EXTERIOR CALCULUS FOR DIFFUSION ON CHANNELS

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Abstract. REVISE We study diffusion processes in regions generated by "sliding" a cross section by the phase flow of vector filed on curved spaces of arbitrary dimension. We do this by studying the effective diffusion coefficient D that arises when trying to reduce the n-dimensional diffusion equation to a 1-dimensional diffusion equation by means of a projection method. We use the mathematical language of exterior calculus to derive a coordinate free formula for this coefficient in both infinite and finite transversal diffusion rate cases. The use of these techniques leads to a formula for D which provides a deeper understanding of effective diffusion than when using a coordinate dependent approach.

1. Introduction

Find all references of Valero, Kalinay and Perkus, Dagdug-Pineda.

EXPLAIN THE NEW THING IS WE DEAL WITH FDRC

The study of diffusion processes in channels have been studied extensively in the literature and have diverse applications: like in the study of artificial nanopores (see [3, 5, 7]) and in biological channels (see [2, 6, 1]). One of the important techniques used in this a projection method that tries to reduce the diffusion in equations in dimensions 2 and 3 to an equation (Fick-Jacobs equation) in 1 dimension (see)

Put REFERENCES COORDS SISTEMS HERE. In this paper we present a coordinate free formulation of the theory of effective diffusion on channels. For this purpose, we use modern tools from differential geometry that provide the following advantages:

(1) Our formulas hold for channels of any dimension in flat and curved spaces, and their geometric content is easier to interpret (see BLA) than when using a coordinate dependent approach. In particular, our work unifies the work for 2-dimensional and 3-dimensional channels in flat and curved spaces.
(2) We identify the Fick-Jacobs equation as a standard diffusion equation (see BLA). We do this by changing the metric in the variable that parameterize the cross sections of the channel, and modifying the definition of effective density function and effective diffusion coefficient that are used in most of the literature.

(3) Our formulas hold channels with cross sections of arbitrary shape; which has lead us to introduce the concepts of natural and imposed projection maps (see BLA). Curvilinear

FINITE AND INFINITE

WHICH ARE THE NEW CONTRIBUTIONS.

EXPLAIN WHY COORDINATE FREE IS GOOD: RIEMANNIAN MANIFOLDS, UNIFICATION OF ALL DIMENSIONS.

1.1. **Plan of the paper.**

The outline of the paper is as follows.

- In section 2 we will explain how to generate channels using vector fields on arbitrary spaces. These vector fields will provide us with cross sections for the generated channel, which will allow us to reduce the diffusion equation on a channel to a diffusion equation with only one spatial variable. We introduce the concepts of natural projection function and fields, which will provide us with the best selection of cross section when studying diffusion processes on channels. Finally, we introduce the concept of flux function of a vector field on a channel, which measure the flux a vector field across the cross section of a channel. These flux functions will be fundamental for writting the formulas for the effective diffusion coefficient in a coordinate free way.
- In section 3 we present formulas for the effective diffusion coefficient (both in the infinite and finite transversal diffusion rate cases) avoiding the use of the language exterior calculus, so that the main results can be understood in a non-technical manner. In fact, the main concept needed in our formulas is simply that of the flux of a vector field across a hyper-surface. We show that there is a special choice of cross section of a channel in which the formulas for the effective diffusion coefficient for the finite and infinite transversal rate cases coincide.
- In Section 4 TODO
- In Section 5 we use exterior calculus to deduce in a rigorous way the coordinate free formulas for the effective diffusion coefficients (presented in Section 3), and we will show how to recover the coordinate dependent formulas from the coordinate free ones.

2. Channel geometry through vector field flows

We will construct a channel-like structures $\mathcal{C}$ in $n-$dimensional space M[1]by the following procedure (see Figure 1). Let $\mathcal{S}_0 \subset M$ be a $(n-1)$-dimensional hyper-surface with boundary and let U be a vector field in M that does not vanish at any point in $\mathcal{S}_0$. For a given scalar u, let $\mathcal{S}_u$ be the hyper-surface obtained by "sliding" $\mathcal{S}_0$ for a duration of u along the *integral curves*[2] of U. We will refer to $\mathcal{S}_u$ as the cross section at u generated by U from $\mathcal{S}_0$. We will say that U generates the channel $\mathcal{C}$ if $\mathcal{C}$ is the union of all these cross sections. For a point x in $\mathcal{C}$ we will let $u(x)$ be equal to the time it takes for a point in $\mathcal{S}_0$ to reach x (by following an integral curve of U); so that $\mathcal{S}_s$ can be characterized as the set of points in $\mathcal{C}$ at

[1]Usually M stands for flat space of dimension either two or three, but our results hold for the general case where M is an arbitrary n-dimensional oriented Riemannian manifold.

[2]An integral curve of U is a curve $x = x(t)$ in M that satisfies $\frac{dx}{dt}(t) = U(x(t))$.

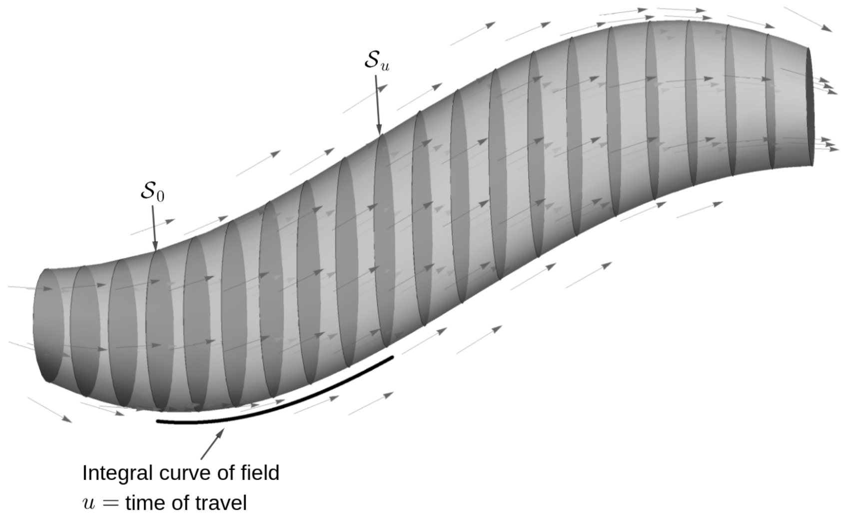

FIGURE 1. A channel $\mathcal{C}$ generated by "sliding" a cross section $\mathcal{S}_0$ along the integral curves of a vector field.

which $u(x) = s$. In this context, we will refer to u as a *projection function*[3] for $\mathcal{C}$. The projection function u is completely characterized the formula

$$\nabla u(x) \cdot U(x) = 1,$$

and the initial condition $u(x) = 0$ for all x in $\mathcal{S}_0$.

We will now illustrate the above concepts by considering *parametric channels.* These channels are constructed by using parametrization maps of the form $x = x(u, v)$, where u is a scalar and v belongs to some region in $(n-1)$-dimensional space. If we let $u(x)$ and $v(x)$ stand for the u and v coordinates of the point x in M, then the field

$$U(x) = \frac{\partial x}{\partial u}(u(x), v(x)) \tag{2.1}$$

generates our parametric channel and $u = u(x)$ is the projection function for this field. Consider the following example for M equal to the plane. Let $c = c(u)$ and $w = w(u)$ be scalar valued functions, which we will refer to as the center and width functions, and consider the channel $\mathcal{C}$ with parametrization map (see Figure 2)

$$x(u, v) = (u, c(u) + vw(u)) \text{ where } -1/2 \leq v \leq 1/2.$$

A simple calculation shows that the vector field 2.1 is given by the formula

$$U(x_1, x_2) = \left(1, c'(x_1) + \left(\frac{x_2 - c(x_1)}{w(x_1)}\right) w'(x_1)\right).$$

The function $u(x_1, x_2) = x_1$ is the projection function for this field, so that the cross section $\mathcal{S}_{x_1}$ is then line segment joining $(x_1, c(x_1) - w(x_1)/2)$ with $(x_1, c(x_1) + w(x_1)/2)$.

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[3]Depending on the context will think u as a scalar or as a function.

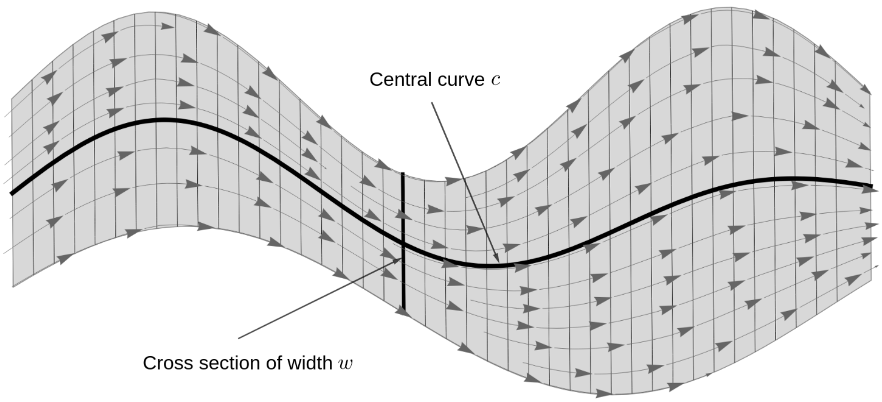
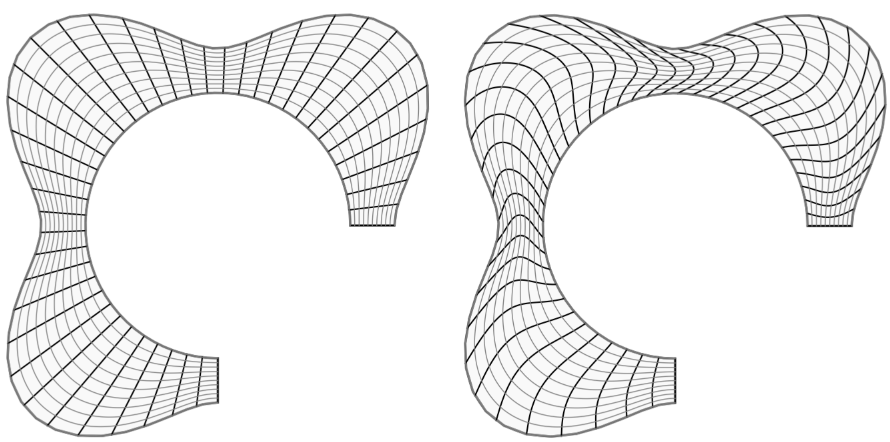


FIGURE 2. Parametric channel with center function $c = c(u)$ and width function $w = w(u)$.

The walls of a channel. We will distinguish between two types of walls in a channel $\mathcal{C}$, side walls and the reflective wall(s). In general, the side walls are two cross sections $\mathcal{A}$ and $\mathcal{B}$ which are at the extreme sides of $\mathcal{C}$. The reflective wall $\mathcal{W}$ consists of rest of border of $\mathcal{C}$ which are not side walls. When we study the diffusion equation in $\mathcal{C}$ we will assume reflective boundary condition on its reflective wall.



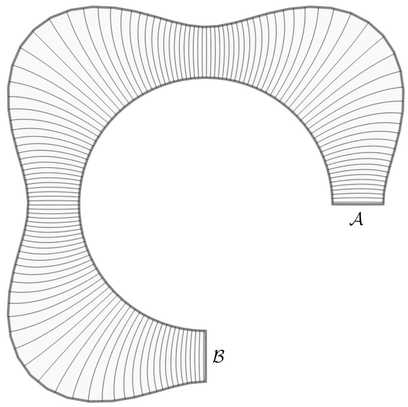
(A) (B)

FIGURE 3. Two sets of cross sections associated with two different generating vector fields of the same channel.

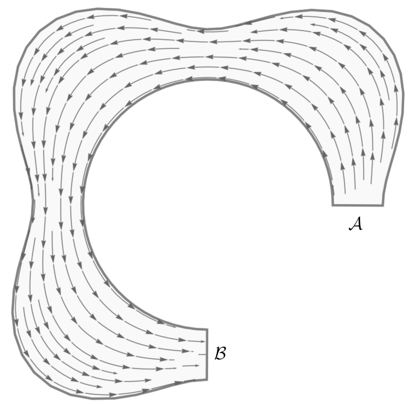
2.1. **Natural projections and fields.** A channel $\mathcal{C}$ can have many generating fields, which in general produce different sets of cross sections (see Figure 3). For a channel $\mathcal{C}$ with fixed side walls $\mathcal{A}$ and $\mathcal{B}$, we want to find a generating vector field U for $\mathcal{C}$ such that

(1) The side walls $\mathcal{A}$ and $\mathcal{B}$ are cross sections of $\mathcal{C}$ generated by U.

(2) The cross sections generated by U "fit" the geometry of $\mathcal{C}$ in a "natural way".



(A) Cross sections



(B) Generating vector field

FIGURE 4. Cross sections and generating field associated to a harmonic function h on a channel. This function takes the values 0 and 1 on $\mathcal{A}$ and $\mathcal{B}$ (respectively), and its gradient has no flux across the the reflective walls of the channel.

In Section 3.2 we will argue that the a vector field U that satisfies these two conditions can be constructed as follows. Let h be the harmonic function (i.e $\Delta h = 0$) on $\mathcal{C}$ such that ∇h has no flux across the reflective wall $\mathcal{W}$, and satisfies the boundary conditions

$$h(x) = \begin{cases} 0 & \text{if } x \text{ is in } \mathcal{A}, \\ 1 & \text{if } x \text{ is in } \mathcal{B}. \end{cases} \tag{2.2}$$

We will let (see Figure 4) $U = H$, where

$$H(x) = \nabla h(x)/||\nabla h(x)||^2. \tag{2.3}$$

This field generates the channel $\mathcal{C}$ and has h as projection function. We will refer to h as the *natural projection function* for $\mathcal{C}$ and the corresponding field H as the *natural generating field* for $\mathcal{C}$. Observe that h depends on the selection of side walls $\mathcal{A}$ and $\mathcal{B}$ for the channel $\mathcal{C}$.

2.2. **Flux functions.** In sections 3.1 and 3.2 we will show that the effective diffusion coefficient of a channel $\mathcal{C}$ can be expressed in terms of the flux of vector fields across its cross sections. The *flux function* of a vector field V in $\mathcal{C}$ is defined as [4]

$$\mathcal{F}_V(u) = \text{flux of } V \text{ across } \mathcal{S}_u.$$

Of particular interest are the flux functions of vector fields the form $V = \lambda U$, where U is a generating field of $\mathcal{C}$ and λ is a scalar valued function in $\mathcal{C}$. If we define (see Figure 5)

$$\mathcal{C}_{[u_0,u_1]} = \text{union of the sets } \mathcal{S}_u \text{ for } u_0 \le u \le u_1$$

[4]This is the integral (over $\mathcal{S}_u$) of the component of V normal to $\mathcal{S}_u$

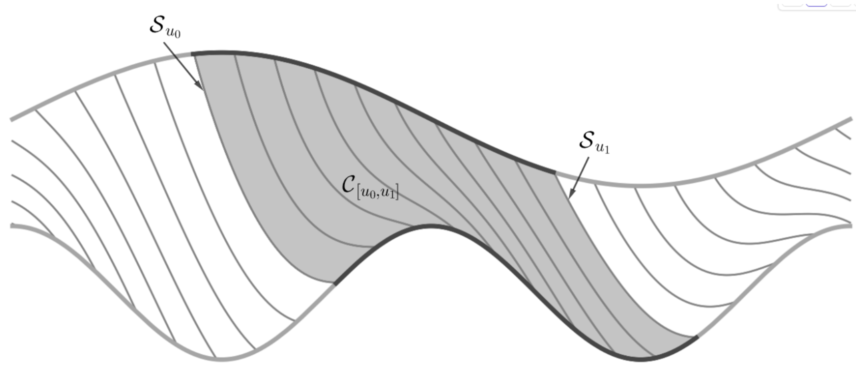


FIGURE 5. Channel region between two cross section

and the total concentration function [5] by

$$c_\lambda(u) = \text{total concentration of } \lambda \text{ in } \mathcal{C}_{[0,u]},$$

we have that

$$\frac{dc_\lambda}{du}(u) = \mathcal{F}_{\lambda U}(u).$$

In particular, if we let $\lambda = 1$ then $c_\lambda = \nu$ where

$$\nu(u) = \text{volume of } \mathcal{C}_{[0,u]},$$

and hence

$$\frac{d\nu}{du}(u) = \mathcal{F}_U(u).$$

An important property of the flux function, that we will use frequently, is that if we can write[6] $\lambda = \lambda(u)$ then

$$\mathcal{F}_{\lambda V}(u) = \lambda(u)\mathcal{F}_V(u)$$

3. EFFECTIVE DIFFUSION ON CHANNELS

We will now study the evolution of a density function $P = P(x, t)$ on a channel $\mathcal{C}$ and such that P obeys the diffusion equation

$$\frac{\partial P}{\partial t}(x, t) = D_0 \Delta P(x, t).$$

We will assume reflective boundary conditions on the reflective wall $\mathcal{W}$ of $\mathcal{C}$, i.e the gradient of P is tangential to $\mathcal{W}$. We will try to reduce the above equation to a diffusion equation in a 1-dimensional spatial variable. To do this, we define the *total concentration function* as

$$c(u, t) = \text{total concentration of density } P \text{ in } \mathcal{C}_{[0,u]} \text{ at time } t,$$

[5]The total concentration is obtained by integrating the function λ in the region $\mathcal{C}_{[0,u]}$.

[6]If we think of λ as a function of x (i.e $\lambda = \lambda(x)$) the expression $\lambda = \lambda(u)$ means that $\lambda(x) = \rho(u(x))$ for a scalar valued function $\rho = \rho(u)$ and $u = u(x)$ the projection function. Our notation has the advantage of avoiding the use the extra function ρ.

and the *effective concentration* as

$$p(u,t) = \frac{\partial c}{\partial u}(u,t)/\frac{d\nu}{du}(u),$$

where the *volume*[7] *function* is given by

$$\nu(u) = \text{volume of } \mathcal{C}_{[0,u]}. \tag{3.1}$$

If we let $u = u(\nu)$ be the value of u that corresponds to volume ν, so that $p(\nu, t) = p(u(\nu), t)$, then

$$p(\nu,t) = \frac{\partial c}{\partial \nu}(\nu,t).$$

Hence, the total concentration of P in the region $\mathcal{C}_{[u_1,u_2]}$ at time t is

$$\int_{\nu_1}^{\nu_2} p(\nu,t)d\nu \text{ for } \nu_i = \nu(u_i).$$

In most of the literature (i.e when studying the Fick-Jacobs equation) the effective concentration is defined as

$$p_f(u,t) = \frac{dc}{du}(u,t), \tag{3.2}$$

so that the total concentration of P in $\mathcal{C}_{[u_1,u_2]}$ is

$$\int_{u_1}^{u_2} p_f(u,t)du.$$

From a mathematical point of view this definition of the effective concentration is not convenient for the following reason. If we introduce a new variable $v = v(u)$, we have

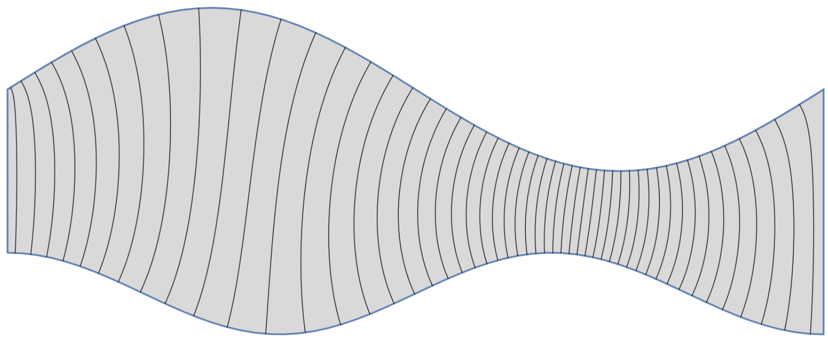
$$p_f(u,t) = \frac{dc}{du}(u,t) = \frac{dv}{du}(u)\frac{dc}{dv}(v(u),t) = \frac{dv}{du}(u)p_f(v(u),t),$$

which is the way vectors (not functions) transform under a change of variable. With our definition of effective concentration we have that

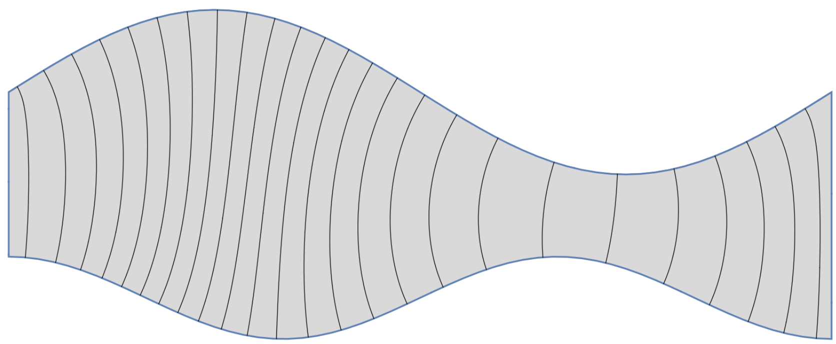
$$\begin{aligned}
p(u,t) &= \frac{\partial c}{\partial u}(u,t)/\left(\frac{d\nu}{du}(u)\right)\\
&= \left(\frac{\partial c}{\partial v}(v(u),t)\frac{dv}{du}(u)\right)/\left(\frac{d\nu}{dv}(v(u))\frac{dv}{du}(u)\right)\\
&= \frac{\partial c}{\partial v}(v(u),t)\frac{d\nu}{dv}(v(u))\\
&= p(v(u),t),
\end{aligned}$$

which the proper formula for the change of variable of a function. Furthermore, if the density function P is constant along the cross sections of the channel then (see Section 5.4)

$$p(u(x),t) = P(x,t).$$



(A) Equidistant cross sections with standard metric on the u variable.



(B) Equidistant cross sections with the volume metric. The regions between consecutive cross sections have equal volume.

FIGURE 6. Two parametrization of the cross sections of a channel with harmonic projection map u

The volume metric. As we progress in our work, we will show that the natural way of measuring the distance between two cross section $\mathcal{S}_{u_1}$ and $\mathcal{S}_{u_2}$ is defined by the formula (see Figure 6)

$$\text{distance}(\mathcal{S}_{u_1}, \mathcal{S}_{u_2}) = \text{volume of } (\mathcal{C}_{[u_1,u_2]}) = \nu(u_2) - \nu(u_1).$$

We can also write this formula as

$$\text{distance}(\mathcal{S}_{u_1}, \mathcal{S}_{u_2}) = \int_{u_1}^{u_2} \sqrt{g(u)}du,$$

where the *volume metric* g is defined by

$$g(u) = \left(\frac{d\nu}{du}(u)\right)^2. \tag{3.3}$$

[7]When we speak of volume in n-dimensional space we are referring to n-dimensional volume, i.e length for $n = 1$, area for $n = 2$, etc.

The expressions for the gradient ∇ and divergence $\nabla\cdot$ operators with respect to this volume metric are[8]

$$\nabla p = \frac{1}{g}\frac{\partial p}{\partial u} \text{ and } \nabla \cdot j = \frac{1}{\sqrt{g}}\frac{\partial}{\partial u}\left(\sqrt{g}j\right). \tag{3.4}$$

We will need these formulas when we study the effective diffusion equation on a channel. Observe that if we let $u = \nu$ then $g = 1$ and

$$\nabla p = \frac{\partial p}{\partial \nu} \text{ and } \nabla \cdot j = \frac{\partial j}{\partial \nu}.$$

3.1. **Infinite transversal diffusion rate.** Let us assume that the density function P stabilizes infinitely fast along the cross sections $\mathcal{S}_u$ of a channel $\mathcal{C}$; which is equivalent to P being constant along each of the $\mathcal{S}_u$'s. Under these conditions, the following *effective diffusion equation*[9] holds (see Section 5.4)

$$\frac{\partial p}{\partial t}(u,t) = \nabla \cdot (\mathcal{D}(u)\nabla p(u,t)), \tag{3.5}$$

where the *effective diffusion coefficient*[10] is given by

$$\mathcal{D}(u) = D_0 \mathcal{F}_{\nabla u}(u)\frac{d\nu}{du}(u). \tag{3.6}$$

The effective diffusion coefficient $\mathcal{D}$ connects the *effective flux*

$$j(u,t) = \mathcal{F}_{J_t}(u)/\frac{d\nu}{du}(u) \text{ where } J_t = D_0 \nabla P_t$$

with the gradient of the effective density function. More concretely, *Fick's first law* establishes that (see sections 5.3 and 5.4)

$$j(u,t) = -\mathcal{D}(u)\nabla p(u,t).$$

In the volume variable ν we have

$$j(\nu,t) = -\mathcal{D}(\nu)\frac{\partial p}{\partial \nu}(\nu,t).$$

Cross section density function. We will now re-write formula 3.6 in a different way, so that we can clarify its geometrical meaning. If we define the area[11] function as

$$\mathcal{A}(u) = \text{area of } \mathcal{S}_u$$

and let

$$\mathcal{G}(u) = \frac{\mathcal{F}_{\nabla u}(u)}{\mathcal{A}(u)},$$

then we can write

$$\mathcal{D}(u) = D_0 \mathcal{A}(u)\mathcal{G}(u)\frac{d\nu}{du}(u). \tag{3.7}$$

[8]When we change the way we measure distances this has to be reflected in the formulas for the divergence and gradient.

[9]The gradient and divergence operators used in formula 3.5 are the ones associated with the volume metric g (see Formulas 3.4)

[10]The gradient operator that appears in formula 3.6 is the one associated to the metric in M.

[11]We refer to area as $(n-1)$-dimensional area. For $n = 2$ this means length, for $n = 3$ this means area in the usual sense, etc. By convention we speak of volume when we want to measure the "extent" of n-dimensional objects in n-dimensional space, and area when we want to measure the "extent" of $(n-1)$-dimensional objects in n-dimensional space.

The vector field ∇u is orthogonal to the cross sections $\mathcal{C}$ (since the cross sections of $\mathcal{C}$ are contained in the level sets of u). Hence, if we orient the cross sections $\mathcal{S}_u$ so that their normal fields have the same direction as ∇u, we have that

$$\mathcal{G}(u) = \text{average value of } |\nabla u| \text{ on } \mathcal{S}_u.$$

This number measures the average density of cross sections near $\mathcal{S}_u$, and we will refer to $\mathcal{G}$ as the *cross section density function* (see Figure 4). If the cross sections of the channel are parametrized by the volume variable ν, we have that

$$\mathcal{D}(\nu) = D_0 \mathcal{A}(\nu)\mathcal{G}(\nu)$$

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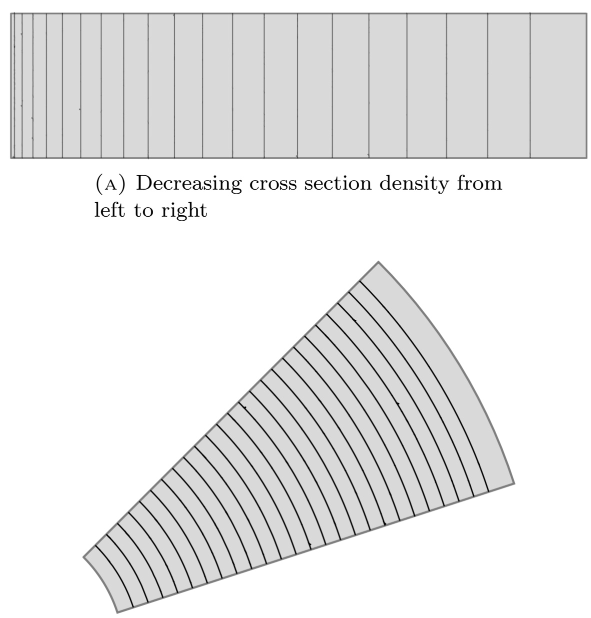

(A) Decreasing cross section density from left to right

(B) Constant cross section density

FIGURE 7. Two channels with different cross section density functions

Comparison with the generalized Fick-Jacobs equation. If we let

$$\sigma(u) = \frac{d\nu}{du}(u) \text{ and } p_f(u,t) = \frac{dc}{du}(u,t),$$

we can write equation 3.5 as a *generalized Fick-Jacobs equation*

$$\frac{dp_f}{dt}(u,t) = \frac{\partial}{\partial u}\left(\sigma(u)\mathcal{D}_f(u)\frac{\partial}{\partial u}\left(\frac{p_f(u,t)}{\sigma(u)}\right)\right), \tag{3.8}$$

where the effective diffusion coefficient is given by

$$\mathcal{D}_f(u) = \frac{D_0 \mathcal{F}_{\nabla u}(u)}{\sigma(u)}.$$

The effective flux

$$j_f(u,t) = \mathcal{F}_{J_t}(u,t)$$

obeys the continuity equation (see 5.3)

$$\frac{\partial p_f}{\partial t} + \frac{\partial j_f}{\partial u} = 0.$$

From the generalized Fick-Jacobs equation we conclude that

$$j_f = -\sigma \mathcal{D}_f \frac{\partial}{\partial u}\left(\frac{p_f}{\sigma}\right).$$

From the above equations and the formulas

$$p = p_f/\sigma \text{ and } j = j_f/\sigma$$

we obtain

$$j(u,t) = -\mathcal{D}_f(u)\frac{\partial p}{\partial u}(u,t).$$

We conclude that the difference between the effective diffusion coefficient in the generalized Fick-Jacobs equation and ours is that: in the first case the gradient we use in Fick's first law is that associated to the metric $g = 1$, and in the second case it is that associated to the metric $g(u) = \sigma(u)^2$. We can relate both coefficients through the formula

$$\mathcal{D}_f(u) = \frac{\mathcal{D}(u)}{\sigma(u)^2}.$$

Observe that when the cross sections of $\mathcal{C}$ are parametrized by the volume variable ν we have that $\sigma(\nu) = 1$, and hence

$$\mathcal{D}_f(\nu) = \mathcal{D}(\nu) = D_0 \mathcal{F}_{\nabla \nu}(\nu).$$

In this case both the effective diffusion equation and the Fick-Jacobs equation become the diffusion equation

$$\frac{\partial p}{\partial t}(\nu,t) = \frac{\partial}{\partial \nu}\left(\mathcal{D}(\nu)\frac{\partial p}{\partial \nu}(\nu,t)\right).$$

3.2. **Finite transversal diffusion rate.** We will now drop the assumption that the density function $P = P(x,t)$ stabilizes infinitely fast along the cross sections of a channel. Let us assume that the channel $\mathcal{C}$ is generated by a vector field U and let u be a projection function for this field. Let H and h be a natural field and projection for $\mathcal{C}$ (see section 2.1), where we chose the side walls of $\mathcal{C}$ to be of the form $\mathcal{A} = \mathcal{S}_{u_0}$ and $\mathcal{B} = \mathcal{S}_{u_1}$(for $u_0 < u_1$). We will refer to the projection function u and the field U as the *imposed projection function and field* (to distinguish them from the natural ones: h and H).

Let ρ be the effective concentration function of h under the projection map u, i.e

$$\rho(u) = \mathcal{F}_{hU}(u)/\frac{d\nu}{du}(u).$$

In section 5.5 we deduce the following formula for the effective diffusion coefficient for the finite transversal diffusion rate case

$$\mathcal{D}(u) = \mathcal{J}\left(\frac{d\nu}{du}(u)\right)^2 / \mathcal{F}_{\lambda U}(u) \tag{3.9}$$

where $\lambda = \lambda(x)$ is a scalar valued function in $\mathcal{C}$ defined by[12]

$$\lambda = \nabla h \cdot U + (h - \rho \circ u)\nabla \cdot U \tag{3.10}$$

and the constant $\mathcal{J}$ is given by[13]

$$\mathcal{J} = D_0 \mathcal{F}_{\nabla h}(u_0).$$

Channels with natural projection map. If we choose the imposed projection function and field to be the natural ones, i.e

$$U = H \text{ and } u = h,$$

then we have that

$$\nabla h \cdot U = \frac{\nabla h \cdot \nabla h}{||\nabla h||^2} = 1.$$

If we use the formula

$$\frac{d\nu}{du}(u) = \mathcal{F}_U(u)$$

we obtain

$$\begin{aligned} \rho(u(x)) &= \mathcal{F}_{hU}(u(x)) / \frac{d\nu}{du}(u(x)) \\ &= h(x)\mathcal{F}_U(u(x)) / \frac{d\nu}{du}(u(x)) \\ &= h(x). \end{aligned}$$

Hence $\lambda = 1$ in formula 3.10, which implies

$$\mathcal{D}(u) = \mathcal{J}\left(\frac{d\nu}{du}(u)\right)^2 (\mathcal{F}_U(u))^{-1} = D_0 \mathcal{F}_{\nabla u}(u)\frac{d\nu}{du}(u).$$

We conclude that *if the imposed projection function and field are the natural the natural ones, then the formulas for the effective diffusion coefficient in the finite and infinite diffusion transversal rate cases coincide.*

4. Effective diffusion for channels of constant width on the sphere

We will now review some basic concepts on spherical geometry that we will need for the computation the effective diffusion coefficients for channels on a sphere. Let $M = S_R^2$ be the sphere of radius R centered at $(0,0,R)$, defined by the equation $x_1^2 + x_2^2 + (x_3 - R)^2 = R^2$. The unit normal at a point $x \in S_R^2$ is the vector $N(x) = (x - (0,0,R))/R$. We can identify S_R^2 with $\mathbb{R}^2 \cup \{\infty\}$ by using the *stereographic projection map*

$$(x_1, x_2, x_3) \mapsto \left(\frac{2R}{2R - x_3}\right)(x_1, x_2),$$

[12]The gradient and divergence operator appearing in this formula are computed with respect to the metric in M.

[13]In fact, the function $u \mapsto D_0\mathcal{F}_{\nabla h}(u)$ is a constant function (see Section 5.5)

whose inverse is the parametrization map

$$(x,y) \mapsto \lambda_R(x,y)\left(x, y, \frac{x^2+y^2}{2R}\right) \text{ where } \lambda_R(x,y) = \left(\frac{4R^2}{4R^2+x^2+y^2}\right).$$

The metric tensor and volume form in S_R^2 can then be written in (x,y)-coordinates as

$$g_R(x,y) = \lambda_R^2(x,y)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \lambda_R^2(x,y)dx \wedge dy.$$

Remark 1. Observe that

$$\lim_{R\mapsto\infty} g_R = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \lim_{R\mapsto\infty} \mu_R = dx \wedge dy.$$

Hence we can recover $\mathbb{R}^2$ as a flat space by letting $R \mapsto \infty$, and we will write

$$g_\infty = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \mu_\infty = dx \wedge dy.$$

4.1. **Effective diffusion on an annulus.** Consider an *annular channel* $\mathcal{A} \subset S_R^2$ defied by (see Figure 8)

$$\mathcal{A} = \{(x_1, x_2, x_3) \in S_R^2 | h_1 \le x_3 \le h_2\},$$

where

$$h_i = R + R\sin(\omega_i) \text{ for } -\pi/2 < \omega_1 < \omega_2 < \pi/2.$$

The border of $\mathcal{A}$ consists of two circles $C_{\omega_1}, C_{\omega_2} \subset S_R^2$, where

$$C_\omega = \{(x_1, x_2, R + R\sin(\omega)) \in \mathbb{R}^3 | \sqrt{x_1^2+x_2^2} = R\cos(\omega)\} \tag{4.1}$$

The stereographic projection of C_ω is a circle in $\mathbb{R}^2$ that is centered at the origin and has radius

$$r(\omega) = \frac{2R\cos(\omega)}{1-\sin(\omega)}. \tag{4.2}$$

Hence, the stereographic projection of $\mathcal{A}$ in the $(x,y)-$plane is the annuls A defined by the inequalities

$$r_1 \le \sqrt{x^2+y^2} \le r_2 \text{ where } r_i = r(\omega_i).$$

The set A is the representation of $\mathcal{A}$ in (x,y)-coordinates.

The effective diffusion coefficient. The functions

$$u(x,y) = \arg(x,y) \text{ and } v(x,y) = \frac{1}{2}\log(x^2+y^2)$$

are conjugate harmonic[14], and we can use u as a natural projection function for $\mathcal{A}$. The metric tensor g_R can be written u,v-coordinates as

$$g_R(u,v) = \left(\frac{4R^2e^v}{e^{2v}+4R^2}\right)^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

[14]They are conjugate harmonic in $\mathbb{R}^2$ since they satisfy the Cauchy-Riemann equations, and they are harmonic in $S_R^2 - \{(0,0,R)\}$ since stereographic projection maps this spaces conformally onto $\mathbb{R}^2$.

and the volume form μ_R as

$$\mu_R(u,v) = \left(\frac{4R^2 e^v}{e^{2v}+4R^2}\right)^2 du \wedge dv.$$

We conclude that (see formula 5.11)

$$\frac{d\nu}{du}(u) = \int_{\log(r(\omega_1))}^{\log(r(\omega_2))} \mu_R dv = \left[-\frac{8R^4}{e^{2v}+4R^2}\right]_{\log(r(\omega_1))}^{\log(r(\omega_2))} = R^2(\sin(\omega_2)-\sin(\omega_1)).$$

Using the fact that v is conjugate harmonic to u we obtain (see Formula 5.10)

$$\mathcal{F}_{\nabla u} = \log(r(\omega_2)/r(\omega_1)),$$

and hence

$$\mathcal{F}_{\nabla u} = \log\left(\frac{\cos(\omega_2)(1-\sin(\omega_1))}{\cos(\omega_1)(1-\sin(\omega_2))}\right).$$

Since u is a natural projection function for $\mathcal{A}$, the effective diffusion coefficient $\mathcal{D}$ for $\mathcal{A}$ in the infinite and finite transversal diffusion coincide. Hence, we can compute $\mathcal{D}$ using formula 3.6 to obtain

$$\mathcal{D} = D_0 R^2(\sin(\omega_2)-\sin(\omega_1))\log\left(\frac{\cos(\omega_2)(1-\sin(\omega_1))}{\cos(\omega_1)(1-\sin(\omega_2))}\right).$$

4.2. **Channels of constant width.** A channel of constant width is made up of segments of great circles of constant length. More precisely, let $\alpha = \alpha(u)$ be a curve in S^2_R and consider a fixed number $w > 0$. For any given u, let $\mathcal{S}_u$ be the segment of great circle[15] of length w that has mid point $\alpha(u)$ and that intersects α perpendicularly at that point (see Figure 9). The union of all the cross sections $\mathcal{S}_u$'s is a channel $\mathcal{C}$ of constant width w over the curve α. If we let

$$\beta(u) = \alpha(u) - (0,0,R),$$
$$\beta_\perp(u) = \beta(u) \times \left(\frac{d\alpha}{du}(u) \Big/ \left|\frac{d\alpha}{du}(u)\right|\right),$$

then we can parametrize $\mathcal{C}$ as

$$p(u,v) = (0,0,R) + \cos(v)\beta(u) + \sin(v)\beta_\perp(u) \text{ for } -\frac{w}{2R} \le v \le \frac{w}{2R},$$

We will now compute the effective diffusion coefficient of a channel of constant width by using an approximation technique by Kalinay and Percus (described in [4]). In our case, the application of this technique consists in approximating $\mathcal{C}$ (at a cross sections $\mathcal{S}_u$) with an annular channel $\mathcal{A}_u$ (see Figure 10). The effective diffusion coefficient $\mathcal{D}(u)$ of $\mathcal{C}$ will then be equal to effective diffusion coefficient of $\mathcal{A}_u$, which we already computed in the previous section.

[15]A great circle on S^2_R is obtained by intersecting a plane through the origin in 3-dimensional space with S^2_R; great circles in S^2_R are geodesics.

Computation of the effective diffusion coefficient. The computation of the effective diffusion coefficient for a channel of constant width depends on the concept of *geodesic curvature*[16] of a curve on surface. We review this concept briefly. Consider an oriented surface $S \subset \mathbb{R}^3$ and let $N = N(p)$ be the unit tangent field to S compatible with its orientation. Let $p = p(s)$ be a curve on S, where s is the arc-length parameter of the curve. The tangent vector

$$T(s) = \frac{dp}{ds}(s)$$

is unitary, and hence

$$\frac{dT}{ds}(s) \cdot T(s) = 0 \text{ for all } s.$$

This conditions implies that we can find scalar valued functions $\lambda = \lambda(s)$ and $\kappa = \kappa(s)$ such that

$$\frac{dT}{ds}(s) = \lambda(s)N(p(s)) + \kappa(s)N(p(s)) \times T(s)$$

where the function

$$\kappa(s) = \frac{dT}{ds}(s) \cdot (N(s)) \times T(s)) \text{ for } N(s) = N(p(s))$$

is known as the geodesic curvature of the curve $p = p(s)$ on the surface S. For a curve $p = p(t)$ not necessarily parametrized by arc-length, we have that

$$\frac{d^2p}{dt^2} = \left(\frac{ds}{dt}\right)^2 \frac{d^2p}{ds^2} + \frac{d^2s}{dt^2}\frac{dp}{ds} = \left(\frac{ds}{dt}\right)^2 \frac{dT}{ds} + \frac{d^2s}{dt^2}T,$$

and hence

$$\kappa = \left(\frac{dp}{dt} \cdot \frac{dp}{dt}\right)^{-3/2} \frac{d^2p}{dt^2} \cdot \left(N \times \frac{dp}{dt}\right) \text{ where } N(t) = N(p(t)).$$

The circle C_ω defined in 4.1 has parametrization

$$t \mapsto (R\cos(\omega)\cos(t), R\cos(\omega)\sin(t), R(1 + \sin(\omega)),$$

from which we obtain that

$$\kappa(\omega) = \tan(\omega)/R,$$

which has as inverse function

$$\omega(\kappa) = \arctan(R\kappa).$$

For a fixed u, we can assume without loss of generality that the vector

$$\frac{d\alpha}{du}(u) \times \frac{d^2\alpha}{du^2}(u)$$

is parallel to the z-axis, since can always achieve this by a rotation in $\mathbb{R}^3$. A circle in S^2_R is the intersection of a plane in $\mathbb{R}^3$ with S^2_R. The circle $C_{\omega(\kappa(u))}$ is the one that best approximates the curve α at $\alpha(u)$; among all the circles in S^2_R that contain

[16]The geodesic curvature is a measure of how far a curve is from being a geodesic on a surface

$\alpha(u)$ and that are tangent to α at that point. Let $\mathcal{A}_u$ be the annulus delimited by the circles $C_{\omega_1(u)}$ and $C_{\omega_2(u)}$, where

$$\omega_1(u) = \arctan(R\kappa(u)) - \frac{w}{2R}, \tag{4.3}$$

$$\omega_2(u) = \arctan(R\kappa(u)) + \frac{w}{2R}. \tag{4.4}$$

By construction $\mathcal{A}_u$is the annulus of width w that best approximates $\mathcal{C}$ at the cross section $\mathcal{S}_u$. Hence, the effective diffusion coefficient for $\mathcal{C}$ is

$$\mathcal{D}_R(u) = D_0 R^2(\sin(\omega_2(u)) - \sin(\omega_1(u))) \log\left(\frac{\cos(\omega_2(u))(1-\sin(\omega_1(u)))}{\cos(\omega_1(u))(1-\sin(\omega_2(u)))}\right), \tag{4.5}$$

where $\omega_1 = \omega_1(u)$ and $\omega_2 = \omega_2(u)$ are defined by formulas 4.3 and 4.4, respectively.

4.3. **Examples.**

Channels of constant width over geodesics. If α is a geodesic we have that $\kappa(u) = 0$ for all u, and hence

$$\omega_1 = -\frac{w}{2R} \text{ and } \omega_2 = \frac{w}{2R}.$$

We conclude that $\mathcal{D}_R$ is constant with value

$$\mathcal{D}_R = 2D_0R^2 \sin\left(\frac{w}{2R}\right) \log\left(\frac{1+\sin\left(\frac{w}{2R}\right)}{1-\sin\left(\frac{w}{2R}\right)}\right).$$

Observe that

$$\lim_{R\mapsto\infty} \mathcal{D}_R = w^2.$$

Flat channels of constant width. The function r defined by 4.2 has inverse

$$\omega(r) = \arctan\left(\frac{r^2-4R^2}{4Rr}\right)$$

so that

$$\sin(\omega(r)) = \frac{r^2-4R^2}{r^2+4R^2} \text{ and } \cos(\omega(r)) = \frac{4Rr}{r^2+4R^2}.$$

From these formulas we obtain

$$\lim_{R\mapsto\infty} R^2(\sin(\omega(r_2)) - \sin(\omega(r_1))) = \frac{1}{2}(r_1+r_2)(r_2-r_1)$$

and

$$\lim_{R\mapsto\infty} \log\left(\frac{\cos(\omega(r_2))(1-\sin(\omega(r_1)))}{\cos(\omega(r_1))(1-\sin(\omega(r_2)))}\right) = \log(r_2/r_1).$$

Since the flat space $\mathbb{R}^2$ is equal S^2_∞ (i.e the limiting case of S^2_R when $R\mapsto\infty$), we conclude that the effective diffusion coefficient of a flat annulus is given by

$$\mathcal{D} = D_0\frac{r_1+r_2}{2}(r_2-r_1)\log(r_2/r_1),$$

where r_1 and r_2 are the inner outer radii of the annulus. If we let

$$r_1 = r_0 - w/2 \text{ and } r_2 = r_0 + w/2$$

we obtain

$$\mathcal{D} = D_0 w r_0 \log\left(\frac{r_0+w/2}{r_0-w/2}\right).$$

Consider a channel of constant width w over a planar curve $\alpha = \alpha(s)$, where s is its arc-length parameter. In this case the Kalinay and Percus approximation technique leads to $r_0(s) = 1/\kappa(s)$, where $\kappa(s)$ is the curvature of α at s. We conclude that

$$\mathcal{D}(s) = D_0 \frac{w}{\kappa(s)} \log\left(\log\left(\frac{1+\kappa(s)w/2}{1-\kappa(s)w/2}\right)\right).$$

To obtain the effective diffusion coefficient $\mathcal{D}_f$ in the Fick-Jacobs equation 3.8 we have to divide $\mathcal{D}$ by

$$\left(\frac{d\nu}{ds}\right)^2 =?.$$

Hence.

$$\mathcal{D}_f(s) = D_0 \frac{1}{w\kappa(s)} \log\left(\frac{1+\kappa(s)w/2}{1-\kappa(s)w/2}\right).$$

We derived this formula in [8] in a different way.

Spiral. JUST PLOT KAPPA AND D.

5. Derivation of the effective diffusion coefficient formula

Let M be an oriented Riemannian manifold of dimension n. We are interested in the diffusion equation

$$\frac{\partial P}{\partial t}(x,t) = \nabla \cdot (D(x)\nabla P(x,t)),$$

where $P : M \times \mathbb{R} \to \mathbb{R}$ is a time dependent function in M and $D(x) : T_xX \to T_xX$ is a linear map for every x in M. The divergence and gradient operators in the above formula can expressed in terms of exterior algebra operations as

$$\nabla \cdot J = *d * J^\flat \text{ and } \nabla P = (dP)^\#,$$

where $d : \bigwedge^k M \to \bigwedge^{k+1} M$ is the exterior derivative, $* : \bigwedge^k M \to \bigwedge^{n-k} M$ is the Hodge star operator, and the musical isomorphisms $\sharp$ and $\flat$ allow us to identify 1-forms and vector fields. If we let g stand for the metric tensor in M and use local coordinates $x_1, \ldots x_n$, we can write

$$\nabla \cdot J = \frac{1}{|g|^{1/2}} \sum_{i=1}^n \frac{\partial}{\partial x_i}\left(|g|^{1/2} J_i\right) \text{ where } |g| = \det(g)$$

for

$$J = \sum_{i=1}^n J_i \frac{\partial}{\partial x_i},$$

and

$$(\nabla P)^i = \sum_{j=1}^n g^{ij} \frac{\partial P}{\partial x_j} \text{ where } (g^{ij}) = (g_{ij})^{-1}.$$

.

In a homogeneous and isotropic medium the diffusion has the form

$$\frac{\partial P}{\partial t}(x,t) = D_0 \Delta P(x,t) \text{ where } \Delta = *d*d \text{ and } D_0 \in \mathbb{R}. \tag{5.1}$$

5.1. **Channels and projection functions.** We will say that $\mathcal{C} \subset M$ is generated by a vector field U, if $\mathcal{C}$ is the union of phase curves of U that have transversal intersection with an $(n-1)$-dimensional compact sub-manifold with boundary $\mathcal{S}_0$. The projection function $u : \mathcal{C} \to \mathbb{R}$ for the field U is defined by the conditions $u(x) = 0$ for all $x \in \mathcal{S}_0$ and $du(U(x)) = 1$ for all $x \in \mathcal{C}$. If $x = x(t)$ is a solution of $\dot{x} = U(x)$ with $x(0) \in \mathcal{S}_0$ then we have that

$$u(x(t)) = \int_0^t du(x(t))\dot{x}(t) = t.$$

In other words, for any $x \in \mathcal{C}$ the scalar $u(x)$ is the time it take for an integral curve of U to reach x from $\mathcal{S}_0$. The cross section $\mathcal{S}_s$ of $\mathcal{C}$ at s is defined by the formula

$$\mathcal{S}_s = u^{-1}(s).$$

Recall that the phase flow $\{\varphi_s : \mathcal{C} \to \mathcal{C}\}_{s\in\mathbb{R}}$ of U is defined by

$$\left.\frac{d}{ds}\right|_{s=0} (\varphi_s(x)) = U(x),$$

and satisfies

$$\varphi_{s_1+s_2} = \varphi_{s_1} \circ \varphi_{s_2}. \tag{5.2}$$

For any $x \in \mathcal{C}$ the condition $du(U) = 1$ implies

$$u(\varphi_s(x)) = u(x) + s,$$

and hence

$$\mathcal{S}_{s+h} = \varphi_h(\mathcal{S}_s).$$

If we let $\mathcal{W} = \partial\mathcal{C}$ then $\mathcal{W}$ is the union of phase curves of U that intersect $\partial\mathcal{S}_0$. We will refer to $\mathcal{W}$ as the reflective wall of $\mathcal{C}$. We define

$$\mathcal{C}_{[s_1,s_2]} = u^{-1}([s_1, s_2]) \text{ and } \mathcal{W}_{[s_1,s_2]} = \mathcal{W} \cap \mathcal{C}_{[s_1,s_2]}.$$

Flux functions. Let $\mu \in \bigwedge^n M$ be the global volume form associated with the metric in M. The orientation in a channel $\mathcal{C}$ will be the one induced by the orientation of M. If we let $\iota_U : \Lambda^k M \to \Lambda^{k-1} M$ be the interior derivative with respect to U, we have the identity

$$\iota_U(\mu) = *U^\flat,$$

and hence

$$du \wedge \iota_U(\mu) = du \wedge (*U^\flat) = < du, U^\flat > \mu = du(U)\mu = \mu. \tag{5.3}$$

If $i_u : \mathcal{S}_u \to \mathcal{C}$ is the inclusion map then $i_u^*(\iota_U(\mu))$ is an $(n-1)$-form in $\mathcal{S}_u$ which vanishes no-where in $\mathcal{S}_u$. We will use this form as an orientation form for $\mathcal{S}_u$. For a vector field V in $\mathcal{C}$ we define the flux function $\mathcal{F}_V : \mathbb{R} \to \mathbb{R}$ as

$$\mathcal{F}_V(u) = \int_{\mathcal{S}_u} \iota_V(\mu) = \int_{\mathcal{S}_u} *(V^\flat).$$

In particular

$$\mathcal{F}_{\nabla P}(u) = \int_{\mathcal{S}_u} *(dP).$$

Change of variable formulas. Let $u : \mathcal{C} \to \mathbb{R}$ be the projection function for U and $f : \mathbb{R} \to \mathbb{R}$ a function with positive derivative and such that $f(0) = 0$. If we let $v = f \circ u$ then

$$dv(x) = f'(u(x))du(x).$$

Hence, if we let $V(x) = U(x)/f'(u(x))$ then $dv(x)(V(x)) = 1$ for all $x \in \mathcal{S}_0$ and $v(x) = 0$ for all $x \in \mathcal{S}_0$, i.e v the projection function for the field V. To simplify notation, we will write the conditions $v = f \circ u$ and $u = f^{-1} \circ v$ as

$$v = v(u) \text{ and } u = u(v),$$

where in the first equation u is seen as a scalar value and v as a function, and on the second formula v is seen as a scalar value and u as a function. If we denote a cross sections at u as $\mathcal{S}_u$ and a cross section at v as $\mathcal{S}_v$, then the formulas $u^{-1}(s) = v^{-1}(f(s))$ and $v^{-1}(s) = u^{-1}(f^{-1}(s))$ can be simply written as $\mathcal{S}_u = \mathcal{S}_{v(u)}$ and $\mathcal{S}_v = \mathcal{S}_{u(v)}$. Furthermore, we have that

$$dv = \left(\frac{dv}{du}\right) du \text{ and } V = \left(\frac{dv}{du}\right)^{-1} U, \tag{5.4}$$

where

$$\frac{dv}{du}(x) = f'(u(x)).$$

5.2. **Some useful identities.** We will now derive some identities that will be useful in our study of effective diffusion on channels. Let $\mathcal{C}$ be a channel generated by a field U and with projection function u. In what follows we will make use of Cartan's magic formula

$$\mathcal{L}_U = \iota_U \circ d + d \circ \iota_U,$$

where $\mathcal{L}_U$ is the Lie derivative operator with respect to U.

Lemma 2. *If α is an $(n-1)$-form in $\mathcal{C}$ and we define*

$$f(u) = \int_{S_u} \alpha,$$

then

$$f'(u) = \int_{S_u} \mathcal{L}_U \alpha.$$

Furthermore, if ω is an n-form in $\mathcal{C}$ and for any $u_0 \in \mathbb{R}$ we define

$$g(u) = \int_{\mathcal{C}_{[u_0,u]}} \omega$$

then

$$g'(u) = \int_{S_u} \iota_U(\omega)$$

and

$$g''(u) = \int_{S_u} (d\lambda(U) + \lambda \nabla \cdot U)\, \iota_U(\mu) \text{ where } \lambda = *\omega.$$

Proof. From the formula $S_{u+h} = \varphi_h(S_u)$ we obtain

$$f(u+h) - f(u) = \int_{S_{u+h}} \alpha - \int_{S_u} \alpha = \int_{S_u} (\varphi_h^* \alpha - \alpha),$$

and hence

$$f'(u) = \lim_{h \mapsto 0} \int_{S_u} \frac{1}{h}(\varphi_h^*(\alpha) - \alpha) = \int_{S_u} \mathcal{L}_U \alpha.$$

To prove the second part of the lemma observe that

$$g(u+h) - g(u) = \int_{\mathcal{C}_{[u,u+h]}} \omega,$$

and hence

$$g'(u) = \lim_{h \mapsto 0} \frac{g(u+h) - g(u)}{h} = \lim_{h \mapsto 0} \frac{1}{h} \int_u^{u+h} \int_{\mathcal{S}_t} (\iota_U(\omega)) dt = \int_{\mathcal{S}_u} \iota_U(\omega).$$

Combining the previous results we obtain

$$g''(u) = \int_{S_u} \mathcal{L}_U(\iota_U(\omega)).$$

Using Cartan's magic formula it is easy to verify that

$$\mathcal{L}_U(\iota_U(\omega)) = \iota_U(\mathcal{L}_U(\omega)).$$

We can write $\omega = \lambda\mu$ for $\lambda = *\omega$, and hence

$$\mathcal{L}_U(\omega) = \mathcal{L}_U(\lambda\mu) = \iota_U(d\lambda)\mu + \lambda \mathcal{L}_U \mu.$$

Using this and the fact that $\mathcal{L}_U \mu = (\nabla \cdot U)\mu$, we conclude that

$$\iota_U(\omega) = (d\lambda(U) + \lambda(\nabla \cdot U))\iota_U(\mu)$$

□

5.3. **The effective continuity equation.** From now on we will assume that metric tensor in the u variable is

$$g(u) = \left(\frac{d\nu}{du}(u)\right)^2.$$

The divergence and gradient operators associated to this metric are given by the formulas

$$\nabla \cdot j = g^{-1/2} \frac{\partial}{\partial u}\left(g^{1/2} j\right) \text{ and } \nabla p = g^{-1} \frac{\partial p}{\partial u}.$$

Consider a concentration function $P = P(x,t)$ and the flux vector field $J = J(x,t)$ on the channel $\mathcal{C}$. Let us write $P_t(x) = P(x,t)$ and $J_t(x) = J(x,t)$, and define the *effective flux function* as

$$j(u,t) = \mathcal{F}_{J_t}(u) / \frac{d\nu}{du}(u) \text{ where } \mathcal{F}_{J_t} = \int_{\mathcal{S}_u} *J_t^\flat.$$

and the *effective concentration* as

$$p(u,t) = \frac{\partial c}{\partial u}(u,t) / \frac{d\nu}{du}(u) \text{ where } c(u,t) = \int_{\mathcal{C}_{[0,u]}} *P_t.$$

By Lemma 2 we have that

$$\frac{\partial c}{\partial u}(u,t) = \int_{\mathcal{S}_u} \iota_U(*P_t)$$

and

$$\frac{d\mathcal{F}_{J_t}}{du}(u) = \int_{\mathcal{S}_u} \mathcal{L}_U(*J_t^\flat) = \int_{\mathcal{S}_u} (d \circ \iota_U + \iota_U \circ d)(*J_t^\flat).$$

If we assume reflective boundary conditions on the wall $\mathcal{W}$ of $\mathcal{C}$, we have that

$$\int_{S_u} d(\iota_U(*J_t^\flat)) = \int_{\partial S_u} \iota_U(*J_t^\flat) = 0.$$

Using the above formulas and the continuity equation

$$*\frac{\partial P}{\partial t}(x,t) + d * J^\flat(x,t) = 0$$

we obtain

$$\frac{d\mathcal{F}_{J_t}}{du}(u) = \int_{S_u} (\iota_U \circ d)(*J_t^\flat) = -\int_{S_u} \iota_U\left(*\frac{\partial P}{\partial t}\right).$$

and

$$\int_{S_u} \iota_U\left(*\frac{\partial P}{\partial t}\right) = \frac{\partial}{\partial t}\int_{S_u} \iota_U(*P_t) = \frac{\partial}{\partial t}\left(\frac{\partial c}{\partial u}(u,t)\right).$$

We conclude that

$$\frac{\partial}{\partial t}\left(\frac{\partial c}{\partial u}(u,t)\right) + \frac{d\mathcal{F}_{J_t}}{du}(u) = 0,$$

which implies that

$$\frac{\partial}{\partial t}\left(g^{-1/2}(u)\frac{\partial c}{\partial u}(u,t)\right) + g^{-1/2}(u)\frac{\partial}{\partial u}\left(g^{1/2}(u)g^{-1/2}(u)\mathcal{F}_{J_t}(u)\right) = 0.$$

This last equation is known *effective continuity equation* and can be re-written as

$$\frac{\partial p}{\partial t}(u,t) + \nabla \cdot j(u,t) = 0. \tag{5.5}$$

5.4. **Infinite transversal diffusion rate.** The assumption of an infinite transversal diffusion rate consists in letting P be constant along the cross sections of the channel. This is equivalent to writing

$$P(x,t) = \rho(u(x),t)$$

for a function $\rho : \mathbb{R}\times\mathbb{R} \to \mathbb{R}$, and where u it the projection function for $\mathcal{C}$. The effective density function can then be written as

$$p(u,t) = g(u)^{-1/2}\int_{S_u} u^*(\rho_t)\iota_U\mu = \rho(u,t)g(u)^{-1/2}\int_{S_u}\iota_U(\mu).$$

From the formula

$$\int_{S_u}\iota_U(\mu) = \frac{d\nu}{du}(u) = g(u)^{1/2},$$

we conclude that

$$p(u,t) = \rho(u,t).$$

Using Fick's law $J_t = -D_0\nabla P_t$, we obtain

$$\mathcal{F}_{J_t}(u) = \int_{S_u} *J_t^\flat = -D_0\int_{S_u} *(dP_t) = -D_0\int_{S_u} *(u^*(d\rho_t)).$$

Since (for s equal to the identity map in $\mathbb{R}$)

$$u^*(d\rho_t) = u^*\left(\frac{\partial \rho_t}{\partial s}ds\right) = u^*\left(\frac{\partial \rho_t}{\partial s}\right)du,$$

we obtain

$$\mathcal{F}_{J_t}(u) = -D_0\frac{\partial \rho}{\partial u}(u,t)\int_{S_u} *(du).$$

Using this last formula and the fact that $\rho = p$, we obtain

$$j(u,t) = g(u)^{-1/2}\mathcal{F}_{J_t}(u) = -\left(D_0 g(u)^{1/2}\int_{S_u} *(du)\right) g(u)^{-1}\frac{\partial p}{\partial u}(u,t).$$

Substitution of this formula for j in the effective continuity equation 5.5 leads to the *effective diffusion formula*

$$\frac{\partial p}{\partial t}(u,t) = \nabla\cdot(\mathcal{D}(u)\nabla p(u,t)), \tag{5.6}$$

where the *effective diffusion coefficient* is given by

$$\begin{aligned}\mathcal{D}(u) &= D_0\left(\int_{S_u} *(du)\right) g(u)^{1/2}.\\ &= D_0\mathcal{F}_{\nabla u}(u)\frac{d\nu}{du}(u).\end{aligned}$$

5.5. **Finite transversal diffusion rate.** We will now consider the case when density function $P = P(x,t)$ is not necessarily constant along the cross sections of the channel. In general it is not possible to define define $\mathcal{D} = \mathcal{D}(u)$ such that the effective density function $p = p(u,t)$ satisfies the 1-dimensional diffusion equation 5.6 exactly, but for many cases of narrow channels it is possible to find $\mathcal{D}$ such that p satisfy 5.6 to a very good approximation. In any case, if such a $\mathcal{D}$ existed we could recover it from of a stable solution $\rho = \rho(u)$ to 5.6. In fact, if ρ is such a function we have that

$$\nabla\cdot(\mathcal{D}\nabla\rho) = 0,$$

which is equivalent to

$$\frac{\partial}{\partial u}\left(\frac{\mathcal{D}}{\sigma}\frac{d\rho}{du}\right) = 0 \text{ where } \sigma = g^{1/2} = \frac{d\nu}{du}. \tag{5.7}$$

Hence, we can find a constant $\mathcal{J}\in\mathbb{R}$ such that

$$\mathcal{D}(u) = \mathcal{J}\sigma(u)\left(\frac{d\rho}{du}(u)\right)^{-1}. \tag{5.8}$$

Remark 3. If we introduce a new variable $v = v(u)$, then we have that

$$\mathcal{D}(v) = \mathcal{D}(u(v)),$$

since

$$\begin{aligned}\mathcal{D}(v) &= \mathcal{J}\frac{d\nu}{dv}(v)\left(\frac{d\rho}{dv}(v)\right)^{-1}\\ &= \mathcal{J}\frac{d\nu}{du}(u(v))\frac{du}{dv}(v)\left(\frac{d\rho}{du}(u(v))\frac{du}{dv}(v)\right)^{-1}\\ &= \mathcal{D}(u(v)).\end{aligned}$$

We will now assume that ρ is the effective concentration function of a stable solution $h = h(x)$ to the full diffusion equation 5.1 (with reflective boundary conditions on $\mathcal{W}$). We then have that

$$\rho(u) = \frac{1}{\sigma(u)}\int_{\mathcal{S}_u} h\iota_U(\mu) = \frac{1}{\sigma(u)}\frac{dc}{du}(u)$$

for

$$c(u) = \int_{\mathcal{C}_{[0,u]}} h\mu,$$

and hence

$$\frac{d\rho}{du} = \frac{d}{du}\left(\frac{1}{\sigma}\frac{dc}{du}\right) = \frac{1}{\sigma}\left(\frac{d^2c}{du^2} - \rho\frac{d^2\nu}{du^2}\right).$$

Using Lemma 2 we obtain

$$\frac{d^2c}{du^2} = \int_{\mathcal{S}_u} (dh(U) + h\nabla\cdot U)\iota_U(\mu),$$

and since

$$\nu(u) = \int_{\mathcal{C}_{[0,u]}} \mu$$

then

$$\frac{d^2\nu}{du^2} = \int_{\mathcal{S}_u} (\nabla\cdot U)\iota_U(\mu).$$

We conclude that

$$\mathcal{D}(u) = \mathcal{J}\sigma^2(u)/\mathcal{F}_{\lambda U}(u) = \mathcal{J}\mathcal{F}_U(u)\left(\frac{\mathcal{F}_U(u)}{\mathcal{F}_{\lambda U}(u)}\right)$$

where

$$\lambda = dh(U) + (h - u^*(\rho))\nabla\cdot U.$$

Computation of $\mathcal{J}$. By definition, we have[17]

$$\mathcal{J}(u) = \frac{\mathcal{D}(u)}{\sigma(u)}\frac{d\rho}{du}(u).$$

Using Fick's laws

$$j(u) = -\mathcal{D}(u)\nabla\rho(u)$$
$$J(x) = -D_0\nabla h(x)$$

and the formulas

$$j(u) = \frac{1}{\sigma(u)}\int_{\mathcal{S}_u} *J^\flat$$
$$\nabla\rho(u) = \frac{1}{\sigma(u)^2}\frac{d\rho}{du}(u)$$

we obtain

$$\mathcal{J}(u) = D_0\int_{\mathcal{S}_u} *(dh) = D_0\mathcal{F}_{\nabla h}(u).$$

The function $\mathcal{J} = \mathcal{J}(u)$ is in fact a constant function (i.e independent of u), since for any two values u_1 and u_2 we have that (by Stokes Theorem and the reflective boundary conditions on $\mathcal{W}$)

$$\mathcal{J}(u_2) - \mathcal{J}(u_1) = D_0\int_{S_{u_2}-S_{u_1}} (*dh) = \int_{\mathcal{C}_{[u_1,u_2]}} d*dh = \int_{\mathcal{C}_{[u_1,u_2]}} *\Delta h = 0.$$

[17]Apparently $\mathcal{J}$ depends on u, but we will show below that $\mathcal{J}$ is actually a constant function (as required for the formula we computed for the effective diffusion coefficient $\mathcal{D}$)

Lateral boundary conditions. It is *important* to notice that formula 5.8 holds only under the assumption that $\rho'(u) \neq 0$ for all $u \in \mathbb{R}$. We can achieve this if for $\alpha \neq \beta$ we fix boundary the conditions

$$\rho(a) = \alpha \text{ and } \rho(b) = \beta. \tag{5.9}$$

For fixed values of α and β we will denote the stable solution to 5.6 satisfying these boundary conditions by $\rho_{\alpha,\beta}$. Using the linearity of equation 5.7 we obtain

$$\rho_{\alpha,\beta} = \alpha + (\beta - \alpha)\rho_{0,1}.$$

If we denote the constant $\mathcal{J}$ associated to $\rho_{\alpha,\beta}$ by $\mathcal{J}(\alpha, \beta)$ then

$$\mathcal{D} = \sigma \mathcal{J}(\alpha, \beta) \left(\frac{d\rho_{\alpha,\beta}}{du}\right)^{-1}.$$

Since $\mathcal{D}$ is independent of the choice of α and β we must have

$$\mathcal{J}(\alpha, \beta) \left(\frac{d\rho_{\alpha,\beta}}{du}\right)^{-1} = \mathcal{J}(0,1) \left(\frac{d\rho_{0,1}}{du}\right)^{-1},$$

from which we obtain the formula

$$\mathcal{J}(\alpha, \beta) = (\beta - \alpha)\mathcal{J}(0,1).$$

The boundary conditions 5.9 can be written in terms of H (using Lemma 2) as

$$\begin{aligned} \frac{1}{\sigma(a)} \int_{\mathcal{S}_a} h\iota_U(\mu) = \alpha, \\ \frac{1}{\sigma(b)} \int_{\mathcal{S}_b} h\iota_U(\mu) = \beta. \end{aligned}$$

If we choose h so that it is has constant value h_a in $\mathcal{S}_a$ and constant value h_b in $\mathcal{S}_b$, the above conditions become

$$h_a = \alpha \text{ and } h_b = \beta.$$

5.6. **Channels defined by harmonic conjugate functions.** Let M be a 2-dimensional oriented surface. We will say that $u, v : M \to \mathbb{R}$ are harmonic conjugate if

$$dv = *du,$$

or equivalently

$$\nabla v = i\nabla u.$$

Observe that in this case

$$*dv = **\,du = -du.$$

The existence of a harmonic conjugate v for u implies that u and v are harmonic, since

$$\begin{aligned} \Delta u &= *d*du = *(d^2 v) = 0, \\ \Delta v &= *d*dv = -*(d^2 u) = 0. \end{aligned}$$

For fixed value $v_1, v_2 \in \mathbb{R}$, consider a channel $\mathcal{C}$ defined as

$$\mathcal{C} = \{x \in M | v_1 \leq v(x) \leq v_2\},$$

If we use a harmonic conjugate u of v as projection function for this channel, then u is a harmonic function with reflective boundary conditions on $\mathcal{W}$. The channels $\mathcal{C}$ has generating field

$$U = \frac{\nabla u}{|\nabla u|^2}.$$

The effective diffusion coefficient both in the infinite and finite transversal diffusion rate cases coincide and is given by the formula

$$\mathcal{D}(u) = \mathcal{J}\frac{d\nu}{du}(u),$$

where

$$\mathcal{J} = \int_{\mathcal{S}_u} *du = \int_{\mathcal{S}_u} dv = v_2 - v_1 \tag{5.10}$$

and

$$\frac{d\nu}{du}(u) = \int_{\mathcal{S}_u} \frac{*du}{|\nabla u|^2} = \int_{\mathcal{S}_u} \frac{dv}{|\nabla v|^2}.$$

Observe that we can parametrize a cross section $\mathcal{S}_u$ with a curve $x : [t_1, t_2] \to \mathcal{C}$ with

$$\dot{x}(t) = \nabla v(x(t)),$$

so that

$$\mathcal{A}(u) = \int_{t_1}^{t_2} |\dot{x}(t)| = \int_{t_1}^{t_2} \frac{|\nabla v(x(t))|^2}{|\nabla v(x(t)|}.$$

Hence

$$\mathcal{A}(u) = \int_{\mathcal{S}_u} \frac{dv}{|\nabla v|}.$$

5.7. **Parametric channels.** In this section we will assume that the channel $\mathcal{C} \subset M$ can be parametrized by a map

$$\varphi : [a, b] \times \Omega \to M,$$

where Ω is a $(n-1)$-dimensional sub-manifold with boundary of $\mathbb{R}^{n-1}$. In local coordinates we will write the elements of $[a, b] \times \Omega$ as (u, v) for $u \in [a, b]$ and $v = (v_1, \ldots, v_{n-1}) \in \mathbb{R}^{n-1}$. If denote the of points in $\mathcal{C}$ by x then we have that $x = \varphi(u, v)$, which we will simply write as $x = x(u, v)$. We will let the generating vector field for $\mathcal{C}$ be

$$U = \varphi_* \left(\frac{\partial}{\partial u}\right),$$

which has u as a projection function. To compute the effective diffusion coefficient for $\mathcal{C}$ (in both the finite and infinite transversal diffusion rate cases) we will need to compute

$$\frac{d\nu}{du}, \mathcal{F}_{\nabla u}, \rho, dh(U) \text{ and } \nabla \cdot U,$$

where h is a natural projection function for $\mathcal{C}$ and ρ its corresponding effective density function. To compute the above quantities in (u, v)-coordinates we will make use of the metric tensor $g = \varphi^*(g_M)$, where g_M is the metric in M. We have that

$$g = \begin{pmatrix} \frac{\partial x}{\partial u}\cdot\frac{\partial x}{\partial u} & \frac{\partial x}{\partial u}\cdot\frac{\partial x}{\partial v} \\ \left(\frac{\partial x}{\partial u}\cdot\frac{\partial x}{\partial v}\right)^T & g_v \end{pmatrix},$$

where

$$\frac{\partial x}{\partial u}\cdot\frac{\partial x}{\partial v}=\left(\frac{\partial x}{\partial u}\cdot\frac{\partial x}{\partial v_1},\dots,\frac{\partial x}{\partial u}\cdot\frac{\partial x}{\partial v_{n-1}}\right)$$

and g_v is the matrix with entries

$$(g_v)_{i,j}=\frac{\partial x}{\partial v_i}\cdot\frac{\partial x}{\partial v_j}.$$

The volume form in $\mathcal{C}$ is given by

$$\mu=\det(g)^{1/2}du\wedge dv,$$

and hence

$$\frac{d\nu}{du}(u)=\int_\Omega \iota_{\frac{\partial}{\partial u}}(\mu)=\int_\Omega \det(g(u,v))^{1/2}dv \tag{5.11}$$

$$\mathcal{A}(u)=\int_\Omega \det(g_v(u,v))^{1/2}dv$$

Observe that

$$\nabla u=a_0\frac{\partial}{\partial u}+\sum_{i=1}^{n-1}a_i\frac{\partial}{\partial v_i}$$

where

$$\begin{pmatrix} a_0\\ a_1\\ \vdots\\ a_{n-1}\end{pmatrix}=g^{-1}\begin{pmatrix}1\\0\\ \vdots\\ 0\end{pmatrix}.$$

Since

$$a_0=\frac{\det(g_v)}{\det(g)},$$

we conclude that

$$\begin{aligned}\mathcal{F}_{\nabla u}(u)&=\int_\Omega \det(g(u,v))^{\frac12}\iota_{\nabla u}(du\wedge dv)\\ &=\int_\Omega\left(\frac{\det(g_v(u,v))}{\det(g(u,v))^{\frac12}}\right)dv.\end{aligned}\tag{5.12}$$

The divergence of U can be computed using the the formula $d(\iota_U(\mu))=(\nabla\cdot U)\mu$. In our case we have that

$$d(\iota_U(\mu))=d(\det(g)^{1/2}dv)=\frac{\partial\det(g)^{1/2}}{\partial u}du\wedge dv,$$

and hence

$$\nabla\cdot U=\frac{\frac{\partial}{\partial u}\left(\det(g)^{1/2}\right)}{\det(g)^{1/2}}=\frac12\frac{\partial}{\partial u}\left(\log(\det(g))\right).$$

If h is the natural projection map on the channel then

$$dh(U)=\frac{\partial h}{\partial u}$$

and

$$\rho=\left(\int_\Omega h(u,v)\det(g(u,v))^{1/2}dv\right)/\left(\int_\Omega \det(g(u,v))^{1/2}dv\right)$$

6. * Conclusions and future work

TODO

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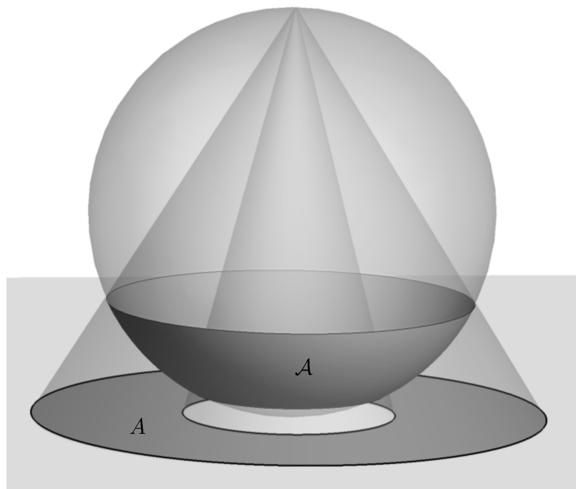
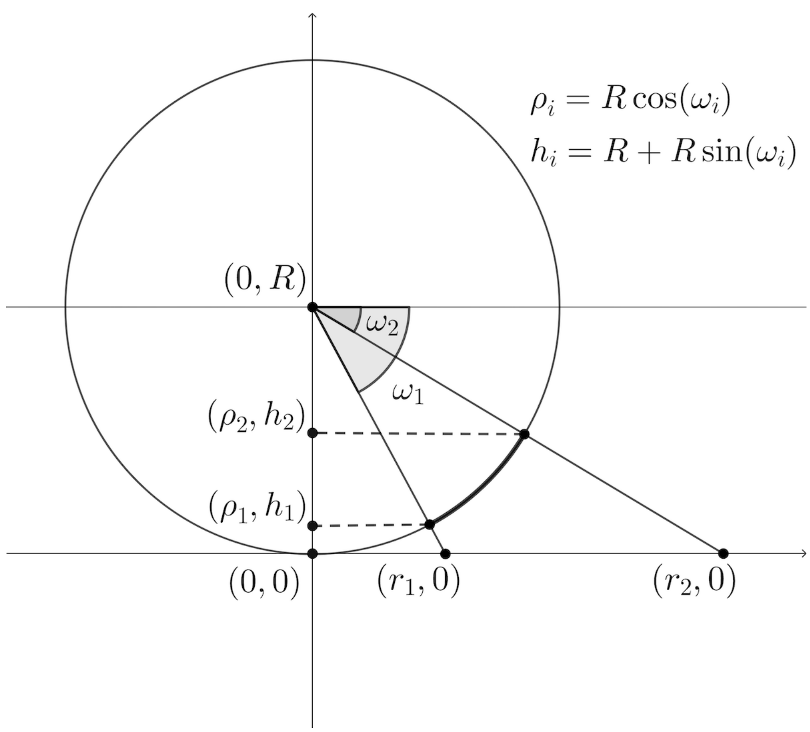


(A) Stereographic projection of annulus $\mathcal{A}$



(B) Annulus projection seen in the (x_1, x_3)-plane

FIGURE 8. Stereographic projection of spherical annulus $\mathcal{A}$ onto planar annulus in A

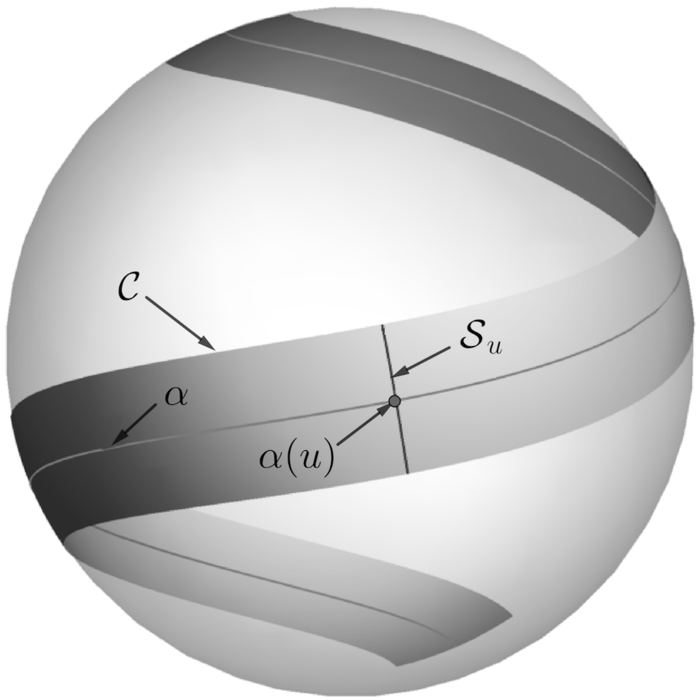


FIGURE 9. Channel of constant width on a sphere

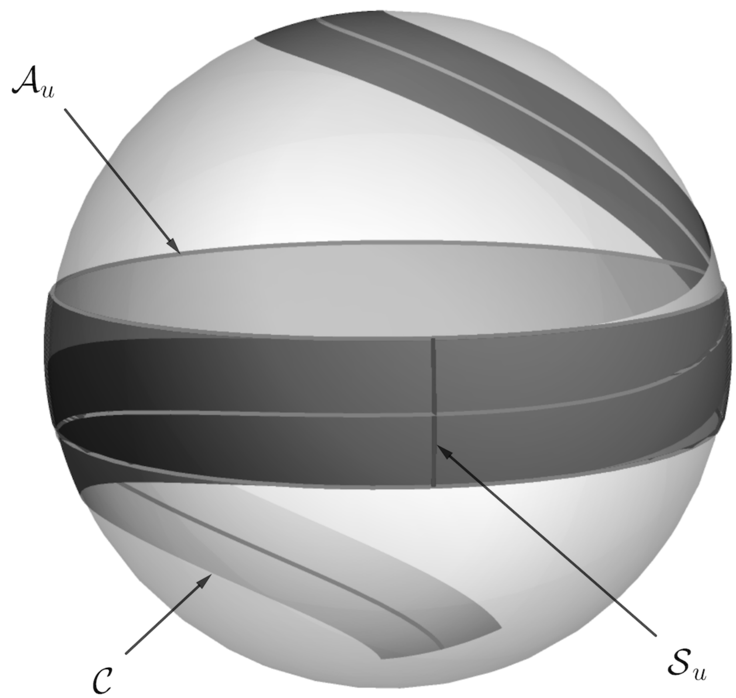


FIGURE 10. Approximation of a channel $\mathcal{C}$ of constant width with an annuls $\mathcal{A}_u$ at a cross section $\mathcal{S}_u$.