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by

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Modelling with measures: Approximation of a mass-emitting object by a point source

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Abstract

We consider a linear diffusion equation on $\Omega := \mathbb{R}^2 \setminus \Omega_{\mathcal{O}}$, where $\Omega_{\mathcal{O}}$ is a bounded domain. The (time-dependent) flux on the boundary $\Gamma := \partial\Omega_{\mathcal{O}}$ is prescribed. The aim of the paper is to approximate the dynamics by the solution of the diffusion equation on the whole of $\mathbb{R}^2$ with a measure-valued point source in the origin and provide estimates for the quality of approximation. For all time t, we derive an $L^2(0, t; L^2(\Gamma))$-bound on the difference in flux on the boundary. Moreover, we derive for all t an $L^2(\Omega)$-bound and an $L^2(0, t; H^1(\Omega))$-bound for the difference of the solutions to the two models.

Keywords : Point source, model reduction, boundary exchange, diffusion, quantitative flux estimates, modelling with measures.

MSC 2010 : Primary: 35K05, 35A35; Secondary: 35B45.

1   Introduction

"What is the force on a test charge due to a single point charge q which is at rest a distance r away?" is a common type of question in textbooks about electromagnetism (e.g. [8], p. 59). In reality there is of course no such thing as a point charge having no volume. This is just a simplification due to the fact that the volume of the charged particle is very small compared to the other typical length scales in the system. Throughout physics it is common practice to replace objects of negligible size by point masses. For instance, cf. grains or colloids in a solution, crowd dynamics [9], electrostatics [12], defects in crystalline structures [5, 17]. Of particular interest is the setting in which exchange of mass, energy etc. between the interior and the exterior of the object takes place at its boundary. In this case the object is approximated not by a mere point mass, but by a point source. Experimental evidence suggests that this example of 'modelling with measures' is often a good approximation to the original (spatially extended) system. In this paper we consider the problem of quantifying the accuracy

of this type of approximation, focussing on such scenario, that is stripped of all superfluous details and shows the essence of the problem.

In $\mathbb{R}^2$, we consider an object of fixed shape and position and of finite size. Outside the object there is a concentration of mass that evolves due to diffusion. On the boundary of the object there is a given mass flux in normal direction. This prescribed flux is a simplistic way of describing the result of processes that occur in the interior of the object. We wish to approximate this object by a point source. To that aim we replace the original diffusion equation on the exterior domain by a diffusion equation on the whole of $\mathbb{R}^2$ with a Dirac measure included at its right-hand side. The exact formulation of the equations will be made clear in Section 2.

This is a first step towards modelling and analysing the mass distribution dynamics in the realistic setting of a large number of these objects in a bounded domain, moving around while exchanging mass. Our motivation comes from the intracellular transport of chemical compounds in vesicles, like neurotransmitters in neurons (cf. [15]) or the hypothetical vesicular transport mechanism for the plant hormone auxin proposed in [2] as an alternative to the conventional auxin transport paradigm (in analogy to neurotransmitters). Auxin is a crucial molecule regulating growth and shape in plants. The vesicles are small membrane-bound balls covered by specific transmembrane transporter proteins that take up auxin from the surrounding cytoplasm. The vesicles are driven by molecular motors over a network of intracellular filaments [11, 19], e.g. from one end of the cell to the other as in Polar Auxin Transport (PAT). Experimental investigations of PAT in *Chara* species [4] revealed that neither diffusion nor cytoplasmic streaming can be the driving mechanism of PAT in the long (3-8 cm) internodal *Chara* cells. See [4, 19] for further discussion and an overview.

A substantial amount of mathematical modelling efforts on PAT have focussed on pattern formation in plant cell tissues (see [3, 13, 16] and the references cited therein). Upscaling to an effective macroscopic continuum description for transport at tissue level was considered in [6]. All models are based however on the assumption of diffusion as intracellular transport mechanism for auxin. Ultimately, we aim at obtaining a convenient mathematical description of the vesicle-driven transport dynamics *within* a cell, in particular in terms of an effective continuum model, which is needed to replace diffusion in an upscaling argument similar to [6]. In view of (the absence of) relevant mathematical literature, this perspective seems to be rather unexplored.

Why do we insist on introducing measures to this problem? This is especially useful once we wish to describe the interaction between multiple moving objects (vesicles). We expect the mathematical description to be much simpler in terms of discrete measures (i.e. the weighted sum of Dirac measures) and the analysis and numerical approximation likewise (see, for instance, [20, 21] for a related case). But before we can go to this advanced setting, we first need to investigate the quality of the approximation for a simple reference scenario; this is the main concern of this paper.

After the aforementioned overview of model equations in Section 2, we summarize some useful preliminary results in Section 3. In Section 4 we show boundedness of the difference in the flux of the full problem (including the finite-size object) and the flux of the reduced

problem (including the point source). This result is used in Section 5, where we estimate the difference between the two problems' solutions on the exterior domain.

2 Two problems

Let $\Omega_{\mathcal{O}} \in \mathbb{R}^2$ be a connected, compact set, such that its boundary $\Gamma := \partial\Omega_{\mathcal{O}}$ is piecewise C^1 and has finite length.[1] This set denotes the interior of the object $\mathcal{O}$ with mass-exchange at its boundary. We also assume that 0 is an interior point of $\Omega_{\mathcal{O}}$. Let Ω denote the exterior of $\mathcal{O}$. That is, $\Omega := \mathbb{R}^2 \setminus \Omega_{\mathcal{O}}$. See Figure 2.1a.

For given initial condition $u_0 \in L^2(\Omega)$ and given flux $\phi \in L^2(0, t; L^2(\Gamma))$ for all $t \in \mathbb{R}^+$, we consider the problem

$$\begin{cases} \dfrac{\partial u}{\partial t} = d\Delta u, & \text{on } \Omega \times \mathbb{R}^+; \\ u(0) = u_0, & \text{on } \Omega; \\ d\nabla u \cdot n = \phi, & \text{on } \Gamma \times \mathbb{R}^+. \end{cases} \tag{2.1}$$

Here, d denotes the diffusion coefficient, which is fixed throughout this paper. The vector n denotes the unit normal pointing outwards on Γ (so *into* $\Omega_{\mathcal{O}}$), and ϕ is the *influx* of u w.r.t. Ω. Positive ϕ corresponds to flux in the direction of $-n$.

Let $\hat{u}_0$ denote an extension of u_0 in $L^2(\mathbb{R}^2)$, given by

$$\hat{u}_0 := \begin{cases} u_0, & \text{on } \Omega; \\ v_0, & \text{on } \Omega_{\mathcal{O}}. \end{cases} \tag{2.2}$$

The aim of the paper is to approximate (2.1) by the reduced problem:

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial t} = d\Delta \hat{u} + \bar{\phi}\delta_0, & \text{on } \mathbb{R}^2 \times \mathbb{R}^+; \\ \hat{u}(0) = \hat{u}_0, & \text{on } \mathbb{R}^2. \end{cases} \tag{2.3}$$

Note that such measure-valued source was treated, for instance, in [21] from the approximation point of view; see also [14] for more background on the solvability of such evolution equations. We remark here that (2.3) is posed on the whole of $\mathbb{R}^2$. The boundary Γ has no physical meaning in this problem; see Figure 2.1b. However, the flux on this imaginary curve will be used in later estimates.

3 Preliminaries

The solution of (2.3) is

$$\hat{u}(x, t) = \int_{\mathbb{R}^2} G_t(x - y)\hat{u}_0(y)\, dy + \int_0^t G_{t-s}(x)\bar{\phi}(s)\, ds$$

$$=: (G *_x \hat{u}_0)(x, t) + (G *_t \bar{\phi})(x, t). \tag{3.1}$$

---

[1]The results of this paper can be derived also under weaker conditions on Γ, but this is not our main focus.

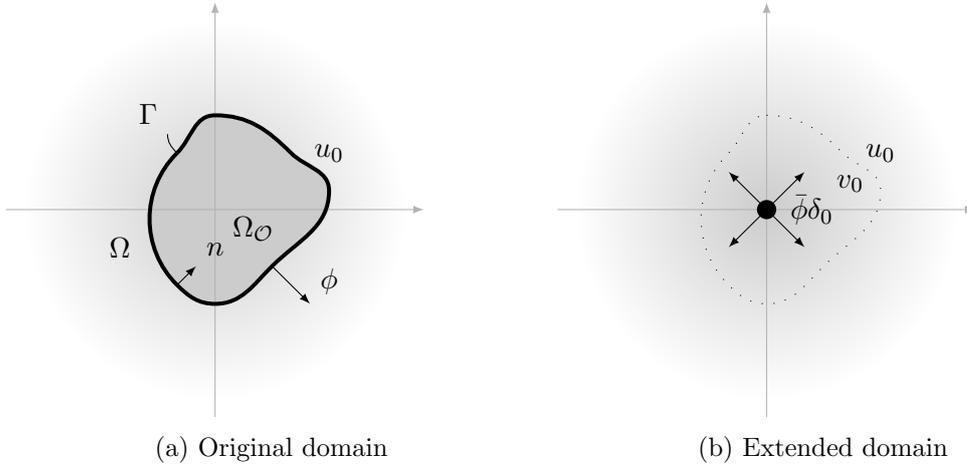(a) Original domain   (b) Extended domain

Figure 2.1: (a): Typical example of the original domain Ω outside the object $\mathcal{O}$, on which u evolves according to (2.1) starting from initial condition u_0. Also, ϕ and n, related to the boundary condition on Γ, are indicated. (b): Domain for the reduced problem associated to (a). Γ is now an imaginary curve within the domain (to be used later). The initial conditions u_0 and v_0 hold outside and inside Γ, respectively. The point source of magnitude $\bar{\phi}$ is indicated in the origin.

for all $(x,t) \in \mathbb{R}^2 \times \mathbb{R}^+$. Here G denotes the Green's function of the diffusion operator, given (for general dimension n) by

$$G_t(x) := (4\pi dt)^{-n/2} \mathrm{e}^{-|x|^2/4dt}. \tag{3.2}$$

Lemma 3.1 (Properties of the convolution, [7] Proposition 8.8, p. 241). *Let $p, q \geq 1$ be such that $1/p + 1/q = 1$. If $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$, then*

    1. $(f * g)(x)$ exists for all $x \in \mathbb{R}^n$;

    2. $f * g$ is bounded and uniformly continuous;

    3. $\|f * g\|_{L^\infty(R^n)} \leq \|f\|_{L^p(\mathbb{R}^n)} \|g\|_{L^q(\mathbb{R}^n)}$.

If $p, q \in (1, \infty)$, then

    4. $f * g \in C_0(\mathbb{R}^n)$.

Proof. The proof can be found in [7], p. 241.   □

Lemma 3.2 (Properties of the Green's function). *Consider the Green's function (3.2) for dimension $n = 2$.*

    1. The gradient of the Green's function satisfies

$$\|\nabla G_{\cdot}(x)\|_{L^\infty(0,\infty)} := \sup_{\tau \in (0,\infty)} \|\nabla G_\tau(x)\| = \begin{cases} 0, & x = 0; \\ \dfrac{8\mathrm{e}^{-2}}{\pi} |x|^{-3}, & x \in \mathbb{R}^2 \setminus \{0\}. \end{cases} \tag{3.3}$$

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2. *For all $1 \leq p \leq \infty$ there is a constant c such that for all $t \in \mathbb{R}^+$*

$$\|G_t(\cdot)\|_{L^p(\mathbb{R}^2)} \leq c\, t^{\frac{1}{p}-1}. \tag{3.4}$$

The constant depends on p and d.

Proof. 1. For all $x \in \mathbb{R}^2$ and all $\tau \in \mathbb{R}^+$

$$\|\nabla G_\tau(x)\| = \frac{|x|}{8\pi d^2 \tau^2}\, \mathrm{e}^{-|x|^2/4d\tau}, \tag{3.5}$$

where $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^2$. For $x = 0$ we have that $\|\nabla G_\tau(0)\| = 0$ for all $\tau \in (0, \infty)$, thus the corresponding part of (3.3) follows.

Next, we consider $x \neq 0$. Note that for all such x we have that $\|\nabla G_\tau(x)\| \geq 0$ for all τ and

$$\lim_{\tau \to 0} \|\nabla G_\tau(x)\| = 0, \tag{3.6}$$

$$\lim_{\tau \to \infty} \|\nabla G_\tau(x)\| = 0. \tag{3.7}$$

Since the right-hand side in (3.5) is differentiable for all $\tau \in \mathbb{R}^+$, its maximum on $\mathbb{R}^+$ is attained where

$$\frac{\partial}{\partial \tau} \|\nabla G_\tau(x)\| = \frac{|x|}{4\pi d^2 \tau^3} \left(\frac{|x|^2}{8dt} - 1 \right) \mathrm{e}^{-|x|^2/4dt} = 0, \tag{3.8}$$

i.e. at $\tau = |x|^2/8d$. Now the statement of the lemma follows:

$$\|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)} = \|\nabla G_\tau(x)\|\Big|_{\tau=|x|^2/8d} = \frac{8\mathrm{e}^{-2}}{\pi}\, |x|^{-3}. \tag{3.9}$$

2. The proof is a direct consequence of the statement in [10] at the bottom of p. 432. $\qquad\square$

4 Flux estimates

In this section we present in Theorem 4.5 a bound on the difference between the fluxes on Γ in (2.1) and (2.3). Before getting at this theorem, we derive auxiliary results in Lemmas 4.1 and 4.2.

Lemma 4.1. *Assume that $\hat{u}_0 \equiv 0$, and that for all $t > 0$*

$$\int_0^t \|\bar{\phi}\|^2_{L^1(0,\tau)}\, d\tau < \infty. \tag{4.1}$$

Then, for all $t > 0$ we have

$$\int_0^t \|d\nabla \hat{u} \cdot n\|^2_{L^2(\Gamma)} < \infty. \tag{4.2}$$

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Proof. For $\hat{u}_0 \equiv 0$, the solution (3.1) of (2.3) is given by

$$\hat{u}(x,t) = \int_0^t G_{t-s}(x)\bar{\phi}(s)\,ds. \tag{4.3}$$

Note that on Γ we have

$$
\begin{aligned}
|d\nabla\hat{u}(x,\tau)\cdot n(x)| &= \left| d\int_0^\tau \nabla G_{\tau-s}(x)\bar{\phi}(s)\,ds \cdot n(x) \right| \\
&\leq \left\| d\int_0^\tau \nabla G_{\tau-s}(x)\bar{\phi}(s)\,ds \right\| \\
&\leq d\,\|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)} \int_0^\tau |\bar{\phi}(s)|\,ds \\
&= d\,\|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)} \|\bar{\phi}\|_{L^1(0,\tau)}.
\end{aligned}
\tag{4.4}
$$

We emphasize here that the infinity norm $\|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)}$ denotes the supremum in the time domain for fixed x, cf. (3.3). This observation leads to the following estimate

$$
\int_0^t \|d\nabla\hat{u}(x,\tau)\cdot n(x)\|_{L^2(\Gamma)}^2\,d\tau = \int_0^t\int_\Gamma |d\nabla\hat{u}(x,\tau)\cdot n(x)|^2\,d\sigma\,d\tau \tag{4.5}
$$

$$
\leq d^2 \int_0^t\int_\Gamma \|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)}^2 \|\bar{\phi}\|_{L^1(0,\tau)}^2\,d\sigma\,d\tau, \tag{4.6}
$$

where (4.4) is used in the second step. Thus

$$
\int_0^t \|d\nabla\hat{u}(x,\tau)\cdot n(x)\|_{L^2(\Gamma)}^2\,d\tau \leq d^2 \int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2\,d\tau \int_\Gamma \|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)}^2\,d\sigma. \tag{4.7}
$$

By hypothesis (4.1) of the lemma, the first integral on the right-hand side is finite. Since Γ is the boundary of a compact set, of which 0 is an interior point, it follows from (3.3) in Lemma 3.2 that the second integral on the right-hand side of (4.7) is also finite. This finishes the proof. $\qquad\square$

In the next lemma we generalize this result to nonzero initial conditions.

Lemma 4.2. *If $\nabla\hat{u}_0 \in L^p(\mathbb{R}^2)$, $2 < p \leq \infty$, and if for all $t > 0$*

$$\int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2\,d\tau < \infty, \tag{4.8}$$

then, for all $t > 0$

$$\int_0^t \|d\nabla\hat{u}\cdot n\|_{L^2(\Gamma)}^2 < \infty. \tag{4.9}$$

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Proof. In this case, the solution of (2.3) is – cf. (3.1) – given by

$$\hat{u}(x,t) = \int_{\mathbb{R}^2} G_t(x-y)\hat{u}_0(y)\,dy + \int_0^t G_{t-s}(x)\bar{\phi}(s)\,ds. \tag{4.10}$$

We start with the following estimate

$$\int_0^t \|d\nabla\hat{u}(x,\tau)\cdot n(x)\|_{L^2(\Gamma)}^2\,d\tau \leq 2\int_0^t\int_\Gamma \left|d\nabla\int_{\mathbb{R}^2} G_\tau(x-y)\hat{u}_0(y)\,dy\cdot n(x)\right|^2\,d\sigma\,d\tau$$

$$+ 2\int_0^t\int_\Gamma \left|d\nabla\int_0^\tau G_{\tau-s}(x)\bar{\phi}(s)\,ds\cdot n(x)\right|^2\,d\sigma\,d\tau, \tag{4.11}$$

of which the second term on the right-hand side was treated in Lemma 4.1 and its proof. Regarding the first term, we remark that, due to properties of the convolution,

$$\left|d\nabla\int_{\mathbb{R}^2} G_\tau(x-y)\hat{u}_0(y)\,dy\cdot n(x)\right| = \left|d\int_{\mathbb{R}^2} G_\tau(y)\nabla\hat{u}_0(x-y)\,dy\cdot n(x)\right|. \tag{4.12}$$

We use Part 3 of Lemma 3.1 to estimate the right-hand side

$$\left|d\int_{\mathbb{R}^2} G_\tau(y)\nabla\hat{u}_0(x-y)\,dy\cdot n(x)\right| \leq d\left\|\int_{\mathbb{R}^2} G_\tau(y)\nabla\hat{u}_0(\cdot-y)\,dy\right\|_{L^\infty(\mathbb{R}^2)}$$

$$\leq d\,\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}\,\|G_\tau\|_{L^q(\mathbb{R}^2)}, \tag{4.13}$$

with $q := (p-1)/p$.

It follows from (4.12)–(4.13) and Part 2 of Lemma 3.2 that

$$\int_0^t\int_\Gamma \left|d\nabla\int_{\mathbb{R}^2} G_\tau(x-y)\hat{u}_0(y)\,dy\cdot n(x)\right|^2\,d\sigma\,d\tau \leq d^2\,\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2 \int_0^t\int_\Gamma \|G_\tau\|_{L^q(\mathbb{R}^2)}^2\,d\sigma\,d\tau$$

$$\leq c^2\,d^2\,|\Gamma|\,\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2 \int_0^t \tau^{\frac{2}{q}-2}\,d\tau$$

$$= \frac{q\,c^2\,d^2\,|\Gamma|}{2-q}\,t^{\frac{2}{q}-1}\,\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2, \tag{4.14}$$

where c depends on q and d. We can perform the integration in time in the last step of (4.14) since the hypothesis $p > 2$ implies $q < 2$. The desired result follows by (4.11) and the calculations in the proof of Lemma 4.1:

$$\int_0^t \|d\nabla\hat{u}(x,\tau)\cdot n(x)\|_{L^2(\Gamma)}^2\,d\tau \leq \frac{2q\,c^2\,d^2\,|\Gamma|}{2-q}\,t^{\frac{2}{q}-1}\,\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2$$

$$+ 2d^2\int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2\,d\tau\int_\Gamma \|\nabla G_\cdot(x)\|_{L^\infty(0,\infty)}^2\,d\sigma, \tag{4.15}$$

of which the right-hand side is finite for all finite t. $\square$

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Remark 4.3. A sufficient condition for $\nabla \hat{u}_0 \in L^p(\mathbb{R}^2)$ to hold, is $\hat{u}_0 \in W^{1,p}(\mathbb{R}^2)$. To this aim, we require $u_0 \in W^{1,p}(\Omega)$ to hold for the *given* initial data. The remaining question is whether it is possible to find an extension v_0 on $\Omega_{\mathcal{O}}$ as in (2.2) such that $\hat{u}_0 \in W^{1,p}(\mathbb{R}^2)$. This, however is guaranteed by Theorem 5.22 on p. 151 of [1].

Remark 4.4. It is crucial that the gradient is applied to the initial condition in (4.12) and further. Instead of (4.12)–(4.13), we could, along the same lines, have estimated

$$\left| d \nabla \int_{\mathbb{R}^2} G_\tau(x - y)\hat{u}_0(y)\, dy \cdot n(x) \right| \le d\, \|\hat{u}_0\|_{L^p(\mathbb{R}^2)} \, \|\nabla G_\tau\|_{L^q(\mathbb{R}^2)}, \tag{4.16}$$

which requires only a condition on $\hat{u}_0$, not on its gradient, for the lemma. It follows from [10] (p. 432, bottom) that for some constant C

$$\|\nabla G_\tau\|_{L^q(\mathbb{R}^2)} \le C\, \tau^{\frac{1}{q} - \frac{3}{2}}. \tag{4.17}$$

This is a problem however, since similar arguments as in (4.14) would lead to

$$\int_0^t \|\nabla G_\tau\|_{L^q(\mathbb{R}^2)}^2 \, d\tau \le C \int_0^t \tau^{\frac{2}{q} - 3} \, d\tau, \tag{4.18}$$

of which the right-hand side is not integrable for any $1 \le q \le \infty$.

We now come to the summarizing result of this section.

Theorem 4.5. *Assume that the hypotheses of Lemma 4.2 hold. Then, for all $t > 0$*

$$c^*(t) := \int_0^t \|\phi - d\nabla \hat{u} \cdot n\|_{L^2(\Gamma)}^2 < \infty. \tag{4.19}$$

Proof. The statement of this theorem is a direct consequence of the observation

$$\int_0^t \|\phi - d\nabla \hat{u} \cdot n\|_{L^2(\Gamma)}^2 \le 2 \int_0^t \|\phi\|_{L^2(\Gamma)}^2 + 2 \int_0^t \|d\nabla \hat{u} \cdot n\|_{L^2(\Gamma)}^2. \tag{4.20}$$

The first term is finite due to the assumption that $\phi \in L^2(0, t; L^2(\Gamma))$ for all $t \in \mathbb{R}^+$ (see Section 2). The second term was estimated in Lemma 4.2. $\qquad \square$

Remark 4.6. Note that the proof of Lemma 4.2, apart from just the finiteness of the second term in (4.20), also shows (part of) the exact behaviour in time.

Remark 4.7. The estimate (4.20) is a very crude way to find an upper bound on $c^*(t)$. In the following (deliberately vague) conjecture, we express under which conditions we expect $c^*(t)$ to be smaller than the upper bound of Theorem 4.5 suggests.

Conjecture 4.8. *The upper bound c^* can be much smaller than Theorem 4.5 suggests. Ideally it goes to zero.*

Conjecture 4.8 is based on the following considerations:

- Once the geometry and ϕ on Γ are given, there still is a lot of freedom in dealing with the reduced problem (2.3). We can choose $\bar{\phi}$ and v_0. Our conjecture is that a smart choice of $\bar{\phi}$ and v_0 can produce a flux on Γ that mimics well ϕ and gives more than merely a *bounded* difference.

- Initially, during a small time interval, the initial condition should induce a sufficiently close flux. To this aim an appropriate v_0 is to be provided.

- At a certain moment, mass originating from the source starts reaching the boundary. From then onwards, the mimicking flux should be – with some delay – mainly due to $\bar{\phi}$.

- Let $|\Omega_{\mathcal{O}}|$ denote a typical length scale of the object $\mathcal{O}$ (e.g. its diameter). The quantity $|\Omega_{\mathcal{O}}|^2/d$ is a typical timescale for points to travel the distance from source to boundary. This is also the timescale at which the transition between the above two bullet points takes place.

- The shape of object $\mathcal{O}$ is important. An intuitive guess is that a small object $\mathcal{O}$ can be better approximated. As the point source emits mass at the same rate in all directions, we expect a better approximation also to be possible if Γ is radially symmetric with respect to the origin, and ϕ is constant on Γ (in space, not necessarily in time). A generalization of the latter condition would be to have ϕ defined on a more general Γ, but to have an extension to a ball $B(0,R)$ such that $\Gamma \subset B(0,R) \subset \mathbb{R}^2$, and this extension is radially symmetric around the origin on $B(0,R)$.

The above was written under the assumption that in general the (normal component of the) flux is directed outward on Γ. For a mass sink, *mutatis mutandis* the same considerations hold.

5 Estimates in the interior

Theorem 5.1. *For all $t \geq 0$ and for all $\varepsilon \in (0, 2d)$ there are $c_1, c_2 > 0$ such that*

$$\|u(\cdot, t) - \hat{u}(\cdot, t)\|_{L^2(\Omega)}^2 \leq c_1 \, c^*(t) \, e^{\varepsilon t}, \ and \tag{5.1}$$

$$\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \leq c_2 \, c^*(t) \, e^{\varepsilon t}. \tag{5.2}$$

The constants depend on Ω, d and ε.

Proof. Let $\langle \cdot, \cdot \rangle$ denote the inner product on $L^2(\Omega)$. Let $\psi \in H^1(\Omega)$ be an arbitrary test function. Then

$$\langle \partial_t u - \partial_t \hat{u}, \psi \rangle = d \, \langle \Delta u - \Delta \hat{u}, \psi \rangle$$

$$= \int_{\Gamma} (\phi - d \nabla \hat{u} \cdot n) \, \psi - d \int_{\Omega} (\nabla u - \nabla \hat{u}) \cdot \nabla \psi . \tag{5.3}$$

Take $\psi := u - \hat{u}$, then (5.3) can be rewritten as

$$\frac{1}{2}\frac{d}{dt}\|u - \hat{u}\|^2_{L^2(\Omega)} + d\|\nabla u - \nabla\hat{u}\|^2_{L^2(\Omega)} = \int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n). \tag{5.4}$$

Add $d\|u - \hat{u}\|^2_{L^2(\Omega)}$ to both sides and integrate in time from 0 to arbitrary t:

$$\frac{1}{2}\|u - \hat{u}\|^2_{L^2(\Omega)} + d\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)} = \int_0^t\int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) + d\int_0^t \|u - \hat{u}\|^2_{L^2(\Omega)}, \tag{5.5}$$

where we have used that u and $\hat{u}$ are initially equal on Ω. Apply the Cauchy-Schwarz inequality and use the result of Theorem 4.5 to obtain

$$\int_0^t\int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) \leq \left(\int_0^t \|u - \hat{u}\|^2_{L^2(\Gamma)}\right)^{\frac{1}{2}} \left(\int_0^t \|\phi - d\nabla\hat{u}\cdot n\|^2_{L^2(\Gamma)}\right)^{\frac{1}{2}}$$

$$= \sqrt{c^*(t)}\left(\int_0^t \|u - \hat{u}\|^2_{L^2(\Gamma)}\right)^{\frac{1}{2}}. \tag{5.6}$$

Since $H^1(\Omega) \hookrightarrow L^2(\Gamma)$, according to the Boundary Trace Imbedding Theorem (cf. [1], Theorem 5.36, p. 164) there is a constant $\bar{c} = \bar{c}(\Omega) > 0$ such that

$$\|u - \hat{u}\|_{L^2(\Gamma)} \leq \bar{c}\,\|u - \hat{u}\|_{H^1(\Omega)}, \tag{5.7}$$

which can be used to further estimate (5.6):

$$\int_0^t\int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) \leq \sqrt{c^*(t)}\,\bar{c}\left(\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)}\right)^{\frac{1}{2}}. \tag{5.8}$$

For arbitrary $\varepsilon > 0$, Young's inequality yields the following estimate on the right-hand side:

$$\sqrt{c^*(t)}\,\bar{c}\left(\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)}\right)^{\frac{1}{2}} \leq \frac{1}{2\varepsilon}c^*(t)\bar{c}^2 + \frac{\varepsilon}{2}\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)}. \tag{5.9}$$

Take $\varepsilon \in (0, 2d)$. Then (5.5)–(5.9) together yield

$$\|u - \hat{u}\|^2_{L^2(\Omega)} + (2d - \varepsilon)\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)} \leq \frac{1}{\varepsilon}c^*(t)\bar{c}^2 + 2d\int_0^t \|u - \hat{u}\|^2_{L^2(\Omega)}, \tag{5.10}$$

or

$$\|u - \hat{u}\|^2_{L^2(\Omega)} + \underbrace{(2d - \varepsilon)\int_0^t \|\nabla u - \nabla\hat{u}\|^2_{L^2(\Omega)}}_{\geq 0} \leq \frac{1}{\varepsilon}c^*(t)\bar{c}^2 + \varepsilon\int_0^t \|u - \hat{u}\|^2_{L^2(\Omega)}. \tag{5.11}$$

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It follows that

$$\|u - \hat{u}\|_{L^2(\Omega)}^2 \leq \frac{1}{\varepsilon} c^*(t) \bar{c}^2 + \varepsilon \int_0^t \|u - \hat{u}\|_{L^2(\Omega)}^2 \,, \tag{5.12}$$

and due to a version of Gronwall's lemma[2]

$$\|u - \hat{u}\|_{L^2(\Omega)}^2 \leq \frac{1}{\varepsilon} c^*(t) \bar{c}^2 \, \mathrm{e}^{\varepsilon t}, \tag{5.13}$$

where we use that $c^*(\cdot)$ is (by definition) non-decreasing. Note that ε is arbitrary but fixed[3], thus $1/\varepsilon < \infty$. We obtain (5.1) by defining $c_1 := \bar{c}^2 / \varepsilon$.

It also follows from (5.10) that

$$\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \leq \frac{1}{\varepsilon(2d - \varepsilon)} c^*(t) \bar{c}^2 + \frac{2d}{2d - \varepsilon} \int_0^t \|u - \hat{u}\|_{L^2(\Omega)}^2 \,. \tag{5.14}$$

The upper bound (5.13) now implies

$$\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \leq \frac{1}{\varepsilon(2d - \varepsilon)} c^*(t) \bar{c}^2 + \frac{2d}{\varepsilon^2(2d - \varepsilon)} c^*(t) \bar{c}^2 \, (\mathrm{e}^{\varepsilon t} - 1)$$

$$\leq \frac{2d}{\varepsilon^2(2d - \varepsilon)} c^*(t) \bar{c}^2 \, \mathrm{e}^{\varepsilon t}, \tag{5.15}$$

where we use that $\varepsilon < 2d$ in the second step. The second statement of the theorem now follows by defining $c_2 := 2d\bar{c}^2 / (\varepsilon^2(2d - \varepsilon))$. $\qquad\square$

Remark 5.2. In principle, (5.15) can be optimized in ε for every t separately, which gives an optimal $\varepsilon = \varepsilon(t)$. After substitution of this $\varepsilon(t)$, (5.2) becomes independent of ε. However, its t-dependence obviously becomes more complicated. Further details are omitted here.

Remark 5.3. The fact that the estimates in Theorem 5.1 are linear in c^* relates nicely to our Conjecture 4.8. If indeed c^* is small or even goes to zero, then the same holds for $\|u(\cdot, t) - \hat{u}(\cdot, t)\|_{L^2(\Omega)}^2$ and $\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2$.

Acknowledgments

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[2] A specific form of Theorem 1 on p. 356 of [18].

[3] Although the use of the letter ε might misleadingly suggest that we intend to take the limit $\varepsilon \to 0$, this is not the case.

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