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Finite-Time Transport in Volume-Preserving Flows

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Finite-time transport between distinct flow regions is of great relevance to many scientific applications, yet quantitative studies remain scarce to date. The primary obstacle is computing the evolution of material volumes, which is often infeasible due to extreme interfacial stretching. We present a framework for describing and computing finite-time transport in n -dimensional (chaotic) volume-preserving flows that relies on the reduced dynamics of an $(n - 2)$ -dimensional “minimal set” of fundamental trajectories. This approach has essential advantages over existing methods: the regions between which transport is investigated can be arbitrarily specified; no knowledge of the flow outside the finite transport interval is needed; and computational effort is substantially reduced. We demonstrate our framework in 2D for an industrial mixing device.

Introduction—Lagrangian transport, in its most general sense, consists of the transfer of material from one region to another over time. It is of fundamental importance to a wide variety of scientific and engineering disciplines, including fluid dynamics [1, 2], chemical kinetics [3], heat transfer [4], and plasma confinement [5]. Here we focus on volume-preserving flows, which include compressible steady flows, incompressible (un)steady flows, magneto-hydrodynamic representations of plasmas, and all Hamiltonian flows. Transport in such flows is notoriously difficult to quantify, particularly in the presence of chaos. Methods exist for computing transport across boundaries of approximately invariant flow regions of steady or periodic systems [6–10], but these fail in the presence of aperiodic time dependence. Recent studies of aperiodic systems give new techniques for identifying finite-time coherent sets [11–14], but few quantify transport between them [15–18]. A generic framework for computing transport was proposed in [19, 20], but was restricted to the case of transitory flows, i.e., two autonomous flow states connected by a time-dependent transition. Notwithstanding these efforts, describing and computing finite-time transport in general aperiodic systems remains largely an open problem.

The primary obstacle is the enormous cost of computing the required trajectories. An initial material volume deforms under the action of a dynamical system, and a Lagrangian transport analysis consists of characterizing its evolution with respect to a second distinct region at some later time (see Fig. 1). In chaotic flows, the initial region typically stretches exponentially fast as it evolves, resulting in a rapid growth of the number of trajectories required to track it [21, 22]. Computing these trajectories can be costly, especially in multi-dimensional systems, making associated transport computations extremely expensive or, in some cases, precluding them altogether.

Here we present a general framework for describing and computing finite-time transport in (chaotic) n -dimensional volume-preserving flows. Our technique minimizes the number of required trajectories, thereby greatly reducing the computational effort compared to

existing methods. It is also independent of any infinite-time asymptotic quantities (e.g., hyperbolic manifolds or elliptic islands); only knowledge of the dynamics inside the finite transport interval is required. Moreover, the regions between which transport is computed can be specified arbitrarily. These qualities greatly extend the scope of our framework compared to existing methods, enabling an analysis of transport (i) in systems known only for finite time and (ii) distinct from measures of mixing by chaotic advection.

Finite-Time Transport—Finite-time transport in “transitory” volume-preserving flows was computed in [19, 20]; however, these methods relied on the steadiness of the flow outside the compact transport interval itself, and this precluded application to systems known only for finite time. In addition the initial and final transport regions were assumed invariant under the steady flow. Here, we remove these restrictions, providing a general framework for the computation of finite-time transport in any volume-preserving flow.

Let φ be a volume-preserving flow on an n -dimensional (n D) phase space M and a finite-time interval $T = [0, \tau]$. In particular, the associated vector field V is also volume-preserving, with $\nabla \cdot V = 0$ with respect to a volume form Ω . We consider the problem of computing the volume Φ of the set of trajectories transported from a region \mathcal{P}_0 to a region \mathcal{F}_τ (see Fig. 1 for the case $n = 2$). The subscripts denote time-slices of orbits in the extended phase space $M \times T$; e.g. \mathcal{P}_τ denotes the evolution of \mathcal{P}_0 under φ from $t = 0$ to $t = \tau$. We assume that the boundaries $\partial\mathcal{P}_0$ and $\partial\mathcal{F}_\tau$ are known explicitly.

Assuming that $\Omega = d\alpha$ is exact on M (e.g., $\Omega = dx_1 \wedge dx_2 \dots \wedge dx_n$ and $\alpha = x_1 dx_2 \wedge \dots \wedge dx_n$ for $M \subseteq \mathbb{R}^n$) and defining $\mathcal{R}_\tau = \mathcal{P}_\tau \cap \mathcal{F}_\tau$, the total transported volume is

$$\Phi = \text{Vol}(\mathcal{R}_\tau) = \int_{\mathcal{R}_\tau} \Omega = \int_{\partial\mathcal{R}_\tau} \alpha, \quad (1)$$

by Stokes’s Theorem. Thus, computing finite-time transport amounts to computing the integral of the $(n - 1)$ -form α along the boundary of the intersection set \mathcal{R}_τ .

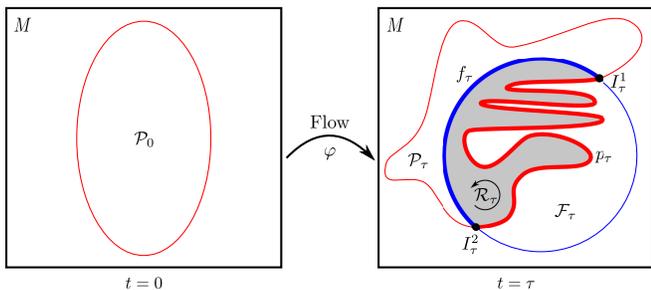


FIG. 1. The lobe \mathcal{R}_τ (shaded) comprises the Lagrangian transport from \mathcal{P}_0 at $t = 0$ to \mathcal{F}_τ at $t = \tau$ under the flow φ .

Whenever $\partial\mathcal{P}_\tau$ intersects $\partial\mathcal{F}_\tau$ transversely, $\Phi \neq 0$. In this case, the boundary $\partial\mathcal{R}_\tau$ can always be decomposed into two sets: $p_\tau = \partial\mathcal{R}_\tau \cap \partial\mathcal{P}_\tau$ and $f_\tau = \partial\mathcal{R}_\tau \cap \partial\mathcal{F}_\tau$. Their $(n - 2)$ -dimensional intersection, \mathcal{I}_τ , is nonempty, and continuity implies that

$$\mathcal{I}_\tau = \partial\mathcal{P}_\tau \cap \partial\mathcal{F}_\tau = p_\tau \cap f_\tau = \partial p_\tau = \partial f_\tau. \quad (2)$$

For example, p_τ and f_τ are curve segments in the 2D case depicted in Fig. 1, and \mathcal{I}_τ consists of the two points I_τ^1 and I_τ^2 . In chaotic flows, computing p_τ is costly due to the exponential stretching of $\partial\mathcal{P}_0$ in time. However, if the flow is volume-preserving, p_τ need not be computed explicitly to evaluate (1); indeed, the necessary trajectory information for computing Φ is concentrated in the orbit of the lower-dimensional set \mathcal{I}_τ .

The reason is that, for volume-preserving flows, the integral of α over $\partial\mathcal{R}_\tau$ is related to the “action” of the trajectories in $\mathcal{I}_\tau = \partial p_\tau = \partial f_\tau$ [20, Theorem 3.1]. In particular,

$$\int_{p_\tau} \alpha = \int_{p_0} \alpha + \int_0^\tau \int_{\partial p_s} \lambda ds, \quad (3)$$

where λ is the *Lagrangian form*; it is defined such that its differential, $d\lambda$, is the time-derivative of α along the flow (i.e., the Lie derivative). The differential form λ is a generalization of the (phase space) Lagrangian of classical mechanics, and the two coincide in 2D. For example, taking $M = \mathbb{R}^2$, $\Omega = dx \wedge dy$, and $\alpha = y dx$, the Lie derivative of α along the incompressible vector field $V = (\partial_y \psi, -\partial_x \psi)$ with stream function ψ is given by $\mathcal{L}_V \alpha = \iota_V(d\alpha) + d(\iota_V \alpha) = d(y \partial_y \psi - \psi) := d\lambda$ (cf. [20] for more details).

Essentially, (3) allows the integral of α to be performed over the simpler set p_0 instead of integrating over $p_\tau \subset \partial\mathcal{R}_\tau$, provided a Lagrangian “adjustment” term is added. Combining (3) with (1), the total finite-time transport becomes

$$\Phi = \int_{f_\tau} \alpha + \int_{p_0} \alpha + \int_0^\tau \int_{\partial p_s} \lambda ds. \quad (4)$$

Since $\partial\mathcal{P}_0$ and $\partial\mathcal{F}_\tau$ are known a priori, the only trajectories needed for this computation are those of $\partial p_\tau = \mathcal{I}_\tau$.

A key advantage of (4) is that the dimension of the required trajectory information is reduced compared to direct evaluation of (1). To see this, consider again the 2D example of Fig. 1. From (1), $\Phi = \int_{f_\tau} \alpha + \int_{p_\tau} \alpha$. To evaluate the second integral, one must track the evolution of p_0 over the interval T , since only $\partial\mathcal{P}_0$ is known a priori. The associated cost (i.e., number of trajectories computed) is directly related to the length, curvature, and desired resolution of the final curve, p_τ , and the computed set covers a surface in the extended phase space $M \times T$. However, in (4), $\partial p_\tau = \mathcal{I}_\tau$ can be computed much more efficiently; we use a root-finding method to identify the intersections [19, 20]. In this case, the number of trajectories that must be computed *decouples* from the length, curvature, and resolution of p_τ . It depends only on the number of points in \mathcal{I}_τ , and these trajectories form only a 1D set in the extended phase space. Thus, the Lagrangian information required to compute the orbit of \mathcal{I}_τ is one dimension less than that required to compute p_τ . This dimension-reduction also generalizes to the case of $n > 2$; the dimension of the set of trajectories required to compute Φ using (4) will always be one less than that using (1) and two less than that using a naive volume integration.

Once the orbit of \mathcal{I}_τ is known, the third integral in (4) is immediately computable since $\partial p_s = \mathcal{I}_s$ and λ is derived directly from the flow. Two factors contribute to the ease of computing the first two integrals in (4). First, the regions \mathcal{P}_0 and \mathcal{F}_τ between which transport is studied are typically quite regular, and integrals along portions of their boundaries are often analytically tractable or otherwise easily computed. Naturally, integrating over p_0 is much easier than integrating over p_τ , which can be exponentially stretched and folded by a chaotic flow.

Secondly, since both $\partial\mathcal{P}_0$ and $\partial\mathcal{F}_\tau$ are known, $p_0 \subset \partial\mathcal{P}_0$ and $f_\tau \subset \partial\mathcal{F}_\tau$ may be specified by just their oriented boundaries (endpoints when $n = 2$). From (2), these are precisely \mathcal{I}_0 and \mathcal{I}_τ , respectively. Thus, once the orbit of \mathcal{I}_τ is known, (4) may be evaluated without computing any additional trajectories. Furthermore, it would be impossible to compute Φ from *fewer* trajectories; this would amount to determining a line segment from a single point. Hence, the cardinality of \mathcal{I}_τ is a lower bound on the trajectory count—i.e., computational effort—needed to compute Φ , and (4) achieves this lower bound.

It should be noted that the dimension reduction and trajectory minimization arguments outlined above are independent both of numerical implementation and of any aspect of the dynamics outside the interval T . In particular, they are independent of the asymptotic notions of hyperbolicity and invariant manifolds (key components of existing formalisms), and the flow need not even be volume-preserving outside T . The framework for computing transport we present here is truly a consequence of the finite-time volume-preserving dynamics [23].

Example: Rotated Arc Mixer—As a simple illustrative

example, we compute transport in a 2D unsteady model of the Rotated Arc Mixer (RAM), a novel industrial mixing device developed on the basis of scientific insight into chaotic advection. Though previous studies have investigated global asymptotic mixing in periodic versions of the RAM [24, 25], none have considered local transport or finite-time effects, both of which have important practical design implications for the device.

The RAM consists of a stationary inner cylinder, punctured by windows, and a rotating outer cylinder that fits snugly over the inner one (see Fig. 2a). As fluid

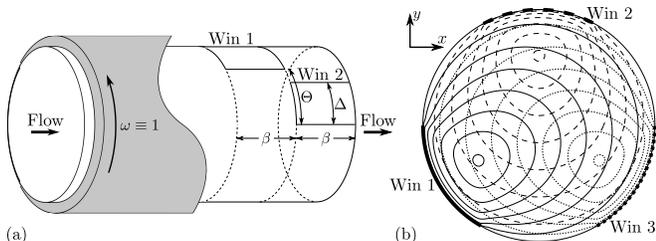


FIG. 2. (a) Schematic of the RAM. (b) Cross section of the RAM and streamline overlay for three different window configurations.

flows axially through the RAM, it contacts the rotating outer cylinder through the windows, inducing a secondary transverse flow (see Fig. 2b). Successive repositioning of the windows in the axial direction effectively reorients this transverse flow, enabling chaotic dynamics and highly efficient mixing [25].

The effect of window reorientation along the RAM's main axis can be modeled in cross-section by a 2D, unsteady, cellular flow [24, 25], assuming a unit uniform axial velocity profile [26]. Each flow cell is a reorientation of a steady base flow and corresponds to a single window of axial length β ; assuming a Stokes flow regime, the analytical stream function ψ from [27] describes its dynamics. The resulting flow is thus volume-preserving and the vector field is given by $(\dot{x}, \dot{y}) = (\partial_y \psi, -\partial_x \psi)$. We assume a unit rotation rate of the outer cylinder, fix the window opening angle $\Delta = \pi/3$, and reorient successive window locations by $\Theta = -2\pi/3$ around the RAM's circumference. This results in a periodic flow of period length 3β and three distinct flow cells whose streamlines are overlaid in Fig. 2b.

The axial window length, β , and the (possibly non-integer) number, k , of windows over the device length are the primary control parameters for the full cellular flow. For the 2D model, β denotes the time duration of each flow cell, and the flow is active for a total transport time $\tau = k\beta$. In the infinite-time case, β was shown to strongly influence global flow topology and asymptotic mixing in the RAM [25]; here we illustrate its importance to finite-time transport. We study transport outward from the core of the RAM, letting \mathcal{P}_0 be the central disk containing half the cross-sectional area and letting the target, \mathcal{F}_τ , be the surrounding annulus (see Fig. 3,

$\tau = 0$). The total transport between \mathcal{P}_0 and \mathcal{F}_τ is com-

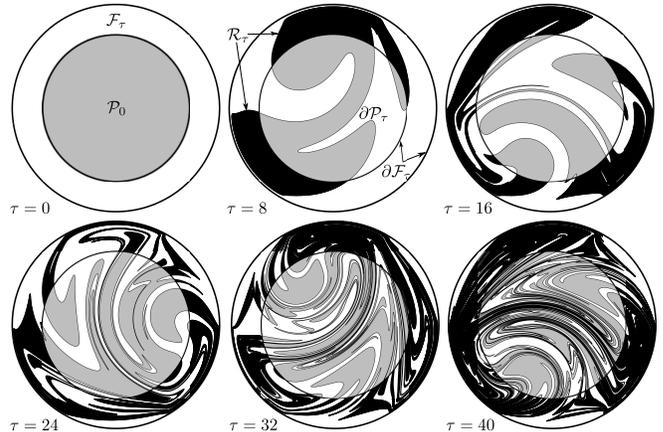


FIG. 3. \mathcal{P}_τ (shaded) and $\mathcal{R}_\tau \subset \mathcal{P}_\tau$ (black) for $\beta = 4$, various τ .

puted via (4) as a function of both β and τ . Note that, despite the periodicity of the flow cells, the flow must be treated as aperiodic since only finitely many periods are encountered on $[0, \tau]$ for any nonzero β .

The length of $\partial\mathcal{P}_\tau$, the number of lobes comprising \mathcal{R}_τ , and the number of intersection points in \mathcal{I}_τ all typically grow exponentially with τ . For the case $\beta = 4$ of Fig. 3, they all grow as $e^{0.12\tau}$. Nonetheless, Φ can still be computed over a large range of τ by employing (4). As noted above, the number of points in \mathcal{I}_τ represents a lower bound on the trajectories required to compute Φ . Of course, to determine \mathcal{I}_τ we must compute some trial trajectories outside the set itself; these are then refined by root-finding methods to determine the true intersections. By choosing the trials appropriately, the number of trajectories needed to compute Φ can be close to the theoretical lower bound. We note that when $n > 2$, $\dim(\mathcal{I}_\tau) > 0$, and so \mathcal{I}_τ must be approximated numerically; this contributes computational error to Φ . In 2D, however, \mathcal{I}_τ comprises finitely many discrete points and such approximation error is absent. In this case, \mathcal{I}_τ and its orbit—and thus Φ itself—are computed accurately and efficiently using standard root-finding and integration techniques, as described in [19, 20].

By contrast, there is effectively no upper bound on the number of trajectories necessary to compute Φ according to (1): finite-resolution effects must be accounted for even when $n = 2$. That is, under (1), the accuracy of the computed transport is *always* tied directly to the numerical resolution of $\partial\mathcal{P}_\tau$. Both the global length and the local curvature of this set typically increase dramatically with τ , resulting in a corresponding increase in the number of trajectories needed for accurate numerics [22]. In the cases we examined, the number of trajectories required to resolve $\partial\mathcal{P}_\tau$ was about two orders of magnitude greater than the number of points in \mathcal{I}_τ . For example, when $\beta = 4$ and $\tau = 35$, about 16,000 points were needed

to resolve $\partial\mathcal{P}_\tau$ whereas \mathcal{I}_τ contains only 166 points.

The results of our transport computations are shown in Fig. 4, displayed as the fraction of the area of \mathcal{P}_τ that intersects \mathcal{F}_τ for various β and τ . Solid lines indicate

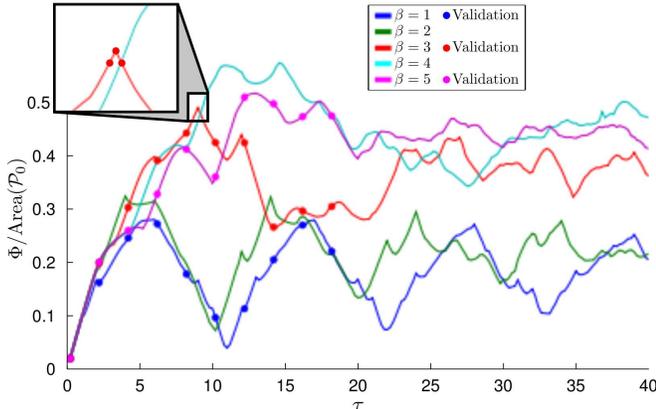


FIG. 4. Relative transport between \mathcal{P}_0 and \mathcal{F}_τ for various β , τ . Sharp peaks result from instantaneous switching between flow cells; they are not numerical artifacts (see inset). (Color Online).

evaluation of (4) and dots represent validation by Monte-Carlo (MC) sampling as described in [19, 20]. Notably, transport depends non-monotonically on both τ and β , and identifying local and global transport maxima could have important design implications. We also note that MC validation was computationally infeasible for large τ . For example, the single MC data point at $\beta = 5$ and $\tau = 18.2$ took about 20 cpu hours, while evaluating (4) took less than 2 minutes. Moreover, the statistical error in the MC computations is around 0.1%. Computing $\Phi = \text{Area}(\mathcal{P}_\tau \cap \{M \setminus \mathcal{F}_\tau\})$ according to (4), the error in the computation of Φ can be estimated by $\frac{1}{2}(\pi/2 - \Phi - \bar{\Phi})$. This error is less than 0.003% for most values of τ and β in Fig. 4, and is everywhere less than the MC error.

Conclusions—We have presented a theoretical framework for describing and efficiently computing finite-time transport between arbitrary regions in n D, volume-preserving flows with arbitrary time dependence. Its essence is the reduction of the transport problem to the dynamics of an $(n - 2)$ D “minimal set” of fundamental trajectories. Our framework requires no knowledge of the flow outside the finite transport interval and is independent of any notions of hyperbolicity or invariant manifolds. Moreover, it offers a tremendous reduction in computational effort compared to existing methods.

We have demonstrated the theory and its various advantages via a study of transport in a 2D unsteady model of a realistic mixing flow, and have exposed nontrivial dependence of the transport on the control parameters. The generality of the theory facilitates similar Lagrangian transport studies in generic n D systems. Additionally, efforts to extend the framework to diffusive processes, such

as those involved in heat transfer and chemical kinetics applications, are currently underway. The Lagrangian formalism for advective-diffusive transport proposed in [4] may offer some indications on how to proceed.

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