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Bock, Andreas; Cotter, Colin J.; Kirby, Robert C.

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Planar curve registration using Bayesian inversion



(1)

Andreas Bock^{a,*}, Colin J. Cotter^b, Robert C. Kirby^c

^a Department of Applied Mathematics and Computer Science, Technical University of Denmark, Richard Petersens Plads, Building 324, Kongens Lyngby, 2800, Denmark

^b Department of Mathematics, Imperial College London, 180 Queen's Gate, South Kensington, London, SW72RH, United Kingdom

^c Department of Mathematics, Baylor University, 1410 S.4th Street, Sid Richardson Science Building, Waco, 76706, TX, United States of America

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ABSTRACT

Keywords: Closed curve matching Nonconforming finite element method Bayesian inverse problem We study parameterisation-independent closed planar curve matching as a Bayesian inverse problem. The motion of the curve is modelled via a curve on the diffeomorphism group acting on the ambient space, leading to a *large deformation diffeomorphic metric mapping* (LDDMM) functional penalising the kinetic energy of the deformation. We solve Hamilton's equations for the curve matching problem using the Wu-Xu element (Wu and Xu (2019) [12]) which provides mesh-independent Lipschitz constants for the forward motion of the curve, and solve the inverse problem for the momentum using Bayesian inversion. Since this element is not affine-equivalent we provide a *pullback theory* which expedites the implementation and efficiency of the forward map. We adopt ensemble Kalman inversion (EKI) using a negative Sobolev norm mismatch penalty to measure the discrepancy between the target and the ensemble mean shape. We provide several numerical examples to validate the approach.

1. Introduction

Closed curve matching is a central problem in shape analysis where the goal is to bring into alignment two closed curves in $\text{Emb}(S^1, \mathbb{R}^d)$ called the *template* and the *target* [1]. This has numerous practical applications in biology [2] and medical image analysis [3] as *shape changes* can model disease progression or lead to an understanding of the variability of the data [4]. Other examples of applications include nuclear analysis, see e.g. [5] where the variation of HeLA cells was studied, and archaeology, where shape analysis has been used for artifact classification [6]. As the resolution of the data captured in all fields of science continues to increase there is a demand for novel scalable methods to be developed for continuous shape matching. Curve shapes are invariant under arbitrary reparameterisation, so in this paper we consider unparameterised planar curves. The shape space for these objects is $Q = \text{Emb}(S^1, \mathbb{R}^d) \setminus \text{Diff}_+(S^1)$ [7,8]. This quotient space disassociates the curve from arbitrary reparameterisation since they do not affect the range of the curves in question. This gives rise to studying the commuting left and right actions of two Lie groups, $G = \text{Diff}_+(\mathbb{R}^2)$ and $H = \text{Diff}_+(S^1)$ as in [9]:

$$GQ = \operatorname{Emb}(S^1, G.\mathbb{R}^2), \qquad HQ = \operatorname{Emb}(H.S^1, \mathbb{R}^2).$$

In the context of developing algorithms for planar curve matching, these group actions must be explicitly discretised. In this paper we equip our shape space with the so-called *outer* metric inherited by *G* which acts on the ambient space. This is in contrast to inner metrics intrinsically defined on the embedded shape [10], see [7] for a comparison. To treat the parameterisation, one can parameterise elements of *H* using its Lie algebra and exploit its vector space structure. In this paper we consider a mismatch penalty that eliminates the need to treat *H* explicitly. We note that two closed curves c_1 and c_2 are similar when the difference between the indicator function $\mathbb{1}$ evaluated on their interiors is small. For some linear differential operator *C* we therefore define the mismatch, or *misfit*, between them as:

$$\mathfrak{G}(c_1, c_2) = \|\mathbb{1}_{c_1} - \mathbb{1}_{c_2}\|_C^2, \tag{2}$$

* Corresponding author.

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E-mail addresses: aasbo@dtu.dk (A. Bock), colin.cotter@imperial.ac.uk (C.J. Cotter), robert_kirby@baylor.edu (R.C. Kirby).

where $||f||_{C}^{2} = \langle C^{-1}f, C^{-1}f \rangle_{L^{2}}$ over some computational domain described later. For the outer metric we take the LDDMM approach [11] and consider a one-parameter family of velocities $t \mapsto u_{t}$ encoding the motion of the ambient space (and therefore the shape) which simultaneously provides a distance measure. We discretise the velocity field using finite elements, specifically the Wu-Xu element [12]. This element provides a nonconforming discretisation for sixth order operators; sixth order is necessary for the diffeomorphism to be sufficiently smooth for the computations that we undertake. The implementation of this element in Firedrake [13] is made possible by applying the theory of [14] and techniques for code generation in [15]. Given certain assumptions on the structure of our problem we can identify this entire family of velocities with a single initial momentum defined as a function over the template. We eliminate its evolution equation by using the analytical solution, and restrict the initial conditions to only generate geodesics in the space of unparameterised curves. This results in a *forward map*, taking as input the initial momentum and providing the diffeomorphism whose action maps the template to the target curve. While adjoint-based methods are popular in variational problems such as the one treated here, the implementation of the Fréchet derivative of the forward map may be difficult if a degree of automation is not available. Instead, we approach the matching problem as a Bayesian inverse problem to apply ensemble Kalman inversion (EKI) [16,17] and invert the forward map for the initial momentum determining the geodesic motion of the curve aligning the template with the target. The aim here is a method which is highly scalable and parallelisable.

We summarise our main contributions in this paper. We provide a formulation of curve matching using an outer metric based on the Lipschitzconforming Wu-Xu element which preserves the diffeomorphic evolution of the curve at any level of mesh refinement. In addition, the formulation removes the need to integrate the momentum equation which otherwise requires additional regularity of the velocity field. In order to carry out the computations efficiently we also provide a pull-back theory for the Wu-Xu element which has not been explored before in the literature. The resulting forward map is mesh-based which easily facilitates parallel computation, a feature that is particularly valuable as forward solves are typically expensive to compute. Not only is our proposed method derivative-free, it is also based on EKI, which is trivially parallelisable. While the use of EKI in shape analysis has been studied before for landmarks [18] (but not curves), this is to the authors' knowledge the first approach allowing a high degree of parallelisation in both the forward map and the inversion method. Since we discretise an outer metric the proposed method is scalable for other types of data allowing for e.g. truly large-scale parallel image LDDMM.

1.1. Previous work

Diffeomorphic registration has enjoyed a rich literature since the seminal works [19,20]. For curves specifically, [21,22] present the first algorithms for modelling curve matching via gradient descent methods. [11] represents curves as measures onto which a Hilbert structure is endowed, and computations of both the outer metric and the curves are done via radial reproducing kernels producing C^{∞} velocities. In particular, curves were represented as geometric currents. [23] studies such a varifold-based loss function for elastic metrics, see also [24–26] for numerical frameworks for H^2 metrics. [27] contains a review of methods related to elastic curves.

In this paper we are concerned with higher-order metrics using finite elements. While there is typically a loss of regularity incurred by these methods, they can offer more computationally efficient methods than e.g. kernel methods. Finite elements also benefit from spatial adaptivity allowing for local refinement e.g. close to embedded curves. Closest to our approach in terms of discretisation are [28,29] where a *particle-mesh* method is employed for curve matching where the curve was discretised into a finite set of particles, acted on by an outer metric. However, we consider instead an outer metric *finite element* discretisation (as opposed to the intrinsic metric in [10]). [30] presents an adaptive Eulerian FEM discretisation of the velocity field for LDDMM using C^1 cubic Hermite elements and compares the deformations generated using C^{∞} fields to assess the effect of the loss of regularity. Smooth mesh deformations are also of interest in shape optimisation where the aim is to transform a mesh such that some functional is minimised. Finite element methods are also adopted here, with deformation fields being discretised using B-splines [31], harmonic polynomials or Lagrange finite elements depending the desired resolution or order [32]. Using the finite element space introduced in [12] we can guarantee that the Lipschitz norm remains bounded under mesh refinement without resorting to spline or kernel discretisations. As mentioned, we use Firedrake [13] for all our numerical experiments, see also [33] for an extension of this package for shape optimisation.

Our formulation eliminates the need to integrate the momentum equation via its analytical solution thereby improving on the typically larger cost of Hamiltonian shooting based methods [34] compared to an LDDMM formulation [11]. We only need to solve an elliptic equation to obtain the velocity and use a simple variational Euler scheme to evolve the diffeomorphism. Traditional approaches in numerical shape analysis often apply shooting procedures to determine the initial momentum transporting the image or landmarks to the desiderata, see e.g. [35,36]. Bayesian approaches have been employed before in the context of shape analysis, see e.g. [37] where function space Markov Chain Monte Carlo is used to characterise the posterior density of momenta generating a given shape. Similar to our approach is [18] in which EKI is applied to recover the momentum for landmark matching.

1.2. Organisation

Section 2 contains an introduction to diffeomorphic curve matching and the associated Hamiltonian systems, we also discuss the application of the finite element approach using the Wu-Xu element from [12] and the discretisation of the velocity equation. Section 3 contains the transformation theory for the Wu-Xu element, and Section 4 contains details of the discretisation of the Hamiltonian equations. Next, Section 5 discusses the Bayesian inverse problem, and Section 6 contains numerical results. Section 7 contains a summary.

2. Diffeomorphic registration

Let Ω be a convex subset of \mathbb{R}^d , d = 2, with polygonal boundary $\partial \Omega$. We study maps $q \in Q = H^1(S^1, \mathbb{R}^d)$ from a template curve $\Gamma_0 \in \text{Emb}(S^1, \Omega)$ to a target curve $\Gamma_1 \in \text{Emb}(S^1, \Omega)$ whose motion is restricted by the differential equation:

$$\dot{q}_t = u_t \circ q_t \,, \tag{3}$$

where u_i , $t \in [0,1]$ is a family of time-dependent vector fields on Ω with some prescribed spatial smoothness. A *geodesic path* between two such parameterised curves Γ_0 and Γ_1 is defined as a path minimising the associated kinetic energy in u:

$$\frac{1}{2}\int_{0}^{1}\|u_{t}\|^{2} dt,$$
(4)

where $\|\cdot\|$ dominates the Lipschitz norm. In fact, since u_t is supported on Ω it generates a curve on Diff(Ω) [1] of the entire ambient space via:

$$\dot{\varphi}_t = u_t \circ \varphi_t, \quad \varphi_0 = \mathbf{id}, \tag{5}$$

whose motion restricted to the curve $q_0 \circ S^1$ equals the $q_t \circ S^1$ at time $t \in [0, 1]$. As the kinetic energy measures distances between two elements of $\text{Emb}(S^1, \mathbb{R}^d)$ via velocity defined over the entire field Ω , we refer to this associated distance measure as an *outer* metric on the shape space $\operatorname{Emb}(S^1, \mathbb{R}^d).$

2.1. Hamiltonian system

Here we take a Hamiltonian approach [38] and introduce the momentum $p_i \in T^*Q$ occupying the linear cotangent space, which we assume has enough regularity so that it has a Fréchet-Riesz representer in $L^2(S^1)$ (also denoted p_i , with some abuse of notation). We extremise the following the functional:

$$S = \int_{0}^{1} \frac{1}{2} ||u_t||^2 + \langle p_t, \dot{q}_t - u_t \circ q_t \rangle \, \mathrm{d}t,$$

where $\langle h, g \rangle = \int_{S^1} h \cdot g \, d\theta$. Taking variations i.e. $\delta S = 0$ leads to Hamilton's equations for curve matching for $t \in [0, 1]$:

$$\int_{0} \langle \delta p, \dot{q}_{t} - u_{t} \circ q_{t} \rangle \, \mathrm{d}t = 0, \qquad \forall \delta p \in L^{2}(S^{1}), \tag{6a}$$

$$\dot{p}_t - \nabla u_t^{\mathsf{T}} \circ q_t p_t, \delta q \rangle \, \mathrm{d}t = 0, \qquad \qquad \forall \delta q \in Q, \tag{6b}$$

$$\frac{1}{2}\frac{\delta \|\boldsymbol{u}_t\|^2}{\delta \boldsymbol{u}} - \langle \boldsymbol{p}_t, \delta \boldsymbol{u} \circ \boldsymbol{q}_t \rangle = 0, \tag{6c}$$

where δp , δu and δq are space-time test functions. The following theorem shows that we can solve (6b) analytically:

Theorem 1. The solution p_t to (6b) is at all times $t \ge 0$ given by $p_t = \nabla \varphi_t^{-\top} \circ q_0 p_0$.

Proof. See Appendix A.

To generate parameterisation-independent geodesics as in [9] we replace the initial condition q_0 by $q_0 \circ \eta$, where $\eta \in \text{Diff}_+(S^1)$ in the case of planar curves is an arbitrary reparameterisation. As a result of this quotient representation $\text{Emb}(S^1, \mathbb{R}^d) \setminus \text{Diff}_+(S^1)$ of curves we minimise over all η leading to the horizontality condition on the momentum. This means that the momentum p_0 has no tangential component and can therefore be described by a one-dimensional signal, $\tilde{p}_0 : S^1 \mapsto \mathbb{R}$:

$$p_0 = \mathbf{n}_{q_0} \tilde{p}_0$$

where \mathbf{n}_{a_0} : $S^1 \to \mathbb{R}^2$ is the outward normal of the template. Thus, along with Theorem 1 we have the following characterisation,

$$p_t = \varphi_t^{-\top} \circ q_0^{-\top} \mathbf{n}_{q_0} \tilde{p}_0.$$
⁽⁷⁾

This generates trajectories of geodesics between unparameterised curves. The entire geodesic motion of the curve can therefore be determined by a one-dimensional signal along the initial curve q_0 . To summarise this section we are concerned with integration of the following reduced Hamiltonian system for $t \in [0, 1]$:

$$\frac{1}{2} \frac{\delta \|\boldsymbol{u}_t\|^2}{\delta \boldsymbol{u}} = \langle \boldsymbol{\varphi}_t^{-\mathsf{T}} \circ \boldsymbol{q}_0 \mathbf{n}_{\boldsymbol{q}_0} \tilde{\boldsymbol{p}}_0, \delta \boldsymbol{u} \circ \boldsymbol{q}_t \rangle, \tag{8a}$$
$$\dot{\boldsymbol{q}}_t = \boldsymbol{u}_t \circ \boldsymbol{q}_t, \tag{8b}$$

with q_0 and \tilde{p}_0 fixed and boundary conditions $u_t|_{\partial\Omega} = 0$ for all $t \in [0, 1]$. Next we discuss a discretisation of (8).

2.2. Outer metric via finite elements

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From Picard-Lindelhöf analysis it is clear that the Banach space ordinary differential equation (ODE) (8b) requires a pointwise Lipschitz condition on u_t . As such, u_t must occupy at least $W^{1,\infty}(\Omega)^d$ when $q_0 \in L^{\infty}(S^1)$, see [37, Theorem 5] (see also Corollary 7 in this reference for other host spaces). Dupuis [20] establishes sufficient conditions accomplishing the same in a Hilbertian setting. The Hilbertian setting is better suited to finite element methods. This is in contrast with $W^{1,\infty}(\Omega)^d$ which is only a Banach space and, to the best of the authors' ability, is not easy to approximate numerically.¹ We therefore request a norm $\|\cdot\|$ such a way that a solution to (8a) ensures that this condition is met, which in turn

¹ [39] approximates by means of a fixed point linearisation solutions to the nonlinear ∞ -harmonic equation [40].



Fig. 1. Affine mapping to a reference cell \hat{K} from a typical cell K. Note that here F maps from the physical cell K to the reference cell \hat{K} rather than the other way around.

implies global existence and uniqueness of (8b) by the references above. For $d = 2, 3, H_0^3(\Omega)$ is contained in $C^1(\overline{\Omega})$ and so is Lipschitz on the interior [41, Theorem 2.5.1]. As such, we want to describe a discretisation of (8a) ensuring a type of H^3 regularity as the follow theorem shows.

Theorem 2. Let *O* be a convex bounded Lipschitz domain in \mathbb{R}^d with polygonal boundary and O_h a shape-regular, quasi-uniform triangulation thereof [42] for some mesh size h > 0. Suppose further that *u* is continuous on \overline{O} , $u|_K \in H^3(K)^d$ for $K \in O_h$ and that there exists an operator *B* inducing the norm $||u||_B^2 = \sum_{K \in O_h} ||u||_{B(K)}^2$, where we define $||u||_{B(K)}^2 = \int_K Bu \cdot u \, dx$ such that $||u||_{H^3(K)^d} \leq ||u||_{B(K)}$. Then $u \in W^{1,\infty}(O)^d$.

Proof. The embedding theorem for homogeneous Sobolev spaces (i.e. with zero traces) into the space $C^{j}(\bar{O})$ is well-known. However, since the trace $\gamma_{K}u$ of u on ∂K , $K \in O_{h}$ may not be zero. By [43, Theorem 4.12], $H^{3}(K) \hookrightarrow C^{1}_{R}(K)$, where:

 $C_{R}^{1}(K) = \{ u \in C^{1}(K) \mid D^{\alpha}u \text{ is bounded on } K, |\alpha| \leq 1 \}.$

This means any $H^3(K)$ function has a continuous representative with almost everywhere bounded first derivatives on *K*. Since $u \in C^0(\bar{O})$, *u* is a continuous function with its first derivative a.e. bounded, implying a Lipschitz condition. To summarise:

$$\|u\|_{W^{1,\infty}(K)^d}^2 \lesssim \|u\|_{H^3(K)^d}^2 \lesssim \|u\|_{B(K)}^2$$

Summing over the elements $K \in \Omega$ and squaring:

 $||u||^2_{W^{1,\infty}(\Omega)^d} \lesssim ||u||^2_B,$

where we have used that u is a continuous function with essentially bounded gradient. \Box

In light of this theorem we approximate the space of velocity fields by a nonconforming finite element space (see e.g. [44, Section 10.3]). This way we can guarantee the necessary Lipschitz properties of our functions without having to impose higher-order *global* continuity of the finite-dimensional solution spaces.

In Section 4 we use the H^3 -nonconforming finite element space presented in [12, Section 4] in a discretisation of (8). We choose the operator $B = (\mathbf{id} - \alpha \Delta)^{2m}$ for a given positive constant α leading to the following bilinear form:

$$a_{\Omega}(u,v) = \sum_{i=1}^{d} \int_{\Omega} \sum_{j=0}^{m} \alpha^{j} \binom{m}{j} D^{j} u^{i} \cdot D^{j} v^{j} \, \mathrm{d}x = \int_{\Omega} Bu \cdot v \, \mathrm{d}x,\tag{9}$$

where $x \cdot y$ is the Euclidean inner product, $D^0 = \mathbf{id}$, and

$$D^{j} = \begin{cases} \nabla D^{j-1} & j \text{ is odd,} \\ \nabla \cdot D^{j-1} & j \text{ is even.} \end{cases}$$

3. A pullback theory for the Wu-Xu element

The Wu-Xu element provides an opportunity to tackle this problem in a (nonconforming) H^3 setting, but it presents implementation challenges. Although we can construct its basis on a reference element, say, using the FIAT package [45], the Wu-Xu elements do not form an affine equivalent family [44] under pullback. Consequently, we apply the theory developed in [14], which gives a generalisation of techniques developed for the C^1 conforming Argyris element [46,47]. The main contribution of this section is to derive a pullback theory for the Wu-Xu elements so that their basis functions may be constructed once on a reference domain rather than constructed individually on each cell in the mesh.

3.1. Some general considerations

To fix ideas, put a reference triangle \hat{K} with vertices by $\{\hat{\mathbf{v}}_i\}_{i=1}^3$. For any nondegenerate triangle K with vertices $\{\mathbf{v}_i\}_{i=1}^3$, we let $F: T \to \hat{K}$ denote the affine mapping sending each \mathbf{v}_i to the corresponding $\hat{\mathbf{v}}_i$ and J_T its Jacobian matrix. (See Fig. 1.)

We adopt the ordering convention used in [48], where edge e_i of any triangle connects the vertices other than *i*. We take the unit tangent $\mathbf{t}_i = \begin{bmatrix} t_i^x & t_i^y \end{bmatrix}^T$ to from the vertex of lower number to the higher one. The normal to edge *i* is defined by counterclockwise rotation of the tangent, so that $\mathbf{n}_i = R\mathbf{t}_i$, where $R = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$. The normals, tangents, and edge midpoints for the reference element \hat{K} will include hats: $\hat{\mathbf{n}}_i$, $\hat{\mathbf{t}}_i$, and $\hat{\mathbf{e}}_i$. The pull-back of any function \hat{f} defined on \hat{K} is given by

$$F^*(\hat{f}) = \hat{f} \circ F,$$

and the push-forward of functionals *n* acting on functions defined over *K* is

$$F_*(n) = n \circ F^*, \tag{11}$$

so that

$$F_{*}(n)(\hat{f}) = (n \circ F^{*})(\hat{f}) = n(\hat{f} \circ F).$$
(12)

A finite element implementation requires local shape functions $\{\psi_i^K\}_{i=1}^N$ that are restrictions of the global basis to cell K. These are taken dual to a set of nodes or degrees of freedom $\{n_i^K\}_{i=1}^N$ in the sense that

$$n_i^K(\psi_i^K) = \delta_{ij}$$

In practice, one typically computes the basis $\{\hat{\psi}_i\}_{i=1}^N$ dual to some nodes $\{\hat{n}_i\}_{i=1}^N$ over the reference element \hat{K} . For affine equivalent families (like the Lagrange basis), the physical basis functions are the pullbacks of reference element shape functions, so that

$$\psi_i^K = F^*(\widehat{\psi}_i).$$

Equivalently, the nodes are preserved under push-forward, with

$$F_*(n_i^K) = \hat{n}_i$$

We may express these relations in a kind of vector-notation. If $\hat{\Psi}$ is a vector whose entries are $\hat{\psi}_i$, then in the affine equivalent case, $F^*(\hat{\Psi})$ contains the basis on cell K, and also $F_*(\mathcal{N}) = \widehat{\mathcal{N}}$. For non-equivalent families, these relations fail, but we can hope to construct a matrix M such

$$\Psi = M F^*(\hat{\Psi}) \tag{13}$$

contains the correct vector of basis functions on T. The matrix M will depend on the particular geometry of each cell, but if it is sparse this amounts to a considerable savings over directly constructing the basis on each triangle. Our theory in [14] proceeds by transforming the actions of the functionals on the finite element space. The finite element functionals are defined on some infinite-dimensional space (e.g. twice-continuously differentiable functions), and we let π denote the restriction of functionals to the finite-element space and $\hat{\pi}$ the corresponding restriction on the reference element. Then, we look for a matrix V such that

$$VF_*(\pi\mathcal{N}) = \hat{\pi}\widehat{\mathcal{N}},\tag{14}$$

and can prove [14, Theorem 3.1] that

$$M = V^T.$$
(15)

3.2. The Wu-Xu element

For any triangle K and integer $k \ge 0$, we let $\mathcal{P}^k(K)$ denote the space of polynomials of degree no greater than k over K. Letting λ_i be the barycentric coordinates for *K* (equivalently, the Lagrange basis for $\mathcal{P}^1(K)$), we let $b_K = \lambda_1 \lambda_2 \lambda_3$ be the standard cubic bubble function over *K*. We also need notation for the linear functionals defining degrees of freedom. We let δ_x denote pointwise evaluation of some (continuous) function:

 $\delta_{\mathbf{x}}(p) = p(\mathbf{x}).$ (16)

We let $\delta_{\mathbf{x}}^{\mathbf{x}}$ denote the derivative in some direction **s** at a point **x**:

$$\delta_{\mathbf{x}}^{\mathbf{s}}(p) = \mathbf{s}^T \nabla p(\mathbf{x}) \tag{17}$$

Repeated superscripts will indicate higher derivatives. We use block notation for gradients and sets of second-order derivatives, such as

$$\nabla_{\mathbf{x}} = \begin{bmatrix} \delta_{\mathbf{x}}^{\mathbf{x}} & \delta_{\mathbf{x}}^{\mathbf{y}} \end{bmatrix}^T \tag{18}$$

for the gradient in Cartesian coordinates at a point x, and

$$\Delta_{\mathbf{x}} = \begin{bmatrix} \delta_{\mathbf{x}}^{\mathbf{xx}} & \delta_{\mathbf{x}}^{\mathbf{xy}} & \delta_{\mathbf{x}}^{\mathbf{yy}} \end{bmatrix}^{T}$$
(19)

for the unique components of the Hessian matrix. We will use superscripts in the block notation to indicate the derivatives taken in directions other than the Cartesian ones, such as ∇^{nt} containing the derivatives with respect to a normal vector **n** and tangent vector **t** for some part of the boundary. Similarly, \triangle^{nt} will contain the second partials in each direction and the mixed partial in both directions.

The Wu-Xu elements also utilise integral moments of normal derivatives, and we shall also need averages of tangential and mixed derivatives over edges to perform the transformations. Given any directional vector s, we define the moment of the derivative in the direction s over edge e by:

$$\mu_{\mathbf{e}}^{\mathbf{s}}(f) = \int_{\mathbf{e}} \mathbf{s} \cdot \nabla f \, ds. \tag{20}$$

Similarly, we let $\mu_e^{s_1s_2}$ to denote the functionals computing moments of second (possibly mixed) directional derivatives over an edge. Now, we define the pair of H^3 nonconforming triangles considered in [12]. Note that there are two spaces given: a space compatible with sixth-order problems, and a robust space that is stable for second, fourth and sixth-order problems. We define function space $\mathcal{W}(K)$ over some triangle K by

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Fig. 2. Degrees of freedom for the Wu-Xu (left) and robust Wu-Xu (right) elements. Point values are given by dots, gradients by circles, while averages of first and second normal derivatives are given by thin and thick arrows, respectively.



Fig. 3. Compatible nodal completions for the Wu-Xu and robust Wu-Xu elements.

$$\mathcal{W}(K) = \mathcal{P}^3 + b_K \mathcal{P}^1,\tag{21}$$

and the function space for the robust element will be

$$\mathcal{W}_r(K) = \mathcal{P}^3 + b_K \mathcal{P}^1 + b_K^2 \mathcal{P}^1, \tag{22}$$

where \mathcal{P}^k is the standard space of polynomials of degree k. Note that we have dim $\mathcal{W}(K) = 12$ and dim $\mathcal{W}_r(K) = 15$ since $b_K \in \mathcal{P}^3 \cap b_K \mathcal{P}^1$. The degrees of freedom for the two elements are quite similar. We can parametrise $\mathcal{W}_r(K)$ by

$$\mathcal{N} = \begin{bmatrix} \delta_{\mathbf{v}_1} & \nabla_{\mathbf{v}_1}^T & \delta_{\mathbf{v}_2} & \nabla_{\mathbf{v}_2}^T & \delta_{\mathbf{v}_3} & \nabla_{\mathbf{v}_3}^T & \mu_{\mathbf{e}_1}^{\mathbf{n}_1 \mathbf{n}_1} & \mu_{\mathbf{e}_2}^{\mathbf{n}_2 \mathbf{n}_2} & \mu_{\mathbf{e}_3}^{\mathbf{n}_3 \mathbf{n}_3} \end{bmatrix}^T.$$
(23)

That is, the degrees of freedom consist of point values and gradients at each vertex, together with moments of the second normal derivative along edges. For the robust element, we also use the moments of the first normal derivatives, so that

$$\mathcal{N}_{r} = \begin{bmatrix} \delta_{\mathbf{v}_{1}} & \nabla_{\mathbf{v}_{1}}^{T} & \delta_{\mathbf{v}_{2}} & \nabla_{\mathbf{v}_{2}}^{T} & \delta_{\mathbf{v}_{3}} & \nabla_{\mathbf{v}_{3}}^{T} & \mu_{\mathbf{e}_{1}}^{\mathbf{n}_{1}} & \mu_{\mathbf{e}_{2}}^{\mathbf{n}_{2}} & \mu_{\mathbf{e}_{3}}^{\mathbf{n}_{3}\mathbf{n}_{1}\mathbf{n}_{1}} & \mu_{\mathbf{e}_{2}}^{\mathbf{n}_{2}\mathbf{n}_{2}} & \mu_{\mathbf{e}_{3}}^{\mathbf{n}_{3}\mathbf{n}_{3}} \end{bmatrix}^{T}.$$
(24)

Wu and Xu actually define the degrees of freedom as average of these moments over the relevant facets, although this does not affect unisolvence or other essential properties. For the reference element, it will be helpful to use their original definition. For some edge e of \hat{K} , define

$$\hat{\mu}_{\hat{\mathbf{e}}}^{\hat{\mathbf{s}}}(f) = \frac{1}{|\hat{\mathbf{e}}|} \int\limits_{\hat{\mathbf{e}}} \hat{\mathbf{s}} \cdot \hat{\nabla} f \, d\hat{s},\tag{25}$$

and similarly define moments second directional derivatives over reference element edges. The reference element nodes for $\mathcal{W}(\hat{K})$ will be taken as

$$\widehat{\mathcal{N}} = \begin{bmatrix} \delta_{\hat{\mathbf{v}}_1} & \hat{\nabla}_{\hat{\mathbf{v}}_1}^T & \delta_{\hat{\mathbf{v}}_2} & \hat{\nabla}_{\hat{\mathbf{v}}_2}^T & \delta_{\hat{\mathbf{v}}_3} & \hat{\nabla}_{\hat{\mathbf{v}}_3}^T & \hat{\mu}_{\hat{\mathbf{e}}_1}^{\hat{\mathbf{n}}_1 \hat{\mathbf{n}}_1} & \hat{\mu}_{\hat{\mathbf{e}}_2}^{\hat{\mathbf{n}}_2 \hat{\mathbf{n}}_2} & \hat{\mu}_{\hat{\mathbf{e}}_3}^{\hat{\mathbf{n}}_3 \hat{\mathbf{n}}_3} \end{bmatrix}^T,$$
(26)

and for $\mathcal{W}_r(\hat{K})$ we will use

$$\widehat{\mathcal{N}} = \begin{bmatrix} \delta_{\hat{\mathbf{v}}_1} & \widehat{\mathbf{v}}_{\hat{\mathbf{v}}_1}^T & \delta_{\hat{\mathbf{v}}_2} & \widehat{\mathbf{v}}_{\hat{\mathbf{v}}_2}^T & \delta_{\hat{\mathbf{v}}_3} & \widehat{\mathbf{v}}_{\hat{\mathbf{v}}_3}^T & \hat{\mu}_{\hat{\mathbf{e}}_1}^{\hat{\mathbf{n}}_1} & \hat{\mu}_{\hat{\mathbf{e}}_2}^{\hat{\mathbf{n}}_2} & \hat{\mu}_{\hat{\mathbf{e}}_3}^{\hat{\mathbf{n}}_1 \hat{\mathbf{n}}_1} & \hat{\mu}_{\hat{\mathbf{e}}_2}^{\hat{\mathbf{n}}_2 \hat{\mathbf{n}}_2} & \hat{\mu}_{\hat{\mathbf{e}}_3}^{\hat{\mathbf{n}}_3 \hat{\mathbf{n}}_3} \end{bmatrix}^T.$$
(27)

Note that this redefinition has no effect in the case of an equilateral reference triangle with unit edge length. For the more common case of a right isosceles reference triangle, however, this will eliminate the need for logic indicating to which reference element edges the edges of each triangle correspond.

3.3. Mapping the Wu-Xu element

The derivative degrees of freedom in both Wu-Xu elements are not preserved under push-forward, and since we have only normal derivatives on the edges, we cannot immediately obtain the correct nodes by taking linear combinations (see Fig. 2). Consequently, we must develop a *compatible nodal completion* [14, Definition 3.4]. For the Wu-Xu elements, this contains all the original degrees of freedom plus the integrals of tangential and mixed normal/tangential derivatives. Such a completion is shown for the standard Wu-Xu element in Fig. 3a. A completion for the robust element includes the first normal moments and tangential moments as well, as shown in Fig. 3b.

We define

$$\mathcal{M}_{1,i} = \left[\mu_{\mathbf{e}_i}^{\mathbf{n}_i} \quad \mu_{\mathbf{e}_i}^{\mathbf{t}_i} \right]^T \tag{28}$$

to be the vector of the moments of the normal and tangential derivatives on a particular edge. We also let $\widehat{\mathcal{M}_{1,i}}$ contain the corresponding reference element nodes. We only need $\mathcal{M}_{1,i}$ and $\widehat{\mathcal{M}_{1,i}}$ for the robust element. Both elements require

$$\mathcal{M}_{2,i} = \begin{bmatrix} \mu_{\mathbf{e}_i}^{\mathbf{n}_i \mathbf{n}_i} & \mu_{\mathbf{e}_i}^{\mathbf{t}_i t_i} & \mu_{\mathbf{e}_i}^{\mathbf{n}_i t_i} \end{bmatrix}^T$$
(29)

containing the unique second derivative moments on each edge. We similarly define $\widehat{\mathcal{M}_{2,i}}$ to contain the reference element integral averages. The compatible nodal completion for $(K, \mathcal{P}(K), \mathcal{N})$ is

$$\mathcal{N}^{C} = \begin{bmatrix} \delta_{\mathbf{v}_{1}} & \nabla_{\mathbf{v}_{1}}^{T} & \delta_{\mathbf{v}_{2}} & \nabla_{\mathbf{v}_{2}}^{T} & \delta_{\mathbf{v}_{3}} & \nabla_{\mathbf{v}_{3}}^{T} & \mathcal{M}_{2,1}^{T} & \mathcal{M}_{2,2}^{T} & \mathcal{M}_{2,3}^{T} \end{bmatrix}^{T},$$
(30)

with the hatted equivalents comprising $\hat{\mathcal{N}}^C$ on the reference cell. The completed set of nodes for the robust element is

$$\mathcal{N}_{r}^{C} = \begin{bmatrix} \delta_{\mathbf{v}_{1}} & \nabla_{\mathbf{v}_{1}}^{T} & \delta_{\mathbf{v}_{2}} & \nabla_{\mathbf{v}_{2}}^{T} & \delta_{\mathbf{v}_{3}} & \nabla_{\mathbf{v}_{3}}^{T} & \mathcal{M}_{1,1}^{T} & \mathcal{M}_{1,2}^{T} & \mathcal{M}_{1,3}^{T} & \mathcal{M}_{2,1}^{T} & \mathcal{M}_{2,3}^{T} \end{bmatrix}^{T}.$$
(31)

Now, the matrix V from (14) will be obtained in factored form

$$V = EV^c D, \tag{32}$$

where each matrix plays a particular role. *D* is a rectangular matrix expressing the completed nodes in terms of the given physical nodes. V^c is a block diagonal matrix relating the push-forward of the reference nodal completion to the physical nodal completion, and *E* is a Boolean matrix selecting actual finite element nodes from the completion. For the Wu-Xu element, *D* is 18×12 , V^c is 18×18 , and *E* is 12×18 . For the robust element, *D* is 24×15 , V^c is 24×24 , and *E* is 15×24 .

Now, we define the matrix D, which expresses the members of \mathcal{N}^C as linear combinations of the members of \mathcal{N} . Clearly, the rows corresponding to members of \mathcal{N}^C also appearing in \mathcal{N} will just have a single nonzero in the appropriate column. For the Wu-Xu element, the remaining nodes are all integrals of quantities over edges, and we can use the Fundamental Theorem of Calculus to perform this task. Let \mathbf{e} be an edge running from vertex \mathbf{v}_a to \mathbf{v}_b with unit tangent and normal \mathbf{t} and \mathbf{n} , respectively. We have

$$\mu_{\mathbf{e}}^{\mathbf{t}}(f) = \int_{\mathbf{e}} \mathbf{t}^{T} \nabla f \, ds = f(\mathbf{v}_{b}) - f(\mathbf{v}_{a}) = \delta_{\mathbf{v}_{b}}(f) - \delta_{\mathbf{v}_{a}}(f). \tag{33}$$

In a similar way, the moments of the second tangential and mixed derivatives on **e** can be expressed as differences between components of the gradients at endpoints by:

$$\mu_{\mathbf{e}}^{\mathbf{nt}}(f) = \mathbf{n}^{T} \left(\nabla_{\mathbf{v}_{b}} f - \nabla_{\mathbf{v}_{a}} f \right),$$

$$\mu_{\mathbf{e}}^{\mathbf{tt}}(f) = \mathbf{t}^{T} \left(\nabla_{\mathbf{v}_{b}} f - \nabla_{\mathbf{v}_{a}} f \right),$$
(34)

and we have that $\mathcal{N}^C = D\mathcal{N}$, or

гс ¬

$o_{\mathbf{v}_1}$															
$\delta^{\mathbf{x}}_{\mathbf{v}_1}$															
$\delta^{\mathbf{y}}_{\mathbf{v}_1}$		Гı	0	0	0	0	0	0	0	0	0	0	0]	1	
δ			1	0	0	0	0	0	0	0	0	0	0	г	
v_2		0	1	0	0	0	0	0	0	0	0	0	0	$\delta_{\mathbf{v}_1}$	
$\delta_{\mathbf{v}_2}^{\mathbf{x}}$		0	0	1	0	0	0	0	0	0	0	0	0	δ ^x	
۶y		0	0	0	1	0	0	0	0	0	0	0	0	• v ₁	
$v_{\mathbf{v}_2}$		0	0	0	0	1	0	0	0	0	0	0	0	$\delta_{\mathbf{v}_1}^{\mathbf{y}}$	
$\delta_{\mathbf{v}_3}$		0	0	0	0	0	1	0	0	0	0	0	0	δ.	
δx		0	0	0	0	0	0	1	0	0	0	0	0	sx	
• • 3 • • •		0	0	0	0	0	0	0	1	0	0	0	0	$o_{\mathbf{v}_2}$	
$\delta_{\mathbf{v}_3}$		0	0	0	0	0	0	0	0	1	0	0	0	$\delta_{\mathbf{v}_2}^{\mathbf{y}}$	
$\mu_{\mathbf{e}_1}^{\mathbf{n}_1\mathbf{n}_1}$	=	0	0	0	0	0	0	0	0	0	1	0	0	$\delta_{\mathbf{v}_3}$	ŀ
$\mu_{a}^{\mathbf{n}_{1}\mathbf{t}_{1}}$		0	0	0	0	$-n_{1,x}$	$-n_{1,v}$	0	$n_{1,x}$	$n_{1,v}$	0	0	0	$\delta_{u}^{\mathbf{x}}$	
<i>r</i> ^r e ₁		0	0	0	0	$-t_{1,x}$	$-t_{1,v}$	0	$t_{1,x}$	$t_{1,v}$	0	0	0		
$\mu_{\mathbf{e}_1}^{\mathbf{e}_1\mathbf{e}_1}$		0	0	0	0	0	0	0	0	0	0	1	0	$\delta_{\mathbf{v}_3}$	
$\mu_{\mathbf{e}_2}^{\mathbf{n}_2\mathbf{n}_2}$		0	$-n_{2,x}$	$-n_{2,v}$	0	0	0	0	$n_{2,x}$	$n_{2,v}$	0	0	0	$n_1 n_1$	
n ₂ t ₂		0	$-t_{2,x}$	$-t_{2,v}$	0	0	0	0	$t_{2,x}$	$t_{2,v}$	0	0	0	$n_2 \mathbf{n}_2$	
$\mu_{\mathbf{e}_2}$		0	0	0	0	0	0	0	0	Ő	0	0	1	$\mu_{\mathbf{e}_2}$	
$\mu_{\mathbf{e}_2}^{\mathbf{t}_2\mathbf{t}_2}$		0	$-n_{3,x}$	$-n_{3,v}$	0	$n_{3,x}$	$n_{3,v}$	0	0	0	0	0	0	$\mu_{\mathbf{e}_3}^{\mathbf{n}_3\mathbf{n}_3}$	
$\mu_{\mathbf{e}_3}^{\mathbf{n}_3\mathbf{n}_3}$		0	$-t_{3,x}$	$-t_{3,y}$	0	$t_{3,x}$	$t_{3,y}$	0	0	0	0	0	0		
$\mu_{\mathbf{n}_3}^{\mathbf{n}_3 \mathbf{t}_3}$															
toto															
$\left[\mu_{\mathbf{e}_3}^{\mathbf{c}_3\mathbf{c}_3} \right]$															

The matrix V^{C} is obtained by relating the push-forwards of the nodal completion to their reference counterparts.

We can convert between the Cartesian and other orthogonal coordinate systems (e.g. normal/tangential) representations as follows. Given a pair of orthogonal unit vectors \mathbf{n} and \mathbf{t} , we can define an orthogonal matrix G by:

(35)

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(36)

 $G = \begin{bmatrix} \mathbf{n} & \mathbf{t} \end{bmatrix}^T$.

In particular, we will use G_i to have the normal and tangential vectors to edge *i* of triangle *K* and \hat{G}_i those for triangle \hat{K} . The multivariate chain rule readily shows that

$$\nabla_{\mathbf{x}} = G^T \nabla_{\mathbf{x}}^{\mathbf{n}\mathbf{t}}.$$
(37)

Similarly, letting $\mathbf{n} = \begin{bmatrix} n_x & n_y \end{bmatrix}^T$ and $\mathbf{t} = \begin{bmatrix} t_x & t_y \end{bmatrix}^T$, we define the matrix Γ by

$$\Gamma = \begin{bmatrix} n_x^2 & 2n_x t_x & t_x^2 \\ n_x n_y & n_x t_y + n_y t_x & t_x t_y \\ n_y^2 & 2n_y t_y & t_y^2 \end{bmatrix},$$
(38)

and the chain rule gives

$$\bigwedge_{x} = \Gamma \bigwedge_{x}^{\text{nt}}.$$
 (39)

Although *G* is an orthogonal matrix, Γ is not. A similar calculation also shows gives that: $\Delta_x^{nt} = \Gamma^{-1} \Delta_x$, where

$$\Gamma^{-1} = \begin{bmatrix} n_x^2 & 2n_x n_y & n_y^2 \\ n_x t_x & n_x t_y + n_y t_x & n_y t_y \\ t_x^2 & 2t_x t_y & t_y^2 \end{bmatrix}.$$
(40)

We will also need to transform derivatives under pull-back. Using the chain rule,

$$\nabla(\hat{\psi} \circ F) = J^T \hat{\nabla} \hat{\psi} \circ F.$$
(41)

Combining this with (37) lets us relate the normal and tangential derivatives in physical space to the normal and tangential derivatives in reference space.

$$\nabla_{\mathbf{x}}^{\mathbf{n}\mathbf{t}} = GJ^T \hat{G}^T \hat{\nabla}_{\hat{\mathbf{x}}}^{\hat{\mathbf{h}}\hat{\mathbf{t}}}.$$
(42)

We can perform a similar calculation for second derivatives. With the entries of the Jacobian matrix as:

$$J = \begin{bmatrix} \frac{\partial x}{\partial \hat{x}} & \frac{\partial x}{\partial \hat{y}} \\ \frac{\partial y}{\partial \hat{x}} & \frac{\partial y}{\partial \hat{y}} \end{bmatrix},\tag{43}$$

we define the matrix

$$\Theta = \begin{bmatrix} \left(\frac{\partial \hat{x}}{\partial x}\right)^2 & 2\frac{\partial \hat{x}}{\partial x}\frac{\partial \hat{y}}{\partial x} & \left(\frac{\partial \hat{y}}{\partial x}\right)^2 \\ \frac{\partial \hat{x}}{\partial y}\frac{\partial \hat{x}}{\partial x} & \frac{\partial \hat{x}}{\partial y}\frac{\partial \hat{y}}{\partial x} + \frac{\partial \hat{x}}{\partial x}\frac{\partial \hat{y}}{\partial y} & \frac{\partial \hat{y}}{\partial x}\frac{\partial \hat{y}}{\partial y} \\ \left(\frac{\partial \hat{x}}{\partial y}\right)^2 & 2\frac{\partial \hat{x}}{\partial y}\frac{\partial \hat{y}}{\partial y} & \left(\frac{\partial \hat{y}}{\partial y}\right)^2 \end{bmatrix},$$
(44)

so that for $\mathbf{x} = F(\hat{\mathbf{x}})$,

$$\bigwedge_{\mathbf{x}} = \Theta \hat{\triangle}_{\hat{\mathbf{x}}}.$$
 (45)

The inverse of Θ follows by reversing the roles of reference and physical variables:

$$\Theta^{-1} = \begin{bmatrix} \left(\frac{\partial x}{\partial \hat{x}}\right)^2 & 2\frac{\partial x}{\partial \hat{x}}\frac{\partial y}{\partial \hat{x}} & \left(\frac{\partial y}{\partial \hat{x}}\right)^2 \\ \frac{\partial x}{\partial \hat{y}}\frac{\partial x}{\partial \hat{x}} & \frac{\partial x}{\partial \hat{y}}\frac{\partial y}{\partial \hat{x}} + \frac{\partial x}{\partial \hat{x}}\frac{\partial y}{\partial \hat{y}} & \frac{\partial y}{\partial \hat{x}}\frac{\partial y}{\partial \hat{y}} \\ \left(\frac{\partial x}{\partial \hat{y}}\right)^2 & 2\frac{\partial x}{\partial \hat{y}}\frac{\partial y}{\partial \hat{y}} & \left(\frac{\partial y}{\partial \hat{y}}\right)^2 \end{bmatrix}$$
(46)

We can also relate the second-order derivatives in normal/tangential coordinates under pullback by

$$\frac{nt}{x} = \Gamma \Theta \hat{\Gamma}^{-1} \frac{\hat{nt}}{\hat{x}}.$$
(47)

From here, we will let G_i and \hat{G}_i denote the matrices containing normal and tangent vectors to edge \mathbf{e}_i of a generic triangle T and the reference triangle \hat{T} , respectively, with similar convention for the other geometric quantities Γ and Θ . For any vector **s**, edge **e**, and smooth function $f = f \circ F$, we have

$$\int_{\mathbf{e}} \mathbf{s}^T \nabla f \, ds = \int_{\mathbf{e}} \mathbf{s}^T \hat{\nabla} f \circ F \, ds = \int_{\hat{\mathbf{e}}} \mathbf{s}^T \hat{\nabla} f \, J_{\mathbf{e}, \hat{\mathbf{e}}} \, d\hat{s}, \tag{48}$$

where the Jacobian $J_{e,\hat{e}}$ is just the ratio of the length of e to that of the corresponding reference element edge \hat{e} . Applying this to the normal and tangential moments and using (42), we have that:

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 $\mathcal{M}_{1,i} = |\mathbf{e}_i| G_i J^T \hat{G}_i^{-1} \widehat{\mathcal{M}}_{1,i},$

(49)

where the factor of $|\hat{\mathbf{e}}_i|$ in the denominator of the Jacobian is merged with the reference element moments to produce $\widehat{\mathcal{M}_{1,i}}$. Hence, the slight modification of reference element nodes avoids extra data structures or logic in identifying reference element edge numbers. Then, we can use (47) to express each $\mathcal{M}_{2,i}$ in terms of the reference element nodes

$$\mathcal{M}_{2,i} = |\mathbf{e}|\Gamma_i \Theta \widehat{\Gamma}_i^{-1} \widehat{\mathcal{M}}_{2,i}.$$
(50)

We define vectors

$$B^{1,i} = \frac{1}{|\mathbf{e}_i|} \hat{G}_i J^{-T} G_i^T, \quad B^{2,i} = \frac{1}{|\mathbf{e}_i|} \hat{\Gamma}_i \Theta^{-1} \Gamma_i^{-1}, \tag{51}$$

and hence V^C is the block-diagonal matrix



with zeros of the appropriate shapes in the off-diagonal blocks. The extraction matrix *E* is just the 12×18 Boolean matrix selecting the members of *N* from N^C :

	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0]
E =	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0

Multiplying EV^CD out and defining

$$\begin{split} \beta^{i,x} &= n_x^i B_{12}^{2,i} + t_x^i B_{13}^{2,i}, \\ \beta^{i,y} &= n_y^i B_{12}^{2,i} + t_y^i B_{13}^{2,i}, \end{split}$$

we obtain for V

	Γ1	0	0	0	0	0	0	0	0	0	0	0]	
	0	$\frac{\partial x}{\partial \hat{x}}$	$\frac{\partial y}{\partial \hat{x}}$	0	0	0	0	0	0	0	0	0	
	0	$\frac{\partial x}{\partial \hat{y}}$	$\frac{\partial y}{\partial \hat{y}}$	0	0	0	0	0	0	0	0	0	
	0	0	0	1	0	0	0	0	0	0	0	0	
	0	0	0	0	$\frac{\partial x}{\partial \hat{x}}$	$\frac{\partial y}{\partial \hat{x}}$	0	0	0	0	0	0	
V _	0	0	0	0	$\frac{\partial x}{\partial \hat{y}}$	$\frac{\partial y}{\partial \hat{y}}$	0	0	0	0	0	0	
<i>v</i> –	0	0	0	0	Ó	Ó	1	0	0	0	0	0	
	0	0	0	0	0	0	0	$\frac{\partial x}{\partial \hat{x}}$	$\frac{\partial y}{\partial \hat{x}}$	0	0	0	
	0	0	0	0	0	0	0	$\frac{\partial x}{\partial \hat{y}}$	$\frac{\partial y}{\partial \hat{y}}$	0	0	0	
	0	0	0	0	$-\beta^{1,x}$	$-\beta^{1,y}$	0	$\beta^{1,x}$	$\beta^{1,y}$	$B_{11}^{2,1}$	0	0	
	0	$-\beta^{2,x}$	$-\beta^{2,y}$	0	0	0	0	$\beta^{2,x}$	$\beta^{2,y}$	0	$B_{11}^{2,2}$	0	
	0	$-\beta^{3,x}$	$-\beta^{3,y}$	0	$\beta^{3,x}$	$\beta^{3,y}$	0	0	0	0	0	$B_{11}^{2,3}$	

(54)

(53)

(55)

The same considerations lead to a similar derivation of E, V^c , and D for the robust element, resulting in

	1	0 dr	0 du	0	0	0	0	0	0	0	0	0	0	0	0
	0	$\frac{\partial x}{\partial \hat{x}}$	$\frac{\partial y}{\partial \hat{x}}$	0	0	0	0	0	0	0	0	0	0	0	0
	0	$\frac{\partial x}{\partial \hat{v}}$	$\frac{\partial y}{\partial \hat{y}}$	0	0	0	0	0	0	0	0	0	0	0	0
	0	Ő	Ŏ	1	0	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	$\frac{\partial x}{\partial \hat{x}}$	$\frac{\partial y}{\partial \hat{x}}$	0	0	0	0	0	0	0	0	0
	0	0	0	0	$\frac{\partial \hat{x}}{\partial \hat{y}}$	$\frac{\partial \hat{y}}{\partial \hat{y}}$	0	0	0	0	0	0	0	0	0
	0	0	0	0	Ő	Ő	1	0	0	0	0	0	0	0	0
V =	0	0	0	0	0	0	0	$\frac{\partial x}{\partial \hat{x}}$	$\frac{\partial y}{\partial \hat{x}}$	0	0	0	0	0	0
	0	0	0	0	0	0	0	$\frac{\partial \hat{x}}{\partial \hat{v}}$	$\frac{\partial \hat{y}}{\partial \hat{y}}$	0	0	0	0	0	0
	0	0	0	$-B_{12}^{1,1}$	0	0	$B_{12}^{1,1}$	0	0	$B_{11}^{1,1}$	0	0	0	0	0
	$-B_{12}^{1,2}$	0	0	0	0	0	$B_{12}^{1,2}$	0	0	0	$B_{11}^{1,2}$	0	0	0	0
	$-B_{12}^{1,3}$	0	0	$B_{12}^{1,3}$	0	0	0	0	0	0	0	$B_{11}^{1,3}$	0	0	0
	0	0	0	0	$-\beta^{1,x}$	$-\beta^{1,y}$	0	$\beta^{1,x}$	$\beta^{1,y}$	0	0	0	$B_{11}^{2,1}$	0	0
	0	$-\beta^{2,x}$	$-\beta^{2,y}$	0	0	0	0	$\beta^{2,x}$	$\beta^{2,y}$	0	0	0	0	$B_{11}^{2,2}$	0
	Lo	$-\beta^{3,x}$	$-\beta^{3,y}$	0	$\beta^{3,x}$	$\beta^{3,y}$	0	0	0	0	0	0	0	0	$B_{11}^{2,}$

(56)

for *V*, where β is as defined in (54).

4. Discretisation

We now describe the discretisations of the Hamiltonian system (8) using a function space introduced in the previous section. Letting Ω_0 denote a convex subset of \mathbb{R}^2 with polygonal boundary, smooth solutions to (8a) defined on Ω_0 generate the following curve of diffeomorphisms:

$$\dot{\varphi}_l = u_l \circ \varphi_l, \quad \varphi_0 = \mathrm{id}, \tag{57}$$

where the domain of φ_t is Ω_0 . This subsumes the left action on the curve q_0 in (8b). Our approach is therefore to solve (8a) for an *outer metric* in tandem with integrating the diffeomorphism defined over the entire domain and moving the mesh, thereby automatically providing a solution to a discrete analogue of (8b). We denote by \mathcal{T}_0 a shape-regular, quasi-uniform triangulation of the template domain Ω_0 . Let \mathcal{E}_h denote the *mesh skeleton* of \mathcal{T}_0 and \mathcal{E}_h the subset of \mathcal{E}_h whose elements do not intersect $\partial\Omega_0$. We place the following assumption on the initial triangulation \mathcal{T}_0 :

Assumption 1. \mathcal{T}_0 is constructed such that the range of q_0 is described by a subset of $\mathring{\mathcal{E}}_h$.

Using the function space $\mathcal{W}(K)$ introduced in (21) we define the vector-valued Wu-Xu space defined over Ω_0 :

$$V(\Omega_0) = \{ v \in L^2(\Omega)^2 \mid v_i \mid_K \in \mathcal{W}(K), K \in \mathcal{T}_0, i = 1, 2 \}.$$

Further, let $0 = t_0, t_{\Delta T}, \dots, t_{T-1} = 1$ denote *T* uniformly distributed points and use an Euler discretisation of the time derivate in (5), where we let $\varphi_{t_k} \in V(\Omega_0), u_{t_k} \in V(\Omega_0)$:

$$\varphi_{t_{k+1}} = \varphi_{t_k} + u_{t_k} \circ \varphi_{t_k} \Delta T.$$
(58)

For sufficiently small ΔT , φ_{t_k} is a diffeomorphism of Ω [49]. Using the notation $\Omega_{t_k} = \varphi_{t_k} \circ \Omega_0$, $V(\Omega_{t_k}) := \{f \mid f \circ \varphi_{t_k}^{-1} \in V(\Omega_0)\}$ and by noting that $q_{t_k} = \varphi_{t_k} \circ q_0$ we obtain a discrete analogue of (8) where $\hat{u}_{t_k} \in V(\Omega_{t_k})$:

$$a_{\Omega_{t_k}}(\hat{u}_{t_k}, \hat{v}) = \int_{S^1} \nabla \varphi_{t_k}^{-\mathsf{T}} \circ q_0 \mathbf{n}_{q_0} \tilde{p}_0 \cdot \hat{v} \circ q_0 \, \mathrm{d}s, \qquad \forall \hat{v} \in V(\Omega_{t_k}),$$

$$\varphi_{t_{k+1}} = \varphi_{t_k} + \hat{u}_{t_k} \Delta T,$$
(59b)

for k = 0, ..., T - 1, where $\varphi_{t_k} \circ \partial \Omega_0 = \mathbf{id}$ owing to the homogeneous Dirichlet boundary conditions implied by (59a). At each time step k after the solution of (59a), the mesh is moved according to (58) upon which the equation (60):

$$q_{t_{k+1}} = q_{t_k} + u_{t_k} \circ q_{t_k} \Delta T, \tag{60}$$

is automatically satisfied. The underlying coordinate field of the mesh itself is chosen to be a Lagrange subspace of $V(\Omega_0)$, so that the map $q_0 \mapsto \varphi_{t_k} \circ q_0$ is a diffeomorphism. At k = 0, the assembly of the right-hand side is in practice done by integration over $q_0 \circ S^1$, which means that we can supply an initial "momentum" signal $\mathbf{p}_0 \in \tilde{p}_0 \circ q_0^{-1} \in L^2(q_0 \circ S^1)$ (now defined over initial curve) to encode the entire geodesic flow of φ , and thereby of the embedded curve. We believe this is the first formulation of a Lipschitz-conforming finite element discretisation of the curve matching equations. Fig. 4 show examples of forward integration of this system for two \mathbf{p}_0 and $q_0 \circ S^1$ (the initial meshes were generated using gmsh [50]). Note that the norm of the velocity present in (8) is confined to certain energy levels determined by the initial momentum as the system is integrated. In the fully discrete analogue we can only hope to establish approximate conservation of the Hamiltonian. The importance of this is nebulous since we only integrate over fixed time intervals, and is subject to future work.

The computational cost of integrating (59) is dominated by the inversion of the discrete bilinear form. Mesh-based methods readily facilitate parallel computations (e.g. matrix-vector products in a Krylov subspace method), which along with preconditioning strategies are competitive with fast multipole methods. They also offer flexibility in choosing the bilinear form (9), which can be altered according to an informed modelling choice



Fig. 4. Top row: two template domains Ω_0 with curves highlighted. Bottom row: $\varphi_1 \circ \Omega_1$ computed by integrating (59) from the two templates with different initial momenta.

or application. Finally, mesh adaptivity is also an option. For the application at hand a *graded* mesh with a fine resolution in the vicinity of the curve and coarser elements closer to the boundary can both increase accuracy and the computational burden of the method.

5. Inverse problem

We now consider the matching problem using the data misfit functional in (2). We wish to estimate the momentum $\mathbf{p}_0 := \tilde{p}_0 \circ q_0^{-1} \in \mathbf{P}$ that generates the curve $t \mapsto q_t$. That is, \mathbf{p}_0 is the momentum object defined on the computational domain $q_0 \circ S^1$. We drop explicit dependence on the template as it remains fixed during computation as well as the time dimension of the initial momentum. To ease the notation we use boldface τ to represent the smoothed version of the indicator function on the interior of a curve q,

$$\boldsymbol{\tau} = \boldsymbol{C}^{-1} \mathbb{1}_q,$$

where *C* is a linear elliptic differential operator. We define the *forward operator*:

$$\mathbf{p} \mapsto \mathcal{F}(\mathbf{p}) = \mathbf{\tau} := \mathcal{C}^{-1} \mathbb{1}_{q_1},\tag{61}$$

where q_1 is the solution at t = 1 given by solving (59) using q_0 and **p** as initial conditions, i.e. the time-1 flow map of the initial curve. Given a target shape τ_{target} the inverse problem of interest is therefore to recover the momentum **p**^{*} such that:

$$\tau_{\text{target}} = \mathcal{F}(\mathbf{p}^*) + \eta, \tag{62}$$

where $\eta \in \text{dom}(C)$ represents noise in the data. The targets we consider in this paper are known, and the noise is therefore deterministic. The use of a probability distribution is, however, essential for the sampling of an initial ensemble.

To tackle this inverse problem we use EKI. We let *N* denote the number of ensemble members and let \mathbf{p}^{j} , j = 1, ..., N denote the momenta corresponding to ensemble member *j*. The ensemble mean momentum and the mean predicted shape are:

$$\bar{\mathbf{p}} := N^{-1} \sum_{j=1}^{N} \mathbf{p}_{j}, \qquad \bar{\boldsymbol{\tau}} := N^{-1} \sum_{j=1}^{N} \boldsymbol{\tau}^{j},$$
(63)

where $\tau^{j} = C^{-1} \mathbb{1}_{\mathcal{F}(\mathbf{p}^{j})}$. The Kalman update operator (or Kalman *gain*) is defined by:

$$\widehat{\mathbf{x}}_{\mathbf{P}} = \operatorname{Cov}_{PQ}[\operatorname{Cov}_{QQ} + \xi I]^{-1},\tag{64}$$

where *I* is the identity operator and ξ is a regularisation parameter that determines the influence of the prediction covariance Cov_{QQ} on $\Re_{\mathbf{P}}$. The actions above are given by:

$$\operatorname{Cov}_{QQ}[\cdot] = \frac{1}{N-1} \sum_{j=1}^{N} (\tau^{j} - \bar{\tau}) \langle \tau^{j} - \bar{\tau}, \cdot \rangle_{L^{2}},$$
(65a)

$$\operatorname{Cov}_{\mathbf{P}Q}[\cdot] = \frac{1}{N-1} \sum_{j=1}^{N} (\mathbf{p}^{j} - \bar{\mathbf{p}}) \langle \boldsymbol{\tau}^{j} - \bar{\boldsymbol{\tau}}, \cdot \rangle_{L^{2}}.$$
(65b)

The data misfit at iteration k of the EKI algorithm is defined as:

$$\mathfrak{E}^{k} = \|\boldsymbol{\tau}_{\text{target}} - \bar{\boldsymbol{\tau}}\|_{L^{2}(\Omega)}^{2}.$$
(66)

The prediction and analysis steps are summarised below:



Fig. 5. Template used in our numerical experiments. On the left we show the initial mesh with the embedded curve q_0 , on the right we show $\mathbb{1}_{q_0 \circ S^1}$.



Fig. 6. Synthetic targets generated using the momenta in (67). From left to right: a simple contraction, a squeezed shape with a right bias, a star and a teardrop shape. In each panel the curve divides the two coloured regions; we choose this representation for visualisation purposes.

- 1. *Prediction*: For each ensemble member *j*, compute $\tau^j = C^{-1} \mathbb{1}_{\mathcal{F}(\mathbf{p}^j)}$ and the average $\bar{\tau}$ using (63).
- 2. Analysis: Update each ensemble momentum:

$$\mathbf{p}^{j+1} = \mathbf{p}^j + \mathfrak{K}_{\mathbf{P}}(\boldsymbol{\tau}_{\text{target}} - \boldsymbol{\tau}^j).$$

6. Numerical experiments

We present numerical experiments showing that the EKI algorithm is able to find suitable approximations of a target given a random initial ensemble. Section 6.1 describes how we generate the synthetic target that we will use as matching targets. Section 6.2 summarises the parameters that we have chosen to in our experiments to match the synthetic data, and section 6.3 contains the numerical results.

6.1. Synthetic data

For simplicity we fix the template curve throughout our experiments and choose the unit circle seen in Fig. 5.

We define $\Omega_0 = [-10, 10]^2$ and let the computational domain be a triangulation \mathcal{T}_0 of Ω_0 with mesh resolution² h = 1. We have taken $\alpha = 0.5$ in (9), T = 15 time steps and have used piecewise constant finite elements on the mesh skeleton to represent **P** (although we compute only with functions supported over the submanifold $q_0 \circ S^1 \subset \mathcal{E}_h$). We use the forward operator described previously to generate synthetic targets for this set of parameters. We produce the four targets in Fig. 6 by applying the forward operator \mathcal{F} to the following four momenta:

$$\mathbf{p}_{\text{contract}}^{\dagger} = -1.38\pi, \tag{67a}$$

$$\mathbf{p}_{\text{squeeze}}^{\dagger} = \begin{cases} 5.05 \, \text{ke}^{-1} \, x < 0.05 \\ \frac{5}{2} \pi \sin(x/5) |y| & \text{otherwise} \end{cases}, \tag{67b}$$

$$\mathbf{p}_{\text{star}}^{\dagger} = 2.6\pi \cos(2\pi x/5),$$
 (67c)

$$\mathbf{p}_{\text{teardrop}}^{\dagger} = \begin{cases} -3\pi \operatorname{sign}(y) & y < 0\\ 3\pi e^{-x^2/5} & \text{otherwise} \end{cases}$$
(67d)

An example of the evolution of the template to one of the targets is shown in Fig. 7. With \mathbf{p}^{\dagger} we associate the following relative error at each iterate *k*:

$$\mathcal{R}^{k} = \|\bar{\mathbf{p}}^{k} - \mathbf{p}^{\dagger}\|_{L^{2}(q_{0} \circ S^{1})} / \|\mathbf{p}^{\dagger}\|_{L^{2}(q_{0} \circ S^{1})}.$$
(68)

The consensus deviation S^k of an ensemble at iteration k in equation (69) is defined below:

$$S^{k} = N^{-1} \sum_{j=1}^{N} \|\mathbf{p}^{j,k} - \bar{\mathbf{p}}^{k}\|_{L^{2}(q_{0} \circ S^{1})},$$
(69)

² This is the maximum diameter h_K of any triangle *K* in the triangulation.



Fig. 7. Evolution of the template in Fig. 5. The panels show the interior of the curve $\varphi_{t_k} \circ q_0$ for 12 time steps 0 < k < T using the initial momentum $\mathbf{p}^{\dagger}_{\text{teardrop}}$ in (67).

where $\mathbf{p}^{j,k}$ denotes the momentum of ensemble member *j* at iteration *k*. This quantity is a useful diagnostic which measures the information remaining in the ensemble after iteration *k*. Since EKI relies on estimates of the forecast covariance, consensus is reached when S^k approaches zero, at which point the algorithm can be stopped.

In all our simulations we invert the system in (59a) using the direct solver MUMPS [51]; investigating a preconditioned iterative solver is subject to future work. For details on the validation of the implementation of the Wu-Xu element in Firedrake, see [52, Appendix B] and the Zenodo entry [53].

6.2. Experimental setup

We now describe the setup we have used to test the EKI. Firstly, we consider the noise in (62) to be deterministic, i.e., $\eta \equiv 0$. We have taken T = 10 and $\alpha = 1$ so the parameters differ from those used to generate the synthetic targets. Recall that EKI requires an initial ensemble, in this case of momenta. The basis coefficients of the momenta was sampled from a uniform distribution over the interval [-25, 25], with different realisations for each ensemble member. We set $\xi = 10^{-3}$ in (64), although adaptive tuning of this parameter to avoid overfitting is possible; an early termination rule is suggested in [17, Equation 10]. We choose $C = i\mathbf{d} - \kappa\Delta$, $\kappa = 10$ in (66), as this smoothes out the mismatch sufficiently for our computational domain. The quality of the matching is directly related to the size and variance of the ensemble as the solution is sought as a linear combination of its members. We conduct experiments for two ensemble sizes, N = 20, N = 40 and N = 80. These were chosen since, with the parameter set as above, dim $\mathbf{P} = 48$ in order to develop an understanding of how EKI performs when the ensemble size is smaller than, similar to, and larger than the dimension of the state, while still keeping the overall computational cost such that the experiments can be done in a reasonable amount of time. The case where $N \ll \dim \mathbf{P}$ is the de facto situation for ensemble methods as the MC approximation allows for a computationally feasible method. In general, small ensemble sizes can lead to filter inbreeding (the forecast covariance is underestimated), filter divergence (the gain does not adequately correct the ensemble), or spurious correlations [54]. We comment on each of these later.

6.3. Results

We have run EKI 10 times for each value of N with different draws for the initial ensemble to assess the robustness of the algorithm with respect to the starting point. Fig. 8 shows examples of the numerical results we obtain for curve matching using EKI. Note that only five iterations of EKI were necessary to produce the results shown in this section to reach a relative tolerance below 3%. Fig. 9 shows the progression of the EKI algorithm for one of these instances. Qualitatively a larger ensemble size leads to a better match, which is to be expected. Ensemble methods such as EKI offer a practical advantage to gradient methods given their inherent parallelisability. Indeed, the *prediction* step discussed in Section 5 can be done in parallel for each ensemble member. We therefore start N processes corresponding to each member, and used a Message Passing Interface (MPI) [55] implementation to exchange information between them (the MPI *reduce* operation, specifically). Thanks to this parallelisation, five iterations of EKI take less than two minutes for N = 20, five minutes for N = 40 and 14 minutes for N = 80 on a 2021 MacBook Pro.³

Fig. 10, 11 and 12 show the relative errors, data misfits and consensus deviations for our experiments across the selected targets and ensemble sizes. These all decrease at various rates in the early iterations after which they stagnate. As the Kalman gain corrects the ensemble members, and therefore the motion of their respective curves, the data misfit decreases meaning that each member improves its prediction. This increases consensus in the ensemble, which explains what is seen in Fig. 12. We notice from the data misfits and the momentum consensus that higher values of N provide a more accurate approximation of the true momentum, which explains the accuracy of the matches seen in Fig. 8. Note that the

³ Apple M1 Pro chip, 16 GB of memory.



Fig. 8. Final reconstruction of the targets in Fig. 6 produced by EKI for N = 20 (left column), N = 40 (middle column) and N = 80 (right column).



Fig. 9. An example of EKI progression for N = 40. The algorithm takes one iteration to produce a recognisable approximation of the desired target while later iterations serve to smooth out localised mismatches.

relative error, which is a surrogate for posterior consistency, also decreases (albeit not with a clear pattern across shapes and ensemble sizes). Since the forward operator in use is heavily nonlinear, theoretical convergence results are not readily obtained at this stage. We highlight that the Kalman gain is very efficient in correcting the ensemble momenta, with the consensus decreasing exponentially in the early stages of the algorithm. We comment on this later. The conclusion is therefore that even at a modest ensemble size, EKI performs well. It is not certain that the same behaviour that we see above (i.e. few iterations are needed) will scale with N and the size of the problem, but the results are promising for research in this direction.

Higher values of ξ were found to slow the convergence of the algorithm compared to the selected value, which is consistent with the behaviour for landmark-based EKI [18], and we do not comment on it further. We noticed that the value of κ also influences the convergence of the EKI; for small values the operator $\mathbf{id} - \kappa \Delta$ approaches the identity, and since the mismatch is computed from point evaluations of the finite element function, information can be lost if the grid is not sufficiently refined. A larger value of κ "spreads out" the mismatch which improves convergence for coarser grids.

7. Summary and outlook

In this paper we have presented a parameterisation- and derivative-free method for matching closed planar curves. A moving mesh discretisation of Hamilton's equations for curves was described using the induced diffeomorphism of a vector field occupying the Wu-Xu finite element space. We also describe a transformation theory for this element facilitating a computationally performant forward model for use in the associated inverse problem. Finding the momentum encoding the forward motion of the template matches a desired curve was treated as a Bayesian inverse problem in section 5 and EKI was used to approximate its solution. The numerical results presented in section 6 suggests that the method shows great promise.

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Fig. 10. Relative error (equation (68)) as a function of EKI iterate. The columns correspond to N = 20, N = 40 and N = 80 and the rows to the targets in Fig. 6.

Not only is it easy to implement, the EKI is shown to quickly reach ensemble consensus meaning that it is efficient in exploring the subspace spanned by the initial ensemble. This is in part thanks to the momentum being a one-dimensional signal on the template. Treating the mismatch term in a negative Sobolev norm was shown to increase both accuracy of our results and robustness to mesh resolution. Further, assuming the forward operator is scalable as the mesh is refined (large-scale PDE solves are common in many areas of scientific computing), the computational burden of our approach stems from the inverse needed in the Kalman gain as it scales cubically in N [56]. However, our results showed that the proposed method is not only robust to the choice of initial ensemble but also effective even when the N is less than half the dimension of the forward problem. Therefore, only a moderate sized ensemble may be required for accurate results.

Future work includes proving convergence of the finite element discretisation for (59) and subsequently using these error estimates to quantify error in a rigorous treatment of the Bayesian inverse problem [57]. As indicated in [58], some challenges exist for nonconforming finite element methods with singular source terms. The template considered in this paper is a piece-wise linear curve. An obvious extension would be to apply isoparametric methods to cater for piece-wise higher-order polynomial curves. The effect of this would only affect the right-hand side and would

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Fig. 11. Data misfits (equation (66)) as a function of EKI iterate. The columns correspond to N = 20, N = 40 and N = 80 and the rows to the targets in Fig. 6.

not affect regularity results for the velocity. An advantage of the finite element method for curves is also that it allows for adaptivity e.g. refinement of the mesh only in the vicinity of the embedded template. We considered problems of modest size to illustrate the discretisation and the EKI. As the mesh is refined, it is likely the case that the dimension of the forward operator dwarfs the size of the ensemble and effects of the MC approximation are more pronounced. This is the case for ensemble methods for e.g. numerical weather prediction and several techniques exist to counter these effects [54] (e.g. localisation or covariance inflation). In particular, localisation methods may be suitable to assume conditional independence between separated states (i.e. parts of the shape that are distant in physical space) so as to counter spurious correlations.

Data availability

No data was used for the research described in the article.

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Fig. 12. Momentum consensus deviation (equation (69)) as a function of EKI iterate. The columns correspond to N = 20, N = 40 and N = 80 and the rows to the targets in Fig. 6.

Appendix A. Proof of Theorem 1

The momentum satisfies

$$\dot{p}_t + \nabla u_t^{\mathsf{T}} \circ q_t p_t = 0.$$

Using the ansatz we verify:

$$\begin{split} \dot{p}_t + \nabla u_t^\top \circ q_t p_t &= J_t^{-\top} p_0 + \nabla u_t^\top J_t^{-\top} p_0 \\ &= -J_t^{-\top} d(J_t^\top) J_t^{-\top} p_0 + \nabla u_t^\top \circ q_t J_t^{-\top} p_0 \end{split}$$

$$\begin{split} &= -J_t^{-\top} (dJ_t)^{\top} J_t^{-\top} p_0 + \nabla u_t^{\top} \circ q_t J_t^{-\top} p_0 \\ &= -J_t^{-\top} (\nabla u_t \circ q_t J_t)^{\top} J_t^{-\top} p_0 + \nabla u_t^{\top} \circ q_t J_t^{-\top} p_0 \\ &= -J_t^{-\top} J_t^{\top} \nabla u_t^{\top} \circ q_t J_t^{-\top} p_0 + \nabla u_t^{\top} \circ q_t J_t^{-\top} p_0 \\ &= -\nabla u_t^{\top} J_t^{-\top} p_0 + \nabla u_t^{\top} \circ q_t J_t^{-\top} p_0 \\ &= 0 \,. \end{split}$$

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