$

from which we get

$$\mu = \left(\frac{c^2}{C'(\gamma)}\right)^{\frac{\gamma-1}{2}} \hat{\lambda}^{\frac{\gamma-1}{2}}. \quad (4.12)$$

We want to understand how the cost function τ depends on the flux $\hat{\lambda}$. Using the relations (4.10) and (4.11) obtained evaluating the Euler-Lagrange equations for (4.8), in the cost definition, we get

$$\tau(\hat{\lambda}) = \int_{\mathbb{R}} \frac{2}{\gamma} \zeta^{2\gamma} dx,$$

with $\int_{\mathbb{R}} \frac{\mu}{2c^2} \zeta^2 dx = \hat{\lambda}$.

With the same change of variable previously performed, and again thanks to the assumptions of

symmetry and decrease on the structure of the function ζ , we are able to evaluate the cost function. In particular,

$$\begin{aligned} \int_{\mathbb{R}} \zeta^{2\gamma} dx &= 2 \int_0^{\zeta_{max}} \frac{\zeta^{2\gamma}}{\sqrt{\frac{\zeta^{2\gamma}}{\gamma} - \frac{\mu^2 \zeta^2}{4c^2}}} d\zeta = \\ 2\mu^{\frac{1}{\gamma-1}} \int_0^{v_{max}} \mu^{\frac{2\gamma}{\gamma-1}} \frac{v^{2\gamma}}{\mu^{\frac{\gamma}{\gamma-1}} \sqrt{\frac{v^{2\gamma}}{\gamma} - \frac{v^2}{4c^2}}} dv &= a(\gamma) \mu^{\frac{\gamma+1}{\gamma-1}}, \end{aligned}$$

where

$$a(\gamma) = 2 \int_0^{v_{max}} \frac{v^{2\gamma}}{\sqrt{\frac{v^{2\gamma}}{\gamma} - \frac{v^2}{4c^2}}} dv.$$

The constant $a(\gamma)$ is finite for every $\gamma \in (\frac{1}{2}, 1)$.

Using the structure of the Lagrange multiplier evaluated in (4.12), we obtain

$$\tau(\hat{\lambda}) = \overline{C}(\gamma) \hat{\lambda}^{\frac{1+\gamma}{2}}, \quad (4.13)$$

where $\overline{C}(\gamma)$ is a finite constant, independent from the flux $\hat{\lambda}$, and defined as $\overline{C}(\gamma) = \frac{2}{\gamma} a(\gamma) \left(\frac{c^2}{\overline{C}'(\gamma)} \right)^{\frac{\gamma+1}{2}}$.

Some observations on the structure of the solution

- The minimising function has just one bump and it has compact support. Indeed, the minimising function ζ satisfies the differential equation (4.11), and as its value approximate zero, the derivative can be approximate by $\zeta' \simeq \zeta^\gamma$, which solutions are known to have compact support.

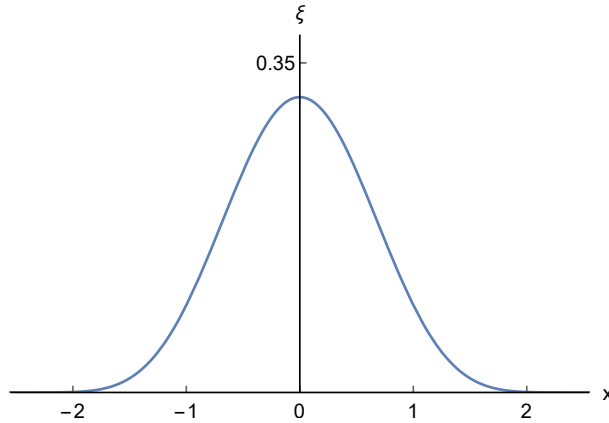


Figure 4.3: Example of the profile of the minimiser regularised flux, with $c = 0.5$, $\gamma = 2/3$, $\hat{\lambda} = 1/2$.

- Behaviour of the profile of the regularised flux as $\hat{\lambda}$ changes:
for each fixed value of $\gamma \in (\frac{1}{2}, 1)$, the support of the solution gets smaller, as the flux gets smaller

$$|supp(u)| = 2 \int_0^{x_{max}} 1 \, dx = \int_0^{u_{max}} \frac{1}{\sqrt{\frac{u^{2\gamma}}{\gamma} - \frac{\mu^2 u^2}{4c^2}}} \, du = 2C(\gamma) \hat{\lambda}^{\frac{1-\gamma}{2}}.$$

The same applies for the maximum value $\xi_{max} \simeq C(\gamma, c) \hat{\lambda}^{\frac{1+\gamma}{2}}$.

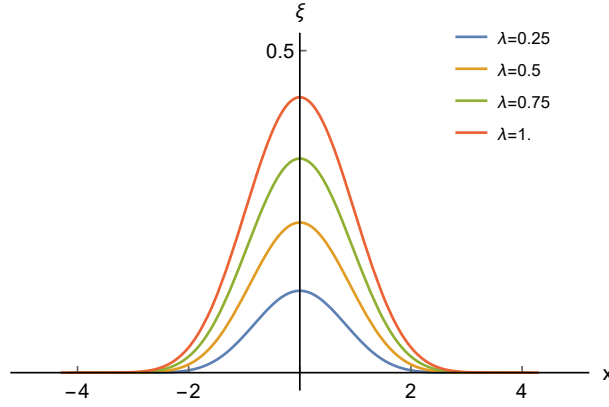


Figure 4.4: Profile of the minimising regularised flux as the intensity of the flux increases, with $c = \frac{1}{2}$, $\gamma = \frac{3}{4}$.

- The solution gets less concentrated as γ approaches 1:

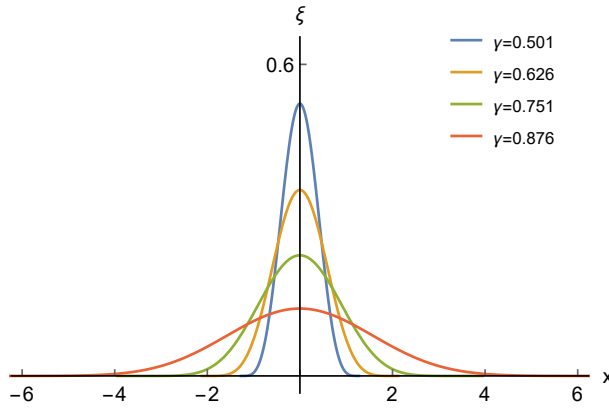


Figure 4.5: Behaviour of the profile of the minimising regularised flux as γ increases, with $c = \frac{1}{2}$, $\hat{\lambda} = \frac{1}{2}$.

For the rest of the chapter, we will denote by τ the cost function $\tau(\lambda) = \overline{C}(\gamma) \lambda^{\frac{\gamma+1}{2}}$, where $\overline{C}(\gamma)$ is a constant depending just on γ and introduced in (4.13).

4.3 Model summary

4.3.1 Notation

In the following, $\Omega \subset \mathbb{R}^2$ will denote an open, bounded set, with Lipschitz boundary. Moreover, we denote by $\mathcal{M}(\overline{\Omega})$, and $\mathcal{M}(\overline{\Omega}; \mathbb{R}^2)$ the space of scalar and $\mathbb{R}^2$ -valued Radon measures, equipped with the total variation norm. With $\mathcal{P}(\overline{\Omega}) \subset \mathcal{M}(\overline{\Omega})$ we indicate the subset of probability measures (i.e. non-negative Radon measures with total variation 1). The weak-* convergence in the measures space is denoted by $\xrightarrow{*}$, while the total variation of $\mu \in \mathcal{M}(\overline{\Omega})$ is denoted by $|\mu|$. The restriction of the measure μ to the subset $A \subset \Omega$ is denoted by $\mu \llcorner A$. The n -dimensional Hausdorff measure is denoted by $\mathcal{H}^n$. Finally, for a given collection $A = \{C_1, \dots, C_K\}$ of subsets of $\mathbb{R}$, for the sake of simplicity, and with a slight abuse of notation, we will also denote by A the set $\cup_{C \in A} C$.

4.3.2 Introduction of the energies

Definition 4.6. (*Divergence measure vector field and mass flux*)

1. A divergence measure vector field is a measure $q \in \mathcal{M}(\overline{\Omega}; \mathbb{R}^2)$ whose weak divergence is a Radon measure, i.e. $\operatorname{div} q \in \mathcal{M}(\overline{\Omega})$. The weak divergence is defined as

$$\int_{\Omega} \psi \operatorname{div} q = \int_{\Omega} \nabla \psi \cdot dq \quad \text{for all } \psi \in C^1(\Omega) \text{ with compact support.}$$

By [67], any divergence measure vector field can be decomposed as

$$q = \lambda_q \theta_q \mathcal{H}^1 \llcorner \Sigma_q + q^\perp,$$

where $\Sigma_q \subset \Omega$ is countably 1-rectifiable, $\lambda_q : \Sigma_q \rightarrow [0, \infty]$ is a $\mathcal{H}^1 \llcorner \Sigma_q$ -measurable function, $\theta_q : \Sigma_q \rightarrow S^1$ is $\mathcal{H}^1 \llcorner \Sigma_q$ -measurable and it is oriented in the direction of the tangent space of Σ_q , and $q^\perp$ is $\mathcal{H}^1$ -diffuse, that is, singular with respect to the one-dimensional Hausdorff measure on any countable 1-rectifiable set.

Given a vector-valued test function ψ , the measure acts on it as follow

$$\int_{\Omega} \psi \cdot dq = \int_{\Sigma_q} \psi(s) \cdot \theta_q(s) d\mathcal{H}^1 + \int_{\Omega} \psi \cdot q^\perp$$

2. Given $S \in \mathcal{M}(\overline{\Omega})$, with compact support, and such that $S(\overline{\Omega}) = 0$, a mass flux between S^+ and S^- is a divergence measure vector field q with $\operatorname{div} q = S$. The set of mass fluxes between μ^+ and μ^- is denoted by

$$X^S = \left\{ q \in \mathcal{M}(\overline{\Omega}; \mathbb{R}^2) \mid \operatorname{div} q = S \right\}.$$

Definition 4.7. 1. We call the function $S \in \mathcal{M}(\overline{\Omega})$ admissible source if it has compact support in Ω , it consists of a finite sum of deltas, and $S(\overline{\Omega}) = 0$.

2. Given an admissible source $S \in \mathcal{M}(\overline{\Omega})$, we define the cost functional $\mathcal{E} : X^S \rightarrow [0, \infty]$ as

$$\mathcal{E}^{\mu^+, \mu^-}[q] = \begin{cases} \int_{\Sigma_q} \tau(m_q) d\mathcal{H}^1 & \text{if } q^\perp = 0 \\ \infty & \text{else.} \end{cases}$$

Definition 4.8 (Phase field cost functional). Let $D > 0$, and $\rho : \mathbb{R}^2 \rightarrow [0, \infty)$ be a fixed smooth convolution kernel with compact support in the unit disk and $\int_{\mathbb{R}^2} \rho dx = 1$.

1. Given an admissible source $S \in \mathcal{M}(\overline{\Omega})$, the smoothed source is defined as

$$S_D := S * \rho_D, \quad \text{where } \rho_D = \frac{1}{D^2} \rho\left(\frac{\cdot}{D}\right).$$

2. The set of admissible functions is

$$X_D^S = \left\{ (q, u) \in L^1(\Omega, \mathbb{R}^2) \times W^{1,2}(\Omega) \mid \operatorname{div} q = S, \text{ on } \partial\Omega \right\}$$

3. The phase field cost functional is denoted by $\mathcal{E}_D : X_D^S \rightarrow [0, \infty)$, and defined as

$$\mathcal{E}_D[q, u] = D^{\frac{\gamma-1}{2}} \int_{\Omega} D^2 |\nabla u|^2 + \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} dx.$$

In order to prove the Γ -convergence result, both the cost functional and the phase field cost functional have to be defined on a common space. Moreover, while we have two variables in the definition of the phase field cost functional, the cost functional is defined as a single-variable functional. We then introduce the space $\mathcal{M}(\Omega; \mathbb{R}^2) \times L^1(\Omega)$, and we define both functionals as followed:

$$E^S[q, u] = \begin{cases} \mathcal{E}^S[q] & \text{if } q \in X^S \text{ and } u = 0 \text{ a.e.,} \\ \infty & \text{else,} \end{cases} \quad (4.14)$$

$$E_D^S[q, u] = \begin{cases} \mathcal{E}_D^S[q] & \text{if } (q, u) \in X_D^S, \\ \infty & \text{else.} \end{cases} \quad (4.15)$$

We start proving that there exist points in which the phase field functional assumes a finite value, and that it admits minimisers.

Proposition 4.9. *The functional (4.15) admits a minimiser $(q, u) \in X_D^S$ satisfying $E_D^S[q, u] < \infty$.*

Proof. We prove first the existence of an element $(q, u) \in L^1(\Omega) \times W^{1,2}(\Omega)$ in which $E_D^{\mu^+, \mu^-}[q, u] < \infty$. Let ω be an open set with regular boundary such that $\operatorname{supp} S \subset \omega \subset\subset \Omega$. For D small enough, it also holds $\operatorname{supp} S_D \subset \omega$. We consider a function $u \in W^{1,2}(\Omega)$ such that $u = 1$ on ω , $u = 0$ on $\partial\Omega$, and it smoothly goes between these two values.

We then consider a function $p \in W^{1,2}(\omega)$ that satisfies

$$\begin{cases} -\Delta p = S_D & \text{in } \omega \\ \partial_n p = 0 & \text{on } \partial\omega. \end{cases}$$

This problem admits a solution that is unique up to an additive constant. We then extend the gradient of such a function on the all set Ω , defining

$$q = \begin{cases} -\nabla p & \text{on } \omega \\ 0 & \text{otherwise.} \end{cases}$$

Such a function belongs to the space $L^1(\Omega)$, and satisfies the constraint $\operatorname{div} q = S_D$. Moreover, it holds $E_D[q, u] < \infty$, proving that the infimum of the energy (4.15) is finite.

Let now $\{(q_n, u_n)\} \in L^1(\Omega) \times W^{1,2}(\Omega)$ be a minimising sequence. It exists a constant $K > 0$ such that

$$E_D[q_n, u_n] \leq K.$$

This implies

$$\|u_n\|_{W^{1,2}} \leq C E_D[q_n, u_n] \leq CK.$$

We introduce the elements $f_n := \frac{|q_n|}{u_n}$. The uniform bounds on the energy along this sequence gives

$$\int_{\Omega} c^2 \frac{|q_n|^2}{u_n^2} dx \leq E_D[q_n, u_n],$$

implying uniform estimates on the L^2 -norm of the sequence $\{f_n\}$. Let $r \in (1, 2)$ be fixed, from Young's inequality follows

$$\begin{aligned} \int_{\Omega} |q_n|^r dx &= \int_{\Omega} f_n^r u_n^r dx \leq \\ &\left(\int_{\Omega} f_n^{rs} dx \right)^{\frac{1}{s}} \left(\int_{\Omega} u_n^{r \frac{s}{s-1}} dx \right)^{\frac{s-1}{s}} = \|f_n\|_2^r \|u_n\|_{\frac{2r}{2-r}}^r, \end{aligned}$$

where in the last equality we set $s = \frac{2}{r}$. Since the sequence $\{u_n\}$ is uniformly bounded in $W^{1,2}(\Omega)$, the L^p -norm of the sequence is uniformly bounded for any $p \in [1, \infty)$. Thus, the L^r -norm of the sequence $\{q_n\}$ is bounded for any $r \in (1, 2)$. There exists a subsequence weakly-converging in this space to an element q , and consequentially in $L^1(\Omega)$. Moreover, the sequence $\{u_n\}$ admits a subsequence weakly converging to an element $u \in W^{1,2}(\Omega)$.

To conclude, it is enough to prove weak-lowersemicontinuity of the energy.

We recall that, because of the assumption $\gamma \in [\frac{1}{2}, 1)$, the term $\int_{\Omega} D^2 |\nabla u|^2 + \frac{|u|^{2\gamma}}{2\gamma} dx$ is convex in the u variable. This implies lower-semicontinuity with respect the $W^{1,2}$ -norm, and then with respect the weak-convergence.

The uniform bound on the $W^{1,2}(\Omega)$ -norm of the sequence $\{u_n\}$, implies uniform bounds on the L^p -norm of the sequence for each $p \in (1, \infty)$ (see [15]). Moreover, up to a subsequence, that we will denote with the same notation, $\{u_n\}$ strongly converges in $L^2(\Omega)$, and then, again up to a subsequence, to u . This gives uniform bound on the L^p -norm of the sequence $\{u_n^2\}$ for each $p \in [1, \infty)$, hence existence of a subsequence weakly-converging in such a space. The limit can be identified with u^2 , thanks to the a.e.-pointwise convergence of $\{u_n^2\}$ to u^2 .

We introduce the map $(q, g) \mapsto \int_{\Omega} \frac{|q|}{g} dx$, which is convex in both variables. Weak convergence of the sequence $\{(q_n, u_n^2)\}$ to (q, u^2) ensure the lower-semicontinuity of the last term along the sequence $\{(q_n, u_n)\}$.

The inequality

$$\inf E_D \leq E_D[q, u] \leq \liminf E_D[q_n, u_n] = \inf E_D,$$

is then satisfied, proving the existence of a minimiser for the regularised energy. ■

4.4 The Γ -liminf result

The Γ -liminf result will be proved via the *slicing method*. The main idea is to study the problem at first in a 1-dimensional setting, by examine the behaviour of the functionals on sections obtained by intersection the set Ω with hyperplanes. Once the Γ -limit is proven in a 1-dimensional environment, Fubini's Theorem and Fatou's Lemma are used in order to recover the result in the whole space. For

a thorough introduction to the method, see for example [13, Chapter 15].

In the following, we first introduce and prove the dimension-reduced problem, then we present some essential results for the slicing method for divergence measure vector fields, and finally we prove the Γ -liminf inequality.

4.4.1 Γ -liminf inequality for the dimension-reduced problem

Definition 4.10 (Reduced functionals). *Let $I \subset \mathbb{R}$ be an open interval.*

1. *The decomposition of a measure $q \in \mathcal{M}(\bar{I})$ into its atoms and the remainder is denoted by*

$$q = \lambda_q \mathcal{H}^0 \llcorner \Sigma_q + q^\perp,$$

where $\Sigma_q \subset \bar{I}$ is the set of atoms of q , $\lambda_q : \Sigma_q \rightarrow \mathbb{R}$ is $\mathcal{H}^0 \llcorner \Sigma_q$ -measurable, and $q^\perp$ contains no atoms.

2. *We define the reduced cost functional on the interval I as $\mathcal{F}[\cdot; I] : \mathcal{M}(\bar{I}) \rightarrow [0, \infty)$*

$$\mathcal{F}[q; I] = \begin{cases} \sum_{x \in \Sigma_q \cap I} \tau(|\lambda_q(x)|) & \text{if } q^\perp = 0, \\ \infty & \text{else.} \end{cases}$$

Its extension to $\mathcal{M}(\bar{I}) \times L^1(I)$ is denoted by $F[\cdot; I] : \mathcal{M}(\bar{I}) \times L^1(I) \rightarrow [0, \infty)$ and defined as

$$F[q, u; I] = \begin{cases} \mathcal{F}[q; I] & \text{if } u = 0 \text{ a.e.}, \\ \infty & \text{otherwise.} \end{cases}$$

3. *For any $(q, u) \in L^1(I) \times W^{1,2}(I)$ we define the reduced phase field functional on I as*

$$\mathcal{F}_D[q, u; I] = D^{\frac{\gamma-1}{2}} \int_I D^2 |u'|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \, dx.$$

Likewise, we define $F_D[\cdot; I] : \mathcal{M}(\bar{I}) \times L^1(I) \rightarrow [0, \infty)$,

$$F_D[q, u; I] = \begin{cases} \mathcal{F}_D[q, u; I] & \text{if } (q, u) \in L^1(I) \times W^{1,2}(I), \\ \infty & \text{else.} \end{cases}$$

Lemma 4.11. *Let $C \subset \mathbb{R}$ be a closed interval, $\gamma \in [\frac{1}{2}; 1)$, and $\eta > 0$. Then,*

$$\begin{aligned} & \inf \left\{ \int_C |\zeta'|^2 + c^2 \frac{\xi^2}{|\zeta|^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dx \mid \int_C \xi \, dx = Q, \, \zeta|_{\partial J} \leq \eta, \, \exists z \in J, \zeta(z) \geq \eta \right\} \\ & \geq C \min \left\{ \eta^{\gamma-1} Q; \, \tau(Q) \right\}. \end{aligned}$$

Proof. Let $\eta > 0$, $\xi \in L^1(C)$ be such that $\int_C \xi \, dx = Q$, and $z \in C$ such that $\max_C \zeta = \zeta(z)$. Without

loss of generality, we can assume $C = [a, b]$.

$$\begin{aligned}
A &:= \int_C |\zeta'|^2 + c^2 \frac{\xi^2}{|\zeta|^2} + \frac{\zeta^{2\gamma}}{\gamma} dx = \int_C |\zeta'|^2 + \frac{\zeta^{2\gamma}}{2\gamma} + \frac{\zeta^{2\gamma}}{2\gamma} + c^2 \frac{\xi^2}{|\zeta|^2} dx \\
&\geq \int_C \sqrt{\frac{2}{\gamma}} |\zeta'| |\zeta|^\gamma dx + \int_C c \sqrt{\frac{2}{\gamma}} \frac{\xi}{|\zeta|} |\zeta|^\gamma dx \\
&\geq \int_a^z \sqrt{\frac{2}{\gamma}} \frac{(\zeta^{\gamma+1})'}{\gamma+1} dy + \int_b^z \sqrt{\frac{2}{\gamma}} \frac{(\zeta^{\gamma+1})'}{\gamma+1} dx + \sqrt{\frac{2}{\gamma}} \int_C c \frac{\xi}{\zeta(z)^{1-\gamma}} dx \\
&= \sqrt{\frac{2}{\gamma}} \left[\frac{2}{\gamma+1} \zeta(z)^{\gamma+1} - \frac{2}{\gamma+1} \eta^{\gamma+1} + \frac{c}{\zeta(z)^{1-\gamma}} Q \right].
\end{aligned}$$

The expression is minimized, under the constraint $\zeta \geq \eta$, by

$$\zeta(z) = \max \left\{ \eta; \sqrt{\frac{c(1-\gamma)}{2}} Q \right\},$$

giving

$$A \geq \begin{cases} \sqrt{\frac{2}{\gamma}} c \eta^{\gamma-1} Q & \text{if } \eta \geq \sqrt{\frac{c(1-\gamma)}{2}} Q, \\ \sqrt{\frac{2}{\gamma}} c \frac{1}{(\sqrt{\frac{c}{2}}(1-\gamma)Q)^{1-\gamma}} Q & \text{else.} \end{cases}$$

We then get

$$A \geq c \sqrt{\frac{2}{\gamma}} \min \left\{ \eta^{\gamma-1} Q; \left(\frac{2}{c(1-\gamma)} \right)^{\frac{1-\gamma}{2}} (Q)^{\frac{1+\gamma}{2}} \right\}.$$

■

Proposition 4.12 (Lower bound on reduced phase field functional). *Let $I = (a, b) \subset \mathbb{R}$ and $\eta > 0$. Let $I_\eta = \{x \in I \mid |u(x)| \leq \eta\}$, and $\mathcal{C}_\eta$ be the collection of connected components of $I \setminus I_\eta$. Moreover, we assume $u(a), u(b) \leq \eta$. It holds*

$$\mathcal{F}_D[q, u; I] \geq \frac{c^2}{D^{\frac{1-\gamma}{2}} \eta^2 \mathcal{H}^1(I)} \left(\int_{I_\eta} |q| dx \right)^2 + \sum_{C \in \mathcal{C}_\eta} \max \left\{ 0, \tau \left(\int_C |q| dx \right) - K \eta^{1+\gamma} \right\}, \quad (4.16)$$

for a constant $K = K(\gamma) > 0$ depending only on γ .

Proof. Restricting the integral in the energy definition, we observe that

$$\begin{aligned}
D^{\frac{\gamma-1}{2}} \int_{I_\eta} D^2 |u'|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} dx &\geq D^{\frac{\gamma-1}{2}} \int_{I_\eta} c^2 \frac{|q|^2}{u^2} dx \\
&\geq \frac{c^2}{D^{\frac{1-\gamma}{2}} \eta^2} \int_{I_\eta} |q|^2 dx \geq \frac{c^2}{D^{\frac{1-\gamma}{2}} \eta^2 \mathcal{H}^1(I_\eta)} \left(\int_{I_\eta} |q| dx \right)^2,
\end{aligned}$$

where the last relation follows from Jensen's inequality.

Furthermore, for any fixed connected set $C \in \mathcal{C}_\eta$, it holds

$$D^{\frac{\gamma-1}{2}} \int_C D^2 |u'|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} dx \geq 0.$$

Moreover,

$$\begin{aligned}
& D^{\frac{\gamma-1}{2}} \int_C D^2 |u'|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \, dx \\
& \geq \inf \left\{ D^{\frac{\gamma-1}{2}} \int_C D^2 |u'|^2 + c^2 \frac{|v|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \, dx \left| \int_C v \, dx = \int_C |q| \, dx, u|_{\partial C} \leq \eta \right\} \\
& = \inf \left\{ \int_{C/D^{(\gamma+1)/2}} |\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dx \left| \int_{C/D^{(\gamma+1)/2}} \xi \, dy = \int_C |q| \, dx, \zeta|_{\partial C/D^{(\gamma+1)/2}} \leq \eta \right\},
\end{aligned}$$

where we performed the same change of variables $y = D^{-\frac{\gamma+1}{2}} x$, $\xi = D^{\frac{\gamma+1}{2}} v$, $\zeta = D^{\frac{1}{2}} u$ used in Section 4.2. Let now extend the functional to $\mathbb{R}$. We define ξ as zero outside the set $C/D^{(\gamma+1)/2}$, and extend continuously the function ζ from the value η to zero on both sides of the interval $C/D^{(\gamma+1)/2}$, minimising the cost to pay. This is possible since the functional $\int_0^\infty |\zeta'|^2 + \frac{|\zeta|^{2\gamma}}{\gamma} \, dy$ is weak-l.s.c. and coercive.

It then holds

$$\begin{aligned}
& \inf \left\{ \int_{C/D^{(\gamma+1)/2}} |\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dx \left| \int_{C/D^{(\gamma+1)/2}} \xi \, dx = \int_C |q| \, dx, \zeta|_{\partial C/D^{(\gamma+1)/2}} \leq \eta \right\} \\
& = \inf \left\{ \int_{\mathbb{R}} |\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dx - \int_{\mathbb{R} \setminus C/(D^{(\gamma+1)/2})} |\zeta'|^2 + 0 + \frac{|\zeta|^{2\gamma}}{\gamma} \, dy \left| \int_{C/D^{(\gamma+1)/2}} \xi \, dx = \int_C |q| \, dx, \right. \right. \\
& \quad \left. \left. \zeta|_{\partial C/D^{(\gamma+1)/2}} \leq \eta \right\} \\
& \geq \inf \int_{\mathbb{R}} |\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dx - g(\eta) \left| \int_{C/D^{(\gamma+1)/2}} \xi \, dy = \int_C |q| \, dx, \zeta|_{\partial C/D^{(\gamma+1)/2}} \leq \eta \right\}
\end{aligned}$$

where the constant $g(\eta)$ is defined as

$$g(\eta) = \inf \left\{ \int_{\mathbb{R} \setminus C/(D^{(\gamma+1)/2})} |\zeta'|^2 + c^2 \frac{|0|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dy \left| \zeta|_{\partial C/D^{(\gamma+1)/2}} \leq \eta \right\}.$$

Considering the extension $\hat{\zeta}(y) = \eta y/L$ for some $L > 0$, the value of $g(\eta)$ can be estimated as

$$\begin{aligned}
g(\eta) & = \inf \left\{ \int_{\mathbb{R} \setminus C/(D^{(\gamma+1)/2})} |\zeta'|^2 + c^2 \frac{|0|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dy \left| \zeta|_{\partial C/D^{(\gamma+1)/2}} \leq \eta \right\} \\
& \leq 2 \int_0^L |\hat{\zeta}'|^2 + \frac{|\hat{\zeta}|^{2\gamma}}{\gamma} \, dy \\
& = 2 \left(\frac{\eta^2}{L} + \frac{\eta^{2\gamma}}{\gamma} \frac{L}{2\gamma+1} \right) \\
& = K \eta^{1+\gamma},
\end{aligned}$$

where $K(\gamma) = \frac{\gamma(2\gamma+1)+1}{\gamma(2\gamma+1)}$, and we chose $L = \eta^{\frac{1-\gamma}{1+\gamma}}$. Thus, from we proved in Section 4.2, follows

$$\begin{aligned}
& D^{\frac{\gamma-1}{2}} \int_C D^2 |u'|^2 + c^2 \frac{|q|^2}{u^2} + \frac{|u|^{2\gamma}}{\gamma} \, dx \geq \inf \left\{ \int_{\mathbb{R}} |\zeta'|^2 + c^2 \frac{|\xi|^2}{\zeta^2} + \frac{|\zeta|^{2\gamma}}{\gamma} \, dy \left| \int_{\mathbb{R}} \xi \, dy = \int_C |q| \, dx \right\} - g(\eta) \\
& \geq \tau \left(\int_C |q| \, dx \right) - K \eta^{1+\gamma}.
\end{aligned}$$

■

Applying the results in Lemma 4.11 to each element $C \in C_\eta$, and assuming $|u| \leq \eta$ on ∂I , the inequality (4.16) can be refine as follows

$$F_D[q, u; I] \geq \frac{c^2}{D^{\frac{1-\gamma}{2}} \eta^2 \mathcal{H}^1(I)} \left(\int_{I_\eta} |q| \, dx \right)^2 + \sum_{C \in C_\eta} \max \left\{ \min \left\{ \eta^{\gamma-1} \int_C |q| \, dx; \tau \left(\int_C |q| \, dx \right) \right\}; \tau \left(\int_C |q| \, dx \right) - K \eta^{1+\gamma} \right\}. \quad (4.17)$$

Between the elements in the set C_η , we now focus our attention on the ones where the flux is small, i.e.

$$C_\eta^{\leq} = \{C \in C_\eta, \int_C |q| \, dx \leq \eta\}.$$

Similarly, we denote $C_\eta^> = \{C \in C_\eta, \int_C |q| \, dx > \eta\}$.

The concavity of the cost function $\tau(s) = \overline{C}(\gamma) s^{\frac{\gamma+1}{2}}$ implies that, for each $s \in [0, \eta]$, it holds $\tau(s) \geq \frac{\tau(\eta)}{\eta} s$. For each $C \in C_\eta^{\leq}$ it then holds

$$\tau \left(\int_C |q| \, dx \right) \geq \frac{\tau(\eta)}{\eta} \int_C |q| \, dx = \overline{C}(\gamma) \eta^{\frac{(\gamma-1)}{2}} \int_C |q| \, dx.$$

Thus,

$$F_D[q, u; I] \geq \sum_{C \in C_\eta^{\leq}} C \min \left\{ \eta^{\gamma-1}, \eta^{\frac{(\gamma-1)}{2}} \right\} \int_C |q| \, dx,$$

from which follows

$$\int_{C_\eta^{\leq}} |q| \, dx \leq \frac{C F_D[q, u; I]}{\min \left\{ \eta^{\gamma-1}, \eta^{\frac{(\gamma-1)}{2}} \right\}}. \quad (4.18)$$

Lemma 4.13. *Let $q_D \xrightarrow{*} q$ in $\mathcal{M}(\overline{I})$, $u_D \rightarrow u$ in $L^1(I)$, be such that $F_D[q_D, u_D; I]$ is uniformly bounded. Further, we assume $u_D|_{\partial I} \rightarrow 0$, as $D \rightarrow 0$. For any $\eta = \eta(D) \rightarrow 0$, satisfying $\eta(D) \geq \max u_D|_{\partial I}$, we define $\tilde{q}_D := q_D \llcorner C_\eta^>$. It follows that $\tilde{q}_D \xrightarrow{*} q$. Moreover, $q^\perp = 0$.*

Proof. The result obtained in Proposition 4.12 implies

$$\left(\int_{I_\eta} |q_D| \, dx \right)^2 \leq \frac{\sup_D F_D[q_D, u_D; I]}{c^2} D^{\frac{1-\gamma}{2}} \eta^2 \mathcal{H}^1(I).$$

It follows that as $D \rightarrow 0$, it holds $\int_{I_\eta} |q_D| \, dx \rightarrow 0$. Moreover, inequality (4.18) implies also $\int_{C_\eta^{\leq}} |q_D| \, dx \rightarrow 0$.

We obtain then

$$\tilde{q}_D := q_D \llcorner C_\eta^> \xrightarrow{*} q.$$

It remains to prove that $q^\perp = 0$. In order to do so, we will consider a specific subsequence $\{\eta(D_k)\}$. From Egorov's theorem follows that, for each $k \in \mathbb{N}$, there exists a set $\tilde{I}^k$ that satisfies $\mathcal{H}^1(I \setminus \tilde{I}^k) \leq \alpha_k$, and on which the sequence $\{u_D\}$ uniformly converges to zero. For each fixed $k \in \mathbb{N}$, we select D_k

small enough such that $u_{D_k} \leq \frac{1}{k}$ on $\tilde{I}^k$. Moreover, the sequence $\{D_k\}$ can be assumed to be strictly decreasing and converging to zero. Let us define $\eta_k = \eta(D_k) := \max\{\frac{1}{k}, \max u_{D_k}|_{\partial I}\}$. It satisfies $\eta_k \rightarrow 0$, and as proved above, it holds $\tilde{q}_k := \tilde{q}_{D_k} \xrightarrow{*} q$. To simplify the notation, we use for the rest of the proof the convention $u_k := u_{D_k}$, $q_k := q_{D_k}$ and for the functional $F_k[q_k, u_k; I] := F_{D_k}[q_{D_k}, u_{D_k}; I]$. Let $\eta_0 \in \mathbb{R}$ be such that, for every $0 \leq \eta \leq \eta_0$, the inequality $\tau(\eta) > 2K\eta^{1+\gamma}$ is satisfied. For η_k small enough it holds

$$\begin{aligned} F_k[q_k, u_k; I] &\geq F_k[\tilde{q}_k, u_k; I] \geq \sum_{C \in C_{\eta_k}^>} \left[\tau \left(\int_C |\tilde{q}_k| dx \right) - K\eta_k^{1+\gamma} \right] \\ &\geq \frac{1}{2} \sum_{C \in C_{\eta_k}^>} \tau \left(\int_C |\tilde{q}_k| dx \right). \end{aligned}$$

Let us now assume, by contradiction, that $q^\perp \neq 0$, and set $M := \|q^\perp\| > 0$. Further, we introduce the constant

$$r = \left(\frac{\overline{C}M}{4 \sup_k F_k[q_k, u_k; I]} \right)^{\frac{2}{1-\gamma}},$$

where we $\overline{C} = \overline{C}(\gamma)$ was defined in Section 4.2, and we consider the set $K_k^r := \{C \in C_{\eta_k}^>, \int_C |q\tilde{D}_k| dx \geq r\}$. We denote by $\tilde{q}_k^r := \tilde{q}_k \llcorner K_k^r$. It holds

$$F_k[q_k, u_k; I] \geq F_k[\tilde{q}_k^r, u_k; I] \geq \frac{1}{2} \sum_{C \in K_k^r} \tau \left(\int_C |\tilde{q}_k^r| dx \right) \geq \frac{1}{2} \sum_{C \in K_k^r} \tau(r),$$

for all η_k small enough. The number of elements in the set K_k^r is then uniformly bounded in k . Up to a subsequence, we can assume that the set K_k^r consists of exactly P elements for each $k > 0$, and that the middle points of this sets converge to $\{x_1, \dots, x_P\} \in \bar{I}$. For each element $C \in K_k^r$, it then holds, $\mathcal{H}^1(C) \leq \mathcal{H}^1(I \setminus I_{\eta_k}) \leq \mathcal{H}^1(I \setminus \tilde{I}^k) \leq \frac{1}{k}$, implying that every element in K_k^r lies in the closed set $\overline{B}_{\frac{1}{k}}(x_1, \dots, x_P)$. The measures $\tilde{q}_k^r$ satisfy then, $|\tilde{q}_k^r|(I \setminus B_{\frac{1}{k}}(x_1, \dots, x_K)) = 0$. Since the total variation of the measures $\{\tilde{q}_k^r\}$ is uniformly bounded, it admits a subsequence converging weakly- $\star$ in the space $\mathcal{M}(\bar{I})$, to a measure that we denote by $\tilde{q}^r$. In the following we will consider such a subsequence, and will denote it with the same notation. Passing to the limit in k , we get $|\tilde{q}^r|(I \setminus \{x_1, \dots, x_K\}) = 0$, i.e. the sequence $\{\tilde{q}_k^r\}$ converges to an atomic measure. It then holds

$$\tilde{q}_k \llcorner (I \setminus K_k^r) = \tilde{q}_k \llcorner (C_{\eta_k}^> \setminus K_k^r) = \tilde{q}_k - \tilde{q}_k^r \xrightarrow{*} q - \sum_i^P a_i \delta_{x_i} = q^\perp + \mu,$$

where μ is a measure singular to $q^\perp$. However, the total variation of the right-hand side is bigger or equal than M , while the measure on the left hand side satisfies

$$\begin{aligned} \int_{C_{\eta_k}^> \setminus K_k^r} |\tilde{q}_k| dx &= \sum_{C \in C_{\eta_k}^> \setminus K_k^r} \int_C |\tilde{q}_k| dx \leq \sum_{C \in C_{\eta_k}^> \setminus K_k^r} \frac{r}{\tau(r)} \tau \left(\int_C |\tilde{q}_k| \right) \\ &\leq \frac{2r}{\tau(r)} F_k[q_k, u_k; I] \leq \frac{2}{\overline{C}(\gamma)} \sup_k F_k[q_k, u_k; I] r^{\frac{1-\gamma}{2}} = \frac{M}{4}, \end{aligned}$$

which is in contradiction with weakly- $\star$ lower semicontinuity of the mass. ■

Theorem 4.14. (*Γ -liminf inequality for reduced functionals*) Let $J \subset \mathbb{R}$ be open and bounded, $q \in \mathcal{M}(\bar{J})$ and $u \in L^1(J)$. Then,

$$\Gamma - \liminf F_D[q, u; J] \geq F[q, u; J]$$

with respect to the topology of weak-* convergence in $\mathcal{M}(\bar{J})$, and strong convergence in $L^1(J)$.

Proof. Let $(q, u) \in \mathcal{M}(\bar{J}) \times L^1(J)$ be a fixed element, and let $\{(q_D, u_D)\}$ be a sequence converging to it in the considered topology. Without loss of generality, the $\liminf F_D[q_D, u_D; J]$ can be assumed (up to a subsequence) to be a finite limit. Indeed, if this would not be the case, the result would trivially hold. Moreover, it is enough to show the result separately for each connected component $\tilde{I} = (a, b) \subset J$.

The inequality

$$D^{\frac{\gamma-1}{2}} \int_{\tilde{I}} \frac{|u_D|^{2\gamma}}{2} dx \leq F_D[q_D, u_D; \tilde{I}],$$

implies that the sequence $\{u_D\}$ converges to zero in the space $L^{2\gamma}(\tilde{I})$, and thus in $L^1(\tilde{I})$, so that $u = 0$. Moreover, up to a subsequence, we can assume $\{u_D\}$ to convergence almost everywhere to u . For each $\xi > 0$, it then exists an interval $(a + \xi, b - \xi) \subset I \subset \tilde{I}$, such that $u_D|_{\partial I} \rightarrow 0$.

Moreover, since $F_D[q_D, u_D; I]$ is uniformly bounded, Lemma 4.13 implies $q^\perp = 0$, so that q is an atomic measure on the set I . Let $\Sigma_q \subset I$ denote the set of points on which the Dirac masses of q are situated, so that we can write

$$q \llcorner I = \sum_{x \in \Sigma_q} \lambda_q(x) \delta_x.$$

Additionally, for each $m > 0$, we denote by S_m the subset of points $x \in \Sigma_q$ in which $|\lambda_q(x)| \geq m$. Since the total variation of q is finite, for each fixed $m > 0$, the set S_m consists of a finite number of elements. Let $d = \frac{1}{4} \min_{x, y \in S_m} |x - y|$, for each $0 < \zeta < d$, the sets $\{B_\zeta(x)\}_{x \in S_m}$ are disjoint and the distance between them is greater or equal than d . To prove the result, it is sufficient to show that, for any fixed $m > 0$, and ζ small enough, it holds

$$\liminf F_D[q_D, u_D; I] \geq \sum_{x \in S_m \cap I} \tau(|q|(B_\zeta(x))). \quad (4.19)$$

Indeed, if the right-hand side diverges as $m \rightarrow 0$, it would imply $\liminf F_D[q_D, u_D; I] = \infty$, and the inequality would hold.

Following a strategy similar to the one adopted in Lemma 4.13, we consider a subsequence of $\{q_D\}$. For each $k \in \mathbb{N}$, Egorov's theorem ensure us that there exist a set $\tilde{I}^k \subset I$ on which $\{u_D\}$ converges uniformly to zero, and such that $\mathcal{H}^1(I \setminus \tilde{I}^k) \leq \frac{1}{k}$. We select a sequence $\{D_k\}$, strictly decreasing and converging to zero, along which it holds $|u_k| \leq \frac{1}{k}$ on the set $\tilde{I}^k$. To simplify the notation, we will use the convention $u_k := u_{D_k}$. Let us now define $\eta_k = \eta(D_k) = \max\{\frac{2}{k}, \max u_{D_k}|_{\partial I}\}$. For each $s \in (0, 1)$, there exists $\eta_0 > 0$ small enough, such that $\tau(\eta) > 1/(1-s)K\eta^{1+\gamma}$ for all $\eta < \eta_0$, where $K = K(\gamma)$ is the constant introduced in Proposition 4.12.

Similarly to what has been done in the previous proof, to simplify the notation, we will denote by $u_k = u_{D_k}$. For η_k small enough, it holds

$$\tau\left(\int_C |q_D| dx\right) - K\eta^{1+\gamma} \geq s\tau\left(\int_C |q_D| dx\right) \text{ for all } C \in C_{\eta_k}^>.$$

For such values of k , from inequality (4.17) follows

$$\begin{aligned} F_k[q_k, u_k; I] &\geq \sum_{C \in C_{\eta_k}^>} \left[\tau \left(\int_C |q_k| dx \right) - K \eta_k^{1+\gamma} \right] \\ &\geq s \sum_{C \in C_{\eta_k}^>} \tau \left(\int_C |q_k| dx \right) \geq s \sum_{x \in S_m \cap I} \sum_{C \in C_{\eta_k}^>, C \cap B_\zeta(x) \neq \emptyset} \tau \left(\int_C |q_k| dx \right). \end{aligned}$$

In the last inequality we assumed $\mathcal{H}^1(I \setminus I_{\eta_k})$ smaller than the distance between the sets $B_\zeta(x)$, so that any set C can intersect at most one element $B_\zeta(x)$. Indeed, for D_k small enough, it holds for each $C \in C_{\eta_k}$, that $\mathcal{H}^1(C) \leq \mathcal{H}^1(I \setminus I_{\eta_k}) \leq \mathcal{H}^1(I \setminus \tilde{I}^k) \leq \frac{1}{k}$.

Due to the subadditivity of the cost function τ , it holds

$$\begin{aligned} F_D[q_D, u_D; I] &\geq s \sum_{x \in S_m \cap I} \tau \left(\sum_{C \in C_{\eta}^>, C \cap B_\zeta(x) \neq \emptyset} \int_C |q_k| dx \right) \\ &\geq s \sum_{x \in S_m \cap I} \tau \left(\int_{B_\zeta(x)} |\tilde{q}_k| dx \right). \end{aligned}$$

As proved in Lemma 4.13, the sequence $\tilde{q}_k := q_k \lfloor (C_{\eta}^>)$ converges weakly- $\star$ to q . Finally, we recall that for each $k \in \mathbb{N}$, and $0 \leq \zeta \leq d$, it holds $|\hat{q}_k|(B_\zeta(x)) \leq |q|(B_\zeta(x)) = m_q(x)$. The arbitrariness of the constant $s \in (0, 1)$, together with the property of the functional cost τ to be non-increasing, inequality (4.19) is proved. Passing to the limit in ξ going to zero, we conclude the proof. $\blacksquare$

4.4.2 Slicing of vector-valued measures

This section consist in an overview on slicing techniques relative to divergence measure vector field. These results are presented in [27, Section 3.2], where the a more thorough discussion, as well as the proofs of the results here presented, can be found.

The slicing will be performed in the direction of a unitary vector $\xi \in S^{d-1}$. The hyperplanes orthogonal to this vector are defined as

$$H_{\xi,t} := \pi_\xi^{-1}(t), \quad \text{where } \pi_\xi : \mathbb{R}^d \rightarrow \mathbb{R}, \quad \pi_\xi(x) = x \cdot \xi.$$

The orthogonal projection on the hyperplane $H_{\xi,t}$ is defined by the function

$$\pi_{H_{\xi,t}}(x) = (I - \xi \otimes \xi) x + t\xi.$$

Let $q \in \mathcal{M}(\mathbb{R}^2)$ be a compactly supported divergence measure vector field. By the Disintegration Theorem [5, Thm. 2.28], for any $\xi \in S^{d-1}$, and almost all $t \in \mathbb{R}$, there exists a unique measure $\nu^{\xi,t} \in \mathcal{M}(H_{\xi,t})$ such that

$$\|\nu^{\xi,t}\|_{\mathcal{M}} = 1, \quad q \cdot \xi = \nu^{\xi,t} \otimes \pi_{\xi\#} |q \cdot \xi|(t).$$

The measure $\pi_{\xi\#} |q \cdot \xi|$ on $\mathbb{R}$ can be decomposed into its absolutely continuous and singular part, as follows:

$$\pi_{\xi\#} |q \cdot \xi| = q_\xi(t) dt + q_\xi^\perp,$$

where dt denoted the Lebesgue measure on $\mathbb{R}$.

Lemma 4.15. *For any $\xi \in S^{d-1}$, and any compactly supported divergence measure vector field q it holds $q_\xi^\perp = 0$, i.e. the measure $\pi_{\xi^\#}|q \cdot \xi| = q_\xi(t) dt$ is absolutely continuous with respect to the Lebesgue measure dt . Moreover, for almost all $t \in \mathbb{R}$, and any compactly supported $\varphi \in C^\infty(\mathbb{R}^2)$, it holds*

$$q_\xi(t) \int_{H^{\xi,t}} \varphi d\nu^{\xi,t} = \int_{\{\xi \cdot x, t\}} \nabla \varphi dq + \int_{\{\xi \cdot x, t\}} \varphi d\text{div } q.$$

Proof. See [27, Lemma 3.1]. ■

The slice of a divergence measure vector field will be defined as the measure obtained via the Disintegration Theorem with respect to the Lebesgue measure on $\mathbb{R}$.

Definition 4.16 (Sliced sets, functions and measures). *Let $\xi \in S^{d-1}$ be a unitary vector, and $t \in \mathbb{R}$.*

1. *For any $A \subset \mathbb{R}^2$, the sliced set is defined as $A^{\xi,t} = A \cap H^{\xi,t}$.*
2. *For any $f : A \rightarrow \mathbb{R}$, the sliced function is defined as $f^{\xi,t} : A^{\xi,t} \rightarrow \mathbb{R}$, $f^{\xi,t} = f|_{A^{\xi,t}}$.
For any $f : A \rightarrow \mathbb{R}^2$, we define $f^{\xi,t} : A^{\xi,t} \rightarrow \mathbb{R}$, $f^{\xi,t} = \xi \cdot f|_{A^{\xi,t}}$.*
3. *The sliced measure of a compactly supported divergence measure vector field q is defined as*

$$q^{\xi,t} = q_\xi(t) \nu^{\xi,t}.$$

By using the Disintegration Theorem, and the result in Lemma 4.15, it can be written $q \cdot \xi = q^{\xi,t} \otimes dt$.

Observation 4.17. *Fubini's theorem implies that for any function $f \in W^{m,p}$, the corresponding sliced function $f^{\xi,t}$ is well-defined and belong to the space $W^{m,p}$ for almost all $(\xi, t) \in S^{n-1} \times \mathbb{R}$.*

Theorem 4.18 (Weak convergence of sliced measures). *Let $q^j \xrightarrow{*} q$, for a sequence $\{q^j\}$ of compactly supported divergence measure vector fields, such that $\|q^j\|_{\mathcal{M}}$ is uniformly bounded. then, for almost all $\xi \in S^{d-1}$, and $t \in \mathbb{R}$, it holds*

$$q_j^{\xi,t} \xrightarrow{*} q^{\xi,t}.$$

Proof. See [27, Theorem 3.1]. ■

Remark 4.19 (Characterisation of sliced measures). *Let q be a 1-rectifiable compactly supported divergence measure vector field, i.e. $q = \theta m \mathcal{H}^1 \llcorner \Sigma$, where $\Sigma \subset \mathbb{R}^2$, and $m : \Sigma \rightarrow [0, \infty)$ and $\theta : \Sigma \rightarrow S^{d-1}$ are $\mathcal{H}^1 \llcorner \Sigma$ -measurable functions, such that θ is tangent to Sigma $\mathcal{H}^1$ -almost everywhere. Then, the coarea formula (see [26, Theorem 3.2.22]) implies $|\theta \cdot \xi| \mathcal{H}^1 \llcorner \Sigma = \mathcal{H}^0 \llcorner \Sigma^{\xi,t} \otimes \mathcal{H}^1(t)$, which gives, for any f Borel function,*

$$\int_{\mathbb{R}^2} f dq \cdot \xi = \int_{\Sigma} f m \theta \cdot \xi d\mathcal{H}^1 = \int_{\mathbb{R}} \int_{\Sigma^{\xi,t}} f m \text{sgn}(\xi \cdot \theta) d\mathcal{H}^0 dt.$$

Therefore, for almost all $t \in \mathbb{R}$, it holds

$$q^{\xi,t} = \text{sgn}(\xi \cdot \theta) m \mathcal{H}^0 \llcorner \Sigma^{\xi,t}.$$

Moreover, by choosing $f = \frac{\tau(m)}{m} \text{sgn}(\xi \cdot \theta)$, we get

$$\int_{\Sigma} \tau(m) |\theta \cdot \xi| d\mathcal{H}^1 = \int_{\mathbb{R}} \int_{\Sigma^{\xi,t}} \tau(m) d\mathcal{H}^0 dt.$$

4.4.3 Final Γ -liminf

Proposition 4.20. *Let $\mu : \mathcal{A}(\mathbb{R}^2) \rightarrow [0, +\infty)$ be an open-set function, superadditive on open sets with disjoint compact closures (i.e. $\mu(A \cup B) \geq \mu(A) + \mu(B)$ if $\overline{A} \cap \overline{B} = \emptyset$, $\overline{A} \cup \overline{B} \subset\subset \Omega$). Let $\lambda \in \mathcal{M}_+(\mathbb{R}^2)$, and ψ_i be positive Borel functions such that $\mu(A) \geq \int_A \psi_i d\lambda$, for every $A \in \mathcal{A}(\mathbb{R}^d)$. We define $\psi(x) := \sup_i \psi_i(x)$. Then*

$$\mu(A) \geq \int_A \psi(x) d\lambda \quad \forall A \in \mathcal{A}(\mathbb{R}^d).$$

Proof. See for example [13, Lemma 15.2]. ■

Theorem 4.21 (Γ - liminf of phase field functional). *Let $\mu^+, \mu^- \in \mathcal{P}(\overline{\Omega})$ be admissible source and sink, it holds*

$$\Gamma - \liminf E_D \geq E$$

with respect the weak- $\star$ topology in $\mathcal{M}(\Omega)$ and the strong convergence in $L^1(\Omega)$.

Proof. Let $(q, u) \in \mathcal{M}(\Omega; \mathbb{R}^2) \times L^1(\Omega)$, and let $\{(q_D, u_D)\}$ be a sequence that converges to it in the considered topology. We extend both u and u_D to zero outside of Ω , and the measures q and q_D to zero on $\mathbb{R}^2 \setminus \overline{\Omega}$. Additionally, we extend the functionals E_D and E on the whole space $\mathbb{R}^2$ in the obvious way.

Without loss of generality, we assume that, up to a subsequence, the $\lim_{D \rightarrow 0} E_D[q_D, u_D]$ exists and it is finite. Indeed, if the limit should not be finite, the inequality would be trivial.

Let $C > 0$ be a constant such that

$$E_D[q_D, u_D; A] = D^{\frac{\gamma-1}{2}} \int_{\Omega} \left(D^2 |\nabla u_D|^2 + c^2 \frac{|q_D|^2}{u_D^2} + \frac{u_D^{2\gamma}}{\gamma} \right) dx \leq C.$$

In particular, the uniform bound on $D^{\frac{\gamma-1}{2}} \int_{\Omega} \frac{u_D^{2\gamma}}{\gamma} dx$, gives that the sequence $\{u_D\}$ converges to zero in $L^{2\gamma}(\Omega)$, and thus in $L^1(\Omega)$, implying that $u = 0$.

Moreover, in order to ensure that the energies are finite, each q_D must satisfy the divergence constraint $\operatorname{div} q_D = S_D$. Its continuity under the weak- $\star$ convergence implies that q satisfies the constraint $\operatorname{div} q = S$.

Let $A \subset \mathbb{R}^2$ be an open and bounded set. The restriction of the functional to this set will be denoted by $E[\cdot, \cdot; A]$. Let $\xi \in S^1$ be fixed, from Fubini's decomposition theorem it follows

$$\begin{aligned} E_D[q_D, u_D; A] &= D^{\frac{\gamma-1}{2}} \int_{\Omega} \left(D^2 |\nabla u_D|^2 + c^2 \frac{|q_D|^2}{u_D^2} + \frac{u_D^{2\gamma}}{\gamma} \right) dx \\ &= D^{\frac{\gamma-1}{2}} \int_{-\infty}^{\infty} \int_{A^{\xi, t}} \left[D^2 |\nabla u_D|^2 + c^2 \frac{|q_D|^2}{u_D^2} + \frac{u_D^{2\gamma}}{\gamma} \right]^{\xi, t} dx dt \\ &\geq D^{\frac{\gamma-1}{2}} \int_{-\infty}^{\infty} \left(\int_{A^{\xi, t}} D^2 |(u_D)^{\xi, t}|^2 + c^2 \frac{|q_D^{\xi, t}|^2}{|u_D^{\xi, t}|^2} + \frac{|u_D^{\xi, t}|^{2\gamma}}{\gamma} dx \right) dt \\ &= \int_{-\infty}^{\infty} \mathcal{F}_D[q_D^{\xi, t}, u_D^{\xi, t}; A^{\xi, t}] dt. \end{aligned}$$

Fatou's lemma implies

$$\int_{-\infty}^{\infty} \liminf_{D \rightarrow 0} \mathcal{F}_D[q_D^{\xi,t}, u_D^{\xi,t}; A^{\xi,t}] dt \leq \liminf_{D \rightarrow 0} E_D[q_D, u_D; A].$$

Since we assumed the $\liminf_{D \rightarrow 0} E_D[q_D, u_D; A]$ to be bounded, for almost each $t \in \mathbb{R}$, it holds that $\liminf_{D \rightarrow 0} \mathcal{F}_D[q_D^{\xi,t}, u_D^{\xi,t}; A^{\xi,t}]$ is finite.

We recall that, as proved in Theorem 4.18, for almost every (ξ, t) , it holds

$$u_D^{\xi,t} \rightarrow u^{\xi,t} \quad \text{in } L^1(A^{\xi,t}), \quad q_D^{\xi,t} \xrightarrow{*} q^{\xi,t} \quad \text{in } \mathcal{M}(A^{\xi,t}).$$

Moreover, from Corollary 4.14 follows that for almost every (ξ, t) , the reduced functionals satisfy

$$\liminf_{D \rightarrow 0} \mathcal{F}_D[q_D^{\xi,t}, u_D^{\xi,t}; A^{\xi,t}] \geq \mathcal{F}[q^{\xi,t}, u^{\xi,t}; A^{\xi,t}].$$

We proceed by denoting

$$\kappa(A) := \liminf_{D \rightarrow 0} E_D[q_D, u_D; A],$$

and introducing the non-negative Borel measure

$$\lambda(A) := \int_{A \cap \Sigma_q} \tau(m_q) d\mathcal{H}^1.$$

Lastly, we fix a sequence of dense elements in S^1 denoted by $\{\xi_j\}$, and we introduce the sequence of $|q|$ -measurable Borel functions $\psi_j : \mathbb{R}^2 \rightarrow \mathbb{R}$, defined as

$$\psi_j := \left| \frac{q}{|q|} \cdot \xi_j \right|.$$

We point out that it holds

$$\int_A \psi_j d\lambda = \int_{A \cap \Sigma_q} \left| \frac{q}{|q|} \cdot \xi_j \right| \tau(\lambda_q) d\mathcal{H}^1.$$

Since q is a divergence measure vector field, it holds for a.e. ξ^j , and any $\alpha > 0$, that

$$\begin{aligned} \kappa(A) &\geq \int_{-\infty}^{\infty} \mathcal{F}[q_{\xi^j,t}, u_{\xi^j,t}; A_{\xi^j,t}] dt = \int_{-\infty}^{\infty} \int_{S_{q_{\xi^j,t}} \cap A_{\xi^j,t}} \tau(|m_{q_{\xi^j,t}}|) d\mathcal{H}^0 dt = \\ &= \int_{S \cap A} \tau(|\lambda_q|) \left| \frac{q}{|q|} \cdot \xi_j \right| d\mathcal{H}^1 \geq \int_A \psi_j d\lambda, \end{aligned}$$

where the last inequality is given by Remark 4.19. Finally, from Proposition 4.20 we get that, for every $A \subset \mathbb{R}^2$, it holds

$$\kappa(A) \geq \int_A \sup_j \psi_j d\lambda.$$

In particular, by choosing A as the 1-neighbourhood of Ω we obtain

$$\begin{aligned} \liminf_{D \rightarrow 0} \mathcal{E}_D[q_D, u_D; A] &\geq \int_A \sup_j \psi_j = \\ &= \int_{\Sigma_q \cap A} \tau(\lambda_q) d\mathcal{H}^1 = \mathcal{E}[q, u; A], \end{aligned}$$

concluding the proof. ■

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