

2 **CONTROLLING TRAJECTORIES GLOBALLY VIA**  
3 **SPATIOTEMPORAL FINITE-TIME OPTIMAL CONTROL\***

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5 **Abstract.** The problems of (i) maximizing or minimizing Lagrangian mixing in fluids via the  
6 introduction of a spatiotemporally varying control velocity, and (ii) globally controlling the finite-  
7 time location of trajectories beginning at all initial conditions in a chaotic system, are considered.  
8 A particular form of solution to these is designed, which uses a new methodology for computing a  
9 spatiotemporally-dependent optimal control. An  $L^2$ -error norm for trajectory locations over a finite-  
10 time horizon is combined with a penalty energy norm for the control velocity in defining the global  
11 cost function. A computational algorithm for cost minimization is developed, and theoretical results  
12 on global error and cost presented. Numerical simulations (using velocities which are specified, and  
13 obtained as data from computational fluid dynamics simulations) are used to demonstrate the efficacy  
14 and validity of the approach in determining the required spatiotemporally-defined control velocity.

15 **Key words.** Global optimal control, Lagrangian trajectory control, chaos control, flow control,  
16 ABC flow, Navier-Stokes flow

17 **AMS subject classifications.** 49J15, 34H10

18 **1. Introduction.** In fluid mechanical systems, particles move according to a  
19 velocity field  $\mathbf{v}$  which is typically dependent on both space  $\mathbf{x}$  and time  $t$ . This field  
20 is often known only numerically, through observational data or computational fluid  
21 dynamics simulations. This has the inevitable consequence that the data is *finite-*  
22 *time*, which has resulted in a preponderance of studies on understanding the flow  
23 characteristics and important moving flow regions (‘coherent structures’) in finite-  
24 time nonautonomous flows [28, 8, 54]. Often, there is a desire to *control* the flow,  
25 usually in order to enhance or suppress mixing (e.g., in optimizing performance in  
26 mixing/combustion devices, or reducing the impact of a spreading pollutant). A  
27 specific example arises in oil recovery, where one might be interested in driving oil  
28 flows to a target region, by using the control strategy of forcing a secondary flow (a  
29 chemical slug) in certain locations [35, 62]. Current theoretical developments in the  
30 area of mixing optimization/suppression area are varied (e.g., parametric investigation  
31 of flow protocols in specific geometries in zero-flow situations [57, 45, 41], maximizing  
32 mixing [48, 24], controlling particular trajectories [5, 9] or optimizing fluid mixing  
33 across flow barriers [7, 4]). Most do not utilize *optimal control* theory to control  
34 particle trajectories, but rely on other aspects of optimization, control, or numerical  
35 methods. (Some exceptions: controlling the Navier-Stokes equations [43, 31] and  
36 multiobjective mixing control [48].) Here, we specifically examine globally controlling  
37 *trajectories* of an existing flow, whose nonautonomous velocities may only know from

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38 observational or experimental data. This is ‘one step before’ the issue of controlling  
 39 *mixing* [41, 45, 48, 24], in which diffusion also needs to be taken into account. In  
 40 this case, we are able to specify the targetted locations of *all* initial conditions after  
 41 a finite-time flow, and seek an added spatio-temporally dependent control velocity  
 42 which helps achieve this target globally.

43 Physically, the flow can be controlled by introducing additional velocities which  
 44 are spatiotemporally-dependent, e.g., by moving a solid or flexible boundary in some  
 45 specified way [19, 58], introducing fluid inlets/outlets at various locations [46, 60, 29],  
 46 displacement by chemical slugs [35, 62], or via microtransducers [32]. Thus, a control  
 47 velocity which is both spatially- and temporally-dependent is achievable physically. In  
 48 this case, since we specify eventual trajectory locations, we build a cost function which  
 49 includes both a distance norm (which captures how closely *all* particles reached the  
 50 targetted location) and a penalty term (which limits the size of the control velocity).  
 51 Assuming that the original velocity field is given (possibly in terms of data), in this  
 52 paper we develop a method for determining the spatio-temporally varying control  
 53 velocity field which minimizes the cost function. This is achieved by modifying and  
 54 adapting optimal control methods to this setting, while providing both theoretical  
 55 results and computational strategies for using our technique.

56 Many methods have been suggested in the fluid mechanics literature for different  
 57 types of flow control. These include turbulence control in various ways by conditioning  
 58 velocity gradients, energy or enstrophy [11, 31, 43, 53], drag forces [11], or boundary  
 59 layers and skin friction [34, 38]. In most of these cases, the issue is to control the  
 60 (Eulerian) velocity field, which evolves according to the Navier-Stokes equation (or  
 61 some approximation/modification). This is a challenging infinite-dimensional situa-  
 62 tion, often requiring geometry-specific methods and projections into finite dimensions  
 63 (e.g. Fourier modes or orthogonal decompositions [34, 53]). Of course, in highly  
 64 turbulent situations in which gradients are large over small scales, achieving such a  
 65 control would require velocity modifications at smaller and smaller scales, which is  
 66 impractical. Moreover, difficulties in achieving control over long-term time-horizons  
 67 are well-established [11]. In contrast to controlling Eulerian velocities which are so-  
 68 lutions to the Navier-Stokes equations, what we study in this paper is the control  
 69 of *Lagrangian trajectories* associated with such Eulerian velocity field. Given that  
 70 Lagrangian trajectories are solutions to an ordinary differential equation associated  
 71 with the Eulerian velocity, the control problem is now a *low-dimensional* one, with  
 72 dimensionality given by the spatial dimension of the flow. However, the difficulty  
 73 here is that we seek spatially *global* trajectory control at a final time, which we are  
 74 able to achieve in a certain way while taking advantage of the low-dimensionality of  
 75 the control problem. Given that control velocities can in reality be achieved only at  
 76 some spatial resolution, our methods are expected to have accuracy if the turbulence  
 77 is moderate, but not excessive.

78 While fluid mechanics is the motivation for this paper, our development is in-  
 79 dependent of it. Our methodology applies to *general systems* of ordinary differential  
 80 equations in any dimension, which are moreover either autonomous or nonautonomous  
 81 and subject to a state equation governed by a vector field  $\mathbf{v}$ . However—pertinent to  
 82 the fact that fluid mechanical systems are confined to two or three dimensions—we  
 83 only claim efficiency at low dimensions. A particular application is to the control of  
 84 chaos [42, 22, 51, 55]. Generally, chaotic systems have unpredictable trajectories, and  
 85 classical methods for chaos control include the determination of controls which result  
 86 in chaotic synchronization [30, 14] or which locally push trajectories towards unstable  
 87 ones [22, 51, 27, 52]. Since we seek to push trajectories globally over the given time

88 period, our method can be construed as a *global* control framework, in which we simul-  
 89 taneously specify the required fate of *all* trajectories in our phase space. Additionally,  
 90 we will not confine attention to equilibria (which generically do not exist anyway for  
 91 nonautonomous systems) or invariant sets such as periodic orbits, and neither will we  
 92 be concerned about the stability of such sets. Thus, instead of working within this  
 93 realm of ‘classical chaos control,’ our method targets the fate of all trajectories after  
 94 a given finite time.

95 Some background to our work comes from optimal control theory. Optimal control  
 96 methods for determining a time-dependent control function for *individual* tra-  
 97 jectories is a mature research area [33, 49, 2, 61, 1]. One class of this focuses on  
 98 obtaining different laws, e.g., feedback control theory as coverage control with dif-  
 99 fusive term [44], sliding control with mismatched uncertainties [33], synchronization  
 100 for non-autonomous chaotic system using integral control [40], global criteria via linear  
 101 state error equation [17], and via delayed term [15]. Another aspect is that of  
 102 nonautonomous system, e.g., minimum time control [13]. Classically, optimal control  
 103 methods focus on a single trajectory of an autonomous system, and often relate to  
 104 stabilizing unstable equilibria [16, 18, 25, 37]. The theoretical results are usually based  
 105 on the Pontryagin minimum (or maximum) principle and the associated Hamilton-  
 106 Jacobi-Bellman partial differential equations. In this work, we extend optimal control  
 107 to the problem of determining a *spatiotemporally-dependent* control, to *globally* control  
 108 trajectories over a finite time. By ‘globally,’ we mean that we can specify the fate of  
 109 initial conditions as a global function on the initial space, rather than, for example,  
 110 insisting that all initial conditions go to *one* invariant set [22, 51, 52, e.g.]. Moreover,  
 111 the method works for general nonautonomous (unsteady) vector fields, and thus is  
 112 not dependent on the presence of fixed points, periodic orbits or chaotic attractors.

113 The remainder of this paper is organized as follows. The problem and its theoret-  
 114 ical solution is outlined in Section 2. We develop both the computational methodol-  
 115 ogy for determining a spatiotemporal optimal control function, as well as theoretical  
 116 results indicating the robustness of the procedure and error analyses on the achieve-  
 117 ment of the finite-horizon target. The algorithm we develop includes novel uses of  
 118 the Newton-Raphson algorithm and an ‘approximant’ [20] method to determine the  
 119 control function spatiotemporally. Section 3 demonstrates the efficacy of the spa-  
 120 tiotemporal optimal control in several examples. We demonstrate the ease of imple-  
 121 mentation of our algorithm, as well as validate the theoretical results concerning the  
 122 target achievement, and the cost function. The proofs of the theoretical results of  
 123 Section 2 are separated out for easy readability of the paper, and given in Section A.  
 124 Finally, in Section 4 we briefly remark on potential extensions of this work.

125 **2. Spatiotemporal optimal control.** Suppose we are given a nonautonomous  
 126 nonlinear state equation

$$127 \quad (2.1) \quad \dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t) \quad ; \quad t \in [0, T],$$

128 where  $\mathbf{x} \in \Omega$ , and  $\Omega$  is an open and bounded subset of  $\mathbb{R}^n$ . We will assume that  
 129  $\mathbf{v}$  is smooth, and that solutions to (2.1) exist for all  $t \in [0, T]$  (thereby precluding  
 130 issues such as ‘blow-up in finite-time’ [56]). For  $\mathbf{v}$  obtained on a spatio-temporal grid  
 131 instead, we imagine that  $\mathbf{v}$  is smoothly extended to the subgrid level (a strategy that  
 132 is usually done when computing trajectories in such cases; see the citations in [8, 28]).  
 133 Since such an extension may give values of  $\mathbf{v}$  which are in reality inaccurate, we will  
 134 (in Theorem 2.4) establish that our method is robust towards these errors.

135 Our goal is to find an additive spatiotemporal control  $\mathbf{c}(\mathbf{x}, t)$  such that initial

136 conditions  $\mathbf{x}_0$  at  $t = 0$ , in a restricted domain  $\Omega_0 \subseteq \Omega$ , approach at the final time  $T$   
 137 specified target locations, which are identified via a globally defined target function  
 138  $\Theta : \Omega_0 \rightarrow \mathbb{R}^n$ . This target function must be *achievable* in that it is generated by a flow  
 139 (i.e., there exists a velocity field  $\mathbf{u}(\mathbf{x}, t)$  such that the flow map of  $\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t)$  from time  
 140 0 to  $T$  is  $\Theta(\mathbf{x})$ ). In particular,  $\Theta$  cannot demand flow trajectories which must cross  
 141 each other, or reverse orientation in other ways. (For example, setting  $\Theta(x) = -x$   
 142 if  $x \in \mathbb{R}$  is unachievable, since this requires trajectories to cross each other—which  
 143 is impossible for a flow.) However, we may specify  $\Theta$  to have jump discontinuities,  
 144 enabling for example steering trajectories into three different target locations. We  
 145 emphasize that there is no restriction to equilibria or other specialized trajectories of  
 146 (2.1), but we rather seek to steer *all* trajectories globally to *any* achievable specified  
 147 locations by time  $T$ . The controlled nonautonomous state equation will take the form

$$148 \quad (2.2) \quad \dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t) + \mathbf{c}(\mathbf{x}, t) \quad ; \quad t \in [0, T],$$

149 where we use the notation  $\mathbf{c}(\mathbf{x}, t)$  for the control. In the standard language of fluid  
 150 mechanics, this represents the control velocity in the ‘natural’ Eulerian coordinate  $\mathbf{x}$ ,  
 151 based on information from the Lagrangian trajectories of (2.1). We will denote by  
 152  $\mathbf{x}(\mathbf{x}_0, t)$  solutions of (2.2) at time  $t \in [0, T]$  subject to the initial condition  $\mathbf{x}_0$  at time  
 153 0. The optimal control problem globally on the  $t = 0$  spatial domain  $\Omega_0$  can then  
 154 be posed as the determination of the control  $\mathbf{c}$  (defined on a spatiotemporal domain  
 155  $(\mathbf{x}, t)$ ) which minimizes the cost function

$$156 \quad (2.3) \quad G := \int_{\Omega_0} \left[ \|\mathbf{x}(\mathbf{x}_0, T) - \Theta(\mathbf{x}_0)\|^2 + \eta \int_0^T \|\mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t)\|^2 dt \right] d\mathbf{x}_0,$$

157 in which  $\|\cdot\|$  is the standard Euclidean norm and  $\eta > 0$  encapsulates the penalty for  
 158 the energy contained in  $\mathbf{c}$  over the time period  $[0, T]$ . This regularizes the problem  
 159 (and hence jump discontinuities are specifiable in  $\Theta$ ; these will be approximately  
 160 achieved when minimizing  $G$  for small but nonzero  $\eta$ ).

161 We will develop a method for solving the minimization problem numerically for  
 162 any given initial domain  $\Omega_0$ , final time  $T$ , evolution law  $\mathbf{v}$  defined on  $[0, T]$ , target  
 163 function  $\Theta$ , and energy parameter  $\eta$ . We will moreover provide theoretical estimates  
 164 on how the error in achieving the target decays with time and  $\eta$ . We also remark  
 165 that within this formulation (specifically attempting to find a control velocity in  
 166 the form  $\mathbf{c}(\mathbf{x}, t)$  for minimizing the spatially-integrated cost function  $G$ ), proceed-  
 167 ing through the Hamilton-Jacobi-Bellman approach directly is unfeasible because a  
 168 numerical minimization is required within the partial differential equation. We instead  
 169 adopt an approach which uses different established methods (from optimal control,  
 170 fluid mechanics, differential equations theory, computer visualization) in an unusual  
 171 way.

172 For  $\mathbf{x}_0 \in \Omega$ , we define

$$173 \quad (2.4) \quad g(\mathbf{x}_0) := \|\mathbf{x}(\mathbf{x}_0, T) - \Theta(\mathbf{x}_0)\|^2 + \eta \int_0^T \|\mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t)\|^2 dt,$$

174 and note that  $G = \int_{\Omega_0} g(\mathbf{x}_0) d\mathbf{x}_0$ . Since  $g \geq 0$  for all  $\mathbf{x}_0 \in \Omega$ , minimizing  $G$  can be  
 175 accomplished by minimizing  $g$  at each  $\mathbf{x}_0$ —a canonical optimal control problem—and  
 176 then combining the results. (There is a caveat to this statement, which we will return  
 177 to in describing the process in more detail subsequently.) Now, once minimizing  $g$  has  
 178 been achieved for a particular initial condition  $\mathbf{x}_0$ , it will result in a control  $\mathbf{c}$  defined

179 along the specific trajectory  $(\mathbf{x}(\mathbf{x}_0, t), t)$  of spacetime. Subsequently, we will detail a  
 180 method for concatenating the results for each such  $\mathbf{x}_0$  to be able to define  $\mathbf{c}$  across all  
 181 (relevant) spacetime  $(\mathbf{x}, t)$ .

182 **THEOREM 2.1** (Single-trajectory optimal control). *For  $\mathbf{x}_0$  fixed in  $\Omega$ , any opti-*  
 183 *mal control  $\mathbf{c}$  locally minimizing (2.4) is representible as*

$$184 \quad (2.5) \quad \mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t) = -\frac{1}{2\eta}\mathbf{p}(t) \quad ; \quad t \in [0, T],$$

185 *in which the conjugate momentum  $\mathbf{p}$  obeys the coupled system*

$$186 \quad (2.6) \quad \left. \begin{aligned} \dot{\mathbf{x}} &= \mathbf{v}(\mathbf{x}, t) - \frac{1}{2\eta}\mathbf{p} \\ \dot{\mathbf{p}} &= -[\nabla\mathbf{v}(\mathbf{x}, t)]^\top \mathbf{p} \end{aligned} \right\}$$

187 *subject to the implicitly-defined initial and end conditions*

$$188 \quad (2.7) \quad \left. \begin{aligned} \mathbf{x}(0) &= \mathbf{x}_0 \\ \mathbf{p}(T) &= 2(\mathbf{x}(T) - \Theta(\mathbf{x}_0)) \end{aligned} \right\}.$$

189 Here,  $[\cdot]^\top$  denotes the matrix transpose, and  $\nabla\mathbf{v}$  is the  $n \times n$  matrix derivative of  $\mathbf{v}$   
 190 with respect to the spatial variable  $\mathbf{x}$ .

191 *Proof.* See Section A.1; this is an elementary application of optimal control.  $\square$

192 The fact that the condition on  $\mathbf{p}$  in (2.7) is an *end* condition (while that of  $\mathbf{x}$   
 193 is an initial condition), and moreover depends on the unknown value  $\mathbf{x}(T)$ , neces-  
 194 sitates some care when solving (2.6)-(2.7) numerically. Methods such as indirect  
 195 shooting, multiple shooting, collocation approaches, as well as sequential, simultane-  
 196 ous or direct transcription have been suggested for this well-known problem. While  
 197 indirect methods suffer difficulties in acquiring a good initial guess and in repeated  
 198 differentiation, the discretization associated with direct methods tends to obtain less  
 199 accurate solutions. Here, we opt for a Newton-Raphson based (indirect) method  
 200 which, as we demonstrate, has quick convergence. Having guessed an initial condition  
 201  $\mathbf{q} := \mathbf{p}(0) \in \mathbb{R}^{2n}$ , we implement (2.6) in forward time (in this case, we use the built-  
 202 in ordinary differential equation solvers in Matlab<sup>TM</sup>), and consequently, determine  
 203  $\mathbf{x}(T)$  and  $\mathbf{p}(T)$  for that initial choice. Given that these depend on the initial guess  $\mathbf{q}$ ,  
 204 we use the notation  $\mathbf{x}(T, \mathbf{q})$  and  $\mathbf{p}(T, \mathbf{q})$  respectively, and define

$$205 \quad (2.8) \quad \mathbf{F}(\mathbf{q}) := \mathbf{p}(T, \mathbf{q}) - 2\mathbf{x}(T, \mathbf{q}) + 2\Theta(\mathbf{x}_0).$$

206 If we find a root  $\mathbf{q}$  of  $\mathbf{F}$ , this is a correct initial condition  $\mathbf{p}(0)$  to use to generate  $\mathbf{c}$   
 207 from (2.5). To find such a  $\mathbf{q}$ , we make an initial guess  $\mathbf{q}_0$ , and choose a small quantity  
 208  $\delta$ . We then take the  $2n$  ‘nearest neighbors’ of  $\mathbf{q}_0$ , i.e.,  $\mathbf{q}_0 \pm \delta\mathbf{e}_i$  for  $i = 1, 2, \dots, n$   
 209 where the  $\mathbf{e}_i$ s are the rectangular basis elements on  $\mathbb{R}^{2n}$ . Given  $\mathbf{x}(0) = \mathbf{x}_0$  and each  
 210 of these initial conditions for  $\mathbf{p}$ , we then advect (2.6) numerically forward to time  $T$ .  
 211 We can now calculate the value of  $\mathbf{F}$  using  $\mathbf{q} = \mathbf{q}_0$ , and can use the results of all the  
 212 nearest neighbor advections to numerically evaluate each of the values  $\mathbf{F}(\mathbf{q}_0 \pm \delta\mathbf{e}_i)$ ,  
 213 and hence estimate the matrix  $\nabla\mathbf{F}(\mathbf{q}_0)$  using standard finite-differencing. We then  
 214 make an improved guess for the root  $\mathbf{q}$  (which we call  $\mathbf{q}_1$ ) using the Newton-Raphson  
 215 method. More concretely, we go from our  $j$ th guess to the  $(j + 1)$ st guess by

$$216 \quad (2.9) \quad \mathbf{q}_{j+1} = \mathbf{q}_j - \left([\nabla\mathbf{F}(\mathbf{q}_j)]^{-1}\right)^\top \mathbf{F}(\mathbf{q}_j),$$

217 and stop the process once  $\|\mathbf{F}(\mathbf{q}_j)\|$  is smaller than a specified threshold. The corre-  
 218 sponding solution  $\mathbf{p}(t)$  then gives us the required (single-trajectory) control  $\mathbf{c}$  using  
 219 (2.5).

220 Thus, for any  $\mathbf{x}_0 \in \Omega_0$ , we can determine the solution trajectories  $\mathbf{x}(\mathbf{x}_0, t)$ . To  
 221 quantify how we approach the target at time  $T$ , we define the global target error

$$222 \quad (2.10) \quad E(t) := \left( \int_{\Omega_0} \|\mathbf{x}(\mathbf{x}_0, t) - \Theta(\mathbf{x}_0)\|^2 d\mathbf{x}_0 \right)^{1/2}$$

223 for times  $t \in [0, T]$ . We note that  $E(0)$  is the  $L^2(\Omega_0)$ -norm of the function  $\mathbf{x}_0 - \Theta(\mathbf{x}_0)$ ,  
 224 and can be assumed known from the problem statement. We now characterize, in  
 225 terms of ‘given’ quantities (i.e., information about  $\mathbf{v}$ ,  $\Omega$ ,  $T$ ,  $\eta$  and  $\Theta$ ), the rate at  
 226 which  $E(t)$  approaches its final value  $E(T)$ . We first require to define some norms for  
 227 functions  $\mathbf{h} : \Omega \times [0, T] \rightarrow \Omega$ . If  $\|\cdot\|$  is the standard Euclidean norm in  $\mathbb{R}^n$ , let

$$228 \quad (2.11) \quad \|\mathbf{h}\|_a := \sup_{(\mathbf{x}, t) \in \Omega \times [0, T]} \|\mathbf{h}(\mathbf{x}, t)\|, \text{ and}$$

$$229 \quad (2.12) \quad \|\mathbf{h}\|_b := \sup_{(\mathbf{x}, t) \in \Omega \times [0, T]} \sup_{\mathbf{y} \in \Omega, \mathbf{y} \neq \mathbf{0}} \frac{\|\nabla \mathbf{h}^\top(\mathbf{x}, t) \mathbf{y}\|}{\|\mathbf{y}\|}.$$

230 **THEOREM 2.2** (Global error decay). *If there exists constants  $A$  and  $B$  such that*  
 231  $\|\mathbf{v}\|_a \leq A < \infty$  *and*  $\|\mathbf{v}\|_b \leq B < \infty$ , *then the rate of decay of*  $E(t)$  *to*  $E(T)$  *obeys*

$$232 \quad (2.13) \quad |E(t) - E(T)| \leq \sqrt{2} \left[ A \sqrt{\mu(\Omega_0)}(T-t) + \frac{E(T)}{\eta} \frac{(e^{B(T-t)} - 1)}{B} \right],$$

233 where  $\mu(\Omega_0)$  is the standard Lebesgue measure on  $\Omega_0$ .

234 *Proof.* See Section A.2. □

235 As  $t$  approaches  $T$ ,  $E(t)$  approaches  $E(T)$  due to two effects: a linear rate which  
 236 is characterized by  $\|\mathbf{v}\|_a$ , and an exponential rate which is characterized by  $\|\mathbf{v}\|_b$ . We  
 237 emphasize that these results hold even if  $\Theta$  is discontinuous (as we will demonstrate  
 238 in Section 3).

239 Next, we address  $\eta$ -dependence in the cost and global error. By choosing  $\eta$  smaller  
 240 and smaller, since the penalization of the control velocity  $\mathbf{c}$  is reduced in (2.3), one  
 241 can achieve a target  $\Theta$  with infinitesimal accuracy by choosing  $\mathbf{c}$  closer and closer to  
 242 the exact value  $\mathbf{u} - \mathbf{v}$ , where  $\mathbf{u}$  is the velocity field which engenders the flow map  $\Theta$   
 243 when considering the flow from time 0 to  $T$ . Thus,  $E(T)$  decreases with  $\eta$ . We now  
 244 establish a relationship with the decay of the total cost  $G$ .

245 **THEOREM 2.3** (Comparative  $\eta$ -dependence). *Suppose the hypotheses of Theo-*  
 246 *rem 2.2 are satisfied. If there exists*  $\alpha > 1/2$  *such that*

$$247 \quad \lim_{\eta \downarrow 0} \frac{E(T)}{\eta^\alpha} < \infty, \text{ then } \lim_{\eta \downarrow 0} \frac{G}{\eta^{2\alpha-1}} < \infty.$$

248 *Proof.* See Section A.3. □

249 If we know that the global error decays as  $\mathcal{O}(\eta^\alpha)$ , then the total cost will decay  
 250 as  $\mathcal{O}(\eta^{2\alpha-1})$ . We note that if  $\alpha = 1$ , Theorem 2.3 implies that  $E(T)$ ’s  $\mathcal{O}(\eta)$  decay  
 251 implies that  $G$  also has  $\mathcal{O}(\eta)$  decay. We will demonstrate this particular behavior in  
 252 our numerical simulations.

253 Next, we address the issue of how to determine  $\mathbf{c}$  as a spatiotemporal function.  
 254 By the process associated with using Theorem 2.1 and the Newton-Raphson method  
 255 (2.9), given any initial condition  $\mathbf{x}_0 \in \Omega$ , we can find the optimal control function  
 256  $\mathbf{c}$ 's values along the spacetime curve  $(\mathbf{x}(\mathbf{x}_0, t), t)$ . By doing this for a grid of initial  
 257 conditions  $\mathbf{x}_0 \in \Omega_0$ , we generate a collection of such spacetime curves along which we  
 258 know the value of  $\mathbf{c}$ . We now seek  $\mathbf{c}$  as a spatiotemporal function (i.e., as a function on  
 259  $(\mathbf{x}, t)$ ). In doing so, we make the assumption that the generated spacetime curves are  
 260 *consistent*, that is, should any two curves intersect in spacetime, the determined values  
 261 of  $\mathbf{c}$  at the point of intersection by following along either of the curves should give the  
 262 identical value. (Since numerical approximation is being used, exactly identical is not  
 263 necessary, but rather these should agree to within the resolution sought.) This is the  
 264 caveat necessary to ensure that minimizing  $g$  and then extending to all spacetime is  
 265 equivalent to minimizing the global cost  $G$ .

266 Now, performing numerical interpolation proves to be ineffective and difficult be-  
 267 cause the spacetime curves do not uniformly traverse spacetime. Moreover, given the  
 268 possibility that the function  $\Theta$  is nonsmooth (e.g., if different collections of initial con-  
 269 ditions are steered towards, say, two different points—this example shall be shown in  
 270 our simulations in Section 3), the consequent roughness of  $\mathbf{c}$  results in wild oscillations  
 271 in the interpolants. Thus, we instead use an *approximant* for  $\mathbf{c}$  based on knowledge  
 272 of the values of  $\mathbf{c}$  along the collection of nonuniformly distributed spacetime curves.  
 273 This is achieved easily in two-dimensions in Matlab<sup>TM</sup> by using the package `gridfit`  
 274 [20], which regularizes the interpolation problem in seeking a smoother surface fitting  
 275 for  $\mathbf{c} = \mathbf{c}(\mathbf{x}, t)$ . (The basic idea, described in detail in [20], is to fit an elastic plate  
 276 approximately through the given points, with a stiffness parameter which penalizes  
 277 deviation from the points.) Throughout this work we use the Laplacian as the regu-  
 278 larizer (the Laplacian integrated over the fitted surface is to be kept small [20]). An  
 279  $N$ -dimensional version of this, `regularizeNd`, has also been developed [47], and is  
 280 what we use when we consider higher-dimensional situations in our examples.

281 Using our theoretical results, we can comment on the robustness of the process  
 282 in the following sense. Suppose that instead of  $\mathbf{v}$ , the true governing vector field is  $\tilde{\mathbf{v}}$ ,  
 283 where while  $\tilde{\mathbf{v}}$  is unknown, we know that it is ‘close’ to  $\mathbf{v}$  (for estimates on Lagrangian  
 284 trajectory uncertainty resulting from this, see [6]). This is inevitable if  $\mathbf{v}$  were known  
 285 from data; even if know *exactly* at the gridpoints,  $\mathbf{v}$  would need to be interpolated  
 286 in some way at the subgrid level when performing trajectory calculations. Moreover,  
 287 the values at the gridpoints, if obtained from experimental or observational data, will  
 288 carry their own measurement errors. Thus, there will always be an error in  $\mathbf{v}$  when  
 289 considered over the domain  $\Omega \times [0, T]$ .

290 **THEOREM 2.4** (Robustness to uncertainties in  $\mathbf{v}$ ). *Suppose there exists  $\epsilon > 0$*   
 291 *such that  $\|\mathbf{v} - \tilde{\mathbf{v}}\|_a < \epsilon$  and  $\|\mathbf{v} - \tilde{\mathbf{v}}\|_b < \epsilon$ . If the ‘tilde’ variables are the quantities*  
 292 *associated with using  $\tilde{\mathbf{v}}$  rather than  $\mathbf{v}$  in calculations of the control velocity, global*  
 293 *error, and cost, then*

$$294 \quad (2.14) \quad \left. \begin{aligned} \mathbf{c}(\mathbf{x}, t) &= \tilde{\mathbf{c}}(\mathbf{x}, t) + \mathcal{O}(\epsilon) \quad \text{in } \Omega \times [0, T], \\ E(T) &= \tilde{E}(T) + \mathcal{O}(\epsilon) \quad \text{and} \\ G &= \tilde{G} + \mathcal{O}(\epsilon). \end{aligned} \right\}$$

295 *Proof.* See Section A.4. □

296 Theorem 2.4 ensures that, since we follow our procedure by using  $\mathbf{v}$  rather than  
 297 the unknown (but  $\mathcal{O}(\epsilon)$ -close)  $\tilde{\mathbf{v}}$ , all relevant computed quantities are similarly  $\mathcal{O}(\epsilon)$ -  
 298 close to the ‘true’ values. This suggests a (specific type) of robustness of the procedure:

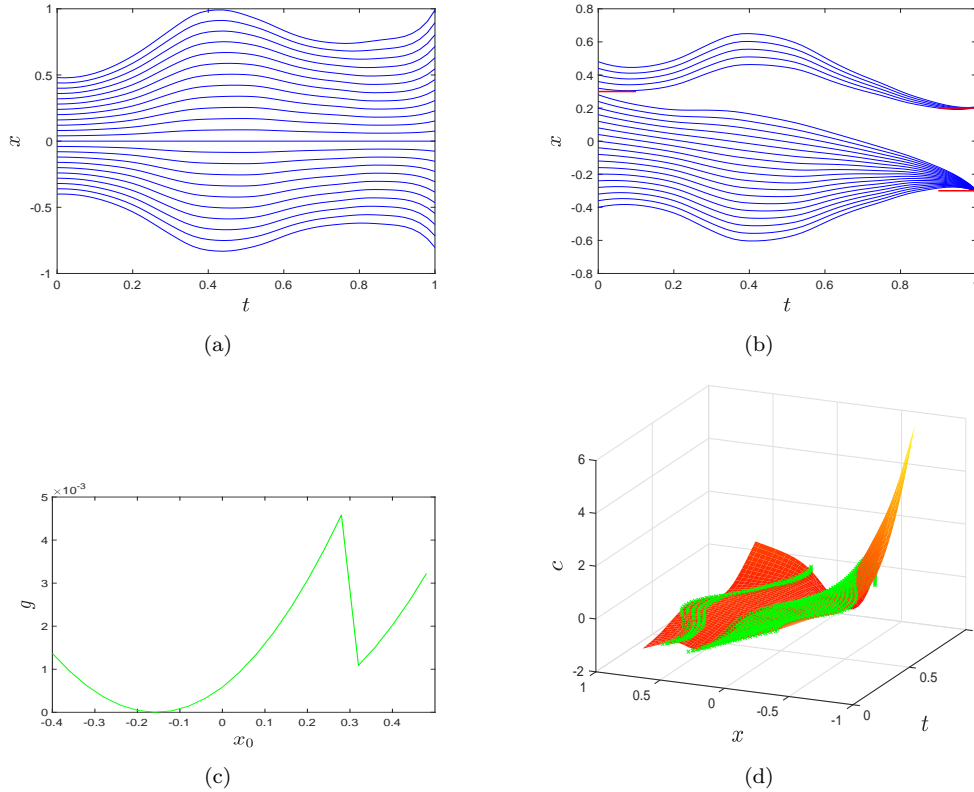


FIG. 1. Spatiotemporal control for (3.1). (a) uncontrolled, (b) controlled to approach two points, (c) cost distribution, and (d) spatiotemporal control function.

299 results will be correct to the same order of uncertainty as in  $\mathbf{v}$ .

300 We have thus developed a methodology for determining a spatiotemporal control  
 301 in finite-time, in relation to globally defined targets, by a process of utilizing an  
 302 unusual viewpoint and methodology to the optimal control discipline. Our algorithm  
 303 is summarized below.

- 304 1. Reduce the spatiotemporal minimization problem (2.3) to individual single-  
 305 trajectory optimal control problems related to minimization of (2.4);
- 306 2. Solve the resulting initial/end-condition problem (as identified in Theorem 2.1) ■  
 307 by using the Newton-Raphson algorithm detailed in (2.9) for each initial con-  
 308 dition, thereby determining the trajectory  $\mathbf{x}(\mathbf{x}_0, t)$  and the control  $\mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t)$ ; ■
- 309 3. Amalgamate the results for each initial condition by applying the `gridfit`  
 310 [20] or `regularizeNd` [47] method to approximate the spatiotemporal control  
 311  $\mathbf{c}$  as a function of  $(\mathbf{x}, t)$ ;
- 312 4. This algorithm is supported by the theoretical conditions on the decay of  
 313  $|E(t) - E(T)|$ , and the  $\eta$ -dependence of  $E(T)$  and  $G$ , and robustness towards  
 314 deviations in  $\mathbf{v}$ .

315 **3. Simulations.** In this Section, we present several simulations which demon-  
 316 strate the ease at which the spatiotemporal control can be computed, and moreover  
 317 validate the theoretical results on  $\eta$ -dependence and decay rates.



318 **3.1. A one-dimensional example.** For  $x \in \mathbb{R}$ , and  $t \in [0, 1]$ , let

$$319 \quad (3.1) \quad v(x, t) = x \sin(7t + 0.3) w_1(t) - 4x^3 \cos(5t) w_2(t),$$

320 in which some roughness to the velocity is obtained by implementing on a time-scale  
 321  $\Delta t = 0.02$  a specific realization of stochasticity via  $w_1(t) = 3U_1(t) + 0.5$  and  $w_2(t) =$   
 322  $2U_2(t) - 2$ , where the  $U_i(t)$  are independently chosen from the uniform distribution on  
 323  $[0, 1]$ . We show in Fig. 1(a) the result of implementing (2.1) for  $x_0 \in \Omega_0 = [-0.4, 0.5]$ .  
 324 We first define  $\Theta(x_0) = 0.2$  for  $x_0 \geq 0.3$  and  $\Theta(x_0) = -0.3$  for  $x_0 < 0.3$ , which  
 325 separates  $\Omega_0$  at 0.3, and aims to send each segment of initial conditions towards a  
 326 different target point. By using  $\eta = 0.01$  and  $\delta = 10^{-5}$  and implementing part (2)  
 327 of our algorithm, we obtain excellent approach to our targets (red lines near  $t = 1$ ),  
 328 as shown in Fig. 1(b). The desired separation point at  $x_0 = 0.3$  is shown by the red  
 329 line near  $t = 0$ . The distribution of the required costs for each initial condition  $x_0$   
 330 (i.e., (2.4) is shown in Fig. 1(c); the trajectory beginning near  $-0.15$  requires hardly  
 331 any adjustment, and there is a sharp transition in the cost near  $x_0 = 0.3$  because  
 332 it is necessary to split the trajectories in different directions. The computed control  
 333  $\mathbf{c}$  for each trajectory is shown in spacetime as the green curves in Fig. 1(d). The  
 334 red surface—which approximates  $c(x, t)$  across the spacetime domain based on the  
 335 information at the green values—is obtained by applying `gridfit` with its default  
 336 parameters. We note from Figs. 1(b) and (d) that although this process allows us to  
 337 determine  $c$  on a connected spatiotemporal domain (i.e., the domain associated with  
 338 the red surface in Fig. 1(d)), in reality its values on the wedge into which trajectories  
 339 do not enter (because of the separation achieved by the process) are irrelevant.

340 In Fig. 2(a), we show by the red circles the cost  $G$  as  $\eta$  is varied. Performing linear  
 341 regression on the 10 smallest values of  $\eta$  yields the green line, whose slope indicates  
 342 that  $G \sim \eta^{1.0782}$ . We similarly analyze the final target error  $E(T)$ 's decay with  $\eta$  in  
 343 Fig. 2(b), and regression reveals that  $E \sim \eta^{0.9447}$ . Thus, these are consistent with  
 344 choosing  $\alpha \approx 1$  in Theorem 2.3. We next demonstrate the error decay with time in  
 345 Fig. 2(c). Rapid decay as  $t \rightarrow T$  is displayed, and in all other implementations (not  
 346 shown), as predicted by (2.13).

347 We finally briefly illustrate the impact of choosing different target functions  $\Theta$   
 348 in Fig. 3, noting that  $\Theta$  must be a monotonic function to avoid trajectories having  
 349 to cross each other. Excellent results are achieved with these parameters, with costs  
 350  $G \sim 10^{-3}$  in both instances.

351 **3.2. A two-dimensional example.** For  $\mathbf{x} = (x, y) \in \mathbb{R}^2$ , suppose that

$$352 \quad (3.2) \quad \mathbf{v}(\mathbf{x}, t) = \begin{pmatrix} v_1(x, y, t) \\ v_2(x, y, t) \end{pmatrix} = \begin{pmatrix} 2x + ty \\ \sin y - t \end{pmatrix},$$

353 and let the initial time set be  $\Omega_0 = [-1, 1] \times [0, 1]$ , to be advected to time  $T = 1$ . We  
 354 specify as our target function

$$355 \quad (3.3) \quad \Theta(\mathbf{x}_0) = \begin{pmatrix} \frac{x_0^2}{4} + y_0 \\ \cos x_0 - 2x_0y_0 \end{pmatrix}.$$

356 There is no difficulty in implementing our methodology in this two-dimensional situa-  
 357 tion (once again, our default values are  $\eta = 0.01$  and  $\delta = 10^{-5}$ ). We show in Fig. 4(a)  
 358 and (b) the uncontrolled and controlled trajectory evolution respectively; this imple-  
 359 mentation incurs a cost of  $G = 0.0317$ , and the target error  $E(T) = 0.0069$ . As a

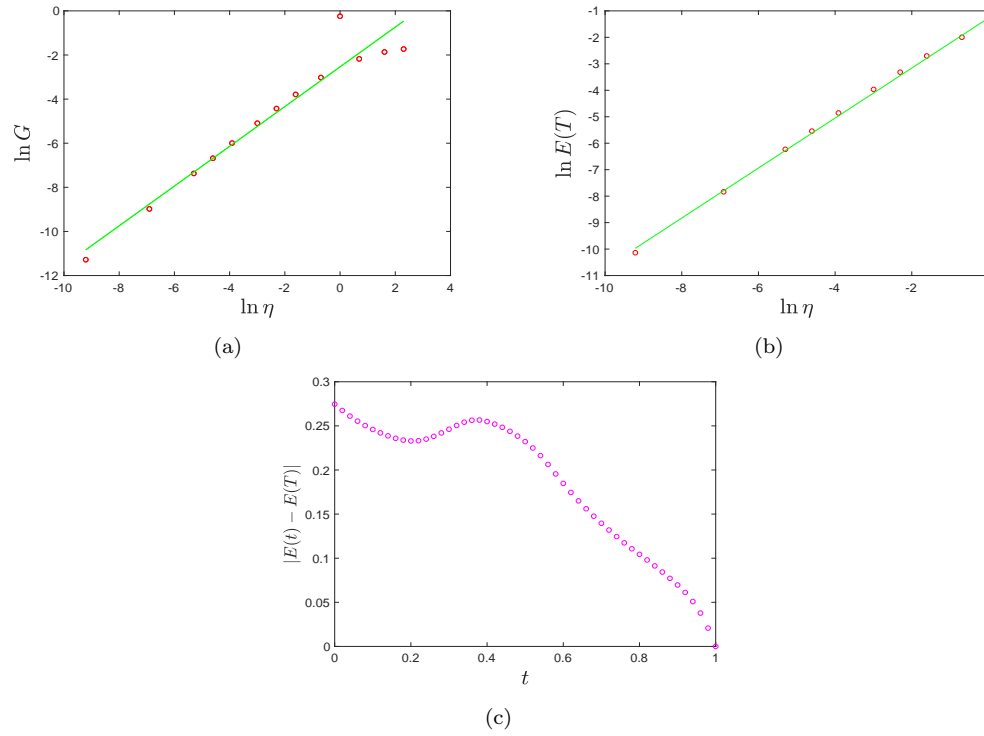


FIG. 2. Analysis for the optimal control associated with Fig. 1: (a) dependence of cost on  $\eta$ , (b) decay of  $E(T)$  as  $\eta$  is reduced, and (c) error decay as per Theorem 2.2.

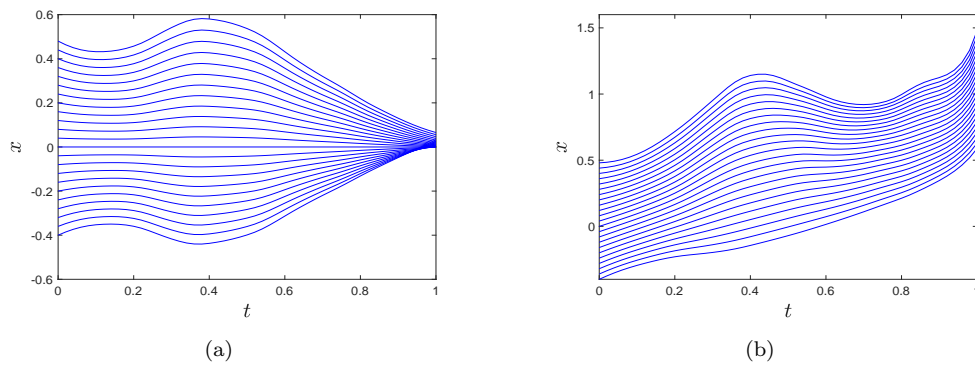


FIG. 3. Different target functions applied to (3.1). (a)  $\Theta(x_0) = x_0^2/4$  ( $G = 0.00134$ ), and (b)  $\Theta(x_0) = x_0 + 1$  ( $G = 0.00477$ ).

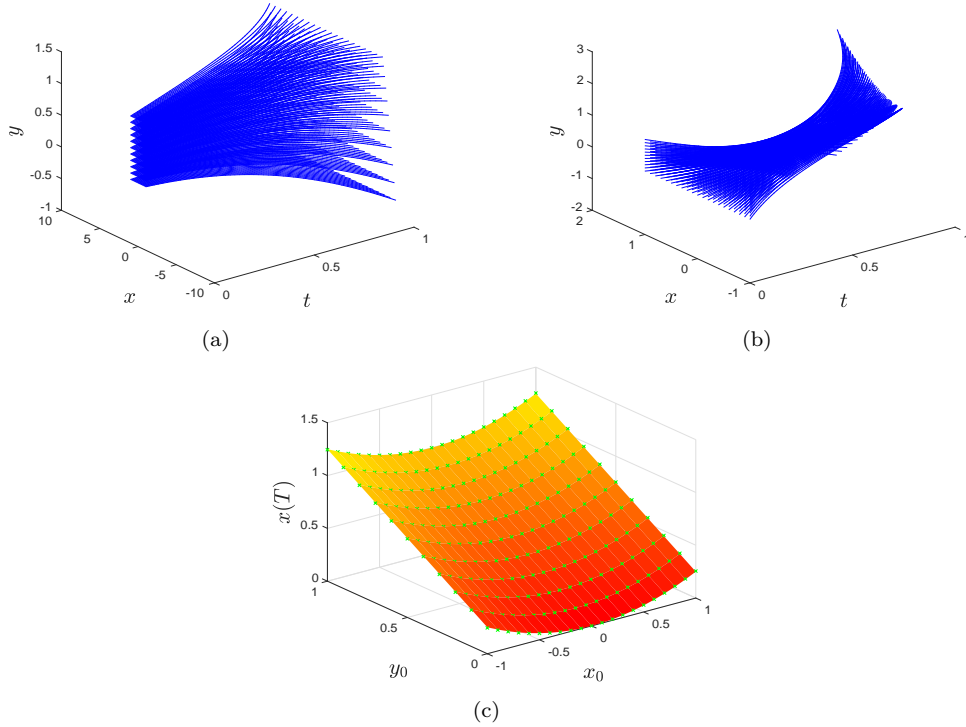


FIG. 4. (a) Flow associated with (3.2); (b) the controlled flow from our algorithm subject to the target function (3.3); (c) target  $x$ -value surface [orange], and achieved values [green crosses].

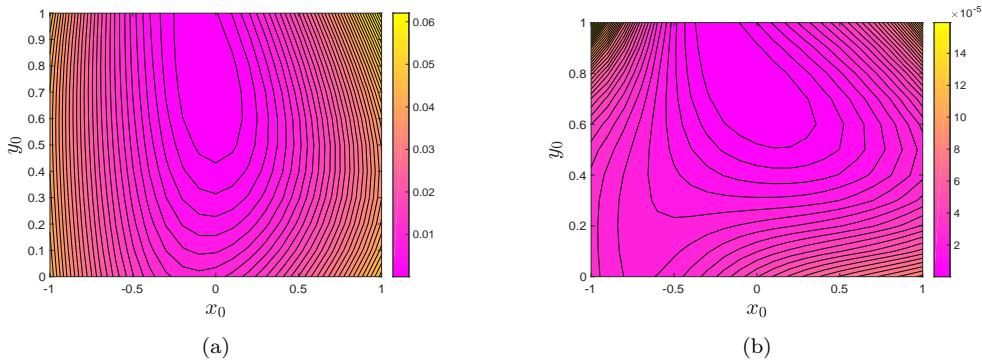


FIG. 5. The distribution of contributions to (a) the cost  $G$ , and (b) the total error  $E(T)$ , over points  $(x_0, y_0) \in \Omega$  for the two-dimensional example.

360 sample to demonstrate the achievement of the target locations, we shown in Fig. 4(c)  
 361 how the controlled final location (green crosses) is close to the target  $x$ -coordinate  
 362 (orange surface) for  $(x_0, y_0) \in \Omega_0$ .

363 The total cost  $G$  and final target error  $E(T)$  are composed by integrating over  
 364  $\Omega_0$ . The distribution of the contributions to each of these integrals with  $(x_0, y_0) \in \Omega_0$   
 365 are shown in Fig. 5. The largest contributions to each of these occurs along the sides  
 366 of  $\Omega_0$ ; this is since the middle regions require the least effort to control for this chosen

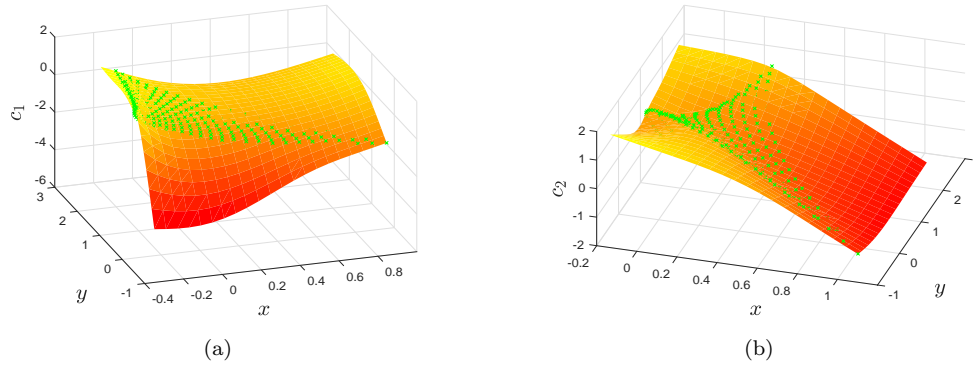


FIG. 6. Computed control function  $\mathbf{c} = (c_1, c_2)$  illustrated by green crosses, with the orange surfaces indicating its approximant: (a)  $c_1(x, y, t = 0.58)$  and (b)  $c_2(x, y, t = 0.78)$ . Different viewing angles are used for better visibility.

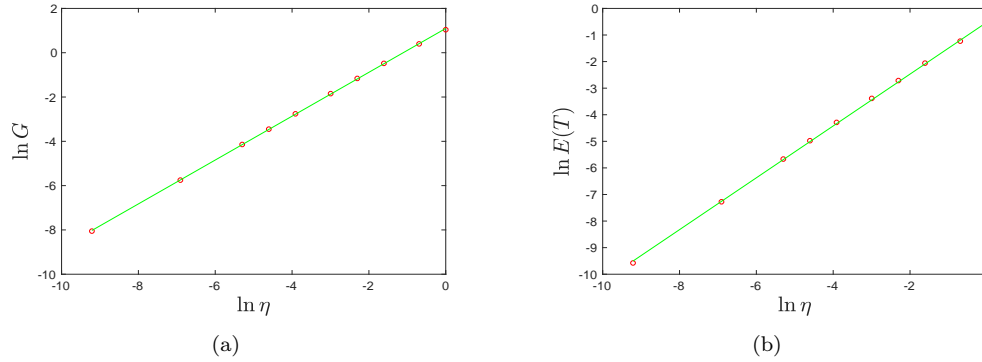


FIG. 7. The variation of (a) the cost  $G$  and (b) the error  $E(T)$  with  $\eta$  for the two-dimensional example.

367 target function.

368 Visualizing the control  $\mathbf{c} = (c_1, c_2)$  as a function of  $(x, y, t)$  requires higher-  
 369 dimensions. Instead, in Fig. 6, we show computed values of  $c_1$  and  $c_2$  at different  
 370 instances in time. The green crosses are the computed values based on our algorithm  
 371 for single-trajectory optimal control, while the orange surface indicates the result of  
 372 applying `gridfit` [20] to obtain approximating functions. While visualizing the full  
 373 control is difficult, the computations did not present any significant difficulty.

374 Finally, we validate  $\eta \rightarrow 0$  behavior in Fig. 7. The fitted regression lines (green)  
 375 give the facts that  $G \sim \eta^{0.990}$  and  $E(T) \sim \eta^{0.975}$ . Thus, both the cost  $G$  and the final  
 376 error  $E(T)$  demonstrate the behavior as intimated in Theorem 2.3 with  $\alpha \approx 1$ .

377 **3.3. ABC flow.** Having validated our theorems in several elementary flows, we  
 378 next investigate the flow associated with an exact solution to the three-dimensional  
 379 steady Euler equations of fluid motion: Arnold-Beltrami-Childress (ABC) flow, whose  
 380 velocity field is given by [3, 21]

$$381 \quad (3.4) \quad \mathbf{v}(\mathbf{x}) = \begin{pmatrix} v_1(x, y, z) \\ v_2(x, y, z) \\ v_2(x, y, z) \end{pmatrix} = \begin{pmatrix} A \sin z + C \cos y \\ B \sin x + A \cos z \\ C \sin y + B \cos x \end{pmatrix},$$

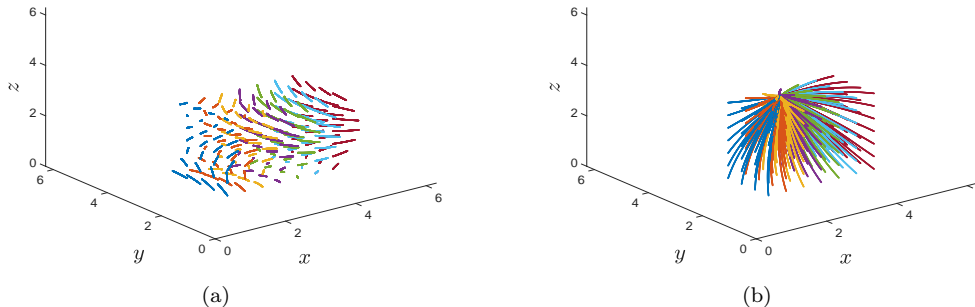


FIG. 8. ABC-flow trajectories from time 0 to 0.4: (a) uncontrolled, and (b) controlled using  $\eta = 0.00001$ , all with a target destination  $(\pi, \pi, \pi)$  for all trajectories.

382 where  $\mathbf{x} = (x, y, z)$ . When considered on the cell  $[0, 2\pi) \times [0, 2\pi) \times [0, 2\pi)$  with  
 383 triply-periodic boundary conditions, the resulting trajectories are well-known to be  
 384 chaotic [21]; Arnold’s criterion for generic integrability of trajectories arising from  
 385 steady Euler flow [3] fails in this instance because the velocity and vorticity fields are  
 386 collinear. The ABC velocity field (3.4) is also an exact solution to the Navier-Stokes  
 387 equation under a particular choice of body force [21]. We use the parameter values  
 388  $A = 1$ ,  $B = 2/3$  and  $C = 1/3$  (also considered in [21]) for our simulations. In the  
 389 spirit of chaos control [42, 22, 51, 55], we seek here to make trajectories all approach  
 390 the same final destination  $(\pi, \pi, \pi)$ .

391 In using our algorithm, since the problem is spatially three-dimensional, we need  
 392 to use a seven-point stencil at each point  $\mathbf{p}$  (the central point, plus points adjacent  
 393 to this in all three coordinate directions) in conjugate momentum space to estimate  
 394 the gradient of the flow map with respect to  $\mathbf{p}$ , and then have to invert the  $3 \times 3$   
 395 matrix in the Newton-Raphson step. Additionally, we require the usage of the higher-  
 396 dimensional `regularizeNd` [47] rather than `gridfit` [20] in determining the control  
 397 velocity globally. We demonstrate in Fig. 8(a) the trajectories in  $(x, y, z)$ -space for a  
 398 grid of initial conditions, evolved from time 0 to  $T = 0.4$  using the ABC velocity (3.4),  
 399 using an Euler method with  $\Delta t = 0.001$ . Our control algorithm is then applied with  
 400 the identical time-spacing, and with  $\eta = 0.0001$ , thereby desiring the achievement of  
 401 the target at a high level of accuracy. The controlled trajectories are displayed in  
 402 Fig. 8(b) with each trajectory shown in a different color. All trajectories are seen to  
 403 approach  $(\pi, \pi, \pi)$  as required.

404 The control velocity  $\mathbf{c} = (c_1, c_2, c_3)$  has three components, with each component  
 405 being a function of  $(x, y, z, t)$ . Illustrating the computed control in a complete way is  
 406 therefore difficult. We show several time-slices, in several  $z = \text{constant}$  planes, for one  
 407 of the components in Fig. 9. These are shown as contour fields. We note that since  
 408 these are computed based on where trajectories are at each time-instance (i.e., from  
 409 the trajectory data in Fig. 8(b)), we can only obtain reliable information in sets which  
 410 are within a convex domain of the existing data points. That is, extrapolation in the  
 411  $(xy)$ -plane beyond the available data points is unreasonable. Hence, the information  
 412 at each time is confined to the current locations of the controlled trajectories. At  
 413 each time-frame, for the demonstration of the control  $c_2(x, y, z, t)$  in Fig. 9, we choose  
 414 a  $z$ -plane which is exactly in the middle of the  $z$ -range of all the current trajectory

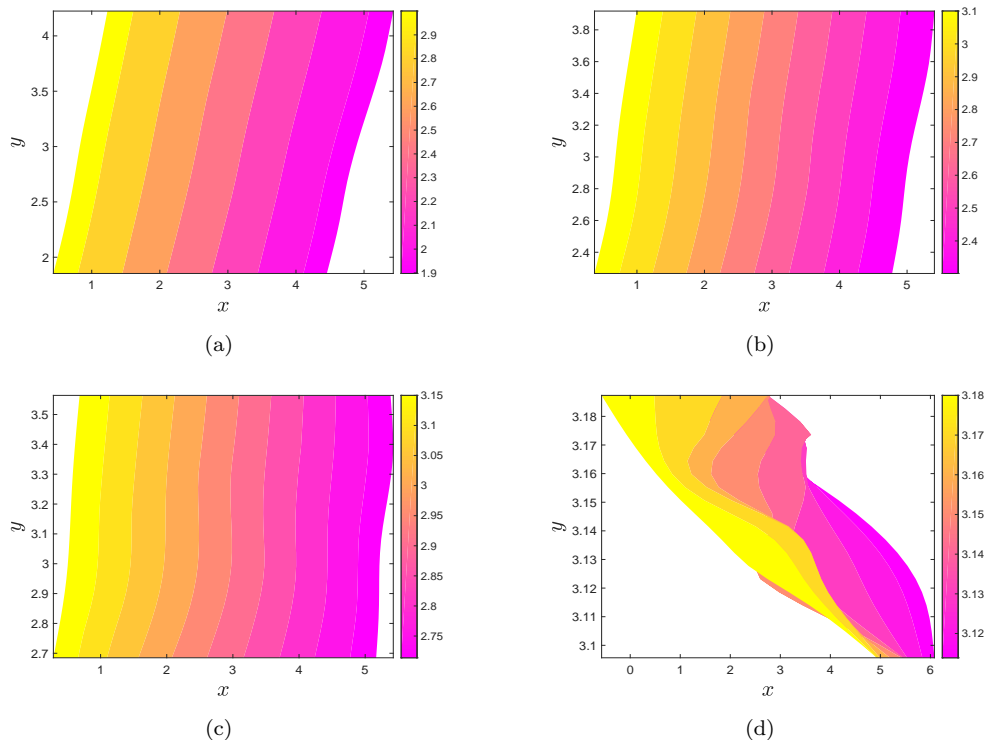


FIG. 9. Displaying the control velocity component  $c_2(x, y, z, t)$  for the ABC-flow control at several time- and  $z$ -slices: (a)  $t = 0.1$  and  $z = 2.3106$ , (b)  $t = 0.2$  and  $z = 2.599$ , (c)  $t = 0.3$  and  $z = 2.869$ , and (d)  $t = 0.4$  and  $z = 3.139$ .

415 locations. At  $t = 0.4$ , since the trajectories have all closely approached  $(\pi, \pi, \pi)$ ,  
 416 information is only available in a small neighborhood near this.

417 **3.4. A Navier-Stokes data example.** Finally, we demonstrate applicability  
 418 when velocities are genuinely given by data, by generating them from a computa-  
 419 tional fluid dynamics simulation of the Navier-Stokes equations. The spatial do-  
 420 main  $[0, 1] \times [0, 1]$  is used, with periodic boundary conditions in both directions. The  
 421 Reynolds number is moderate at 5000, and 100 equally spaced intervals are used  
 422 in each direction to define a spatial grid. The Navier-Stokes equations are solved  
 423 in this case using the vorticity formulation, with a specified forcing function and a  
 424 randomly generated initial vorticity distribution. A pseudo-spectral code is used:  
 425 discrete Fourier transforms in space, and a Crank-Nicholson algorithm in time, with  
 426  $\Delta t = 0.01$ . The equations are numerically solved from an initial time  $t = 0$  to a final  
 427 time  $T = 2$ . Thus, the two components of the velocity field  $\mathbf{v} = (v_1, v_2)$  are generated  
 428 on a spatiotemporal grid. To get a sense of the computed velocity, we show in Fig. 10  
 429 the components  $v_1$  and  $v_2$  at a couple of instances in time.

430 The velocity data from the Navier-Stokes simulation is then stored, and used as  
 431 input into a spatiotemporal control strategy. We take an equally-spaced grid of 25  
 432 initial points  $(x_0, y_0)$ , and first plot their evolution under the uncontrolled unsteady  
 433 velocity data in Fig. 11(a). Our control aim in this instance is to have these approach

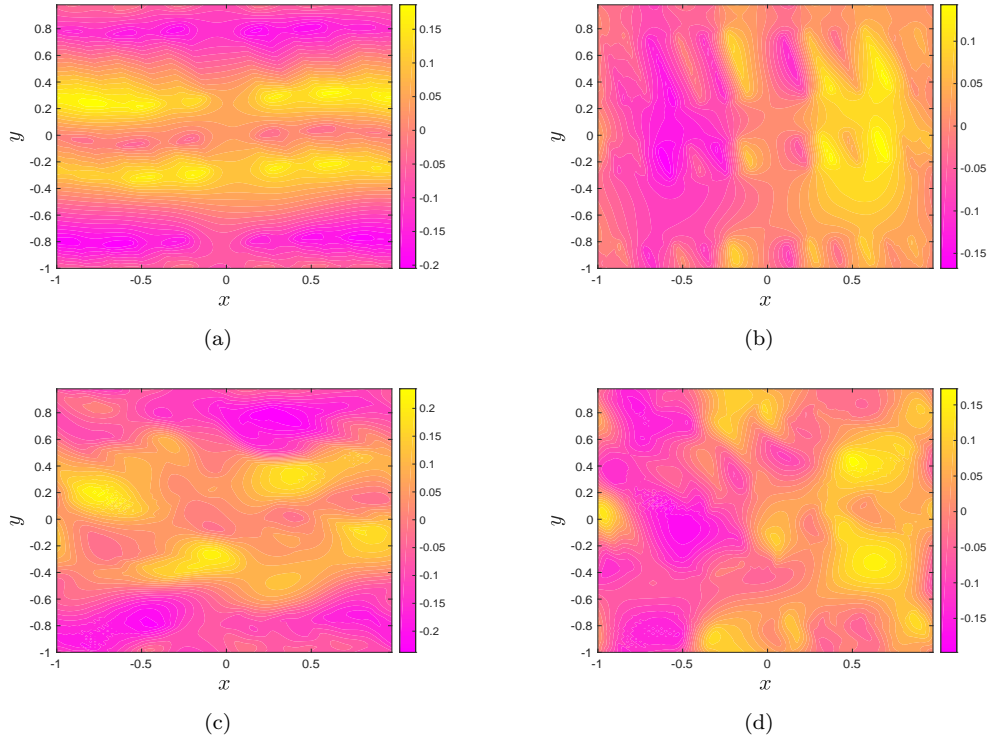


FIG. 10. The velocity components  $v_1$  (left) and  $v_2$  (right), computed at times 0.5 (top row) and 2.0 (bottom row), as generated from the Navier-Stokes computational fluid dynamics solver.

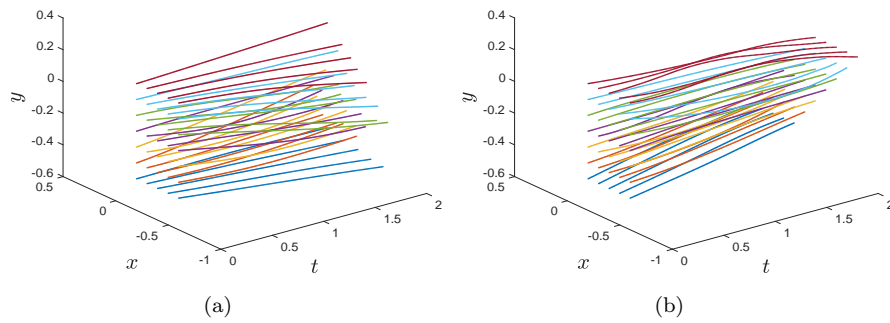


FIG. 11. The (a) uncontrolled, and (b) controlled, trajectories from the Navier-Stokes example.

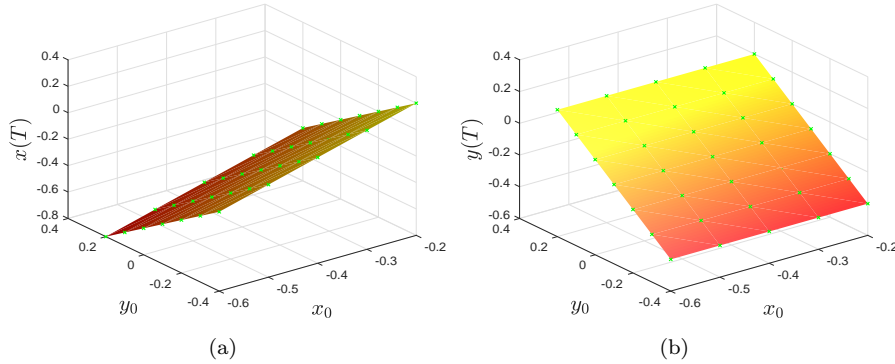


FIG. 12. The (a)  $x$ -coordinate, and (b) the  $y$ -coordinate, of the controlled trajectories at the final time  $T = 2$  (green crosses), along with the relevant target surface (3.5) (orange planes).

434 the target destination function

435 (3.5) 
$$\Theta(\mathbf{x}_0) = \begin{pmatrix} x_0 - y_0 \\ y_0 \end{pmatrix}.$$

436 by the final time ( $T = 2$ ), and we choose  $\eta = 0.0001$ . Applying the methodology that  
 437 we have described is now straightforward. Even though the velocity is given purely in  
 438 terms of data on a discrete grid, it is possible to approximate quantities such as  $\nabla \mathbf{v}$  (as  
 439 needed for implementation of (2.6) by standard finite-differencing, and interpolating  
 440 as needed when trajectories are off the grid. The controlled trajectories derived from  
 441 this process are shown in Fig. 11(b). To verify that the desired targets have been  
 442 achieved, in Fig. 12 we illustrate with green crosses the  $x$ - and  $y$ -coordinates of the  
 443 final locations as functions of the initial location  $(x_0, y_0)$ . The planes displayed are  
 444 the exact target functions given in (3.5). Clearly, the targets have been achieved to  
 445 excellent accuracy. It turns out that the global error  $E(T)$  in (2.10) is 0.00184, and  
 446 the total cost (2.3) is  $4.26 \times 10^{-6}$ .

447 Finally, we demonstrate the computed control velocity  $\mathbf{c}(x, y) = (c_1, c_2)$  at several  
 448 intermediate time-instances in Fig. 13. As before, the green crosses indicate the  
 449 computed value of the control velocity from the integration along trajectories, while  
 450 the orange surface (the global control velocity) is obtained by applying the `gridfit`  
 451 technique. In all cases, the  $(x, y)$  domain is automatically limited here to the spatial  
 452 regions the relevant trajectories traverse, and not the full domain of the Navier-Stokes  
 453 simulation (which would entail spurious extrapolation). We have thus demonstrated  
 454 the applicability of our optimal control technique to computational fluid dynamics  
 455 data as well.

456 **4. Discussion and conclusions.** By combining and adapting different tech-  
 457 niques (Hamiltonian formulation of optimal control, Newton-Raphson method, ap-  
 458 proximating surfaces using `gridfit` [20] and/or `regularizeNd` [47] and the applied  
 459 analysis of differential equations), we have developed a methodology for determining  
 460 a spatiotemporal optimal control function for a finite-horizon globally-specified tar-  
 461 get achievement. With this specific focus in mind, the cost function we chose takes  
 462 the most amenable convex form (2.3); however, the algorithm we propose can be ex-  
 463 tended to more general forms of  $G$ . For this cost function, we were able to provide  
 464 theoretical estimates which show the rate of decay of the error, and the comparative



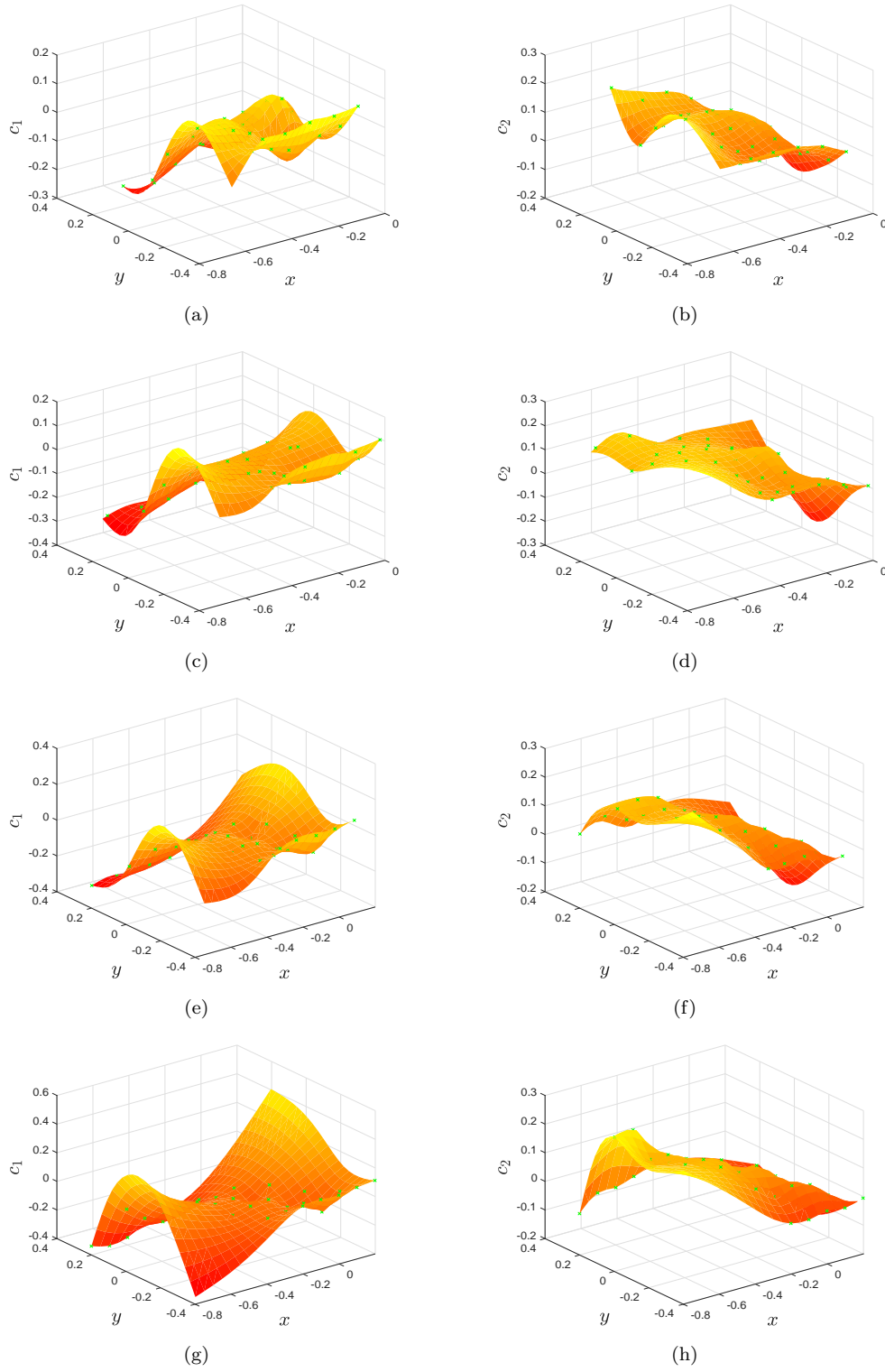


FIG. 13. The control velocity components  $c_1$  (left) and  $c_2$  (right), computed at times 0.5, 1.0 1.5 and 2.0 (in order of rows). The green crosses are computed from the controlled trajectories, while the orange surface extends these globally using `gridfit`.

465  $\eta$ -dependence on the error and cost, in elementary ways, avoiding elaborate functional  
 466 analytic arguments.

467 We have highlighted that our formulation is particularly relevant to fluid mechan-  
 468 ical systems in which  $\mathbf{v}$  is a observed/computationally-determined velocity field, and  
 469 then the spatiotemporal control  $\mathbf{c}$  will be something physically realizable by imposing  
 470 additional flow conditions such as boundary vibration [19, 58], or sinks/sources posi-  
 471 tioned at strategic locations [11, 53, 46, 60, 29]. Often, fluid mixing is to be controlled  
 472 or enhanced by pushing fluid trajectories in some specified way over a time duration;  
 473 our assumptions in this paper (i.e., that  $\Theta$  is specified) is particularly suited to this  
 474 situation. Significant future applications of this method in fluid mechanical systems  
 475 is therefore anticipated.

476 Controlling the Navier-Stokes equations of fluid mechanics is mature research  
 477 field (see the reviews [11, 31]), in which principal difficulties arise in the infinite-  
 478 dimensionality of the control problem, finite-dimensional projections also being of  
 479 sufficiently large dimension to make the control procedure computationally expensive,  
 480 highly turbulent situations requiring highly resolved information, and unpredictability  
 481 over longer time-horizons. Generally, the task is to control the Eulerian velocity by  
 482 limiting its ‘turbulence level’ as measured in terms of its gradients, vorticity, enstrophy,  
 483 etc. Controllability is usually via the boundary, thereby restricting the nature of  
 484 the control. Our approach is different, instead targeting the eventual Lagrangian  
 485 locations of trajectories, while seeking a spatiotemporally distributed control velocity.  
 486 Consequently, our control problem has a dimensionality equal to that of the physical  
 487 space in which the fluid resides (i.e., no more than three), allowing the effective usage  
 488 of a Hamiltonian formulation of optimal control. We recover the spatiotemporal  
 489 nature of the control velocity by using an approximant based on the control algorithm  
 490 applied to an ensemble of trajectories. Of course, we would expect the method to face  
 491 greater difficulties when the turbulence or the time-horizon is large; these require  
 492 higher resolutions spatially and temporally.

493 Our framework can also be thought of as an interesting approach for controlling  
 494 chaotic systems which may be autonomous or nonautonomous [10, 59, 63]. We have  
 495 the ability to steer trajectories *globally* over some finite time using our method. We  
 496 have demonstrated the application of this to an example from fluid mechanics—ABC  
 497 flow. Thus, this provides a contribution to chaos control theory which is different  
 498 from standard ones such as chaotic synchronization [50, 12, 36] and local control near  
 499 chaotic saddles [23, 26]. The smoothness our theorems require in  $\mathbf{v}$  is consonant  
 500 with chaotic systems; the unpredictability of corresponding Lagrangian trajectories  
 501 because of sensitivity to initial conditions is apparently not an impediment to our  
 502 theory and algorithm. As in the turbulent flow situation, the difficulty will be that  
 503 the control velocity would need to be specified on finer and finer scales, and the  
 504 control will be achievable for times which are not too large. We also note that the  
 505 criteria we have developed apply even for nonsmooth  $\Theta$  allowing, for example, the  
 506 separation of trajectories into specified clusters. Thus, we expect this methodology  
 507 to be a promising new approach for chaos control.

508 The numerical simulations we presented in Section 3 demonstrated the power of  
 509 the method. We have illustrated the usage in both analytically-defined velocities, and  
 510 velocities on a spatio-temporal grid obtained from a computational fluid dynamics  
 511 simulation of the Navier-Stokes equation. While we showed one- two- and three-  
 512 dimensional examples, the method works in any spatial dimension. However, the  
 513 computational complexity does increase with the dimension, rendering the method  
 514 impractical in large dimensions. Moreover, in instances in which the initial velocity

515 field is highly turbulent, the presence of large velocity gradients will mean that the  
 516 control velocities may become difficult to compute. Put another way, highly turbu-  
 517 lent situations will have large  $\|\cdot\|_b$  norms in the velocity fields, and thus our theorems  
 518 which provide decay rates and robustness of the optimal control methodology have  
 519 less value because the size of this norm is relevant. There is also a subtle issue which  
 520 requires further exploration: the implicit assumption that an optimal control  $\mathbf{c}$  *exists*  
 521 *as a function of*  $(\mathbf{x}, t)$ . Should different trajectories give different predictions for  $\mathbf{c}$  at  
 522 a point of intersection of spacetime curves, determining  $\mathbf{c}$  as a genuine spatiotemporal  
 523 function becomes problematic. We plan to explore this issue, and seek an alternative  
 524 formulation which is both analytically and physically reasonable, in future work. Ad-  
 525 ditionally, we are seeking improvements in computational efficiency of the algorithm,  
 526 for improved performance on densely defined and/or higher-dimensional data.

### 527 **Appendix A. Proofs of theorems.**

528 Here, we provide the proofs of the theorems of Section 2.

529 **A.1. Proof of Theorem 2.1.** This is a result emerging from classical optimal  
 530 control theory [39], which works even when the evolution law is nonautonomous. We  
 531 first use the following standard result (e.g., see Sections 2.5–2.6 in [39]), and written  
 532 here in our notation. The notation  $\nabla_{\mathbf{y}}$  represents the  $n \times n$  matrix derivative with  
 533 respect to the variable  $\mathbf{y} \in \mathbb{R}^n$ .

534 **THEOREM A.1** (Nonautonomous optimal control). *Consider for  $\mathbf{x} \in \mathbb{R}^n$  a system*

$$535 \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{c}, t) \quad ; \quad t \in [0, T]$$

536 *in which  $\mathbf{c}$  is the control, and the optimization of a quantity*

$$537 \quad g = h_1(\mathbf{x}(T)) + \int_0^T h_2(\mathbf{x}(t), \mathbf{c}, t) dt$$

538 *is sought. Upon definition of the Hamiltonian*

$$539 \quad H(\mathbf{x}, \mathbf{c}, \mathbf{p}, t) := h_2(\mathbf{x}, \mathbf{c}, t) + \mathbf{f}(\mathbf{x}, \mathbf{c}, t)^\top \mathbf{p},$$

540 *a necessary condition for  $\mathbf{c}$  to be a local optimizer of  $g$  is  $\nabla_{\mathbf{c}} H = 0$ , in which  $\mathbf{x} = \mathbf{x}(t)$   
 541 and  $\mathbf{p} = \mathbf{p}(t)$  are solutions to the system*

$$542 \quad \left. \begin{array}{l} \dot{\mathbf{x}} = \nabla_{\mathbf{p}} H \\ \dot{\mathbf{p}} = -\nabla_{\mathbf{x}} H \end{array} \right\}, \text{ where } \left. \begin{array}{l} \mathbf{x}(0) = \mathbf{x}_0 \\ \mathbf{p}(T) = \nabla_{\mathbf{x}} h_1(\mathbf{x}(T)) \end{array} \right\}.$$

543 *Moreover, the solution corresponds to a minimizer if  $\frac{\partial^2}{\partial \mathbf{c}^2} H$  is positive definite.*

544 To prove Theorem 2.1, we apply Theorem A.1 with the choice  $\mathbf{f}(\mathbf{x}, \mathbf{c}, t) = \mathbf{v}(\mathbf{x}, t) +$   
 545  $\mathbf{c}$ ,  $h_1(\mathbf{x}) = \|\mathbf{x} - \Theta(\mathbf{x}_0)\|^2$  and  $h_2(\mathbf{x}, \mathbf{c}, t) = \eta \|\mathbf{c}\|^2$ . Then, the Hamiltonian is

$$546 \quad H(\mathbf{x}, \mathbf{c}, \mathbf{p}, t) = \eta \|\mathbf{c}\|^2 + (\mathbf{v}(\mathbf{x}, t) + \mathbf{c})^\top \mathbf{p}.$$

547 The condition  $\nabla_{\mathbf{c}} H = 0$  yields  $\eta 2\mathbf{c} + \mathbf{p} = 0$ , and thus  $\mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t) = -1/(2\eta)\mathbf{p}(t)$ .  
 548 Now, since

$$549 \quad \nabla_{\mathbf{x}} H = [\nabla_{\mathbf{x}} \mathbf{v}]^\top \mathbf{p} \quad \text{and} \quad \nabla_{\mathbf{p}} H = \mathbf{v}(\mathbf{x}, t) + \mathbf{c},$$

550 the differential equations (2.6) emerge immediately. Moreover,  $\nabla_{\mathbf{x}} h_1(\mathbf{x}(T)) = 2(\mathbf{x}(T) - \Theta(\mathbf{x}_0))$ ,  
 551 which gives the end condition for  $\mathbf{p}$  in (2.7). To establish that this critical  $\mathbf{c}$  corre-  
 552 sponds to a minimizer of  $g$ , we observe that  $\frac{\partial^2}{\partial \mathbf{c}^2} H = 2\eta \mathbb{I}$ , where  $\mathbb{I}$  is the  $n \times n$  identity  
 553 matrix. Since  $\eta > 0$ , this is positive definite. (More simply, the convexity of  $H$  in  $\mathbf{c}$   
 554 in fact ensures that this is a global minimizer.)

555 **A.2. Proof of Theorem 2.2.** By taking the  $t$ -derivative of  $E(t)^2$ , we get

$$556 \quad \frac{d}{dt} [E(t)^2] = 2 \int_{\Omega_0} \frac{d}{dt} [\mathbf{x}(\mathbf{x}_0, t)]^\top [\mathbf{x}(\mathbf{x}_0, t) - \Theta(\mathbf{x}_0)] d\mathbf{x}_0$$

557 Now, using the fact that  $(d/dt)\mathbf{x} = \mathbf{v} + \mathbf{c}$ , and subsequently applying the Cauchy-  
558 Schwarz inequality on the right-hand side, we get

$$\begin{aligned} 559 \quad \left| \frac{d}{dt} [E(t)^2] \right| &\leq 2 \left( \int_{\Omega_0} \|\mathbf{v} + \mathbf{c}\|^2 d\mathbf{x}_0 \right)^{1/2} E(t) \\ 560 &\leq 2 \left( 2 \int_{\Omega_0} \|\mathbf{v}\|^2 d\mathbf{x}_0 + 2 \int_{\Omega_0} \|\mathbf{c}\|^2 d\mathbf{x}_0 \right)^{1/2} E(t) \\ 561 &\leq 2\sqrt{2} \left[ \left( \int_{\Omega_0} \|\mathbf{v}\|^2 d\mathbf{x}_0 \right)^{1/2} + \left( \int_{\Omega_0} \|\mathbf{c}\|^2 d\mathbf{x}_0 \right)^{1/2} \right] E(t) \\ 562 \quad (\text{A.1}) \quad &\leq 2\sqrt{2} \left[ A\sqrt{\mu(\Omega_0)} + \left( \int_{\Omega_0} \|\mathbf{c}\|^2 d\mathbf{x}_0 \right)^{1/2} \right] E(t). \end{aligned}$$

563 In the above, we have suppressed the arguments  $(\mathbf{x}(\mathbf{x}_0, t), t)$  in both  $\mathbf{v}$  and  $\mathbf{c}$  for  
564 brevity, and at the last step used the bound on  $\|\mathbf{v}\|_a$ . Now from Theorem 2.1, for any  
565 fixed  $\mathbf{x}_0$ , we know that  $\mathbf{c} = -\mathbf{p}/(2\eta)$  with  $\mathbf{p}$  obeying (2.6) with condition for  $\mathbf{p}(T)$   
566 given in (2.7). Using the abuse of notation  $\mathbf{c}(t) := \mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t)$ , this means that

$$567 \quad \dot{\mathbf{c}} = -[\nabla \mathbf{v}(\mathbf{x}(\mathbf{x}_0, t), t)]^\top \mathbf{c}$$

568 subject to the condition  $\mathbf{c}(T) = -[\mathbf{x}(\mathbf{x}_0, T) - \Theta(\mathbf{x}_0)]/\eta$ . We rewrite this in a new in-  
569 dependent variable  $\tau = T - t$ , and let  $\hat{\mathbf{c}}(\tau) = \mathbf{c}(t)$ . Setting  $L(\tau) := [\nabla \mathbf{v}(\mathbf{x}(\mathbf{x}_0, t), t)]^\top$ ,  
570 we have

$$571 \quad \frac{\partial}{\partial \tau} \hat{\mathbf{c}} = L(\tau) \hat{\mathbf{c}} ; \quad \hat{\mathbf{c}}(0) = -\frac{\mathbf{x}(\mathbf{x}_0, T) - \Theta(\mathbf{x}_0)}{\eta}.$$

572 Premultiplying the differential equation above by  $\hat{\mathbf{c}}^\top$ , we obtain

$$573 \quad \frac{1}{2} \frac{\partial}{\partial \tau} \|\hat{\mathbf{c}}\|^2 = \hat{\mathbf{c}}^\top L(\tau) \hat{\mathbf{c}},$$

574 and consequently

$$\begin{aligned} 575 \quad \frac{\partial}{\partial \tau} \|\hat{\mathbf{c}}\|^2 &\leq 2 \|\hat{\mathbf{c}}^\top\| \|L(\tau) \hat{\mathbf{c}}\| \\ 576 &\leq 2 \|\hat{\mathbf{c}}^\top\| B \|\hat{\mathbf{c}}\| = 2B \|\hat{\mathbf{c}}\|^2 \end{aligned}$$

577 using the bound on  $\|\mathbf{v}\|_b$ . Separating variables and integrating from  $\tau = 0$  to a general  
578  $\tau$  value in  $[0, T]$ , we have

$$579 \quad \ln \frac{\|\hat{\mathbf{c}}(\tau)\|^2}{\|\hat{\mathbf{c}}(0)\|^2} \leq 2B\tau,$$

580 and applying the value of  $\hat{\mathbf{c}}(0)$  we acquire the bound

$$581 \quad \|\hat{\mathbf{c}}(\tau)\|^2 \leq \frac{\|\mathbf{x}(\mathbf{x}_0, T) - \Theta(\mathbf{x}_0)\|^2}{\eta^2} e^{2B\tau}.$$

582 Reverting to  $t \in [0, T]$  as the independent variable, this means that

$$583 \quad (\text{A.2}) \quad \|\mathbf{c}(t)\|^2 \leq \frac{\|\mathbf{x}(\mathbf{x}_0, T) - \Theta(\mathbf{x}_0)\|^2}{\eta^2} e^{2B(T-t)}.$$

584 Inserting this bound into (A.1) yields

$$585 \quad \left| \frac{d}{dt} [E(t)^2] \right| \leq 2\sqrt{2} \left[ A\sqrt{\mu(\Omega_0)} + \frac{E(T)e^{B(T-t)}}{\eta} \right] E(t).$$

586 This means that

$$587 \quad (\text{A.3}) \quad \left| \frac{d}{dt} [E(t)] \right| \leq \sqrt{2} \left[ A\sqrt{\mu(\Omega_0)} + \frac{E(T)e^{B(T-t)}}{\eta} \right],$$

588 and integrating from a general time  $t$  to  $T$  results in

$$589 \quad E(T) - E(t) \leq \sqrt{2} \left[ A\sqrt{\mu(\Omega_0)}(T-t) - \frac{E(T)(1-e^{B(T-t)})}{B\eta} \right].$$

590 Similarly working with the fact that  $(d/dt)E(t)^2$  is greater than negative the term on  
591 the right of (A.3) enables

$$592 \quad E(T) - E(t) \geq -\sqrt{2} \left[ A\sqrt{\mu(\Omega_0)}(T-t) - \frac{E(T)(1-e^{B(T-t)})}{B\eta} \right].$$

593 Combining these two results gives us the required equation (2.13).

594 **A.3. Proof of Theorem 2.3.** We can write (2.3) as

$$595 \quad (\text{A.4}) \quad G = E(T)^2 + \eta \int_{\Omega_0} \int_0^T \|\mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t)\|^2 dt d\mathbf{x}_0.$$

596 Using (A.2) we have

$$597 \quad \int_{\Omega_0} \int_0^T \|\mathbf{c}(\mathbf{x}(\mathbf{x}_0, t), t)\|^2 dt d\mathbf{x}_0 \leq \frac{E(T)^2(e^{2BT} - 1)}{2B\eta^2},$$

598 and so

$$599 \quad G \leq E(T)^2 \left[ 1 + \frac{e^{2BT} - 1}{2B\eta} \right].$$

600 Now if  $E(T) = \mathcal{O}(\eta^\alpha)$  for some  $\alpha > 1/2$ , then

$$601 \quad G \leq \mathcal{O}(\eta^{2\alpha}) \left[ 1 + \frac{e^{2BT} - 1}{2B\eta} \right] = \mathcal{O}(\eta^{2\alpha-1})$$

602 as required.

603 **A.4. Proof of Theorem 2.4.** If we consider the initial system (2.1) with  $\tilde{\mathbf{v}}$   
604 instead of  $\mathbf{v}$ , the procedure outlined will then generate a control  $\tilde{\mathbf{c}}$ , a global error  $\tilde{E}(t)$   
605 at a general time  $t$ , a global error  $\tilde{E}(T)$  at the final time  $T$ , and the minimizing cost  
606  $\tilde{G}$ . Now, since  $\tilde{\mathbf{v}}$  is  $\mathcal{O}(\epsilon)$ -close to  $\mathbf{v}$  in both the norms  $\|\cdot\|_a$  and  $\|\cdot\|_b$ , this Theorem is  
607 a simple consequence that *every* step in the previous theorems inherits this closeness  
608 because  $\Omega_0$  is bounded, and the time-interval  $[0, T]$  over which integration is performed  
609 is finite. Specifically,  $\tilde{\mathbf{x}}(\mathbf{x}_0, t)$  and  $\tilde{\mathbf{p}}$  must be  $\mathcal{O}(\epsilon)$ -close to the variables  $\mathbf{x}(\mathbf{x}_0, t)$  and  
610  $\mathbf{p}$  generated via Theorem 2.1. Since  $\tilde{\mathbf{c}} = -\tilde{\mathbf{p}}/(2\eta)$ , this property transfers to  $\tilde{\mathbf{c}}$ . Then  
611 (2.10) ensures that  $\tilde{E}(t)$  is  $\mathcal{O}(\epsilon)$ -close to  $E(t)$ , and furthermore, (A.4) ensures that  
612  $\tilde{G} = G + \mathcal{O}(\epsilon)$  as well. The decay expression in Theorem 2.2 also remains valid, with  
613 of course the replacements  $A \rightarrow \tilde{A}$  and  $B \rightarrow \tilde{B}$ , thereby only perturbing the results  
614 by  $\mathcal{O}(\epsilon)$ .

615

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