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Characterization and Efficient Computation of Lagrangian Coherent Structures

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Abstract

A wide number of physical systems have been observed to contain Lagrangian structures at large scales that resist (diffusive) transport or mixing. However, a precise characterization of these structures that is amenable to both analysis and computation is elusive. In this cumulative dissertation, we describe some progress made in [55, 56, 57, 42] towards the question of characterization and efficient computation of Lagrangian coherent structures in time-dependent flows. This involves the analysis of connections between different methods in the literature for the computation of Lagrangian coherent structures from the viewpoint of the advection-diffusion equation; in particular the 'geometry' of the low-diffusivity limit (see [40]) of this equation is investigated in some detail. Asymptotic quantities relating to this limit are derived. We strengthen and/or provide new proofs for results already existing in the literature. We also provide proofs of hitherto unproven statements. In connection to this and other research, the `CoherentStructures.jl` Julia package was written in collaboration with others which aims to provide a high-quality implementation of methods for the computation of Lagrangian coherent structures.

Zusammenfassung

In einer großen Anzahl von physikalischen Systemen werden Lagrange'sche Strukturen beobachtet, die auf großen Skalen (diffusivem) Transport bzw Mischung widerstehen. Jedoch ist eine präzise Charakterisierung dieser Strukturen, welche sowohl analytischen als auch rechnerischen Methoden zugänglich ist, schwer fassbar. In dieser kumulativen Dissertation wird Fortschritt aus [55, 56, 57, 42] in diese Richtung beschrieben. Insbesondere werden Lagrange'sche kohärente Strukturen in zeitabhängigen Flüssen betrachtet. Verbindungen zwischen unterschiedlichen Methoden aus der Literatur werden untersucht, dies geschieht mit Hilfe der Advektions-Diffusions-Gleichung und deren 'Geometrie' (siehe auch [40]) im kleindiffusiven Limes. Asymptotische Eigenschaften von diesem Limes werden hergeleitet. Es werden neue und/oder stärkere Beweise für aus der Literatur bekannte Resultate geführt, und bisher unbekannte Resultate bewiesen. In Verbindung mit dieser und anderer Forschung wurde das `CoherentStructures.jl` Julia Softwarepaket in Zusammenarbeit mit anderen geschrieben; dieses hat das Ziel, hochwertige Implementierungen für Methoden für die Berechnung von Lagrange'schen kohärenten Strukturen bereitzustellen.

Index of included publications

Included in this cumulative dissertation are the following publications:

1. The publication [56], "Higher-order finite element approximation of the dynamic Laplacian" that appeared in Volume 54 No 5 of *ESAIM: Mathematical Modelling and Numerical Analysis (ESAIM: M2AN)* in 2020 is included as a 'Core-Publication'. The original publication is available at `www.esaim-m2an.org` and ESAIM M2AN owns the copyright, a permission to include it here is included in the appendix.

2. The publication [55], "Short-Time Heat Content Asymptotics via the Wave and Eikonal Equations" that appeared in Volume 31 of "The Journal of Geometric Analysis" in 2021 is also included as a 'Core-Publication'. It can be found at `https://link.springer.com/article/10.1007/s12220-020-00416-z`, and is licensed under a Creative Commons Attribution 4.0 International License license which can be found at `http://creativecommons.org/licenses/by/4.0/` .

3. The article [57] is included as an additional publication, a version of this article has been previously uploaded to arXiv as a pre-print. This article has been accepted to be published by the IOP Publishing Journal *Nonlinearity*.

4. The article [42] is also included as an additional publication, a version of this article has been previously uploaded to arXiv as a pre-print.

Contents

1 Background and Motivation

This section aims to provide an introduction to the subject matter considered, as well as looking at some methods used. Following a non-technical overview of the subject matter, I will use this section to describe the mathematical underpinnings of a few popular characterizations of "coherent structures". A contribution of this thesis has been to elucidate connections between some of these, and to answer some natural questions that have come up. The aim of this section is also to set the stage for the mathematical description of results of the papers submitted with this document.

1.1 Non-technical overview

Very informally, *coherent structures* can be defined as "interesting" regions of phase space that "stay together" when exposed to some underlying dynamics. An illustrative example is the case where the underlying dynamics is defined by advection by ocean surface velocities which we obtain by interpolating data from Copernicus Marine Environment Monitoring Service[1]. Figure 1.1 shows boundaries of two coherent sets (computed using the method described in [36, 41]), together with their images under the dynamics, on the left hand side. The same sets, when shifted by a small amount – displayed on the right – are no longer coherent but are extremely filamented.

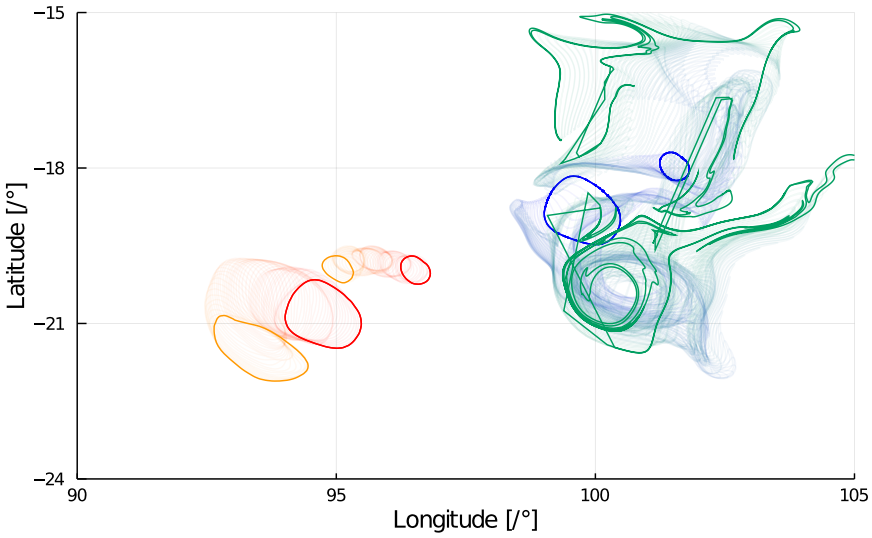

Figure 1.1: Sets on the left hand side (initial position red, advected position orange) are thought of as being *coherent*, in contrast to a set of the same shapes shifted by a small amount to the right (initial position blue, advected position green). Translucent lines show intermediate positions.

Defining coherent sets simply as those that "stay together" under the flow has the benefit of including the wide range of objects in the literature subsumed by the umbrella term "coherent structures", but an obvious drawback is that it is very vague. A large body of work exists trying to find precise, mathematical, characterizations of coherent structures. Much work has also been done to discover how these objects can then be computed.

[1]The velocity fields are publicly available at `https://resources.marine.copernicus.eu/?option=com_csw&view=details&product_id=SEALEVEL_GLO_PHY_L4_REP_OBSERVATIONS_008_047` and were interpolated using the `OceanTools.jl` package [54]

When several methods give similar results, it is natural to wonder if any structural connections between the methods exist. In [40], a geometric framework – the *geometry of mixing* – was introduced that suggested some connections of this form. In this framework, the Lagrangian point of view – in particular related to the advection-diffusion equation – was emphasized.
One contribution of my thesis has been to clarify a number of questions connected to coherent structures and the geometry of mixing. Firstly, in [42], we answered some open questions from [40] relating to the low-diffusivity behavior of the advection-diffusion equation. There, we then investigated the *weighted area form* induced by the geometry of mixing which had previously not been studied in this detail[2]. We were able to show precisely how this area form is closely related to both the methods in [16, 21] as well as those in [36, 37].

Previous works on coherent structures had often considered the action of the advection-diffusion equation, or other closely related mathematical operators, on smooth functions. However, when looking at coherent *sets* (as suggested by the general approach present already in [15, 23], see also [26]), the natural objects to investigate are not smooth functions, but *indicator functions*. My results in [55] and [57] can be seen as working on this idea. The result in [57] is a precise characterization — based on the area form in the geometry of mixing — of certain small-diffusion asymptotics related to indicator functions.

A significant portion of my time during in the past years was devoted to programming. Together with my colleagues, we developed the `CoherentStructures.jl` package, which currently contains some of the fastest and most efficient implementations of algorithms for computing coherent structures. Moreover, I wrote the `OceanTools.jl` package for dealing with large oceanographic datasets. A number of publications have used the `CoherentStructures.jl` such as [40, 37, 1] and possibly [58]), my master's thesis [41] (which also used `OceanTools.jl`), and [56] which is included here. In [56], we looked at a specific family of methods implemented in the `CoherentStructures.jl` package based on the work in [18] and investigated both theoretical and practical properties.

[2] This weighted area form does however appear in the published version of [40], which references [42], and the area form was eluded to in previous preprints of [40] also.

1.2 Flow Maps and Transfer Operators

Let us recap some basic definitions and concepts. References for the material here (section 1.2) include [45, 6, 2, 40].

Nonautonomous flows: The mathematical setting in which coherent structures can be found starts with the ordinary differential equation

$$x' = V(t, x), \tag{1.1}$$

defined by a smooth time-dependent vector field V on a smooth manifold M. In this work, we are interested in *finite time* behavior, i.e. we may take without loss $t \in [0, 1]$. We will implicitly assume that all further objects are smooth whenever this is possible and take M to be compact unless stated otherwise to avoid sensitive technical issues related to well-definedness. There is a *flow map* associated to eq. (1.1) which we denote by $\Phi_{t_0}^t$ for $t_0, t \in [0, 1]$. This flow map can be thought of as being a smooth function

$$(t, x) \mapsto \Phi_0^t(x)\,, \tag{1.2}$$

moreover $\Phi_0^t : M \to M$ is a diffeomorphism for every $t \in [0, 1]$.

Lagrangian coherent structures: A coherent set/structure[3] is a space-time subset $S \subset [0, 1] \times M$ that is in some way distinguished with regards to the underlying dynamics defined by eq. (1.2) - the precise details will depend on which definition is used [33, 16, 5, 34]. For such a set S, we denote the time-t slice by $S_t \subset M$, that is $\{t\} \times S_t = S \cap (\{t\} \times M)$. A large family of definitions for coherent structures have in common that they a priori restrict the space of Lagrangian subsets. Such definitions are the focus of this work. We call a set $S \subset [0, 1] \times M$ *Lagrangian* (or *material*, both terms are frequently used in the continuum dynamics literature), if it is invariant under the flow $\Phi_{t_0}^t$, i.e. if $S_t = \Phi_0^t(S_0)$ for all $t \in [0, 1]$. Clearly, a Lagrangian set is uniquely specified by any time-t slice. We will in this context make the identification of the whole (space-time) Lagrangian set $S \subset [0, 1] \times M$ with its time-0 slice $S_0 \subset M$. Given that Lagrangian sets are naturally in bijective correspondence with subsets of M, the restriction to Lagrangian sets still leaves a very large number of sets, and is not alone sufficient as a useful definition of coherent structures (see also [40, 34]).

[3] We treat the terms 'coherent sets' and 'coherent structures' as synonyms in this work, this is not always done in the literature.

1.2.1 The transfer operator

After fixing the initial time, eq. (1.2) induces a one-parameter family of linear operators $(P_t)_{t\in[0,1]}$ on differential forms by the formula

$$P_t(f) \coloneqq (\Phi_0^t)_* f\,, \tag{1.3}$$

where $(\Phi_0^t)_*$ is the differential geometric pushforward acting on k-forms $f \in \Gamma(\wedge^k T^*M) =: \Omega^k(M)$ for each value of $k = 0, \dots, n \coloneqq \dim(M)$. In the case that f is a function (i.e $k = 0$), the pushforward satisfies $(\Phi_0^t)_* f = f \circ (\Phi_0^t)^{-1}$, and the resulting operator $P_t : C^\infty(M) \to C^\infty(M)$ is called the *Koopman* operator for $(\Phi_0^t)^{-1}$. For top-level (volume) forms, P_t is called the *transfer* (or *Frobenius-Perron*) operator. This somewhat unconventional (though appearing in the literature in various forms) characterization of the transfer operator, has the advantage that it is mathematically very simple, we will now proceed to show the connection with the more common definition. In what follows, $(\Phi_0^t)^*$ denotes the pullback, which is the inverse to $(\Phi_0^t)_*$ because Φ_0^t is a diffeomorphism. When $f \in \Omega^n(M)$ and $h \in C^\infty(M)$, then $fh = f \wedge h$. As pullbacks commute with the wedge product,

$$\begin{aligned}\int_M h \wedge (\Phi_0^t)_* f &= \int_M (\Phi_0^t)_* (\Phi_0^t)^* h \wedge (\Phi_0^t)_* f \\ &= \int_M (\Phi_0^t)_* \left((\Phi_0^t)^* h \wedge f \right) \\ &= \int_M (\Phi_0^t)^* h \wedge f\,, \end{aligned} \tag{1.4}$$

where we used in the last step that $\Phi_0^t : M \to M$ is a diffeomorphism and so $\Phi_0^t(M) = M$. We will require a distinguished nondegenerate volume-form ω in order to now define a transfer operator on functions. The correspondence $f \leftrightarrow f\,\omega$ gives a bijection between smooth functions and volume forms[4], both directions of which we denote by $*$. For $t \in [0,1]$, an operator T_t – which we call the 'transfer operator on functions' – is defined by the commutative diagram

$$\begin{array}{ccc} \Omega^n(M) & \xrightarrow{P_t} & \Omega^n(M) \\ \updownarrow{\scriptstyle *} & & \updownarrow{\scriptstyle *} \\ C^\infty(M) & \xrightarrow{T_t} & C^\infty(M)\,. \end{array}$$

which is equivalent to requiring that $T_t(f)\,\omega = P_t(f\,\omega)$. Writing $\tilde{f} \coloneqq *f$, Equation (1.4) yields

$$\int_M h\; T_t \tilde{f}\;\; \omega = \int_M (h \circ \Phi_0^t)\;\; \tilde{f}\;\; \omega\,,$$

[4] When ω is the volume form of a Riemannian metric, then this bijection is well-known as the Hodge-$*$ operator [45, chap. X(§4)].

showing that T_t agrees with the conventional definition of the transfer operator [6, chapter 4]. As T_t *is* $P_t : \Omega^n(M) \to \Omega^n(M)$, modulo a bijection, we may think of either of these operators as the transfer operator. In some sense, P_t is the more 'natural' choice as no distinguished volume form is required. There is of course also the well-known generalization from volume-forms to pushforwards on measures, which is the same idea but in measure-theoretic language [6].

The dynamics defined by the transfer operator in function space (or, more generally, by eq. (1.3)) are linear even if the dynamical system Φ_0^t is not. As there is a large body of work related to discretisations of linear systems, this is convenient from the standpoint of numerical analysis.

A particularly interesting and well-known special case is the *volume-preserving* case, i.e. when $P_t\,\omega = \omega$. Here, it is straightforward to verify that $T_t \mathbb{1}_M = \mathbb{1}_M$, and the transfer operator T_t agrees with the differential geometric pushforward P_t on the space of functions.

Generalization to arbitrary diffeomorphisms: All of the preceding arguments make sense even if $(\Phi_0^t)_{t\in[0,1]}$ is just some one-parameter family of diffeomorphisms, there is no requirement for it to be a flow induced by an ODE. Similarly, Φ_0^t is not required to be a diffeomorphism from a space to *itself*, the generalization $\Phi_0^t : M_0 \to M_t$ with $M_0 \neq M_t$ (as featured, for example, in [16]; see also [21]) just requires that each manifold in $(M_t)_{t\in[0,1]}$ be equipped with some nondegenerate volume-form $\omega_t \in \Omega^n(M_t)$ for $t \in [0,1]$. The generalization of volume-preservation, i.e. $T_t \mathbb{1}_{M_0} = \mathbb{1}_{M_t}$ is readily seen to be equivalent to $\omega_t = (\Phi_0^t)_*\,\omega_0$. This is called *mass-preservation* (see [37, 40, 21] and the references therein) to highlight that the volume-forms $(\omega_t)_{t\in[0,1]}$ in general are not preserved (even when $\Phi_0^t(M) = M$), but there are close conceptual connections to the volume-preserving case as again $T_t = P_t$ on functions. *Any* system can be made into a mass-preserving one by choosing $(\omega_t)_{t\in[0,1]}$ appropriately.

1.2.2 The advection equation

Writing $u(t,x) = (P_t u_0)(x)$, differentiating eq. (1.3) immediately shows that

$$\partial_t u = -\mathcal{L}_V u \tag{1.5}$$

where $\mathcal{L}_V$ denotes the Lie derivative. This gives a PDE-theoretic approach related to the operators $(P_t)_{t\in[0,1]}$ which is well-known in the literature.

1.2.3 Lagrangian coordinates

Given that we are interested in *Lagrangian* sets, we wish to adopt a point of view in which the Lagrangian sets are constant over time. In differential geometric language, this means that we choose Φ_0^t as our (time-dependent) coordinate charts,

which is equivalent to pulling back any objects at time t by the diffeomorphism Φ_0^t. These coordinate charts are called *Lagrangian coordinates* and are well-known in the literature. By an abuse of notation, we will use the same symbols for the pulled back objects in Lagrangian coordinates as we did previously, i.e. we will write "u in Lagrangian coordinates" to refer to the object $(\Phi_0^t)^* u$.

Consistently with the continuum-mechanical convention, we call other non-time-dependent coordinates *Eulerian*. In Eulerian coordinates, the u appearing in eq. (1.5) is in general not constant with time. However, in Lagrangian coordinates it is - indeed, taking the PDE-theoretic perspective, using [45, Chapter V, Prop. 5.2] one sees that eq. (1.5) in Lagrangian coordinates becomes

$$\partial_t u = 0\,. \tag{1.6}$$

We will adopt a similar notation for a number of objects whenever it makes sense to do so. Thus if, for example, $S' = \Phi_0^1(S)$ for some subset $S \subset M$, then we may say that "S' is S in Lagrangian coordinates" as implicitly S' is an object in the codomain of Φ_0^1 and S in its domain. Likewise, the set $\Phi_0^1(S)$ may be called "S at time 1 in Eulerian coordinates". Typically, however, we will use this notation for functions that are explicitly defined on the space $[0,1] \times M$ or operators on such functions. As we did previously with sets, we can also identify a function $f : M \to \mathbb{R}$ with the function $f : [0,1] \times M \to \mathbb{R}$ defined via $(t,x) \mapsto \Phi_0^t(x)$ in Eulerian coordinates, in Lagrangian coordinates this is the function $(t,x) \mapsto f(x)$. The preceding example shows also that the pushforward operator is the identity in Lagrangian coordinates; indeed this is exactly how Lagrangian coordinates were defined. More precisely, for $f : M \to \mathbb{R}$, the function $f \mapsto (t, P_t f)$ in Eulerian coordinates is the function $f \mapsto (t, f)$ in Lagrangian coordinates. Typically the parameter t will be implicit and clear from the context and may therefore be omitted in what follows.

1.3 Transfer operator-based methods

Properties of discretizations of the linear operators $(T_t)_{t\in(0,1]}$ have a long history of use for the computation of 'dynamically interesting' features in phase space like coherent structures. This was initially done in the autonomous, non-Lagrangian case, i.e. when the vector field V in eq. (1.1) does not depend on time. In the volume-preserving case, each $(T_t)_{t\in[0,1]}$ is unitary [6, chapter 4], so its spectrum is contained in the unit circle. In practice, however, discretizations of T_t are typically *not* unitary, and "dynamically interesting" features can be found by looking at eigenvectors corresponding to largest-magnitude eigenvalues of the operator. Recognizing this, a common approach in the literature for analyzing such discretizations is to look at perturbations of transfer operators [11, 19, 15, 23]. In the sequel, we will look at some specific perturbations of transfer operators more closely. In some cases in the literature, the exact perturbation is not always made explicit and it is sometimes assumed that the numerical scheme used introduces sufficient "numerical diffusion" precluding the necessity of an explicit perturbation; cf. [19, 15].

An early example of this kind of transfer operator based approach is [11], which describes a Galerkin numerical method (a generalization of "Ulam's method" introduced in [63, Chapter VI.4]) based on box coverings for discretizing transfer operators of stochastic systems. In this case[5], the SRB-measures of suitable stochastically perturbed systems converge to the SRB-measure of the unperturbed system; moreover the discretisation yields a measure converging to the SRB-measure when applied to each of the stochastic systems[11]. Their definition of an *almost-invariant* set can be (conceptually) thought of as being the autonomous precursor to coherent structures; or conversely we may define coherent sets to be almost-invariant sets of a suitable perturbation in Lagrangian coordinates [40]. The connection between almost invariant sets and eigenvectors of the transfer operator (for suitably perturbed systems) was also made in [11].

A different approach to perturbation appears in [19]. Here, in the volume-preserving setting, eq. (1.5) in Euclidean space is perturbed to the *advection-diffusion equation*

$$\partial_t u = -\mathcal{L}_V u + \varepsilon \Delta u,$$

and, as we are in the autonomous setting, the (unbounded) operator $-\mathcal{L}_V u + \varepsilon\Delta u$ generates a semi-group of compact operators when $\varepsilon > 0$. This generator can be discretized, leading to computational methods in [15] for almost-invariant sets based on the eigenvectors and eigenvalues of this discretisation.

Similar issues arise when considering nonautonomous systems where eigenvalues/vectors must be replaced by singular values/vectors with respect to some Hilbert-spaces. Without a perturbation, the only singular value (on $L^2(M,\omega)$)

[5] The details are subject to some underlying assumptions as described in section 4 of [11].

in a mass-preserving system is 1. However, after a suitable perturbation, singular values/vectors again result in interesting quantities. This is the approach explored in [23], see also [22, 15]. In that work, adapted and here to our setting and notation, a quantity we refer to here (the same terminology appears in [58] for this quantity; see also the discussion in [5, 12]) as the *coherence ratio* (for a perturbation L_ε of the transfer operator) induced by function $\Phi_0^1 : M_0 \to M_1$ with ω_0, ω_1 being volume-forms on M_0, M_1 respectively) of two sets S, S' is defined in Eulerian coordinates as

$$\rho_\varepsilon(S, S') \coloneqq \frac{\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_{S'} \rangle_{L^2(M_1,\omega_1)}}{\omega_0(S)} + \frac{\langle L_\varepsilon \mathbb{1}_{M_0 \setminus S}, \mathbb{1}_{M_1 \setminus S'} \rangle_{L^2(M_1,\omega_1)}}{\omega_0(M_0 \setminus S)}, \tag{1.7}$$

where we recall that in the mass-preserving setting, $\omega_1 = (\Phi_0^1)_* \, \omega_0$. Maximizers of this ratio are known as *coherent pairs* (cf. also the discussion in [5, 23]; the idea is that coherent pairs formalize the idea of a coherent (space-time) set which does not lose much mass from the diffusion). Though typically this is not done in the transfer-operator literature, one may restrict to the Lagrangian case in which S and S' as the time-0 and time-1 slices respectively of a single Lagrangian space-time set, i.e. $S' = \Phi_0^1(S)$. This is also a particularly natural point of view as the coherence ratio for S without diffusion, i.e. $\rho_0(S, \cdot)$, is maximized by this choice of S'. This suggests the Lagrangian coherence ratio[57] , $\rho(S, \Phi_0^1(S))$, which can in the mass-preserving setting be written in Lagrangian coordinates as

$$\tilde{\rho}_\varepsilon(S) \coloneqq \frac{\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle_{L^2(M,\,\omega)}}{\omega(S)} + \frac{\langle L_\varepsilon \mathbb{1}_{M \setminus S}, \mathbb{1}_{M \setminus S} \rangle_{L^2(M,\omega)}}{\omega(M \setminus S)}, \tag{1.8}$$

and $M \coloneqq M_0, \omega \coloneqq \omega_0$ as an appropriate object to study in the Lagrangian setting. We remind the reader that eq. (1.8) is simply a special case of eq. (1.7), but our notation in Lagrangian coordinates identifies M_0, M_1 using Φ_0^1 and therefore only one manifold appears in eq. (1.8). In Eulerian coordinates, $L_\varepsilon : M_0 \to M_1$, which corresponds in Lagrangian coordinates to $L_\varepsilon : M \to M$ (recall that we defined $M = M_0$).

1.4 Some perturbations of transfer operators

The previous chapter has described ways in which perturbations of transfer operators are important. We include below some details of some particularly natural perturbations that can be found in the literature and were studied in greater detail in my work.

1.4.1 The advection-diffusion equation

In Eulerian coordinates, a singular perturbation of eq. (1.5) is the advection-diffusion equation

$$\partial_t u = -\mathcal{L}_V u + \varepsilon \Delta u \,, \tag{1.9}$$

where Δ is a Laplace operator acting on differential forms. We have mentioned this equation above in the autonomous case, but the equation remains well-defined when the vector-field V is time-dependent and/or the Laplacian in eq. (1.9) depends on time.

In Lagrangian coordinates, with some differential geometry [45, Chapter V, Prop. 5.2] one sees that eq. (1.9) becomes

$$\partial_t u = \varepsilon [(\Phi_0^t)^* \Delta] u \,, \tag{1.10}$$

which is a time-dependent heat equation; the advection-diffusion equation in Lagrangian coordinates is studied in [62]. Recall that the operator P_t is the time-t solution operator to eq. (1.5). Likewise, there is a time-t solution operator associated to eq. (1.9), which we write as $P_{t,\varepsilon}$. In Lagrangian coordinates, P_t is the identity; this is in marked contrast to $P_{t,\varepsilon}$ for positive t, ε – these are well-known to be compact operators on $L^2(M, \omega)$.

This PDE-theoretic point of view is particularly rich for the transfer operator on functions in the volume preserving setting. We also assume that Δ takes the form $\Delta = \operatorname{div}_\omega \circ \nabla$ – here the divergence $\operatorname{div}_\omega$ is defined via $(\operatorname{div}_\omega W)\,\omega = \mathcal{L}_W \omega$ for smooth vector fields W, and ∇u is the Riemannian gradient induced by some metric. Then, eq. (1.10) (still in Lagrangian coordinates) becomes

$$\partial_t u = \varepsilon \operatorname{div}_\omega \nabla_t u = \varepsilon \operatorname{div}_\omega g_t^{-1} \mathrm{d}u \,, \tag{1.11}$$

where ∇_t is a Riemannian gradient for a *time-dependent* metric[6] $(g_t)_{t\in[0,1]}$ obtained by pulling back the metric of the Laplacian in eq. (1.9) by Φ_0^t [40]. We have also used that $\nabla_t u = g_t^{-1} \mathrm{d}u$ and d is the exterior derivative; the notation g_s^{-1} appearing in eq. (1.11) should be understood as the well-known identification of the metric tensor with an isomorphism from tangent to cotangent space, see e.g. [45]. Even

[6] With *time-dependent metric* we simply mean a one-parameter family of metrics indexed by the time parameter.

if the Laplacian in eq. (1.9) does not depend on time, changing to Lagrangian coordinates will (in general) result in a time-dependent metric as featured in eq. (1.10).

This reasoning extends in a straightforward way to the mass-preserving case, for further details on this and on the steps outlined above, see [40, 42].

Averaging and the dynamic Laplacian, the geometry of mixing: In [40] it was suggested to (in Lagrangian coordinates) replace eq. (1.11) by the much simpler equation

$$\partial_t \overline{u} = \varepsilon \operatorname{div}_\omega \left(\int_0^1 g_s^{-1} \mathrm{d}s \right) \mathrm{d}\overline{u} \,, \tag{1.12}$$

which is the heat equation on a weighted Riemannian manifold (see [50, 30, 4]; we have collected some basic differential geometric definitions and results also in the appendix of [42]), whose Laplace operator is the *dynamic Laplacian* from [16]. The time-t solution operator for this equation, denoted here (in Lagrangian coordinates) by $\overline{P}_{t,\varepsilon} = \exp(t\varepsilon\overline{\Delta})$ is also a perturbation of P_t. A marked advantage of $\overline{P}_{t,\varepsilon}$ over $P_{t,\varepsilon}$ is that the former is self-adjoint in Lagrangian coordinates [40, 53], whereas the latter is not, in general.

The weighted Riemannian manifold $(M, \overline{g}, \omega)$ with Laplace operator $\overline{\Delta}$ was dubbed the *geometry of mixing* in [40]. The Riemannian metric of this manifold is readily seen to be given by $\overline{g} = \left(\int_0^1 g_t^{-1} \mathrm{d}t \right)^{-1}$ and the volume-form is the mass-form conserved by the advection/diffusion equation. In [42], which is included here, we look at the geometry of mixing – in particular its induced area form (cf. [51, section 18.1]) – in more detail. We are unaware of conceptually prior study of this area form in the literature; though there is some further discussion on the approach used in [42] in [40] and the (unweighted) area in $(M, \overline{g})$ had been previously mentioned in [42] also.

1.4.2 Averaging over geodesic balls

Another perturbation of the transfer operator can be found in works like [15], the idea is to (pre/post) compose the transfer operator with a convolution-like operator. A possible choice of this form is averaging over geodesic balls, i.e. the operator

$$(I_{g,\omega,\varepsilon} f)(x) \coloneqq \frac{1}{\omega(B_g(x,\varepsilon))} \int_{B_g(x,\varepsilon)} f(y) \mathrm{d}\,\omega(y) \,, \tag{1.13}$$

where ω is some (finite) measure/volume-form and $B_g(x,\varepsilon)$ is the geodesic ball of radius ε centered at x defined using the metric g on the smooth complete (but not necessarily compact) Riemannian manifold M. We have identified the volume-form ω with its induced measure in the equation above. The operators $I_{g,\omega,\varepsilon}$,

being of Hilbert-Schmidt-type [44], are compact on $L^2(M,\omega)$. In the literature, more general convolutions of the transfer operator are also present, but this is an interesting special case.

In order to understand this operator better, we present an amalgam of ideas from [46, 29, 61], see also [16, 21]. This interesting Fourier/functional analytic point of view has not been prominently featured in the coherent structures literature, so I present it here in more detail. This will become relevant in the sequel where we sketch how methods used in [55] are applicable not only to the heat flow, but also to $I_{g,\omega,\varepsilon}$.

As noted in [46], the operator $I_{g,\omega,\varepsilon}$ can be written as function of $\sqrt{-\Delta}$ when (M,g) and ω come from the flat torus, the same reasoning works for n-dimensional Euclidean space. To see this, observe that $I_{g,\omega,\varepsilon}$ is convolution with (the scaled indicator function of) a ball

$$F_\varepsilon(x) = \mathbb{1}_{B(0,1)}(\varepsilon^{-1}x)/\,\omega(B(0,\varepsilon))\,.$$

Writing c_n as the volume of the n-dimensional unit ball, we calculate that in Fourier-space,

$$\begin{aligned}\hat{F}_1(\xi) &= \frac{2(2\pi)^{-n/2}}{c_n}\int_0^1 c_{n-1}\cos(|\xi|t)\left(1-t^2\right)^{\frac{n-1}{2}}\mathrm{d}t\\ \hat{F}_\varepsilon(\xi) &= \hat{F}_1(\varepsilon\xi)\,.\end{aligned}$$

We know that convolution corresponds to (suitably scaled) multiplication in Fourier space. It thus follows directly via the functional calculus that

$$I_{g,\omega,\varepsilon} = \frac{2c_{n-1}}{c_n}\int_0^1 \cos(t\sqrt{-\varepsilon^2\Delta})(1-t^2)^{\frac{n-1}{2}}\mathrm{d}t\,. \tag{1.14}$$

This is because the spectrum of the Euclidean Laplacian Δ is the negative real line, and eigenfunctions of eigenvalue $-|k|^2$ are trigonometrical functions of frequency k, convolution operators with radial functions (which correspond to multiplication by a radial function in Fourier-space) can be expressed in terms of functions of Δ; see [61, Eq. 3.5.26]. By Taylor-expanding the cosine in the equation above, well-known results on the beta function [61, Eq. 3.A.24] yield (at least formally, see also [46] (in particular Eq. 1.6 and 1.14 there) which is in the same vein and goes on to prove much stronger results), that

$$I_{g,\omega,\varepsilon} = \mathrm{Id} + \frac{\varepsilon^2}{2(n+2)}\Delta + O(\varepsilon^4)\,; \tag{1.15}$$

this result – including its generalization to Riemannian manifolds – has already been mentioned in the coherent structures context in [40]. By explicitly looking

at the remainder in the Taylor expansion we can say even more about the convergence of eq. (1.15). To do so, let us write $\cos(x) = 1 - \frac{x^2}{2} + x^4 r(x)$ where $r(x)$ is a bounded function. Thus, evidently

$$I_{g,\omega,\varepsilon} f = f + \frac{\varepsilon^2}{2(n+2)} \Delta f + \underbrace{\int_0^1 (t\sqrt{-\varepsilon^2\Delta})^4 r(t\sqrt{-\varepsilon^2\Delta})(1-t^2)^{\frac{n-1}{2}} f \mathrm{d}t}_{:= R_f(\varepsilon)} .$$

Denoting the Fourier-transform of the function $R_f(\varepsilon)$ by $\hat{R}_f(\varepsilon)$, observe that directly from the definition of $R_f(\varepsilon)$

$$\hat{R}_f(\varepsilon)(\xi) = \varepsilon^4 \int_0^1 t^4 |\xi|^4 r(t\varepsilon|\xi|)(1-t^2)^{\frac{n-1}{2}} \hat{f}(\xi) \mathrm{d}t \,,$$

and as a consequence,

$$|\hat{R}_f(\varepsilon)(\xi)| \leq C\varepsilon^4 |\xi|^4 |\hat{f}(\xi)| \tag{1.16}$$

for suitable $C > 0$. Indeed, recall that the Sobolev spaces $H^k(\mathbb{R}^n)$ can be defined using growth rates of the Fourier-transform at infinity [61, chapter 4], and thus eq. (1.16) can be used to bound weak derivatives of the remainder $R_f(\varepsilon)$ in terms of weak derivatives of f. More precisely, this shows that if f has $k \geq 4$ weak derivatives in L^2 (i.e. $f \in H^k$), then the convergence in eq. (1.15) is in the Sobolev space H^{k-4}; this also locally gives uniform convergence of all derivatives for sufficiently smooth f by the Sobolev embedding theorems.

Though we do not make us of this fact yet, we mention that $\cos(t\sqrt{-\Delta})$ is the solution-operator for the *wave-equation* [61] which means eq. (1.14) can also be interpreted as an integral over the solution to an appropriate wave equation.

Unfortunately, eq. (1.14) no longer holds exactly on general Riemannian manifolds, but results relating to eq. (1.15) including certain spectral results are obtained in [46]. The ideas used in [29, chap. 11] on a similar quantity offer a simpler way of seeing why eq. (1.15) holds, and we will use them to make a slight generalization to the *weighted* manifold setting in what follows. For a point p in a complete smooth (not necessarily compact) Riemannian manifold (M, g), we follow [29, chap. 11] and pull the Euclidean metric on $\mathbb{R}^n$ to M via the geodesic normal coordinates at p, and write $\tilde{g}$ for this metric. By construction, the $\tilde{g}$-geodesic-normal-coordinates centered at p agree with those for g. The associated Laplace operator and volume-form to the Riemannian manifold $(M, \tilde{g})$ are denoted by $\tilde{\Delta}$ and $\tilde{\omega}$ respectively. To reduce clutter we omit the dependence on p in the notation. It is well-known that $\tilde{\Delta} = \Delta$ at p, here Δ refers to the Laplace operator on the Riemannian manifold (M, g). If we write $\tilde{\theta}\tilde{\omega} = \omega$, then $I_{g,\omega,\varepsilon} f = I_{\tilde{g},\tilde{\omega},\varepsilon}(f\tilde{\theta}) / I_{\tilde{g},\tilde{\omega},\varepsilon}(\tilde{\theta})$ and applying eq. (1.15) to denominator and numerator together with the quotient rule for derivatives yields

$$I_{g,\omega,\varepsilon} f = f + \frac{\varepsilon^2}{2(n+2)} \left(\Delta f + \frac{2\nabla f \cdot \nabla \tilde{\theta}}{\tilde{\theta}} \right) + o(\varepsilon^2) \,. \tag{1.17}$$

We would like to replace $\tilde{\theta}$ with θ in the formula above. To see that this can be done, observe that g agrees with $\tilde{g}$ near p up to a second-order error in the geodesic normal coordinate representation [29, Corollary 9.8]; for $\tilde{g}$ this is trivial as it has been *defined* to have coordinate representation equal to the identity. If ϱ is the Riemannian volume of g, then the coordinate representation of ϱ will agree with $\tilde{\omega}$ with the same asymptotic error [29, Corollary 9.9]. Writing $\omega = \theta\varrho$, the same may be said of $\tilde{\theta}$ and θ. Thus we may replace $\tilde{\theta}$ with θ in eq. (1.17), which leads to the somewhat surprising[7] conclusion that on smooth functions,

$$I_{g,\sqrt{\theta}\varrho,\varepsilon} = \mathrm{Id} + \frac{\varepsilon^2}{2(n+2)}\Delta_{\omega,g} + o(\varepsilon^2),$$

where $\Delta_{\omega,g} = \mathrm{div}_\omega \circ \nabla_g$. A more explicit examination of this setup shows that the locally uniform convergence of any derivatives carries over from the Euclidean setting to the general weighted manifold case given sufficient smoothness.

[7] This is surprising as $\sqrt{\theta}$ appears in the left hand side instead of θ, see also the connection to [30, Equation (2.4)].

1.5 Dynamic isoperimetry and the dynamic Laplace

As described in section 1.3, the introduction of a perturbation of the transfer operator has the advantage of sidestepping certain technical difficulties. However, a marked disadvantage is the fact that one introduces a new parameter ε to control the strength of the perturbation. It is not clear what value of $\varepsilon > 0$ should be chosen, so a natural approach when lacking a clear physical model for the perturbation is to consider the limit $\varepsilon \to 0$. Such limits are present – sometimes more explicitly and sometimes less explicitly – in a number of places in the coherent structures literature[16, 5, 36].

When choosing a perturbation like that of pre/post-averaging over suitably scaled ε-geodesic balls, this perturbation is closely related to a Laplace-type operator (see previous chapter). In [16], similar questions are investigated for the perturbation of the time-1 transfer operator T_1 defined in Eulerian coordinates (with our notation) by

$$\mathcal{L}_\varepsilon = I_{(\Phi_0^1)_* g_1, \mathrm{d}g, \varepsilon}\ T_1\ I_{g, \mathrm{d}g, \varepsilon} \tag{1.18}$$

where g, g_1 are flat metrics in the domain and codomain respectively of a volume-preserving flow Φ_0^1 and the volume form induced by g is denoted by $\mathrm{d}g$. Consistent with the asymptotics described in section 1.4.2, they find that (for sufficiently smooth functions f),

$$\mathcal{L}_\varepsilon^* \mathcal{L}_\varepsilon f = \left(\mathrm{Id} + C\varepsilon^2 \left(\frac{\Delta + (\Phi_0^1)^* \Delta}{2}\right)\right) f + o(\varepsilon^2)$$

pointwise as $\varepsilon \to 0$, here C is a constant depending only on the dimension. The setup in [16] is slightly more general and includes other convolutional operators. Extensions to non-flat manifolds are in [21]; though their approach appears to use a slightly different generalization to the one considered here. The operator $\frac{1}{2}\left(\Delta + (\Phi_0^1)^* \Delta\right)$ was coined the *dynamic Laplacian* for Φ_0^1, with natural extensions to multiple time-steps and/or the setting of continuous time which has already been mentioned. Being similar to the usual Laplace operator, a number of interesting results make it possible to prove statements related to dynamical systems with this object.

Definition of coherent structures: Coherent structures, in the dynamic Laplace approach of [16], come from minimizing the functional

$$F(\Gamma) := \frac{\mathrm{hypearea}(\Gamma) + \mathrm{hyperarea}(\Phi_0^1(\Gamma))}{2 \min\{\mathrm{vol}(M_1), \mathrm{vol}(M_2)\}}$$

over smooth surfaces Γ that partition M into submanifolds M_1, M_2. It is typically not feasible to compute a minimizer exactly, but the minimal value can be bounded using the first nontrivial eigenvalue of the dynamic Laplacian, this is

the *dynamic Cheeger Inequality* of [16, 21] which states that the leading nonzero eigenvalue λ_2 of the dynamic Laplacian satisfies

$$\min_{\Gamma} F(\Gamma) \leq 2\sqrt{-\lambda_2}\,,$$

where Γ takes the form described above. We provide a different proof of the dynamic Cheeger inequality in [42], which yields a slightly stronger result than the one present in [24, 21]. This is done by a reduction to the Cheeger inequality on weighted manifolds by making use of the area-form in the geometry of mixing.

Eigenfunctions of the dynamic Laplacian *are* again computationally tractable [16, 17, 18], and these are used (sometimes in conjunction with other methods like [25]) when computing coherent structures (see also [58]).

As observed in [40], the dynamic Laplacian is the Laplace-operator on a weighted Riemannian manifold, and the connection to the classical Laplace-operator also (as again observed in [40]) means that results such as [10], which may be relevant to extending ideas like the dynamical Cheeger inequality to n-partitions, can be applied.

In terms of computation, discretization of the dynamic Laplace operator is in some sense easier than of the transfer-operator. This is because the dynamic Laplacian is an uniformly-elliptic second-order differential operator, for which finite element methods are well-suited [13]. Methods based on finite-elements have been used in [18], but there are also approaches to discretization based on radial basis functions [17]; there is also a trajectory-based method with close connections to the dynamic Laplacian in [5]. The publication [56] included here looks at the discretizations from [18] in more detail. There, we go beyond [18] by looking at higher-order finite-element methods for this problem and by proving convergence for some methods that were previously not known to converge.

1.6 Material barriers/Black-hole vortices

The *geodesic vortex* methods at first glance appear to be completely unrelated to other methods for computing coherent structures. Our presentation here takes an abstract point of view (as already partially present in [41]) summarizing some aspects of methods appearing in [35, 59, 36, 37]. The bottom line of this family of approaches is that there are a number of variational problems in two dimensions[8] whose solutions correspond to curves of constant "strain". Such curves can be computed efficiently, and on very large domains [39, 41].

The first source of such variational problems arises from the fact that if a time-independent Lagrangian L only depends on the *direction* of the velocity component (i.e. $L(\gamma, \gamma') = L(\gamma, c\gamma')$ for all $c > 0$), then Noether's theorem immediately yields that L is a conserved quantity along stationary points $\gamma : [a, b] \to M$ of the action functional

$$\mathcal{L}_0(\gamma) \coloneqq \int_a^b L(\gamma(t), \gamma'(t))\mathrm{d}t\,. \tag{1.19}$$

Such an L may be constructed, for example, from a pair of covariant symmetric rank-2 tensor-fields (i.e. sections of $\otimes^2 T^*M$) T_0 and $\mathbf{T}$ with $L(\gamma, \gamma') \coloneqq f(\mathbf{T}(\gamma', \gamma')/T_0(\gamma', \gamma'))$ for some invertible smooth function f, provided that T_0 is Riemannian. We have left the dependence of $\mathbf{T}(\gamma', \gamma')$ and $T_0(\gamma', \gamma')$ on $\gamma(t)$ implicit in the notation. As L is conserved, the $(\mathbf{T}, T_0)$-strain, defined as

$$\sqrt{\mathbf{T}(\gamma', \gamma')/T_0(\gamma', \gamma')}$$

, is also conserved by stationary points of eq. (1.19), for more details related to specific constructions of this form see the reasoning in [35, 59].

Another source of such variational problems, again given Riemannian metric T_0 and $\mathbf{T}$ as above, is the functional

$$\mathcal{L}_1(\gamma) \coloneqq \frac{\int_\gamma \mathbf{T}(\gamma', \gamma')/T_0(\gamma', \gamma')\mathrm{d}A}{\int_\gamma \mathrm{d}A} \tag{1.20}$$

where $\mathrm{d}A$ is the Riemannian area from T_0. As observed in [36], stationary points γ with $\lambda \coloneqq \mathbf{L}_1(\gamma))$ are stationary points of

$$\mathcal{L}_2(\gamma) \coloneqq \int_\gamma (\mathbf{T}(\gamma', \gamma')/T_0(\gamma', \gamma') - \lambda)\,\mathrm{d}A\,, \tag{1.21}$$

but applying Noether's theorem to the time-invariance of the Lagrangian in $\mathcal{L}_3$ does not yield a non-trivial conserved quantity. Incidentally, this is not entirely

[8] Some of the theory, such as that in [36] can be extended to higher dimensions, but there are hitherto unsolved challenges related to proving existence of minimizers and their computation.

surprising given the reparametrisation invariance of the Lagragian (see [27]), this is an example of gauge-symmetry as defined in [3]. However, it is shown in [36] for Riemannian $\mathbf{T}$ that $\mathbf{T}(\gamma', \gamma')/T_0(\gamma', \gamma')$ is nevertheless a conserved quantity along stationary points of the functional. This general approach is taken in [36, 37] to define coherent structures.

Definition of coherent structures: *Closed*[9] curves γ that are stationary points of eq. (1.19), are conceptually seen as boundaries of coherent structures. The tensor-field T_0 is typically the standard Euclidean metric in some choice of coordinates, and curves of constant $(\mathbf{T}, T_0)$-strain can be computed using an eigendecomposition of the coordinate representation of $\mathbf{T}$ in the T_0 Euclidean standard basis [35, 39, 41].

A specific choice of $\mathbf{T}$ is of particular relevance here. In [36], where $M \subset \mathbb{R}^n$, an expression was derived for the leading-order term of the Lagrangian diffusive transport through a hypersurface Γ in the volume-preserving advection-diffusion equation for sufficiently smooth initial conditions. If u is the solution to the advection-diffusion equation eq. (1.10) then this *diffusive transport* out of the Lagrangian set S can be written (in Lagrangian coordinates) as

$$T(u_0, \varepsilon, S) \coloneqq \int_0^1 \int_{\partial S} \nabla u(t, x) \cdot (\mathbf{T}_0^t(x)\nu(x)) \mathrm{d}A(x) \mathrm{d}t \,, \tag{1.22}$$

Here $\mathrm{d}A$ is the Euclidean area, ν is unit-normal to ∂S and $\mathbf{T}_0^t$ are some tensors. Choosing $\overline{\mathbf{T}} = \int_0^1 \mathbf{T}_0^t \mathrm{d}t$, it is shown in [36] (we are summarizing here to make the connections to other methods clearer, they prove a slightly stronger and more general claim, see there also for technical assumptions needed) that this quantity is given by

$$T(u_0, \varepsilon, S) = \varepsilon \int_{\partial S} \nabla u(0, x) \cdot (\overline{\mathbf{T}}(x)\nu(x)) \mathrm{d}A(x) + o(\varepsilon). \tag{1.23}$$

This quantity naturally depends on the initial condition $u(0, \cdot)$. In [36], normalizing by the length of this gradient (at initial time), by taking $u(0, \cdot)$ to be a function with a uniform length gradient in the metric at initial time yields a leading-order term usable for the numerator in $\mathcal{L}_1$ even if the length of this gradient is arbitrarily large. The geodesic vortices for this case are called *material barriers (to diffusive transport)*, extensions to the non-volume-preserving case are given in [37]. We describe a new connection between eq. (1.23) and the dynamic Laplace operator/geometry of mixing in [40].

[9] The curve $\gamma : [a, b] \to M$ is *closed* if $\gamma(a) = \gamma(b)$.

1.7 Relaxation to (smooth) functions

Though conceptually one is typically interested in *sets*, a common approach, shared by the methods described above, is to formulate an approach based on (often smooth) functions, which in some cases can be seen as a *relaxation* step [12, 15]. For example, the reasoning in [36] described in the previous section can be read as investigating the diffusive outflow of a set using a smooth functions with arbitrarily larger gradient; which is calls to mind the idea of a function with discontinuity at the boundary of the set. Similarly, [16] looks at the dynamic Laplace, which is only defined classically on sufficiently smooth functions, while mentioning "mass lost through the boundary [...] via continually-present small-scale-diffusion"[16, p. 2], which suggests that the advection-diffusion equation, with an *indicator function* as the initial condition is relevant to questions related to coherent sets.

The mathematical analysis of properties of indicator functions under the kinds of perturbed transfer operators we have seen so far is much more difficult as indicator functions are not smooth. In the case that there is no advection, the advection-diffusion equation reduces to the heat-equation on a Riemannian manifold. The diffusive outflow from a set can then be calculated; a generalization of this quantity is referred to the *heat content out of a manifold* by [65] who use methods using pseudodifferential operators and invariance theory, to investigate this quantity, see also [49]. There is also a large literature on a different kind of heat content – which looks at the action of the heat equation with constant initial condition on a manifold with boundary [64].

In [55], which is included here, we present a different proof for some small-time asymptotic quantities related to a form of the heat content out of a manifold. Though [55] is less general than [65] in some ways, more general manifolds are considered there as the results apply to any complete Riemannian manifold. It also states its results for a more general class of functions $k(\sqrt{-t\Delta})$ and not only the heat flow; though it should be noted that these generalizations are in some sense straightforward once one takes into account the well-known relationship between the heat– and wave– equations (as featured for example in [9, 61]).

In [57] we derive leading-order asymptotics (in the low-diffusivity limit) of a form of the heat-flow in time-dependent heat flows. To the best of our knowledge, this has hitherto not been done in the literature. This also yields new asymptotics for the diffusive transport out of a material set in the setting that the initial condition is an indicator function.

Our approach in [57] makes use of stochastic analysis. Indeed, via the well-known Kolmogorov backwards equation [14] it becomes possible to reason about certain partial differential equations using stochastic differential equations (and vice versa). On the other hand, the classical result from [7] allows for stochastic differential equations to be approximated by other (simpler) stochastic differential equations in certain settings. This kind of reasoning (being well-known in the

literature), makes it possible to use stochastic differential equations to reason about partial differential equations. In [57], we use it to reduce the leading-order behavior of the diffusive outflow from a material set to the diffusive outflow from the same material set in the heat flow of the geometry of mixing. This, in turn, is known from [65, 55] to be equivalent to the short-time diffusive outflow from a set. For more details on the specific methods used there, we refer to [57].

1.8 Other methods

For the sake of completeness, we mention that there is a plethora of further methods sometimes included under the umbrella term "coherent structures". A comparison of a large number of methods can be found in [32]. There are also a number of methods that work directly on trajectories (see e.g. [5]), which we have not looked at here further.

2 Results

Before describing the publications included in more detail, recall the earlier adaption of the *coherence ratio* appearing in [23] to the Lagrangian setting. With L_ε being a perturbation of T_1, the expression from eq. (1.7) in Lagrangian coordinates is

$$\tilde{\rho}_\varepsilon(S) \coloneqq \frac{\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle}{\omega(S)} + \frac{\langle L_\varepsilon \mathbb{1}_{M\setminus S}, \mathbb{1}_{M\setminus S} \rangle}{\omega(M \setminus S)}\,, \tag{2.1}$$

where $\langle \cdot, \cdot \rangle$ is the $L^2(M, \omega)$ inner product. Naturally, the asymptotics of $\tilde{\rho}$, as $\varepsilon \to 0$, depend on which perturbation of the transfer-operator T_1 (or, equivalently, the identity in Lagrangian coordinates) is chosen. We restrict ourselves here and in what follows to the mass-preserving case, i.e. $\omega \coloneqq \omega_0$ and $\omega_t = P_t\, \omega_0$.

As is done in the literature, relaxing the numerator of the first term from sets (i.e. indicator functions) to smooth functions readily yields the term $\langle L_\varepsilon f, f \rangle$ (in Eulerian coordinates this would be $\langle L_\varepsilon f, T_1 f \rangle_{L^2(M_1,\omega_1)}$). We now turn to looking at specific choices for the perturbation L_ε:

1. Let us define (depending on a metric g and the volume-form ω) the operators $J_{g,\omega,\varepsilon} \coloneqq \exp(\varepsilon \Delta_{g,\omega})$. In Eulerian coordinates, $L_\varepsilon = J_{g,\omega_1,\varepsilon} \circ T_1$ is a perturbation of the transfer operator, in Lagrangian coordinates this perturbation reads $L_\varepsilon = J_{(\Phi_0^1)^* g,\omega,\varepsilon}$. For a time-independent metric g, defining $g_1 \coloneqq (\Phi_0^1)^* g$, the $\varepsilon \to 0$ asymptotics are readily found by Taylor expansion of the heat-flow $J_{g_1,\omega,\varepsilon}$ at $\varepsilon = 0$, so the leading-order behavior is $\mathrm{Id} + \varepsilon \Delta_{g_1,\omega} + O(\varepsilon^2)$, i.e. this case is nothing but applying well-known results on the heat flow.

2. The averaging-over-geodesic-balls operator $I_{g,\omega,\varepsilon}$ also has a $\varepsilon \to 0$ Taylor-expansion on smooth functions which we described in a previous section (see also the references given there). Replacing $J_{g_1,\omega,\varepsilon}$ with $I_{g_1,\omega,\varepsilon}$ in item 1. is thus also straightforward.

In both cases, the leading-order deviation from the identity depends on a Laplacian. We are thus firmly in the classical theory when it comes to minimizers of the $\varepsilon \to 0$ limit of suitably relaxed expressions like eq. (2.1) over smooth functions. The same reasoning extends also to the setting where we both pre- and post-compose (as opposed to merely post-composing) a suitable perturbation by applying a Taylor-expansion to each; the resulting operator in the ε^2 coefficient

will be the dynamic Laplace operator. In case of item 1. above, the permissibility of doing so follows from the fact that for sufficiently smooth f, the error term implicit in the $O(\varepsilon^2)$ notation is smooth and sufficiently many derivatives can be uniformly bounded as $\varepsilon \to 0$ using standard methods from the theory of heat flow. This result appears for flat manifolds in [21]. The permissibility for the analogous modification in point 2. can be derived from the machinery outlined in section 1.4.2 in the general case of Riemannian manifolds. It is possible that the methods in [21] can also be applied to this question, though it appears that the averaging operator there is of a slightly different form than the one used here.

2.1 Summary of [42]

We have already mentioned that an alternative to the perturbations considered in 1.–2. above is given by choosing L_ε to be the time-1 solution operator $P_{1,\varepsilon}$ of the mass-preserving advection-diffusion equation. In Lagrangian coordinates, this is the time-1 solution operator to the time-dependent heat equation

$$\partial_t u = \varepsilon \Delta_t u \,,$$

where $\Delta_t \coloneqq (\Phi_0^t)^* \Delta$ takes the form $\Delta_t = \operatorname{div}_\omega g_t^{-1}$ for a time-dependent family of metrics $(g_t)_{t\in[0,1]}$.

We considered the $\varepsilon \to 0$ behavior of eq. (2.1) relaxed to smooth functions. Using the methods from a very similar proof in the literature, we show in [42] that for sufficiently smooth f, subject to some technical conditions,

$$P_{1,\varepsilon} f = f + \overline{\Delta} f + O(\varepsilon^2) \,. \tag{2.2}$$

Here $\overline{\Delta} u \coloneqq \operatorname{div}_\omega \left(\int_0^1 g_s^{-1} \mathrm{d}s \, \mathrm{d}u \right)$ is the dynamic Laplacian. This is the same asymptotic behavior as that of $\overline{P}_{1,\varepsilon} \coloneqq \exp(\varepsilon \overline{\Delta})$, for which the $\varepsilon \to 0$ behavior is well-known from semi-group theory [53].

As $\overline{P}_{1,\varepsilon}$ comes from a semi-group generated by the dynamic Laplacian, the spectral mapping theorem for semi-groups (see [53]) applies and can be used to yield statements about the singular values of $\overline{P}_{1,\varepsilon}$ based on those of $\overline{\Delta}$. This is not true for $P_{1,\varepsilon}$. We are able to nevertheless show in [42] that the leading singular values of $P_{1,\varepsilon}$ obey $\varepsilon \to 0$ asymptotics similar to those of $\overline{P}_{1,\varepsilon}$, with the corresponding singular vectors converging (as $\varepsilon \to 0$) to eigenvectors of the dynamic Laplacian. This is done using some PDE-theoretic arguments that rely on a periodisation approach like the one employed in [20] and a proof using ideas similar to the well-known direct method from the calculus of variations.

As conjectured in [40], the geometry of mixing thus is intimately connected to the small-ε asymptotics of $P_{1,\varepsilon}$ via the dynamic Laplacian. As a (weighted) geometry, there exist further geometrical structures apart from the Laplacian. Looking in particular at the *(hyper)area-form* defined by this geometry, which we write as $\mathrm{d}\overline{A}$, is shown in [42] to be a fruitful endeavor. From an expression for this object, we are able to recover (and even strengthen) the dynamic Cheeger inequality of [16, 21] directly from the classical one on weighted manifolds.

We are also able to prove a result on the *diffusive outflow* from a set (in Lagrangian coordinates) in the advection-diffusion equation, which was proven originally in [36] and which was mentioned above as eq. (1.23). The diffusive outflow out of a set S may be defined as $T(f,\varepsilon,S) = \langle P_{1,\varepsilon} f, \mathbb{1}_{M\setminus S}\rangle - \langle f, \mathbb{1}_{M\setminus S}\rangle$, so applying eq. (2.2) yields

$$T(f,\varepsilon,S) = -\varepsilon \int_S \overline{\Delta} \mathrm{d}\,\omega + O(\varepsilon^2) = \varepsilon \int_{\partial S} \overline{\nu}(\mathrm{d}f) \mathrm{d}\overline{A} + O(\varepsilon^2)$$

where $\overline{g}$ is the metric in the geometry of mixing and $\overline{\nu}$ is $\overline{g}$-unit normal to ∂S. The last step is the divergence theorem. This shows deep connections between the material-barriers of [36] and the dynamic Laplacian of [16, 21]. Indeed, the expression in the numerator of the functional in [36] is

$$\int_{\partial S} \langle \overline{\nu}, \nu_0 \rangle_{\overline{g}} \, \mathrm{d}\overline{A} \,,$$

where ν_0 is g_0-unit normal to ∂S.

Clarification of contributions: The work [42] was written jointly with Daniel Karrasch. Daniel Karrasch had suggested in [40] that the results of [43] could be relevant to the averaging result, the details were worked out by me; I would like to thank Alvaro de Diego for frequent discussions about this subject matter; Oliver Junge also contributed some helpful suggestions. The generalization to eigenvectors/eigenvalues has also been worked out by me. The relevance of the classical Cheeger inequality on weighted manifolds to the dynamic Cheeger inequality was conjectured by Daniel Karrasch, I worked out the details but not as clearly as they are now in the paper. The formulation of section 2.1 and 2.2 was initially that of Daniel Karrasch. Together with Daniel Karrasch we then revised all sections of the paper (some even multiple times), so it is impossible to clearly specify individual responsibilities with respect to the presentation.

2.2 Summary of [55]

So far, we have looked at small-ε behavior of the perturbed transfer-operators in the relaxed setting of smooth functions. However, the relaxation step is somewhat unsatisfying as it is not clear how to recover *sets* from a smooth function. Therefore I looked at quantities related to $L_\varepsilon \mathbb{1}_S$ and eq. (2.1) for various choices of L_ε.

If there is no advection, and $L_\varepsilon = J_{g,\omega,\varepsilon} (= \exp(\varepsilon \Delta_{g,\omega}))$, then asymptotics of the diffusive outflow $\langle J_{g,\omega,\varepsilon} \mathbb{1}_S, \mathbb{1}_{S^c} \rangle$ have been derived in [65] using methods from the theory of pseudodifferential operators and invariance theory to obtain asymptotics of the more general *heat content*. In [55], I showed how to recover asymptotics of a form of the heat content with different (and arguably simpler) methods in the general setting of complete Riemannian manifolds. The idea used there was that if $k \colon \mathbb{R} \to \mathbb{R}$ is sufficiently regular, f is smooth and $L_\varepsilon = k(\sqrt{-\varepsilon\Delta})$, then

$$\langle L_\varepsilon (f \mathbb{1}_S), \mathbb{1}_S \rangle = \int_0^\infty \hat{k}(s) \langle \cos\left(s\sqrt{-\varepsilon\Delta}\right)(f\mathbb{1}_S), \mathbb{1}_S \rangle \mathrm{d}s \tag{2.3}$$

for a suitable choice of $\hat{k}$. This follows from the functional calculus and is well-known (see [9, 61]). Now the operator $\cos(\sqrt{-t\Delta})$ is a solution-operator for the wave-equation, which has *finite propagation speed*, and can be approximated using geometrical optics (see [61, Sect. 6.6]) near ∂S. This yields the small-ε asymptotics of $\langle \cos(\sqrt{-t\Delta}) \mathbb{1}_S, \mathbb{1}_S \rangle$, and thus also of $\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle$.

The leading-order asymptotics (though the proof extends to higher orders also) obtained are of order $\varepsilon^{\frac{1}{2}}$, with the constant being proportional to the *(hyper)-area* of ∂S in the weighted geometry (M, g, ω) which we denote by $\mathrm{d}A(\partial S)$. To be more precise, when $L_\varepsilon = J_{g,\omega,\varepsilon}$, then

$$\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle = \omega(S) - \sqrt{\frac{\varepsilon}{\pi}} \mathrm{d}A(\partial S) + O(\varepsilon).$$

As mentioned above, similar results extend to other values of k also. For example (and we have corrected a typo appearing in the published version in what follows), when $k(x) = \exp(-x^{2m})$, $m \in \mathbb{N}_{\geq 2}$, then as $t \to 0^+$,

$$\langle \exp(-(-t\Delta)^m)(f\mathbb{1}_S), \mathbb{1}_S \rangle = \int_S f \mathrm{d}V - \left(\pi^{-1} \Gamma\left(\frac{2m-1}{2m}\right) \int_{\partial S} f \mathrm{d}A \right) \sqrt{t} + o(t),$$

where $\mathrm{d}V$ is the Riemannian volume, and $\langle \cdot, \cdot \rangle$ is the L^2 inner product with respect to this volume.

Though not noticed in [55], the case $L_\varepsilon = I_{g,\mathrm{d}g,\varepsilon}$ can also be treated using methods used in that work. In the Euclidean case, the formula eq. (1.14), i.e.

$$I_{g,\omega,\varepsilon} = \frac{2c_{n-1}}{c_n} \int_0^1 \cos(t\sqrt{-\varepsilon^2\Delta})(1-t^2)^{\frac{n-1}{2}} \mathrm{d}t\,, \tag{2.4}$$

was derived in section 1.4.2 (see references there, recall that c_n is the volume of the n-dimensional unit ball with n being the dimension of M), which (up to various scalings) means that $\langle I_{g,\omega,\varepsilon}\mathbb{1}_S, \mathbb{1}_S\rangle$ can be brought into the form eq. (2.3) . Thus applying calculations like in [55], it follows that for smooth f,

$$\langle L_\varepsilon(f\mathbb{1}_S), \mathbb{1}_S\rangle = \int_S f \mathrm{d}x + \varepsilon \frac{c_{n-1}}{c_n(n+1)} \int_{\partial S} f \mathrm{d}A + o(\varepsilon)\,, \tag{2.5}$$

where $\mathrm{d}x$ and $\mathrm{d}A$ are Euclidean volume and (hyper)area respectively. With some work, this generalizes to the case that (M, g, ω) is a weighted Riemannian manifold:

Proof of eq. (2.5) in weighted Riemannian manifolds: To see this, start with the claim (whose proof we postpone briefly) that $I_{g,\omega,\varepsilon}\mathbb{1}_S = I_{\tilde{g},\omega,\varepsilon}\mathbb{1}_S + O(\varepsilon)$ uniformly locally, where $\tilde{g}$ is the Euclidean metric in Fermi coordinates [29, chap. 2] of ∂S near ∂S; that is a coordinate system where the n-th coordinate is a unit normal field orthogonal to ∂S. Since both $I_{\tilde{g},\mathrm{d}\tilde{g},\varepsilon}\mathbb{1}_S$ and $I_{\tilde{g},\omega,\varepsilon}\mathbb{1}_S$ disappear on $M \setminus S$ outside of an $O(\varepsilon)$-neighborhood of ∂S, from the claim we conclude that $\langle I_{g,\omega,\varepsilon}\mathbb{1}_S, \mathbb{1}_{M\setminus S}\rangle_{L^2(M,\omega)} = \langle I_{\tilde{g},\mathrm{d}\tilde{g},\varepsilon}\mathbb{1}_S, \mathbb{1}_{M\setminus S}\rangle_{L^2(M,\omega} + o(\varepsilon)$. Moreover, $I_{\tilde{g},\mathrm{d}\tilde{g},\varepsilon}$ is self-adjoint with respect to $L^2(M, \mathrm{d}\tilde{g})$, where we have assumed without loss of generality[1] that the coordinates cover the entire manifold. We write $\theta \mathrm{d}\tilde{g} = \omega$, and $\mathrm{d}\tilde{A}$ as the (hyper)area induced by $\tilde{g}$, with $\mathrm{d}A$ denoting the area form in the weighted geometry (M, g, ω). Then by self-adjointness, and using the expansion eq. (2.5),

$$\begin{aligned}
\langle I_{\tilde{g},\mathrm{d}\tilde{g},\varepsilon}\mathbb{1}_{M\setminus S}, \mathbb{1}_S\rangle_{L^2(M,\omega)} &= \langle \mathbb{1}_S, I_{\tilde{g},\mathrm{d}\tilde{g},\varepsilon}(\theta\mathbb{1}_{M\setminus S})\rangle_{L^2(M,\mathrm{d}\tilde{g})} \\
&= \frac{c_{n-1}}{c_n(n+1)}\varepsilon \int_{\partial(M\setminus S)} \theta \mathrm{d}\tilde{A} + o(\varepsilon) \\
&= C\varepsilon\ \mathrm{d}A(\partial S) + o(\varepsilon)
\end{aligned}$$

as the $\tilde{g}$ and g-unit normals at ∂S agree. This generalizes eq. (2.4) to weighted manifolds. It remains to prove the claim we assumed, which we only sketch. For $x \in M \setminus S$, denote by π_x the orthogonal projection (in Fermi-coordinates) to ∂S of x. Given that we may restrict ourselves to a sufficiently small neighborhood of ∂S, this is always possible. Clearly,

$$I_{g,\omega,\varepsilon}(\mathbb{1}_S f)(x) = f(\pi_x)\frac{\int_{B(x,\varepsilon)\cap S} \mathrm{d}\,\omega}{\int_{B(x,\varepsilon)} \mathrm{d}\,\omega} + O(\varepsilon) \tag{2.6}$$

by Taylor-expansion of f. Likewise, we may choose $\mathrm{d}\tilde{g}$ in place of ω in the integrals by Taylor-expansion of a coordinate representation of ω without making an error larger than $O(\varepsilon)$.

[1] All of the operations involved can be suitably localized for sufficiently small ε, so this is permissible.

With the n-dimensional Lebesgue measure λ^n, define

$$c(\varepsilon, r) \coloneqq \lambda^n(\{x; x_n \geq r \wedge \|x\|_2 \leq \varepsilon)\})/\lambda^n(\{x; \|x\|_2 \leq \varepsilon\})$$

as the volume of the intersection of a ε-ball with a (shifted) half-space. We claim that

$$\frac{\int_{B(x,\varepsilon)\cap S} \mathrm{d}\,\omega}{\int_B (x, \varepsilon) \mathrm{d}\,\omega} = c(\varepsilon, \mathrm{dist}(x, \partial S)) + O(\varepsilon), \tag{2.7}$$

regardless of whether g or $\tilde{g}$ is used to measure metric balls and distances in eq. (2.7). To see this, let H_x be the half-space not containing x whose boundary is tangent to ∂S at π_x in geodesic normal coordinates. By Gauss' lemma, we may choose these coordinates so that the n-th coordinate is orthogonal to ∂S and H_x is orthogonal to the geodesic from x to π_x. We can replace S with H_x on the left hand side of eq. (2.7) and incur only a $O(\varepsilon)$ error as ∂H_x is tangent to ∂S at x, this can be seen by writing ∂S as a graph over ∂H_x near π_x. Likewise, we may replace ω with the Euclidean volume form in these geodesic normal coordinates and only incur an $O(\varepsilon)$ error, leaving us with $c(\varepsilon, \mathrm{dist}(x, \pi_x))$ which proves eq. (2.7). All constant implicit in the $O(\varepsilon)$ notation depend only on quantities like the curvature of ∂S and the curvature of g and $\tilde{g}$, and can therefore be chosen uniformly in x. Together with eq. (2.6) this proves the claim.

Clarification of contributions: The paper [55] was completely written by me, though I benefited from feedback of Oliver Junge and Daniel Karrasch with regards to the presentation. The anonymous reviewer at the Journal of Geometric Analysis (where [55] appeared) also helped to improve the argument.

2.3 Summary of [57]

We return to the setting of the mass-preserving advection-diffusion equation on a manifold M with mass ω in Lagrangian coordinates; as before $\langle \cdot, \cdot \rangle$ denotes the $L^2(M, \omega)$ inner product. In the previous section, we looked at [55] in which the quantity $\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle$ was analyzed in the setting of no advection. We now turn to the case where advection is present; i.e. the metric in Lagrangian coordinates depends on time.

Choosing, $L_\varepsilon = P_{1,\varepsilon}$ as the solution-operator to the advection-diffusion equation, we obtain in [57] a formula in Lagrangian coordinates for $\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle$.

Equivalently, in Eulerian coordinates this quantity is given by $\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_{\Phi_0^1(S)} \rangle$ and may be seen to represent the diffusive outflow out of a material set. In contrast to some of the other perturbations considered here, even though only a single application of the flow map Φ_0^1 is considered, the fact that the diffusion in the advection-diffusion equation does not take place only at a single instant means that *all* times $t \in [0, 1]$ contribute to this quantity. By crafting a suitable time-dependent metric, the methods there may be seen to also apply to perturbations like $L_\varepsilon = J_{g_1,\omega,\varepsilon} J_{g_0,\omega,\varepsilon}$ in Lagrangian coordinates, where g_0, g_1 are different metrics; such perturbations represent pre and post-composition of the transfer-operator by different heat flows.

Our main result – letting $\mathrm{d}\overline{A}$ denote the (weighted) area form in the geometry of mixing – is that

$$\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_S \rangle = \omega(S) - \sqrt{\frac{\varepsilon}{\pi}} \mathrm{d}\overline{A}(\partial S) + o(\varepsilon^{\frac{1}{2}})$$

like in [55]; except that here also time-dependent metrics are permitted. The proof is mostly via stochastic methods to reduce the problem to the case discussed in [55]. This is done with the help of the well-known Kolmogorov backwards equation and a classical approximation result for stochastic differential equations from [7].

We also observe that when looking at the coherence ratio without relaxing to smooth functions, we can nevertheless connect to classical theory by looking at (weighted) area forms. Stationary points of such weighted area forms with respect to various perturbations are well-known to be closely connected to surfaces of a generalized constant mean curvature; see [31, Section 9.4E].

Clarification of contributions: I was responsible for the proof in [57] initially. Daniel Karrasch and Oliver Junge were strongly involved with improving the clarity of the paper and to overhaul it into a better form. In particular, the presentation of section 4 is that of a rewrite attributable in large part to Daniel Karrasch.

2.4 Summary of [56]

As mentioned in previous chapters, discretizations of the dynamical Laplace can be used to compute coherent sets. In [56], we looked at theoretical and practical properties of various generalizations of some discretizations described in [18].

I consider the main contribution of this work in clarifying the role of the weak-form of various discretizations from [18]. In [18], the construction of the discretized dynamic Laplace was presented in terms of a Galerkin-type approach involving point-masses. In [56], we we introduce the idea that computations of eigenvalues with the "TO approach" schema of [18] is equivalent to computing minimizers of bilinear forms

$$a_h(u, v) = \sum_{i=1}^{N} a_i(I_{h,i}u, I_{h,i}v) \tag{2.8}$$

where $I_{h,i}$ is an interpolation operator defined on (some subset of) weakly differentiable functions and h is a mesh-parameter related to the mesh width. Viewed this way, it becomes possible to reason about minimizers of these bilinear forms using tools from the theory of partial differential equations. We prove convergence results under appropriate hypotheses using a proof based on the well-known direct method in the calculus of variations (see [28] for an introduction). The convergence theory for the standard Galerkin discretization of the weak-form of the dynamic Laplacian is a special case of the well-known general theory; see for example[13, 60]. Using this fact we obtain one of the bounds in the converge proof for the "TO approach"; the other direction requires the fact that the sum in eq. (2.8) is finite and therefore does not generalize in a straightforward way to non-finite sums. For the case that the $I_{h,i}$ operators mentioned earlier are nodal interpolation operators on a suitably regular mesh, we adapt a proof from [8] in order to bound certain operator norms required in the proof.

In [56], we also investigate whether or not the use of higher-order (P^2-Lagrange as opposed to P^1-Lagrange) finite elements yield better results numerically. This is done by numerical experiments. Our experiments, using an implementation from the `CoherentStructures.jl` package, suggest that while this is the case for the straightforward finite-element weak-form of the dynamic Laplacian, no evidence is found that suggests that it remains true for the "non-adaptive TO" discretization introduced in [18].

Clarification of contributions: In [56], I contributed the convergence proofs as well as the numerical experiments. Throughout this, I was in frequent discussions with Oliver Junge and Gary Froyland (who formulated the research topic) about the results and how to formulate the resulting form of the paper, including the Introduction. I would also like to thank Christian Ludwig for pointing me to a paper that was crucial for an important case of the convergence result.

2.5 Software packages

I am a co-author of the `CoherentStructures.jl` software package, to which I contributed a lot of code during the past years. This software package contains state of the art Julia implementations of various methods for computing coherent structures, together with an extensive documentation. I also wrote the `OceanTools.jl` package, both packages are available on github, both packages were also used in my master's thesis.

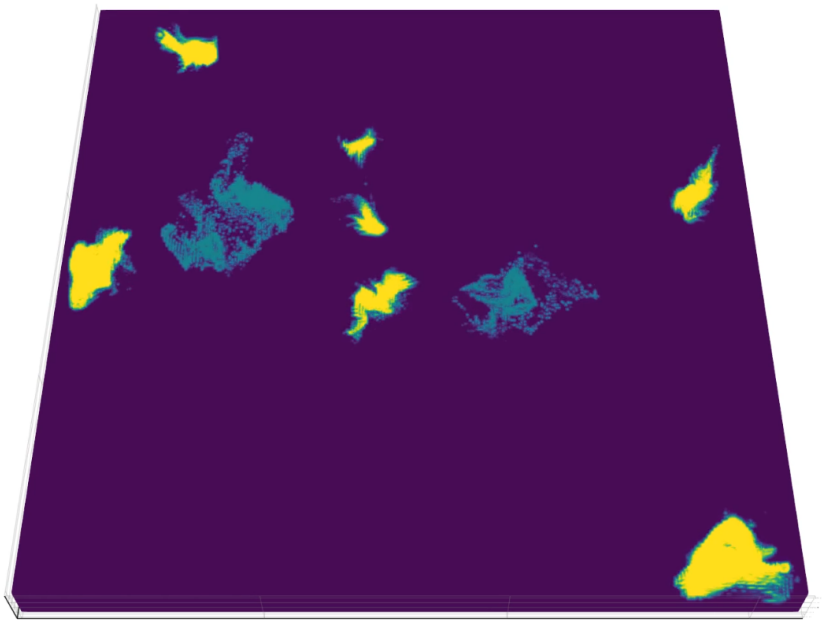

Figure 2.1: A method from [18] implemented in `CoherentStructures.jl` applied to a time-dependent 3D velocity field obtained from direct numerical simulation of Rayleigh-Bénard convection obtained from the authors of [52]. The yellow blobs are images of computed coherent sets under the flow; the blue ones are some non coherent sets displayed as a comparison.

3 Open Questions

A number of interesting questions related to those explored above remain. We sketch here one direction that I was not able to explore in more detail.

Recall that the pushforward operators $(P_t)_{t\in[0,1]}$ are defined not only for functions, but also for differential forms of higher orders. The advection-diffusion equation in Lagrangian coordinates,

$$\partial_t u = \varepsilon \Delta_t u \tag{3.1}$$

remains similarly well-defined, with $\Delta_t = (\Phi_0^t)^* \Delta$ if $\Delta = \mathrm{d}\mathrm{d}^* + \mathrm{d}^*\mathrm{d}$ is a de Rham-Laplacian, possibly on a weighted Riemannian manifold. We may still average to define a generalized dynamic Laplacian $\overline{\Delta} = \int_0^1 \Delta_t \mathrm{d}t$. Are spectral properties of this operator of relevance to the computation of coherent structures? Is this the 'natural' de Rham-Laplacian of some (generalized) geometry? Are its spectral properties relevant to the study of sets in this geometry? I conjecture that we will need to generalize here from weighted manifolds to the *superconnections* as featured in [48].

If $M = M_a \uplus M_b$ is the disjoint union of two connected components, the 0-eigenspace of of the Laplacian on functions (with Neumann boundary) is 2-dimensional. Now if M is "almost" the sum of two such connected components (in the sense that there is cut of small area that separates M into two parts of somewhat balanced volume), then there are two eigenvalues close to zero (including the zero-eigenvalue) – this is the Cheeger inequality[47]; see also the extension to multiple eigenvalues in [10]; see also also [38]. As zero eigenvalues of the Laplacian on functions are well-known to correspond to the 0th cohomology on M, we may informally think of the existence of such a cut as resulting in the manifold "almost" having 2-dimensional 0th (de Rham) cohomology. The connection to dynamical systems is via the geometry of mixing.

But what about other cohomology groups, i.e. those of higher degree? If $M = M_a \uplus M_b$ and M_a is homeomorphic to $\mathbb{S}^1 \times \mathbb{D}_2$ (where $\mathbb{S}^1$ is the one-dimensional sphere, and $\mathbb{D}_2$ is the unit ball/disk in two dimensions) and M_b to a $[0,1]\times\mathbb{D}_2$, then the 1-cohomology of M is 1-dimensional, and the Hodge Laplacian on 1-forms has 1-dimensional kernel. Does this mean that if M is in some sense "almost" such a disjoint union, that the Hodge Laplacian has a 1-dimensional eigenspace corresponding to an almost-zero eigenvalue? If so, it is possible that small eigenvalues of the (generalized) dynamic Laplace on 1-forms yield information about $\mathbb{S}^1 \times \mathbb{D}_2$-shaped Lagrangian coherent structures like smoke-rings in 3 dimensions. This is

particularly interesting from a physical perspective, given that smoke-ring-shaped Lagrangian coherent structures are known to exist in turbulent 3d flows. I would also like to thank David Hien for interesting discussions on such ideas.

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Appendices

We include here the following documents:

1. The publication [56], "Higher-order finite element approximation of the dynamic Laplacian" that appeared in Volume 54 No 5 of *ESAIM: Mathematical Modelling and Numerical Analysis (ESAIM: M2AN)* in 2020.

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5. The pre-print " A Lagrangian perspective on nonautonomous advection-diffusion processes in the low-diffusivity limit ", a version of which was previously uploaded to arXiv.

6. The submitted pre-print "Heat-content and diffusive leakage from material sets in the low-diffusivity limit", a version of which was previously uploaded to arXiv. This article has been accepted to appear in the IOP Publishing journal *Nonlinearity*, the version included here is not the final journal article and may deviate from it e.g. when it comes to formatting.

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HIGHER-ORDER FINITE ELEMENT APPROXIMATION OF THE DYNAMIC LAPLACIAN

Nathanael Schilling[1,*], Gary Froyland[2] and Oliver Junge[1]

Abstract. The dynamic Laplace operator arises from extending problems of isoperimetry from fixed manifolds to manifolds evolved by general nonlinear dynamics. Eigenfunctions of this operator are used to identify and track finite-time coherent sets, which physically manifest in fluid flows as jets, vortices, and more complicated structures. Two robust and efficient finite-element discretisation schemes for numerically computing the dynamic Laplacian were proposed in Froyland and Junge [*SIAM J. Appl. Dyn. Syst.* **17** (2018) 1891–1924]. In this work we consider higher-order versions of these two numerical schemes and analyse them experimentally. We also prove the numerically computed eigenvalues and eigenvectors converge to the true objects for both schemes under certain assumptions. We provide an efficient implementation of the higher-order element schemes in an accompanying Julia package.

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1. Introduction

The dynamic Laplacian is a second-order partial differential operator underlying a range of methods for computing finite-time coherent sets in finite-time non-autonomous dynamical systems. It was introduced in [12] in the context of defining sets that remain coherent in a Lagrangian sense *via* dynamic isoperimetry. Coherent sets are time-dependent families of sets whose boundaries remain small relative to the volume of the set as the family evolves according to the nonlinear dynamics; extensions to weighted, curved manifolds and non-volume-preserving dynamics were made in [15]. Coherent sets are captured by the eigenvectors of the dynamic Laplacian corresponding to the leading eigenvalues (*i.e.* those closest to 0). In particular, level sets of the eigenvector corresponding to the first nontrivial eigenvalue can be used to partition the domain into two coherent sets. A dynamic Cheeger inequality [12, 15] links this eigenvalue to the ratio of boundary size to volume. Moreover, if n eigenvalues are close to zero followed by a spectral gap, this forces the eigenvectors to be close to linear combinations of indicator functions on an n-partition [6]. We note that the dynamic Laplacian is the Laplace–Beltrami operator of a weighted manifold [20] and therefore can be used as the time-independent generator of a diffusion process approximating the given (time-dependent) advection-diffusion process. Eigenvectors corresponding to small eigenvalues decay slowest under this diffusion process and yield almost-invariant sets in the

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sense of [7]. Algorithmically, coherent sets can be extracted from the eigenvectors of the dynamic Laplacian *via*, *e.g.* clustering techniques [11], optimising eigenbasis separation [8], optimising sublevel sets [16], or sparse eigenbasis approximation [18].

In most cases, the dynamic Laplacian eigenproblem must be solved numerically. To this end, a scheme based on radial basis functions had been proposed [13], which showed high order of convergence, but suffered from a number of drawbacks like high sensitivity with respect to the radius parameter, a non-real spectrum and non-sparseness of the discretized operator. In [14], two finite element schemes were proposed (the "Cauchy-Green" (CG) and the "Transfer Operator" (TO) approach), which eliminated each of these drawbacks.

Experimentally, only piecewise linear elements were considered in [14]. In this paper, we consider higher-order (and in particular quadratic) elements and analyse convergence properties both theoretically and experimentally. We provide an efficient implementation in the Julia package `CoherentStructures.jl`. We find that using P^2 elements can give a higher asymptotic order of convergence compared to P^1 elements in the "CG" approach. For the "CG" approach, classical theory concerning eigenproblems in FEM applies. We also provide some test cases where using P^2 elements can greatly reduce the amount of information needed to calculate partitions of the domain that show important dynamical features. The question of convergence in the "TO" approaches is more subtle. We prove convergence of eigenvalues and eigenvectors for a family of TO approaches with P^1 elements, but the proof does not give any insight into the convergence rates that should be expected. For P^2 elements we do not observe asymptotically higher orders of convergence even for the simple example of a one-dimensional shift-map on the torus. This suggests that using P^2 elements does not have substantial benefits when using the "TO" approach and that one should use the simpler and well-performing linear P^1 elements in the "TO" schemes.

This paper is organized as follows. In Section 2 we recall the definition of the dynamic Laplacian. In Section 3 we look at convergence rates for the "CG" approach which follow directly from the standard FEM theory for eigenproblems. Section 4 deals with convergence of the "TO" approach, with some of the proofs relegated to Appendix A.

2. The dynamic Laplacian

Let $\mathcal{I} \subset \mathbb{R}$ denote a finite subset of time and consider a finite family $(\Omega_t)_{t\in\mathcal{I}}$ of open bounded subsets of $\mathbb{R}^d$ with Lipschitz boundary. For each $t \in \mathcal{I}$ let $T_t : \Omega_0 \to \Omega_t$ be a volume-preserving diffeomorphism. We assume that T_t is sufficiently regular so that T_t and T_t^{-1} can be smoothly extended to the boundary, and that $0 \in \mathcal{I}$ with T_0 being the identity. A typical setting in which these conditions apply are T_t taken to be time-t flow maps of a divergence-free vector-field.

Denote the Laplace operator on Ω_t by Δ_t for each $t \in \mathcal{I}$. Then the *dynamic Laplacian* (an operator on Ω_0) is given by

$$\Delta^{\mathrm{dyn}} := \frac{1}{|\mathcal{I}|}\sum_{t\in\mathcal{I}} T_t^* \Delta_t T_{t,*}$$

where $T_t^* : L^2(\Omega_t) \to L^2(\Omega_0)$ denotes the pullback by T_t defined by $T_t^* f = f \circ T_t$, and $T_{t,*} : L^2(\Omega_0) \to L^2(\Omega_t)$ is the pushforward defined by $T_{t,*} f = f \circ T_t^{-1}$.

Standard PDE-theoretic arguments can be used to show that Δ^{dyn} is a uniformly elliptic second-order partial-differential operator [10,12], with weak form [14]

$$a(u,v) := \frac{1}{|\mathcal{I}|}\sum_{t\in\mathcal{I}} \int_\Omega \nabla u \cdot [DT_t]^{-1} \left([DT_t]^{-1}\right)^T \nabla v \,\mathrm{d}\ell^d, \tag{2.1}$$

where ℓ^d is the d-dimensional Lebesgue measure. The time set $\mathcal{I}$ can also be a compact interval, and the dynamic Laplacian can be defined by means of an integral over $\mathcal{I}$ [12,15]

$$\Delta^{\mathrm{dyn}} := \frac{1}{|\mathcal{I}|}\int_{\mathcal{I}} T_t^* \Delta_t T_{t,*} \,\mathrm{d}t,$$

where $|\mathcal{I}|$ now denotes the length of the interval $\mathcal{I}$, we do not consider this generalization further here.

The uniform ellipticity of the dynamic Laplacian ensures that the bilinear form in (2.1) is coercive under suitable boundary conditions. These are determined by the choice of the underlying space S on which (2.1) acts. For natural (Neumann) boundary conditions, we look at a on $\hat{H}^1 \times \hat{H}^1$, where $\hat{H}^1 = \hat{H}^1(\Omega_0) := \left\{v \in H^1(\Omega_0) : \int f \, \mathrm{d}\ell^d = 0\right\}$ is the space of mean-free H^1 functions. For homogeneous Dirichlet boundary conditions, a must be taken to act on $H^1_0 \times H^1_0$. With either choice of boundary conditions, the variational form of the eigenproblem $\Delta^{\mathrm{dyn}} u = \lambda u$ becomes

$$a(u, v) = \lambda \langle u, v \rangle_{L^2} \quad \text{for all} \quad v \in S. \tag{2.2}$$

In both cases, ellipticity ensures that there exists a countable sequence of pairwise orthogonal eigenvectors $u_0, u_1, \ldots$ corresponding to real eigenvalues $0 \geq \lambda_0 \geq \lambda_1 \geq \cdots$. Furthermore, the span of the eigenvectors is dense in L^2 (Dirichlet) and mean-free L^2 functions (Neumann) [10,12].

2.1. Discretisation with finite elements

A natural discretisation of the eigenproblem (2.2) is by using a finite element method (FEM) [14]. In the standard Galerkin discretization of (2.2), $S' \subset S$ is taken to be a finite dimensional approximation space spanned by some basis $(\varphi_1, \ldots, \varphi_n)$. We now find approximate solutions $u \in S'$, $\lambda \in \mathbb{R}$, that satisfy (2.2) with S' taking the place of S. In matrix form, the coefficients $\mathbf{u} = (\mathbf{u}_1, \ldots, \mathbf{u}_n)$ of u with respect to the basis $(\varphi_1, \ldots, \varphi_n)$ are found by solving the generalized eigenvalue problem

$$D\mathbf{u} = \lambda M \mathbf{u}. \tag{2.3}$$

Here, $D = (D_{i,j}) = a(\varphi_i, \varphi_j)$ is referred to as the *stiffness matrix* and $M = (M_{i,j}) = \langle \varphi_i, \varphi_j \rangle_{L^2}$ as the *mass matrix*. We use P^k Lagrange nodal basis functions on some (triangular or simplicial) mesh for $\varphi_1, \ldots, \varphi_n$, but other choices are also possible in general (see [9]).

Using a finite element method for approximating Δ^{dyn} has a number of advantages: The matrix formulation (2.3) inherits self-adjointness from the continuous problem and thus the computed eigenpairs are always real. With a suitably localized basis, D and M are both sparse. Sparse Hermitian generalized eigenproblems are well known in the literature, and a number of algorithms exist for efficiently solving them [1]. Also, finite element methods have been widely studied, and there are a range of theoretical results regarding convergence (*cf.* [9]) that are applicable to some solution approaches.

While the entries of the mass matrix can be computed exactly, the integrand in (2.1) in the entries of the stiffness matrix can be of extremely high variation locally, making an accurate computation possibly expensive. Several approaches for approximating D were suggested in [14], which we investigate further in the following sections.

3. Convergence for the CG approach

In the "CG approach" of [14], a quadrature formula is used to approximate (2.1). This is the standard way of solving elliptic eigenproblems with finite elements.

We work on P^k-Lagrange finite element spaces for a family of quasi-uniform[3] triangulations (in 2 or 3 dimensions) $\left\{\mathcal{T}_h^0\right\}_{h>0}$ of Ω_0, where the family parameter h is related to the mesh size. Let $\varphi_h^1, \ldots, \varphi_h^{N(h)}$ be the associated nodal basis, $S_h^0 := \operatorname{span}\left\{\varphi_h^1, \ldots, \varphi_h^{N(h)}\right\}$ the finite element approximation space, and $\hat{S}_h^0 := \hat{H}^1 \cap S_h^0$. Moreover, let $\lambda_{i,h}$ be the Ritz-values with corresponding Ritz-vectors $v_{i,h}$ in $\hat{S}_h^0$, *i.e.* $\lambda_{i,h}$ is the minimum

[3] A family $\{\mathcal{T}_h\}_{h>0}$ of meshes is *quasi-uniform*, if it is shape-regular and there exists a constant $c > 0$ so that for any $h > 0$ and any element $K \in \mathcal{T}_h$ one has that $h_K \geq ch$, where h_K is the diameter of the element K. Shape regularity means that there is a constant σ_0 so that uniformly for all K it holds that $\sigma = \frac{h_K}{\rho_K} \leq \sigma_0$. Here ρ_K is the diameter of the largest ball that can be inscribed in K [9].

value of $a(v,v)$ over the set $\left\{v \in \hat{S}_h^0; \|v\|_{L^2} = 1, \langle v, v_j\rangle = 0 \text{ for } j = 1, \cdots, (i-1)\right\}$ and $v_{i,h}$ is the corresponding minimizer.

Under the assumption that the eigenvectors of $a : \hat{H}^1 \times \hat{H}^1 \to \mathbb{R}$ are in H^{k+1}, classical results from FEM theory [9,25] give that (where C stands for a generic constant):

$$\frac{\lambda_{i,h} - \lambda_i}{\lambda_i} \leq Ch^{2k} \quad (h \to 0). \tag{3.1}$$

Moreover, it holds for simple (and L^2-normalised) eigenvectors that

$$\|v_i - v_{i,h}\|_{H^1} \leq Ch^k \quad (h \to 0). \tag{3.2}$$

In the case that the problem (2.1) satisfies the technical assumption of being *regularizing* [9] (*i.e.* $\|Pu\|_{H^2} \leq C\|u\|_{L^2}$), the "Aubin–Nitsche trick" gives

$$\|v_i - v_{i,h}\|_{L^2} \leq Ch^{k+1} \quad (h \to 0). \tag{3.3}$$

Note that not all elliptic problems are regularizing. We thus cannot expect (3.3) to hold in general.

If the entries of the stiffness and the mass matrix are approximated with a quadrature rule of order $2k-1$, the convergence orders are unaffected, provided that the quadrature points contain a $\mathcal{P}^k$ unisolvent set [2]. Moreover, the results generalize to non-simple eigenspaces and Kato's subspace distance used for the error [2].

3.1. Numerical experiments

We now aim at reproducing the predicted convergence rates in numerical experiments. As a reference, we compute (L^2 normalized) eigenpairs (λ_i, v_i) on a very fine mesh and estimate the error in the eigenvector $v_{i,h}$ by computing the L^2-distance of $v_{i,h}$ to the closest reference eigenvector, given by the expression

$$e_{i,h} := \sqrt{1 - |\langle v_i, v_{i,h}\rangle_{L^2}|^2}. \tag{3.4}$$

The L^2 inner-product is approximated by first interpolating to the fine grid, and then calculating the inner product there using quadrature.

To generalize this to higher-dimensional eigenspaces, let $\tilde{V}$ and V be two m-dimensional subspaces of L^2 with orthonormal bases given by $\{\tilde{v}_1, \ldots, \tilde{v}_m\}$ and $\{v_1, \ldots, v_m\}$. Let $\tilde{P}, P$ be orthogonal projections onto $\tilde{V}$ and V respectively. As a measure of the subspace error [21], we maximize $\|\tilde{v} - P\tilde{v}\|_{L^2}$ over $\tilde{v} \in \tilde{V}$ with $\|\tilde{v}\|_{L^2} = 1$. This is equivalent to maximizing $\sqrt{1 - \|P\tilde{v}\|^2}$, which has maximum given by $\sqrt{1 - \rho_{\min}(P)^2}$ where $\rho_{\min}$ is the smallest singular value of P on $\tilde{V}$ which is also that of the matrix $(\langle \tilde{v}_i, v_j\rangle_{L^2})_{i,j=1}^m$.

In general, one is not directly interested in the eigenvectors themselves, but in a partition of the domain obtained by a suitable post-processing of the eigenvectors (*e.g.* as mentioned, thresholding, clustering or sparse eigenbases). This motivates us making a qualitative comparison of such partitions based on eigenvectors for different approximation spaces. Here, we focus in particular on the question of how well Lagrangian coherent sets can be found with as little information about the flow as possible. Evidently, in this low data case some features may not be accurately resolved even if the eigenvectors clearly give some indication of their existence. We therefore also look at how coarse the grid can be made without affecting the topology of such a partition in some test cases.

In the sequel, mesh sizes of the form $n \times m$ refer to a regular triangular mesh with $n \times m$ (non-inner) nodes in each direction. For all time-integration done in this work we used a relative and absolute tolerance of 10^{-8} and the `DifferentialEquations.jl` Julia package [23] with the `BS5()` solver [3]. Derivatives of flow maps were approximated with second order central finite differences. The stiffness matrix was calculated by approximating the integral in (2.1) on each element with nodal basis functions for u and v using quadrature. The results from

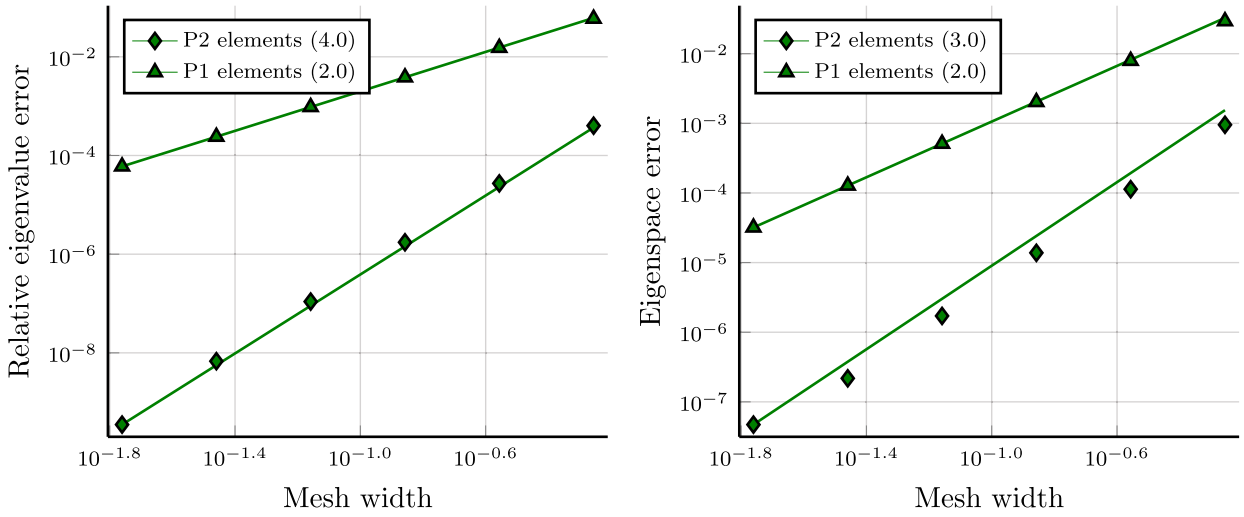

FIGURE 1. Standard map: errors in the first nontrivial eigenvalue (*left*) and 2-dimensional eigenspace corresponding to the two smallest nontrivial eigenvalues (*right*) of the dynamic Laplacian with the CG approach. The slopes of the corresponding lines are given in brackets in the legends.

this were then summed over all elements in the support of a basis function to give the corresponding entry in the stiffness matrix. Similarly, the integral in the mass matrix was also calculated element-wise and then additively combined to give the full mass matrix. The `CoherentStructures.jl` package internally uses the `JuAFEM.jl` package [5].

3.1.1. Standard map

As a simple first example, we consider two iterations of the standard map

$$T(x, y) = (x + y + a\sin(x), y + a\sin(x))$$

on the 2-torus $\mathbb{S}^1 \times \mathbb{S}^1$ with parameter $a = 0.971635$. This is the first example considered in [13] and is a weakly nonlinear map. Figure 1 shows the eigenvalue and eigenspace errors in dependence of the mesh width for triangular P^1 and P^2 Lagrange elements.

The reference solution was computed with P^2 elements on a regular 1025×1025 grid with quadrature order 5. In this case, the experimentally observed rates almost perfectly agree with the predictions (3.1) and (3.3) even for quadrature order 2 in the computation of the entries of stiffness- and mass-matrix. Improvements in errors ranged between one and two orders of magnitude when moving from P^1 to P^2 elements. To be able to directly compare these results with the corresponding plots for TO methods in Figure 5, we used a two-dimensional eigenspace in Figure 1.

3.1.2. Cylinder flow

As a second example, we consider the cylinder flow map used in [13] based on [17]. This is a time-dependent flow on the cylinder $\mathbb{S}^1 \times [0, \pi]$ defined by the non-autonomous ordinary differential equation

$$\begin{aligned}\dot{x}(t) &= c - A(t)\sin(x - \nu t)\cos(y) + \varepsilon G(g(x, y, t))\sin(t/2)\\ \dot{y}(t) &= A(t)\cos(x - \nu t)\sin(y)\end{aligned}$$

where $A(t) = 1 + 0.125\sin\left(2\sqrt{5}t\right)$, $G(\psi) = 1/\left(\psi^2 + 1\right)^2$ and $g(x, y, t) = \sin(x - \nu t)\sin(y) + y/2 - \pi/4$. Here the parameters $c = 0.5, \nu = 0.5, \varepsilon = 0.25$ were used, the time-interval was $[0, 40]$.

The reference solution was computed on a regular mesh on 1025×1025 nodes with triangular P^2-Lagrange elements and quadrature order 8. We used quadrature order 5 for the numerical experiments (since we did not observe the same rates for smaller orders). The results for this numerical experiment are shown in Figure 6.

The orders of convergence observed in Figure 3 for the eigenvalue and eigenvector errors is surprisingly low; the experimental values are almost exactly half of the orders predicted in (3.1), (3.2) or (3.3). The observed order of the eigenvector errors for P^1 elements is particularly poor. We also note that the slopes shown in the figure do not remain consistent when varying the quadrature order.

For this flow (and other highly stretching and highly nonlinear systems), the mean diffusion tensor $A = [DT_t]^{-1}\left([DT_t]^{-1}\right)^T$ used in the weak formulation of the dynamic Laplacian (2.1) has extremely high variation locally (*cf.* Fig. 3). We suspect that even the reference grid of 1025×1025 nodes is not sufficiently resolved to be in a regime where the convergence orders predicted by the theory can be observed.

3.1.3. Bickley jet

The Bickley jet flow is a well-known test case first introduced in [24]. The flow is defined by a stream-function

$$\psi(x,y,t) = -U_0 L \tan h\,(y/L_0) + \sum_{i=1}^{3} A_i U_0 L \sec h^2(y/L)\cos\left(k_i\left(x - c_i t\right)\right) \tag{3.5}$$

with constants U_0, L_0, A_i, k_i, c_i on a cylindrical domain (see [24]). We considered the flow for a timespan of 40 days. 8-partitions were computed by k-means clustering on 200×60 values of the leading eigenvectors of the FEM approximation. The mesh widths in Figure 4 below are the lowest (at the aspect ratio 10 : 3) for which the topology of the clustering result does not change. It is possible to obtain the same result (topologically) with P^2 elements at significantly reduced cost (in terms of the number of quadrature point used) to P^1 elements. In many cases, the computation requiring the most runtime (apart from the clustering) is the computation of diffusion tensors by time-integration at the quadrature points. As shown in Figure 4, in this case this is reduced by a factor of 25 by using P^2 elements.

4. Convergence for the TO approach

The CG approach has the disadvantage of requiring the numerical approximation of the derivative DT_t and a subsequent quadrature which might be challenging if DT_t has high variation locally.

An alternative approach [14] is to rewrite the weak form (2.1) of the dynamic Laplacian operator using the transfer operator T_t. In the sequel we discuss the case $t \in \mathcal{I} := \{0,1\}$, although the results hold for general finite $\mathcal{I}$. Letting a^t be the weak-form of the Laplacian on Ω_t, we have (for $u, v \in H^1(\Omega_0)$)

$$a(u,v) = \frac{1}{2}\left(a^0(u,v) + a^1(Tu,Tv)\right)$$

where we write $T := T_1$, and for brevity overload this notation so that T acts on elements of Ω_0 in the usual way *and* acts on functions in $L^2(\Omega_0)$ as $Tu := T_{1,*}u$. In the transfer operator (TO) approach, we approximate T on a suitable subspace of H^1 by an operator of the form $I_h T$, where I_h is some projection operator. Let $\left\{\mathcal{T}_h^1\right\}_{h>0}$ be a quasi-uniform family of triangulations on Ω_1, S_h^1 the approximation space with Lagrange $P^{k'}$ finite elements and $\hat{S}_h^1 := S_h^1 \cap \hat{H}^1(\Omega_1)$. Note that in general, the collection $\left\{\mathcal{T}_h^0\right\}_{h>0}$ (introduced at the beginning of Sect. 3) and $\left\{\mathcal{T}_h^1\right\}_{h>0}$ are unrelated. We consider the following options for I_h in the sequel:

(1) the L^2-orthogonal projection onto S_h^1 (L^2-*Galerkin*),
(2) the H^1-orthogonal projection onto S_h^1 (H^1-*Galerkin*),
(3) the (Lagrange P^k) nodal interpolation on S_h^1 (*collocation*).

Case 3 corresponds to the "TO approach" from [14], with the difference between the adaptive and non-adaptive approaches being the choice of the mesh $\{\mathcal{T}_h^1\}_{h>0}$.

We now define the (h-dependent) symmetric bilinear form

$$\tilde{a}_h(u,v) := \frac{1}{2}\left(a^0(u,v) + a^1\left(I_hTu, I_hTv\right)\right). \tag{4.1}$$

As in [14], eigenpairs are numerically approximated by calculating generalized eigenpairs of $(\tilde{D}_h, M_h)$ given by

$$\begin{aligned}\left(\tilde{D}_h\right)_{ij} &:= \tilde{a}_h\left(\varphi_h^i, \varphi_h^j\right)\\ \left(M_h\right)_{ij} &= \langle\varphi_h^i, \varphi_h^j\rangle_{L^2}.\end{aligned}$$

As a^0 is elliptic on $\hat{H}^1(\Omega_0)$ and a_1 is non-negative, it follows immediately from (4.1) that $\tilde{a}_h$ is elliptic uniformly in h on $\hat{S}_h^0$, with a lower bound of the ellipticity constant being half the ellipticity constant of a^0.

Hypotheses on I_h and the setup. In order to investigate the convergence of the numerically calculated eigenpairs to those of the dynamic Laplacian, we will require a regularity assumption on the meshes used:

(A0) $\{\mathcal{T}_h^0\}_{h>0}$ and $\{\mathcal{T}_h^1\}_{h>0}$ are families of quasi-uniform triangulations of Ω_0 and Ω_1 respectively that are nested in the sense that $S_{h'} \subset S_h$ for $h < h'$.

We will need to consider the following conditions for I_hT acting on S_h^0:

(A1) exactness for constant functions: $I_hT\chi_{\Omega_0} = \chi_{\Omega_1}$,
(A2) H^1-convergence: $\lim_{h\to 0}\|I_hTf - Tf\|_{H^1} = 0$ for any $f \in \cup_h S_h^0$,
(A3) L^2-stability: For all $h' > 0$ it holds that $\sup_{h<h'}\|I_hT|S_{h'}^0\|_{L^2\to L^2} \le C$, where $C > 0$ is independent of h'.

We now consider whether the conditions (A1)–(A3) are satisfied by the three variants of I_h:

(i) It is easy to see that condition (A1) is satisfied for all three variants, by the fact that $T := T_1$ is volume-preserving and I_h is exact on constant functions.
(ii) Condition (A2) is satisfied by the H^1-Galerkin approach. For the L^2-Galerkin approach, (A0) implies (A2) [9].
(iii) Condition (A3) is trivially satisfied by the L^2-Galerkin approach.

We will show (A2) and (A3) for the case that I_h comes from the collocation approach. In Appendix A, we give proofs of the following two lemmata for P^1-triangular elements under assumption (A0).

Lemma 4.1 (L^2-stability (A3) of P^1-nodal interpolation)**.** *Let $I_h : C\left(\overline{\Omega_1}\right) \to S_h^1$ be the P^1-Lagrange nodal interpolation operator corresponding to $\{\mathcal{T}_h^1\}_{h>0}$. If (A0) holds, then there exists a constant $C > 0$ so that $\|I_hTv\|_{L^2} \le C\|v\|_{L^2}$ for all $v \in S_{h'}^0$ and all $h < h'$.*

Lemma 4.2 (H^1-convergence (A2) of P^1-nodal interpolation)**.** *Let $I_h : C\left(\overline{\Omega_1}\right) \to S_h^1$ be the P^1-Lagrange nodal interpolation operator corresponding to $\{\mathcal{T}_h^1\}_{h>0}$. If (A0) holds, and if v is piecewise C^∞ on Ω_1 then*

$$\|I_hv - v\|_{H^1} \to 0 \quad \text{as} \quad h \to 0.$$

Convergence for homogeneous Neumann Boundary. Let $r(v) = a(v,v)/\langle v,v\rangle_{L^2}$ and $\tilde{r}_h(v) = \tilde{a}_h(v,v)/\langle v,v\rangle_{L^2}$ be the Rayleigh quotients for a and $\tilde{a}_h$ respectively. Assuming (A0), we know that both $r(v)$ and $\tilde{r}_h(v)$ are trivially minimized by a constant function. Going to mean-free functions, we therefore define λ_1 and $\tilde{\lambda}_{h,1}$ to be the corresponding smallest Ritz values on $\hat{H}^1$ and $\hat{S}_h^0$, respectively and v, $\tilde{v}_h$ the corresponding Ritz vectors (normalized to have unit L^2-norm).

We now derive a convergence result for $\tilde{v}_h$ to v in two parts:

Theorem 4.3. *Provided that (A0) holds and I_h satisfies the assumptions (A1) and (A2), then*

$$\limsup_{h\to 0} \tilde{\lambda}_{h,1} \leq \lambda_1.$$

Proof. Pick any sequence h_n with $h_n \to 0$. For arbitrary $w \in \hat{S}^0_{h_n}$, have

$$\begin{aligned}\limsup_{n\to\infty} \tilde{\lambda}_{h_n,1} &= \limsup_{n\to\infty} \tilde{r}_{h_n}(\tilde{v}_{h_n}) \quad \text{(definition of } \tilde{v}_{h_n}\text{)} \\ &\leq \limsup_{n\to\infty} \tilde{r}_{h_n}(w) \qquad \text{(Ritz-values minimize the Rayleigh-quotient).}\end{aligned}$$

Now for arbitrary $\epsilon > 0$, pick[4] some $w \in \hat{S}^0_{h'}$ where $h' = h'(\epsilon)$ with $\|w\|_{L^2} = 1$ so that $r(w) < \lambda_1 + \epsilon$. Then by the assumption that our meshes are nested, w is in the domain of $\tilde{a}_{h_n}$ for sufficiently large n and we have:

$$\begin{aligned}\limsup_{n\to\infty} \tilde{\lambda}_{h_n,1} &\leq \limsup_{n\to\infty} \tilde{r}_{h_n}(w) \\ &= \limsup_{n\to\infty} \tilde{a}_{h_n}(w,w) \qquad \text{(definition of Rayleigh Quotient)} \\ &= \limsup_{n\to\infty} \left(a(w,w) + \tilde{a}_{h_n}(w,w) - a(w,w)\right) \\ &\leq \limsup_{n\to\infty} \left(\lambda_1 + \epsilon + a^1\left(I_{h_n}Tw, I_{h_n}Tw\right) - a^1(Tw,Tw)\right).\end{aligned}$$

For this fixed v we know that $a^1\left(I_{h_n}Tw, I_{h_n}Tw\right) - a^1(Tw,Tw) \to 0$ by the H^1 convergence assumption, and by H^1-continuity of a^1. This gives the result. □

Theorem 4.4. *Provided that (A0) holds and I_h satisfies (A1) and (A3), then*

$$\liminf_{h\to 0} \tilde{\lambda}_{h,1} \geq \lambda_1.$$

Proof. We use an approach reminiscent of the *direct method* in the calculus of variations (*cf.* [19]). Assume that I_h satisfies both properties, but (for the sake of contradiction) that there exists a sequence $h_n \to 0$ monotonically with $\tilde{\lambda}_{h_n,1} \to \beta < \lambda_1$. Note that by positivity of $\tilde{a}_h$ the sequence cannot diverge to $-\infty$, and by Theorem 4.3 it cannot diverge to $+\infty$. Hence, using coercivity of a^0 on $\hat{H}^1$ we get that $|\tilde{v}_{h_n}|_{H^1} \leq C$ for some $C > 0$, otherwise the a^0 term would go to infinity. Here and below, C represents a generic constant independent of h_n. The Poincaré-Friedrichs inequality (*cf.* [9], Lem. B.66) for mean-free functions states that the L^2 norm is uniformly bounded by a constant times the H^1 seminorm, thus it follows that

$$\|\tilde{v}_{h_n}\|_{H^1} \leq C. \tag{4.2}$$

Recall that the Banach–Alaoglu theorem states that the closed unit ball in H^1 is weakly sequentially compact, while the Rellich–Kondrachev theorem asserts that norm-bounded H^1 sets are L^2-precompact. Hence we can assume that (going to a subsequence) $\tilde{v}_{h_n} \rightharpoonup \tilde{v}$ in H^1 and $\tilde{v}_{h_n} \to \tilde{v}$ in L^2 for some $\tilde{v} \in H^1$. Note that the two limits are indeed the same since $\cdot \mapsto \langle \cdot, v\rangle_{L^2}$ is a continuous linear functional on H^1 for all $v \in L^2$.

As $\tilde{v}_{h_n} \in \hat{H}^1$, it follows that $\tilde{v} \in \hat{H}^1$, the L^2-convergence gives us further that $\|\tilde{v}\|_{L^2} = 1$.

Without loss of generality, assume that $\ell^d(\Omega_1) = 1$ and define $J_n : \Omega_0 \to \mathbb{R}$ as the constant function taking the value $\int_{\Omega_1} I_{h_n} T\tilde{v}_{h_n} \mathrm{d}\ell^d$, and observe that

$$a^1\left(I_{h_n}T\tilde{v}_{h_n}, I_{h_n}T\tilde{v}_{h_n}\right) = a^1\left(I_{h_n}T\tilde{v}_{h_n} - J_n, I_{h_n}T\tilde{v}_{h_n} - J_n\right). \tag{4.3}$$

[4]That we can do this follows the classical theory of density of finite-element spaces in Sobolev spaces ([9], Cor. 1.110), or from convergence of eigenvalues of the Galerkin approximation such as equation (3.1) in the case that the eigenvectors are sufficiently smooth at the boundary.

We know from the positivity of a^0 that $a^1\left(TI_{h_n}\tilde{v}_{h_n}, TI_{h_n}\tilde{v}_{h_n}\right) \leq \tilde{r}_{h_n}\left(\tilde{v}_{h_n}\right)$ and as the right hand side converges, the left hand side is bounded by a constant that does not depend on n. Hence, by coercivity of a^1 on mean-free H^1 functions, it follows from (4.3) and the Poincaré–Friedrichs inequality that $\|I_{h_n}T\tilde{v}_{h_n} - J_n\|_{H^1} < C$, yielding that $I_{h_n}T\tilde{v}_{h_n}$ is H^1-bounded as long as J_n is – which is the case by L^2-stability, the L^2–L^2 continuity of T, and the fact that $\|\tilde{v}_{h_n}\|_{L^2} = 1$. Hence $I_{h_n}T\tilde{v}_{h_n}$ is (uniformly in n) H^1-bounded. Going to a subsequence, it is therefore weakly H^1- and strongly L^2-convergent (as above). As the weak-H^1 and L^2-limits coincide, to show that the sequence converges to $T\tilde{v}$ weakly in H^1, it is enough to show L^2-convergence.

Let C_1 be the stability constant from the L^2-stability condition. We know that as $v_{h_n} \to \tilde{v}$ in L^2, it holds that $T\tilde{v}_{h_n} \to T\tilde{v}$. Therefore given $\varepsilon > 0$, pick m so that $\|T\tilde{v}_{h_m} - T\tilde{v}\|_{L^2} \leq \varepsilon/3$ and and $C_1\|\tilde{v}_{h_n} - \tilde{v}_{h_m}\|_{L^2} \leq \varepsilon/3$ for all $n \geq m$. Also, by the nesting property of the meshes $\tilde{v}_{h_n} - \tilde{v}_{h_m} \in \hat{S}^0_{h_n}$ and hence

$$\begin{aligned}\|I_{h_n}T\tilde{v}_{h_n} - T\tilde{v}\|_{L^2} &\leq \|I_{h_n}T\tilde{v}_{h_n} - I_{h_n}T\tilde{v}_{h_m}\|_{L^2} + \|I_{h_n}T\tilde{v}_{h_m} - T\tilde{v}_{h_m}\|_{L^2} + \|T\tilde{v}_{h_m} - T\tilde{v}\|_{L^2}\\ &\leq C_1\|\tilde{v}_{h_n} - \tilde{v}_{h_m}\|_{L^2} + \|I_{h_n}T\tilde{v}_{h_m} - T\tilde{v}_{h_m}\|_{L^2} + \|T\tilde{v}_{h_m} - T\tilde{v}\|_{L^2}\\ &\leq 2\varepsilon/3 + \|I_{h_n}T\tilde{v}_{h_m} - T\tilde{v}_{h_m}\|_{L^2}.\end{aligned}$$

Now using the H^1-convergence property, pick $n_0 \geq m$ so that for $n \geq n_0$, we have

$$\|I_{h_n}T\tilde{v}_{h_m} - T\tilde{v}_{h_m}\|_{L^2} \leq \varepsilon/3.$$

It follows that for all $n \geq n_0$

$$\|I_{h_n}T\tilde{v}_{h_n} - T\tilde{v}\|_{L^2} \leq \epsilon.$$

Summarizing, we now have proved that

(1) $\tilde{v}_{h_n} \rightharpoonup \tilde{v}$ in H^1,
(2) $I_{h_n}T\tilde{v}_{h_n} \rightharpoonup T\tilde{v}$ in H^1, and
(3) $\tilde{v} \in \hat{H}^1$ with $\|\tilde{v}\|_{L^2} = 1$.

The functions $u \mapsto \sqrt{a^0(u,u)}$ and $u \mapsto \sqrt{a^1(u,u)}$ are norms that are equivalent to the $\hat{H}^1$-norm by the Poincaré–Friedrichs inequality[5]. By the Banach–Steinhaus theorem, norms are weakly sequentially lower-semicontinuous. The L^2 convergence of $I_{h_n}Tv_{h_n}$ also gives that $J_n \to 0$ in L^2, and therefore also in H^1 as J_n is constant). Thus we have:

$$\begin{aligned}a^0\left(\tilde{v},\tilde{v}\right) &\leq \liminf_{n\to\infty} a^0\left(\tilde{v}_{h_n},\tilde{v}_{h_n}\right)\\ a^1\left(T\tilde{v},T\tilde{v}\right) &\leq \liminf_{n\to\infty} a^1\left(I_{h_n}T\tilde{v}_{h_n} - J_n, I_{h_n}T\tilde{v}_{h_n} - J_n\right)\\ &= \liminf_{n\to\infty} a^1\left(I_{h_n}T\tilde{v}_{h_n}, I_{h_n}T\tilde{v}_{h_n}\right)\end{aligned}$$

yielding

$$\begin{aligned}a\left(\tilde{v},\tilde{v}\right) &= a^0\left(\tilde{v},\tilde{v}\right) + a^1\left(T\tilde{v},T\tilde{v}\right)\\ &\leq \liminf_{n\to\infty}\left(a^0\left(\tilde{v}_{h_n},\tilde{v}_{h_n}\right) + a^1\left(I_{h_n}T\tilde{v}_{h_n}, I_{h_n}T\tilde{v}_{h_n}\right)\right)\\ &= \liminf_{n\to\infty} \tilde{r}_{h_n}\left(\tilde{v}_{h_n}\right)\\ &= \lim_{n\to\infty} \tilde{\lambda}_{h_n,1} = \beta < \lambda_1.\end{aligned}$$

This is a contradiction to the definition of λ_1, which requires that $a\left(\tilde{v},\tilde{v}\right) \geq \lambda_1$ and thus the claim is proved. □

[5]The weak topologies also coincide, as for any $f \in \hat{H}^1$, the Riesz representation theorem gives a $\tilde{f} \in \hat{H}^1$ so that $\langle\cdot, f\rangle_{H^1} = a_0(\cdot, \tilde{f})$.

Theorem 4.5. *The conclusion of the previous theorem also holds if (A0) is satisfied and I_h comes from the H^1-Galerkin approach.*

Proof. The previous proof required the L^2-stability only in two places. The first was in bounding J_n, this is trivially bounded as $\|I_h\|_{H^1 \to H^1} = 1$ and $\tilde{v}_{h_n}$ is H^1-bounded. The second was in showing that $I_{h_n} T \tilde{v}_{h_n} \rightharpoonup T\tilde{v}$. But this follows from the fact that for $f \in H^1$:

$$\langle I_{h_n} T \tilde{v}_{h_n}, f \rangle_{H^1} = \langle T \tilde{v}_{h_n}, I_{h_n} f \rangle_{H^1}.$$

As $I_h f \to f$ in H^1 and $T\tilde{v}_{h_n} \rightharpoonup T\tilde{v}$, this gives the claim. □

Theorem 4.6 (Eigenvector convergence)**.** *Assume that (A0)–(A3) hold, and that the eigenspace corresponding to λ_1 is one-dimensional. Then $|\langle \tilde{v}_h, v \rangle_{L^2}| \to 1$ for $h \to 0$.*

Proof. The proof of Theorem 4.4 shows that for any monotone sequence $h_n \to 0$ for which λ_{h_n} converges to λ_1, every in L^2 convergent subsequence of $\tilde{v}_{h_n}$ converges to some $\tilde{v} \in H^1$ with $r(\tilde{v}) = \lambda_1$. Theorems 4.4 and 4.3 show that $\lambda_{h_n} \to \lambda_1$ for any $h_n \to 0$. As $\tilde{v}_{h_n}$ is bounded in H^1 and therefore pre-compact in L^2, this means that $\tilde{v}_{h_n} \to \tilde{v}$ in L^2 with $r(\tilde{v}) = \lambda_1$, from which it follows that $\tilde{v} = \pm v$, giving the result for a subsequence. We get the final result by noting that if $\tilde{v}_{h_n}$ has a subsequence $\tilde{v}_{h_{n_k}}$ for which $|\langle \tilde{v}_{h_{n_k}}, v \rangle| \to c \neq 1$, by the above it must have a (further) subsequence that converges to a different value, a contradiction. □

Theorem 4.7 (Higher eigenpairs)**.** *Assuming (A0)–(A3), the results of the previous theorems generalize to the m-th eigenpair for $m > 1$.*

Proof. The generalization of Theorem 4.3 can be proven by the same method as the case $m = 1$: instead of choosing a w with $r(w) < \lambda_1 + \epsilon$, choose a series of pairwise-orthogonal $(w_i)_{i=1\ldots m} \in \hat{S}_h^0$ with the property that $r(w_i) \leq \lambda_i + \epsilon$.

The proof of Theorem 4.4 must only be modified to show that the limit point $\tilde{v}_m$ is L^2-orthogonal to the previous eigenvectors span $\{v_1, \ldots, v_{m-1}\}$. Writing $\tilde{v}_{m,h}$ for the m-th Ritz-vector of $\tilde{a}_h$ on $\hat{S}_h^1$, this readily follows (by induction) from the fact that $\tilde{v}_{m,h_n} \perp \operatorname{span}\{\tilde{v}_{1,h_n}, \ldots, \tilde{v}_{m-1,h_n}\}$ and thus also $\langle \tilde{v}_{i,h_n}, T v_i \rangle \to 0$ in L^2 for $i = 1, \ldots, m-1$.

The proof of the generalization of Theorem 4.6 then follows from the generalization of Theorem 4.4. □

Convergence for homogeneous Dirichlet boundary. For the case of a homogeneous Dirichlet boundary, we must replace $\hat{H}^1$ with H_0^1. Here we require the additional condition:

(A1′) Boundary preservation: for $v \in H_0^1(\Omega_1) \cap S_h^0$ we have that $I_h T v \in H_0^1(\Omega_1)$.

We note that the I_h from collocation and H^1-Galerkin have this property.

Theorem 4.8. *The convergence results of Theorems 4.3, 4.4 and 4.6 hold also for the Ritz-values for homogeneous Dirichlet boundary conditions, provided that (A0) holds and I_h satisfies (A1′) in addition to satisfying (A2) and (A3).*

Proof. Same as the proofs for the Neumann case, except that coercivity of the bilinear forms involved on $\hat{H}^1$ is replaced with that on H_0^1. The boundary preservation property ensures we do not need J_n in the proof of Theorem 4.4, the proof otherwise goes on exactly the same lines. □

4.1. Numerical experiments

The three TO approaches yield a stiffness-matrix D of the form

$$D = D_0 + A^T D_1 A$$

where A is the representation matrix of $I_h T$ and D_0, D_1 result from the bilinear form of the static Laplacian. In the case of the L^2- or H^1-Galerkin approach, the matrix A has the form

$$A = G^{-1}\tilde{A},$$

where $\tilde{A} = \langle \varphi_i, T\varphi_j \rangle$ and $G_{i,j} = \langle \varphi_i, \varphi_j \rangle$. Note that sparsity of G and $\tilde{A}$ does not necessarily imply sparsity of A. A naive calculation of the full matrix A therefore renders the computation of (some) eigenvalues of D too expensive for larger problems. We therefore do not include the Galerkin–TO approaches in the numerical experiments below, further work is needed to determine if the Galerkin–TO methods can be modified to overcome this issue.

All TO results shown below are therefore the collocation-based ones. For the "non-adaptive TO" experiments, we used identical regular meshes for the initial and final triangulations $\mathcal{T}_h^0$ and $\mathcal{T}_h^1$. For the "adaptive TO" experiments, the initial mesh was regular but the final mesh was a Delaunay-triangulation (with the `VoronoiDelaunay.jl` package [22]) of the images of the initial mesh points under the flow map T. The theory outlined above requires (i) nested meshes, and (ii) uniform bounds on shape-regularity and quasi-uniformity constants of the meshes as they are refined; each of these properties is difficult to guarantee in general for the image triangulations. We nevertheless include the adaptive TO in the plots for comparison.

We note that the finest grid used for the TO experiments is 257×257. This is not as fine as the finest grid used in the CG approach (513×513). The reason for this is that the stiffness matrix D from the TO approach does not have the same banded structure as that coming from the CG approach, making a solution of the eigenproblem more expensive (for the example of the cylinder flow: 1 h 28 min for the non-adaptive TO using a P^1 513×513 mesh *vs.* 14 min for the CG approach with P^2 elements on a 1025×1025 mesh). The reference solution here is the same as that used for the CG experiments.

Our numerical experiments appear to be consistent with our theoretical results proven above.

4.1.1. Standard map

We investigate the convergence of collocation-based TO approaches on the Standard map test case.

The results for this numerical experiment are shown in Figure 2. We see an improvement by a full order of magnitude in the errors in both the eigenvalues and the eigenspaces for P^2 elements over P^1 elements. Concerning the convergence order, this experiment suggests that the order for P^2 elements is not higher than for P^1 elements in the TO approach, which match those obtained for eigenvectors based on P^1 elements in the CG approach.

4.1.2. Cylinder flow

We observe a smaller error reduction in the eigenvalue and eigenvector errors for P^2 *vs.* P^1 elements for the cylinder flow (Fig. 6) compared to the standard map example. The reduction in convergence orders compared to the standard map (*i.e.* comparing Fig. 6 to Fig. 5) mirrors the reductions observed in the corresponding CG experiments (*i.e.* comparing Fig. 2 to Fig. 1), where the orders are around half those seen for the standard map. Similarly to the standard map results, the P^2 elements did not perform asymptotically better than P^1 elements.

4.1.3. Bickley jet

We repeat the experiment from Section 3.1.3 with the (non-adaptive) TO approach, see Figure 7. Here we note that this experiment falls outside of the theory described so far as the computational domain is not exactly mapped to itself by the flow, but our attempts to work around this (by *e.g.* having a larger mesh at the final

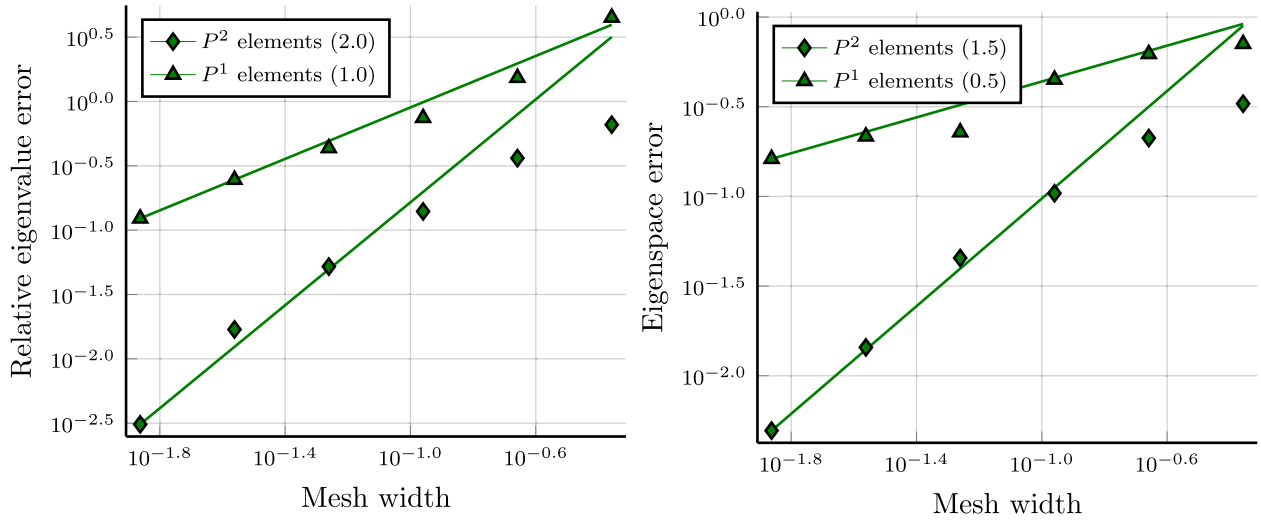

FIGURE 2. Cylinder flow: errors in the first nontrivial eigenvalue (*left*) and corresponding 1-dimensional eigenspace (*right*) of the dynamic Laplacian discretized with CG approach. The slopes of the corresponding lines are given in brackets in the legends.

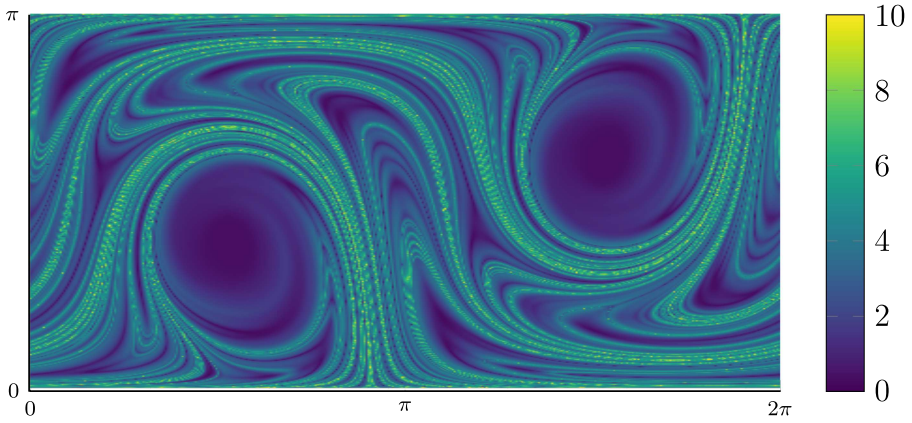

FIGURE 3. Cylinder flow: log of the trace of the mean diffusion tensor, $\log_{10} \operatorname{tr}(A(x))$.

time) did not significantly affect the topology of the clustering result in the low data cases we looked at. We note that on even finer meshes, we also saw clusterings different to those in Figure 7, such as those where the central jet was a separate cluster. We did not concern ourselves with these further as our aim was merely to compare the different discretisations in the low data limit, and it is not clear what the "correct" clustering should be.

As in Section 3.1.3, the mesh widths in Figure 7 below are the lowest at that aspect ratio for which the topology of the clustering result does not change; nodes at the boundaries that are identified due to the periodic boundary conditions are counted twice. Here, the majority of the computational cost (apart from the clustering) is given by the evaluation of the (inverse) flow map, which has to be evaluated once for each basis function of the finite element space. Note that there are three basis functions per element for P^1 and six per element for P^2 elements. While for P^2 elements, a coarser mesh was sufficient, the number of basis functions was comparable (even a little larger) than for the P^1 case – which is in contrast to the corresponding CG experiment.

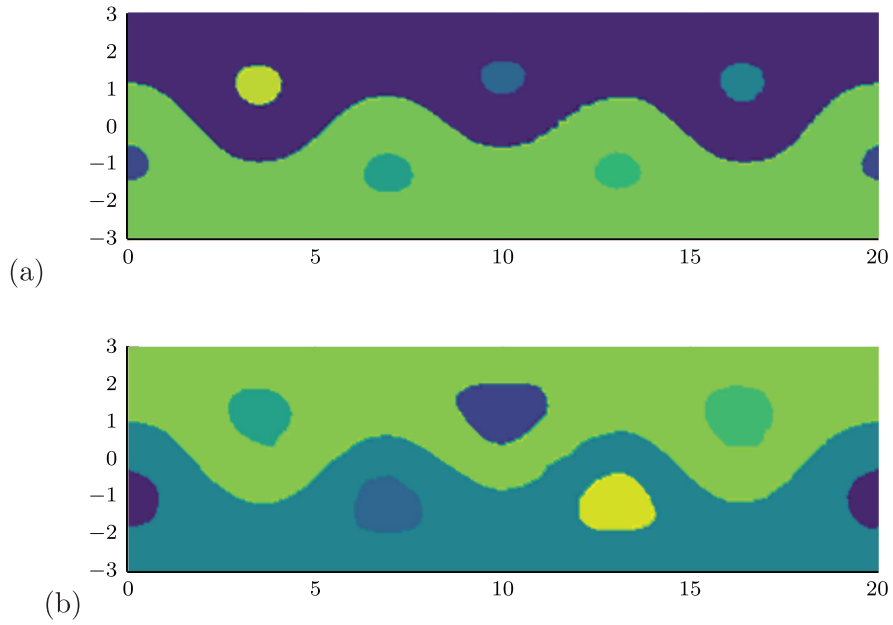

FIGURE 4. Bickley jet: comparison of coherent sets obtained by the CG approach with P^1 *vs.* P^2 elements. (a) P^1 elements on 101×31 mesh (18 000 quadrature points, 6000 triangles). (b) P^2 elements on 21×7 mesh (720 quadrature points, 240 triangles).

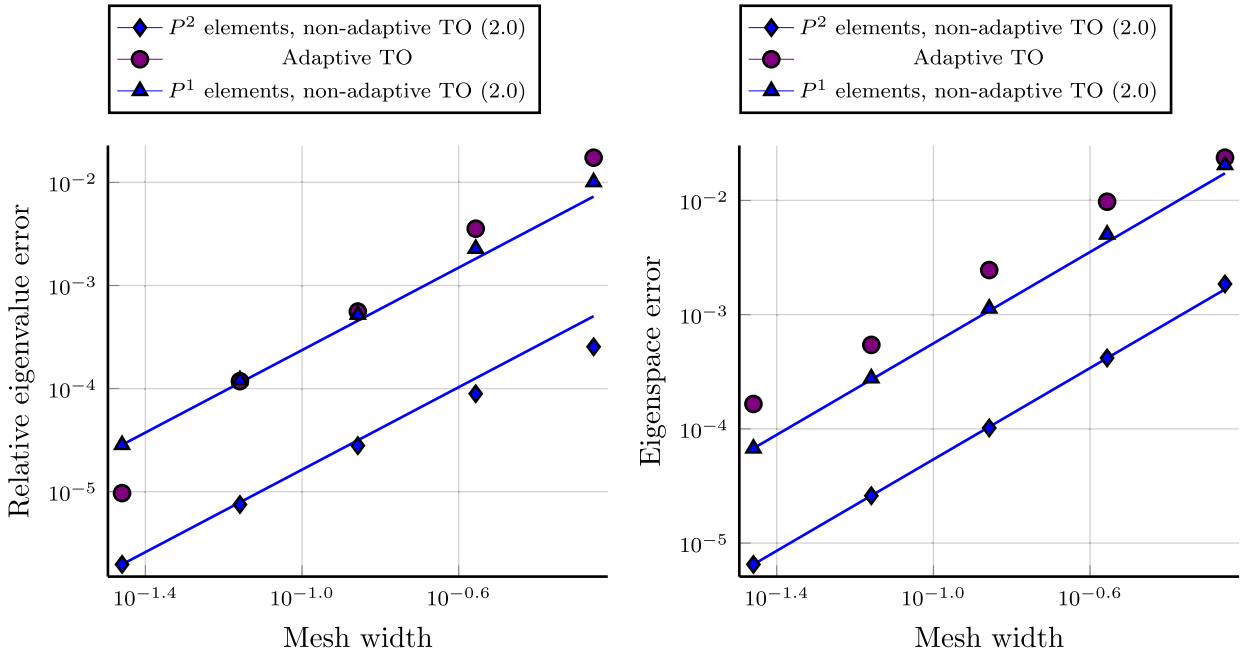

FIGURE 5. Standard map: errors in the first nontrivial eigenvalue (*left*) and 2-dimensional eigenspace spanned by the smallest eigenvectors (*right*) of the dynamic Laplacian discretized with the TO approach. The slopes of the corresponding lines are given in brackets in the legends.

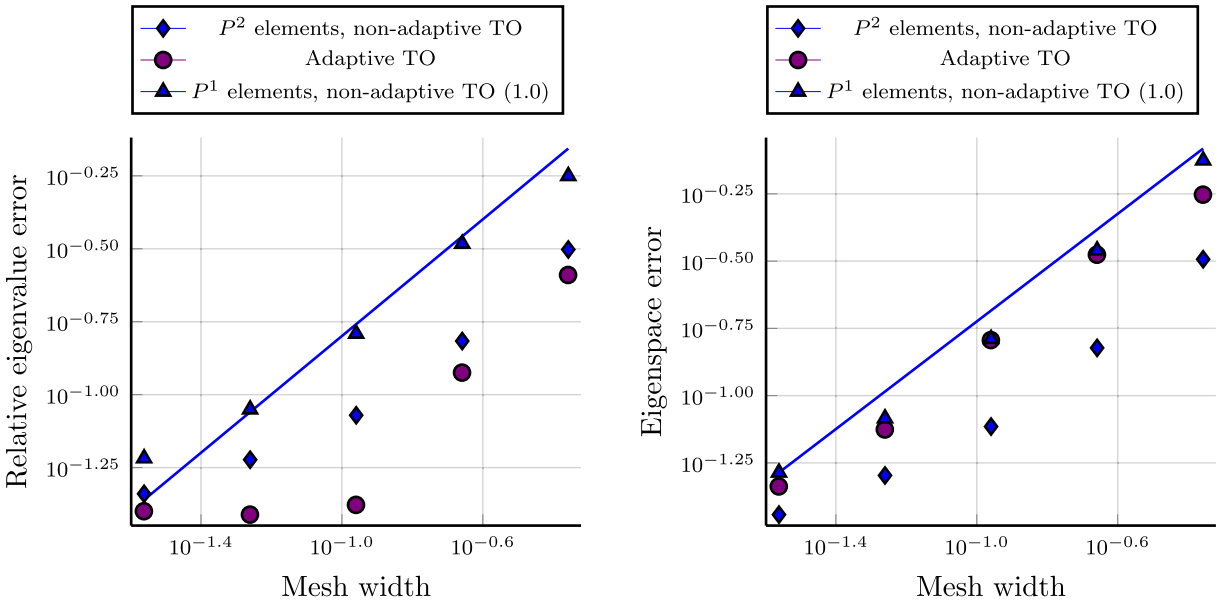

FIGURE 6. Cylinder flow: errors in the first nontrivial eigenvalue (*left*) and corresponding eigenspace (*right*) of the dynamic Laplacian for the TO approaches. The slopes of the corresponding lines are given in brackets in the legends.

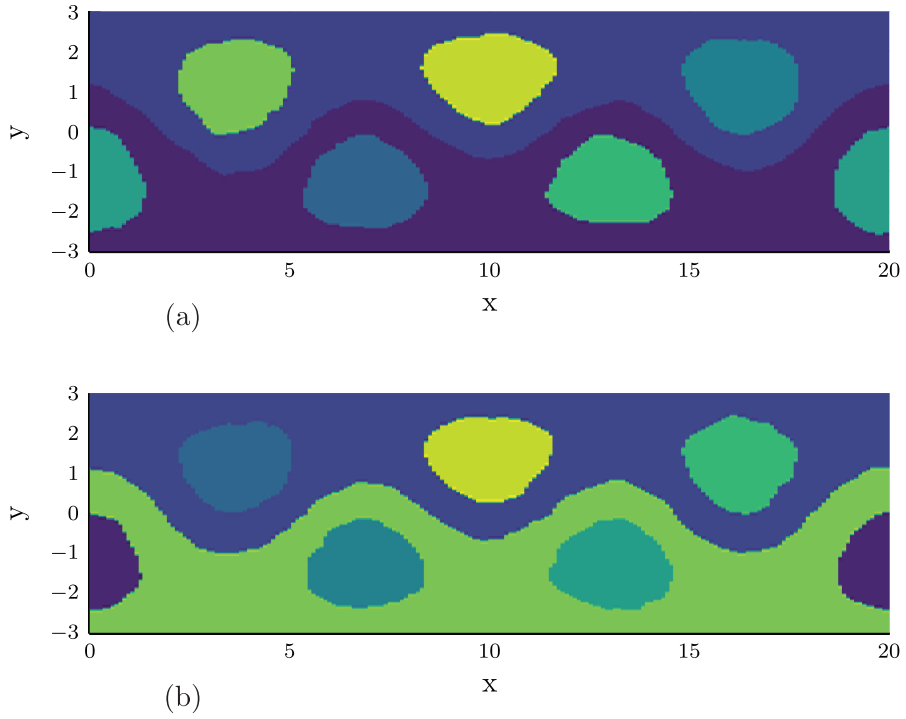

FIGURE 7. Bickley jet: comparison of TO method with P^1 and P^2 elements. (a) P^1 elements on 71×22 mesh (1540 nodes). (b) P^2 elements on 41×13 mesh (2000 nodes).

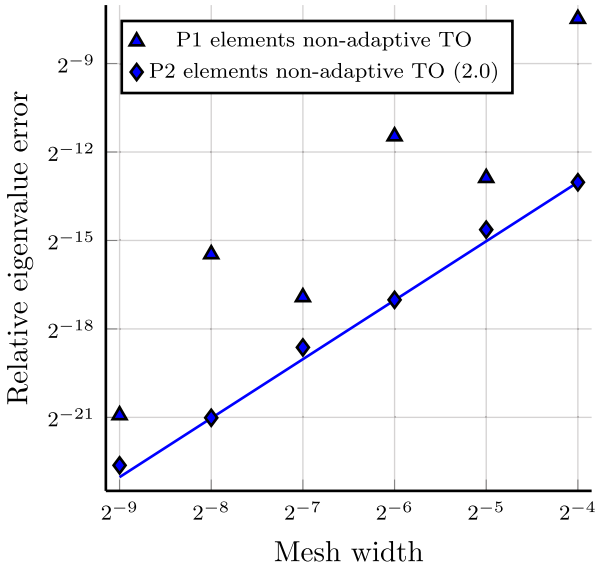

FIGURE 8. 1D shift map: errors in the first calculated eigenvalue. The slope of the corresponding line is given in brackets in the legend.

4.2. TO convergence rates

Determining the theoretical convergence orders of the TO-methods is an outstanding task. In order to investigate whether we can expect higher-order convergence, we consider the collocation-based non-adaptive TO approach on a simple example in one dimension. In this example we can largely isolate the dynamics from the errors to focus on errors arising from translations of the basis functions.

The only volume-preserving diffeomorphisms of the circle $\mathbb{S}^1 = \mathbb{R}/\mathbb{Z}$ to itself are rigid rotations. Let $T : \mathbb{S}^1 \to \mathbb{S}^1$ be given by $T(x) = (x + \alpha) \mod 1$. Rigid rotations commute with the Laplace operator; thus $\Delta^{\text{dyn}} = (\Delta + T_1^* \Delta T_{1,*})/2 = \Delta$, and the dynamic Laplacian is equal to the static Laplacian. The first nontrivial eigenspace of the dynamic Laplacian is therefore spanned by $v(x) = \sqrt{2}\sin(2\pi x)$ and $u(x) = \sqrt{2}\cos(2\pi x)$ which are orthonormal eigenvectors for the eigenvalue $\lambda_1 = 4\pi^2$.

Any errors in the corresponding discrete bilinear form

$$\tilde{a}_h(u, v) = \frac{1}{2}\left(a(u, v) + a\left(I_h T u, I_h T v\right)\right)$$

therefore arise solely from discretisation errors related to the rotation of the φ_i by α. In our experiments, we consider $\alpha = 0.15$. For the non-adaptive collocation TO approach, denote the leading nontrivial eigenvalue of Δ^{dyn} by $\tilde{\lambda}_{h,1}$. We now look at the order of convergence for the error $\frac{|\tilde{\lambda}_{h,1} - \lambda_1|}{\lambda_1}$ as $h \to 0$.

The convergence rates in Figure 8 are identical to those found for the standard map in Figure 5. The CG approach in this example is simply computing the eigenvectors and eigenvectors of the standard Laplace operator and therefore unsurprisingly one recovers the theoretical orders of convergence. These numerical results suggest that when using the non-adaptive TO method, we cannot expect an asymptotically higher convergence rate for P^2 elements in comparison to P^1-elements even for very simple flow maps.

5. CONCLUSION

We compared the use of P^1 and P^2 elements in collocation-based CG and TO approximations of the dynamic Laplacian. In the CG approach applied to weakly nonlinear dynamics, P^2 elements can significantly reduce the

computational cost by providing an asymptotically higher order of convergence. A benefit of P^1 elements for the CG approach is that a first-order method of quadrature can be used in the discretization, whereas using first-order quadrature for P^2 elements results in a singular mass matrix. This does not affect the asymptotic order of convergence, but nevertheless introduces a constant factor which may be relevant in some low-data cases. It seems promising to investigate how to locally adapt the element order and/or the element diameter (in the spirit of *p*- or *hp*-adaptive finite element methods).

In the non-adaptive TO approach, there seems to be little benefit gained by using P^2 as opposed to P^1 elements. The adaptive TO is inherently P^1-based, and thus does not benefit from a P^2 discretization either. In general, numerical experiments suggest that collocation-based TO approaches have equal (or in some cases better) rates of convergence compared to the P^1 CG discretisation.

The P^2 CG discretisation generally had a higher order of convergence, though the numerically observed convergence rates varied significantly when the quadrature order was changed or when applied to more nonlinear and hyperbolic dynamics. It is difficult to compare the CG and TO approaches in general as the former relies on being able to calculate derivatives of the flow map, whereas the latter is purely data based. This makes the TO approach applicable to some cases where the CG approach cannot be used.

A hindrance to using the TO approach for finely resolved meshes is the fact that here the call to `eigs` takes much longer compared to when one uses the CG discretisation on the same mesh. We suspect that this is due to the fact that unlike in the TO approach, the CG discretisation preserves the banded structure of the stiffness matrix. More work is needed to determine how the eigenproblem can be solved efficiently in this case, or whether it is possible to avoid the eigenproblem completely but still be able to compute coherent sets. More work is also needed to determine the true rates of convergence of eigenvalues and eigenvectors. We proved that they do converge for the non-adaptive TO approach, but were only able to conjecture what the true rates are based on numerical experiments. It also remains to be seen whether Galerkin TO approaches can be modified to be computationally efficient.

Appendix A. Proofs

Throughout all proofs, C refers to a constant depending only on the mesh and dimension.

A.1. Proof of Lemma 4.1

The following proof of Lemma 4.1 uses ideas from the proof of Lemma 2.1 from [4]. We start with a helper lemma:

Lemma A.1. *Let $\left\{\mathcal{T}_{h'}^0\right\}_{h'>0}$ and $\left\{\mathcal{T}_h^1\right\}_{h>0}$ be quasi-uniform meshes on d-dimensional open sets Ω_0 and Ω_1 respectively. Let $F:\Omega_0\to\Omega_1$ be smooth on Ω_0 with smooth extension to the boundary. Then there exists $C>0$ so that for all $h,h'>0$ and $\tau'\in\mathcal{T}_{h'}^0$ it holds that:*

$$\mathcal{N}(\tau') := \left|\left\{\tau\in\mathcal{T}_h^1 : F(\tau')\cap\tau\neq\emptyset\right\}\right| \leq C\left(\frac{h'+h}{h}\right)^d.$$

Proof. By quasi-uniformity of the meshes, we can find positive constants a', A' so that for any triangle $\tau'\in\mathcal{T}_{h'}^0$ there is a point τ_x' so that:

$$B\left(\tau_x', a'h'\right) \subset \tau \subset B\left(\tau_x', A'h'\right), \tag{A.1}$$

where $B(x,r)$ is the open ball of radius r centered at x. This gives that where $y := F\left(\tau_x'\right)$:

$$F(\tau') \subset F\left(B\left(\tau_x', A'h'\right)\right) \subset B\left(y, \underbrace{\|DF\|_\infty A'}_{:=E} h'\right) \tag{A.2}$$

where the last inclusion follows from the mean-value theorem, and $\|DF\|_\infty$ exists as F is smoothly extensible to the boundary.

Now write a, A for the shape-regularity/quasi-uniformity constants of $\{\mathcal{T}_h^1\}_{h>0}$, so that a formula like (A.1) holds for $\{\mathcal{T}_h^1\}_{h>0}$ also.

Then if $\tau \in \mathcal{T}_h^1$ intersects $B(y, Eh')$, it must hold that $B(\tau_x, ah) \subset B(\tau_x, Ah) \subset B(y, Eh' + 2Ah) \subset B(y, c(h'+h))$ with $c := \max\{E, 2A\}$. As for different τ, the sets $B(\tau_x, ah)$ are disjoint, we get

$$\mathcal{N}(\tau') \leq \left(\frac{c(h'+h)}{ah}\right)^d$$

which gives the claim. □

Lemma A.2. *Let $\{\mathcal{T}_h\}_{h>0}$ be a family of quasi-uniform meshes on an open subset of d-dimensional space. Let S_h be the space of functions representable by P^k-Lagrange elements on the mesh. Then there exist $C, C' > 0$ so that for all $v \in S^h$:*

$$C_1\|v\|_{L^2}^2 \leq h^d \sum_p |v(p)|^2 \leq C_2\|v\|_{L^2}^2$$

where p ranges over the nodes of the triangulation.

Proof. This follows directly from well-known results about the spectrum of mass-matrices, see p. 386 of [9] □

Proof of Lemma 4.1. Throughout the proof, C refers to a constant that does not depend on h or h' and whose exact value can change from line to line. Let $h' > h > 0$ and $v \in S_{h'}^0$. Then by Lemma A.2, and as F is volume-preserving,

$$\|I_h T v\|_{L^2}^2 \leq Ch^d \sum_p |v\left(F^{-1}(p)\right)|^2 =: (*)$$

where p ranges over the nodes of $\mathcal{T}_h^1$. Using Lemma A.1, we know that for any triangle $\tau' \in \mathcal{T}_h^0$, at most $C\left(\frac{h'+h}{h}\right)^d$ triangles from $\mathcal{T}_{h'}^1$ can intersect with $F(\tau')$; up to a constant factor this therefore bounds the number of vertices p in $\mathcal{T}_h^1$ for which $F^{-1}(p)$ lies in a given triangle. Moreover, as we are using P^1-Lagrange elements, $|v\left(F^{-1}(p)\right)|$ is bounded by $|v(p')|$ for some vertex p' of the triangle that contains $F^{-1}(p)$. This gives, using Lemma A.2 and the fact that $h' > h$, that:

$$\begin{aligned}(*) &\leq Ch^d \left(\frac{h'+h}{h}\right)^d \sum_{p'} |v(p')|^2 \\ &\leq C(h')^d \sum_{p'} |v(p')|^2 \\ &\leq C\|v\|_{L^2}^2\end{aligned}$$

where p' ranges over the nodes of $\mathcal{T}_{h'}^0$. □

A.2. Proof of Lemma 4.2

Proof. Without loss of generality, look at triangles in dimension 2; similar arguments apply to higher-dimensional meshes. Since $\|I_h v - v\|_{L^2} \leq C\|I_h v - v\|_{L^\infty}$ and v is uniformly continuous, we have that

$$\|I_h v - v\|_{L^2} \to 0 \quad \text{as} \quad h \to 0.$$

What remains to be shown is $\|\nabla(I_h v - v)\|_{L^2} \to 0$.

We first show that $\|\nabla I_h v\|_{L^\infty} \leq C\|\nabla v\|_{L^\infty}$ (where C does not depend on h). It is enough to prove this for any triangle τ in the mesh $\mathcal{T}_h^1$. Assume first that the triangle τ has vertices $0, e_1$ and e_2, where e_1, e_2 are the canonical unit vectors in $\mathbb{R}^2$. Without loss of generality also $v(0) = 0$. Then $\nabla I_h v = (v(e_1), v(e_2))^T$.

By a mean value inequality[6], $\max\{|v(e_1)|, |v(e_2)|\} \leq \|\nabla v\|_{L^\infty(\tau)}$. Thus $\|\nabla I_h v\|_{L^\infty(\tau)} \leq \|\nabla v\|_{L^\infty(\tau)}$. Shape regularity immediately gives $\|\nabla I_h v\|_{L^\infty(\tau)} \leq C\|\nabla v\|_{L^\infty(\tau)}$ for general triangles, taking suprema over all triangles gives the claim.

By assumption v is C^2 except for on a nowhere dense set of measure zero. By standard FEM theory, $\|\nabla(I_h v - v)\|_{L^2(\Omega')} \to 0$ on all sub-meshes Ω' on which v is C^∞, and with $h \to 0$ we can choose Ω' so that $\ell^d(\Omega') \to \ell^d(\Omega)$, recalling that ℓ^d was the notation used for d-dimensional Lebesgue measure. Moreover, $|\nabla I_h v| < C$ almost everywhere, and hence discontinuities do not cause problems. It follows that $\|\nabla(I_h v - v)\|_{L^2} \to 0$. □

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Short-Time Heat Content Asymptotics via the Wave and Eikonal Equations

Nathanael Schilling[1]

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Abstract
In this short paper, we derive an alternative proof for some known (van den Berg & Gilkey 2015) short-time asymptotics of the heat content in a compact full-dimensional submanifolds S with smooth boundary. This includes formulae like

$$\int_S \exp(t\Delta)(f\mathbb{1}_S)\,\mathrm{d}V = \int_S f\,\mathrm{d}V - \sqrt{\frac{t}{\pi}}\int_{\partial S} f\,\mathrm{d}A + o(\sqrt{t}), \quad t \to 0^+,$$

and explicit expressions for similar expansions involving other powers of $\sqrt{t}$. By the same method, we also obtain short-time asymptotics of $\int_S \exp(t^m\Delta^m)(f\mathbb{1}_S)\,\mathrm{d}V$, $m \in \mathbb{N}$, and more generally for one-parameter families of operators $t \mapsto k(\sqrt{-t\Delta})$ defined by an even Schwartz function k.

Keywords Heat equation · Heat content · Riemannian manifolds · Geometrical optics

1 Introduction

Let (M, g) be a complete, boundaryless,[1] oriented Riemannian manifold with Laplace–Beltrami operator Δ, and volume $\mathrm{d}V$. On a codimension-1 submanifold of M, we write $\mathrm{d}A$ for the induced surface (hyper)-area form. The *heat semi-group* $T_t := \exp(t\Delta)$ acting on $L^2(M, \mathrm{d}V)$ is well defined (Δ is essentially self-adjoint on $C_c^\infty(M)$ [2]) and its behaviour as $t \to 0^+$ has been extensively investigated in the literature. Specifically, for a set $S \subset M$, the *heat content* of the form

[1] We assume that M has no boundary for the sake of simplicity, and the method presented here can be adapted to more general manifolds with boundary provided that S is compactly contained in the interior of M. If this is not the case, such as in the classical heat content setting as in [13], it should be possible to obtain similar results by modifying the geometrical optics construction used.

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$\Omega_{S,f}(t) := \int_S T_t(f\mathbb{1}_S)\,\mathrm{d}V$, $f \in C^\infty(M)$, has recently received much attention; see, for instance, [7,11,12] and the references therein.

Let us briefly recall some known results. On $\mathbb{R}^n$, sets S of *finite perimeter* $P(S)$ are characterized by [7, Thm. 3.3]

$$\lim_{t\to 0^+} \sqrt{\frac{\pi}{t}}\Big(\Omega_{S,\mathbb{1}_M}(0) - \Omega_{S,\mathbb{1}_M}(t)\Big) = P(S). \tag{1}$$

Extensions of this idea to abstract metric spaces are given in [6]. In the setting of compact manifolds M (or $M = \mathbb{R}^n$) and S a full-dimensional submanifold with smooth boundary ∂S, the authors of [12] show that

$$\Omega_{S,f}(t) = \sum_{j=0}^{\infty} \beta_j t^{\frac{j}{2}}, \quad t \to 0^+, \tag{2}$$

where the coefficients β_j depend on S, f and the geometry of M. The setting of [12] is more general, amongst other things it includes f which have singularities. Some of the coefficients obtained in [12, corollary 1.7] are

$$\beta_0 = \int_S f\,\mathrm{d}V, \quad \beta_1 = -\frac{1}{\sqrt{\pi}}\int_{\partial S} f\,\mathrm{d}A, \quad \beta_2 = \frac{1}{2}\int_S \Delta f\,\mathrm{d}V.$$

Extensions to some non-compact manifolds M and certain non-compact S are in [11].

Both Eqs. (1) and (2) are proven with significant technical effort, yielding strong results. For example, in [7], explicit knowledge of the fundamental solution of the heat equation is used to obtain Eq. (1) for $C^{1,1}$-smooth ∂S, after which geometric measure theory is used. Similarly, [12] requires pseudo-differential calculus and invariance theory.

Our aim is to show that slightly weaker results can be obtained by considerably lower technical effort. In contrast to [7], we treat only compact S with smooth boundary, and do not allow f to have singularities like [12] does. On the other hand, we put no further restrictions than completeness on M. The proof presented here is simple, comparatively short, and provides an alternative differential geometric/functional analytic point of view to questions regarding heat content. Moreover, this approach is readily extended to some other PDEs including the semi-group generated by Δ^m. Observe that $T(t) = k(\sqrt{-t\Delta})$ with $k(x) = \exp(-x^2)$. We allow k to be an arbitrary even Schwarz function, with $\Omega_{S,f}(t) = \int_S k(\sqrt{-t\Delta})(f\mathbb{1}_S)\,\mathrm{d}V$ and will prove:

Theorem 1 *Let M be a complete Riemannian manifold with Laplace–Beltrami operator Δ, Riemannian volume $\mathrm{d}V$ and induced (hyper) area form $\mathrm{d}A$. Let $S \subset M$ be a compact full-dimensional submanifold with smooth boundary. For $f \in C^\infty(M)$ and $N \in \mathbb{N}$,*

$$\Omega_{S,f}(t) = \sum_{j=0}^{N} \beta_j t^{\frac{j}{2}} + o(t^{\frac{N}{2}}), \quad t \to 0^+,$$

for constants $(\beta_j)_{j=0}^N$ described further in the next theorem.

With the jth derivative $k^{(j)}$ (for $j \in \mathbb{N}_0$), let $r_j := (-1)^{j/2}k^{(j)}(0)$ for j even and $r_j := (-1)^{(j-1)/2}\int_0^\infty \frac{2k^j(s)}{-\pi s}\,\mathrm{d}s$ for j odd. Let φ locally be the signed distance function (see also [8, Sect. 3.2.2]) to ∂S with $S = \varphi^{-1}([0,\infty))$, and denote by ∇ and $\cdot$ the gradient and (metric) inner product, respectively. The vector field $\nu := -\nabla\varphi$ is outer unit normal at ∂S.

Theorem 2 *The coefficients of Theorem 1 satisfy $\beta_0 = r_0\int_S f\,\mathrm{d}V$ and $\beta_1 = -\frac{1}{2}r_1\int_{\partial S} f\,\mathrm{d}A$. For even $j \in \mathbb{N}_{\geq 2}$,*

$$\beta_j = \frac{r_j}{j!}\int_S \frac{1}{2}\Delta^{j/2} f\,\mathrm{d}V.$$

Moreover, given the Lie-derivative $\mathcal{L}_\nu$ with respect to ν,

$$\beta_3 = \frac{r_3}{2\cdot 3!}\int_{\partial S}\mathcal{L}_\nu(-\mathcal{L}_\nu + \frac{1}{2}\Delta\varphi)f - \frac{1}{2}\Delta f + \frac{1}{2}(-\mathcal{L}_\nu + \frac{1}{2}\Delta\varphi)^2 f\,\mathrm{d}A,$$

similar expression can be found also for larger odd values of j (see Sect. 3).

The properties of the signed distance function φ may be used to express terms appearing in Theorem 2 using other quantities. For example, its Hessian $\nabla^2\varphi$ is the second fundamental form on the tangent space of ∂S [3, Chap. 3], and thus $\frac{1}{2}\Delta\varphi$ is the mean curvature.

Our approach to prove Theorems 1 and 2 is to combine 3 well-known facts:

(A) The short-time behaviour of the heat flow is related to the short-time behaviour of the wave equation (cf. [1]).
(B) The short-time behaviour of the wave equation with discontinuous initial data is related to the short-time behaviour of the eikonal equation (cf. 'geometrical optics' and the progressing wave expansion [10]).
(C) The short-time behaviour of the wave and eikonal equations with initial data $f\mathbb{1}_S$ is directly related to the geometry of M near ∂S.

Though points (A)-(C) are well known in the literature, they have (to the best of our knowledge) not been applied to the study of heat content so far.

A significant portion of (C) will rest on an application of the Reynolds transport theorem. Here, denote by Φ^s the time-s flow of the vector field $\nu = -\nabla\varphi$. For small s, the (half) tubular neighbourhood

$$S^{-s} := \{x \in M \setminus S : \mathrm{dist}(x, \partial S) \leq s\} \tag{3}$$

satisfies $S \cup S^{-s} = \Phi^s(S)$. For $a \in C^\infty((-\varepsilon,\varepsilon)\times M)$, by [5, Chap. V, Prop. 5.2],

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}\int_{S^{-s}} a(s,\cdot)\,\mathrm{d}V\Big|_{s=0} &= \frac{\mathrm{d}}{\mathrm{d}s}\left(\int_{S^{-s}\cup S} a(s,\cdot)\,\mathrm{d}V - \int_S a(s,\cdot)\,\mathrm{d}V\right)\Big|_{s=0}\\ &= \int_S \mathcal{L}_{\tilde{\nu}}[a(0,\cdot)\,\mathrm{d}V] = \int_{\partial S} a(0,\cdot)\,\mathrm{d}A.\end{aligned} \tag{4}$$

The last equation is a consequence of Cartan's magic formula and Stokes' theorem, where we use that $\mathrm{d}V(\nu, \cdot) = \mathrm{d}A(\cdot)$ on ∂S.

2 Proof for β_0, β_1

By Fourier theory (for non-Gaussian k, the formulae must be adapted),

$$k(t) = \exp(-t^2) = \int_0^\infty \hat{k}(s)\cos(ts)\,\mathrm{d}s \quad \text{with} \quad \hat{k}(s) := \frac{1}{\sqrt{\pi}}\exp\left(\frac{-s^2}{4}\right).$$

On the operator level, this yields the well-known formula [10, Sect. 6.2]

$$T_t = \exp(t\Delta) = \int_0^\infty \hat{k}(s)\cos(s\sqrt{-t\Delta})\,\mathrm{d}s. \tag{5}$$

The operator $W^s := \cos(s\sqrt{-\Delta})$ is the time-s solution operator for the wave equation with zero initial velocity, in particular $u(s, x) := (W^s f\mathbb{1}_S)(x)$ (weakly) satisfies $(\partial_t^2 - \Delta)u = 0$. Let $\langle\cdot,\cdot\rangle$ denote the $L^2(M, \mathrm{d}V)$ inner product. Using Eq. (5),

$$\langle T_t f\mathbb{1}_S, \mathbb{1}_S\rangle = \int_0^\infty \hat{k}(s)\langle W_{s\sqrt{t}} f\mathbb{1}_S, \mathbb{1}_S\rangle\,\mathrm{d}s.$$

Similar reasoning has been used to great effect in [1] to derive heat-kernel bounds by making use of the *finite propagation speed* of the wave equation. As in [1], finite propagation speed yields for $s \geq 0$ that $\langle W_s f\mathbb{1}_S, \mathbb{1}_{M\setminus S}\rangle = \langle W_s f\mathbb{1}_{S^s}, \mathbb{1}_{S^{-s}}\rangle$, where $S^s := (M \setminus S)^{-s}$ is defined like Eq. (3). Even if $\mathbb{1}_{M\setminus S} \notin L^2(M, \mathrm{d}V)$, we have just seen that the inner product $\langle W_s f\mathbb{1}_S, \mathbb{1}_{M\setminus S}\rangle$ is nevertheless well defined. In [1], it is further observed that $\|W_s\| \leq 1$. Using the Cauchy–Schwarz inequality and assuming $f = \mathbb{1}_M$, Eq. (4) yields

$$h(s) := \langle W_s f\mathbb{1}_{S^s}, \mathbb{1}_{S^{-s}}\rangle \leq \|\mathbb{1}_{S^s}\|_2\|\mathbb{1}_{S^{-s}}\|_2 \leq s\int_{\partial S}\mathrm{d}A + o(s), \quad s \to 0^+. \tag{6}$$

In addition, $|\langle W_s f\mathbb{1}_S, \mathbb{1}_S\rangle| \leq \|f\mathbb{1}_S\|_2\|\mathbb{1}_S\|_2$ for all $s \geq 0$, in particular as $s \to \infty$. We conclude with some calculations (cf. Lemma 3), that

$$\begin{aligned}\langle T_t\mathbb{1}_S, \mathbb{1}_S\rangle &= \int_0^\infty \hat{k}(s)\left(\langle W_{s\sqrt{t}}\mathbb{1}_S, \mathbb{1}_M\rangle - \langle W_{s\sqrt{t}}\mathbb{1}_S, \mathbb{1}_{M\setminus S}\rangle\right)\mathrm{d}s \\ &= \langle\mathbb{1}_S, \mathbb{1}_M\rangle - \int_0^\infty \hat{k}(s)h(s\sqrt{t})\,\mathrm{d}s \\ &\geq \int_S \mathrm{d}V - 2\sqrt{\frac{t}{\pi}}\int_{\partial S}\mathrm{d}A + o(\sqrt{t}), \qquad t \to 0^+.\end{aligned} \tag{7}$$

This is weaker than the desired estimate, and restricts to $f = \mathbb{1}_M$. The problem is that the estimates in Eq. (6) are too crude. To improve them, we instead approximate

the solution u to the wave equation with geometrical optics, using the "progressing wave" construction described in [10, Sect. 6.6], some details of which we recall here. The basic idea is that u is in general discontinuous, with an outward—and an inward—moving discontinuity given by the zero level-set of functions φ^+ and φ^-, respectively. The functions $\varphi^\pm$ satisfy the eikonal equation $\partial_t\varphi = \pm|\nabla\varphi^\pm|$ with initial value $\varphi^\pm(0,\cdot) = \varphi(\cdot)$. Equivalently, using the (nonlinear) operator $Ew := (\partial_t w)^2 - |\nabla w|^2$, the functions $\varphi^\pm$ satisfy $E(\varphi^\pm) = 0$. Our analysis is greatly simplified by choosing the initial φ to (locally) be the signed distance function to ∂S. The eikonal equation is then $\partial_t\varphi^\pm = \pm|\nabla\varphi| = \pm|-\nu| = \pm 1$, i.e. $\varphi^\pm(x,t) = \varphi(x) \pm t$.

The progressing wave construction further makes use of two (locally existing and smooth) solutions $a_0^\pm$ to the first-order transport equations $\pm\partial_t a_0^\pm(t,\cdot) + \nu \cdot \nabla a_0^\pm(t,x) = \frac{1}{2}a_0^\pm\Delta\varphi^\pm$. Observe that with the Heaviside function $\theta\colon \mathbb{R} \to \mathbb{R}$, and $\Box := \partial_t^2 - \Delta$, the expression $\Box(a_0^\pm\theta(\varphi^\pm))$ is given by

$$(\theta''(\varphi^\pm)E\varphi^\pm + \Box\varphi^\pm\theta'(\varphi^\pm))a_0^\pm + 2\left(\partial_t a_0^\pm\partial_t\varphi^\pm - \nabla a_0^\pm\cdot\nabla\varphi^\pm\right)\theta'(\varphi^\pm) + \Box a_0^\pm\theta(\varphi^\pm).$$

The functions $\varphi^\pm$ and $a_0^\pm$ have been chosen so the above simplifies to

$$\begin{aligned}\Box(a_0^\pm\theta(\varphi^\pm)) &= 2\left(\pm\partial_t a_0^\pm + \nabla a_0^\pm\cdot\nu - \frac{1}{2}\Delta\varphi a_0^\pm\right)\theta'(\varphi^\pm) + \Box a_0^\pm\theta(\varphi^\pm)\\ &= \Box a_0^\pm\theta(\varphi^\pm).\end{aligned} \tag{8}$$

Thus $\Box(a_0^\pm\theta(\varphi^\pm))$ is as smooth as θ is. We use

$$\tilde{u}(t,x) := a_0^+(t,x)\theta(\varphi^+(t,x)) + a_0^-(t,x)\theta(\varphi^-(t,x))$$

as an approximation to the discontinuity of the solution u to the wave equation. To maintain consistency with the initial values of u, the initial values of the approximation $\tilde{u}$ are chosen to coincide with those of u at $t = 0$, this is achieved by setting $a_0^\pm(0,\cdot) = \frac{1}{2}f$ so that (at least formally) $\partial_t\tilde{u}(0,\cdot) = 0$ and also $\tilde{u}(0,\cdot) = \mathbb{1}_S f$.

The function $\tilde{u}$ approximates the discontinuous solution u of the wave equation well enough that the function $(s,x) \mapsto u(s,x) - \tilde{u}(s,x)$ is continuous on $[-T,T]\times M$, see [10, Sect. 6.6, eq. 6.35]. By construction, $\tilde{u}(0,\cdot) = u(0,\cdot)$. Hence $|(u(s,x) - \tilde{u}(s,x)| = o(1)$ as $s \to 0^+$, which implies

$$|\langle u(s,\cdot), \mathbb{1}_{S^{-s}}\rangle - \langle\tilde{u}(s,\cdot), \mathbb{1}_{S^{-s}}\rangle| = o(s) \quad s \to 0^+. \tag{9}$$

As $\nabla\varphi = -\nu$, for sufficiently small t the sets $\{x \in M : \varphi^+(t,x) = 0\}$ (resp. $\{x : \varphi^-(t,x) = 0\}$) are level sets of φ on the outside (resp. inside) of S (see also [10, Sect. 6.6]). By construction, $\theta(\varphi^-)$ vanishes outside of S for $t > 0$. Consequently,

using Eq. (4), we see that as $s \to 0^+$,

$$\begin{aligned}\langle \tilde{u}(s,\cdot), \mathbb{1}_{S^{-s}} \rangle &= \int_{S^{-s}} a_0^+(s,x)\mathbb{1}_{\{\varphi^+(s,\cdot)\geq 0\}} + a_0^-(s,x)\mathbb{1}_{\{\varphi^-(s,x)\geq 0\}}\,\mathrm{d}V(x) \\ &= s\int_{\partial S} a_0^+(0,x)\,\mathrm{d}A(x) + o(s) = \frac{s}{2}\int_{\partial S} f\,\mathrm{d}A + o(s). \end{aligned} \tag{10}$$

Combining Eqs. (9) and (10),

$$h(s) = \langle W_s f\mathbb{1}_S, \mathbb{1}_{S^{-s}}\rangle = \langle u(s,\cdot), \mathbb{1}_{S^{-s}}\rangle = \frac{s}{2}\int_{\partial S} f\,\mathrm{d}A + o(s), \quad s \to 0^+.$$

Calculations along the lines of Lemma 3 and Eq. (7) yield

$$\langle T_t f\mathbb{1}_S, \mathbb{1}_S\rangle = \int_S f\,\mathrm{d}V - \sqrt{\frac{t}{\pi}}\int_{\partial S} f\,\mathrm{d}A + o(\sqrt{t}), \qquad t \to 0^+,$$

as claimed.

Lemma 3 *Let $j \in \mathbb{N}$ and $\gamma : \mathbb{R}_{\geq 0} \to \mathbb{R}$. Let $\gamma(s) = s^j + o(s^j)$ for $s \to 0$ and $\gamma(s) = O(1)$ for $s \to \infty$. Then for $t \to 0^+$,*

$$\int_0^\infty \gamma(s\sqrt{t})\hat{k}(s)\,\mathrm{d}s = t^{\frac{j}{2}}\begin{cases}(-1)^{\frac{j}{2}}k^{(j)}(0) & j \text{ even}\\ (-1)^{\frac{j-1}{2}}\int_0^\infty \frac{2k^{(j)}(s)}{-\pi s}\,\mathrm{d}s & j \text{ odd}\end{cases} + o\left(t^{\frac{j}{2}}\right). \tag{11}$$

With $k(s) = \exp(-s^2)$ and $h(s) = c_0 + c_1 s + c_2 s^2 + o(s^2)$, this implies

$$\int_0^\infty h(s\sqrt{t})\hat{k}(s)\,\mathrm{d}s = c_0 + \frac{2c_1}{\sqrt{\pi}}\sqrt{t} + 2c_2 t + o(t). \tag{12}$$

Proof For even j, we obtain Eq. (11) by the Fourier-transform formula for jth derivatives. If j is odd, we also need to multiply by the sign function in frequency space, and then use that the inverse Fourier-transform (unnormalized) of the sign function is given by the principal value p.v. $\left(\frac{2i}{x}\right)$ [10, Sect. 4], see also [9, Chap. 7]. Equation 11 holds more generally, e.g. if k is an even Schwarz function. Equation 12 may also be verified directly without Eq. (11). □

3 Proof for $\beta_2, \beta_3, \ldots$

We now turn to calculating β_j for $j \geq 2$. We use the Nth order progressing wave construction with sufficiently large $N \gg j$. For the sake of simplicity, we write $O(t^\infty)$ for quantities that can be made $O(t^k)$ for any $k \in \mathbb{N}$ by choosing sufficiently large N. As in the previous section, the construction is from [10, Sect. 6.6]. With

$\theta_0 := \theta$, and $\theta_i(t) := \int_{-\infty}^t \theta_{i-1}(s)\mathrm{d}s$ we write

$$\tilde{u}^{\pm}(t,x) := \sum_{i=0}^{N} a_i^{\pm}(t,x)\theta_i(\varphi^{\pm}(t,x)).$$

Here the functions $a_0^{\pm}$ are defined as before, and for $i \geq 1$ the ith order transport equations $\pm\partial_t a_i^{\pm} = -\nu\cdot\nabla a_i^{\pm} + \frac{1}{2}a_i^{\pm}\Delta\varphi^{\pm} - \frac{1}{2}\Box a_{i-1}^{\pm}$ define $a_i^{\pm}$ together with initial data $a_i^{\pm}(0,\cdot) = -\frac{1}{2}(\partial_t a_{i-1}^{+}(0,\cdot) + \partial_t a_{i-1}^{-}(0,\cdot))$. As in Eq. (8), one may verify that $\Box\tilde{u}^{\pm} = \Box a_i\theta_N(\varphi^{\pm})$. Writing $\tilde{u} = \tilde{u}^{+} + \tilde{u}^{-}$ and

$$u(t,x) = \tilde{u}^{+}(t,x) + \tilde{u}^{-}(t,x) + R_N(t,x),$$

the remainder satisfies $R_N \in C^{(N,1)}([-T,T]\times M)$ and $R_N(t,\cdot)$ vanishes at $t=0$, see [10, Sect. 6.6, eq. 6.35]. Moreover, R_N is supported on $\{(x,t) : \mathrm{dist}(x,S) \leq |t|\}$, all of this implies that, as $t \to 0^+$,

$$h(t) = \int_{M\setminus S} u(t,x)\,\mathrm{d}V(x) = \int_{M\setminus S} \tilde{u}^{+}(t,x)\,\mathrm{d}V(x) + O(t^{\infty}) \tag{13}$$

and moreover $h \in C^{\infty}([0,T])$. The structure of R_N implies that $\Box\tilde{u}^{+}(t,x) = O(t^{\infty})$ on $M\setminus S$, provided that this expression is interpreted in a sufficiently weak sense. Formally, therefore

$$\begin{aligned}\partial_t^2 \int_{M\setminus S} \tilde{u}^{+}(\cdot,t)\,\mathrm{d}V &= \int_{M\setminus S} \Delta\tilde{u}^{+}(\cdot,t)\,\mathrm{d}V + O(t^{\infty}) \\ &= -\int_{\partial S} \nabla\tilde{u}^{+}(\cdot,t)\cdot\nu\,\mathrm{d}A + O(t^{\infty}),\end{aligned} \tag{14}$$

where the last step is the divergence theorem. One may verify Eq. (14) rigorously by either doing the above steps in the sense of distributions, or by a (somewhat tedious) manual computation. Combining this with Eq. (13),

$$h''(t) = -\int_{\partial S} \nabla\tilde{u}^{+}(\cdot,t)\cdot\nu\,\mathrm{d}A + O(t^{\infty}). \tag{15}$$

The quantity $h^{(j)}(0)$ may thus be seen to depend $\tilde{u}^{+}(0,\cdot)$ at ∂S, which in turn depends on $a_i^{\pm}$ at $t=0$. Defining $\mathbf{S}_i := a_i^{+} + a_i^{-}$ and $\mathbf{D}_i := a_i^{+} - a_i^{-}$ for $i = 0, 1, \ldots$, let L be the (spatial) differential operator defined for $w \in C^{\infty}(M)$ by $Lw := \frac{1}{2}\Delta\varphi w - \nu\cdot\nabla w$. For $i \in \mathbb{N}_0$, the transport equations imply

$$\partial_t\mathbf{S}_0 = L\mathbf{D}_0, \qquad \partial_t\mathbf{D}_0 = L\mathbf{S}_0, \tag{16}$$

$$\partial_t\mathbf{S}_{i+1} = L\mathbf{D}_{i+1} - \frac{1}{2}\Box\mathbf{D}_i, \qquad \partial_t\mathbf{D}_{i+1} = L\mathbf{S}_{i+1} - \frac{1}{2}\Box S_i \quad \text{for} \quad i \geq 0, \tag{17}$$

with initial values satisfying

$$a_0^+(0,\cdot) = \frac{1}{2}\mathbf{S}_0(0,\cdot) = \frac{1}{2}f(\cdot), \qquad \mathbf{D}_0(0,\cdot) = 0, \tag{18}$$

$$a_{i+1}^+(0,\cdot) = \frac{1}{2}\mathbf{D}_{i+1}(0,\cdot) = -\frac{1}{2}\partial_t \mathbf{S}_i(0,\cdot), \quad \mathbf{S}_{i+1}(0,\cdot) = 0. \tag{19}$$

Lemma 4 *For $i, n \in \mathbb{N}_0$ it holds that $\partial_t^{2n}\mathbf{D}_i(0,\cdot) = 0$ (note that as a consequence, also $a_{i+1}(0,\cdot)$, $L\mathbf{D}_i(0,\cdot)$, and $\Box^n\mathbf{D}_i(0,\cdot)$ are zero).*

Proof We will proceed by induction over i and use the identities Eqs. (16)–(19). For $i = 0$, $\mathbf{D}_0(0,\cdot) = 0$ is trivially satisfied. Moreover, $\partial_t^{2n}\mathbf{D}_0 = R^n\mathbf{D}_0$, which is zero at $t = 0$. For $i = 1$, observe that $a_1^+(0,\cdot) = -\frac{1}{2}\partial_t\mathbf{S}_0(0,\cdot) = -\frac{1}{2}L\mathbf{D}_0(0,\cdot) = 0$, and thus $\mathbf{D}_1(0,\cdot) = 0$. Likewise, $\partial_t^2\mathbf{D}_1 = \partial_t(L\mathbf{S}_1 - \frac{1}{2}\Box\mathbf{S}_0) = L(L\mathbf{D}_1 - \frac{1}{2}\Box\mathbf{D}_0) - \frac{1}{2}\Box L\mathbf{D}_0$. As the operator L commutes with ∂_t^2, this expression vanishes at $t = 0$. Induction over n proves the remainder of the statement for $i = 1$. For the general case, we assume the induction hypothesis for i and $i + 1$ and start by noting that $\mathbf{D}_{i+2}(0,\cdot) = 2a_{i+2}^+(0,\cdot) = -\partial_t\mathbf{S}_{i+1}(0,\cdot) = -\left(L\mathbf{D}_{i+1}(0,\cdot) - \frac{1}{2}\Box\mathbf{D}_i(0,\cdot)\right) = 0$. Moreover, $\partial_t^2\mathbf{D}_{i+2} = \partial_t(L\mathbf{S}_{i+2} - \frac{1}{2}\Box\mathbf{S}_{i+1}) = L(L\mathbf{D}_{i+2} - \frac{1}{2}\Box\mathbf{D}_{i+1}) - \frac{1}{2}\Box\left(L\mathbf{D}_{i+1} - \frac{1}{2}\Box\mathbf{D}_i\right)$, which again vanishes at $t = 0$; the case $n > 1$ may again be proven by induction over n. □

Corollary 5 *For even $j \in \mathbb{N}_{\geq 2}$, the jth derivative of h satisfies*

$$h^{(j)}(0) = -\frac{1}{2}\int_S \Delta^{j/2} f \,\mathrm{d}V.$$

Proof Lemma 4 shows that for $i \geq 1$, $a_i^+(0,x) = 0$. Together with Eq. (15), thus $h''(0) = -\int_{\partial S}\nabla a_0^+(0,\cdot)\cdot\nu\,\mathrm{d}A = -\frac{1}{2}\int_{\partial S}\nabla f\cdot\nu\,\mathrm{d}A$. This is the case $j = 2$. More generally, for $j = 2k$ with $k \in \mathbb{N}_{\geq 2}$, we use that (for $x \in \partial S$), $\tilde{u}^+$ satisfies $\partial_t^2\tilde{u}^+(t,x) = \Delta\tilde{u}^+(t,x) + O(t^\infty)$. Equation 15 ensures that as $t \to 0^+$,

$$h^{(2k)}(t) = \int_{\partial S}\nabla(\Delta^{k-1}\tilde{u}^+(t,\cdot))\cdot\nu\,\mathrm{d}A + O(t^\infty).$$

As for the case $k = 1$, it follows that $h^{(2k)}(0) = -\int_{\partial S}\nabla(\Delta^{k-1}a_0^+)\cdot\nu\,\mathrm{d}A$, the divergence theorem yields the claim. □

The odd coefficients are trickier, we only compute the case $j = 3$. We start with the observation that for $x \in \partial S$, $\varphi^+(t,x) = t$ and therefore

$$\tilde{u}^+(t,x) = \sum_{i=0}^{N}\frac{1}{i!}t^i a_i^+(t,x) \quad \text{for } t \geq 0, \quad x \in \partial S.$$

Recall that the Lie-derivative acts on functions $w \in C^\infty(M)$ by $\mathcal{L}_\nu w = \nabla w \cdot \nu$. Thus $\mathcal{L}_\nu \theta_{i+1}(\varphi^+(t,x)) = -\theta_i(\varphi^+(t,x))$, so for $x \in \partial S$,

$$\mathcal{L}_\nu \tilde{u}^+(t,x) = \sum_{i=0}^{N-1} \frac{t^i}{i!}(\mathcal{L}_\nu a_i^+(t,x) - a_{i+1}(t,x)) + O(t^\infty).$$

Therefore $\partial_t \mathcal{L}_\nu \tilde{u}^+(0,x) = \partial_t(\mathcal{L}_\nu a_0^+(0,x) - a_1^+(t,x)) + (\mathcal{L}_\nu a_1^+(0,x) - a_2^+(0,x))$, but the second term is zero as a_1^+ and a_2^+ vanish at $t = 0$ by Lemma 4. Substituting the transport equations and removing further zero terms leaves $\partial_t \mathcal{L}_\nu \tilde{u}^+(0,x) = \mathcal{L}_\nu L a_0^+(0,x) + \frac{1}{2}\Box a_0(0,x) = \frac{1}{2}\left(\mathcal{L}_\nu L f(x) - \frac{1}{2}\Delta f(x) + \frac{1}{2}L^2 f(x)\right)$. Thus (recall that $L = -\mathcal{L}_\nu + \frac{1}{2}\Delta\varphi$) directly from Eq. (15),

$$h^{(3)}(0) = -\frac{1}{2}\int_{\partial S} \mathcal{L}_\nu L f(x) - \frac{1}{2}\Delta f(x) + \frac{1}{2}L^2 f(x)\,\mathrm{d}A(x).$$

The formula

$$\Omega_{S,f}(t) = \int_0^\infty \hat{k}(s)\left(\int_S f\,\mathrm{d}V - h(s\sqrt{t})\right)\mathrm{d}s \tag{20}$$

established in the previous section, together with Lemma 3, yields the asymptotic behaviour of $\Omega_{S,f}(t)$ by taking the Taylor expansion of h using Corollary 5. This gives the remainder of the claims of theorem 2.

4 Discussion

The above-said is not specific to the heat equation. Taking $k(x) = \exp(-x^{2m}), m \in \mathbb{N}$, we may, for example, study the one-parameter operator family $\exp(-t^m \Delta^m)$. The wave equation estimates needed are the same. For $m \geq 2$, a brief calculation yields the explicit $t \to 0^+$ asymptotics

$$\langle \exp(t^m\Delta^m) f \mathbb{1}_S, \mathbb{1}_S\rangle = \int_S f\,\mathrm{d}V - \left(\pi^{-1}\Gamma\left(\frac{2m-1}{2m}\right)\int_{\partial S} f\,\mathrm{d}A\right)\sqrt{t} + o(t).$$

We conclude with the observation that the generalization of this paper to *weighted* Riemannian manifolds (cf. [4]) is straightforward.

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A Lagrangian perspective on nonautonomous advection-diffusion processes in the low-diffusivity limit

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Abstract

We study mass preserving transport of passive tracers in the low-diffusivity limit using Lagrangian coordinates. Over finite-time intervals, the solution-operator of the nonautonomous diffusion equation is approximated by that of a time-averaged diffusion equation. We show that leading order asymptotics that hold for functions based on [Krol, 1991] extend to the dominant nontrivial singular value. The generator of the time-averaged diffusion/heat semigroup is a Laplace operator associated to a weighted manifold structure on the material manifold. We show how geometrical properties of this weighted manifold directly lead to physical transport quantities of the *nonautonomous* equation in the low-diffusivity limit.

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1 Introduction

We begin by sketching the outlines of this paper, a more comprehensive introduction with more detailed references is given in section 2. We are concerned with the problem of transport and mixing in nonautonomous advection-diffusion processes in the vanishing-diffusivity limit. Such processes are, in the simplest case, described by the *advection-diffusion equation*,

$$\partial_t u_\varepsilon(x,t) + \operatorname{div}(u_\varepsilon(x,t)\, V(x,t)) = \varepsilon \Delta u_\varepsilon(x,t)\,, \tag{1}$$

where V is a time-dependent, smooth velocity field, u_ε the density of a weakly diffusive passive scalar, and $\varepsilon > 0$ is referred to as the (strength of) *diffusivity*. We sometimes omit the explicit ε in our notation when referring to u_ε for the sake of clarity. In this work, we are interested in the *finite-time* setting, i.e., without loss $t \in \mathcal{I} = [0,1]$.

Lagrangian coordinates can be obtained from the advection-only version of eq. (1) with $\varepsilon = 0$. With p denoting an arbitrary point in these coordinates, it is known that eq. (1) takes the form of a time-dependent diffusion (or heat) equation

$$\partial_t u_\varepsilon(p,t) = \varepsilon \Delta_t u_\varepsilon(p,t)\,. \tag{2}$$

The smoothly varying family of operators $(\Delta_t)_{t\in\mathcal{I}}$ may be viewed as Laplace operators on a suitably defined time-dependent family of weighted manifolds. We want to compare the solution u_ε of eq. (2) to the solution $\overline{u}_\varepsilon$ of the *time-averaged* equation

$$\partial_t \overline{u}_\varepsilon(p,t) = \varepsilon \overline{\Delta}\, \overline{u}_\varepsilon(p,t)\,, \qquad\qquad \overline{\Delta} \coloneqq \int_0^1 \Delta_t \,\mathrm{d}t\,, \tag{3}$$

as $\varepsilon \to 0$ at the final time $t = 1$. To the best of our knowledge, an averaging approach like this has been first taken in [35], albeit in an infinite-time setting. The operator $\overline{\Delta}$ has also been introduced by Froyland in his recent work on *dynamic* isoperimetry [10]. Consistently with his work, we will refer to $\overline{\Delta}$ as the *dynamic Laplacian*.

In the present work, we prove two results in the spirit of averaging theory, whose precise formulation we defer to section 3. First, for fixed initial condition u_0 the final density $u_\varepsilon(1,\cdot)$ (of eq. (2)) is uniformly approximated by $\overline{u}_\varepsilon(1,\cdot)$ (of eq. (3)) in leading order as $\varepsilon \to 0$; see proposition 3.1. This result follows directly from prior work by Krol [24] on the averaging method

applied to time-periodic advection-diffusion equations, in which, by the way, the transformation to *standard averaging form* is what is known as the transformation from Eulerian to Lagrangian coordinates in continuum mechanics. Second, we show that the largest (nontrivial) singular value/vector of the time-1 solution operator converge in a suitable sense to the largest (nontrivial) eigenvalue/eigenfunction of the averaged heat semigroup defined by eq. (3); see theorem 3.5.

In section 4, we work towards a geometric interpretation of our averaging results within the framework of the *geometry of mixing*, as introduced in [22]. This leads to a strengthened version of Froyland's dynamic Cheeger inequality [10]; we also draw a connection to the notion of *material barriers to diffusive transport* as developed in [19, 20]. A by-product of our averaging result is an alternative and simplified proof of a low-diffusivity approximation result for the diffusive transport across boundaries of full-dimensional material subsets; see eq. (6) of [19] and corollary 4.2. Diffusive flux or material leakage has long been implicit in different approaches in finding so-called *Lagrangian coherent structures (LCSs)*; see, for instance, [18, 10, 16] and [17] for a general review. It has been identified as the potentially unifying perspective on LCSs as *diffusion barriers* in [22], and finally became the central object in the variational approach to *material barriers to diffusive transport* in [19, 20].

Our main motivation stems from transport and mixing problems as studied in physical oceanography and the atmospheric sciences. There, a typical problem is that presumably purely advective transport processes are observed only up to some finite scale. The effect of unresolved (small) scales is then often modelled via a weak diffusion with spatiotemporal inhomogeneity; see, for instance, [44]. To address such problems, we treat advection-diffusion processes on (compact) smooth manifolds, and include general time-dependent, spatially inhomogeneous and anisotropic diffusion.

We would like to emphasize that we are interested in the details of spatial inhomogeneity of mixing, that would allow to explain significant differences in the mixing ability of different flow regions (transport/diffusion barriers vs. enhancers). This is in contrast to asymptotic or statistical information, like decay rates to equilibrium or spatially homogeneous effective diffusion tensors, typically obtained in homogenization theory; see, for instance, [8, 33].

The advection-diffusion equation (2) has been extensively studied in the literature. The time-periodic case has been investigated in the low-diffusivity limit by Krol [24], cf. also [39, 45]. Time-periodic advection-diffusion prob-

lems have also been studied by Liu & Haller [30] from the Eulerian perspective. They developed mathematical theory for observed time-periodic patterns, *strange eigenmodes*, in periodically driven advection-diffusion processes. The time-periodic setting is closely related to this work, as one may construct a time-periodic advection-diffusion process from the finite-time setting by appending its ajoint equation (which is again of advection-diffusion type) and time-periodic extension. This resulting equation is then periodic with continuous coefficients. Such a time-periodic extension procedure has been employed recently by Froyland *et al.* [11] to the Fokker–Planck equation associated to a stochastic differential equation, in order to find approximations to Eulerian, spatiotemporal sets with small exponential escape rates of stochastic trajectories.

In the *autonomous* case—where V in eq. (2) does not depend on time—semi-group theory may be applied, and many results have been obtained in this case. For instance, Kifer [23, Chapter III] studies asymptotics of spectra in the low-diffusivity limit; see also [9, Chapter 6.7]. Further autonomous, non-finite-time results were obtained in [3, 6].

2 Diffusion-induced Lagrangian geometries

This section is meant to be both a motivation and a gentle recall of the geometric interpretation of advection-diffusion processes, as developed in [22, 19]. For a recall of fundamental differential geometry concepts and notation used, we refer to appendix A.

2.1 Advection processes

We recall some basic properties of advection processes that preserve mass; see also [20]. These generalize the notion of volume-preservation to vector fields whose flows do not preserve volume; this is done by constructing a time-dependent volume-form ϱ, the (fluid) *mass form*, that has precisely the property that it is preserved by the flow of a time-dependent velocity field V. Readers who are only interested in volume-preserving flows (with respect to a volume ω, such as the usual Euclidean volume) may set $\varrho(t, x) \equiv \omega(x)$ everywhere below.

Recall that, in a fixed spatial frame, the evolution of the passively advected mass-form ϱ, with initial value ω, is given by the advection equa-

tion/conservation law

$$\partial_t \varrho = -\mathcal{L}_V \varrho \tag{4}$$

$$\varrho(0,\cdot) = \omega \ . \tag{5}$$

Here, V is the sufficiently regular time-dependent fluid (bulk) velocity. We consider eq. (4) on an orientable smooth manifold M, potentially with a sufficiently regular boundary, over a (finite subset of the) finite time interval $\mathcal{I} \subset \mathbb{R}$. For notational simplicity, we assume w.l.o.g. that $\mathcal{I} = [0,1]$.

Equation (4) is well-known as a hyperbolic partial differential equation (PDE) that can be solved by the *method of lines/characteristics*. That is, consider the associated ordinary differential equation (ODE)

$$\dot{x} = v(t,x), \qquad\qquad x(0) = x_0 \in M, \tag{6}$$

on $\mathcal{I}$. Let ϕ denote the *flow map* associated to eq. (6), i.e., $t \mapsto \phi_0^t(x_0)$ is the unique solution of eq. (6) satisfying the initial condition $\phi_0^0(x_0) = x_0$. The solutions of eq. (6) are then known as the *characteristics* of eq. (4), and each characteristic is also referred to as the *trajectory* of a *(fluid) particle*. Now, with the formula for time-derivatives along trajectories, [27, Chapter V, Prop. 5.2], eq. (4) becomes

$$(\tau \mapsto (\phi_0^\tau)^* \varrho)'(t) = (\phi_0^t)^* (\mathcal{L}_V \varrho) + (\phi_0^t)^* \partial_t \rho = 0 \,,$$

where $(\phi_0^t)^*$ is the pullback by ϕ_0^t. For its push-forward $(\phi_0^t)_*$ this implies

$$\rho(t,\cdot) = (\phi_0^t)_* \, \omega \ . \tag{7}$$

In particular, the mass-form along a trajectory is uniquely determined by its value anywhere on the trajectory.

In addition to the mass form ϱ, we would like to model the evolution of a passive tracer that is advected by the fluid. This passive tracer is described by a (time-dependent) function/density u such that the volume form $u\varrho$, integrated against any (measurable) $S \subset M$, returns the total amount of the tracer in S. Here,

$$\partial_t u = -\mathrm{d}u(V) = -\mathcal{L}_V u \,, \qquad\qquad u(0,\cdot) = u_0 \,. \tag{8}$$

As above, along characteristics we obtain

$$\frac{d}{dt}\left((\phi_0^t)^* u\right) = (\phi_0^t)^* (\mathcal{L}_V u) + (\phi_0^t)^* \partial_t u = 0 \,,$$

therefore u is constant along characteristics.

One important consequence is the following intimate relation between the PDE formulation of transport, eqs. (4) and (8), and its ODE formulation, eq. (6). For any (measurable) set $S \subset M$ and any (measurable) initial scalar density u_0 one has

$$\int_S u_0 \, \omega = \int_{\phi_0^t(S)} u(t,\cdot)\varrho(t,\cdot)\,. \tag{9}$$

Note that eq. (9) contains both the densities ϱ and u *and* the flow map ϕ, which otherwise do not occur simultaneously in eqs. (4), (6) and (8).

Next, assume the scalar is confined to some set $S \subset M$, e.g., $u_0 = \mathbb{1}_S$. Then, as a direct consequence of eq. (9), we have

$$\int_{\phi_0^t(S)^\mathrm{c}} u(t,\cdot)\varrho(t,\cdot) = 0\,, \tag{10}$$

where A^c denotes the complement of A (in M). In other words, none of u leaks out of the spatiotemporal tube $\bigcup_{t\in[0,1]} \phi_0^t(S)$. For later reference and in accordance with continuum mechanics, we call any flow-invariant spatiotemporal set $S = \bigcup_{t\in[0,1]} \phi_0^t(S_0)$ a *material set*. So far, all considerations were relative to some spatial or, synonymously, some *Eulerian* frame. Besides different spatial frames, however, which can be related to different observers of the physical transport process, there exists the *Lagrangian* frame that is related only to the characteristics/particles of the underlying process. Changing from *some* Eulerian to *the* Lagrangian frame is essentially applying the method of lines, where one additionally declares the initial conditions of eq. (6), i.e., the particles, as *coordinates*, and represents all physical equations w.r.t. those.

Briefly, in Lagrangian coordinates that are co-moving with the trajectories, eq. (4) becomes

$$\partial_t \varrho = 0\,, \qquad\qquad \partial_t u = 0\,;$$

eq. (6) reads as

$$\dot{x} = 0\,, \tag{11}$$

and, as a consequence, the "flow map" is the identity map for all times. Equation (10) then states that no scalar mass leaks out of any material set into the respective complementary material set; likewise the Lagrangian advective transport through any material surface vanishes.

2.2 Advection-diffusion processes

In the following, we will consider advection-diffusion processes and re-inspect our above considerations in this framework in order to summarize the construction appearing in [22].

Recall that, in a fixed spatial frame, the evolution of a weakly diffusive scalar, given by its density u, passively advected by a (possibly compressible) fluid described with mass form ϱ is given by the *advection-diffusion equation* [25, 42]

$$\partial_t u = -\mathcal{L}_V u + \varepsilon \operatorname{div}_\varrho(D\,\mathrm{d}u)\,, \tag{12a}$$

$$\partial_t \varrho = -\mathcal{L}_V \varrho\,. \tag{12b}$$

Here, $\varepsilon > 0$ is the *diffusivity* (or the inverse Péclet number in non-dimensionalized units), which is assumed to be small, and $D\colon T^*M \to TM$ is a (possibly time-dependent) bundle morphism satisfying the following property: for given $(t, x) \in \mathcal{I} \times M$ identify D with a bilinear form $\tilde{g}_t^{-1}$ on T^*M, then this bilinear form is symmetric and positive-definite. In particular, D gives rise to a dual metric, inducing a Riemannian metric $\tilde{g}_t$ on M. Viewed in this sense, D is a *diffusion tensor field*, modeling possibly (spatially and temporally) inhomogeneous, anisotropic diffusion; for further details on the aforementioned steps, see also [22]. It is also necessary to impose suitable boundary conditions in the case that the manifold M has nonempty boundary ∂M. We will focus on homogeneous boundary conditions of Dirichlet–, and for only some of our results, Neumann form.

Taking a closer look at eq. (12a), we directly recognize $D\,\mathrm{d}u$ as the gradient of u w.r.t. the metric $\tilde{g}$. As a consequence, the diffusion term can then be elegantly represented via the Laplace operators on the family of weighted manifolds $(M, \tilde{g}_t, \theta)$,

$$\partial_t u = -\mathcal{L}_V u + \varepsilon \Delta_{\tilde{\theta}_t, \tilde{g}_t} u\,, \tag{13a}$$

$$\partial_t \varrho = -\mathcal{L}_V \varrho\,, \tag{13b}$$

where $\tilde{\theta}_t$ is the density of ϱ w.r.t. $\mathrm{d}\tilde{g}_t$, i.e., $\tilde{\theta}_t\,\mathrm{d}\tilde{g}_t = \varrho(t, \cdot)$.

In stark contrast to the advection equations, eqs. (4), (12b) and (13b), the advection-diffusion equation, eq. (13a), is not amenable to the method of characteristics, and, therefore does *not* introduce a concept of deterministic particles, trajectories, or Lagrangian coordinates for the scalar u. On the other hand, it is a singular perturbation of a hyperbolic PDE: namely

eq. (13a) with $\varepsilon = 0$ as considered before. Hence, we may introduce Lagrangian coordinates based on the characteristics of its singular limit (cf. [42]), or, equivalently, based on eq. (13b). In these Lagrangian coordinates, the advective terms in eq. (13) vanish as in section 2.1, and we obtain from the well-known pullback transformation rules

$$\partial_t u = \varepsilon \Delta_{\theta_t, g_t} u = \varepsilon \operatorname{div}_\omega(g_t^{-1} \, \mathrm{d}u) \,, \tag{14}$$

which is an evolution equation on the material manifold M. Here, $g_t \coloneqq (\phi_0^t)^* \tilde{g}_t$ is the diffusion-adapted pullback metric on M and $\theta_t = (\phi_0^t)^* \theta$. As a consequence of mass preservation, the volume form ω—w.r.t. which we compute the divergence—does not depend on time. Henceforth, we write div without a subscript whenever we refer to $\operatorname{div}_\omega$. Moreover, let $\Delta_t \coloneqq \operatorname{div}(g_t^{-1} \mathrm{d}u)$, then with this notation eq. (14) simplifies to

$$\partial_t u = \varepsilon \Delta_t u \,. \tag{15}$$

The lack of characteristics for the advection-diffusion equation has another, crucial consequence: given a (proper) material subset $S \subset M$, the amount of u is in general no longer constant over time, or, equivalently

$$T_0^t(S, u_0) \coloneqq \int_S u_0 \; \omega - \int_{\phi_0^t(S)} u(t, \cdot) \, \varrho(t, \cdot) \neq 0 \,. \tag{16}$$

In simple words, there is leakage of u out of or into material sets. For given scalar fields and material subsets, the associated scalar leakage is an nontrivial and interesting quantity when regarded as a function of material sets S, see [19, 20].

In Lagrangian coordinates, eq. (16) reads as

$$T_0^t(S, u_0) = \int_S (u_0 - u(t, \cdot)) \; \omega \;. \tag{17}$$

Furthermore, assuming for the moment that all involved functions are sufficiently smooth, differentiating with respect to t and applying the fundamental theorem of calculus yields

$$T_0^t(S, u_0) = -\varepsilon \int_0^t \left(\int_S \Delta_\tau u(\tau, \cdot) \; \omega \right) \mathrm{d}\tau \,. \tag{18}$$

Heuristically, for very small ε we have $u \approx u_0$ which suggests that

$$\frac{T_0^t(S,u_0)}{\varepsilon} \approx -\int_0^t \int_S \Delta_\tau u_0 \; \omega \; \mathrm{d}\tau \; =: \overline{T}_0^t(S,u_0)\,. \tag{19}$$

Indeed, it was shown in [19, 20] for the case that $M \subset \mathbb{R}^n$ and homogeneous Neumann boundary condition that

$$T_0^t(S,u_0) = \varepsilon \overline{T}_0^t(S,u_0) + o(\varepsilon), \quad \varepsilon \to 0\,. \tag{20}$$

In section 3, we develop an alternative proof of eq. (20) on compact manifolds with Dirichlet boundary; see corollary 3.4.

By Fubini's theorem, we have that

$$\overline{T}_0^t(S,u_0) = -\int_S \int_0^t \Delta_\tau u_0 \,\mathrm{d}\tau \; \omega = -\int_S \int_0^t \Delta_\tau \,\mathrm{d}\tau \; u_0 \, \omega \;.$$

For $t = 1$, this suggests the definition

$$\overline{\Delta} \coloneqq \int_0^1 \Delta_t \,\mathrm{d}t\,. \tag{21}$$

This operator was recently introduced in [10, 12] and coined *dynamic Laplacian*. With this notation, eq. (20) reads as

$$T_0^1(S,u_0) = -\varepsilon \int_S \overline{\Delta} u_0 \; \omega + o(\varepsilon)\,,$$

and combines mathematical tools from recent work on material surfaces that extremize diffusive flux [19, 20] on the one hand, and dynamic isoperimetry [10, 12] on the other hand. A goal of this work is to investigate these connections rigorously; see corollary 4.2.

2.3 The geometry of mixing and diffusive permeability

Our study is centered around the *geometry of mixing* as induced by $\overline{\Delta}$ and introduced in [22]. There, it was observed that $\overline{\Delta}$ is the Laplace operator of a specific *weighted* (Riemannian) manifold. With the above notation, let us define

$$\overline{g} = \left(\int_{\mathcal{I}} g_t^{-1} \mathrm{d}t \right)^{-1}\,. \tag{22}$$

Lemma 2.1 ([22, Prop. 3])**.** *The dynamic Laplacian $\overline{\Delta}$ is the Laplace operator associated to the weighted manifold $(M, \overline{g}, \theta)$, where $\theta \, \mathrm{d}\overline{g} = \omega$.*

As in [22], we refer to the material manifold M, equipped with the metric $\overline{g}$ and density θ as the *geometry of mixing*. This, together with appendix A, shows that the geometry of mixing is constructed to have the following elegant properties: (i) volume/fluid mass is given by ω, the differential form preserved by the flow, and (ii) diffusion is given by averaged pullback diffusion tensors as featured in the dynamic Laplacian. It was further observed in [22] that

$$\partial_t \overline{u} = \varepsilon \overline{\Delta} \overline{u}, \qquad \overline{u}(0, \cdot) = u_0 \,, \tag{23}$$

is an *averaged* (cf. [38, 33]) form of eq. (15). It was conjectured that eq. (23) approximates eq. (15) in the vanishing diffusivity limit, leaving open the concrete nature of the approximation and the required assumptions. We prove this in section 3 building on a similar result in the classic, i.e., time-periodic, averaging context [24]. A by-product of our averaging result is a new proof of eq. (20), as mentioned above. We also prove that the convergence extends to singular values/vectors, addressing an open question from [22].

To summarize the previous sections: eq. (20) shows that in leading order as $\varepsilon \to 0$, the diffusive transport out of a material set is determined by

$$\overline{T}^1_0(S, u_0) = -\int_S \overline{\Delta} u_0 \; \omega \; .$$

By the divergence theorem, we have

$$\overline{T}^1_0(S, u_0) = -\int_{\partial S} \mathrm{d}u_0(\overline{\nu}) \, \mathrm{d}\overline{A} \,, \tag{24}$$

where $\overline{\nu}$ is the outward-pointing $\overline{g}$-unit normal vector field on ∂S and $\mathrm{d}\overline{A} = \theta \mathrm{d}A_{\overline{g}}$ is the induced area form on ∂S in the geometry of mixing.

Of course, $\overline{T}^1_0(S, u_0)$ could be represented similarly in other weighted geometries on M: choose any metric $\widetilde{g}$, compute the density $\widetilde{\theta}$ of the fluid mass relative to the induced volume $\mathrm{d}g$, denote the induced area form and the $\widetilde{g}$-unit normal vector field on ∂S by $\mathrm{d}\widetilde{A}$ and $\widetilde{\nu}$, respectively, then one obtains analogously to eq. (24)

$$\overline{T}^1_0(S, u_0) = -\int_{\partial S} \mathrm{d}u_0(H\widetilde{\nu}) \, \mathrm{d}\widetilde{A} \,, \tag{25}$$

where $H = \overline{g}^{-1}\widetilde{g}$ is a tangent space isomorphism; cf. also section 4.1 below and references [19, 20], in which $\overline{T}^1_0(S, u_0)$ is represented in the usual Euclidean/physical geometry, and H is coined the *transport tensor* (denoted by $\mathbf{T}^{t_1}_{t_0}$ there). It is exactly the absence of any additional tensor in eq. (24) that makes arguably the geometry of mixing the "best-adapted" or "most natural" geometry in which to look at leading-order diffusive flux in Lagrangian coordinates.

Equation (24) emphasizes that, in leading order, the diffusive transport $T^1_0(S, u_0)$ out of a material set S depends on (i) the differential/gradient of the initial concentration u_0 along ∂S, and (ii) properties of the geometry of mixing via the surface measure $\mathrm{d}\overline{A}$ and unit normal vector field $\overline{\nu}$. As argued in [22], $\mathrm{d}\overline{A}$ is particularly interesting as an intrinsic measure of the "diffusive permeability" of the material boundary ∂S. In many physical applications, it is of great interest to diagnose the mixing structure of an advection-dominated transport process *independent* of any specific scalar quantity; cf. the discussion in [19].

3 Finite-time averaging of the advection-diffusion equation

We now show that in the setting of the advection-diffusion equation, the diffusion process induced by the dynamic Laplacian approximates the diffusion of the advection-diffusion equation in Lagrangian coordinates, in the limit of vanishing diffusivity.

In this section, we restrict to those M that are compact manifolds whose boundary, if it is nonempty, is smooth. The proof can be extended to other classes of manifolds also, provided there is a suitable maximum principle.

3.1 Uniform convergence

Let $u_\varepsilon \colon M \times [0,1] \to \mathbb{R}$ solve the advection-diffusion equation in Lagrangian coordinates for diffusivity ε with initial condition $u_0 \colon M \to \mathbb{R}$ with—if there is a boundary—homogeneous Dirichlet or Neumann[1] boundary conditions.

[1] Given a metric for each time $t \in [0,1]$, we also have a g_t unit-normal vector ν_t field on ∂M for each $t \in [0,1]$. The natural homogeneous Neumann condition is thus $\mathrm{d}u_\varepsilon(t,\cdot)(\nu_t) = 0$ for each $t \in [0,1]$ on ∂M.

Thus, in the interior of M, u_ε satisfies

$$\partial_t u_\varepsilon = \varepsilon \Delta_t u_\varepsilon \,. \tag{26}$$

Similarly, let $\overline{u}_\varepsilon \colon M \times [0,1] \to \mathbb{R}$ be the solution of the heat flow generated by the dynamic Laplacian $\overline{\Delta}$, with initial condition u_0 and diffusivity ε, i.e.,

$$\partial_t \overline{u}_\varepsilon = \varepsilon \overline{\Delta} \overline{u}_\varepsilon \tag{27}$$

and—if there is a boundary—homogeneous Dirichlet or Neumann[2] boundary conditions of the corresponding type. We will focus mainly on the case of Dirichlet boundary, and refer to appendix D for a recall of results regarding existence, uniqueness and regularity of solutions. We expect analogous existence, uniqueness and regularity results to hold in the Neumann case on manifolds, but could not find a reference.

Definition. Depending on the boundary condition used, we call an initial value $u_0 \in C^\infty(M)$ *admissible* if (i) u_0 is compactly supported in the interior of M (Dirichlet case), (ii) if u_0 is constant in a neighborhood of the spatial boundary ∂M (Neumann case).

This definition is motivated by the fact that the time-dependent parabolic eqs. (26) and (27) may not be smooth at $t = 0$ if the initial value u_0 does not satisfy certain compatibility conditions at the boundary; see [7, Sect. 7.1, Thm. 6]; cf. also [24]. These may differ between eq. (26) and eq. (27). Our definition of admissibility guarantees that the compatibility conditions of both the time-dependent and the averaged equations are satisfied simultaneously.

Proposition 3.1. *With u_ε and $\overline{u}_\varepsilon$ as above, let u_0 be an admissible initial value. Then*

$$u_\varepsilon(1, x) = \overline{u}_\varepsilon(1, x) + O(\varepsilon^2) \,, \qquad \varepsilon \to 0, \tag{28}$$

uniformly in x.

Proof. The proof is a simplification of the one given in [24]. Let

$$\widetilde{u}_\varepsilon = u_0 + \varepsilon \int_0^t \Delta_\tau u_0 \, \mathrm{d}\tau \,.$$

[2]Here, we require $\mathrm{d}\overline{u}_\varepsilon(t, \cdot)(\overline{\nu}) = 0$ independent of t, where $\overline{\nu}$ is unit normal field for $\overline{g}$ on ∂M.

We start with the Dirichlet boundary condition case. Let $\mathcal{L}^\varepsilon \coloneqq \partial_t - \varepsilon\Delta_t$ and observe that $\mathcal{L}^\varepsilon \widetilde{u}_\varepsilon = -\varepsilon^2 \int_0^t \Delta_t \Delta_s u_0 \,\mathrm{d}s$. As u_0 is smooth and M compact,

$$C \coloneqq \sup_{t\in[0,1]} \left\| \left(\int_0^t \Delta_t \Delta_\tau u_0 \,\mathrm{d}\tau \right) \right\|_{L^\infty(M)} < \infty \,.$$

By definition, $\mathcal{L}^\varepsilon u^\varepsilon = 0$. Thus, $\mathcal{L}^\varepsilon(\widetilde{u}_\varepsilon - u_\varepsilon - C\varepsilon^2 t) \leq 0$; u_ε and $\widetilde{u}_\varepsilon$ agree at $t = 0$; and (by the admissibility of the initial value) both satisfy Dirichlet boundary conditions. The weak maximum principle (lemma D.4) therefore yields that

$$\max_{[0,1]\times M} (\widetilde{u}_\varepsilon - u_\varepsilon - C\varepsilon^2 t) = \max_{[0,1]\times \partial M \cup \{0\}\times M} (-C\varepsilon^2 t) \leq 0 \,.$$

As a consequence, we have $\max_{[0,1]\times M}(\widetilde{u}_\varepsilon - u_\varepsilon) \leq C\varepsilon^2$.

One may prove $(u_\varepsilon - \widetilde{u}_\varepsilon) \leq C\varepsilon^2$ along the same lines. Thus, $\|u_\varepsilon - \widetilde{u}_\varepsilon\|_{L^\infty([0,1]\times M)} = O(\varepsilon^2)$. For $t = 1$, this implies the uniform expansion

$$u_\varepsilon(1,\cdot) = \widetilde{u}_\varepsilon(1,\cdot) + O(\varepsilon^2) = u_0 + \varepsilon\overline{\Delta} u_0 + O(\varepsilon^2) \,. \tag{29}$$

The right-hand side coincides up to second order with the expansion of $\overline{u}_\varepsilon(1,\cdot)(= \exp(\varepsilon\overline{\Delta})u_0)$ which yields the claim.

For Neumann boundary conditions, the proof goes along the same lines, where the weak maximum principle must be augmented with the parabolic Hopf boundary point lemma (see [36, Chapter 3, Thm. 6]) to ensure that a strict maximum cannot be achieved at positive time. □

We restate eq. (29) for further reference, and also observe that it can be interpreted as the time-continuous generalization of [10, Thm. 5.1].

Corollary 3.2. *Under the assumptions of proposition 3.1,*

$$u_\varepsilon(1,x) = u_0(x) + \varepsilon\overline{\Delta} u_0(x) + O(\varepsilon^2) \,, \tag{30}$$

uniformly in x.

Corollary 3.3. *Under the assumptions of proposition 3.1,*

$$u_\varepsilon(1,\cdot) = u_0 + \varepsilon\overline{\Delta} u_0 + O(\varepsilon^2) \,,$$

in $L^p(M,\omega)$ for all $p \in [1,\infty]$.

Proof. For $p = \infty$, our claim corresponds to corollary 3.2. For $p \in [1, \infty)$, the natural injection $L^\infty(M, \omega) \hookrightarrow L^p(M, \omega)$ is well-defined and continuous since $\omega(M)$ is finite, which yields the claim. □

Corollary 3.4. *Under the assumptions of proposition 3.1,*

$$T_0^1(S, u_0) = \int_S u_0(x)\ \omega - \int_S u_\varepsilon(x, 1)\ \omega = -\varepsilon \int_S \overline{\Delta} u_0\ \omega + O(\varepsilon^2)\,. \tag{31}$$

Proof. This follows by integrating eq. (29) over S. □

3.2 Convergence of singular values

We denote by P_t^ε and $\overline{P}_t^\varepsilon$ the time-t solution operators of eqs. (26) and (27), respectively, i.e., $u_\varepsilon(t, \cdot) = P_t^\varepsilon u_0$ and $\overline{u}_\varepsilon(t, \cdot) = \overline{P}^\varepsilon u_0$. To reduce notational clutter, we write $P^\varepsilon \coloneqq P_1^\varepsilon$ and $\overline{P}^\varepsilon \coloneqq \overline{P}_1^\varepsilon$. We only treat homogeneous Dirichlet boundary in this section.

The previous section dealt with the relationship of P^ε and $\overline{P}^\varepsilon$ in the limit $\varepsilon \to 0$. In particular, proposition 3.1, with this notation, is

$$\|(P^\varepsilon - \overline{P}^\varepsilon) u_0\|_{L^\infty(M)} = O(\varepsilon^2) \quad \text{for all } u_0 \in \mathrm{C}_\mathrm{c}^\infty(\mathring{\mathrm{M}})\ . \tag{32}$$

Recall that as P^ε is compact (cf. appendix D), the first singular value of P^ε is given by the operator norm of $P^\varepsilon \colon L^2(M, \omega) \to L^2(M, \omega)$. By lemma C.2, P^ε is a contraction on $L^2(M, \omega)$, hence $\|P^\varepsilon\| \leq 1$.

If M is boundaryless, then $P^\varepsilon \mathbb{1}_M = \mathbb{1}_M$, and, as a consequence, $\|P^\varepsilon\| = 1$ for any $\varepsilon > 0$. Since the subspace of constant functions is a trivial invariant subspace, we restrict the domain of P^ε to its orthogonal complement, the space of mean-free functions. If M has a boundary, we consider P^ε with its domain the entire $L^2(M, \omega)$.

With these preparations, we denote the largest *nontrivial* singular value by σ^ε, and a corresponding (normalized) left singular vector by v^ε, i.e.,

$$\|v^\varepsilon\|_{L^2(M,\omega)} = 1, \qquad \|P^\varepsilon\| = \|P^\varepsilon v^\varepsilon\|_{L^2(M,\omega)} = \sigma^\varepsilon\,.$$

For the sake of brevity, let $\|\cdot\|_0 \coloneqq \|\cdot\|_{L^2(M,\omega)}$ and $\langle \cdot, \cdot \rangle_0 = \langle \cdot, \cdot \rangle_{L^2(M,\omega)}$. Equation (32) suggests the conjecture that

$$|\|P^\varepsilon\| - \|\overline{P}^\varepsilon\|| = o(\varepsilon)\,, \tag{33}$$

where the norm is the operator norm. By the spectral mapping theorem (see, for instance, [34, Sect. 1, Thm. 2.4(c)]),

$$\|\overline{P}^{\varepsilon}\| = \mathrm{e}^{\varepsilon\overline{\lambda}} = 1 + \varepsilon\overline{\lambda} + o(\varepsilon)\,,$$

where $\overline{\lambda} < 0$ is the largest, i.e., smallest in absolute value, nontrivial eigenvalue of the dynamic Laplacian. Thus, eq. (33) is equivalent to

$$\|P^{\varepsilon}\| = 1 + \varepsilon\overline{\lambda} + o(\varepsilon)\,. \tag{34}$$

It can be interpreted as an expansion of the first singular value of P^{ε} in ε, in analogy to the expansion obtained in corollary 3.2. We will prove the following equivalent statement.

Theorem 3.5. *With the above notation and assuming a Dirichlet boundary, one has*

$$\lim_{\varepsilon\to 0} \frac{\sigma^{\varepsilon} - 1}{\varepsilon} = \overline{\lambda}\,. \tag{35}$$

Proof. We split the proof into several steps.

Step 1: We start by proving the lower bound

$$\liminf_{\varepsilon\to 0} \frac{\sigma^{\varepsilon} - 1}{\varepsilon} \geq \overline{\lambda}\,. \tag{36}$$

To this end, the operator-norm definition of σ^{ε} shows that $\sigma^{\varepsilon} \geq \|P^{\varepsilon}u\|_0$ for all $u \in \mathrm{C}_{\mathrm{c}}^{\infty}(\mathring{\mathrm{M}})$ in the domain of P^{ε} which have $\|u\|_0 = 1$. Applying corollary 3.3 to such u yields $P^{\varepsilon}u = u + \varepsilon\overline{\Delta}u + o(\varepsilon)$ in $L^2(M,\omega)$. Therefore, we also have $\|P^{\varepsilon}u\|_0^2 = \|u\|_0^2 + 2\varepsilon\langle u, \overline{\Delta}u\rangle + o(\varepsilon)$. Since $\|u\|_0 = 1$, we obtain $\liminf_{\varepsilon\to 0} \frac{(\sigma^{\varepsilon})^2-1}{\varepsilon} \geq 2\langle u, \overline{\Delta}u\rangle$. The right hand side can be made arbitrarily close to $2\overline{\lambda}$, which shows

$$\liminf_{\varepsilon\to 0} \frac{(\sigma^{\varepsilon})^2 - 1}{\varepsilon} \geq 2\overline{\lambda}\,. \tag{37}$$

From lemma C.2 it follows that $0 \leq \sigma^{\varepsilon} \leq 1$. Thus $\sigma^{\varepsilon} \to 1$ for $\varepsilon \to 0$. Finally, as $(\sigma^{\varepsilon})^2 - 1 = (\sigma^{\varepsilon} - 1)(\sigma^{\varepsilon} + 1)$, we deduce eq. (36) from eq. (37).

Step 2: We now prove the upper bound,

$$\limsup_{\varepsilon\to 0} \frac{\sigma^{\varepsilon} - 1}{\varepsilon} \leq \overline{\lambda}\,, \tag{38}$$

which is somewhat more involved. It is based on the identity:

$$\frac{(\sigma^\varepsilon - 1)(\sigma^\varepsilon + 1)}{\varepsilon} = \frac{\|P^\varepsilon v^\varepsilon\|_0^2 - \|v^\varepsilon\|_0^2}{\varepsilon} = 2\int_0^1 \langle v^\varepsilon(t), \Delta_t v^\varepsilon(t)\rangle_0 \,\mathrm{d}t\,, \tag{39}$$

where the first equality is satisfied as v^ε is first non-trivial singular vector, $v^\varepsilon(t) \coloneqq P_t^\varepsilon(v^\varepsilon)$, and the second equality is a direct consequence of the fundamental theorem of calculus applied to $f^\varepsilon(t) \coloneqq \langle v^\varepsilon(t), v^\varepsilon(t)\rangle_0$. To connect eq. (39) to the theory of elliptic partial differential equations, in analogy to [7] we introduce the bilinear form

$$a_t(u, w) \coloneqq -\langle u, \Delta_t w\rangle\,,$$

defined (by unique continuous extension) for $u, w \in H_0^1(M, g, \omega)$, where g is an arbitrary fixed metric (e.g. g_0) used to measure lengths and angles. The Sobolev space $H_0^1(M, g, \omega) \subset L^2(M, \omega)$ is defined as the Hilbert space with norm $\|\cdot\|_1^2 \coloneqq \|\cdot\|_0^2 + |\cdot|_1^2$, here $|\cdot|_1$ is induced by the bilinear form

$$\langle u, v\rangle_1 \coloneqq \int_M g(\mathrm{grad}_g\, u, \mathrm{grad}_g\, v)\ \omega \tag{40}$$

using the metric g and volume-form ω. This norm is equivalent to the usual $H^1(M, g, \mathrm{d}g)$ Sobolev norm since ω is smooth and nonvanishing on the compact manifold M. As usual, $H_0^1(M, g, \omega)$ is defined as the completion of $\mathrm{C}_\mathrm{c}^\infty(\mathring{\mathrm{M}})$ w.r.t. the norm $\|\cdot\|_1$. We have shown in Step 1 that $\sigma^\varepsilon \to 1$ for $\varepsilon \to 0$. As a consequence, eq. (39) is equivalent to

$$\beta \coloneqq \liminf_{\varepsilon\to 0} \frac{1 - \sigma^\varepsilon}{\varepsilon} = \liminf_{\varepsilon\to 0} \int_0^1 a_t(v^\varepsilon(t), v^\varepsilon(t))\,\mathrm{d}t\,. \tag{41}$$

Equation (41) is the negative of the left hand side of eq. (38). The bilinear form $a_t(\cdot,\cdot)$ on $H_0^1(M, g, \omega)$ is positive, continuous and coercive (cf. lemma C.1), and thus induces a norm $\|\cdot\|_{a_t}$that is equivalent to $|\cdot|_1$. In particular, $\|\cdot\|_{a_t}$-continuous functionals are $|\cdot|_1$-continuous functionals and vice versa. Therefore, the weak topologies for these norms coincide. The Banach-Steinhaus theorem, with the norm $\|\cdot\|_{a_t}$, thus states that if $u_n \to u$ weakly in $H_0^1(M, g, \omega)$, then

$$a_t(u, u) \leq \liminf_{n\to 0} a_t(u_n, u_n)\,. \tag{42}$$

We are now in a position to prove eq. (35) by contradiction. To do so, we will employ a construction similar to the "direct method" from the calculus of variations; cf. [14]. To this end, we take a null sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ for which $\int_0^1 a_t(v^{\varepsilon_n}(t), v^{\varepsilon_n}(t))\,\mathrm{d}t$ converges to β. Assume, for the sake of contradiction, that

$$\beta = \lim_{n\to\infty} \int_0^1 a_t(v^{\varepsilon_n}(t), v^{\varepsilon_n}(t)) \; < -\overline{\lambda}\,. \tag{43}$$

We will use a claim whose proof we defer:

Claim. *There exist $v \in H_0^1(M, g, \omega)$ with $\|v\|_0 = 1$ and a subsequence of $(\varepsilon_n)_n$, for simplicity again denoted by $(\varepsilon_n)_n$, for which the sequences $(v^{\varepsilon_n}(t))_n$ converge weakly in $H_0^1(M, g, \omega)$ to v for every $t \in [0, 1]$.*

For this specific v, Fatou's lemma and eq. (42) imply that

$$\int_0^1 a_t(v, v)\,\mathrm{d}t \le \liminf_{n\to\infty} \int_0^1 a_t(v^{\varepsilon_n}(t), v^{\varepsilon_n}(t))\,\mathrm{d}t = \beta < -\overline{\lambda}\,. \tag{44}$$

The left hand side, in a weak sense, is equal to $-\langle v, \overline{\Delta} v\rangle_0$, the bilinear form associated to the weak form of the dynamic Laplacian. It is well-known that the Rayleigh quotient $v \mapsto -\langle v, \overline{\Delta} v\rangle_0 / \langle v, v\rangle_0$ is minimized by $-\overline{\lambda}$ on $H_0^1(M, g, \omega)$; see, for instance, [7, Sect. 6.5, Thm. 2]. With $\|v\|_0 = 1$, eq. (44) states that v's Rayleigh quotient is strictly lower, hence a contradiction.

It follows that $\beta \ge -\overline{\lambda}$, we conclude using eq. (41) that

$$\liminf_{\varepsilon\to 0} \frac{1 - \sigma^\varepsilon}{\varepsilon} \ge -\overline{\lambda}\,,$$

which proves Step 2.

Step 3, proof of claim: Our proof requires that there exists $\varepsilon_0 > 0$ such that $C \coloneqq \sup_{0\le\epsilon<\varepsilon_0, t\in[0,1]} |v^\varepsilon(t)|_1$ is finite, this part is done in appendix C.

Assuming that C is finite, the Rellich-Kondrachev theorem [41, Sect. 4, Prop. 3.4], states that $v^{\varepsilon_n}(0) \to v$ in $L^2(M, \omega)$ (up to passing to a subsequence if necessary), and therefore $\|v\|_0 = 1$. After again passing to a subsequence if necessary, we may assume $v^{\varepsilon_n}(0) \to v \in H_0^1(M, g, \omega)$ weakly in $H^1(M, g, \omega)$ by the (sequential) Banach-Alaoglu theorem; see, for instance, [5, Thm. 3.2.1].

To show that this limit is attained by $v^\varepsilon(t)$ also for $t \neq 0$ as $\varepsilon \to 0$, we differentiate $h^\varepsilon(t) \coloneqq \|v^\varepsilon(t) - v^\varepsilon(0)\|_0^2$, and apply the fundamental theorem of calculus to yield

$$\|v^\varepsilon(t) - v^\varepsilon(0)\|_0^2 = 2\varepsilon \left| \int_0^t a_\tau(v^\varepsilon(\tau), v^\varepsilon(\tau) - v^\varepsilon) \,\mathrm{d}\tau \right| \leq 4\varepsilon C^2 C' \,,$$

where

$$C' \coloneqq \sup_{t\in[0,1],\ u,w\in H_0^1(M,g,\omega)} |a_t(u,w)|/(|u|_1|w|_1) < \infty \,;$$

see lemma C.1. We may apply the fundamental theorem of calculus due to the absolute continouity ensured by [7, Sect. 5.9, Thm. 3], see also appendix D. As $v^{\varepsilon_n}(0) \to v$, it follows that $v^{\varepsilon_n}(t) \to v$ in $L^2(M,\omega)$ for all $t \in [0,1]$. In particular, v is the only $L^2(M,g,\omega)$ accumulation point in the set $F \coloneqq \{v^{\varepsilon_n}(t)\}_{n\in\mathbb{N},t\in[0,1]}$, therefore also the only weak $H^1(M,g,\omega)$ accumulation point. The sequential Banach-Alaoglu theorem guarantees that the set F is weakly sequentially compact in $H^1(M,g,\omega)$. Combining this with the fact that v is its only accumulation point yields weak convergence of $v^\varepsilon(t) \to v$ in $H^1(M,g,\omega)$ for all $t \in [0,1]$.

This finishes the proof of theorem 3.5. □

3.2.1 Convergence of eigenvectors

The proof of theorem 3.5 also shows that the corresponding eigenvectors must converge in L^2 (in fact, even weakly in H^1). Since, in general, the singular vectors of P^ε satisfy different compatibility conditions at the boundary to those of $\overline{P}^\varepsilon$, this is somewhat surprising.

4 Diffusive transport and surface area

In this section, we look at properties of the surface area form $\mathrm{d}\overline{A}$ in the geometry of mixing, and how it relates to other, similar, area forms obtained from different types of averaging.

In the setting of the advection-diffusion equation, we have assumed that the time set $\mathcal{I}$ is the unit interval equipped with the Lebesgue measure. For the purpose of this section (only), we may weaken this assumption towards $(\mathcal{I}, \mathrm{d}t)$ being a probability space, such as a finite set of numbers equipped with the normalized counting measure, or a compact interval equipped with the

Lebesgue measure normalized by the interval's length. By the term *surface*, we refer to a smooth, oriented, embedded (codimension-1) submanifold.

4.1 Surface area in the geometry of mixing

Let g be any metric on the material manifold M, we call g the "reference metric". This could be, for instance, some "universal" spatial metric (the way we measure lengths and volume), defined on M, or any of the diffusion-adapted metrics from $(g_t)_{t\in\mathcal{I}}$. The choice of g is in analogy to the choice of local coordinates in differential geometry – we will derive expressions for various quantities in terms of g. The metric g is in no way required to be related to the physical transport process under consideration. In particular, if g is the Euclidean metric in some coordinate chart, we obtain coordinate representations in that chart.

As before, define a mass-induced surface area form $\mathrm{d}A$ on any surface $\Gamma \subset M$ via $\iota_\nu\,\omega$, where ν is the g-unit normal vector field[3]

With this notation, $\overline{C} \coloneqq \overline{g}^{-1}g$ and $C_t \coloneqq g_t^{-1}g$ are tangent bundle isomorphisms, i.e., $\overline{C}, C_t \colon TM \to TM$. Then

$$\overline{C} = \left(\int_{\mathcal{I}} g_t^{-1}\,\mathrm{d}t\right) g = \int_{\mathcal{I}} C_t\,\mathrm{d}t\,.$$

For $v \in T_xM \subset TM$, we have that

$$\left\|\overline{C}v\right\|_{\overline{g}}^2 = \overline{g}\left(\overline{C}v, \overline{C}v\right) = \left[\overline{g}\left(\overline{C}v\right)\right]\left(\overline{C}v\right) = \left[\overline{g}\,\overline{g}^{-1}gv\right]\left(\overline{C}v\right) = g(v)\left(\overline{C}v\right) = g\left(v, \overline{C}v\right).$$

Denote by ν_t, $t \in [0,1]$, and $\overline{\nu}$ the unit normal vector fields w.r.t. g_t and $\overline{g}$ on Γ. As with the reference metric, we define

$$\mathrm{d}A_t \coloneqq \iota_{\nu_t}\,\omega\,, \qquad\qquad \mathrm{d}\overline{A} \coloneqq \iota_{\overline{\nu}}\,\omega\,. \tag{45}$$

In other words, corresponding to the three types of metrics—reference g, time-dependent $(g_t)_t$ and time-averaged $\overline{g}$—we derive three area forms ($\mathrm{d}A$, $\mathrm{d}A_t$, and $\mathrm{d}\overline{A}$) from the mass form.

We now show how to relate to each other area form that are induced by the mass form via different metrics on a surface Γ.

[3]If Γ is the boundary of a full-dimensional submanifold, we take the outward-pointing unit normal

Lemma 4.1. *Let $g, \tilde{g}$ be metrics on M. Let Γ be a surface in M, $\tilde{C} \coloneqq \tilde{g}^{-1}g$, and ν and $\tilde{\nu}$ their respective (consistently oriented) unit normal vector fields on Γ. Then*

$$\iota_{\tilde{\nu}}\,\omega = g(\nu,\tilde{\nu})\,\iota_\nu\,\omega = g\left(\nu,\tilde{C}\nu\right)^{1/2}\ \iota_\nu\,\omega\ .$$

Proof. The first equality is trivial, because we may represent $\tilde{\nu}$ as the linear combination of $g(\nu,\tilde{\nu})\nu$ and its projection onto $T_p\Gamma$. But the latter does not contribute to the result. It remains to show $g(\nu,\tilde{\nu}) = g(\nu,\tilde{C}\nu)^{1/2}$. To this end, we show that $\tilde{\nu} = g(\nu,\tilde{C}\nu)^{-1/2}\,\tilde{C}\nu$. First, observe that $\tilde{C}\nu$ is $\tilde{g}$-normal to $T_p\Gamma$, since for any $v \in T_p\Gamma$ we have

$$\tilde{g}(\tilde{C}\nu, v) = (\tilde{g}\tilde{g}^{-1}g\nu)(v) = g(\nu,v) = 0\,.$$

Now, $\|\tilde{C}\nu\|_{\tilde{g}}^2 = \tilde{g}\left(\tilde{C}\nu,\tilde{C}\nu\right) = g\left(\nu,\tilde{C}\nu\right)$, which means that $g(\nu,\tilde{C}\nu)^{-1/2}\,\tilde{C}\nu$ is also $\tilde{g}$-normalized. Finally, $g(\nu,\tilde{C}\nu)^{-1/2}\,\tilde{C}\nu = \tilde{\nu}$ necessarily as they share the same orientation: $g(\nu,\tilde{\nu}) = \tilde{g}(\tilde{C}\nu,\tilde{C}\nu) > 0$. □

Applying lemma 4.1 to the metrics g and g_t, we obtain

$$\mathrm{d}A_t = \sqrt{g(\nu, C_t\nu)}\,\mathrm{d}A\,, \tag{46}$$

and for g and $\overline{g}$,

$$\mathrm{d}\overline{A} = \sqrt{g\left(\nu,\overline{C}\nu\right)}\,\mathrm{d}A\,. \tag{47}$$

By combining lemma 4.1 with corollary 3.4, we obtain the approximation result for accumulated diffusive flux through boundaries of full-dimensional material submanifolds.

Corollary 4.2 ([19, eq. (6)][4])**.** *Let $S \subset M$ be a full-dimensional submanifold with smooth boundary, and u_0 an admissible initial condition. Then*

$$T_0^1(S,u_0) = -\varepsilon\int_0^1\int_{\partial S}\mathrm{d}u_0(C_t\nu)\,\mathrm{d}A\,\mathrm{d}t + O(\varepsilon^2)\,.$$

[4]Recall that $C_t = g_t^{-1}g$, where g is here the Euclidean metric on the flat state space, and corresponds to the transport tensor in [19, 20]; and ν is the outward-pointing g-unit normal vector field on ∂S. In [19], material surfaces are considered that are not necessarily the boundary of a full-dimensional set. In case they are, [19, Eq. (6)] measures the *influx*, which explains the opposite sign to ours. They also require weaker technical assumptions and obtain a slightly weaker result than that $O(\varepsilon^2)$ error appearing here.

Proof. We calculate with lemma 4.1

$$\varepsilon \int_0^1 \int_{\partial S} \mathrm{d}u_0(C_t\nu)\,\mathrm{d}A\,\mathrm{d}t = \varepsilon \int_0^1 \int_{\partial S} \mathrm{d}u_0(\nu_t)\,g(\nu, C_t\nu)^{1/2}\,\mathrm{d}A\,\mathrm{d}t,$$
$$= \varepsilon \int_0^1 \int_{\partial S} \mathrm{d}u_0(\nu_t)\,\mathrm{d}A_t\,\mathrm{d}t\,,$$

and conclude with the divergence theorem and Fubini's theorem

$$= \varepsilon \int_0^1 \int_S \Delta_t u_0\ \omega\ \mathrm{d}t = \varepsilon \int_S \overline{\Delta} u_0\ \omega\ .$$

The claim now follows from corollary 3.4. □

Using the transformation rules for normal vectors and surface forms from lemma 4.1 we can find the representation of (the negative of) the leading-order total diffusive transport through a material boundary w.r.t. an arbitrary weighted manifold structure on the material manifold $(M, \tilde{g}, \frac{\omega}{\mathrm{d}\tilde{g}})$:

$$-\lim_{\varepsilon\to 0} \tfrac{1}{\varepsilon} T_0^1(S, u_0) = -\overline{T}_0^1(S, u_0) = \int_0^1 \int_{\partial S} \mathrm{d}u_0(C_t\nu)\,\mathrm{d}A\,\mathrm{d}t =$$
$$\int_{\partial S} \mathrm{d}u_0(\overline{C}\nu)\,\mathrm{d}A = \int_{\partial S} \mathrm{d}u_0(\overline{C}\tilde{C}^{-1}\tilde{\nu})\,\mathrm{d}\tilde{A} =$$
$$\int_{\partial S} \mathrm{d}u_0(H\tilde{\nu})\,\mathrm{d}\tilde{A} = \int_{\partial S} \tilde{g}(\mathrm{grad}_{\tilde{g}}\,u_0, H\tilde{\nu})\,\mathrm{d}\tilde{A}\,, \quad (48)$$

where $H = \overline{g}^{-1}\tilde{g}$ as claimed in eq. (25).

4.2 Relations to other dynamic surface areas

On a surface $\Gamma \subset M$ with g-unit normal vector field ν, we compute

$$\mathrm{d}\overline{A} = \sqrt{g\left(\nu, \overline{C}\nu\right)}\,\mathrm{d}A =$$
$$= g\left(\nu, \left(\int_{\mathcal{I}} C_t\,\mathrm{d}t\right)\nu\right)^{1/2}\,\mathrm{d}A = \left(\int_{\mathcal{I}} g(\nu, C_t\nu)\,\mathrm{d}t\right)^{1/2}\,\mathrm{d}A\,.$$

Plugging in eq. (46) gives:

$$\mathrm{d}\overline{A} = \left(\int_{\mathcal{I}} \left(\frac{\mathrm{d}A_t}{\mathrm{d}A}\right)^2\,\mathrm{d}t\right)^{1/2}\,\mathrm{d}A\,.$$

This shows that the density of the surface element in the geometry of mixing w.r.t. $\mathrm{d}A$ is an L^2-average of the densities of the time-t surface elements. Relating this with the interpretation in terms of diffusive transport, this is consistent with the observation made in [13, Sect. III.A], "that the rate of mass transport from an element of a material interface is related to the square of the relative change of the surface area".

Proposition 4.3 (Comparison to averages of surface areas)**.** *Let* Γ *be a compact surface, and* $\mathrm{d}\overline{A}(\Gamma)$ *and* $\mathrm{d}A_t(\Gamma)$ *be its surface area as measured by* $d\overline{A}$ *and* $\mathrm{d}A_t$*, respectively; i.e.,*

$$\mathrm{d}\overline{A}(\Gamma) = \int_\Gamma \mathrm{d}\overline{A}, \qquad\qquad \mathrm{d}A_t(\Gamma) = \int_\Gamma \mathrm{d}A_t.$$

Then

$$\mathrm{d}\overline{A}(\Gamma) \geq \left(\int_{\mathcal{I}} \mathrm{d}A_t(\Gamma)^2 \,\mathrm{d}t\right)^{\frac{1}{2}} \geq \int_{\mathcal{I}} \mathrm{d}A_t(\Gamma)\,\mathrm{d}t =: \overline{\mathrm{d}A_t(\Gamma)}\,.$$

Proof. For convenience, we denote $\xi(t,p) = \frac{\mathrm{d}A_t}{\mathrm{d}A}(p)$ and compute

$$\begin{aligned}
\mathrm{d}\overline{A}(\Gamma) &= \int_\Gamma \left(\int_{\mathcal{I}} \xi(t,p)^2\,\mathrm{d}t\right)^{1/2} \mathrm{d}A(p) = \int_\Gamma \|\xi(\cdot,p)\|_{L^2(\mathcal{I})}\,\mathrm{d}A(p) \\
&\geq \|\int_\Gamma \xi(\cdot,p)\,\mathrm{d}A(p)\|_{L^2(\mathcal{I})} \qquad (49) \\
&= \left(\int_{\mathcal{I}} \left(\int_\Gamma \xi(t,p)\,\mathrm{d}A(p)\right)^2 \mathrm{d}t\right)^{1/2} = \left(\int_{\mathcal{I}} \mathrm{d}A_t(\Gamma)^2\,\mathrm{d}t\right)^{1/2},
\end{aligned}$$

where eq. (49) is the triangle inequality for Banach-space valued maps (e.g. for the Bochner integral see [26, Sect. VI]). The second claimed inequality is a direct consequence of Jensen's inequality applied to the expression in eq. (49). □

Notably, $\overline{\mathrm{d}A_t(\Gamma)}$ appears in the definition of the *dynamic Cheeger constant* in [10, Eq. (4)]. Moreover, by means of the Cheeger inequality for weighted manifolds, proposition B.1 in appendix B, we may strengthen the dynamic Cheeger inequality [10, Thm. 3.2], where it was shown that

$$\inf_\Gamma \frac{\overline{\mathrm{d}A_t(\Gamma)})}{\min\{\omega(M_1),\omega(M_2)\}} \leq 2\sqrt{-\lambda_2}\,,$$

for the case that $\omega = \mathrm{d}g_t$ for all $t \in \mathcal{I}$. In this case, $\mathrm{d}A_t$ is the g_t-Riemannian area. Flat Riemannian manifolds were considered in [10], an extension to more general geometries was made in [12].

Corollary 4.4 (Strong dynamic Cheeger inequality)**.** *It holds*

$$\inf_{\Gamma} \frac{\overline{\mathrm{d}A_t(\Gamma)})}{\min\{\omega(M_1), \omega(M_2)\}} \leq \inf_{\Gamma} \frac{\mathrm{d}\overline{A}(\Gamma)}{\min\{\omega(M_1), \omega(M_2)\}} \leq 2\sqrt{-\lambda_2}\,,$$

where $\inf_\Gamma$ *denotes the infimum over all dividing surfaces* Γ *that split* M *into two sets* M_1 *and* M_2*, and* $\lambda_2 < 0$ *is the first non-trivial eigenvalue of* $\overline{\Delta}$*.*

Proof. The first estimate follows from proposition 4.3, the second from proposition B.1, since $\mathrm{d}\overline{A}(\Gamma)/\min\{\omega(M_1), \omega(M_2)\}$ is the Cheeger constant for the geometry of mixing. □

4.3 Relation to total Lagrangian diffusive transport

The authors of [19] establish the approximation of the total diffusive flux as in corollary 3.4 in order to define a measure of diffusive permeability for a generic material surface Γ. Here, the ("diffusive transport") response $\overline{T}^1_0(\Gamma, u_0)$ to a "diffusion stress" given by some virtual initial condition u_0—of which Γ is supposed to be a level set—is computed. As a consequence, the gradient of u_0 along Γ is normal to Γ.

To make this construction comparable among different surfaces, they require that the norm is uniformly constant along the entire Γ, which specifies u_0 in a neighborhood of Γ to first order. It remains to choose a norm w.r.t. which to measure the gradient and thereby require constancy. Since the response depends linearly on this constant in the stress, one may take this constant to be equal to 1 without loss of generality. The requirement on u_0 then reads as $\mathrm{grad}_g\, u_0 = \nu$, with ν the g-unit normal along Γ. We set

$$\overline{T}^1_0(\Gamma; g) \coloneqq -\int_\Gamma \mathrm{g}(\nu, \overline{C}\nu)\,\mathrm{d}A\,, \tag{50}$$

where, notationally, we replace the dependence of $\overline{T}^1_0$ on u_0 by a dependence on the metric g which determines (i) the gradient of u_0; (ii) the unit normal vector; and (iii) the area element $\mathrm{d}A$. By corollary 4.2, the previous definition equals the leading-order coefficient of $T^1_0(S, u_0)$ in the case that $\partial S = \Gamma$ and u_0 is chosen as described above.

In [19], the reference metric g is chosen as the one induced by the initial spatial configuration of the fluid. For this choice, the norm of the gradient of u_0 is constant as measured in the spatial metric. This choice suggests itself, but is by no means natural. For instance, if at the initial time instance the diffusion is not spatially homogeneous (along Γ), a u_0 chosen with constant gradient measured w.r.t. g may have non-constant gradient w.r.t. g_0, the initial, diffusion-adapted metric. As a consequence, it will have non-constant instantaneous diffusive flux, which puts different diffusion stress on different subsets of Γ, and hence makes them incomparable.

Alternatively, one could argue that the gradient should be measured in the "effective" diffusion-adapted norm $\overline{g}$, the norm in the geometry of mixing, and request uniform constancy w.r.t. this norm; i.e. $\operatorname{grad}_{\overline{g}} u_0 = \overline{\nu}$. The diffusive transport represented in the geometry of mixing ($g = \overline{g}$), where H is the identity (see eq. (48)), reduces to

$$\overline{T}^1_0(\Gamma;\, \overline{g}) = -\int_\Gamma \overline{g}(\overline{\nu}, \overline{\nu})\, \mathrm{d}\overline{A} = -\int_\Gamma \mathrm{d}\overline{A}\,, \tag{51}$$

the (negative of the) surface area of Γ in the geometry of mixing. For comparison, we represent the surface area in the the geometry of the initial configuration using lemma 4.1, and obtain

$$\overline{T}^1_0(\Gamma;\, \overline{g}) = -\int_\Gamma \sqrt{g(\nu, \overline{C}\nu)}\, \mathrm{d}A\,. \tag{52}$$

and find that the different uniformization choices for (the gradient of) u_0 lead to integrands that are the square and square root of each other, respectively.

Noticeably, within the $\overline{T}^1_0(\Gamma;\, \overline{g})$ setting, the problem of finding closed material surfaces that minimize leading-order diffusive transport normalized by the enclosed fluid mass is exactly the isoperimetric problem posed in the geometry of mixing; cf. [10, 12] for a related but different approach (recall also corollary 4.4, and the surrounding discussion).

5 Conclusions

In the above, we have investigated the $O(\varepsilon)$ asymptotics of finite-time, time-dependent heat flow on manifolds as the diffusivity ε goes to zero. Such time-dependent heat flows arise naturally when studying (possibly time-dependent) advection-diffusion equations in Lagrangian coordinates. When

the initial concentration u_0 is smooth with support compactly contained in M, the behaviour of the advection-diffusion equation in leading order is described by the time-averaged heat equation or, equivalently, the heat flow in the geometry of mixing.

The advection-diffusion equation remains well-defined even with non-smooth initial data u_0. In particular, it seems natural to investigate $T_0^1(S, \mathbb{1}_S)$, the diffusive transport out of a material set S when the initial density is uniformly distributed on S. The theory developed in this work does not apply to this quantity. Here, the leading order asymptotics is no longer of order ε, as even in the autonomous heat flow context $T_0^1(S, \mathbb{1}_S)$ is of order $\varepsilon^{1/2}$; see, e.g., [43, 40]. There, the leading-order coefficient is proportional to the surface area of the boundary of S. In the time-dependent, finite-time heat flow case, a similar result can be shown, where the relevant surface area is the one in the geometry of mixing. This will be published in forthcoming work.

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A Differential geometric preliminaries

In this section, we briefly recall some fundamental concepts from differential geometry and fix our notation. General references include [29, 15]. Throughout, let M be a smooth, oriented, compact manifold of dimension $\dim M = n$, possibly with smooth boundary.

A *(Riemannian) metric* g on M is a symmetric, positive-definite, contravariant tensor field of rank 2, i.e., $g\colon TM \times TM \to \mathbb{R}$. For any tangent vector $v \in T_xM$, a metric g induces a linear form $g_x(v, \cdot)$ on T_xM. Correspondingly, for any vector field v, the metric g induces a one-form on M. With the *contraction operation/interior multiplication* on forms, denoted by ι, i.e.,

$$(\iota_F \alpha)(v_1, \dots, v_{k-1}) = \alpha(F, v_1, \dots, v_{k-1}) \,,$$

for any k-form α, the induced one-form can be written as $w = \iota_v g$. Henceforth, we identify a metric g with its interpretation as the linear transforma-

tion $g_x \colon T_xM \to T_x^*M$, $v \mapsto \iota_v g_x$, often referred to as the *canonical/musical isomorphism* between T_xM and T_x^*M. Moreover, we will often suppress the subscript x and regard g as a vector-bundle morphism $g \colon TM \to T^*M$; cf., for instance, [27].

Non-degeneracy of g implies its invertibility, and we may interpret its inverse $g^{-1} \colon T^*M \to TM$ by a similar identification as above with a symmetric, positive-definite, covariant tensor field of rank 2, i.e., $g^{-1} \colon T^*M \times T^*M \to \mathbb{R}$. This can be interpreted as an inner product on one-forms, and is known in the literature as the *dual metric (to g)*.

With this notation, the gradient (induced by g) $\operatorname{grad}_g f$ is defined as the vector field (a section of TM) obtained from transforming the one-form $\mathrm{d}f$ by $g^{-1} \colon T^*M \to TM$,

$$\operatorname{grad}_g f = g^{-1}\,\mathrm{d}f\,. \tag{53}$$

For any volume form ω on M, the induced *divergence* $\operatorname{div}_\omega$ of a smooth vector field $F \colon M \to TM$ is defined via

$$(\operatorname{div}_\omega F)\,\omega \coloneqq d(\iota_F \omega) = \mathcal{L}_V \omega,$$

where $\operatorname{div}_\omega F \in C^\infty(M)$, and $\mathcal{L}$ is the Lie-derivative.

The induced *(Riemannian) volume element* is the unique volume form, denoted by $\mathrm{d}g$ (the d here does *not* refer to the exterior derivative we used before), that returns 1 when applied to an oriented, orthonormal set of tangent vectors $v_1, \dots, v_n \in T_xM$. It holds that $\operatorname{div}_{\mathrm{d}g}$ is the usual Riemannian divergence.

Next, let Γ be an oriented codimension-1 surface in M. Then the metric g induces a *surface element* $\mathrm{d}A_g$ on Γ via the volume element on M as follows. For given, oriented linearly independent $v_1, \dots v_{n-1} \in T_p\Gamma$, let $\nu_g \perp_g \operatorname{span}\{v_1, \dots, v_{n-1}\}$ with $\|\nu_g\|_g = 1$ be such that $(\nu_g, v_1, \dots, v_{n-1})$ is positively oriented in M. We call such ν *the* unit normal vector to Γ at p. Then the action of the surface element is given by

$$\mathrm{d}A_g(v_1, \dots, v_{n-1}) = \mathrm{d}g(\nu, v_1, \dots, v_{n-1}), \qquad v_1, \dots, v_{n-1} \in T_p\Gamma\,. \tag{54}$$

Intuitively, $(v_1, \dots, v_{n-1})$ span a parallelepiped of area 1 if, when expanded by the unit normal ν, the resulting parallelepiped has volume 1. By construction, a surface Γ has non-negative *surface area*

$$\mathrm{d}A_g(\Gamma) \coloneqq \int_\Gamma \mathrm{d}A_g\,.$$

The surface element $\mathrm{d}A_g$ is a top-degree form on Γ and can be hence regarded as the volume element there.

A natural differential operator on Riemannian manifolds is the *Laplace-Beltrami operator* Δ_g defined as

$$\Delta_g \coloneqq \mathrm{div}_{\mathrm{d}g} \circ \mathrm{grad}_g \,.$$

It will turn out that for an elegant description and study of a suitably general class of advection-diffusion processes, *weighted manifolds* (also known as *manifolds with density* [31]) are very helpful. A weighted manifold (M, g, θ) is a Riemannian manifold (M, g), on which the volume form and—as a consequence—the induced surface area forms are weighted by a (strictly) positive smooth function $\theta\colon M \to \mathbb{R}$ w.r.t. the canonical volume $\mathrm{d}g$ or surface area $\mathrm{d}A_g$ forms [32, Sect. 18.1]. For the induced surface area the same intuition and formalism applies: measure the volume of a higher-dimensional parallelepiped as obtained by expansion with a suitably oriented unit normal vector, and the result is the area of the base parallelepiped.

On a weighted manifold (M, g, θ), the *Laplace operator* $\Delta_{\theta,g}$ is defined analogously to the classic Riemannian case by composition of the associated divergence and gradient,

$$\Delta_{\theta,g} \coloneqq \mathrm{div}_{\theta\,\mathrm{d}g} \circ \mathrm{grad}_g \,.$$

B Cheeger inequality on weighted manifolds

Proposition B.1 (Cheeger inequality for weighted manifolds)**.** *Let (M, g, θ) be a compact weighted manifold with Laplace operator Δ. We denote the (weighted) volume form by $\omega \coloneqq \theta \mathrm{d}g$, the (weighted) surface measure by $\mathrm{d}\overline{A}$, and the first nontrivial eigenvalue of Δ by λ. Furthermore* $\mathrm{grad} \coloneqq \mathrm{grad}_g$*, and $\|\cdot\| \coloneqq \|\cdot\|_g$. Then the Cheeger inequality holds:*

$$h \coloneqq \inf_{\Gamma \text{ disconnects } M \text{ into } M_1, M_2} \frac{\mathrm{d}\overline{A}(\Gamma)}{\min\{\omega(M_1), \omega(M_2)\}} \leq 2\sqrt{-\lambda}\,. \tag{55}$$

Proof. The proof of the classical Cheeger inequality given in [28] applies—with obvious modifications—to the weighted manifold case. □

C Spectral convergence

Recall that we used the notation $\langle \cdot, \cdot \rangle_0$ for the $L^2(M, \omega)$ scalar product and $\langle \cdot, \cdot \rangle_1$ for the $H^1(M, g, \omega)$ scalar product; furthermore, we introduced g as some reference metric on M and $\mathrm{grad} = \mathrm{grad}_g$. For later reference, we first prove estimates on solutions.

Lemma C.1 (Uniform parabolicity)**.** *There exist constants $C_1, C_2 > 0$ independent of t so that $C_1 |u|_1^2 \leq -\langle u, \Delta_t u \rangle_0 \leq C_2 |u|_1^2$ for all $u \in H_0^1(M, g, \omega)$. Moreover, for $u_1, u_2 \in H_0^1(M, g, \omega)$ it holds that $\langle u_1, \Delta_t u_2 \rangle \leq C_2 |u_1|_1 |u_2|_1$.*

Proof. This is well-known to follow directly from uniform ellipticity of the smooth, t-dependent family of operators Δ_t, defined on the compact $[0, 1]$, which are in divergence form w.r.t. the volume form ω. □

For reference, we state the following well-known result/proof.

Lemma C.2 (L^2 contractivity; [7, Sect. 7.1, Thm. 2])**.** *Let $u_0 \in L^2(M, \omega)$. Then $\|P_t^\varepsilon u_0\|_0 \leq \|u_0\|_0$.*

Proof. To see this, note that

$$\partial_t \|P_t^\varepsilon u\|_0^2 = 2\varepsilon \langle P_t^\varepsilon u, \Delta_t P_t^\varepsilon u \rangle_0 \leq 0 \,,$$

since Δ_t is non-positive. Absolute continuity of $t \mapsto \|P_t^\varepsilon u\|_0^2$ is established in lemma D.1, appendix D. □

Lemma C.3 (Uniform H^1 boundedness; cf. [30, Prop. 2(iii)])**.** *For $t \in [0, 1]$ and $u_0 \in H_0^1$, we have $|P_t^\varepsilon u_0|_1 \leq C_3 |u_0|_1$ for some constant C_3 that does not depend on u_0, t or ε.*

Proof. Our proof conceptually closely follows [30, App. B], which is given in Eulerian coordinates, and therefore takes a seemingly different form because of the presence of the advection term in the evolution PDE.

We start with the case that u_0 is in the domain of Δ_0. By uniform parabolicity it suffices to find bounds on $f^\varepsilon(t) \coloneqq -\langle u_\varepsilon(t), \Delta_t u_\varepsilon(t) \rangle_0$. Using lemma D.2, see see that $f^\varepsilon(t)$ is absolutely continuous, and moreover

$$\begin{aligned} \partial_t \langle u_\varepsilon(t), \Delta_t u_\varepsilon(t) \rangle_0 &= 2\varepsilon \langle \Delta_t u_\varepsilon(t), \Delta_t u_\varepsilon(t) \rangle_0 + \langle u_\varepsilon(t), \partial_t(\Delta_t) u_\varepsilon(t) \rangle_0 \\ &\geq \langle u_\varepsilon(t), \partial_t(\Delta_t) u_\varepsilon(t) \rangle_0 \,. \end{aligned}$$

The operator $\partial_t(\Delta_t)$ is given via its action on $u \in C^\infty(M)$ as

$$\partial_t(\Delta_t)u = \mathrm{div}_\omega(\partial_t(g_t^{-1})\mathrm{d}u)\,,$$

recalling that $\Delta_t u = \mathrm{div}_\omega(g_t^{-1}\mathrm{d}u)$ is the action of Δ_t. Hence, $\partial_t(\Delta_t)$ is a well-defined second-order partial differential operator with smooth coefficients. Arguments as in the proof of lemma C.1 yield that

$$C \coloneqq \sup_{u \in H_0^1(M,\omega,g)} |\langle \partial_t(\Delta_t)u, u\rangle_0|/|u|_1^2 < \infty\,.$$

Therefore

$$-\partial_t \langle u_\varepsilon(t), \Delta_t u_\varepsilon(t)\rangle_0 \leq C|u_\varepsilon(t)|_1^2\,.$$

Due to uniform parabolicity we have that $|u_\varepsilon(t)|_1^2 \leq C_1^{-1} f^\varepsilon(t)$. Hence by Grönwall's lemma ([7, Appendix B.2]), $f^\varepsilon(t) \leq \mathrm{e}^{CC_1^{-1}} f^\varepsilon(0)$, which finishes the proof. Since the domain of Δ_0 is dense in H_0^1, the general result is a consequence of this special case (using the results in appendix D). □

Recall the well-known fact that the L^2-adjoint of P^ε is the time-1 solution operator associated to the Lagrangian advection-diffusion equation with the same Dirichlet boundary conditions, but with reversed time[5], i.e.,

$$\partial_t u(t,x) = \varepsilon \Delta_{(1-t)} u(t,x)\,. \tag{56}$$

The range of $(P^\varepsilon)^*$ is a subset of $H_0^1(M,g,\omega)$; see appendix D. Therefore, the left singular vectors of P^ε, or equivalently the eigenvectors of $(P^\varepsilon)^* P^\varepsilon$, are in $H_0^1(M,g,\omega)$. Recall that the constant C_3 from lemma C.3 depends (i) on the uniform parabolicity bounds C_1 and C_2 from lemma C.1, and (ii) on bounds on $\partial_t(\Delta_t)$. All of these bounds equally apply to eq. (56). Therefore, we conclude with lemma C.3 that

$$|P^* u|_1 \leq C_3 |u|_1\,, \tag{57}$$

for $u \in H_0^1(M,g,\omega)$. Furthermore, the same estimate

$$|P_{t,1} u|_1 \leq C_3 |u|_1\,, \tag{58}$$

[5]See, for example, the proof of [1, Prop. 2.9] and appendix D

applies to the solution operator (from time t to time 1) of the Lagrangian advection-diffusion equation, considered on the time interval $[t, 1]$. By construction,

$$P_1^\varepsilon = P_{t,1}^\varepsilon P_t^\varepsilon$$

for any $t \in (0, 1)$.

Lemma C.4. *There exists $C_4 > 0$, independent from ε, satisfying*

$$|v^\varepsilon|_1 \leq \max_{t\in[0,1]} |v^\varepsilon(t)|_1 \leq C_4 \min_{t\in[0,1]} |v^\varepsilon(t)|_1 \leq C_4 |v^\varepsilon|_1$$

for sufficiently small ε and the singular vector v^ε. Recall that $v^\varepsilon(t) \coloneqq P_t^\varepsilon v^\varepsilon$.

Proof. The rightmost and leftmost inequalities are trivial. For the middle inequality, by lemma C.3 we have

$$\max_{t\in[0,1]} |v^\varepsilon(t)|_1 \leq C_3 |v^\varepsilon|_1 \,. \tag{59}$$

Thus it is enough to show

$$|v^\varepsilon|_1 \leq C |v^\varepsilon(t)|_1 \tag{60}$$

for all $t \in [0, 1]$, with some $C > 0$ independent from t or ε. Since the square of singular values of P^ε are eigenvalues of $(P^\varepsilon)^* P^\varepsilon$, we have

$$(\sigma^\varepsilon)^2 v^\varepsilon(0) = (P^\varepsilon)^* P_1^\varepsilon v^\varepsilon(0) = (P^\varepsilon)^* v^\varepsilon(1) \,. \tag{61}$$

Applying eq. (58) to $v^\varepsilon(1) = P_{t,1}^\varepsilon v^\varepsilon(t)$ yields $|v^\varepsilon(1)|_1 \leq C_3 |v^\varepsilon(t)|_1$. Equations (57) and (61) yield that $(\sigma^\varepsilon)^2 |v^\varepsilon|_1 \leq C_3 |v^\varepsilon(1)|_1$. Combining these inequalities, we obtain $|v^\varepsilon(0)|_1 \leq (\sigma^\varepsilon)^{-2} C_3^2 |v^\varepsilon(t)|_1$. We know that (step 1 of theorem 3.5) $\sigma^\varepsilon \to 1$ for $\varepsilon \to 0$, and is thus bounded away from zero for sufficiently small ε. This proves eq. (60), and the claim is shown. □

Lemma C.5 (H^1 bound on singular vectors)**.** *There exists a constant $C > 0$, independent of ε and t, for which $|v^\varepsilon(t)|_1 \leq C$ holds for $t \in [0, 1]$ and sufficiently small ε.*

Proof. With eq. (39) and lemmas C.1 and C.4 we obtain for any $t \in (0,1]$ and sufficiently small ε that:

$$\begin{aligned}\frac{(1-(\sigma^\varepsilon)^2)}{2\varepsilon} &= -\int_0^1 \langle v^\varepsilon(t), \Delta_t v^\varepsilon(t)\rangle_0 \,\mathrm{d}t \\ &\geq \min_{t\in[0,1]} -\langle v^\varepsilon(t), \Delta_t v^\varepsilon(t)\rangle_0 \\ &\geq C_1 \min_{t\in[0,1]} |v^\varepsilon(t)|_1^2 \\ &\geq C_1 C_4^{-1} |v^\varepsilon(0)|_1^2 \,.\end{aligned}$$

In eq. (37) we have already shown that the limit superior of the left hand side is less than or equal to $-\overline{\lambda}$, and, therefore, it may be bounded from above by, say, $-2\overline{\lambda}$ for sufficiently small ε. This shows that $|v^\varepsilon|_1^2 \leq -2\overline{\lambda} C_4 C_1^{-1}$, proving the claim for $t = 0$. The case $t \neq 0$ is now a consequence of lemma C.3. □

D Parabolic PDEs on compact manifolds with boundary

We briefly collect some properties of second-order parabolic PDEs on compact and orientable smooth Riemannian manifolds with (potentially empty) C^2 boundary. These properties are well known when the domain is an open subset of $\mathbb{R}^n$ [7, 37] and the straightforward extension to compact manifolds seems to be folklore knowledge , though rarely explicitly treated; see [2]. We describe below some properties of the the Galerkin-approach described in [7][37, Chapter 11.1] with straightforward modification to the time-dependent mass-preserving setting on a compact manifold; the reasoning below is included only in order to (a) demonstrate that well-known results on $\mathbb{R}^n$ indeed extend to compact manifolds in a straightforward way because we could not find a reference and (b) collect some technical results arising directly in the standard Galerkin approach that we require elsewhere.

Let ω be a smooth, nonvanishing volume-form on M. For convenience, we will use a metric g such that $\mathrm{d}g = \omega$. The metric may be constructed by any metric on M after suitable rescaling. We need this metric only for defining a norm on $H^1(M,g)$, given by

$$\|u\|^2_{H^1(M,g)} \coloneqq \int_M g(\operatorname{grad} u, \operatorname{grad} u)\,\omega + \int_M |u|^2\,\omega\,,$$

where $\operatorname{grad} u$ is interpreted in a suitably weak sense. Since M is compact, the specific choice of g will not affect the topology of $H^1(M,g)$. The space $H^1_0(M,g)$ is defined as the completion of $\mathrm{C}^\infty_\mathrm{c}(\mathring{\mathrm{M}})$ w.r.t. $\|\cdot\|_{H^1(M,g)}$ [15, 21].

We will describe the parabolic PDE theory needed for the equation

$$\partial_t u = \operatorname{div}_\omega(D(t)\mathrm{d}u)\,, \tag{62}$$

with $D\colon [0,1]\times T^*M \to TM$ a smooth—including at the boundary—family of nonvanishing bundle morphisms that are symmetric in the sense that $D(t,u)(v) = D(t,v)(u)$ for $t \in [0,1]$ and all vector fields u and v. Let $L(t)v \coloneqq \operatorname{div}_\omega(D(t)\mathrm{d}u)$. The tensor field D is bounded—due to its smoothness and compactness of M—and nonvanishing, hence the operator $\partial_t - L$ is *uniformly parabolic*, i.e., there exists $\alpha > 0$ such that for any $v \in H^1_0(M,g)$

$$\alpha^{-1}\|\operatorname{grad}_g v\|^2_{L^2(M,\omega)} \leq -\langle v, L(t)v\rangle_{L^2(M,\omega)} \leq \alpha\|\operatorname{grad}_g v\|^2_{L^2(M,\omega)}\,. \tag{63}$$

For what follows, we require the well-known theory of vector-valued Sobolev spaces, and our notation essentially follows [37]; see also [4, Appendix A] for proofs of fundamental results. For a Hilbert space X, we write X^* for its dual, and $H^{-1}(M,g) \coloneqq H^1_0(M,g)^*$.

As in [37], to each $t \in [0,1]$ we associate an operator $L(t)\colon H^1_0(\omega) \mapsto H^{-1}(M,g)$, defined by

$$(L(t)u)v = \langle \mathrm{d}u, D(t)\mathrm{d}v\rangle_{L^2(M,\omega)} = \int_M \mathrm{d}u(D(t)\mathrm{d}v)\ \omega\ .$$

The space $L^2(M,\omega)$ embeds continuously into H^{-1} by the identification of a function $f \in L^2(M,\omega)$ with the functional $\langle f, \cdot\rangle_{L^2(M,\omega)}$. By a slight abuse of notation, for $f \in H^{-1}(M,g)$ and $g \in H^1_0(M,g)$ we will write $\langle f, g\rangle_{L^2(M,\omega)} \coloneqq f(g)$, even if f is not contained in the image of the embedding.

Lemma D.1. *Equation* (62) *has a unique weak solution*

$$u \in C([0,1]; L^2(M,\omega)) \cap L^2((0,1); H^1_0(M,g)),$$

given an initial value $u(0,\cdot) \in L^2(M,\omega)$*. Moreover, the function* $t \mapsto \|u(t,\cdot)\|^2_{L^2(U)}$ *is absolutely continuous, with*

$$\frac{d}{dt}\|u(t)\|^2_{L^2(M,\omega)} = 2\langle L(t)u(t), u(t)\rangle_{L^2(M,\omega)} \tag{64}$$

for almost all t*, where the right hand side must be interpreted in a weak sense.*

Proof. The L^2-Galerkin approach described in [7, Sect. 7.1, Thms. 3 & 4] yields existence and uniqueness for the compact manifold case just like for $M \subset \mathbb{R}^n$ compact. Theorem 3 in [7, Sect. 5.9] proves the remaining claims. □

These arguments show that for $t \in [0,1]$, the time-t solution operator to eq. (62) is well-defined when viewed as an operator $P_t \colon L^2 \to L^2$. Arguments as in lemma C.2 establish its continuity.

Let the domain of $L(t)$ be the collection of $f \in H_0^1(M,g) \subset L^2(M,\omega)$ satisfying $L(t)f \in L^2(M,\omega)$. As a consequence of elliptic regularity theory and the fact that we are working with homogeneous Dirichlet boundary (see [7, Chapters 6.3 & 7.4]), this function space does not depend on t. By arguments as in [34, Chapter 7], one sees that for $t \in (0,1]$, the image of the time-t solution operator P_t is in the domain of $L(t)$. Hence, the image of P_t is in $H_0^1(M,g)$ for all $t \in (0,1]$. Thus, the operator $P_t \colon L^2(M,\omega) \to H_0^1(M,g)$ is well-defined, and by the closed graph theorem it is continuous. By the Rellich-Kondrachev theorem, P_t is therefore compact when viewed as an operator from $L^2(M,\omega)$ to itself.

Lemma D.2. *Provided that the initial value u_0 is in the domain of $L(0)$, the solution from lemma D.1 is sufficiently regular such that*

(i) $u \in H^1\left((0,1); H_0^1(M,g)\right)$,

(ii) $L(t)u \in H^1\left((0,1); H^{-1}(M,g)\right)$, *and*

(iii) $L(t)u \in C\left([0,1]; L^2(M,\omega)\right)$.

The function $\langle u, L(t)u\rangle_{L^2(M,\omega)}$ is absolutely continuous with

$$\frac{d}{dt}\langle u(t), L(t)u(t)\rangle_{L^2(M,\omega)} = 2\langle L(t)u(t), L(t)u(t)\rangle_{L^2(M,\omega)} + \langle L'(t)u(t), u(t)\rangle_{L^2(M,\omega)} \quad (65)$$

for almost all $t \in [0,1]$.

Proof. Proceed as in [37, Sect. 11.1.4], for the last statement a result like [4, Cor. A.4] is required. □

Lemma D.3. *If $u_0 \in \mathrm{C}_\mathrm{c}^\infty(\mathring{\mathrm{M}})$, then the solution u from lemma D.1 is in $C^\infty([0,1] \times M)$.*

Proof. Certainly u_0 is in the domain of all powers of $L(t)$. Iterating the construction of [37, Sect. 11.1.4] together with Sobolev embedding and elliptic-regularity results yields the claim. See also [7, Sect. 7.1, Thm. 7] for a proof of the nonautonomous case on open subsets of $\mathbb{R}^n$. □

We conclude with a well-known property of smooth solutions to parabolic equations.

Lemma D.4 (Weak maximum principle on manifolds; [21, Thm. A.3.1] or [7, Sect. 7.1, Thm. 8])**.** *Let $u \in C^{1,2}([0,1]\times M)\cap C([0,1]\times\overline{M})$. If $\mathcal{L}^\varepsilon u \leq 0$ on $[0,1]\times\operatorname{int}(M)$, then for the "parabolic boundary" $B \coloneqq [0,1]\times\partial M \cup \{0\}\times M$ one has*

$$\max_{[0,1]\times M} u = \max_B u\,. \tag{66}$$

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Heat-content and diffusive leakage from material sets in the low-diffusivity limit*

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We generalize leading-order asymptotics of a form of the *heat content of a submanifold* (van den Berg & Gilkey 2015) to the setting of time-dependent diffusion processes in the limit of vanishing diffusivity. Such diffusion processes arise naturally when advection-diffusion processes are viewed in Lagrangian coordinates. We prove that as diffusivity ε goes to zero, the diffusive transport out of a material set S under the time-dependent, mass-preserving advection-diffusion equation with initial condition given by the characteristic function $\mathbb{1}_S$, is $\sqrt{\varepsilon/\pi}\,\mathrm{d}\overline{A}(\partial S) + o(\sqrt{\varepsilon})$. The surface measure $\mathrm{d}\overline{A}$ is that of the so-called *geometry of mixing*, as introduced in (Karrasch & Keller 2020). We apply our result to the characterisation of coherent structures in time-dependent dynamical systems.

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1. Motivation

Consider the advection-diffusion process of a passive scalar u by a sufficiently regular, possibly time-dependent, volume-preserving vector field V as described by the advection-diffusion equation

$$\partial_t u = -\operatorname{div}(uV) + \varepsilon\Delta u\,, \tag{1}$$

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and some initial condition $u(0,\cdot) = u_0$. Let Φ_0^t denote the flow map (from time 0 to time t) induced by V. For $\varepsilon = 0$, there is only advection and the time-t solution operator mapping $u(0,\cdot)$ to $u(t,\cdot)$ under eq. (1) is given by a coordinate change by the flow map of V, i.e., $u(t, \Phi_0^t(x)) = u_0(x)$. The coordinates induced by the flow map Φ_0^t are well known as *Lagrangian* coordinates. We refer to flow-invariant space-time sets as *material sets*.

For any non-negative ε, we are interested in the leakage of $u = u_\varepsilon$ from a full-dimensional material set S with smooth boundary over the time interval $[0,t]$ under eq. (1). Let us denote this *material outflow* by

$$T_0^t(S, u_0, \varepsilon) \coloneqq \int_S u_0 \, \mathrm{d}x - \int_{\Phi_0^t(S)} u_\varepsilon(t,x) \, \mathrm{d}x \,.$$

In the advection-only case, flow-invariance directly implies

$$T_0^t(S, u_0, 0) = 0 \,, \tag{2}$$

regardless of the initial condition u_0 and set S. In simple terms, no mass can leak out of a material set if there is no diffusion.

For $\varepsilon > 0$, however, the situation is different: In general, $T_0^t(S, u_0, \varepsilon)$ does not vanish, and the asymptotics of $T_0^t(S, u_0, \varepsilon)$ as $\varepsilon \to 0$ are nontrivial and of both scientific and practical interest. In [15], leading-order asymptotics of $T_0^t(S, u_0, \varepsilon)$ for smooth u_0 compactly supported in the interior of the domain were derived, and in [20] they were additionally studied from a geometric point of view. In this work, we further expand the theory towards the natural case $u_0 = \mathbb{1}_S$.

Let $\tilde{u}_\varepsilon$ denote u_ε in Lagrangian coordinates, i.e., $\tilde{u}_\varepsilon(t,\cdot) = u_\varepsilon(t,\cdot) \circ \Phi_0^t$. Then eq. (1) reads as

$$\partial_t \tilde{u}_\varepsilon = \varepsilon \Delta_t \tilde{u}_\varepsilon \,, \tag{3}$$

where Δ_t is the differential geometrical pullback of the Laplace operator by Φ_0^t; see, for instance, [22, 27, 19]. With a common, slight abuse of notation, we will omit the tilde in eq. (3) henceforth as we work in Lagrangian coordinates exclusively. Here,

$$T_0^t(S, \mathbb{1}_S, \varepsilon) = \int_S \mathrm{d}x - \int_S u_\varepsilon(t,x) \, \mathrm{d}x = \int_{M \setminus S} u_\varepsilon(t,x) \, \mathrm{d}x \,,$$

since $\int_M u_\varepsilon(t,x) \, \mathrm{d}x = \int_M u_0(x) \, \mathrm{d}x = \int_S \mathrm{d}x$ for all $t \in [0,1]$ by mass preservation. If eq. (3) were the classical autonomous heat equation, then the leading-order coefficient (of order $\sqrt{\varepsilon}$) in $T_0^1(S, \mathbb{1}_S, \varepsilon)$ is proportional to the surface area of ∂S; see [28]. For a generalization to the nonautonomous case as in eq. (3), it is *a priori* unclear whether one should again expect some kind of surface measure of ∂S in the leading-order coefficient: in the Lagrangian pullback geometry, ∂S has—in general—a different surface area at each time instance t. Recently, [19] proposed a (weighted) geometry—the *geometry of mixing* to be recalled below—which was developed to specifically analyze advection-diffusion processes on finite-time intervals. This geometry, which has the mathematical structure of a weighted (Riemannian) manifold [19, 20], admits an area form $\mathrm{d}\overline{A}$ about

which we show in this work that it, indeed, determines the leading-order asymptotics of material leakage out of material sets, namely

$$T_0^1(S, \mathbb{1}_S, \varepsilon) = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} \mathrm{d}\overline{A} + o\left(\sqrt{\varepsilon}\right) .$$

In our proof, we will work with a generalized form of the time-dependent Lagrangian heat equation eq. (3), and do not assume that it is necessarily given as some advection-diffusion equation in Lagrangian coordinates.

2. Mathematical setting

Let M be a smooth compact manifold (possibly with smooth boundary), and ω a non-vanishing volume form on M. Recall that ω naturally defines a divergence operator, acting on vector fields $V \in \Gamma(TM)$, by $(\mathrm{div}_\omega V)\,\omega = \mathcal{L}_V\,\omega$. Here, $\Gamma(TM)$ denotes smooth sections of the tangent bundle and $\mathcal{L}$ is the Lie derivative. If $(g_t)_{t\in[0,1]}$ is a smoothly-varying one-parameter family of Riemannian metrics on M, a *weighted* Laplace operator (cf. [13]), acting on smooth functions $f \in C^\infty(M)$, is defined for each t with the formula

$$\Delta_t f \coloneqq \mathrm{div}_\omega\, g_t^{-1}\, \mathrm{d}f\,.$$

The notation g_t^{-1} shall be interpreted using the well-known natural identification of g_t with a vector bundle morphism mapping a tangent vector v to the cotangent vector $g_t(v,\cdot)$. As g_t is positive definite at each point, this is in fact a vector bundle *isomorphism* and g_t^{-1} is well-defined. Indeed, $f \mapsto g_t^{-1}\,\mathrm{d}f$ is the *gradient* induced by the metric g_t.

As mentioned earlier, our object of study is the time-dependent heat equation with diffusivity $\varepsilon > 0$ and initial value $u_0 \in L^2(M,\omega)$,

$$\partial_t u_\varepsilon = \varepsilon \Delta_t u_\varepsilon\,, \qquad u_\varepsilon(0,\cdot) = u_0\,, \tag{4}$$

which is a generalization of the classical heat equation on M for which g_t is independent from t and ω is the Riemannian volume form. We will look at eq. (4) with boundary conditions given by either (i) $\partial M = \varnothing$, (ii) homogeneous Dirichlet boundary or (iii) homogeneous Neumann boundary. Of course, (i) is a special case of both (ii) and (iii).

3. The geometry of mixing

We write P_t^ε for the the time-t solution operator of eq. (4), and denote by $\langle\cdot,\cdot\rangle_0$ the $L^2(M,\omega)$ inner product. Throughout, we will identify the volume form ω with its induced measure. A *(time) averaged* version of eq. (4) describes the leading-order behaviour of P_1^ε as $\varepsilon \to 0$. Indeed, defining[1]

$$\overline{g} \coloneqq \left(\int_0^1 g_t^{-1}\,\mathrm{d}t\right)^{-1}\,, \quad \overline{\Delta} \coloneqq \mathrm{div}_\omega\, \overline{g}^{-1}\,\mathrm{d}f\,, \quad \text{and} \quad \overline{P}_t^\varepsilon \coloneqq \exp(\varepsilon t\overline{\Delta})\,,$$

[1] The imposed boundary condition type in the definition of the semigroup $\exp(\varepsilon t\overline{\Delta})$ corresponds to the one (homogeneous Dirichlet/Neumann) imposed in eq. (4), see also [20].

it is true [20], see also [21, 15], that for $u_0 \in C_c^\infty(M)$, i.e., $u_0 \in C^\infty(M)$ with compact support in M,

$$\left\| P_1^\varepsilon u_0 - \overline{P}_1^\varepsilon u_0 \right\|_{L^\infty(M)} = O(\varepsilon^2), \quad \varepsilon \to 0\,. \tag{5}$$

The operator $\overline{\Delta}$ was called the *dynamic Laplacian* in [9], and is the natural Laplace operator of the weighted manifold $(M, \overline{g}, \omega)$. This weighted manifold was coined *geometry of mixing* in [19]. On the surface ∂S oriented by the $\overline{g}$-unit outer normal vector field ν, the geometry of mixing has a natural area form given by $\mathrm{d}\overline{A}(\cdot) := \omega(\nu, \cdot)$; see [19, 20].

For non-smooth u_0, such as $u_0 = \mathbb{1}_S$, it is not clear whether we can expect a result like eq. (5): even in the special case of the time-*independent* heat equation on the weighted manifold $(M, \overline{g}, \omega)$, there are now terms of order $\varepsilon^{\frac{1}{2}}$ and its powers (which is in stark contrast to the case of smooth initial values). It is known, for example, that

$$\left\langle \overline{P}_1^\varepsilon \mathbb{1}_S, \mathbb{1}_{M\setminus S} \right\rangle = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} \mathrm{d}\overline{A} + o(\sqrt{\varepsilon})\,, \quad \varepsilon \to 0\,; \tag{6}$$

see [28, 23]. In this paper, we show that eq. (6) remains true if $\overline{P}_1^\varepsilon$ is replaced by P_1^ε, i.e. the following theorem which we prove in section 5.

Theorem 1. *Let S be a compact, full-dimensional submanifold of M with smooth boundary, contained in the interior of M, and let $S^c := M \setminus S$. Then*

$$\left\langle P_1^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c} \right\rangle_0 = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} \mathrm{d}\overline{A} + o(\sqrt{\varepsilon})\,, \quad \varepsilon \to 0\,. \tag{7}$$

4. Eulerian coherent pairs and Lagrangian coherent sets

In [10], the following concept of *coherence* has been introduced. Consider two spatial sets S (at time 0) and S' (at time 1), L_ε a small perturbation of the *transfer operator*, i.e., the solution operator for eq. (1) with $\varepsilon = 0$, where the perturbation strength scales with $\varepsilon > 0$. Then [10] proposed a *coherence ratio*

$$\rho_\varepsilon(S, S') := \frac{\left\langle L_\varepsilon \mathbb{1}_S, \mathbb{1}_{S'} \right\rangle_0}{\omega(S)} + \frac{\left\langle L_\varepsilon \mathbb{1}_{M\setminus S}, \mathbb{1}_{M\setminus S'} \right\rangle_0}{\omega(M \setminus S')}\,, \tag{8}$$

as a measure of *coherence* of the pair (S, S'). Verbally, this measures how much of S is carried to S' and how much of $M \setminus S$ is carried to $M \setminus S'$ by the "perturbed flow". In yet other words, *coherent pairs* (see also [2]) S and S' are pairs of spatial sets such that there is little leakage under the action of L_ε.

Of course, choosing $S' = \Phi_0^1(S)$ results in no leakage (or, equivalently, coherence ratio equal to 1) in the non-diffusive case, notably for any choice of S, see eq. (2). While, in that limit case, the problem of seeking "maximally coherent pairs" becomes meaningless, one would expect that $S' = \Phi_0^1(S)$ is the right condition to perturb from when bringing weak diffusion into consideration.

We thus define the *Lagrangian coherence ratio* as

$$\tilde{\rho}_\varepsilon(S) \coloneqq \rho_\varepsilon(S, \Phi_0^1(S))\,.$$

Seemingly trivial, this has conceptually deep implications. First, it removes one degree of freedom, the choice of S'. As a consequence, it changes the focus from Eulerian coherent pairs (of sets) to individual Lagrangian coherent sets. Moreover, it is clear that, for given S, the Lagrangian coherence ratio depends only on the type and the strength of the perturbation of the transfer operator. One implementation of a perturbation, as done in [10], is to convolve densities both before and after the purely advective transport with an explicitly-defined kernel, whose support is bounded by ε away from 0. Another popular approach is to omit any explicit perturbation, and rely on "numerical diffusion" (e.g., via box discretizations) instead; see [11]. The choice $L_\varepsilon = P_1^\varepsilon$, i.e., the solution operator to the Lagrangian advection-diffusion equation eq. (3) was suggested in [19]—see [5] for the analogous Eulerian approach—as a physically natural perturbation candidate, that can also be given a stochastic interpretation. With this definition of L_ε, we can work with indicator functions directly when maximizing coherence measures like eq. (8), instead of applying a two-step relaxation procedure as is sometimes done; see [17, 10, 4].

By Theorem 1, if ∂S is smooth and $\partial M = \emptyset$ (or with homogeneous Neumann boundary), then as $\varepsilon \to 0$,

$$\rho_\varepsilon(S, \Phi_0^1(S)) = \frac{\omega(S) - \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} \mathrm{d}\overline{A}}{\omega(S)} + \frac{\omega(M \setminus S) - \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} \mathrm{d}\overline{A}}{\omega(M \setminus S)} + o(\sqrt{\varepsilon})\,.$$

In other words, if we fix $\omega(S)$, the coherence ratio depends in leading order as $\varepsilon \to 0$ only on (a constant times) the area of ∂S in the geometry of mixing. Smooth local minimizers of the area functional in a (weighted) manifold with respect to volume-preserving variations are well-known to be surfaces of constant generalized mean curvature; see [14, Sect. 9.4E]. The above considerations hence suggest that sets bounded by such a minimizing surface be viewed as *Lagrangian coherent sets* in the low-diffusivity limit. This connection between the concept of coherent sets and that of the (generalized) isoperimetric problem is closely related to the connection described in [9]. At the same time, it has close ties to the studies of diffusive transport across material surfaces performed in [19, 15, 16].

5. Proof of the main theorem

5.1. Overview

Our proof consists of a reduction of eq. (7) to the time-independent setting so that we can apply eq. (6). In a first step, we perform this reduction for the case $M = \mathbb{R}^n$ in section 5.2 using stochastic methods. This avoids technical complications arising from dealing with manifold-valued stochastic processes. We then treat the general case where M is an arbitrary compact manifold in a second step (section 5.3).

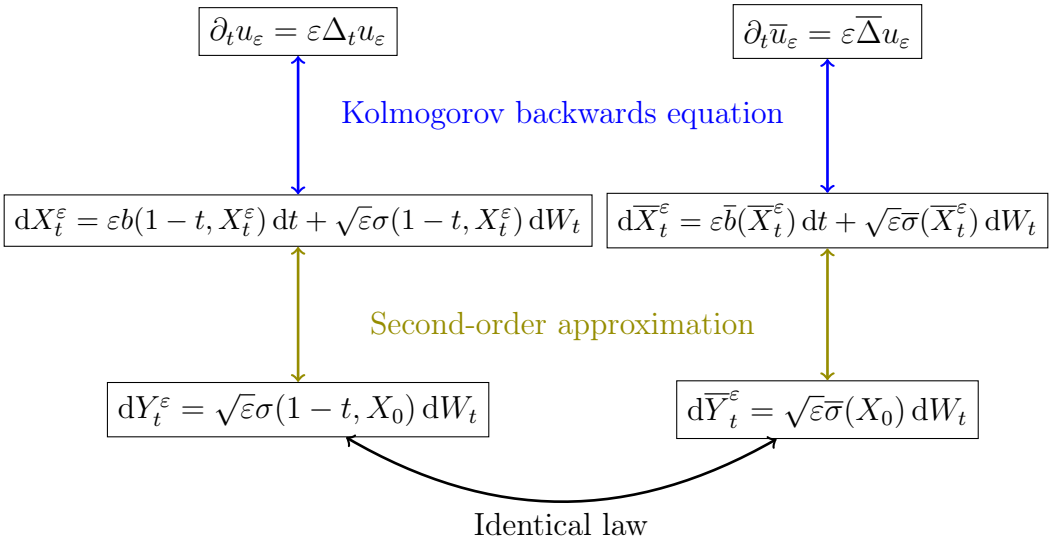

Figure 1: Schematic visualization of the structure of the proof of Theorem 1 on $\mathbb{R}^n$.

The structure of the first step is sketched in Fig. 1. On the top right hand side we depict the averaged, i.e., time-independent, advection-diffusion equation for which we know (eq. (6)) the asymptotic behaviour of $\langle P_1^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c}\rangle_0$ as $\varepsilon \to 0$. On the top left there is the *time-dependent* advection-diffusion equation which is the subject of Theorem 1. Each arrow represents a reduction or approximation step in the proof:

(i) The upper two arrows (blue) connect a stochastic differential equation (SDE) to its Kolmogorov backward PDE above it; see section 5.2.1.

(ii) Central arrows (olive): Each SDE is approximated by another SDE, inheriting the leading-order asymptotics we are interested in, see section 5.2.4. The use of this kind of SDE approximation to obtain PDE approximations is well known in the literature, see, e.g., [7, Section 2.3].

(iii) The lower arrow (black) highlights the fact that Y_t^ε and $\overline{Y}_t^\varepsilon$ have the same law, and, as a consequence, they share the same the leading-order asymptotics of interest.

The reduction as a whole may be conceptualised as going along the arrows from the top right of Fig. 1 to the top left.

Technical issues caused by non-compactness

As $\mathbb{R}^n$ is not compact, it may be that $\mathbb{1}_{\mathbb{R}^n} \notin L^2(\mathbb{R}^n, \omega)$. This means that the $\langle \cdot, \cdot \rangle_0$ notation appearing in eq. (7) must be clarified: we abuse notation by writing $\langle f, g\rangle_0 \coloneqq \int_M f(x)g(x)\,\omega$ whenever $fg \in L^1(\mathbb{R}^n, \omega)$. Similar issues also play a role in the non-compact case. Since in Theorem 1 we assume the set S to be compact anyway, in order to avoid unncessary technical complications, we state the following simplifiying

Assumption A. *There exists a bounded set B (containing S in its interior) so that both g_t and ω are equal to the Euclidean metric and its volume form respectively outside of B for all $t \in [0,1]$.*

5.2. Step 1: The case $M = \mathbb{R}^n$

On $M = \mathbb{R}^n$, the initial value problem eq. (4) takes the form

$$\partial_t u_\varepsilon = \varepsilon \left(\sum_{i=1}^n b_i \partial_i u_\varepsilon + \frac{1}{2} \sum_{i,j=1}^n a_{i,j} \partial_{ij} u_\varepsilon \right), \qquad u_\varepsilon(0,\cdot) = u_0 \,. \tag{9}$$

Here, the space-time-dependent, real-valued functions a_{ij} and b_i depend on the metrics $(g_t)_{t\in[0,1]}$ and the volume form ω. There are no coefficients of lower order because $\Delta_t \mathbb{1}_{\mathbb{R}^n} = 0$ for all $t \in [0,1]$. Assumption A yields that on the complement of B, $a_{i,j} = \delta_{ij}$ and $b_i = 0$ in Cartesian coordinates. We have collected some results from the literature on parabolic PDEs in appendix C adapted to our setting which we will use in the sequel.

5.2.1. The Kolmogorov backwards equation

The time-1 solution operator of eq. (9) is closely linked to the stochastic process governed by the SDE

$$\mathrm{d}X_t^\varepsilon = \varepsilon b(1-t, X_t^\varepsilon)\,\mathrm{d}t + \sqrt{\varepsilon}\sigma(1-t, X_t^\varepsilon)\,\mathrm{d}W_t \,, \tag{10}$$

with $\big(\sigma(t,x)\sigma^\top(t,x)\big)_{ij} = a_{ij}(t,x)$ and initial value $X_{t_0}^\varepsilon = X_{t_0}$ independently of ε. It is well known that for a given n-dimensional Brownian motion $(W_t)_{t\in[0,1]}$, for $t_0 \in [0,1]$ a unique strong solution to eq. (10), starting at time t_0, exists provided that X_{t_0} is independent of $(W_t)_{t\in[t_0,1]}$ and that b and σ satisfy Lipschitz and growth conditions (cf. also section 5.2.4). A direct consequence of smoothness and Assumption A is that the Lipschitz and growth conditions are satisfied, as it is well known that σ may be chosen to be smooth. To explicitly include the dependence of the process $(X_t^\varepsilon)_{t\in[t_0,1]}$ on the random variable X_{t_0}, we will write $E_{t_0,x}[\cdot]$ (given $x \in \mathbb{R}^n$) for the expected value under the assumption that $X_{t_0} = x$ almost surely; in this case X_0 has law given by the Dirac delta measure centered at x. The *Kolmogorov backwards-equation* associated to eq. (10) is a partial differential equation (PDE) for the function

$$w_\varepsilon(t,x) = E_{t,x}[u_0(X_1^\varepsilon)] \,,$$

provided that u_0 is sufficiently smooth, see [8, Thm. 6.1]. This PDE reads

$$\partial_t w_\varepsilon(t,x) = -\varepsilon \left(\sum_{i=1}^n b_i(1-t,x)\partial_i w_\varepsilon(t,x) + \frac{1}{2}\sum_{i,j=1}^n a_{ij}(1-t,x)\partial_{ij} w_\varepsilon(t,x) \right),$$

and moreover $w_\varepsilon(t,x) \to u_0(x)$ as $t \to 1$. Thus, $u_\varepsilon(t,x) = w_\varepsilon(1-t,x)$, as both sides satisfy eq. (9) and solutions to parabolic PDEs are unique. As a consequence,

$$(P_1^\varepsilon u_0)(x) = u_\varepsilon(1,x) = w_\varepsilon(0,x) = E_{0,x}[u_0(X_1^\varepsilon)] \,. \tag{11}$$

This equation provides a probabilistic interpretation of the time-1 solution operator of eq. (9) in terms of the SDE defined by eq. (10).

5.2.2. Probabilistic interpretation of the heat content in a manifold

In eq. (11) we assume the process X_t^ε to start at the constant x almost surely, i.e., we choose the initial value X_0 to have law equal to the point measure at x. We may, however, also treat the case in which the initial value X_0 of eq. (10) is no longer a constant random variable.

Let $h\colon M \to \mathbb{R}_{\geq 0}$ be a measurable function so that $h\,\omega$ is a probability measure. We denote by $E_h[\cdot]$ the expected value in a probability space where X_0 has law $h\,\omega$ independent of the Brownian motion $(W_t)_{t\in[0,1]}$. One may verify that[2]

$$\langle x \mapsto E_{0,x}[u_0(X_1^\varepsilon))], h\rangle_0 = E_h[u_0(X_1^\varepsilon)]$$

holds in the case $u_0 = \mathbb{1}_A$, the extension to all $u_0 \in L^\infty(\mathbb{R}^n)$ follows from linearity and monotone convergence. Using eq. (11) and Theorem 12, it follows that

$$\langle P^\varepsilon u_0, h\rangle_0 = \langle x \mapsto E_{x,0}[u_0(X_1^\varepsilon)], h\rangle_0 = E_h[u_0(X_1^\varepsilon)]\,. \tag{12}$$

We summarize that eq. (12) proves a *probabilistic* interpretation of inner products of the form $\langle P_1^\varepsilon u_0, h\rangle_0$ provided that (i) $u_0 \in L^\infty(\mathbb{R}^n)$, and (ii) $h \in L^1(\mathbb{R}^n, \omega)$ is nonnegative. The inner product appearing in eq. (7) is not of the form just discussed as $\mathbb{1}_{S^c}$ is not in general in $L^1(\mathbb{R}^n, \omega)$. Observe, however, that for compact S,

$$\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c}\rangle_0 = \langle \mathbb{1}_S, P^\varepsilon \mathbb{1}_{S^c}\rangle_0\ ,$$

which is proven in Theorem 14 in appendix B. As a consequence of this and eq. (12), the left hand side of eq. (7) may be re-written as

$$\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c}\rangle_0 = E_{\mathbb{1}_S}[\mathbb{1}_{S^c}(X_1^\varepsilon))]\,, \tag{13}$$

provided that $\omega(S) = 1$, which can be assumed without loss of generality.

5.2.3. Probabilistic interpretation of heat content in the averaged setting

The steps above correspond to the left blue arrow in Fig. 1. The right blue arrow corresponds to repeating the same construction for the *averaged* equation $\partial_t \overline{u}_\varepsilon = \varepsilon \overline{\Delta}\,\overline{u}_\varepsilon$. Here, the PDE of $\overline{u}_\varepsilon$ is given in coordinates by

$$\partial_t \overline{u}_\varepsilon = \varepsilon \left(\sum_{i=1}^n \overline{b}_i \partial_i \overline{u}_\varepsilon + \frac{1}{2} \sum_{i,j=1}^n \overline{a}_{i,j} \partial_{ij} \overline{u}_\varepsilon \right),$$

[2] To see this, we first observe that the Markov property of SDEs [1, Thm. 9.2.3] yields a time-1 transition function p_ε satisfying $p_\varepsilon(x, A) = E_{x,0}[\mathbb{1}_A(X_1^\varepsilon)]$ for $x \in \mathbb{R}^n$ and measurable $A \subset \mathbb{R}^n$. The definition of the inner product $\langle\cdot,\cdot\rangle_0$ yields

$$\langle x \mapsto E_{0,x}[\mathbb{1}_A(X_1^\varepsilon))], h\rangle_0 = \int_{\mathbb{R}^n} p_\varepsilon(\cdot, A) h(\cdot)\,\omega = E_h[\mathbb{1}_A(X_1^\varepsilon)].$$

with $\overline{b}_i(x) = \int_0^1 b(t,x)\,\mathrm{d}t$ and $\overline{a}_{i,j}(x) = \int_0^1 a_{i,j}(t,x)\,\mathrm{d}t$. The associated stochastic process is defined by the SDE

$$\mathrm{d}\overline{X}_t^\varepsilon = \varepsilon\overline{b}(\overline{X}_t^\varepsilon)\,\mathrm{d}t + \sqrt{\varepsilon}\overline{\sigma}(\overline{X}_t^\varepsilon)\,\mathrm{d}W_t\,, \tag{14}$$

with $\overline{\sigma}\overline{\sigma}^\top = \overline{a}$. Given initial value $\overline{X}_0^\varepsilon = X_0$, we see that analogously to eq. (12),

$$\left\langle \overline{P}^\varepsilon u_0, h\right\rangle_0 = E_h[u_0(\overline{X}_1^\varepsilon)]$$

holds when $u_0 \in L^\infty(M,\omega)$ and $h\,\omega$ is a probability measure. Our aim is now to show that

$$E_{\mathbb{1}_S}[\mathbb{1}_{S^c}(X_1^\varepsilon)] = E_{\mathbb{1}_S}[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] + o(\sqrt{\varepsilon})\,, \quad \varepsilon \to 0\,, \tag{15}$$

corresponding to $h = \mathbb{1}_S$. In fact, we generalize to positive

$$h \in C_S^\infty(M) := \{f\mathbb{1}_S;\ f \in C^\infty(M)\}\,,$$

so that $h\,\omega$ is a probability measure, and will look at the quantity $E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)] = \langle P^\varepsilon \mathbb{1}_{S^c}, h\rangle_0$ with the aim of showing

$$E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)] = E_h[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] + o(\sqrt{\varepsilon})\,, \quad \varepsilon \to 0\,. \tag{16}$$

Writing $h = f\mathbb{1}_S$, we know from [28, 23], that

$$E_h[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] = \left\langle \overline{P}^\varepsilon \mathbb{1}_{S^c}, f\mathbb{1}_S\right\rangle_0 = \sqrt{\frac{\varepsilon}{\pi}}\int_{\partial S} f\,\mathrm{d}\overline{A} + o(\sqrt{\varepsilon})\,, \quad \varepsilon \to 0\,, \tag{17}$$

which yields the asymptotic behaviour of the right hand side of eq. (16). Our aim in the next steps will be to prove eq. (16).

5.2.4. Approximation of stochastic processes

We continue with the middle (green) arrows in Fig. 1, starting with the left one. Here, we will construct a family of stochastic processes $(Y_t^\varepsilon)_{t\in[0,1]}$ so that

$$E\left[|X_t^\varepsilon - Y_t^\varepsilon|^2\right] \le K\varepsilon^2 \tag{18}$$

for some $K > 0$ and all $t \in [0,1]$ for sufficiently small ε. In light of the arguments around eq. (16), we will use this approximation to show that:

Proposition 2. *If $(Y_t^\varepsilon)_{t\in[0,1]}$ satisfies eq. (18), then for $h \in C_S^\infty(M)$,*

$$E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)] = E_h[\mathbb{1}_{S^c}(Y_1^\varepsilon)] + o(\sqrt{\varepsilon}). \tag{19}$$

Analogously, corresponding to the the right hand side of Fig. 1, if the family of processes $(\overline{Y}_t^\varepsilon)_{t\in[0,1]}$ satisfies an inequality like eq. (18) but with $\overline{X}_t^\varepsilon$ in place of X_t^ε, then

$$E_h[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] = E_h[\mathbb{1}_{S^c}(\overline{Y}_1^\varepsilon)] + o(\sqrt{\varepsilon})\,. \tag{20}$$

The processes Y_1^ε and $\overline{Y}_1^\varepsilon$ will have the same law (this is the bottom arrow in Fig. 1), after we have proven this we may conclude that $E_h[\mathbb{1}_{S^c}(Y_1^\varepsilon)] = E_h[\mathbb{1}_{S^c}(\overline{Y}_1^\varepsilon)]$, which yields eq. (16), which together with eqs. (19) and (20) shows (here $h = \mathbb{1}_S f$), that

$$E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)] = E_h[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] + o(\sqrt{\varepsilon}) = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} f \, \mathrm{d}\overline{A} + o(\sqrt{\varepsilon}) \,.$$

Before proving Theorem 2, we will state a lemma needed in the proof. Let A be a (Borel) measurable subset of $\mathbb{R}^n$. We denote by $d(x, A) = \inf_{a \in A} |x - a|$ the Euclidean distance between a point $x \in \mathbb{R}^n$ and the set A. Let further $A_\delta \coloneqq \{x \in \mathbb{R}^n;\ d(x, \partial A) \leq \delta\}$ be the δ-neighborhood of the boundary of A.

Lemma 3. *Let $(\Omega, \mathcal{A}, \Pr)$ be some probability space and let $E[X]$ denote the expectation of some random variable X on Ω with respect to $\Pr$. For $\varepsilon \in [0, 1]$, let A^ε and B^ε be $(\mathbb{R}^n, \mathcal{B})$-valued random variables with $E[|A^\varepsilon - B^\varepsilon|^2] \leq C_0^2 \varepsilon^2$ for some $C_0 > 0$. Let $R \in \mathcal{B}$ and assume that $\Pr(A^\varepsilon \in R_\delta) \leq C_1 \delta$ for sufficiently small $\delta > 0$ and some $C_1 > 0$. Then,*

$$|E[\mathbb{1}_R(A^\varepsilon)] - E[\mathbb{1}_R(B^\varepsilon)]| = o(\sqrt{\varepsilon}) \quad \varepsilon \to 0.$$

Proof. The proof is given in appendix B, and is essentially an application of the Markov inequality. □

Proof of Theorem 2. We will apply Theorem 3 twice with $R = S^c$. For the first application, with $A^\varepsilon = X_1^\varepsilon$ (corresponding to eq. (19)), we will need to check that $\Pr[X_1^\varepsilon \in (S^c)_\delta] \leq C_1 \delta$ for some constant $C_1 > 0$. To see this is indeed the case, observe that $(S^c)_\delta = S_\delta$, and furthermore $\Pr(X_1^\varepsilon \in S_\delta) = E[\mathbb{1}_{S_\delta}(X_1^\varepsilon)]$. In the case that X_0 has law $f \mathbb{1}_S \, \omega$, this is equal to $E_{f\mathbb{1}_S}[\mathbb{1}_{S_\delta}(X_1^\varepsilon)]$. Thus, if X_0 has law $f \mathbb{1}_S \, \omega$ we have

$$\begin{aligned}
\Pr(X_1^\varepsilon \in (S^c)_\delta) &= \langle P^\varepsilon \mathbb{1}_{S_\delta}, f \rangle_0 \\
&\leq \|P^\varepsilon \mathbb{1}_{S_\delta}\|_{L^1(M,\omega)} \, \|f\|_\infty && \text{(by Hölder's inequality)} \\
&\leq \omega(S_\delta) \, \|f\|_\infty && \text{(by mass preservation of } P^\varepsilon) \\
&\leq C_1 \delta \,,
\end{aligned}$$

for some $C_1 > 0$, proving the claim. The proof required for the second application (with $A = \overline{X}_1$, i.e., eq. (20)) that $\Pr(\overline{X}_1^\varepsilon \in S_\delta) = O(\delta)$ proceeds along the same lines. □

5.2.5. Approximation by a Gaussian process

We now construct the processes required by Theorem 2 satisfying eq. (18). To this end, let $(Y_t^\varepsilon)_{t \in [0,1]}$ be defined by

$$\mathrm{d}Y_t^\varepsilon = \sqrt{\varepsilon} \sigma(1 - t, X_0) \, \mathrm{d}W_t \,, \qquad Y_0^\varepsilon = X_0 \,,$$

where X_0 is independent of the Wiener process and bounded. Likewise, let $(\overline{Y}_t^\varepsilon)_{t \in [0,1]}$ be defined by

$$\mathrm{d}\overline{Y}_t^\varepsilon = \sqrt{\varepsilon} \overline{\sigma}(X_0) \, \mathrm{d}W_t \,, \qquad \overline{Y}_0^\varepsilon = X_0 \,.$$

Proposition 4 ([3]). *Let $(X_t^\varepsilon)_{t\in[0,1]}$ be the stochastic process satisfying eq. (10). The process $(Y_t^\varepsilon)_{t\in[0,1]}$ approximates $(X_t^\varepsilon)_{t\in[0,1]}$ in the sense that*

$$E\left[|X_t^\varepsilon - Y_t^\varepsilon|^2\right] \leq K\varepsilon^2\,, \qquad \text{for all } t\in[0,1].$$

Similarly, let $(\overline{X}_t^\varepsilon)_{t\in[0,1]}$ by the solution of eq. (14), then $(\overline{Y}_t^\varepsilon)_{t\in[0,1]}$ approximates $(\overline{X}_t^\varepsilon)_{t\in[0,1]}$ in the sense that

$$E\left[\left|\overline{X}_t^\varepsilon - \overline{Y}_t^\varepsilon\right|^2\right] \leq K\varepsilon^2\,, \qquad \text{for all } t\in[0,1]\,.$$

In both cases, $K>0$ is a constant independent of ε and t.

Proof. This is a special case of the result in [3]. We have adapted the proof of this special case in appendix A. □

The processes $(Y_t^\varepsilon)_{t\in[0,1]}$ and $(\overline{Y}_t^\varepsilon)_{t\in[0,1]}$ may be thought of as being second-order approximations to the processes $(X_t^\varepsilon)_{t\in[0,1]}$ and $(\overline{X}_t^\varepsilon)_{t\in[0,1]}$ respectively. With Theorem 2, we conclude the following.

Proposition 5. *With $X_1^\varepsilon, Y_1^\varepsilon, \overline{X}_1^\varepsilon, \overline{Y}_1^\varepsilon$ as defined above and $h\in C_S^\infty(M)$,*

$$\begin{aligned}|E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)] - E_h[\mathbb{1}_{S^c}(Y_1^\varepsilon)]| &= o(\sqrt{\varepsilon})\,,\\ \left|E_h[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] - E_h[\mathbb{1}_{S^c}(\overline{Y}_1^\varepsilon)]\right| &= o(\sqrt{\varepsilon})\,.\end{aligned}$$

While these second-order approximations may differ pointwise, their laws are the same, this is the black arrow in Fig. 1 and the subject of the following lemma.

Lemma 6. *The random variables $Y_1^\varepsilon - X_0$ and $\overline{Y}_1^\varepsilon - X_0$ have the same law, namely that of $\sqrt{\varepsilon}\overline{\sigma}(X_0)W_1$.*

Proof. Recall that $\overline{a}(x) \coloneqq \int_0^1 a(t,x)\,\mathrm{d}t$, $\overline{b}(x)\coloneqq\int_0^1 b(t,x)\,\mathrm{d}t$, and $\overline{\sigma\sigma}^\top = \overline{a}$. As $Y_0 = X_0$, we see that $Y_1^\varepsilon - X_0 = \sqrt{\varepsilon}\int_0^1 \sigma(1-t, X_0)\,\mathrm{d}W_t$. If $X_0 = x$ then by [1, Cor. 4.5.6], the random variable $Y_1^\varepsilon - X_0$ is a normal random variable with zero mean and covariance matrix $\varepsilon\int_0^1 \sigma(t,x)\sigma(t,x)^\top\,\mathrm{d}s = \varepsilon\overline{a}(x)$, which is (by the same argument) also the law of $\overline{Y}^\varepsilon - X_0$. The random variable $\sqrt{\varepsilon}\overline{\sigma}(X_0)W_1$ is a normal random variable with the same mean and covariance matrix, proving the claim for constant X_0. The processes $(Y_t^\varepsilon)_{t\in[0,1]}$ and $(\overline{Y}_t^\varepsilon)_{t\in[0,1]}$ are not memoryless as the right hand side depends on the *initial* value of the process. This can be worked around by suitably augmenting the state space, the claim of the lemma for nonconstant X_0 follows by making use of the Markov property for SDEs in this augmented state space. □

Corollary 7. *For $h\in C_S^\infty(M)$, one has that*

$$E_h\left[\mathbb{1}_{S^c}(Y_1^\varepsilon)\right] = E_h\left[\mathbb{1}_{S^c}(\overline{Y}_1^\varepsilon)\right].$$

Proof. This is a direct result of Theorem 6. □

To summarize the reasoning so far: combining Theorem 7 with Theorem 5 yields for $h \in C_S^\infty(M)$, that

$$E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)] = E_h[\mathbb{1}_{S^c}(\overline{X}_1^\varepsilon)] + o(\sqrt{\varepsilon}), \quad \varepsilon \to 0.$$

We know that $\langle P^\varepsilon \mathbb{1}_{S^c}, h\rangle_0 = E_h[\mathbb{1}_{S^c}(X_1^\varepsilon)]$. Writing $h = \mathbb{1}_S f$, together with eq. (17), we may see that

$$\langle P^\varepsilon \mathbb{1}_{S^c}, h\rangle_0 = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} f \, \mathrm{d}\overline{A} + o(\sqrt{\varepsilon}), \quad \varepsilon \to 0. \tag{21}$$

With $f \equiv 1$, applying Theorem 14 completes the proof of Theorem 1 on $\mathbb{R}^n$ in the setting of Assumption A.

5.3. Step 2: Restriction to local data and geometry

In this section, we write $P^\varepsilon = P_1^\varepsilon$ and $\overline{P}^\varepsilon = \overline{P}_1^\varepsilon$.

5.3.1. Only local data is asymptotically important

Let U be a compact, full-dimensional submanifold of M with smooth boundary and with $S \subset \mathring{U}$. The inner product appearing on the left hand side of eq. (7) may be written as

$$\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c}\rangle_0 = \left\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{U\setminus S}\right\rangle_0 + \langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{U^c}\rangle .$$

We start by showing that discarding the second term yields an error of $o(\varepsilon)$.

Lemma 8. *Let either M be compact, or $M = \mathbb{R}^n$ (together with Assumption A) and S, U as above. Let $f \in L^\infty(M, \omega)$ with $\operatorname{supp}(f) \subset \mathring{U}$. Then*

$$|\langle P^\varepsilon f, \mathbb{1}_{U^c}\rangle_0| = o(\varepsilon), \quad \varepsilon \to 0.$$

Proof. Without loss of generality, assume $f \geq 0$. Pick some $h \in C_c^\infty(\mathring{M})$ with $f \leq h$ and $\operatorname{supp}(h) \subset \mathring{U}$. We compute:

$$\begin{aligned} 0 \leq \langle P^\varepsilon f, \mathbb{1}_{U^c}\rangle_0 &\leq \langle P^\varepsilon h, \mathbb{1}_{U^c}\rangle_0 \\ &= \langle P^\varepsilon h, \mathbb{1}_M\rangle_0 - \langle P^\varepsilon h, \mathbb{1}_U\rangle_0 . \end{aligned} \tag{22}$$

If M is compact we are already done at eq. (22), as by Theorem 13, $P^\varepsilon h = h + \varepsilon\overline{\Delta}h + O(\varepsilon^2)$ and $\mathbb{1}_{U^c} \in L^2(M, \omega)$. If $M = \mathbb{R}^n$, we observe that $\langle P^\varepsilon h, \mathbb{1}_M\rangle_0 = \langle h, \mathbb{1}_M\rangle_0 = \langle h, \mathbb{1}_U\rangle_0$. Using Theorem 13, $\langle P^\varepsilon h, \mathbb{1}_U\rangle_0 = \left\langle h + \varepsilon\overline{\Delta}h + o(\varepsilon), \mathbb{1}_U\right\rangle_0$. Given that h is compactly supported in the interior of U, the term $\left\langle \varepsilon\overline{\Delta}h, \mathbb{1}_U\right\rangle_0$ vanishes by the divergence theorem. We conclude that $\langle P^\varepsilon h, \mathbb{1}_U\rangle_0 = \langle h, \mathbb{1}_U\rangle_0 + o(\varepsilon)$ which yields the claim. □

5.3.2. Only local geometry is asymptotically important

Similarly, only local geometry affects the asymptotic behaviour of $\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c}\rangle_0$.

Lemma 9. *Let M be either compact (with homogeneous Neumann or Dirichlet boundary conditions) or equal to $\mathbb{R}^n$ (together with Assumption A). Let $U \subset M$ be a compact, full-dimensional submanifold. Let $f \in L^\infty(M,\omega)$ with $\operatorname{supp}(f) \subset \mathring{U}$. Let $\tilde{P}^\varepsilon$ be defined the same way as P^ε via eq. (4) but on U with homogeneous Dirichlet boundary, i.e., $\tilde{P}^\varepsilon_t$ is the time-t solution operator to the time-dependent diffusion problem eq. (4) on U with Dirichlet boundary, and $\tilde{P}^\varepsilon := \tilde{P}^\varepsilon_1$. Then,*

$$\left\|(P^\varepsilon - \tilde{P}^\varepsilon)f\right\|_{L^\infty(U)} = o(\varepsilon)\,, \quad \varepsilon \to 0\,.$$

Proof. Let $e_\varepsilon(t) = (P^\varepsilon_t - \tilde{P}^\varepsilon_t)h$ for a generic positive $h \in C^\infty_c(\mathring{U})$. The function $e_\varepsilon(t)$ satisfies the time-dependent heat equation $\partial_t e_\varepsilon = \varepsilon \Delta_t e_\varepsilon$ on U, with nonhomogeneous Dirichlet boundary $e_\varepsilon\big|_{\partial_U} = P^\varepsilon_t h\big|_{\partial U} \geq 0$. By construction (and reasoning like the following is well known in the literature, cf. [12]), $e_\varepsilon(0,\cdot) = 0$, and the weak maximum principle [18, Thm. A.3.1] applied to $-e_\varepsilon(t)$ yields that on U and $t \in [0,1]$,

$$(P^\varepsilon_t - \tilde{P}^\varepsilon_t)h \geq 0\,. \tag{23}$$

By a continuity argument, eq. (23) extends to positive $h \in L^\infty(M,\omega)$ with $\operatorname{supp}(h) \subset U$, including f. Going back to the case of a smooth h, we may pick h so that $h \geq f$, and for this particular choice we get

$$0 \leq (P^\varepsilon_t - \tilde{P}^\varepsilon_t)f \leq (P^\varepsilon_t - \tilde{P}^\varepsilon_t)h = e_\varepsilon(t)\,,$$

where both inequalities are a consequence of eq. (23). We conclude for e_ε, once more with the maximum principle, that

$$0 \leq \|e_\varepsilon\|_{L^\infty([0,1]\times U)} \leq \|P^\varepsilon_t h\|_{L^\infty([0,1]\times \partial U)}\,. \tag{24}$$

With Theorem 13, we see that $\left\|P^\varepsilon_t h - \tilde{h}^\varepsilon\right\|_{L^\infty([0,1]\times M)} = o(\varepsilon)$, where $\tilde{h}^\varepsilon(t,\cdot) := h + \varepsilon \int_0^t \Delta_s h \,\mathrm{d}s$. In particular, this L^∞ bound holds also on $[0,1]\times\partial U$ as required in eq. (24) (by construction, $\tilde{u}^\varepsilon$ vanishes on ∂U). This shows that $\|e_\varepsilon\|_{L^\infty([0,1]\times U)} = o(\varepsilon)$, proving the lemma. □

5.3.3. Remaining steps

The statement of Theorem 1 is thus reduced to one about

$$\langle \mathbb{1}_S, P^\varepsilon \mathbb{1}_{S^c}\rangle_0\,,$$

regardless of what manifold P^ε is defined on, as long as this manifold is isometric to the original one on a neighborhood of S. By taking a smooth partition of unity $(f_i)_{i=1}^N$ so

that $\sum_{i=1}^N f_i = 1$ on S and each f_i is supported in a single coordinate chart it is (by linearity) enough to prove that

$$\langle f_i \mathbb{1}_S, P^\varepsilon \mathbb{1}_{S^c} \rangle_0 = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} f_i \, \mathrm{d}\overline{A} + o(\sqrt{\varepsilon}) \,,$$

for each $i = 1, \ldots, N$. As each f_i is supported in a single coordinate chart, we may pick a local isometry into $\mathbb{R}^n$ and prove the expression there. This is precisely the end result of what was proven in step 1, i.e., eq. (21), so we are done.

A. Approximation of stochastic processes

Let $(\Omega, \mathcal{F}, \Pr)$ be a probability space supporting a classical Wiener process $W_t \colon \Omega \to \mathbb{R}^n$ for $t \in [0,1]$. Let $b \colon [0,1] \times \mathbb{R}^n \to \mathbb{R}^n$ and $\sigma \colon [0,1] \times \mathbb{R}^n \to \mathbb{R}^{n \times n}$ be measurable functions. Consider the stochastic initial value problem

$$\mathrm{d}X_t^\varepsilon = \varepsilon b(t, X_t^\varepsilon) \, \mathrm{d}t + \sqrt{\varepsilon} \sigma(t, X_t^\varepsilon) \, \mathrm{d}W_t \,, \qquad X_0^\varepsilon = X_0 \,, \tag{25}$$

with initial value $X_0 \in L^2(\Pr)$. If there is $K > 0$ such that

$$|b(t,X) - b(t,Y)| + |\sigma(t,X) - \sigma(t,Y)| \leq K \, |X - Y| \,,$$

and

$$|b(t,X)| + |\sigma(t,X)| \leq K \sqrt{1 + |X|^2} \,,$$

for all $t \in [0,1]$, then the initial value problem eq. (25) has a Pr-almost surely unique continuous solution [1, Theorem (6.2.2)].

The following result is a special case of [3], we follow the proof there and track the dependence of constants involved on other values more explicitly. The precise value of C, however, may change from line to line.

Theorem 10. *Let X_t^ε be the unique solution of eq. (25) and Y_t^ε the unique solution of the stochastic initial value problem*

$$\mathrm{d}Y_t^\varepsilon = \sqrt{\varepsilon} \sigma(t, X_0) \, \mathrm{d}W_t \,, \qquad Y_0^\varepsilon = X_0 \,.$$

Then there exists $C > 0$ such that for $\varepsilon \leq 1$:

$$E\left[\sup_{0 \leq t \leq 1} |X_t^\varepsilon - Y_t^\varepsilon|^2 \right] \leq C \varepsilon^2 \,. \tag{26}$$

Proof. For $t \in [0,1]$, let

$$\gamma(t,\varepsilon) \coloneqq \frac{X_t^\varepsilon - Y_t^\varepsilon}{\varepsilon} \,, \qquad \psi(t,\varepsilon) \coloneqq E\left(\sup_{0 \leq s \leq t} |\gamma(s,\varepsilon)|^2 \right) .$$

In order to prove eq. (26), it must be shown that that $\psi(1,\varepsilon) \leq C$. By the definition of γ,

$$\varepsilon\gamma(t,\varepsilon) = \underbrace{\varepsilon \int_0^t b(s, X_s^\varepsilon)\ \mathrm{d}s}_{:=a_1(t,\varepsilon)} + \underbrace{\sqrt{\varepsilon} \int_0^t \sigma(s, X_s^\varepsilon) - \sigma(s, X_0)\ \mathrm{d}W_s}_{:=a_2(t,\varepsilon)},$$

and furthermore

$$\begin{aligned} a_1(t,\varepsilon) &= \varepsilon \left(\int_0^t b(s, X_s^\varepsilon) - b(s, Y_s^\varepsilon)\ \mathrm{d}s + \int_0^t b(s, Y_s^\varepsilon)\ \mathrm{d}s \right), \\ |a_1(t,\varepsilon)| &\leq \varepsilon K \left(\int_0^t \varepsilon\, |\gamma(s,\varepsilon)|\ \mathrm{d}s + \int_0^t \sqrt{1 + |Y_s^\varepsilon|^2}\ \mathrm{d}s \right). \end{aligned}$$

Now, as $t \leq 1$, Jensen's inequality (and $(a+b)^2 \leq 2(a^2+b^2)$ twice) yields

$$\begin{aligned} |a_1(t,\varepsilon)|^2 &\leq 2\varepsilon^2 K^2 \left(\varepsilon^2 \left(\int_0^t |\gamma(s,\varepsilon)|\, \mathrm{d}s \right)^2 + \left(\int_0^t \sqrt{1 + |Y_s^\varepsilon|^2}\ \mathrm{d}s \right)^2 \right) \\ &\leq 2\varepsilon^2 K^2 \left(\varepsilon^2 \int_0^t |\gamma(s,\varepsilon)|^2\ \mathrm{d}s + 1 + 2\,|X_0|^2 + 2\varepsilon \int_0^t \left| \frac{Y_s^\varepsilon - X_0}{\sqrt{\varepsilon}} \right|^2 \mathrm{d}s \right). \end{aligned}$$

By monotonicity of the Lebesgue integral,

$$\begin{aligned} \sup_{0\leq s\leq t} |a_1(s,\varepsilon)|^2 \leq 4\varepsilon^2 K^2 \Bigg(\varepsilon^2 \int_0^t \sup_{0\leq u\leq s} |\gamma(u,\varepsilon)|^2\ \mathrm{d}s + 1 + \\ + |X_0|^2 + \varepsilon \int_0^t \sup_{0\leq u\leq s} \left| \frac{Y_u^\varepsilon - X_0}{\sqrt{\varepsilon}} \right|^2 \mathrm{d}s \Bigg). \end{aligned}$$

Consequently,

$$\begin{aligned} E\left(\sup_{0\leq s\leq t} |a_1(s,\varepsilon)|^2 \right) \leq 4K^2\varepsilon^2 \Bigg(\varepsilon^2 \int_0^t \psi(s,\varepsilon)\ \mathrm{d}s + 1 + \\ + E(|X_0|^2) + \varepsilon E\left(\int_0^t \sup_{0\leq u\leq s} \left| \frac{Y_u^\varepsilon - X_0}{\sqrt{\varepsilon}} \right|^2 \mathrm{d}s \right) \Bigg). \quad (27) \end{aligned}$$

To deal with the a_2 term, we use the Itô isometry:

$$\begin{aligned}
E(|a_2(t,\varepsilon)|^2) &= \varepsilon \int_0^t E\left(|\sigma(s, X_s^\varepsilon) - \sigma(s, X_0)|^2\right) \mathrm{d}s \\
&\leq \varepsilon \int_0^t K^2 E\left(|X_s^\varepsilon - X_0|^2\right) \mathrm{d}s \\
&\leq K^2 \varepsilon \int_0^t E\left(|Y_s^\varepsilon - X_0 + \varepsilon\gamma(s,\varepsilon)|^2\right) \mathrm{d}s \\
&\leq K^2 \varepsilon^2 \int_0^t E\left(\left|\frac{Y_s^\varepsilon - X_0}{\sqrt{\varepsilon}} + \sqrt{\varepsilon}\gamma(s,\varepsilon)\right|^2\right) \mathrm{d}s \\
&\leq 2K^2\varepsilon^2 \left(\int_0^t E\left(\left|\frac{Y_s^\varepsilon - X_0}{\sqrt{\varepsilon}}\right|^2\right) \mathrm{d}s + \varepsilon \int_0^t E(|\gamma(s,\varepsilon)|^2)\, \mathrm{d}s\right) \\
&\leq 2K^2\varepsilon^2 \left(\int_0^t E\left(\left|\frac{Y_s^\varepsilon - X_0}{\sqrt{\varepsilon}}\right|^2\right) \mathrm{d}s + \varepsilon \int_0^t \psi(s,\varepsilon)\ \mathrm{d}s\right).
\end{aligned}$$

As $a_2(t,\varepsilon)$ is a martingale, Doob's maximal inequality for $p = 2$ shows that

$$\begin{aligned}
E\left(\sup_{0\leq s\leq t} |a_2(s,\varepsilon)|^2\right) &\leq 4E(|a_2(t,\varepsilon)|^2) \\
&\leq 8K^2\varepsilon^2 \left(\int_0^t E\left(\left|\frac{Y_s^\varepsilon - X_0}{\sqrt{\varepsilon}}\right|^2\right) \mathrm{d}s + \varepsilon \int_0^t \psi(s,\varepsilon)\ \mathrm{d}s\right). \qquad (28)
\end{aligned}$$

Let $Z_t^\varepsilon = \frac{Y_t^\varepsilon - X_0}{\sqrt{\varepsilon}}$. One may readily verify that Z_t^ε satisfies

$$Z_t^\varepsilon = \int_0^t \sigma(t, X_0)\ \mathrm{d}W_t\,,$$

and hence in particular Z_t^ε does not depend on ε, so we may write Z_t without the superscript ε. Moreover, Z_t is an L^2-martingale. Thus, Doob's inequality ensures that $K_1 := 4E[Z_1^2]$ satisfies $E\left(\sup_{0\leq t\leq 1} |Z_t|^2\right) \leq K_1$. Combining eq. (27) with eq. (28) and $(a+b)^2 \leq 2(a^2+b^2)$, we obtain

$$\begin{aligned}
\varepsilon^2\psi(t,\varepsilon) &\leq 8K^2\varepsilon^2 \left(\varepsilon^2 \int_0^t \psi(s,\varepsilon)\ \mathrm{d}s + 1 + E(|X_0|^2) + \varepsilon E\left(\int_0^t \sup_{0\leq u\leq s} |Z_u|^2\ \mathrm{d}s\right)\right) \\
&\qquad + 16K^2\varepsilon^2 \left(\int_0^t E(|Z_t|^2)\ \mathrm{d}s + \varepsilon \int_0^t \psi(s,\varepsilon)\ \mathrm{d}s\right) \\
&\leq 16K^2\varepsilon^2 \left((\varepsilon+\varepsilon^2) \int_0^t \psi(s,\varepsilon)\ \mathrm{d}s + 1 + E(|X_0|^2) + (1+\varepsilon) \int_0^t E(\sup_{0\leq u\leq s} |Z_u|^2)\right).
\end{aligned}$$

Writing $E(|X_0|^2) = K_2 < \infty$ we see that for suitable $D > 0$,

$$\psi(t,\varepsilon) \leq D \int_0^t \psi(s,\varepsilon)\, \mathrm{d}s + 1 + 2K_1 + K_2\,,$$

assuming $\varepsilon \leq 1$. Grönwall's lemma[3], yields that $\psi(1,\varepsilon)$ is uniformly bounded, proving the claim. □

B. Miscellaneous proofs

Lemma 11. *Let $(\Omega, \mathcal{A}, \Pr)$ be some probability space and let $E[X]$ denote the expectation of some random variable X on Ω. For $\varepsilon \in [0,1]$, let A^ε and B^ε be $(\mathbb{R}^n, \mathcal{B})$-valued random variables with $E\left[|A^\varepsilon - B^\varepsilon|^2\right] \leq C_0^2\varepsilon^2$ for some $C_0 > 0$. Let $R \in \mathcal{B}$ and assume that $\Pr(A^\varepsilon \in R^\delta) \leq C_1\delta$ for sufficiently small $\delta > 0$ and some $C_1 > 0$. Then:*

$$|E[\mathbb{1}_R(A^\varepsilon)] - E[\mathbb{1}_R(B^\varepsilon)]| = o(\sqrt{\varepsilon}), \quad \varepsilon \to 0.$$

Proof. Note that for $\omega \in \Omega$, the condition

$$(A^\varepsilon(\omega) \in R \text{ and } B^\varepsilon(\omega) \in R) \text{ or } (A^\varepsilon(\omega) \notin R \text{ and } B^\varepsilon(\omega) \notin R)$$

implies $\mathbb{1}_R(A^\varepsilon(\omega)) = \mathbb{1}_R(B^\varepsilon(\omega))$. We thus may see that for any $\delta > 0$

$$\begin{aligned}
|E[\mathbb{1}_R(A^\varepsilon)] - E[\mathbb{1}_R(B^\varepsilon)]| &\leq \Pr(A^\varepsilon \in R \,\text{and}\, B^\varepsilon \notin R) \\
&\quad + \Pr(A^\varepsilon \notin R \,\text{and}\, B^\varepsilon \in R) \\
&\leq 2\Pr(A^\varepsilon \in R^\delta \text{ or } |A^\varepsilon - B^\varepsilon| \geq \delta) \\
&\leq 2\left(\Pr(A^\varepsilon \in R^\delta) + \Pr(|A^\varepsilon - B^\varepsilon| \geq \delta)\right).
\end{aligned}$$

Now note that by the Markov inequality

$$\Pr(|A^\varepsilon - B^\varepsilon| \geq \delta) \leq \frac{E\left[|A^\varepsilon - B^\varepsilon|^2\right]}{\delta^2} \leq \frac{C_0^2\varepsilon^2}{\delta^2}.$$

By assumption, we therefore get for sufficiently small δ that

$$|E(\mathbb{1}_R(A^\varepsilon) - E(\mathbb{1}_R(B^\varepsilon)))| \leq 2\left(C_1\delta + C_0^2\varepsilon^2/\delta^2\right).$$

Choosing $\delta = \varepsilon^{0.6}$ makes the first term $o(\sqrt{\varepsilon})$. The second term is then proportional to $\varepsilon^2/\delta^2 = \varepsilon^{0.8} = o(\sqrt{\varepsilon})$, which proves the claim. □

C. Parabolic PDEs

We collect here some useful technical facts about parabolic PDE of the form

$$\partial_t u = \varepsilon\Delta_t u, \quad u(0,\cdot) = u_0(\cdot), \tag{29}$$

[3]Observe that $t \mapsto \psi(t,\varepsilon)$ is monotone (and hence measurable) and finite (cf. [8, Ch. 5, Cor. 1.2]). By the monotone convergence theorem, if $t_n \to t$ from below, then $\psi(t_n,\varepsilon) \to \psi(t,\varepsilon)$. In particular, the almost-everywhere (in t) bound from the integral form of Grönwall's lemma (see [6, app B.2]) holds everywhere.

where $\Delta_t u := \operatorname{div}_\omega g_t^{-1}\, \mathrm{d}u$ is a Laplace-like operator on a manifold M for every $t \in [0,1]$, and $(g_t)_{t\in[0,1]}$ is a smoothly varying nonvanishing family of Riemannian metrics. We write P_t^ε for the time-t solution operator, i.e., $u(\cdot,t) = P_t^\varepsilon u_0$. In the case that M is a compact Riemannian manifold (possibly with Dirichlet boundary), we have summarized some well-known existence and uniqueness results for $u_0 \in L^2(M,\omega)$ in Appendix D of [20]. If $M = \mathbb{R}^n$, we use in this document the assumption (Assumption A) that there exists a bounded set B (containing S in its interior) so that both g_t and ω are equal to the Euclidean metric and its volume form respectively outside of B for all $t \in [0,1]$. Under this restriction, it is well-known that the time-t solution operator P_t^ε is well-defined for $u_0 \in C_b(\mathbb{R}^n)$, and a maximum principle for initial values in $C_0(\mathbb{R}^n)$ (continuous functions vanishing on infinity) holds. The solution $u_\varepsilon(t,x) := P_t^\varepsilon u_0$ satisfies eq. (29) everywhere on $(0,1]\times\mathbb{R}^n$ if u_0 has compact support. Moreover, P_t^ε is of the form $(P_t^\varepsilon u_0)(x) = \int_{\mathbb{R}^n} p_\varepsilon(0,x,t,y)u_0(y)\,\omega$. We have here taken the somewhat unconventional step of using ω instead of the Lebesgue measure for the definition of the fundamental solution as this is the natural measure for problems like eq. (29), recall that ω is equivalent to the n-dimensional Lebesgue measure ℓ^n under Assumption A . As a reference for these statements, see for instance [8, Ch. 3–4], [25, Ch. 3] and [24].

Remark 12. The measure $p_\varepsilon(0,x,t,\cdot)\,\omega$ is a probability measure, so we may extend P_t^ε to act on $u_0 \in L^\infty(\mathbb{R}^n)$. Moreoever, if $u_n \uparrow u$ pointwise everywhere for a sequence of functions $u_n \in L^\infty(\mathbb{R}^n)$, then the monotone convergence theorem yields that $P_t^\varepsilon u_n \uparrow P^\varepsilon u$.

For positive initial data, the time-dependent heat equation preserves the integral with respect to ω. This may be seen by adapting the proof of [8, Sec. 6, Thm. 4.7], but using the $L^2(\mathbb{R}^n,\omega)$ adjoint (as opposed to the $L^2(\mathbb{R}^n,\mathrm{d}\ell^d)$ adjoint considered there) of $\mathcal{M} := \varepsilon\Delta_t - \partial_t$ which is given by $\mathcal{M}^* = \varepsilon\Delta_t + \partial_t$. The fundamental solution for $\mathcal{M}^*$ (adapted to ω instead of the Lebesgue measure as before), denoted by $p^*(x,t,y,\tau)$ satisfies $\mathcal{M}^* p^*(\cdot,\cdot,y,\tau) = 0$ and (by mirroring the aformentioned proof) also $p^*(x,t,y,\tau) = p(y,\tau,x,t)$. As a consequence,

$$\begin{aligned}
\int (P_t^\varepsilon u_0)(x,t)\,\omega(x) &= \int\int p(x,t,y,0)u_0(y)\,\omega(y)\,\omega(x)\\
&= \int\int p^*(y,0,x,t)u_0(y)\,\omega(y)\,\omega(x)\\
&= \int\int p^*(y,0,x,t)\,\omega(x)u_0(y)\,\omega(y)\\
&= \int u_0\,\omega\,,
\end{aligned}$$

as $p^*(y,0,\cdot,t)\,\omega$ is a probability measure. Of course, all of the arguments above may also be applied to $\overline{P}^\varepsilon$. In addition, here it is known that $\overline{\Delta}$ generates an analytic semigroup on $L^p(\mathbb{R}^n)$ for $p \in [1,\infty)$ [26, Sect. 5.4, Thm. 5.6], and on $C^0(\mathbb{R}^n)$ [24].

We will make use of the following approximation result.

Proposition 13 ([21, 20]). *If M is compact (possibly with smooth homogeneous Dirichlet/Neumann boundary) and $u_0 \in C_c^\infty(\mathring{M})$ then*

$$(P_t^\varepsilon u_0)(x) = u_0 + \varepsilon \int_0^t \Delta_\tau u_0(x)\ \mathrm{d}\tau + O(\varepsilon^2)$$

uniformly in $(t, x) \in [0, 1] \times M$ as $\varepsilon \to 0$.

By adapting the proof in [20], this result can be extended to the case that $M = \mathbb{R}^n$ assuming that the boundedness condition mentioned earlier holds. In fact, the case $M = \mathbb{R}^n$ is close to the original setting of [21] on which the proof in [20] is based.

We conclude with the following useful property of P_1^ε.

Lemma 14. *Let $S \subset \mathbb{R}^n$ be compact and measurable. Then*

$$\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c} \rangle_0 = \langle \mathbb{1}_S, P^\varepsilon \mathbb{1}_{S^c} \rangle_0 \ .$$

Note that P_1^ε is generally not self-adjoint.

Proof. Using the properties of P_1^ε mentioned above, we compute

$$\begin{aligned}
\langle P^\varepsilon \mathbb{1}_S, \mathbb{1}_{S^c} \rangle_0 &= \langle (P^\varepsilon(\mathbb{1}_{\mathbb{R}^n} - \mathbb{1}_{S^c}))(\mathbb{1}_{\mathbb{R}^n} - \mathbb{1}_S), \mathbb{1}_{\mathbb{R}^n} \rangle_0 \\
&= \langle (P^\varepsilon \mathbb{1}_{S^c})\mathbb{1}_S + (\mathbb{1}_{\mathbb{R}^n} - P^\varepsilon \mathbb{1}_{S^c} - \mathbb{1}_S), \mathbb{1}_{\mathbb{R}^n} \rangle_0 \\
&= \langle (P^\varepsilon \mathbb{1}_{S^c})\mathbb{1}_S + (P^\varepsilon \mathbb{1}_S - \mathbb{1}_S), \mathbb{1}_{\mathbb{R}^n} \rangle_0 \\
&= \langle P^\varepsilon \mathbb{1}_{S^c}, \mathbb{1}_S \rangle_0 + 0 \,.
\end{aligned}$$

□

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